



# wwPDB X-ray Structure Validation Summary Report ⓘ

May 24, 2017 – 09:08 PM EDT

PDB ID : 1VY4  
Title : Crystal structure of the *Thermus thermophilus* 70S ribosome in the pre-attack state of peptide bond formation containing acylated tRNA-substrates in the A and P sites.  
Authors : Polikanov, Y.S.; Steitz, T.A.; Innis, C.A.  
Deposited on : 2014-05-13  
Resolution : 2.60 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  
Mogul : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20029077  
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) : rb-20029077

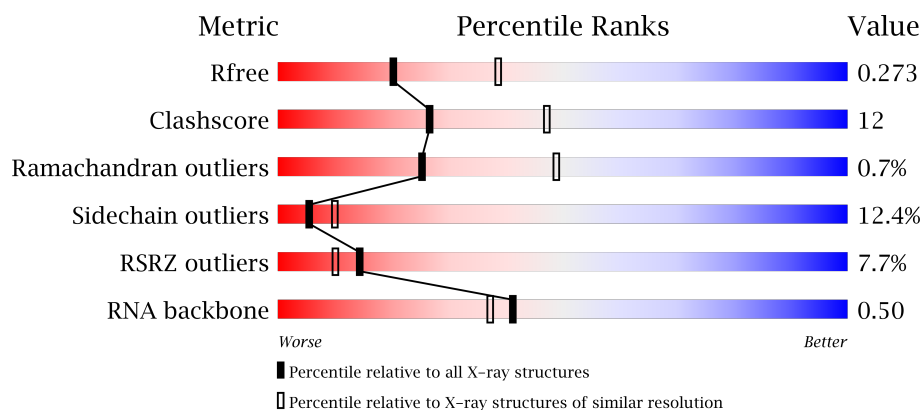
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.60 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	2542 (2.60-2.60)
Clashscore	112137	2895 (2.60-2.60)
Ramachandran outliers	110173	2848 (2.60-2.60)
Sidechain outliers	110143	2848 (2.60-2.60)
RSRZ outliers	101464	2550 (2.60-2.60)
RNA backbone	2435	1140 (3.00-2.20)

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	1521	
1	CA	1521	
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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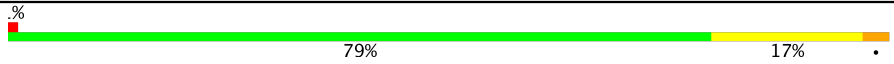

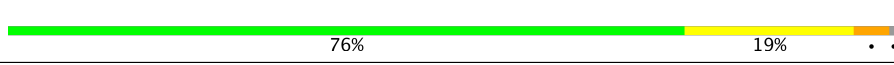

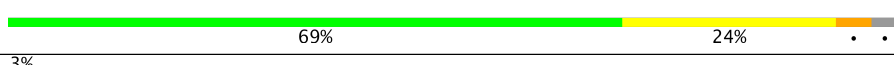
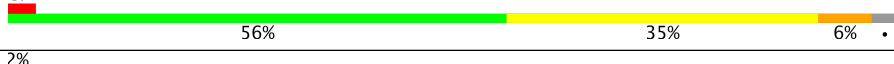
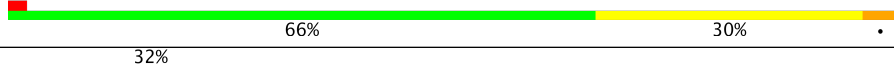
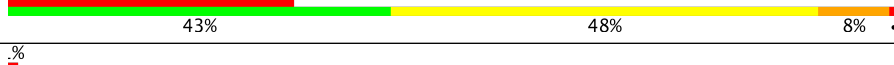
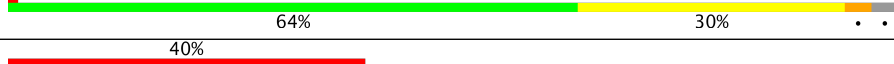


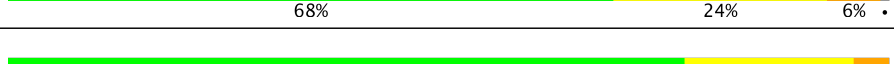
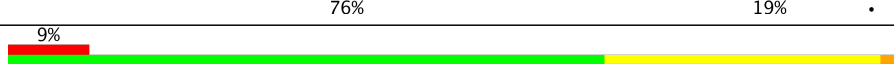
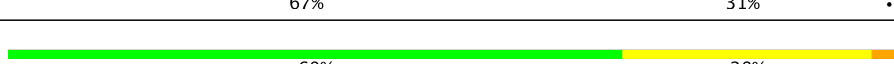

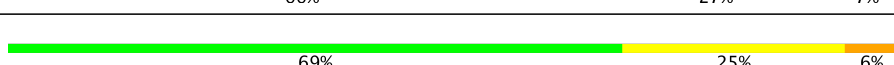
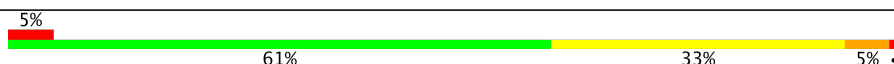
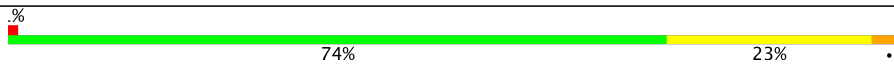
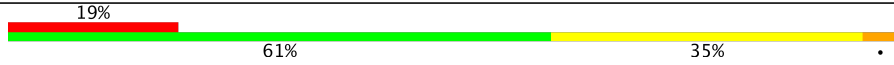


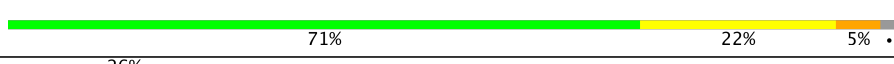
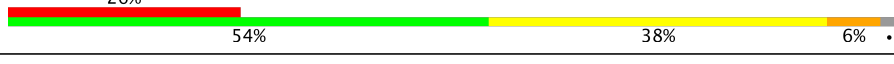


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Mol	Chain	Length	Quality of chain
15	CO	89	
16	AP	88	
16	CP	88	
17	AQ	105	
17	CQ	105	
18	AR	88	
18	CR	88	
19	AS	93	
19	CS	93	
20	AT	106	
20	CT	106	
21	AU	27	
21	CU	27	
22	AV	24	
22	CV	24	
23	AW	76	
23	CW	76	
24	AX	77	
24	CX	77	
25	AY	76	
25	CY	76	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

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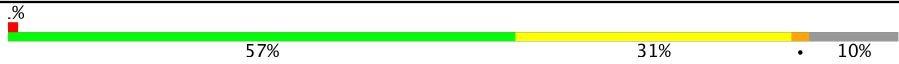

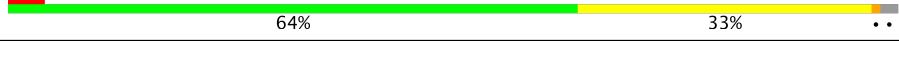
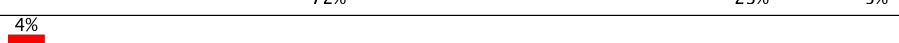
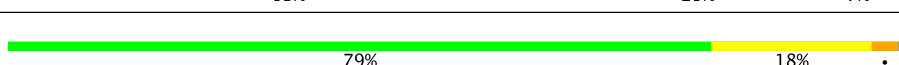


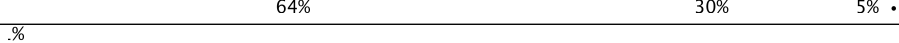
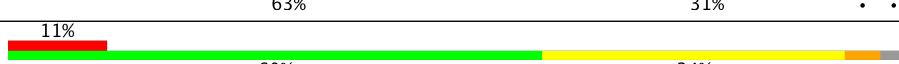

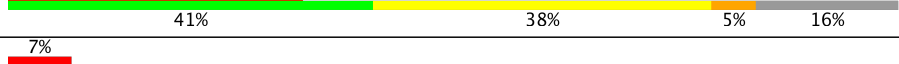
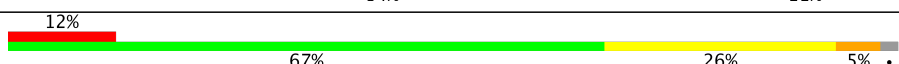

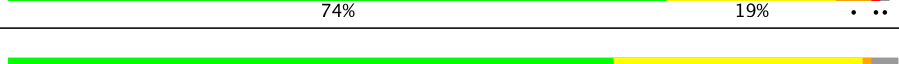
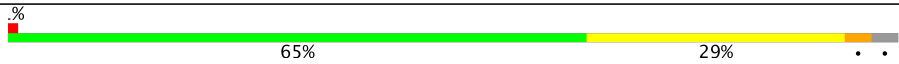









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Mol	Chain	Length	Quality of chain
28	BD	276	
28	DD	276	
29	BE	206	
29	DE	206	
30	BF	210	
30	DF	210	
31	BG	182	
31	DG	182	
32	BH	180	
32	DH	180	
33	BI	148	
33	DI	148	
34	BN	140	
34	DN	140	
35	BO	122	
35	DO	122	
36	BP	150	
36	DP	150	
37	BQ	141	
37	DQ	141	
38	BR	118	
38	DR	118	
39	BS	112	
39	DS	112	
40	BT	146	

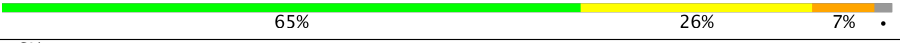




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Mol	Chain	Length	Quality of chain
40	DT	146	
41	BU	118	
41	DU	118	
42	BV	101	
42	DV	101	
43	BW	113	
43	DW	113	
44	BX	96	
44	DX	96	
45	BY	110	
45	DY	110	
46	BZ	206	
46	DZ	206	
47	B0	85	
47	D0	85	
48	B1	98	
48	D1	98	
49	B2	72	
49	D2	72	
50	B3	60	
50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

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

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
25	PSU	CY	39	-	-	X	-
57	MG	AA	1675	-	-	-	X
57	MG	AA	1687	-	-	-	X
57	MG	AA	1702	-	-	-	X
57	MG	AA	1725	-	-	-	X
57	MG	AA	1730	-	-	-	X
57	MG	AA	1756	-	-	-	X
57	MG	AA	1757	-	-	-	X
57	MG	AX	3002	-	-	-	X
57	MG	AX	3003	-	-	-	X
57	MG	BA	3007	-	-	-	X
57	MG	BA	3018	-	-	-	X
57	MG	BA	3033	-	-	-	X
57	MG	BA	3035	-	-	-	X
57	MG	BA	3037	-	-	-	X
57	MG	BA	3041	-	-	-	X
57	MG	BA	3044	-	-	-	X
57	MG	BA	3061	-	-	-	X
57	MG	BA	3070	-	-	-	X
57	MG	BA	3083	-	-	-	X
57	MG	BA	3085	-	-	-	X
57	MG	BA	3100	-	-	-	X
57	MG	BA	3103	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
57	MG	BA	3111	-	-	-	X
57	MG	BA	3121	-	-	-	X
57	MG	BA	3124	-	-	-	X
57	MG	BA	3135	-	-	-	X
57	MG	BA	3136	-	-	-	X
57	MG	BA	3142	-	-	-	X
57	MG	BA	3171	-	-	-	X
57	MG	BA	3174	-	-	-	X
57	MG	BA	3176	-	-	-	X
57	MG	BA	3182	-	-	-	X
57	MG	BA	3186	-	-	-	X
57	MG	BA	3200	-	-	-	X
57	MG	BA	3204	-	-	-	X
57	MG	BA	3210	-	-	-	X
57	MG	BA	3214	-	-	-	X
57	MG	BA	3215	-	-	-	X
57	MG	BA	3216	-	-	-	X
57	MG	BA	3219	-	-	-	X
57	MG	BA	3244	-	-	-	X
57	MG	BA	3256	-	-	-	X
57	MG	BA	3277	-	-	-	X
57	MG	BA	3310	-	-	-	X
57	MG	BA	3369	-	-	-	X
57	MG	BA	3400	-	-	-	X
57	MG	BA	3403	-	-	-	X
57	MG	BA	3424	-	-	-	X
57	MG	BA	3425	-	-	-	X
57	MG	BA	3456	-	-	-	X
57	MG	BA	3507	-	-	-	X
57	MG	BA	3520	-	-	-	X
57	MG	BA	3526	-	-	-	X
57	MG	BA	3529	-	-	-	X
57	MG	BA	3530	-	-	-	X
57	MG	BA	3543	-	-	-	X
57	MG	BA	3561	-	-	-	X
57	MG	BA	3591	-	-	-	X
57	MG	BA	3608	-	-	-	X
57	MG	BA	3648	-	-	-	X
57	MG	BA	3672	-	-	-	X
57	MG	BA	3674	-	-	-	X
57	MG	BA	3680	-	-	-	X
57	MG	BA	3688	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
57	MG	BA	3700	-	-	-	X
57	MG	BA	3710	-	-	-	X
57	MG	BA	3716	-	-	-	X
57	MG	BA	3743	-	-	-	X
57	MG	BA	3770	-	-	-	X
57	MG	BA	3775	-	-	-	X
57	MG	BA	3795	-	-	-	X
57	MG	BA	3807	-	-	-	X
57	MG	BA	3814	-	-	-	X
57	MG	BD	3003	-	-	-	X
57	MG	BD	3007	-	-	-	X
57	MG	BD	3008	-	-	-	X
57	MG	BF	302	-	-	-	X
57	MG	BF	303	-	-	-	X
57	MG	BF	304	-	-	-	X
57	MG	BF	306	-	-	-	X
57	MG	BU	201	-	-	-	X
57	MG	BU	203	-	-	-	X
57	MG	BU	204	-	-	-	X
57	MG	BV	201	-	-	-	X
57	MG	BX	3001	-	-	-	X
57	MG	CA	3067	-	-	-	X
57	MG	CA	3130	-	-	-	X
57	MG	CA	3167	-	-	-	X
57	MG	CA	3168	-	-	-	X
57	MG	DA	3026	-	-	-	X
57	MG	DA	3027	-	-	-	X
57	MG	DA	3029	-	-	-	X
57	MG	DA	3042	-	-	-	X
57	MG	DA	3060	-	-	-	X
57	MG	DA	3070	-	-	-	X
57	MG	DA	3090	-	-	-	X
57	MG	DA	3102	-	-	-	X
57	MG	DA	3103	-	-	-	X
57	MG	DA	3105	-	-	-	X
57	MG	DA	3119	-	-	-	X
57	MG	DA	3160	-	-	-	X
57	MG	DA	3161	-	-	-	X
57	MG	DA	3169	-	-	-	X
57	MG	DA	3191	-	-	-	X
57	MG	DA	3192	-	-	-	X
57	MG	DA	3220	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
57	MG	DA	3274	-	-	-	X
57	MG	DA	3323	-	-	-	X
57	MG	DA	3325	-	-	-	X
57	MG	DA	3362	-	-	-	X
57	MG	DA	3422	-	-	-	X
57	MG	DA	3456	-	-	-	X
57	MG	DA	3464	-	-	-	X
57	MG	DA	3491	-	-	-	X
57	MG	DA	3500	-	-	-	X
57	MG	DA	3503	-	-	-	X
57	MG	DA	3602	-	-	-	X
57	MG	DA	3617	-	-	-	X
57	MG	DA	3621	-	-	-	X
57	MG	DA	3624	-	-	-	X
57	MG	DA	3657	-	-	-	X
57	MG	DA	3660	-	-	-	X
57	MG	DB	3008	-	-	-	X
57	MG	DE	3001	-	-	-	X
57	MG	DF	301	-	-	-	X
57	MG	DF	305	-	-	-	X
57	MG	DQ	3003	-	-	-	X
57	MG	DU	201	-	-	-	X
57	MG	DV	201	-	-	-	X
59	ZN	B6	102	-	-	-	X

## 2 Entry composition

There are 61 unique types of molecules in this entry. The entry contains 297127 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	1497	Total	C	N	O	P	0	0	0
			32185	14324	5968	10396	1497			
1	CA	1503	Total	C	N	O	P	0	0	0
			32312	14381	5990	10438	1503			

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	AC	206	Total	C	N	O	S	0	0	0
			1552	976	302	273	1			
3	CC	206	Total	C	N	O	S	0	0	0
			1544	970	300	273	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	AD	208	Total	C	N	O	S	0	0	0
			1659	1040	326	286	7			
4	CD	208	Total	C	N	O	S	0	0	0
			1678	1052	333	286	7			

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	AF	100	Total	C	N	O	S	0	0	0
			812	514	146	149	3			
6	CF	100	Total	C	N	O	S	0	0	0
			820	518	147	152	3			

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	AI	127	Total	C	N	O		0	0	0
			986	626	193	167				
9	CI	127	Total	C	N	O		0	0	0
			978	619	190	169				

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
13	AM	123	Total	C	N	O	S		
			966	598	200	166	2	0	0
13	CM	122	Total	C	N	O	S		
			950	586	197	165	2	0	0

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	AS	84	Total	C	N	O	S	0	0	0
			661	423	122	114	2			
19	CS	83	Total	C	N	O	S	0	0	0
			646	412	119	113	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	AT	96	Total	C	N	O	S	0	0	0
			728	446	156	124	2			
20	CT	96	Total	C	N	O	S	0	0	0
			731	449	156	124	2			

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

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

- Molecule 22 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	AV	13	Total	C	N	O	P	0	0	0
			277	125	51	88	13			
22	CV	12	Total	C	N	O	P	0	0	0
			252	115	46	80	11			

- Molecule 23 is a RNA chain called A-site tRNA.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
23	AW	74	Total	C	N	O	P	S	0	0	0
			1599	722	287	515	73	2			
23	CW	72	Total	C	N	O	P	S	0	0	0
			1552	697	280	502	72	1			

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

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

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

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
25	AY	74	Total	C	N	O	P	S	0	0	0
			1581	707	285	515	73	1			
25	CY	73	Total	C	N	O	P	S	0	0	0
			1561	698	283	507	72	1			

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
28	BD	275	Total	C	N	O	S	0	0	0
			2136	1349	423	361	3			
28	DD	275	Total	C	N	O	S	0	0	0
			2142	1352	426	361	3			

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
33	BI	146	Total	C	N	O	S	0	0	0
			1085	693	189	202	1			
33	DI	146	Total	C	N	O	S	0	0	0
			1073	688	188	196	1			

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
36	BP	149	Total	C	N	O	S	0	0	0
			1139	709	231	196	3			
36	DP	149	Total	C	N	O	S	0	0	0
			1135	706	230	196	3			

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
51	B4	69	Total	C	N	O	S	0	0	0
			558	352	102	99	5			
51	D4	69	Total	C	N	O	S	0	0	0
			532	339	97	91	5			

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

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

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



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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	B4	1	Total	Mg	0	0
			1	1		
57	BA	814	Total	Mg	0	0
			814	814		
57	AK	1	Total	Mg	0	0
			1	1		
57	DQ	3	Total	Mg	0	0
			3	3		
57	D3	1	Total	Mg	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	AB	1	Total 1	Mg 1	0	0
57	DF	5	Total 5	Mg 5	0	0
57	B8	2	Total 2	Mg 2	0	0
57	BE	6	Total 6	Mg 6	0	0
57	AW	2	Total 2	Mg 2	0	0
57	DU	1	Total 1	Mg 1	0	0
57	AN	2	Total 2	Mg 2	0	0
57	BP	2	Total 2	Mg 2	0	0
57	AX	15	Total 15	Mg 15	0	0
57	DN	1	Total 1	Mg 1	0	0
57	CA	169	Total 169	Mg 169	0	0
57	B5	3	Total 3	Mg 3	0	0
57	BB	23	Total 23	Mg 23	0	0
57	D8	1	Total 1	Mg 1	0	0
57	AE	1	Total 1	Mg 1	0	0
57	DB	13	Total 13	Mg 13	0	0
57	CF	1	Total 1	Mg 1	0	0
57	B9	1	Total 1	Mg 1	0	0
57	BF	11	Total 11	Mg 11	0	0
57	BX	1	Total 1	Mg 1	0	0
57	B2	1	Total 1	Mg 1	0	0

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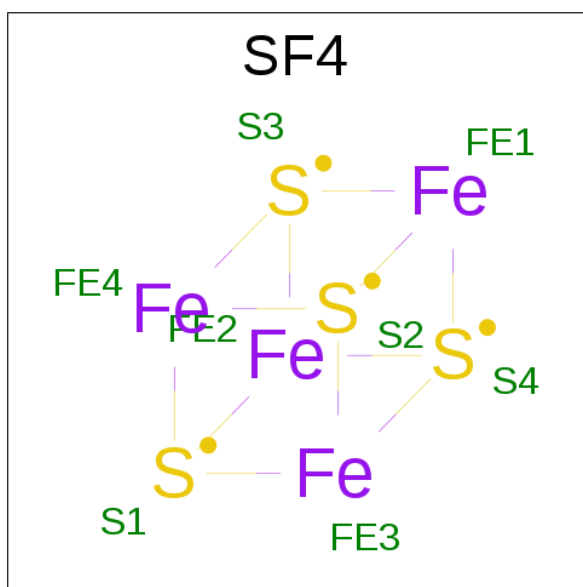
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	AA	216	Total 216	Mg 216	0	0
57	BQ	2	Total 2	Mg 2	0	0
57	CX	2	Total 2	Mg 2	0	0
57	DV	1	Total 1	Mg 1	0	0
57	B6	2	Total 2	Mg 2	0	0
57	AM	2	Total 2	Mg 2	0	0
57	BU	4	Total 4	Mg 4	0	0
57	DR	1	Total 1	Mg 1	0	0
57	BN	3	Total 3	Mg 3	0	0
57	CT	1	Total 1	Mg 1	0	0
57	D0	1	Total 1	Mg 1	0	0
57	BG	2	Total 2	Mg 2	0	0
57	BY	1	Total 1	Mg 1	0	0
57	DE	7	Total 7	Mg 7	0	0
57	CJ	1	Total 1	Mg 1	0	0
57	BR	2	Total 2	Mg 2	0	0
57	DA	664	Total 664	Mg 664	0	0
57	AU	1	Total 1	Mg 1	0	0
57	DW	1	Total 1	Mg 1	0	0
57	B7	5	Total 5	Mg 5	0	0
57	AL	2	Total 2	Mg 2	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	BV	5	Total 5	Mg 5	0	0
57	DP	2	Total 2	Mg 2	0	0
57	DO	2	Total 2	Mg 2	0	0
57	BO	1	Total 1	Mg 1	0	0
57	BZ	2	Total 2	Mg 2	0	0
57	DY	1	Total 1	Mg 1	0	0
57	CW	1	Total 1	Mg 1	0	0
57	DG	1	Total 1	Mg 1	0	0
57	CD	1	Total 1	Mg 1	0	0
57	BD	10	Total 10	Mg 10	0	0
57	AT	1	Total 1	Mg 1	0	0
57	B0	2	Total 2	Mg 2	0	0
57	CE	2	Total 2	Mg 2	0	0
57	BW	4	Total 4	Mg 4	0	0
57	AY	3	Total 3	Mg 3	0	0
57	DD	4	Total 4	Mg 4	0	0
57	CK	1	Total 1	Mg 1	0	0
57	AF	1	Total 1	Mg 1	0	0
57	BH	1	Total 1	Mg 1	0	0

- Molecule 58 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe<sub>4</sub>S<sub>4</sub>).



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

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

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

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

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

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

- Molecule 61 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
61	AA	210	Total 210	O 210	0	0
61	AD	1	Total 1	O 1	0	0
61	AE	2	Total 2	O 2	0	0
61	AJ	1	Total 1	O 1	0	0
61	AL	2	Total 2	O 2	0	0
61	AM	2	Total 2	O 2	0	0
61	AV	2	Total 2	O 2	0	0
61	AW	4	Total 4	O 4	0	0
61	AX	4	Total 4	O 4	0	0
61	AY	1	Total 1	O 1	0	0
61	BA	1405	Total 1406	O 1406	0	1
61	BB	37	Total 37	O 37	0	0
61	BD	15	Total 15	O 15	0	0
61	BE	17	Total 17	O 17	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
61	BF	11	Total 11	O 11	0	0
61	BG	3	Total 3	O 3	0	0
61	BH	1	Total 1	O 1	0	0
61	BI	1	Total 1	O 1	0	0
61	BN	1	Total 1	O 1	0	0
61	BO	2	Total 2	O 2	0	0
61	BP	13	Total 13	O 13	0	0
61	BQ	4	Total 4	O 4	0	0
61	BR	2	Total 2	O 2	0	0
61	BS	2	Total 2	O 2	0	0
61	BT	2	Total 2	O 2	0	0
61	BU	4	Total 4	O 4	0	0
61	BV	2	Total 2	O 2	0	0
61	BW	3	Total 3	O 3	0	0
61	BX	3	Total 3	O 3	0	0
61	BZ	1	Total 1	O 1	0	0
61	B0	6	Total 6	O 6	0	0
61	B1	2	Total 2	O 2	0	0
61	B3	2	Total 2	O 2	0	0
61	B5	4	Total 4	O 4	0	0
61	B6	2	Total 2	O 2	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
61	B7	3	Total 3	O 3	0	0
61	B8	13	Total 13	O 13	0	0
61	B9	1	Total 1	O 1	0	0
61	CA	156	Total 156	O 156	0	0
61	CE	2	Total 2	O 2	0	0
61	CH	1	Total 1	O 1	0	0
61	CJ	1	Total 1	O 1	0	0
61	CK	1	Total 1	O 1	0	0
61	CL	1	Total 1	O 1	0	0
61	CT	1	Total 1	O 1	0	0
61	CW	2	Total 2	O 2	0	0
61	CX	2	Total 2	O 2	0	0
61	CY	1	Total 1	O 1	0	0
61	DA	989	Total 989	O 989	0	0
61	DB	9	Total 9	O 9	0	0
61	DD	18	Total 18	O 18	0	0
61	DE	5	Total 5	O 5	0	0
61	DF	4	Total 4	O 4	0	0
61	DN	2	Total 2	O 2	0	0
61	DP	12	Total 12	O 12	0	0
61	DQ	1	Total 1	O 1	0	0

*Continued on next page...*



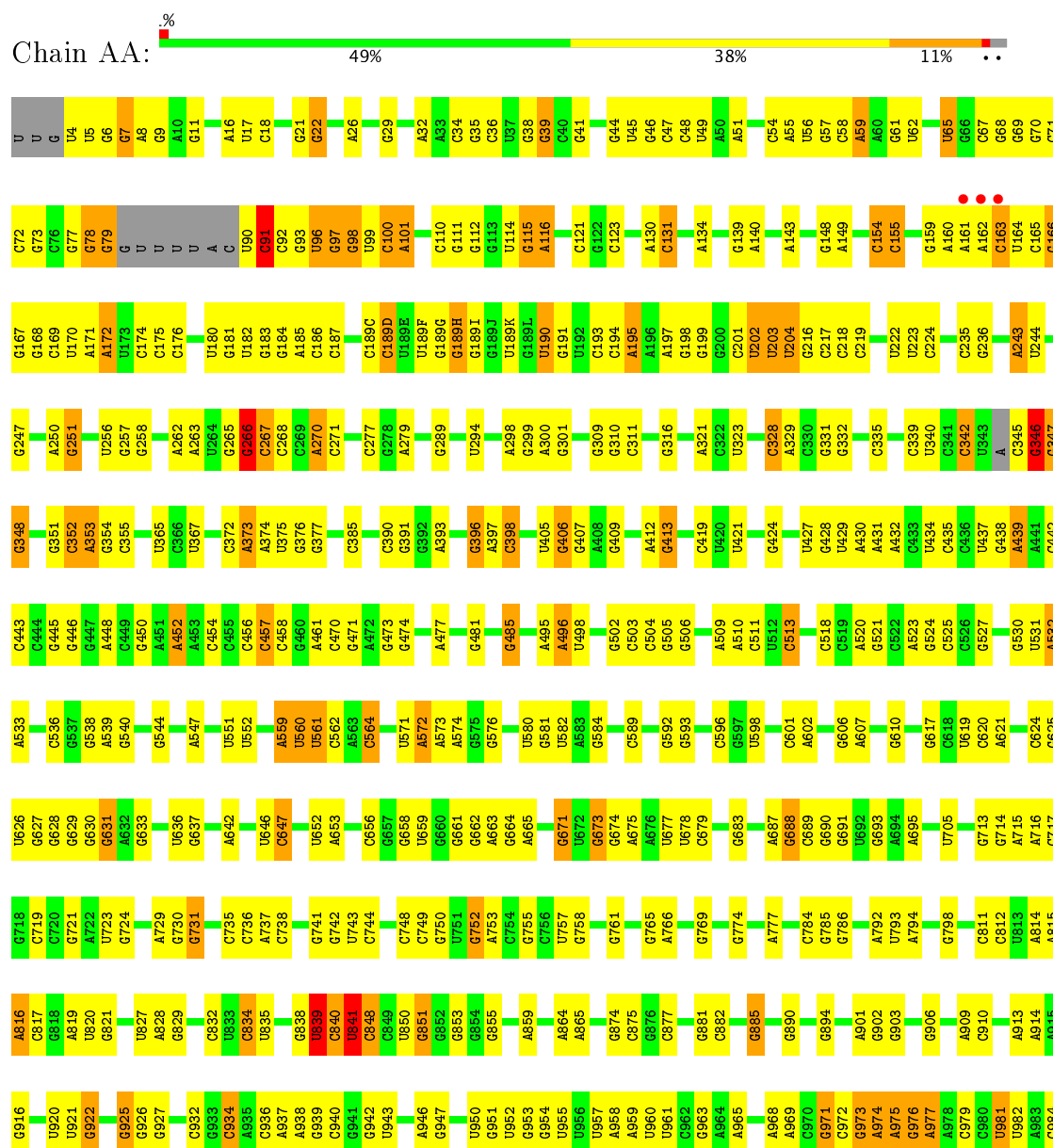
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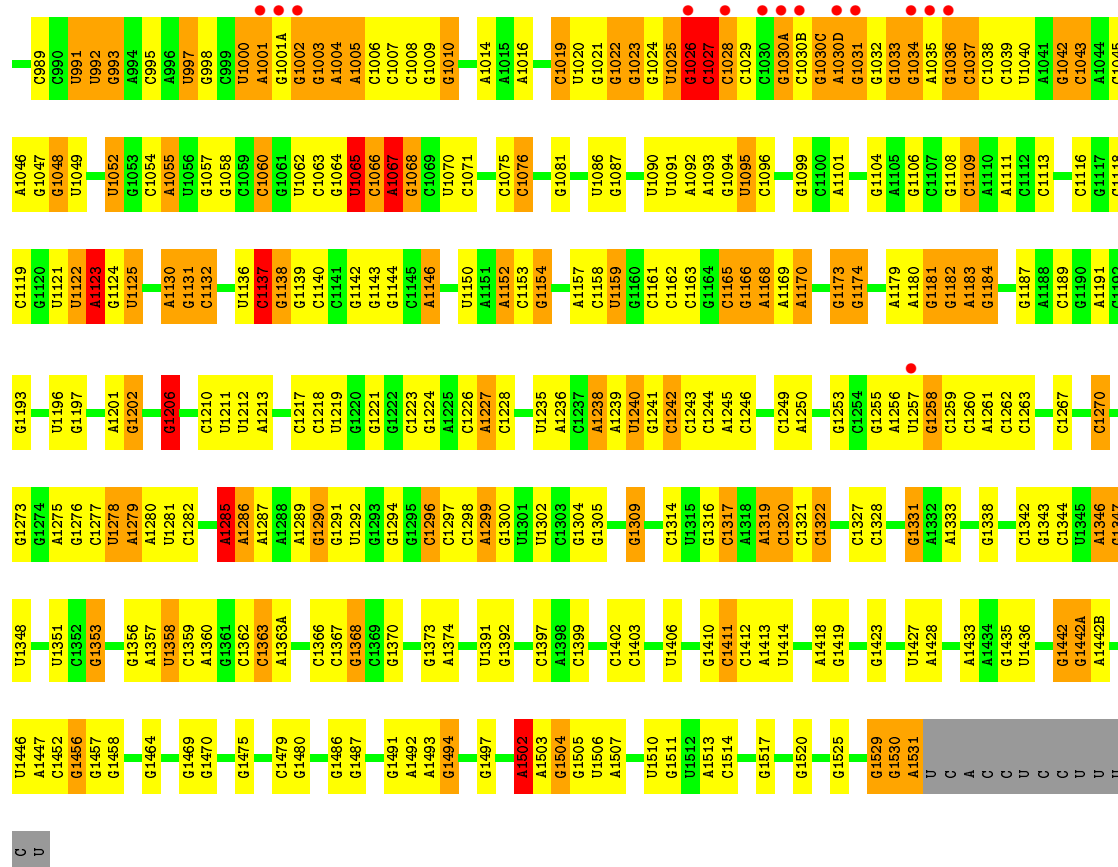
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
61	DT	4	Total 4	O 4	0	0
61	DU	1	Total 1	O 1	0	0
61	DV	1	Total 1	O 1	0	0
61	DW	1	Total 1	O 1	0	0
61	DX	2	Total 2	O 2	0	0
61	DY	1	Total 1	O 1	0	0
61	D0	4	Total 4	O 4	0	0
61	D1	1	Total 1	O 1	0	0
61	D3	2	Total 2	O 2	0	0
61	D5	1	Total 1	O 1	0	0
61	D6	1	Total 1	O 1	0	0
61	D8	3	Total 3	O 3	0	0

### 3 Residue-property plots

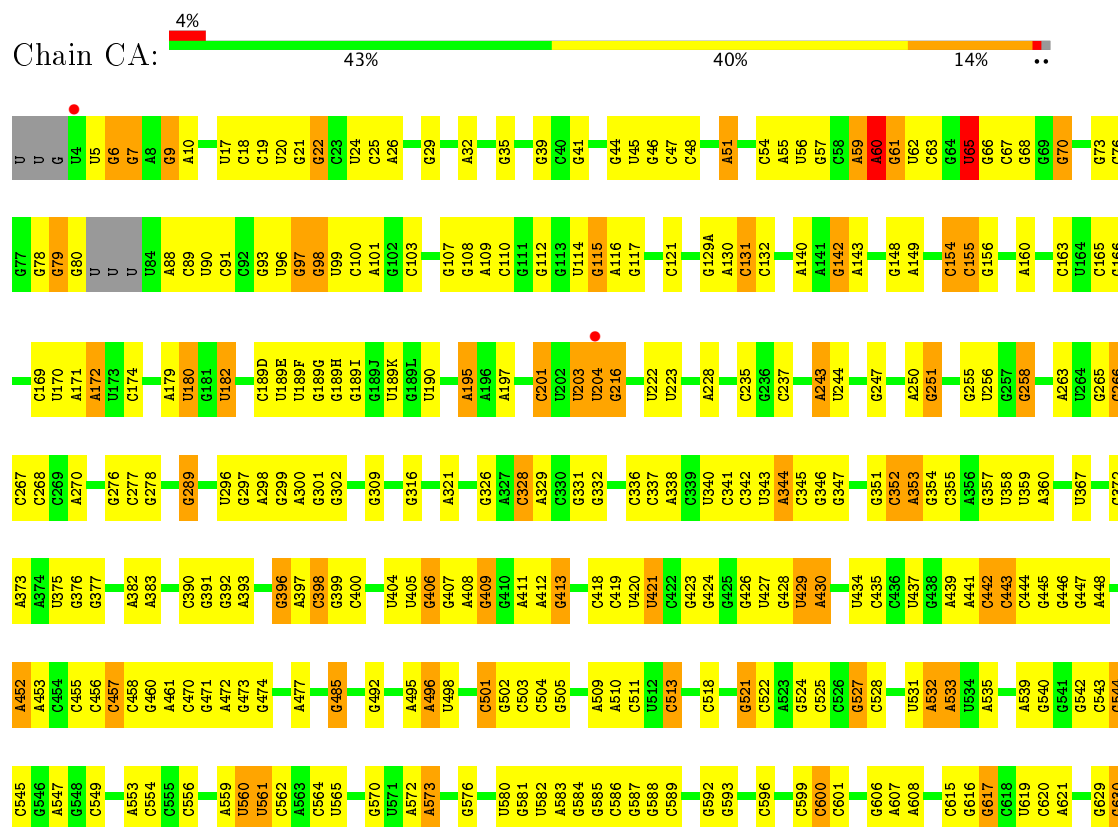
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are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

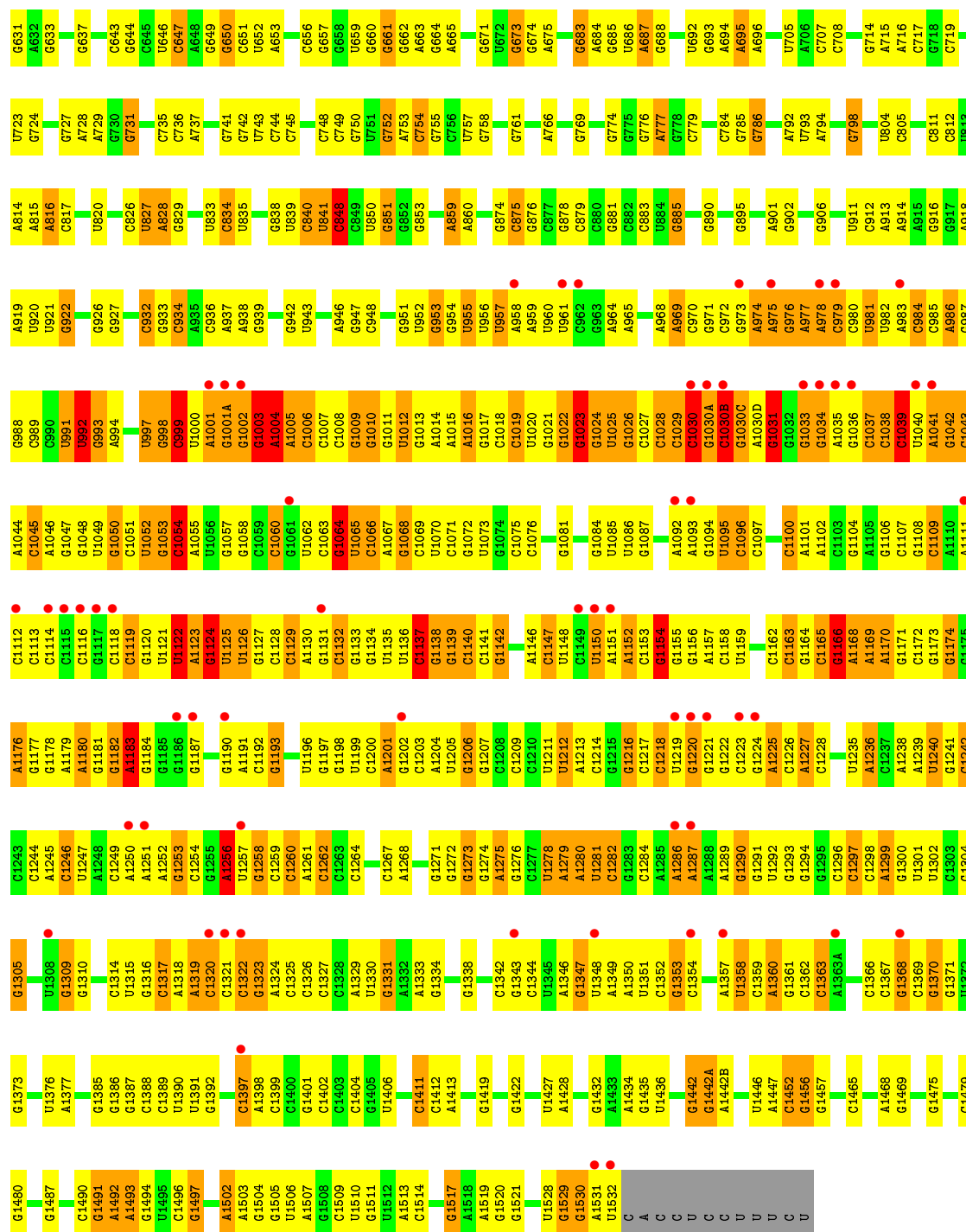
#### • Molecule 1: 16S Ribosomal RNA



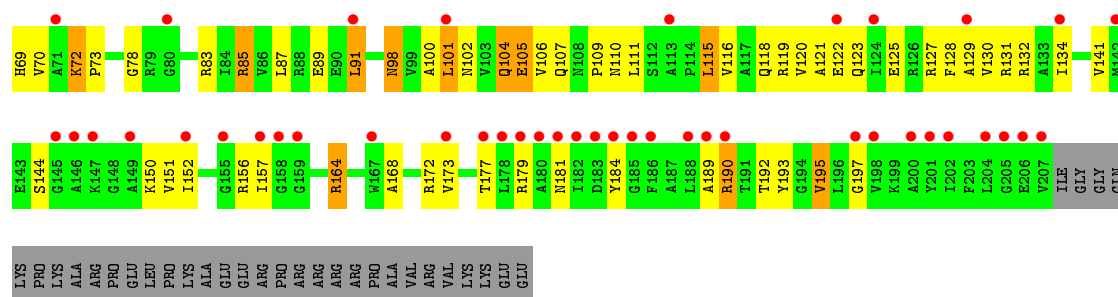


### • Molecule 1: 16S Ribosomal RNA

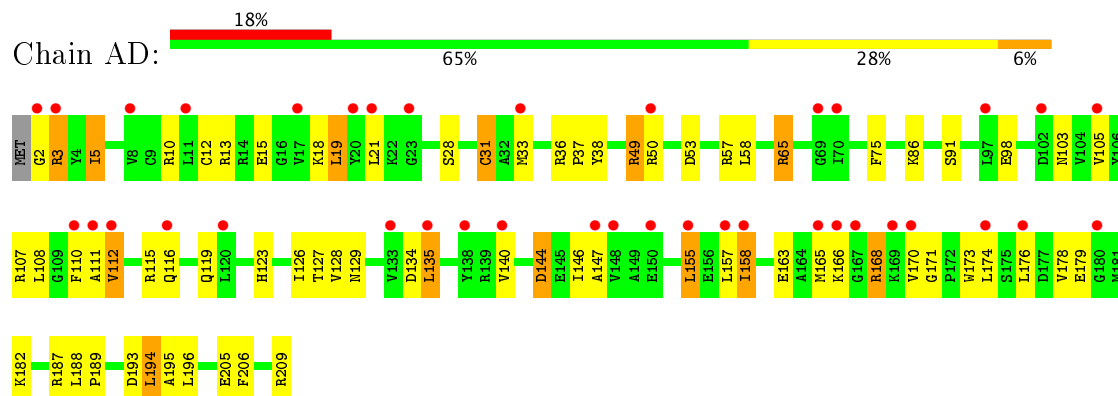




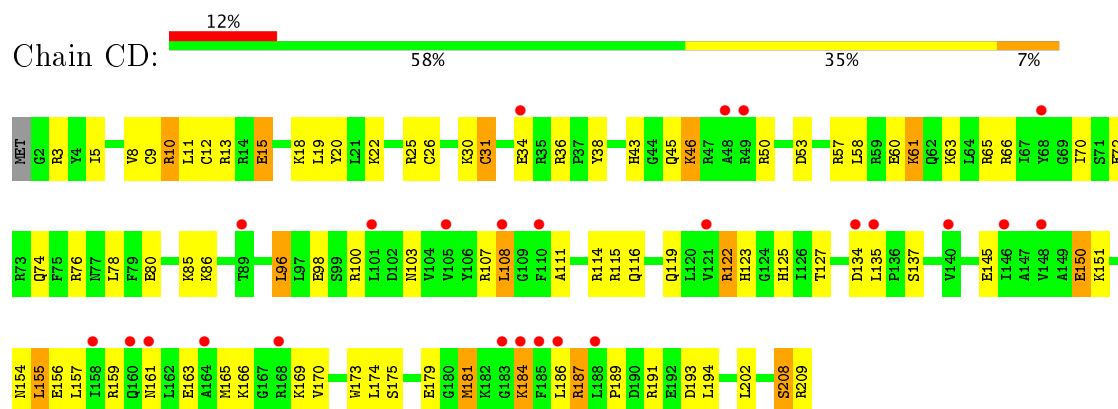




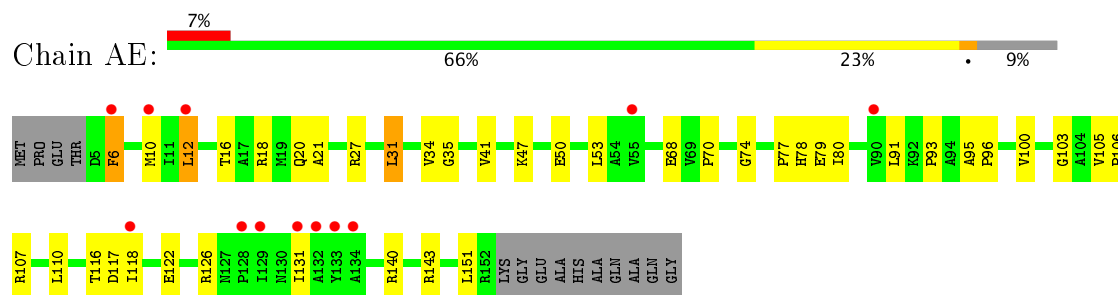
• Molecule 4: 30S ribosomal protein S4



• Molecule 4: 30S ribosomal protein S4

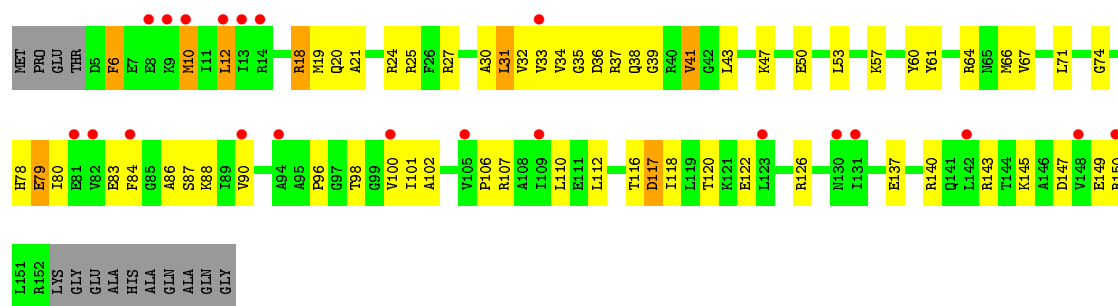


• Molecule 5: 30S ribosomal protein S5

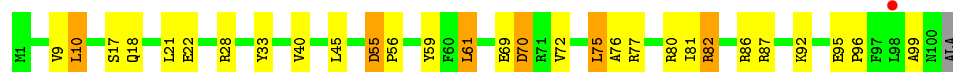


• Molecule 5: 30S ribosomal protein S5

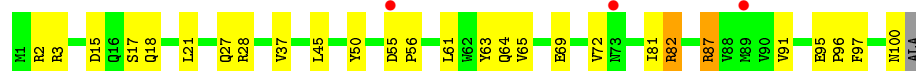
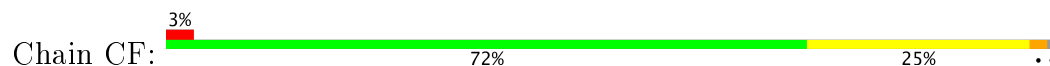




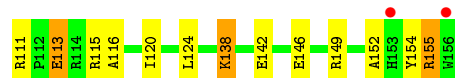
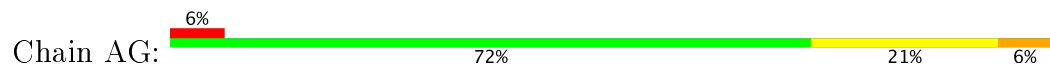
- Molecule 6: 30S ribosomal protein S6



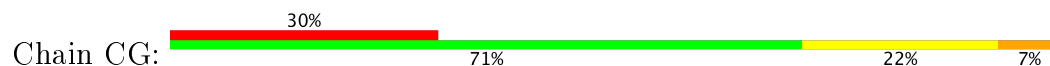
- Molecule 6: 30S ribosomal protein S6



- Molecule 7: 30S ribosomal protein S7

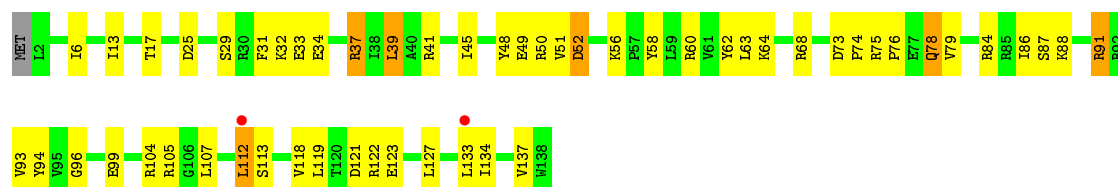


- Molecule 7: 30S ribosomal protein S7

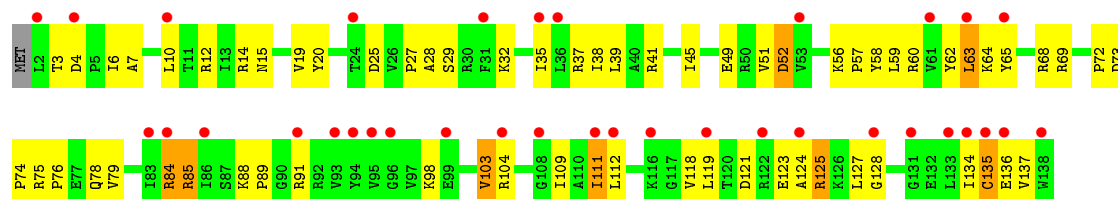


- Molecule 8: 30S ribosomal protein S8

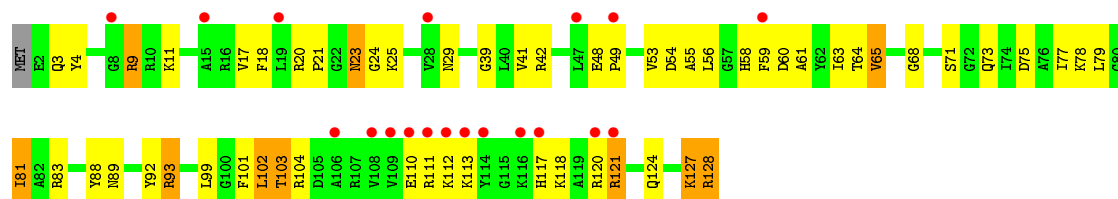




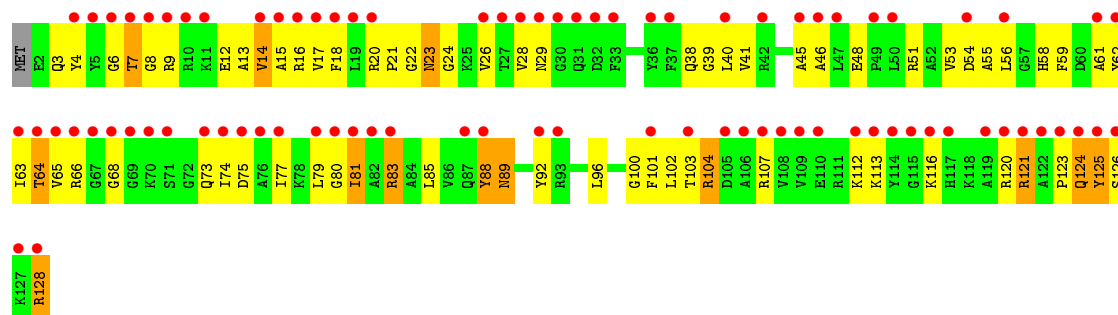
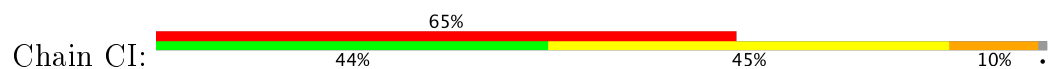
• Molecule 8: 30S ribosomal protein S8



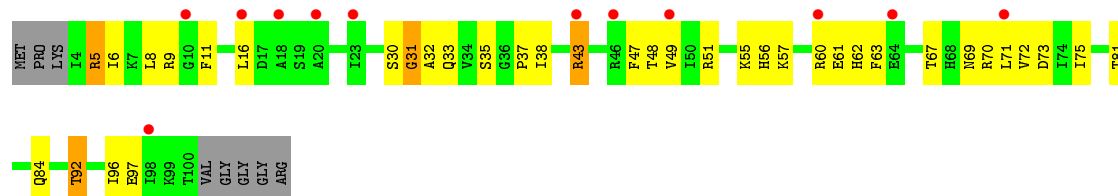
• Molecule 9: 30S ribosomal protein S9



• Molecule 9: 30S ribosomal protein S9

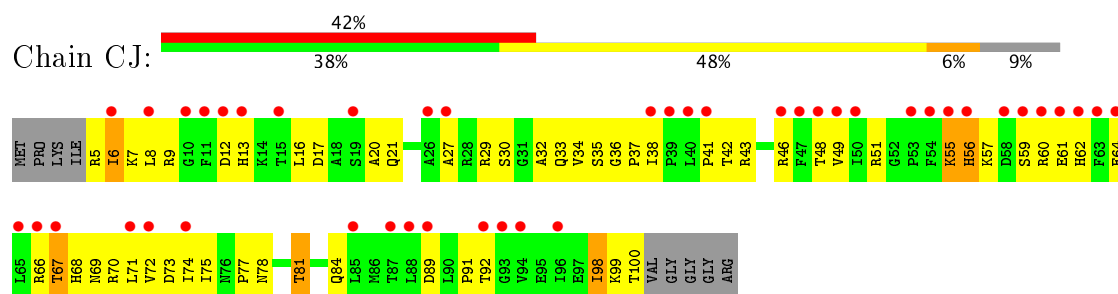


• Molecule 10: 30S ribosomal protein S10

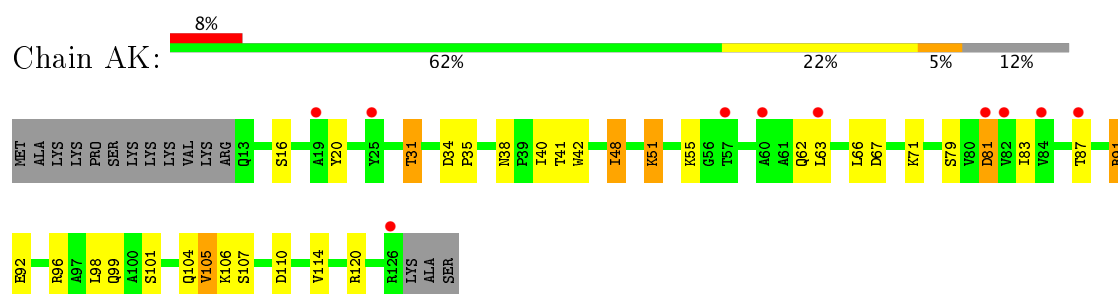




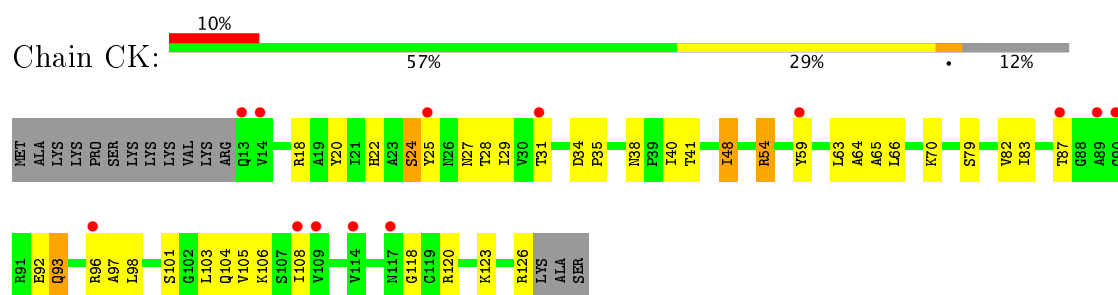
- Molecule 10: 30S ribosomal protein S10



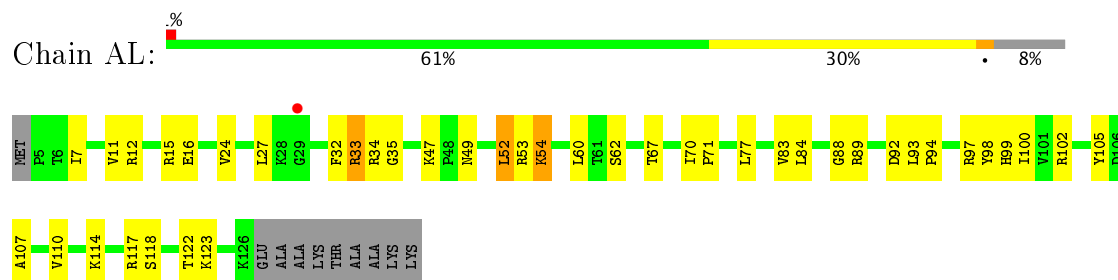
- Molecule 11: 30S ribosomal protein S11



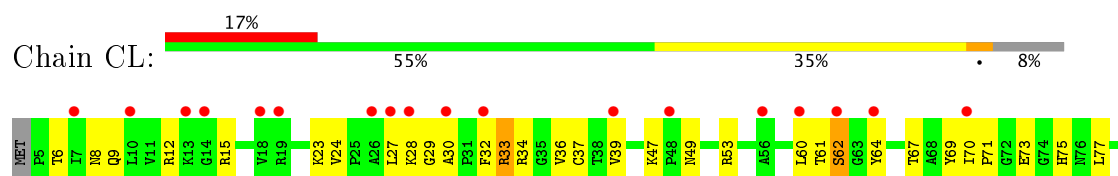
- Molecule 11: 30S ribosomal protein S11



- Molecule 12: 30S ribosomal protein S12

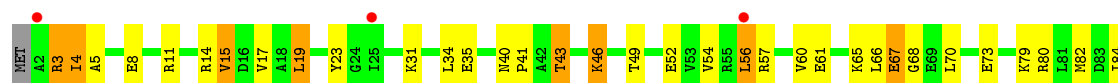


- Molecule 12: 30S ribosomal protein S12

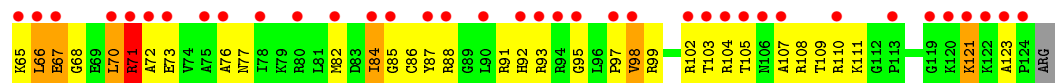




• Molecule 13: 30S ribosomal protein S13



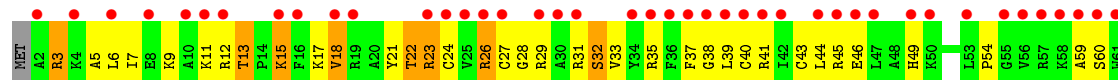
• Molecule 13: 30S ribosomal protein S13



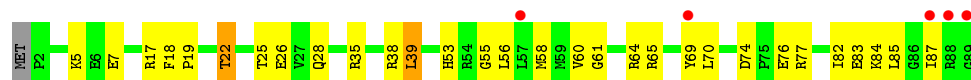
• Molecule 14: 30S ribosomal protein S14 type Z



• Molecule 14: 30S ribosomal protein S14 type Z



• Molecule 15: 30S ribosomal protein S15

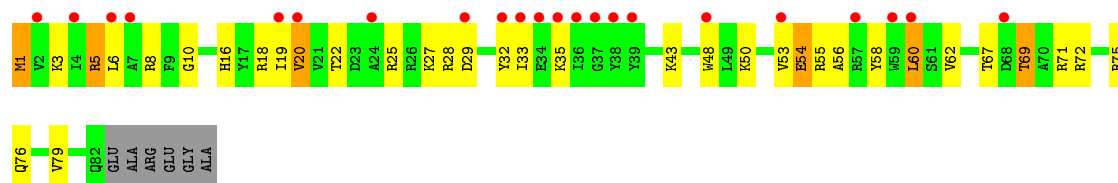


• Molecule 15: 30S ribosomal protein S15

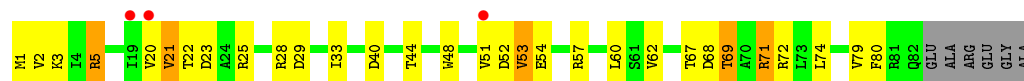




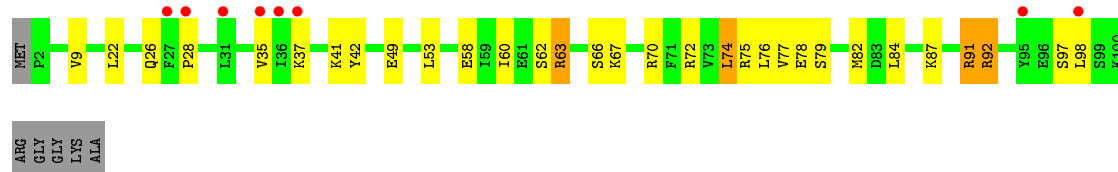
- Molecule 16: 30S ribosomal protein S16



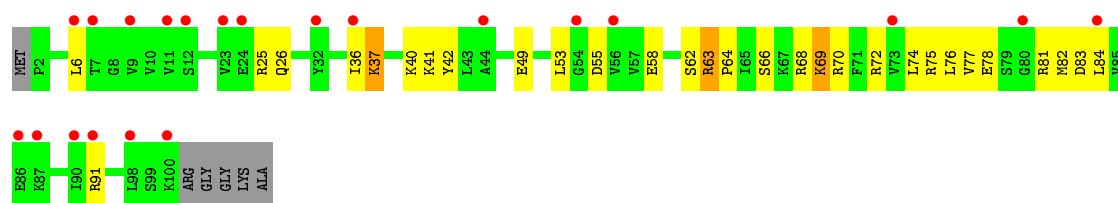
- Molecule 16: 30S ribosomal protein S16



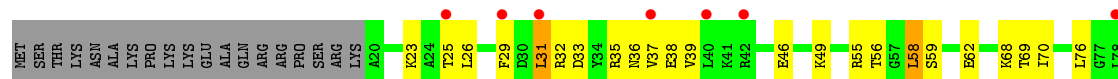
- Molecule 17: 30S ribosomal protein S17

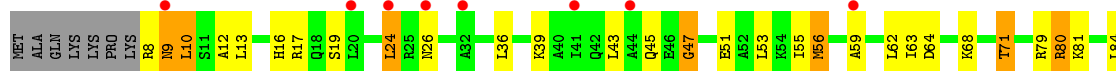


- Molecule 17: 30S ribosomal protein S17



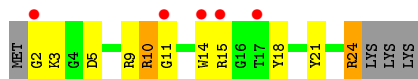
- Molecule 18: 30S ribosomal protein S18



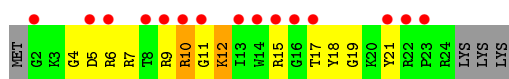
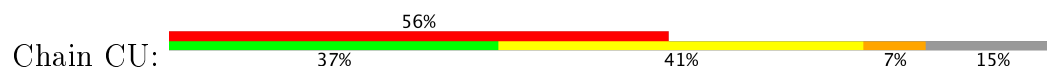




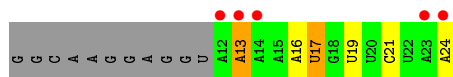
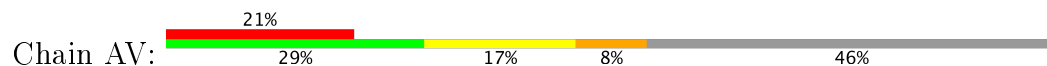
- Molecule 21: 30S ribosomal protein Thx



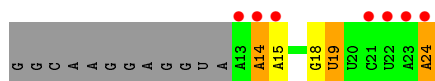
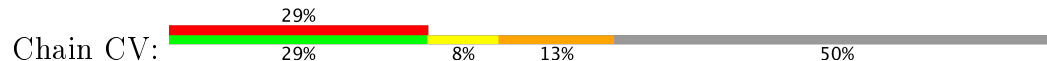
- Molecule 21: 30S ribosomal protein Thx



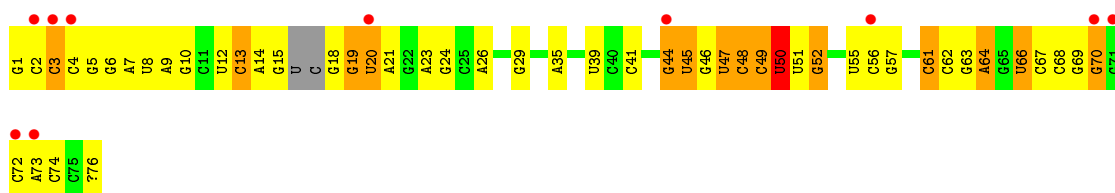
- Molecule 22: mRNA



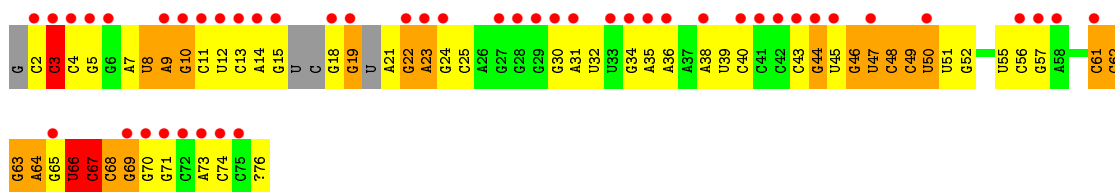
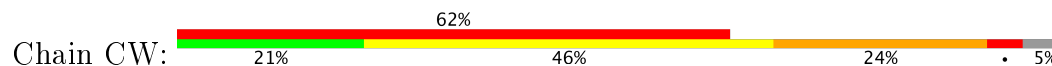
- Molecule 22: mRNA



- Molecule 23: A-site tRNA

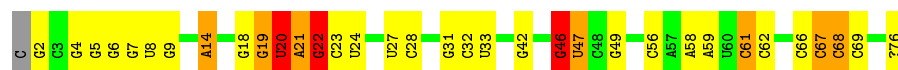


- Molecule 23: A-site tRNA



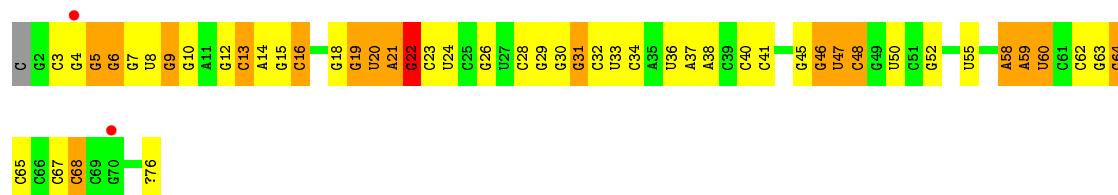
- Molecule 24: P-site tRNA

Chain AX: 



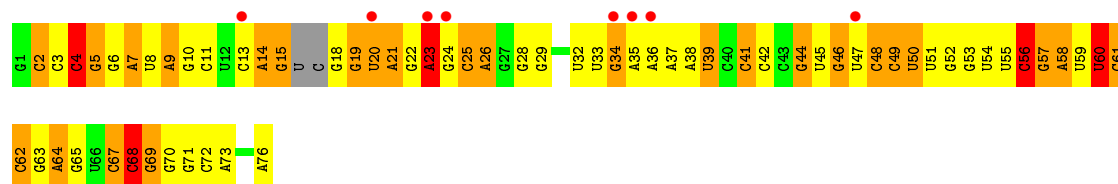
- Molecule 24: P-site tRNA

Chain CX: 



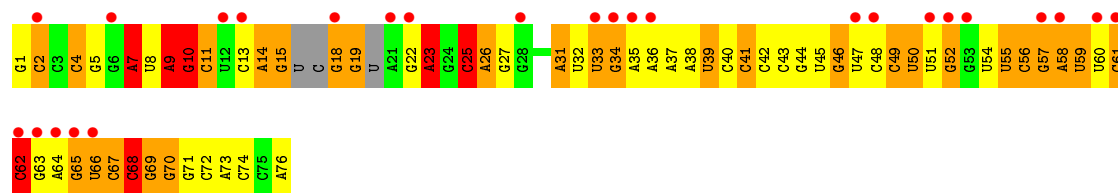
- Molecule 25: E-site tRNA

Chain AY: 



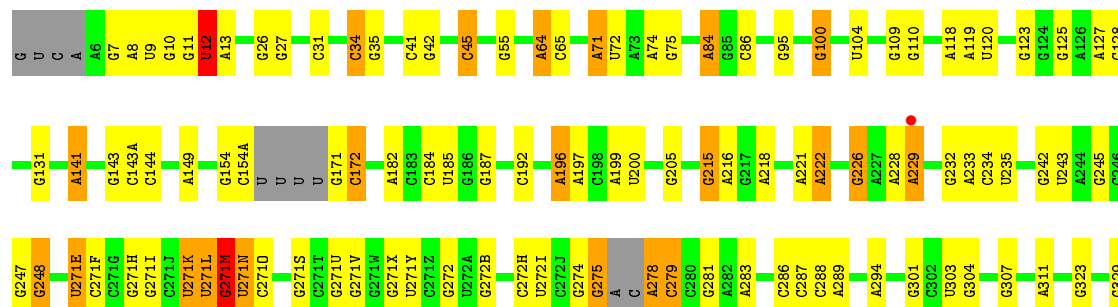
- Molecule 25: E-site tRNA

Chain CY: 

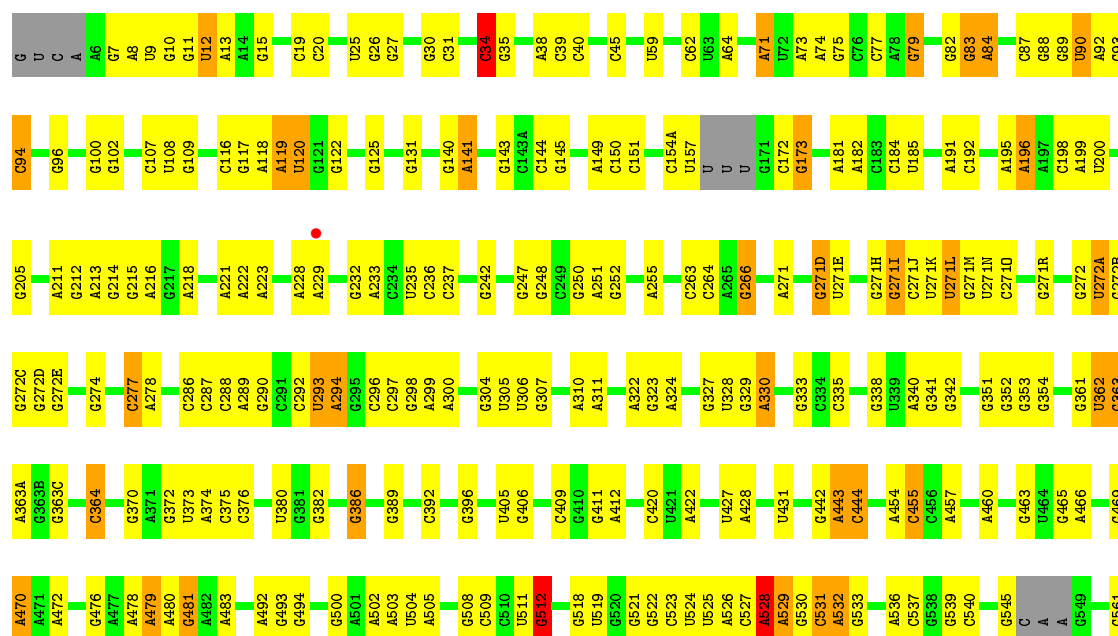


- Molecule 26: 23S Ribosomal RNA

Chain BA: 



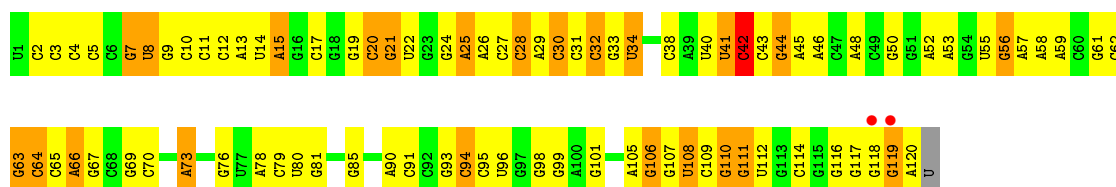
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A1786	A1785	A	G1421	A1275	C1153	C998	C893	G794	C	G577	A472	C335
A1919	G1674	C	G1422	A1276	C1154	U999	C894	G795	U	A578	A473	G352
A1791	C1683	G1537	C1428	U1292	A1155	A1001	U895	G796	C	G579	A474	A359
A1927	C1684	G1538	C1429	C1293	G1156	G1002	A896	C797	C	C580	A475	G360
A1928	C1685	G1539	C1430	C1294	G1157	C1005	G897	A800	C	G581	A476	G361
G1929	C1686	U1540	C1431	C1295	G1158	C1006	C898	A801	G	G582	A477	U362
G1930	C1687	A1541	U1432	C1296	G1159	C1007	C899	A802	C	G583	A478	G363
C1797	U1688	C1542	A1433	C1297	G1160	C1008	G900	G803	C	G584	A479	A363A
U1798	A1689	A1554	G1441	U1300	G1161	A1009	C901	G804	C	G585	A480	G363B
G1799	U1690	A1555	G1442	A1301	G1162	U1012	U902	A805	C	G586	A481	G363C
U1800	U1691	C1557	G1443	A1302	G1163	U1013	A903	G806	C	G587	A482	A359
A1803	G1696	A1558	A1444	G1303	G1164	U1014	A904	A807	C	G588	A483	G360
G1814	G1697	A1559	G1445	G1304	G1165	U1015	U905	A808	C	G589	A484	U361
A1815	G1698	A1560	G1446	U1313	G1166	U1016	A906	A809	C	G590	A485	U362
G1816	G1699	A1561	G1447	C1314	G1167	U1017	A907	A810	C	G591	A486	G372
U1817	A1700	A1562	G1448	C1315	G1168	A1021	A908	A811	C	G592	A487	A505
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A1825	G1702	A1564	G1450	C1317	G1170	G1025	A910	U826	C	G594	A489	U380
U1826	U1578	A1565	A1451	C1318	G1171	U1026	A911	U827	C	G595	A490	U383
G1827	A1579	A1566	U1452	C1319	G1172	A1027	A912	U828	C	G596	A491	G386
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A1829	G1703	A1568	G1454	C1321	G1174	U1029	A914	A830	C	G598	A493	C517
U1830	U1704	A1569	G1455	C1322	G1175	U1030	A915	G831	C	G599	A494	A526
G1831	G1705	A1570	A1456	C1323	G1176	U1031	A916	G832	C	G600	A495	C527
U1832	U1706	A1571	U1457	C1324	G1177	U1032	A917	U833	C	G601	A496	A528
G1833	G1707	A1572	G1458	C1325	G1178	A1033	A918	U834	C	G602	A497	U405
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A1841	U1715	A1580	A1466	C1333	G1186	U1041	A926	U842	C	G610	A505	U534
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G1846	U1720	A1585	G1471	C1338	G1191	U1046	A931	U847	C	G615	A510	G545
A1847	U1721	A1586	G1472	C1339	G1192	U1047	A932	U848	C	G616	A511	C
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G1849	G1723	A1588	G1474	C1341	G1194	U1049	A934	U850	C	G618	A513	A548
U1850	U1724	A1589	G1475	C1342	G1195	U1050	A935	U851	C	G619	A514	G549
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A1858	G1748	A1597	G1483	C1350	G1203	C	A943	U859	C	G627	A522	A
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G1860	U1730	A1599	G1485	C1352	G1205	C	A945	U861	C	G629	A524	A
A1861	C1749A	A1600	G1486	C1353	G1206	C	A946	U862	C	G630	A525	A
U1862	G1746	A1601	G1487	C1354	G1207	C	A947	U863	C	G631	A526	A
G1863	U1731	A1602	G1488	C1355	G1208	C	A948	U864	C	G632	A527	A
A1864	U1732	A1603	G1489	C1356	G1209	C	A949	U865	C	G633	A528	A
U1865	G1747	A1604	G1490	C1357	G1210	C	A950	U866	C	G634	A529	A
G1866	U1733	A1605	G1491	C1358	G1211	C	A951	U867	C	G635	A530	A
A1867	C1750A	A1606	G1492	C1359	G1212	C	A952	U868	C	G636	A531	A
U1868	G1748	A1607	G1493	C1360	G1213	C	A953	U869	C	G637	A532	A
G1869	U1734	A1608	G1494	C1361	G1214	C	A954	U870	C	G638	A533	A
A1870	C1751A	A1609	G1495	C1362	G1215	C	A955	U871	C	G639	A534	A
U1871	G1749	A1610	G1496	C1363	G1216	C	A956	U872	C	G640	A535	A
G1872	U1735	A1611	G1497	C1364	G1217	C	A957	U873	C	G641	A536	A
A1873	U1736	A1612	G1498	C1365	G1218	C	A958	U874	C	G642	A537	A
U1874	C1752A	A1613	G1499	C1366	G1219	C	A959	U875	C	G643	A538	A
G1875	G1750	A1614	G1500	C1367	G1220	C	A960	U876	C	G644	A539	A
A1876	U1737	A1615	G1501	C1368	G1221	C	A961	U877	C	G645	A540	A
U1877	C1753	A1616	G1502	C1369	G1222	C	A962	U878	C	G646	A541	A
G1878	G1751	A1617	G1503	C1370	G1223	C	A963	U879	C	G647	A542	A
A1879	U1738	A1618	G1504	C1371	G1224	C	A964	U880	C	G648	A543	A
U1880	C1754	A1619	G1505	C1372	G1225	C	A965	U881	C	G649	A544	A
G1881	G1752	A1620	G1506	C1373	G1226	C	A966	U882	C	G650	A545	A
A1882	U1739	A1621	G1507	C1374	G1227	C	A967	U883	C	G651	A546	A
U1883	C1755	A1622	G1508	C1375	G1228	C	A968	U884	C	G652	A547	A
G1884	G1753	A1623	G1509	C1376	G1229	C	A969	U885	C	G653	A548	A
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G1887	G1754	A1626	G1512	C1379	G1232	C	A972	U888	C	G656	A551	A
A1888	U1741	A1627	G1513	C1380	G1233	C	A973	U889	C	G657	A552	A
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G1890	G1755	A1629	G1515	C1382	G1235	C	A975	U891	C	G659	A554	A
A1891	U1742	A1630	G1516	C1383	G1236	C	A976	U892	C	G660	A555	A
U1892	C1758	A1631	G1517	C1384	G1237	C	A977	U893	C	G661	A556	A
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A1894	U1743	A1633	G1519	C1386	G1239	C	A979	U895	C	G663	A558	A
U1895	C1759	A1634	G1520	C1387	G1240	C	A980	U896	C	G664	A559	A
G1896	G1757	A1635	G1521	C1388	G1241	C	A981	U897	C	G665	A560	A
A1897	U1744	A1636	G1522	C1389	G1242	C	A982	U898	C	G666	A561	A
U1898	C1760	A1637	G1523	C1390	G1243	C	A983	U899	C	G667	A562	A
G1899	G1758	A1638	G1524	C1391	G1244	C	A984	U900	C	G668	A563	A
A1900	U1745	A1639	G1525	C1392	G1245	C	A985	U901	C	G669	A564	A
U1901	C1761	A1640	G1526	C1393	G1246	C	A986	U902	C	G670	A565	A
G1902	G1759	A1641	G1527	C1394	G1247	C	A987	U903	C	G671	A566	A
A1903	U1746	A1642	G1528	C1395	G1248	C	A988	U904	C	G672	A567	A
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A1906	U1747	A1645	G1531	C1398	G1251	C	A991	U907	C	G675	A570	A
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G1908	G1761	A1647	G1533	C1400	G1253	C	A993	U909	C	G677	A572	A
A1909	U1748	A1648	G1534	C1401	G1254	C	A994	U910	C	G678	A573	A
U1910	C1764	A1649	G1535	C1402	G1255	C	A995	U911	C	G679	A574	A
G1911	G1762	A1650	G1536	C1403	G1256	C	A996	U912	C	G680	A575	A
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U1913	C1765	A1652	G1538	C1405	G1258	C	A998	U914	C	G682	A577	A
G1914	G1763	A1653	G1539	C1406	G1259	C	A999	U915	C	G683	A578	A
A1915	U1750	A1654	G1540	C1407	G1260	C	A1000	U916	C	G684	A579	A
U1916	C1766	A1655	G1541	C1408	G1261	C	A1001	U917	C	G685	A580	A
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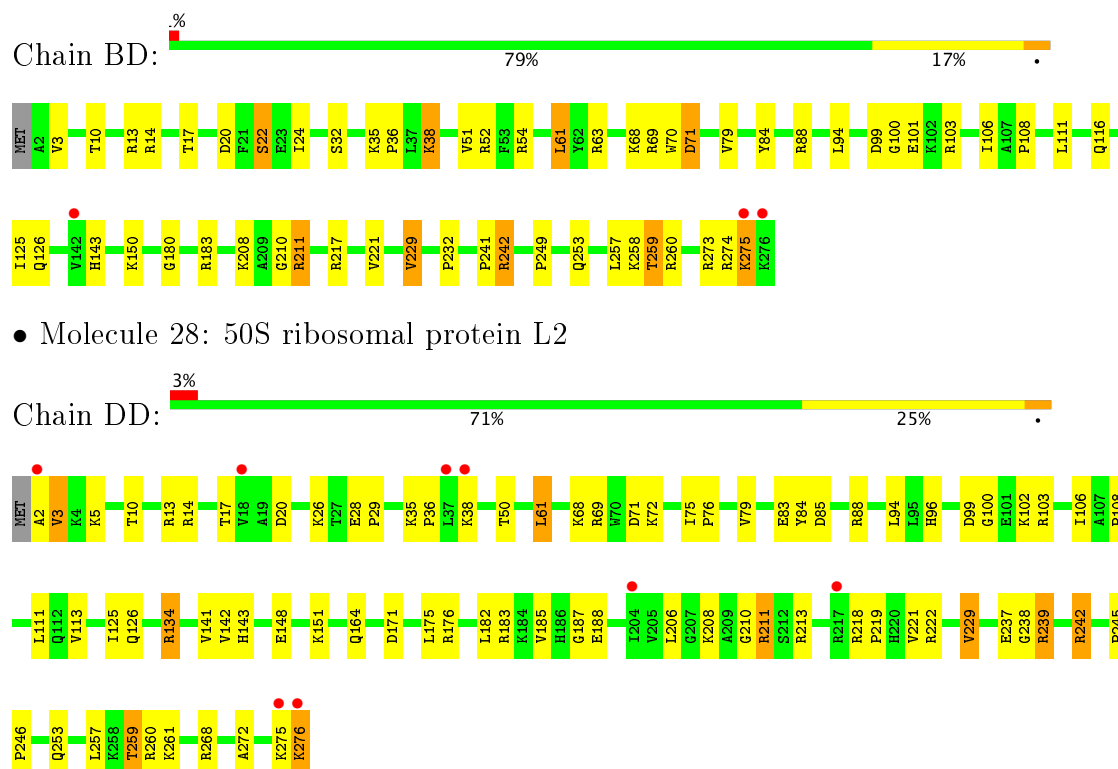


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G1793	G1667	A1567	G1488	C1291	U1205	G1122	G	G987	A901	A820	G723	G642	G563
C1794	A1668	G1568	U1489	U1292	A1210	G1123	U	A988	C902	A821	U724	A643	C564
U1795	A1669	G1569	C1293	C1293	G1211	G1125	G	C992	C903		G725	C645	C565
C1797		C1575	C1407	C1297	G1212	A1126	G	G993	C904	U827	G726	A646	U567
U1798	G1674	U1576	C1408	G1297	A1213	A1127	C	C994	U905	U828		G647	U568
G1799		C1577	C1409	G1298	C1218	A1128	U	C995	C908	A829	G729	G648	U569
C1800	U1688	U1578	G1410	G1299	G1219	A1129	U	A996	A909	U839	C730		G570
G1801	A1689	C1411	U1300	U1300	G1220	A1130	A	G997	A910	C840	C731	G651	A571
A1802	C1501	A1412	A1301	A1412	A1220	G1131	G	A1000	A911		C732	G652	A572
A1803		G1413	A1302	G1221	G1221	U1132	A	A1001	G916	U847	G733	A652A	G573
G1804	C1694		G1303	G1221A	C1135	G1136	A	C1005	A917	C848	A734	A652B	C574
U1805		G1416			G1137	G1138	G	C1006		A849	A735	G652C	A575
	G1695	C1417	A1308	G1229	G1230	G1139	C	A1010	G921	C852	U740		U576
A1812	G1696	C1418	A1309	G1230	G1231	G1140	C	A1011	U922	C853	G741	G652D	G577
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G1816	G1699	C1588	G1420	U1313	G1235	U1142	A	C1013	C925	C856		C	G582
	C1589	G1421	G1421	C1314	G1236	A1142A	U	U1014	A926	C857	A751	C	A586
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C1830		U1431		G1327	A1242	G1152	A	A1020	C936	A863	G765	G	G592
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G1834		C1436	C1436	G1334	G1245	G1155	A	G1025	A941	A866		C652T	G599
C1835		C1437	C1437	U1339	A1246	U1159	U	U1026	G942	C867	A774	G652U	G600
G1836		U1437	U1437	U1340	A1247		U	A1027	U943	U868	G775		C601
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A1848		U1453	U1453	A1359	U1255	G1169	A	A1032	C948	C875		C659	U606
				A1360	G1256	G1170	U	U1033	C949		G785	G660	U607
U1851				G1364	C1257	G1171	U	G1034	U950	A878		G661	
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A1853		G1461	G1461	A1366	C1259	U	C	A953	A954	C880		U667	U614
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		C1467	C1467	U1372	U1267	A1189	U	A	U958	C886			
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A1877		A1471	A1471	A1378	A1269	C1185	U	G	A960	C888			A621
G1878		C1474	C1474	A1379	A1270	G1186	U	A	C961	C889	G805	C692	G622
G1883		G1479	G1479	G1380	G1271	G1187	C	A	C971	A890	C906	G699	G623
A1884		G1480	G1480	A1384	A1272	U1188	A	G	C972	C892	U807		G624
A1885		U1481	U1481	G1385	A1273	A1189	C	C	A973	C893	G808	A706	A627
		A1482	A1482	C1386	A1274	U1199	C	C	G974	U895	G809	G707	
A1889		U1483	U1483	U1394	A1278	G1113	U	A	C975	A896		C812	A631
A1890		C1482	C1482	A1395	A1287	G1114	C	G	A980	C897	U813	G715	A637
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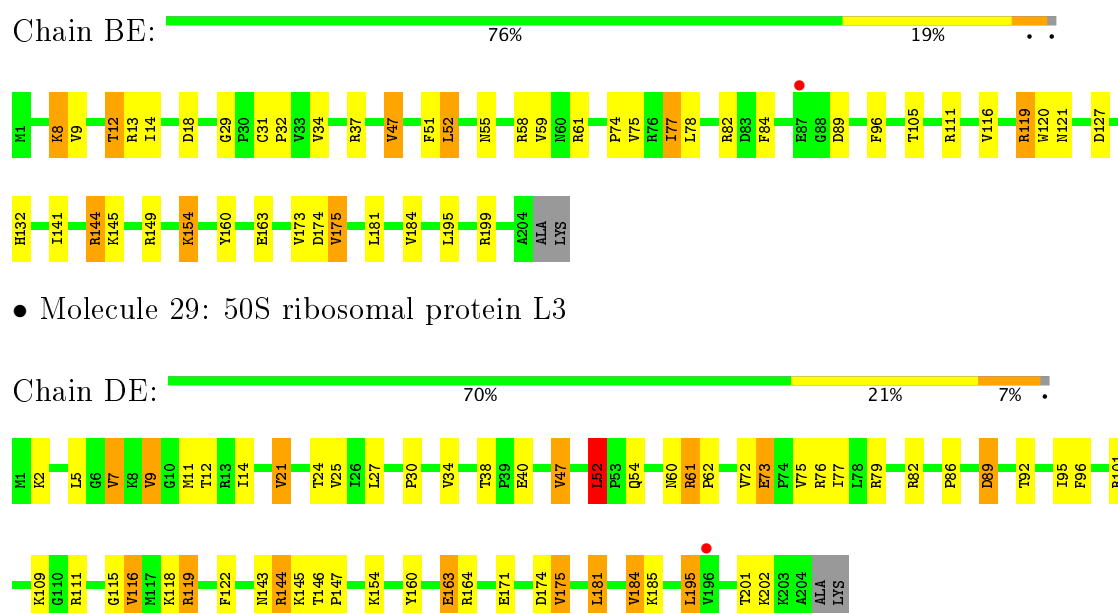




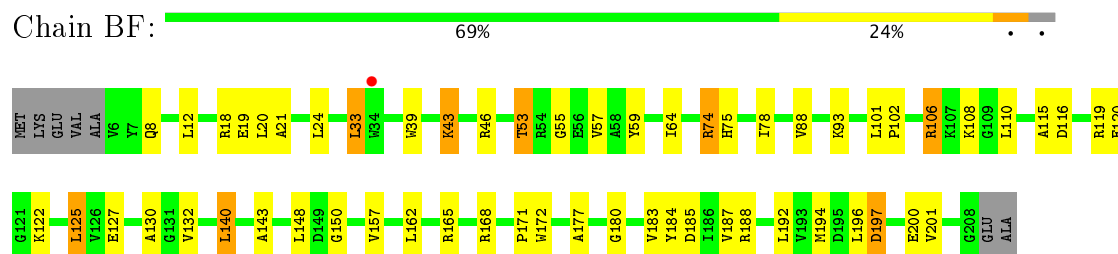
• Molecule 28: 50S ribosomal protein L2



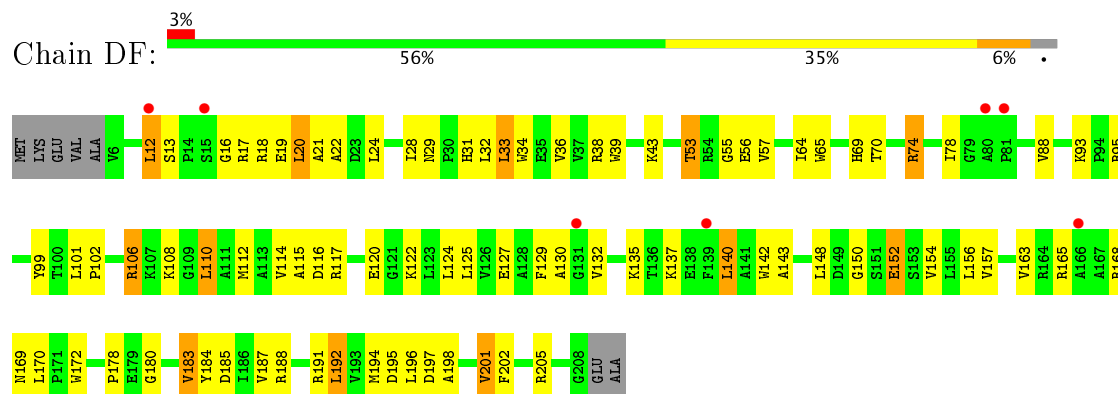
• Molecule 29: 50S ribosomal protein L3



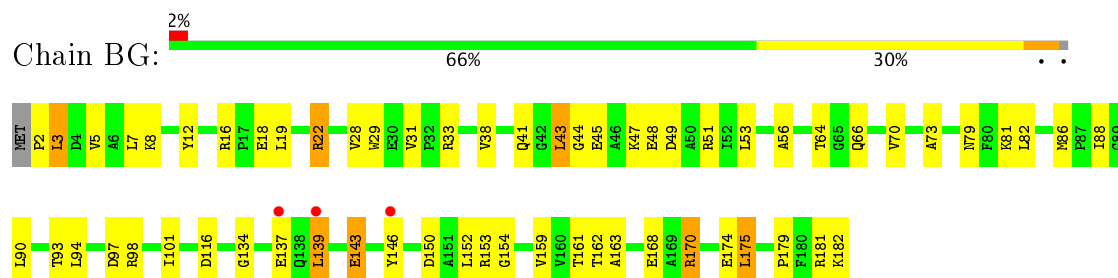
- Molecule 30: 50S ribosomal protein L4



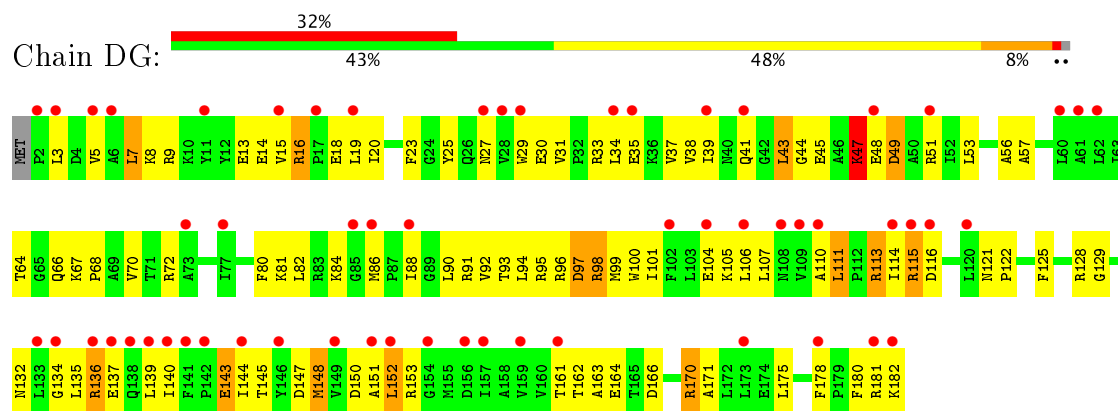
- Molecule 30: 50S ribosomal protein L4



- Molecule 31: 50S ribosomal protein L5

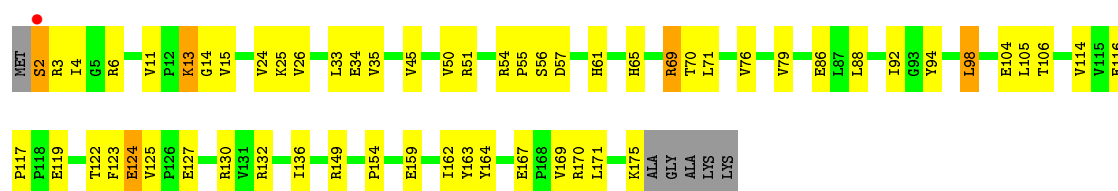


- Molecule 31: 50S ribosomal protein L5

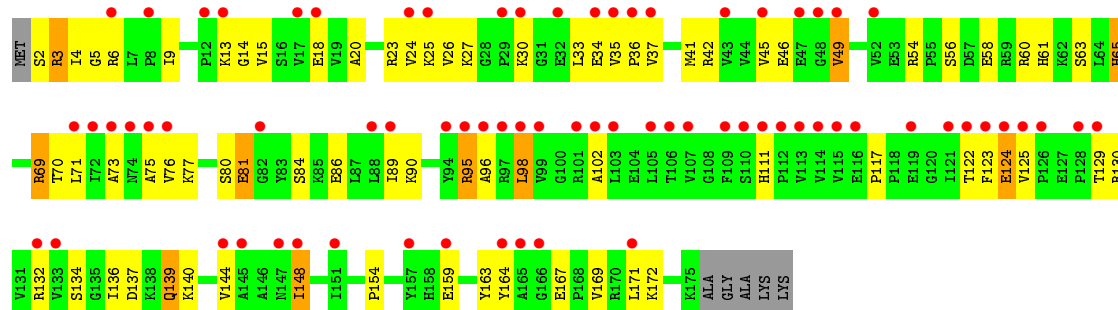
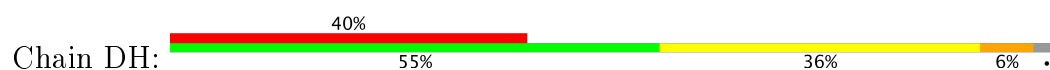


- Molecule 32: 50S ribosomal protein L6

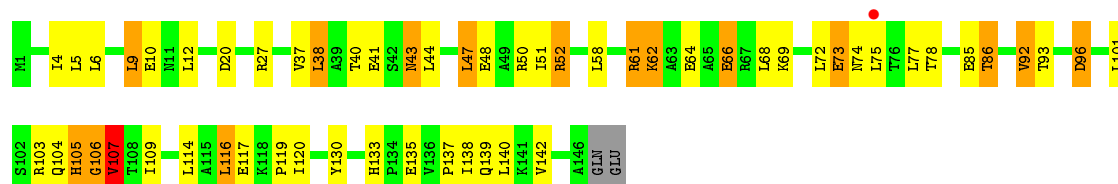




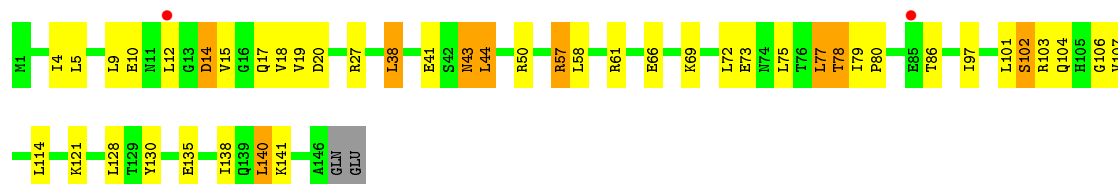
• Molecule 32: 50S ribosomal protein L6



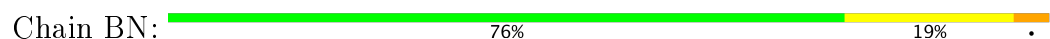
• Molecule 33: 50S ribosomal protein L9



• Molecule 33: 50S ribosomal protein L9

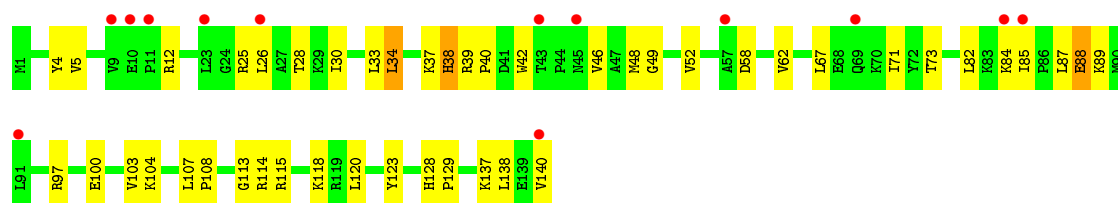


• Molecule 34: 50S ribosomal protein L13



• Molecule 34: 50S ribosomal protein L13





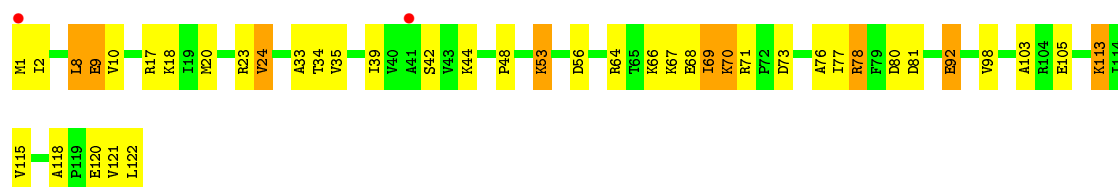
- Molecule 35: 50S ribosomal protein L14

Chain BO: 69% 28% .



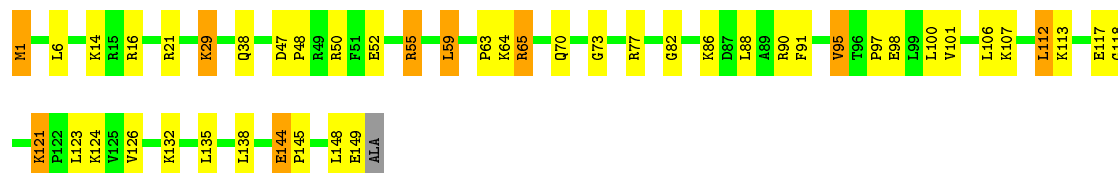
- Molecule 35: 50S ribosomal protein L14

Chain DO: 2% 66% 27% 7%



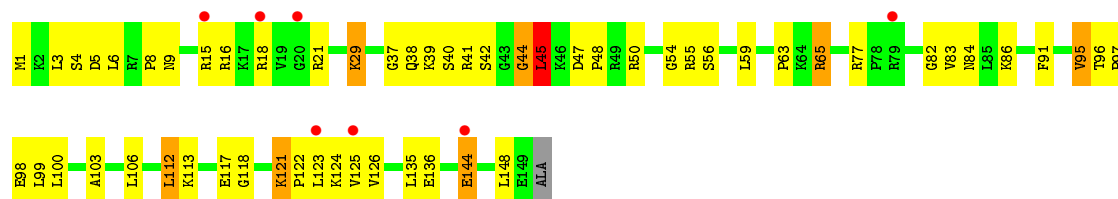
- Molecule 36: 50S ribosomal protein L15

Chain BP: 69% 25% 6% .



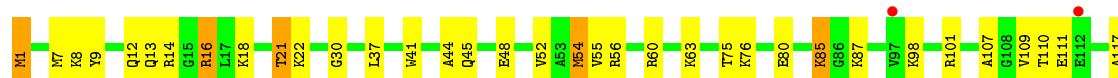
- Molecule 36: 50S ribosomal protein L15

Chain DP: 5% 61% 33% 5% ..



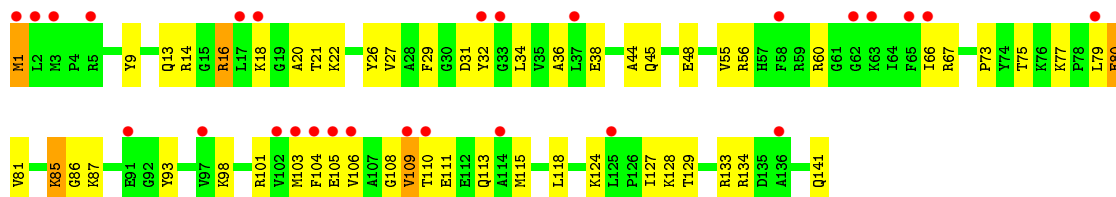
- Molecule 37: 50S ribosomal protein L16

Chain BQ: .% 74% 23% .

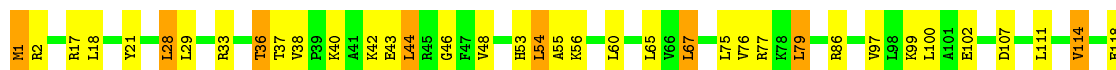




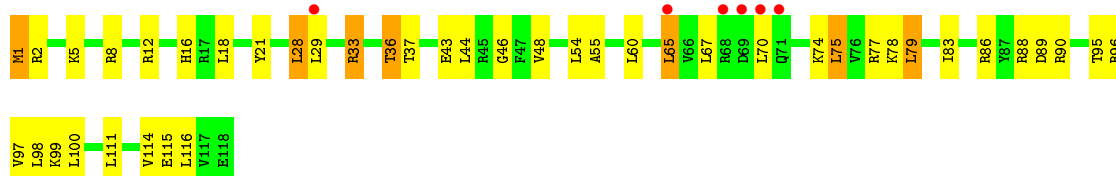
- Molecule 37: 50S ribosomal protein L16



- Molecule 38: 50S ribosomal protein L17



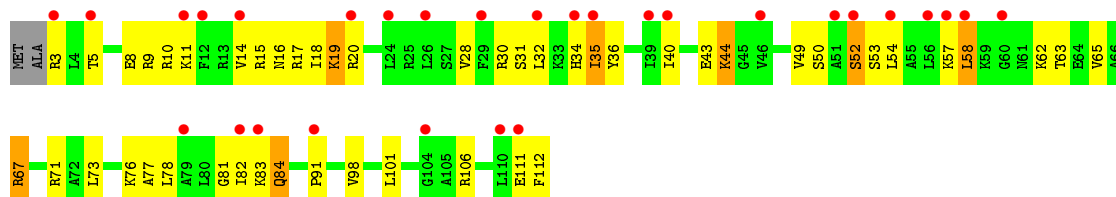
- Molecule 38: 50S ribosomal protein L17



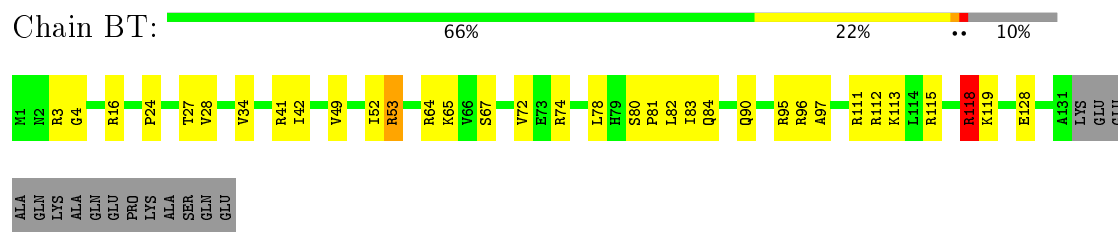
- Molecule 39: 50S ribosomal protein L18



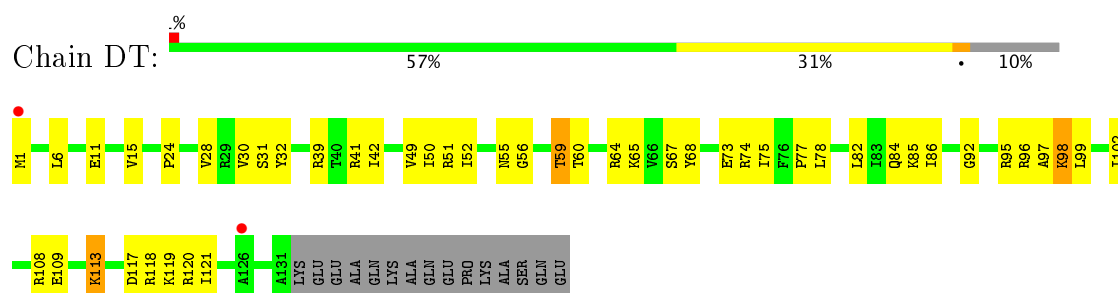
- Molecule 39: 50S ribosomal protein L18



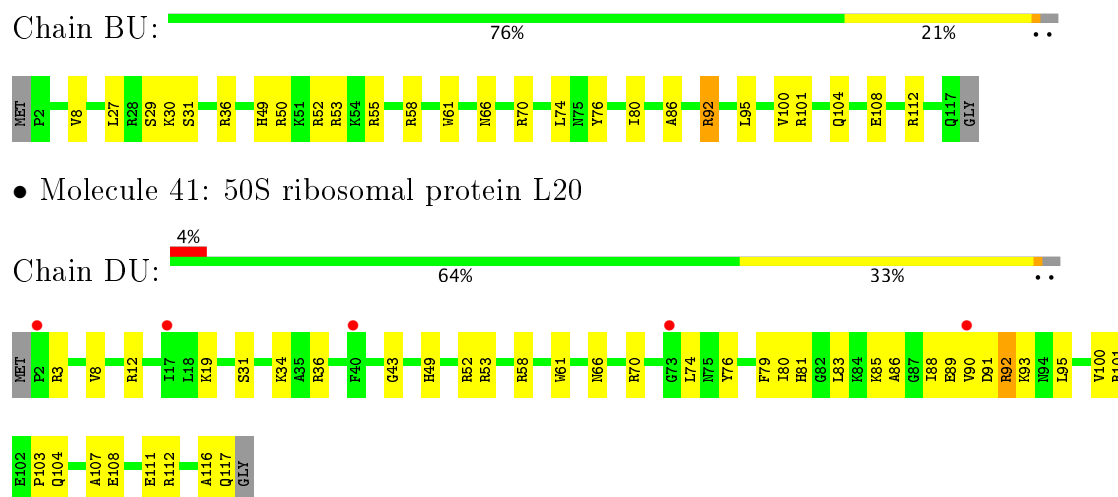
- Molecule 40: 50S ribosomal protein L19



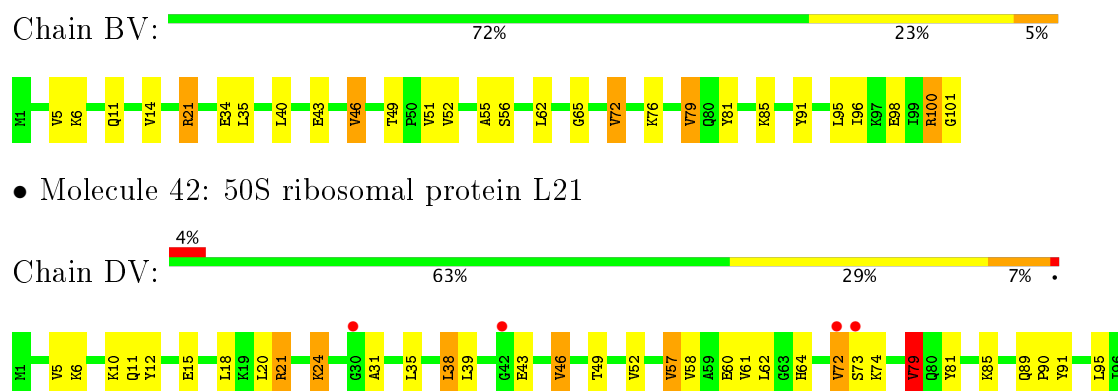
- Molecule 40: 50S ribosomal protein L19



- Molecule 41: 50S ribosomal protein L20



- Molecule 42: 50S ribosomal protein L21

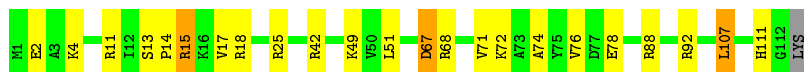






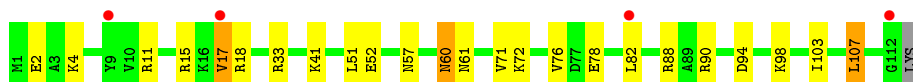
- Molecule 43: 50S ribosomal protein L22

Chain BW: 79% 18% ..



- Molecule 43: 50S ribosomal protein L22

Chain DW: 4% 78% 19% ..



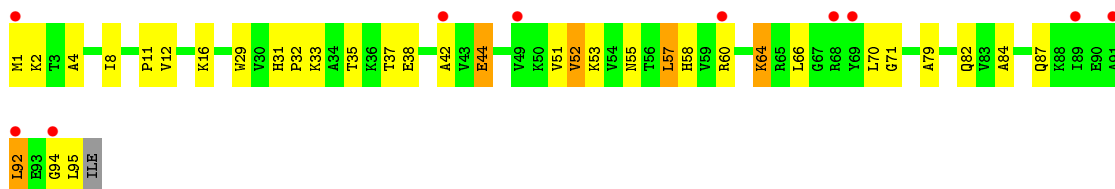
- Molecule 44: 50S ribosomal protein L23

Chain BX: 75% 20% ..



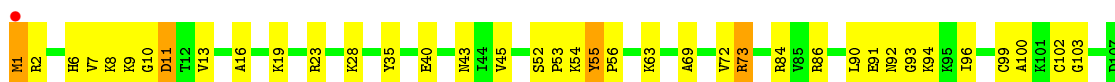
- Molecule 44: 50S ribosomal protein L23

Chain DX: 10% 64% 30% 5% ..



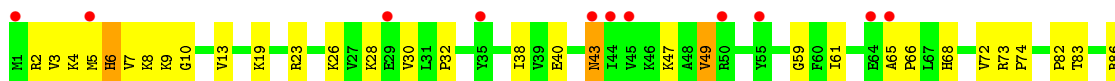
- Molecule 45: 50S ribosomal protein L24

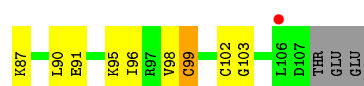
Chain BY: 63% 31% ..



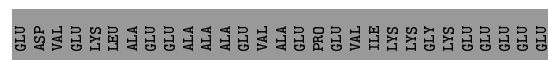
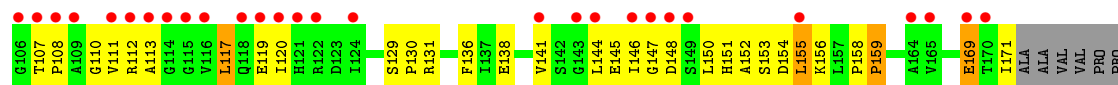
- Molecule 45: 50S ribosomal protein L24

Chain DY: 11% 60% 34% ..

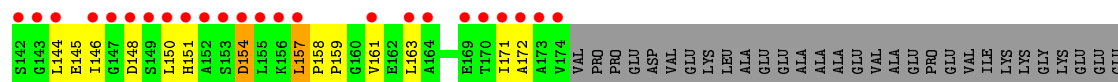
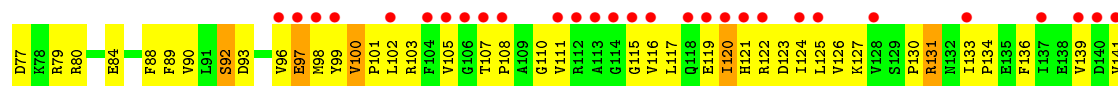
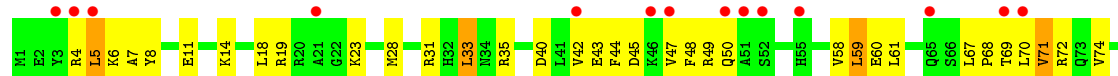
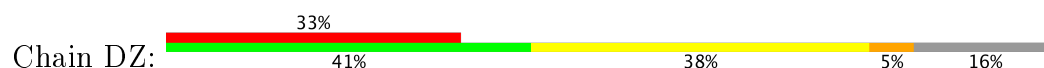




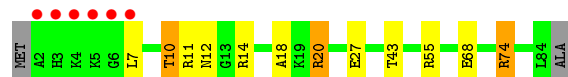
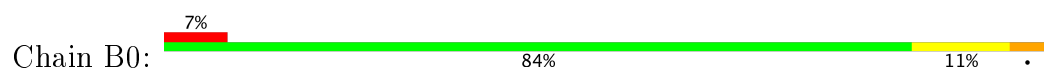
- Molecule 46: 50S ribosomal protein L25



- Molecule 46: 50S ribosomal protein L25



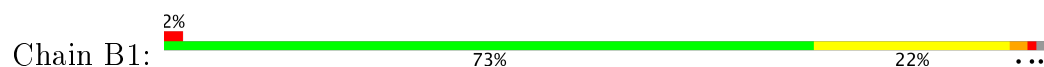
- Molecule 47: 50S ribosomal protein L27

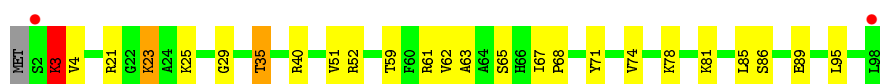


- Molecule 47: 50S ribosomal protein L27

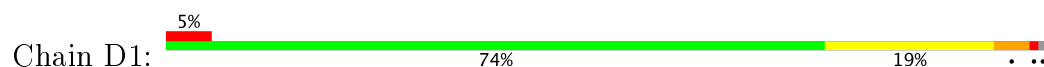


- Molecule 48: 50S ribosomal protein L28





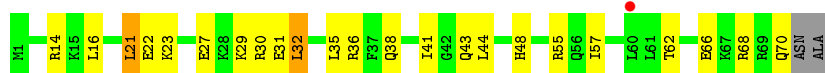
- Molecule 48: 50S ribosomal protein L28



- Molecule 49: 50S ribosomal protein L29



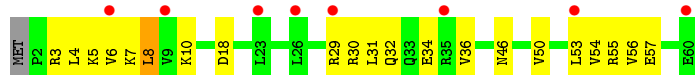
- Molecule 49: 50S ribosomal protein L29



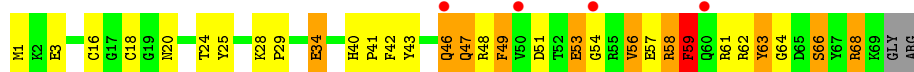
- Molecule 50: 50S ribosomal protein L30



- Molecule 50: 50S ribosomal protein L30

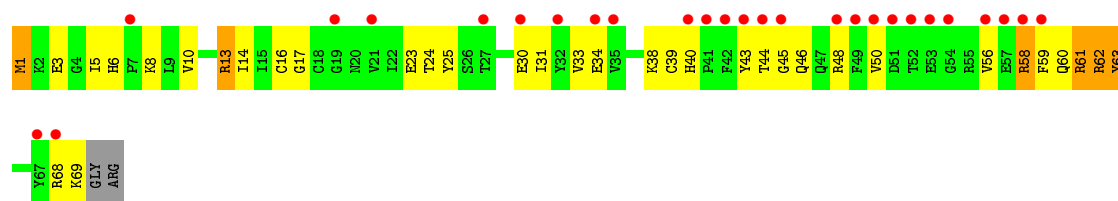


- Molecule 51: 50S ribosomal protein L31

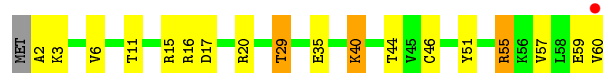


- Molecule 51: 50S ribosomal protein L31





- Molecule 52: 50S ribosomal protein L32



- Molecule 52: 50S ribosomal protein L32



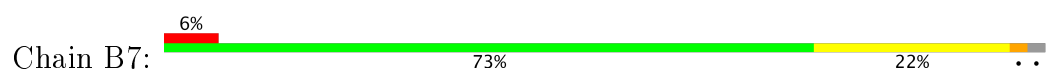
- Molecule 53: 50S ribosomal protein L33



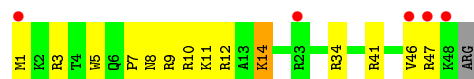
- Molecule 53: 50S ribosomal protein L33



- Molecule 54: 50S ribosomal protein L34



- Molecule 54: 50S ribosomal protein L34



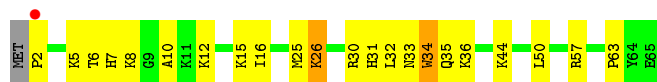
- Molecule 55: 50S ribosomal protein L35

Chain B8:  71% 26% ..




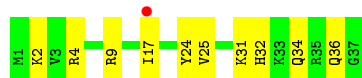
- Molecule 55: 50S ribosomal protein L35

Chain D8:  2% 65% 31% ..



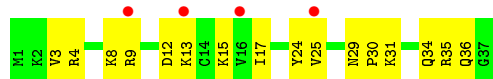
- Molecule 56: 50S ribosomal protein L36

Chain B9:  3% 73% 27%



- Molecule 56: 50S ribosomal protein L36

Chain D9:  11% 57% 43%



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	209.45Å 448.85Å 619.02Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	151.90 – 2.60 224.43 – 2.60	Depositor EDS
% Data completeness (in resolution range)	99.8 (151.90-2.60) 99.9 (224.43-2.60)	Depositor EDS
$R_{merge}$	0.23	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.22 (at 2.62Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.2_1309)	Depositor
R, $R_{free}$	0.223 , 0.264 0.235 , 0.273	Depositor DCC
$R_{free}$ test set	88430 reflections (5.29%)	DCC
Wilson B-factor (Å <sup>2</sup> )	56.4	Xtriage
Anisotropy	0.077	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.28 , 60.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.40$ , $\langle L^2 \rangle = 0.22$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	297127	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	60.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.55% 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: 5MU, ZN, MIA, SF4, MG, F3N, 31H, 5MC, 4SU, 7MG, K, PSU

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z  > 5$	RMSZ	# $ Z  > 5$
1	AA	0.38	0/36027	0.91	43/56227 (0.1%)
1	CA	0.41	8/36170 (0.0%)	1.01	101/56452 (0.2%)
2	AB	0.30	0/1881	0.62	0/2542
2	CB	0.33	0/1860	0.67	2/2518 (0.1%)
3	AC	0.27	0/1576	0.52	0/2130
3	CC	0.31	0/1568	0.61	1/2122 (0.0%)
4	AD	0.29	0/1689	0.55	0/2267
4	CD	0.30	0/1708	0.55	0/2289
5	AE	0.30	0/1145	0.54	0/1543
5	CE	0.33	0/1149	0.61	0/1548
6	AF	0.30	0/825	0.52	0/1118
6	CF	0.32	0/833	0.55	0/1128
7	AG	0.28	0/1250	0.50	0/1679
7	CG	0.27	0/1254	0.53	0/1683
8	AH	0.28	0/1108	0.52	0/1494
8	CH	0.29	0/1108	0.54	0/1494
9	AI	0.29	0/1005	0.57	0/1350
9	CI	0.31	0/997	0.64	0/1343
10	AJ	0.27	0/722	0.54	0/982
10	CJ	0.33	0/727	0.62	0/988
11	AK	0.28	0/848	0.51	0/1149
11	CK	0.28	0/848	0.53	0/1149
12	AL	0.33	0/946	0.52	0/1274
12	CL	0.30	0/946	0.58	0/1274
13	AM	0.31	0/977	0.60	0/1310
13	CM	0.31	0/961	0.62	1/1291 (0.1%)
14	AN	0.32	0/501	0.53	0/664
14	CN	0.33	0/501	0.57	0/664
15	AO	0.28	0/739	0.52	0/985
15	CO	0.29	0/739	0.54	0/985
16	AP	0.31	0/697	0.54	0/939
16	CP	0.29	0/693	0.51	0/935

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
17	AQ	0.29	0/836	0.53	0/1117
17	CQ	0.29	0/836	0.50	0/1117
18	AR	0.27	0/560	0.54	0/746
18	CR	0.29	0/560	0.56	0/746
19	AS	0.30	0/676	0.58	0/911
19	CS	0.33	0/661	0.71	0/893
20	AT	0.29	0/730	0.57	0/965
20	CT	0.28	0/733	0.55	0/969
21	AU	0.27	0/203	0.50	0/266
21	CU	0.33	0/203	0.53	0/266
22	AV	0.39	0/310	0.96	1/480 (0.2%)
22	CV	0.42	0/282	0.99	2/437 (0.5%)
23	AW	0.47	0/1577	1.20	7/2454 (0.3%)
23	CW	0.53	0/1531	1.28	9/2379 (0.4%)
24	AX	0.53	2/1700 (0.1%)	1.20	22/2650 (0.8%)
24	CX	0.46	0/1700	1.15	6/2650 (0.2%)
25	AY	0.58	0/1602	1.35	20/2493 (0.8%)
25	CY	0.59	0/1579	1.40	25/2455 (1.0%)
26	BA	0.50	1/68013 (0.0%)	0.93	91/106165 (0.1%)
26	DA	0.41	1/67542 (0.0%)	0.92	74/105428 (0.1%)
27	BB	0.41	0/2878	0.86	1/4490 (0.0%)
27	DB	0.44	0/2878	0.92	2/4490 (0.0%)
28	BD	0.37	0/2186	0.59	0/2944
28	DD	0.33	0/2192	0.57	0/2951
29	BE	0.37	0/1592	0.57	0/2149
29	DE	0.33	0/1592	0.55	0/2149
30	BF	0.34	0/1619	0.55	0/2193
30	DF	0.32	0/1615	0.55	0/2188
31	BG	0.31	0/1450	0.54	1/1959 (0.1%)
31	DG	0.33	0/1449	0.60	0/1958
32	BH	0.33	0/1356	0.54	0/1834
32	DH	0.29	0/1356	0.54	0/1834
33	BI	0.28	0/1100	0.56	0/1501
33	DI	0.29	0/1088	0.55	0/1484
34	BN	0.34	0/1144	0.53	0/1543
34	DN	0.31	0/1144	0.52	0/1543
35	BO	0.37	0/943	0.57	0/1269
35	DO	0.31	0/943	0.55	1/1269 (0.1%)
36	BP	0.35	0/1156	0.57	0/1537
36	DP	0.32	0/1152	0.61	1/1533 (0.1%)
37	BQ	0.35	0/1143	0.53	0/1527
37	DQ	0.32	0/1143	0.53	0/1527
38	BR	0.36	0/982	0.58	0/1312



Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
38	DR	0.30	0/982	0.53	0/1312
39	BS	0.31	0/887	0.56	0/1180
39	DS	0.28	0/880	0.56	0/1172
40	BT	0.34	0/1105	0.56	1/1477 (0.1%)
40	DT	0.31	0/1097	0.53	0/1468
41	BU	0.39	0/977	0.56	0/1301
41	DU	0.30	0/977	0.54	0/1301
42	BV	0.36	0/782	0.58	0/1049
42	DV	0.32	0/782	0.57	1/1049 (0.1%)
43	BW	0.39	0/897	0.56	0/1205
43	DW	0.31	0/897	0.52	0/1205
44	BX	0.38	0/764	0.57	1/1025 (0.1%)
44	DX	0.33	0/764	0.58	1/1025 (0.1%)
45	BY	0.35	0/819	0.57	0/1095
45	DY	0.32	0/819	0.55	0/1095
46	BZ	0.32	0/1379	0.58	0/1873
46	DZ	0.30	0/1390	0.56	0/1890
47	B0	0.35	0/662	0.55	0/881
47	D0	0.32	0/662	0.53	0/881
48	B1	0.35	0/762	0.54	0/1014
48	D1	0.31	0/762	0.53	0/1014
49	B2	0.31	0/590	0.53	0/781
49	D2	0.28	0/590	0.46	0/781
50	B3	0.34	0/474	0.57	0/635
50	D3	0.27	0/469	0.55	0/630
51	B4	0.31	0/571	0.70	0/768
51	D4	0.32	0/545	0.67	0/737
52	B5	0.35	0/469	0.65	0/635
52	D5	0.31	0/469	0.50	0/635
53	B6	0.37	0/460	0.52	0/613
53	D6	0.29	0/456	0.49	0/608
54	B7	0.40	0/426	0.57	0/561
54	D7	0.33	0/426	0.54	0/561
55	B8	0.37	0/525	0.59	0/691
55	D8	0.32	0/525	0.51	0/691
56	B9	0.37	0/310	0.50	0/407
56	D9	0.33	0/310	0.52	0/407
All	All	0.41	12/316594 (0.0%)	0.87	415/473940 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	AB	0	2
2	CB	0	1
7	AG	0	2
20	CT	0	1
33	BI	0	1
35	BO	0	1
39	BS	0	1
51	B4	0	1
All	All	0	10

The worst 5 of 12 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	CA	1154	G	N1-C2	-10.90	1.29	1.37
1	CA	1119	C	N3-C4	-10.71	1.26	1.33
1	CA	1154	G	C6-N1	-10.47	1.32	1.39
26	DA	528	A	N9-C4	-6.80	1.33	1.37
1	CA	1154	G	N7-C5	-6.78	1.35	1.39

The worst 5 of 415 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	CA	1119	C	N1-C2-O2	35.97	140.48	118.90
1	CA	1154	G	C5-C6-O6	25.44	143.86	128.60
1	CA	1154	G	N3-C2-N2	24.34	136.94	119.90
1	CA	1154	G	N1-C2-N2	-21.83	96.56	116.20
1	CA	1119	C	N3-C2-O2	-21.82	106.63	121.90

There are no chirality outliers.

5 of 10 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	AB	231	GLU	Peptide
2	AB	9	GLU	Peptide
7	AG	78	ARG	Peptide
7	AG	79	ARG	Peptide
33	BI	9	LEU	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	32185	0	16245	536	0
1	CA	32312	0	16307	762	0
2	AB	1846	0	1867	81	0
2	CB	1825	0	1828	119	0
3	AC	1552	0	1546	60	0
3	CC	1544	0	1524	70	0
4	AD	1659	0	1676	56	0
4	CD	1678	0	1718	67	0
5	AE	1129	0	1185	27	0
5	CE	1133	0	1191	46	0
6	AF	812	0	804	18	0
6	CF	820	0	814	19	0
7	AG	1231	0	1238	21	0
7	CG	1235	0	1249	39	0
8	AH	1088	0	1126	35	0
8	CH	1088	0	1126	40	0
9	AI	986	0	995	43	0
9	CI	978	0	966	55	0
10	AJ	709	0	650	34	0
10	CJ	714	0	672	44	0
11	AK	833	0	836	19	0
11	CK	833	0	836	22	0
12	AL	930	0	980	27	0
12	CL	930	0	980	33	0
13	AM	966	0	1024	40	0
13	CM	950	0	988	74	0
14	AN	492	0	529	26	0
14	CN	492	0	529	34	0
15	AO	728	0	760	20	0
15	CO	728	0	760	22	0
16	AP	681	0	697	27	0
16	CP	677	0	686	22	0
17	AQ	823	0	891	26	0
17	CQ	823	0	891	19	0
18	AR	555	0	618	12	0
18	CR	555	0	618	24	0
19	AS	661	0	675	31	0
19	CS	646	0	644	40	0
20	AT	728	0	798	26	0
20	CT	731	0	807	26	0
21	AU	199	0	208	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
21	CU	199	0	208	9	0
22	AV	277	0	140	3	0
22	CV	252	0	130	6	0
23	AW	1599	0	830	42	0
23	CW	1552	0	794	51	0
24	AX	1635	0	839	23	0
24	CX	1635	0	839	36	0
25	AY	1581	0	805	82	0
25	CY	1561	0	796	94	0
26	BA	60729	0	30622	666	0
26	DA	60311	0	30412	876	0
27	BB	2573	0	1306	20	0
27	DB	2573	0	1306	76	0
28	BD	2136	0	2218	42	0
28	DD	2142	0	2229	58	0
29	BE	1559	0	1618	25	0
29	DE	1559	0	1618	39	0
30	BF	1584	0	1625	39	0
30	DF	1580	0	1619	60	0
31	BG	1425	0	1443	38	0
31	DG	1424	0	1434	90	0
32	BH	1330	0	1407	34	0
32	DH	1330	0	1407	44	0
33	BI	1085	0	1114	37	0
33	DI	1073	0	1106	22	0
34	BN	1117	0	1184	23	0
34	DN	1117	0	1184	26	0
35	BO	933	0	996	25	0
35	DO	933	0	996	32	0
36	BP	1139	0	1223	41	0
36	DP	1135	0	1212	52	0
37	BQ	1122	0	1179	28	0
37	DQ	1122	0	1179	40	0
38	BR	968	0	1033	22	0
38	DR	968	0	1033	28	0
39	BS	877	0	938	20	0
39	DS	870	0	923	33	0
40	BT	1091	0	1151	26	0
40	DT	1083	0	1136	37	0
41	BU	959	0	1019	18	0
41	DU	959	0	1018	30	0
42	BV	771	0	830	13	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
42	DV	771	0	830	24	0
43	BW	886	0	940	17	0
43	DW	886	0	940	13	0
44	BX	750	0	814	15	0
44	DX	750	0	814	27	0
45	BY	806	0	881	27	0
45	DY	806	0	881	30	0
46	BZ	1349	0	1355	44	0
46	DZ	1360	0	1363	70	0
47	B0	653	0	674	13	0
47	D0	653	0	674	22	0
48	B1	755	0	826	16	0
48	D1	755	0	826	18	0
49	B2	588	0	643	11	0
49	D2	588	0	643	14	0
50	B3	469	0	518	6	0
50	D3	464	0	514	13	0
51	B4	558	0	544	37	0
51	D4	532	0	503	25	0
52	B5	455	0	465	14	0
52	D5	455	0	465	13	0
53	B6	453	0	473	13	0
53	D6	449	0	469	12	0
54	B7	418	0	467	10	0
54	D7	418	0	467	13	0
55	B8	517	0	582	17	0
55	D8	517	0	582	15	0
56	B9	307	0	335	7	0
56	D9	307	0	335	11	0
57	AA	216	0	0	0	0
57	AB	1	0	0	0	0
57	AE	1	0	0	0	0
57	AF	1	0	0	0	0
57	AK	1	0	0	0	0
57	AL	2	0	0	0	0
57	AM	2	0	0	0	0
57	AN	2	0	0	0	0
57	AT	1	0	0	0	0
57	AU	1	0	0	0	0
57	AW	2	0	0	0	0
57	AX	15	0	0	0	0
57	AY	3	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
57	B0	2	0	0	0	0
57	B2	1	0	0	0	0
57	B4	1	0	0	0	0
57	B5	3	0	0	0	0
57	B6	2	0	0	0	0
57	B7	5	0	0	0	0
57	B8	2	0	0	0	0
57	B9	1	0	0	0	0
57	BA	814	0	0	0	0
57	BB	23	0	0	0	0
57	BD	10	0	0	0	0
57	BE	6	0	0	0	0
57	BF	11	0	0	0	0
57	BG	2	0	0	0	0
57	BH	1	0	0	0	0
57	BN	3	0	0	0	0
57	BO	1	0	0	0	0
57	BP	2	0	0	0	0
57	BQ	2	0	0	0	0
57	BR	2	0	0	0	0
57	BU	4	0	0	0	0
57	BV	5	0	0	0	0
57	BW	4	0	0	0	0
57	BX	1	0	0	0	0
57	BY	1	0	0	0	0
57	BZ	2	0	0	0	0
57	CA	169	0	0	0	0
57	CD	1	0	0	0	0
57	CE	2	0	0	0	0
57	CF	1	0	0	0	0
57	CJ	1	0	0	0	0
57	CK	1	0	0	0	0
57	CT	1	0	0	0	0
57	CW	1	0	0	0	0
57	CX	2	0	0	0	0
57	D0	1	0	0	0	0
57	D3	1	0	0	0	0
57	D8	1	0	0	0	0
57	DA	664	0	0	0	0
57	DB	13	0	0	0	0
57	DD	4	0	0	0	0
57	DE	7	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
57	DF	5	0	0	0	0
57	DG	1	0	0	0	0
57	DN	1	0	0	0	0
57	DO	2	0	0	0	0
57	DP	2	0	0	0	0
57	DQ	3	0	0	0	0
57	DR	1	0	0	0	0
57	DU	1	0	0	0	0
57	DV	1	0	0	0	0
57	DW	1	0	0	0	0
57	DY	1	0	0	0	0
58	AD	8	0	0	1	0
58	CD	8	0	0	1	0
59	AN	1	0	0	0	0
59	B4	1	0	0	0	0
59	B5	1	0	0	0	0
59	B6	1	0	0	0	0
59	B9	1	0	0	0	0
59	BY	1	0	0	0	0
59	CN	1	0	0	0	0
59	D4	1	0	0	0	0
59	D5	1	0	0	0	0
59	D6	1	0	0	0	0
59	D9	1	0	0	0	0
59	DY	1	0	0	0	0
60	AX	1	0	0	0	0
61	AA	210	0	0	13	0
61	AD	1	0	0	0	0
61	AE	2	0	0	0	0
61	AJ	1	0	0	0	0
61	AL	2	0	0	1	0
61	AM	2	0	0	0	0
61	AV	2	0	0	0	0
61	AW	4	0	0	0	0
61	AX	4	0	0	0	0
61	AY	1	0	0	0	0
61	B0	6	0	0	0	0
61	B1	2	0	0	0	0
61	B3	2	0	0	0	0
61	B5	4	0	0	0	0
61	B6	2	0	0	0	0
61	B7	3	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
61	B8	13	0	0	0	0
61	B9	1	0	0	0	0
61	BA	1406	0	0	56	0
61	BB	37	0	0	1	0
61	BD	15	0	0	2	0
61	BE	17	0	0	4	0
61	BF	11	0	0	0	0
61	BG	3	0	0	0	0
61	BH	1	0	0	0	0
61	BI	1	0	0	0	0
61	BN	1	0	0	0	0
61	BO	2	0	0	0	0
61	BP	13	0	0	0	0
61	BQ	4	0	0	0	0
61	BR	2	0	0	0	0
61	BS	2	0	0	0	0
61	BT	2	0	0	0	0
61	BU	4	0	0	0	0
61	BV	2	0	0	0	0
61	BW	3	0	0	1	0
61	BX	3	0	0	0	0
61	BZ	1	0	0	0	0
61	CA	156	0	0	11	0
61	CE	2	0	0	0	0
61	CH	1	0	0	0	0
61	CJ	1	0	0	0	0
61	CK	1	0	0	0	0
61	CL	1	0	0	1	0
61	CT	1	0	0	0	0
61	CW	2	0	0	2	0
61	CX	2	0	0	0	0
61	CY	1	0	0	0	0
61	D0	4	0	0	0	0
61	D1	1	0	0	0	0
61	D3	2	0	0	0	0
61	D5	1	0	0	0	0
61	D6	1	0	0	0	0
61	D8	3	0	0	0	0
61	DA	989	0	0	44	0
61	DB	9	0	0	0	0
61	DD	18	0	0	3	0
61	DE	5	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
61	DF	4	0	0	0	0
61	DN	2	0	0	0	0
61	DP	12	0	0	4	0
61	DQ	1	0	0	0	0
61	DT	4	0	0	0	0
61	DU	1	0	0	0	0
61	DV	1	0	0	0	0
61	DW	1	0	0	0	0
61	DX	2	0	0	0	0
61	DY	1	0	0	0	0
All	All	297127	0	196404	5502	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 12.

The worst 5 of 5502 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)
26:DA:2139:C:N4	26:DA:2152:G:H1	1.46	1.14
1:CA:999:C:N4	1:CA:1042:G:H1	1.48	1.12
25:AY:49:C:N4	25:AY:65:G:H1	1.51	1.09
1:CA:985:C:N4	1:CA:1220:G:H1	1.50	1.09
1:CA:998:G:H1	1:CA:1043:C:N4	1.51	1.09

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

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

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
2	AB	229/256 (90%)	208 (91%)	13 (6%)	8 (4%)	<b>4</b> <b>6</b>
2	CB	229/256 (90%)	208 (91%)	14 (6%)	7 (3%)	<b>5</b> <b>8</b>

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	AC	204/239 (85%)	193 (95%)	10 (5%)	1 (0%)	32	58
3	CC	204/239 (85%)	191 (94%)	13 (6%)	0	100	100
4	AD	206/209 (99%)	197 (96%)	9 (4%)	0	100	100
4	CD	206/209 (99%)	200 (97%)	5 (2%)	1 (0%)	32	58
5	AE	146/162 (90%)	142 (97%)	4 (3%)	0	100	100
5	CE	146/162 (90%)	142 (97%)	3 (2%)	1 (1%)	25	49
6	AF	98/101 (97%)	95 (97%)	3 (3%)	0	100	100
6	CF	98/101 (97%)	95 (97%)	3 (3%)	0	100	100
7	AG	153/156 (98%)	149 (97%)	3 (2%)	1 (1%)	25	49
7	CG	153/156 (98%)	149 (97%)	3 (2%)	1 (1%)	25	49
8	AH	135/138 (98%)	133 (98%)	2 (2%)	0	100	100
8	CH	135/138 (98%)	131 (97%)	4 (3%)	0	100	100
9	AI	125/128 (98%)	119 (95%)	5 (4%)	1 (1%)	22	44
9	CI	125/128 (98%)	120 (96%)	4 (3%)	1 (1%)	22	44
10	AJ	95/105 (90%)	85 (90%)	8 (8%)	2 (2%)	8	15
10	CJ	94/105 (90%)	84 (89%)	6 (6%)	4 (4%)	3	4
11	AK	112/129 (87%)	107 (96%)	4 (4%)	1 (1%)	20	40
11	CK	112/129 (87%)	107 (96%)	4 (4%)	1 (1%)	20	40
12	AL	120/132 (91%)	118 (98%)	2 (2%)	0	100	100
12	CL	120/132 (91%)	117 (98%)	2 (2%)	1 (1%)	22	44
13	AM	121/126 (96%)	116 (96%)	4 (3%)	1 (1%)	22	44
13	CM	120/126 (95%)	113 (94%)	4 (3%)	3 (2%)	6	11
14	AN	58/61 (95%)	57 (98%)	1 (2%)	0	100	100
14	CN	58/61 (95%)	57 (98%)	1 (2%)	0	100	100
15	AO	86/89 (97%)	84 (98%)	2 (2%)	0	100	100
15	CO	86/89 (97%)	83 (96%)	3 (4%)	0	100	100
16	AP	80/88 (91%)	78 (98%)	2 (2%)	0	100	100
16	CP	80/88 (91%)	78 (98%)	1 (1%)	1 (1%)	14	29
17	AQ	97/105 (92%)	94 (97%)	3 (3%)	0	100	100
17	CQ	97/105 (92%)	94 (97%)	3 (3%)	0	100	100
18	AR	66/88 (75%)	64 (97%)	2 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
18	CR	66/88 (75%)	64 (97%)	2 (3%)	0	100	100
19	AS	82/93 (88%)	76 (93%)	5 (6%)	1 (1%)	15	32
19	CS	81/93 (87%)	75 (93%)	6 (7%)	0	100	100
20	AT	94/106 (89%)	85 (90%)	4 (4%)	5 (5%)	2	2
20	CT	94/106 (89%)	85 (90%)	4 (4%)	5 (5%)	2	2
21	AU	21/27 (78%)	20 (95%)	1 (5%)	0	100	100
21	CU	21/27 (78%)	21 (100%)	0	0	100	100
28	BD	273/276 (99%)	263 (96%)	9 (3%)	1 (0%)	38	63
28	DD	273/276 (99%)	261 (96%)	10 (4%)	2 (1%)	25	49
29	BE	202/206 (98%)	196 (97%)	5 (2%)	1 (0%)	32	58
29	DE	202/206 (98%)	196 (97%)	5 (2%)	1 (0%)	32	58
30	BF	201/210 (96%)	197 (98%)	3 (2%)	1 (0%)	32	58
30	DF	201/210 (96%)	197 (98%)	3 (2%)	1 (0%)	32	58
31	BG	179/182 (98%)	171 (96%)	7 (4%)	1 (1%)	28	53
31	DG	179/182 (98%)	168 (94%)	8 (4%)	3 (2%)	11	21
32	BH	172/180 (96%)	166 (96%)	6 (4%)	0	100	100
32	DH	172/180 (96%)	166 (96%)	6 (4%)	0	100	100
33	BI	144/148 (97%)	132 (92%)	7 (5%)	5 (4%)	4	6
33	DI	144/148 (97%)	135 (94%)	8 (6%)	1 (1%)	25	49
34	BN	138/140 (99%)	136 (99%)	2 (1%)	0	100	100
34	DN	138/140 (99%)	135 (98%)	3 (2%)	0	100	100
35	BO	120/122 (98%)	114 (95%)	6 (5%)	0	100	100
35	DO	120/122 (98%)	115 (96%)	5 (4%)	0	100	100
36	BP	147/150 (98%)	142 (97%)	4 (3%)	1 (1%)	25	49
36	DP	147/150 (98%)	139 (95%)	6 (4%)	2 (1%)	13	26
37	BQ	139/141 (99%)	135 (97%)	4 (3%)	0	100	100
37	DQ	139/141 (99%)	134 (96%)	4 (3%)	1 (1%)	25	49
38	BR	116/118 (98%)	115 (99%)	1 (1%)	0	100	100
38	DR	116/118 (98%)	114 (98%)	2 (2%)	0	100	100
39	BS	108/112 (96%)	106 (98%)	2 (2%)	0	100	100
39	DS	108/112 (96%)	107 (99%)	0	1 (1%)	20	40

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
40	BT	129/146 (88%)	123 (95%)	6 (5%)	0	100	100
40	DT	129/146 (88%)	126 (98%)	3 (2%)	0	100	100
41	BU	114/118 (97%)	114 (100%)	0	0	100	100
41	DU	114/118 (97%)	114 (100%)	0	0	100	100
42	BV	99/101 (98%)	93 (94%)	5 (5%)	1 (1%)	18	37
42	DV	99/101 (98%)	96 (97%)	2 (2%)	1 (1%)	18	37
43	BW	110/113 (97%)	110 (100%)	0	0	100	100
43	DW	110/113 (97%)	110 (100%)	0	0	100	100
44	BX	93/96 (97%)	91 (98%)	2 (2%)	0	100	100
44	DX	93/96 (97%)	91 (98%)	1 (1%)	1 (1%)	17	35
45	BY	105/110 (96%)	98 (93%)	7 (7%)	0	100	100
45	DY	105/110 (96%)	101 (96%)	4 (4%)	0	100	100
46	BZ	169/206 (82%)	153 (90%)	15 (9%)	1 (1%)	28	53
46	DZ	172/206 (84%)	159 (92%)	13 (8%)	0	100	100
47	B0	81/85 (95%)	81 (100%)	0	0	100	100
47	D0	81/85 (95%)	79 (98%)	1 (1%)	1 (1%)	15	32
48	B1	95/98 (97%)	93 (98%)	1 (1%)	1 (1%)	17	35
48	D1	95/98 (97%)	92 (97%)	2 (2%)	1 (1%)	17	35
49	B2	68/72 (94%)	68 (100%)	0	0	100	100
49	D2	68/72 (94%)	68 (100%)	0	0	100	100
50	B3	57/60 (95%)	56 (98%)	1 (2%)	0	100	100
50	D3	57/60 (95%)	55 (96%)	2 (4%)	0	100	100
51	B4	67/71 (94%)	54 (81%)	9 (13%)	4 (6%)	2	2
51	D4	67/71 (94%)	53 (79%)	11 (16%)	3 (4%)	3	3
52	B5	57/60 (95%)	55 (96%)	2 (4%)	0	100	100
52	D5	57/60 (95%)	56 (98%)	1 (2%)	0	100	100
53	B6	51/54 (94%)	49 (96%)	2 (4%)	0	100	100
53	D6	51/54 (94%)	49 (96%)	2 (4%)	0	100	100
54	B7	46/49 (94%)	45 (98%)	1 (2%)	0	100	100
54	D7	46/49 (94%)	45 (98%)	0	1 (2%)	8	14
55	B8	62/65 (95%)	62 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
55	D8	62/65 (95%)	62 (100%)	0	0	100	100
56	B9	35/37 (95%)	35 (100%)	0	0	100	100
56	D9	35/37 (95%)	35 (100%)	0	0	100	100
All	All	11410/12128 (94%)	10945 (96%)	381 (3%)	84 (1%)	25	49

5 of 84 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	AB	17	PHE
2	AB	19	HIS
2	AB	231	GLU
9	AI	54	ASP
10	AJ	56	HIS

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	AB	192/220 (87%)	155 (81%)	37 (19%)	1	2
2	CB	187/220 (85%)	151 (81%)	36 (19%)	1	2
3	AC	143/188 (76%)	127 (89%)	16 (11%)	7	12
3	CC	141/188 (75%)	116 (82%)	25 (18%)	2	3
4	AD	170/181 (94%)	147 (86%)	23 (14%)	4	7
4	CD	174/181 (96%)	147 (84%)	27 (16%)	3	5
5	AE	113/123 (92%)	106 (94%)	7 (6%)	21	42
5	CE	114/123 (93%)	99 (87%)	15 (13%)	5	8
6	AF	84/90 (93%)	74 (88%)	10 (12%)	6	11
6	CF	86/90 (96%)	79 (92%)	7 (8%)	14	26
7	AG	119/127 (94%)	99 (83%)	20 (17%)	2	4
7	CG	120/127 (94%)	106 (88%)	14 (12%)	6	11
8	AH	114/119 (96%)	101 (89%)	13 (11%)	7	12

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
8	CH	114/119 (96%)	97 (85%)	17 (15%)	3	6
9	AI	91/99 (92%)	73 (80%)	18 (20%)	1	2
9	CI	89/99 (90%)	69 (78%)	20 (22%)	1	2
10	AJ	66/92 (72%)	60 (91%)	6 (9%)	11	21
10	CJ	69/92 (75%)	61 (88%)	8 (12%)	6	11
11	AK	83/99 (84%)	74 (89%)	9 (11%)	7	14
11	CK	83/99 (84%)	72 (87%)	11 (13%)	4	8
12	AL	97/109 (89%)	88 (91%)	9 (9%)	10	20
12	CL	97/109 (89%)	85 (88%)	12 (12%)	5	10
13	AM	95/101 (94%)	81 (85%)	14 (15%)	3	6
13	CM	92/101 (91%)	74 (80%)	18 (20%)	1	2
14	AN	49/50 (98%)	40 (82%)	9 (18%)	2	3
14	CN	49/50 (98%)	37 (76%)	12 (24%)	1	1
15	AO	78/80 (98%)	70 (90%)	8 (10%)	8	15
15	CO	78/80 (98%)	67 (86%)	11 (14%)	4	7
16	AP	69/74 (93%)	58 (84%)	11 (16%)	3	5
16	CP	68/74 (92%)	59 (87%)	9 (13%)	5	8
17	AQ	94/97 (97%)	87 (93%)	7 (7%)	16	32
17	CQ	94/97 (97%)	84 (89%)	10 (11%)	8	14
18	AR	59/77 (77%)	50 (85%)	9 (15%)	3	5
18	CR	59/77 (77%)	46 (78%)	13 (22%)	1	2
19	AS	70/80 (88%)	59 (84%)	11 (16%)	3	5
19	CS	67/80 (84%)	54 (81%)	13 (19%)	1	2
20	AT	70/82 (85%)	60 (86%)	10 (14%)	4	6
20	CT	71/82 (87%)	62 (87%)	9 (13%)	5	9
21	AU	18/22 (82%)	15 (83%)	3 (17%)	2	4
21	CU	18/22 (82%)	15 (83%)	3 (17%)	2	4
28	BD	215/218 (99%)	196 (91%)	19 (9%)	12	22
28	DD	216/218 (99%)	200 (93%)	16 (7%)	16	32
29	BE	164/166 (99%)	145 (88%)	19 (12%)	6	11
29	DE	164/166 (99%)	141 (86%)	23 (14%)	4	7

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
30	BF	160/166 (96%)	142 (89%)	18 (11%)	7	12
30	DF	159/166 (96%)	138 (87%)	21 (13%)	5	8
31	BG	143/156 (92%)	127 (89%)	16 (11%)	7	12
31	DG	142/156 (91%)	119 (84%)	23 (16%)	3	4
32	BH	144/148 (97%)	129 (90%)	15 (10%)	8	15
32	DH	144/148 (97%)	124 (86%)	20 (14%)	4	7
33	BI	110/124 (89%)	88 (80%)	22 (20%)	1	2
33	DI	107/124 (86%)	87 (81%)	20 (19%)	2	3
34	BN	118/119 (99%)	101 (86%)	17 (14%)	4	6
34	DN	118/119 (99%)	101 (86%)	17 (14%)	4	6
35	BO	100/100 (100%)	92 (92%)	8 (8%)	14	27
35	DO	100/100 (100%)	89 (89%)	11 (11%)	7	13
36	BP	116/116 (100%)	104 (90%)	12 (10%)	8	15
36	DP	115/116 (99%)	103 (90%)	12 (10%)	8	15
37	BQ	111/111 (100%)	95 (86%)	16 (14%)	4	6
37	DQ	111/111 (100%)	97 (87%)	14 (13%)	5	9
38	BR	101/101 (100%)	83 (82%)	18 (18%)	2	3
38	DR	101/101 (100%)	86 (85%)	15 (15%)	3	6
39	BS	87/88 (99%)	79 (91%)	8 (9%)	11	20
39	DS	85/88 (97%)	74 (87%)	11 (13%)	5	9
40	BT	115/127 (91%)	107 (93%)	8 (7%)	18	35
40	DT	113/127 (89%)	105 (93%)	8 (7%)	17	34
41	BU	93/94 (99%)	86 (92%)	7 (8%)	16	31
41	DU	93/94 (99%)	87 (94%)	6 (6%)	20	39
42	BV	80/82 (98%)	70 (88%)	10 (12%)	5	10
42	DV	80/82 (98%)	67 (84%)	13 (16%)	3	4
43	BW	90/92 (98%)	83 (92%)	7 (8%)	15	29
43	DW	90/92 (98%)	84 (93%)	6 (7%)	19	38
44	BX	77/78 (99%)	72 (94%)	5 (6%)	20	39
44	DX	77/78 (99%)	70 (91%)	7 (9%)	11	21
45	BY	85/91 (93%)	77 (91%)	8 (9%)	10	19

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
45	DY	85/91 (93%)	78 (92%)	7 (8%)	13	26
46	BZ	145/179 (81%)	128 (88%)	17 (12%)	6	11
46	DZ	145/179 (81%)	127 (88%)	18 (12%)	5	10
47	B0	65/67 (97%)	61 (94%)	4 (6%)	21	42
47	D0	65/67 (97%)	59 (91%)	6 (9%)	11	20
48	B1	80/83 (96%)	72 (90%)	8 (10%)	9	17
48	D1	80/83 (96%)	71 (89%)	9 (11%)	7	12
49	B2	65/67 (97%)	59 (91%)	6 (9%)	11	20
49	D2	65/67 (97%)	60 (92%)	5 (8%)	15	29
50	B3	51/52 (98%)	47 (92%)	4 (8%)	15	29
50	D3	50/52 (96%)	47 (94%)	3 (6%)	22	44
51	B4	60/63 (95%)	51 (85%)	9 (15%)	3	6
51	D4	53/63 (84%)	38 (72%)	15 (28%)	0	1
52	B5	50/52 (96%)	46 (92%)	4 (8%)	14	27
52	D5	50/52 (96%)	48 (96%)	2 (4%)	36	64
53	B6	51/52 (98%)	45 (88%)	6 (12%)	6	11
53	D6	50/52 (96%)	47 (94%)	3 (6%)	22	44
54	B7	41/42 (98%)	39 (95%)	2 (5%)	29	54
54	D7	41/42 (98%)	39 (95%)	2 (5%)	29	54
55	B8	54/55 (98%)	50 (93%)	4 (7%)	16	32
55	D8	54/55 (98%)	50 (93%)	4 (7%)	16	32
56	B9	34/34 (100%)	33 (97%)	1 (3%)	48	75
56	D9	34/34 (100%)	33 (97%)	1 (3%)	48	75
All	All	9336/10066 (93%)	8180 (88%)	1156 (12%)	5	10

5 of 1156 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
51	B4	3	GLU
5	CE	79	GLU
43	DW	4	LYS
53	B6	28	ARG
3	CC	21	ARG



Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 127 such sidechains are listed below:

Mol	Chain	Res	Type
51	B4	46	GLN
4	CD	77	ASN
42	DV	64	HIS
2	CB	16	HIS
3	CC	3	ASN

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	AA	1494/1521 (98%)	361 (24%)	19 (1%)
1	CA	1501/1521 (98%)	370 (24%)	25 (1%)
22	AV	12/24 (50%)	3 (25%)	0
22	CV	11/24 (45%)	3 (27%)	0
23	AW	70/76 (92%)	27 (38%)	2 (2%)
23	CW	67/76 (88%)	26 (38%)	3 (4%)
24	AX	74/77 (96%)	16 (21%)	0
24	CX	74/77 (96%)	23 (31%)	0
25	AY	71/76 (93%)	37 (52%)	3 (4%)
25	CY	69/76 (90%)	36 (52%)	1 (1%)
26	BA	2812/2915 (96%)	444 (15%)	36 (1%)
26	DA	2791/2915 (95%)	563 (20%)	24 (0%)
27	BB	119/121 (98%)	13 (10%)	0
27	DB	119/121 (98%)	38 (31%)	0
All	All	9284/9620 (96%)	1960 (21%)	113 (1%)

5 of 1960 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	AA	5	U
1	AA	7	G
1	AA	9	G
1	AA	22	G
1	AA	29	G

5 of 113 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
26	BA	2181	G
1	CA	266	G
26	DA	1653	G

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Mol	Chain	Res	Type
26	BA	2183	C
26	BA	2689	U

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z  > 2$	Counts	RMSZ	# $ Z  > 2$
23	PSU	AW	32	57,23	16,21,22	1.32	1 (6%)	20,30,33	3.54	7 (35%)
23	MIA	AW	37	23	23,31,32	1.67	2 (8%)	25,44,47	1.37	4 (16%)
23	PSU	AW	39	23	16,21,22	1.34	1 (6%)	20,30,33	3.58	6 (30%)
23	7MG	AW	46	23	20,26,27	1.67	2 (10%)	22,39,42	2.77	5 (22%)
23	5MU	AW	54	23	14,22,23	0.71	0	16,32,35	2.42	2 (12%)
23	PSU	AW	55	23	16,21,22	1.43	1 (6%)	20,30,33	3.88	6 (30%)
23	F3N	AW	76	23	30,36,37	1.48	4 (13%)	29,51,54	2.01	1 (3%)
23	4SU	AW	8	23	14,21,22	1.30	1 (7%)	15,30,33	1.56	2 (13%)
24	5MC	AX	32	24	15,22,23	1.43	1 (6%)	17,32,35	1.10	2 (11%)
24	5MU	AX	54	24,57	14,22,23	0.78	0	16,32,35	2.30	3 (18%)
24	PSU	AX	55	24	16,21,22	1.66	2 (12%)	20,30,33	3.65	7 (35%)
24	31H	AX	76	24,57	28,34,35	1.18	3 (10%)	24,47,50	2.47	4 (16%)
24	4SU	AX	8	24	14,21,22	1.46	2 (14%)	15,30,33	2.68	2 (13%)
25	PSU	AY	32	25	16,21,22	1.18	1 (6%)	20,30,33	3.56	7 (35%)
25	MIA	AY	37	25	18,24,32	1.25	2 (11%)	17,35,47	1.78	2 (11%)
25	PSU	AY	39	25	16,21,22	1.32	1 (6%)	20,30,33	3.68	7 (35%)
25	7MG	AY	46	25	20,26,27	1.53	2 (10%)	22,39,42	3.24	8 (36%)
25	5MU	AY	54	25	14,22,23	0.83	1 (7%)	16,32,35	2.47	3 (18%)
25	PSU	AY	55	25	16,21,22	1.45	1 (6%)	20,30,33	3.50	6 (30%)
25	4SU	AY	8	25	14,21,22	1.30	1 (7%)	15,30,33	1.36	2 (13%)
23	PSU	CW	32	23	16,21,22	1.35	1 (6%)	20,30,33	3.59	6 (30%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
23	MIA	CW	37	23	18,24,32	1.20	2 (11%)	17,35,47	1.81	2 (11%)
23	PSU	CW	39	23	16,21,22	1.44	1 (6%)	20,30,33	3.93	6 (30%)
23	7MG	CW	46	23	20,26,27	1.81	2 (10%)	22,39,42	2.48	6 (27%)
23	5MU	CW	54	23	14,22,23	0.72	0	16,32,35	2.53	2 (12%)
23	PSU	CW	55	23	16,21,22	1.33	1 (6%)	20,30,33	3.58	6 (30%)
23	F3N	CW	76	23	30,36,37	1.50	5 (16%)	29,51,54	2.01	1 (3%)
23	4SU	CW	8	23	14,21,22	1.26	1 (7%)	15,30,33	1.32	2 (13%)
24	5MC	CX	32	24	15,22,23	1.33	1 (6%)	17,32,35	1.11	1 (5%)
24	5MU	CX	54	24	14,22,23	0.74	0	16,32,35	2.23	3 (18%)
24	PSU	CX	55	24	16,21,22	1.41	1 (6%)	20,30,33	3.53	7 (35%)
24	31H	CX	76	24,57	28,34,35	1.20	2 (7%)	24,47,50	2.56	2 (8%)
24	4SU	CX	8	24	14,21,22	1.24	2 (14%)	15,30,33	2.36	2 (13%)
25	PSU	CY	32	25	16,21,22	1.23	1 (6%)	20,30,33	3.70	7 (35%)
25	MIA	CY	37	25	18,24,32	1.26	2 (11%)	17,35,47	1.77	2 (11%)
25	PSU	CY	39	25	16,21,22	1.72	3 (18%)	20,30,33	3.37	7 (35%)
25	7MG	CY	46	25	20,26,27	1.70	2 (10%)	22,39,42	2.86	7 (31%)
25	5MU	CY	54	25	14,22,23	0.72	0	16,32,35	2.23	3 (18%)
25	PSU	CY	55	25	16,21,22	1.21	2 (12%)	20,30,33	3.61	6 (30%)
25	4SU	CY	8	25	14,21,22	1.35	1 (7%)	15,30,33	1.41	2 (13%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	PSU	AW	32	57,23	-	0/7/25/26	0/2/2/2
23	MIA	AW	37	23	-	0/11/33/34	0/3/3/3
23	PSU	AW	39	23	-	0/7/25/26	0/2/2/2
23	7MG	AW	46	23	-	0/7/37/38	0/3/3/3
23	5MU	AW	54	23	-	0/3/25/26	0/2/2/2
23	PSU	AW	55	23	-	0/7/25/26	0/2/2/2
23	F3N	AW	76	23	-	0/15/37/38	0/4/4/4
23	4SU	AW	8	23	-	0/3/25/26	0/2/2/2
24	5MC	AX	32	24	-	0/3/25/26	0/2/2/2
24	5MU	AX	54	24,57	-	0/3/25/26	0/2/2/2
24	PSU	AX	55	24	-	0/7/25/26	0/2/2/2
24	31H	AX	76	24,57	-	1/18/40/41	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	4SU	AX	8	24	-	0/3/25/26	0/2/2/2
25	PSU	AY	32	25	-	0/7/25/26	0/2/2/2
25	MIA	AY	37	25	-	0/3/25/34	0/3/3/3
25	PSU	AY	39	25	-	0/7/25/26	0/2/2/2
25	7MG	AY	46	25	-	0/7/37/38	0/3/3/3
25	5MU	AY	54	25	-	0/3/25/26	0/2/2/2
25	PSU	AY	55	25	-	0/7/25/26	0/2/2/2
25	4SU	AY	8	25	-	0/3/25/26	0/2/2/2
23	PSU	CW	32	23	-	0/7/25/26	0/2/2/2
23	MIA	CW	37	23	-	0/3/25/34	0/3/3/3
23	PSU	CW	39	23	-	0/7/25/26	0/2/2/2
23	7MG	CW	46	23	-	0/7/37/38	0/3/3/3
23	5MU	CW	54	23	-	0/3/25/26	0/2/2/2
23	PSU	CW	55	23	-	0/7/25/26	0/2/2/2
23	F3N	CW	76	23	-	0/15/37/38	0/4/4/4
23	4SU	CW	8	23	-	0/3/25/26	0/2/2/2
24	5MC	CX	32	24	-	0/3/25/26	0/2/2/2
24	5MU	CX	54	24	-	0/3/25/26	0/2/2/2
24	PSU	CX	55	24	-	0/7/25/26	0/2/2/2
24	31H	CX	76	24,57	-	1/18/40/41	0/3/3/3
24	4SU	CX	8	24	-	0/3/25/26	0/2/2/2
25	PSU	CY	32	25	-	0/7/25/26	0/2/2/2
25	MIA	CY	37	25	-	0/3/25/34	0/3/3/3
25	PSU	CY	39	25	-	0/7/25/26	0/2/2/2
25	7MG	CY	46	25	-	0/7/37/38	0/3/3/3
25	5MU	CY	54	25	-	0/3/25/26	0/2/2/2
25	PSU	CY	55	25	-	0/7/25/26	0/2/2/2
25	4SU	CY	8	25	-	0/3/25/26	0/2/2/2

The worst 5 of 59 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	AW	37	MIA	C2-S10	-6.29	1.70	1.75
24	AX	55	PSU	C5-C1'	-5.30	1.47	1.52
25	CY	39	PSU	C5-C1'	-5.21	1.47	1.52
23	AW	76	F3N	CB-CG	-5.00	1.39	1.51
25	AY	55	PSU	C5-C1'	-4.74	1.48	1.52

The worst 5 of 166 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	CW	39	PSU	N1-C2-N3	-10.64	120.75	128.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	CY	55	PSU	N1-C2-N3	-10.21	121.06	128.40
24	CX	76	31H	N3-C2-N1	-10.12	120.04	128.86
23	CW	76	F3N	N3-C2-N1	-10.11	120.06	128.86
25	AY	39	PSU	N1-C2-N3	-9.99	121.21	128.40

There are no chirality outliers.

All (2) torsion outliers are listed below:

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

There are no ring outliers.

26 monomers are involved in 48 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
23	AW	39	PSU	1	0
23	AW	55	PSU	1	0
23	AW	76	F3N	1	0
24	AX	32	5MC	2	0
24	AX	76	31H	1	0
24	AX	8	4SU	1	0
25	AY	37	MIA	1	0
25	AY	39	PSU	2	0
25	AY	46	7MG	3	0
25	AY	55	PSU	1	0
25	AY	8	4SU	1	0
23	CW	32	PSU	1	0
23	CW	39	PSU	1	0
23	CW	46	7MG	2	0
23	CW	55	PSU	1	0
23	CW	76	F3N	3	0
23	CW	8	4SU	2	0
24	CX	32	5MC	1	0
24	CX	55	PSU	1	0
24	CX	76	31H	1	0
24	CX	8	4SU	3	0
25	CY	37	MIA	3	0
25	CY	39	PSU	8	0
25	CY	46	7MG	4	0
25	CY	55	PSU	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
25	CY	8	4SU	2	0

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 2063 ligands modelled in this entry, 2061 are monoatomic - leaving 2 for Mogul analysis.

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

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

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

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

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 2 short contacts:

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

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data i

### 6.1 Protein, DNA and RNA chains i

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	1497/1521 (98%)	0.04	17 (1%) 80 77	41, 72, 93, 106	0
1	CA	1503/1521 (98%)	0.06	63 (4%) 37 29	43, 75, 94, 106	0
2	AB	231/256 (90%)	0.71	29 (12%) 4 2	68, 82, 89, 95	0
2	CB	231/256 (90%)	1.73	85 (36%) 0 0	68, 83, 90, 96	0
3	AC	206/239 (86%)	0.79	24 (11%) 5 3	69, 79, 87, 94	0
3	CC	206/239 (86%)	1.63	73 (35%) 0 0	70, 82, 90, 94	0
4	AD	208/209 (99%)	1.04	38 (18%) 1 1	57, 72, 81, 87	0
4	CD	208/209 (99%)	0.96	25 (12%) 5 3	60, 72, 81, 89	0
5	AE	148/162 (91%)	0.74	12 (8%) 13 8	58, 71, 81, 85	0
5	CE	148/162 (91%)	1.07	21 (14%) 3 1	60, 74, 83, 86	0
6	AF	100/101 (99%)	0.41	1 (1%) 82 79	52, 67, 75, 85	0
6	CF	100/101 (99%)	0.38	3 (3%) 51 43	57, 71, 81, 85	0
7	AG	155/156 (99%)	0.42	9 (5%) 24 18	66, 76, 85, 96	0
7	CG	155/156 (99%)	1.29	47 (30%) 0 0	68, 77, 86, 97	0
8	AH	137/138 (99%)	0.31	2 (1%) 74 69	62, 72, 79, 83	0
8	CH	137/138 (99%)	1.22	35 (25%) 1 0	64, 74, 80, 85	0
9	AI	127/128 (99%)	0.98	19 (14%) 3 1	62, 80, 87, 89	0
9	CI	127/128 (99%)	2.97	83 (65%) 0 0	69, 82, 89, 91	0
10	AJ	97/105 (92%)	0.81	12 (12%) 4 2	66, 83, 91, 92	0
10	CJ	96/105 (91%)	2.16	44 (45%) 0 0	68, 84, 91, 93	0
11	AK	114/129 (88%)	0.86	10 (8%) 11 7	51, 70, 80, 84	0
11	CK	114/129 (88%)	0.93	13 (11%) 6 3	52, 72, 81, 85	0
12	AL	122/132 (92%)	0.24	1 (0%) 86 83	41, 56, 71, 75	0
12	CL	122/132 (92%)	0.84	23 (18%) 1 1	58, 73, 82, 87	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
13	AM	123/126 (97%)	0.46	7 (5%) 24 18	57, 72, 83, 88	0
13	CM	122/126 (96%)	1.99	51 (41%) 0 0	69, 85, 92, 97	0
14	AN	60/61 (98%)	1.05	8 (13%) 4 2	70, 76, 83, 84	0
14	CN	60/61 (98%)	3.06	42 (70%) 0 0	73, 79, 85, 87	0
15	AO	88/89 (98%)	0.53	5 (5%) 24 18	54, 68, 79, 83	0
15	CO	88/89 (98%)	0.55	6 (6%) 18 13	56, 70, 81, 84	0
16	AP	82/88 (93%)	1.40	22 (26%) 1 0	59, 71, 79, 84	0
16	CP	82/88 (93%)	0.65	3 (3%) 42 34	59, 70, 79, 83	0
17	AQ	99/105 (94%)	0.62	8 (8%) 13 8	57, 70, 79, 84	0
17	CQ	99/105 (94%)	1.09	21 (21%) 1 0	60, 71, 79, 84	0
18	AR	68/88 (77%)	0.77	9 (13%) 4 2	59, 69, 81, 84	0
18	CR	68/88 (77%)	0.91	11 (16%) 2 1	58, 70, 81, 85	0
19	AS	84/93 (90%)	0.32	2 (2%) 59 52	70, 81, 87, 92	0
19	CS	83/93 (89%)	2.06	38 (45%) 0 0	74, 83, 90, 94	0
20	AT	96/106 (90%)	0.37	5 (5%) 28 21	59, 71, 80, 83	0
20	CT	96/106 (90%)	0.58	8 (8%) 12 8	59, 71, 80, 83	0
21	AU	23/27 (85%)	1.18	5 (21%) 1 0	70, 75, 78, 82	0
21	CU	23/27 (85%)	2.83	15 (65%) 0 0	71, 78, 81, 82	0
22	AV	13/24 (54%)	1.82	5 (38%) 0 0	58, 77, 95, 100	0
22	CV	12/24 (50%)	2.34	7 (58%) 0 0	64, 81, 93, 95	0
23	AW	66/76 (86%)	1.03	10 (15%) 2 1	66, 95, 102, 105	0
23	CW	64/76 (84%)	3.09	47 (73%) 0 0	70, 96, 101, 106	0
24	AX	71/77 (92%)	-0.01	0 100 100	42, 73, 90, 96	0
24	CX	71/77 (92%)	0.09	2 (2%) 53 46	55, 86, 95, 98	0
25	AY	67/76 (88%)	0.48	8 (11%) 5 3	44, 97, 101, 105	0
25	CY	66/76 (86%)	1.69	26 (39%) 0 0	48, 98, 102, 103	0
26	BA	2819/2915 (96%)	0.52	17 (0%) 89 88	23, 43, 87, 106	0
26	DA	2800/2915 (96%)	-0.11	60 (2%) 64 58	27, 48, 90, 108	0
27	BB	120/121 (99%)	0.49	0 100 100	41, 64, 76, 88	0
27	DB	120/121 (99%)	-0.08	2 (1%) 70 65	48, 70, 80, 91	0
28	BD	275/276 (99%)	0.46	3 (1%) 80 77	24, 41, 58, 79	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
28	DD	275/276 (99%)	0.40	8 (2%) 52 45	28, 44, 61, 79	0
29	BE	204/206 (99%)	0.59	1 (0%) 90 89	23, 46, 65, 83	0
29	DE	204/206 (99%)	0.25	1 (0%) 90 89	26, 50, 67, 84	0
30	BF	203/210 (96%)	0.61	1 (0%) 90 89	25, 51, 76, 86	0
30	DF	203/210 (96%)	0.43	7 (3%) 46 38	28, 56, 78, 88	0
31	BG	181/182 (99%)	0.51	3 (1%) 70 65	55, 72, 83, 93	0
31	DG	181/182 (99%)	1.53	58 (32%) 0 0	64, 76, 85, 93	0
32	BH	174/180 (96%)	0.51	1 (0%) 89 88	50, 66, 75, 82	0
32	DH	174/180 (96%)	1.75	72 (41%) 0 0	56, 71, 79, 83	0
33	BI	146/148 (98%)	0.34	1 (0%) 87 85	49, 74, 83, 87	0
33	DI	146/148 (98%)	0.12	2 (1%) 75 71	50, 74, 83, 87	0
34	BN	140/140 (100%)	0.67	0 100 100	29, 48, 67, 79	0
34	DN	140/140 (100%)	0.80	13 (9%) 9 6	35, 53, 70, 82	0
35	BO	122/122 (100%)	0.28	0 100 100	25, 40, 57, 67	0
35	DO	122/122 (100%)	0.47	2 (1%) 72 67	44, 58, 74, 79	0
36	BP	149/150 (99%)	0.55	0 100 100	25, 55, 75, 80	0
36	DP	149/150 (99%)	0.59	7 (4%) 32 25	28, 58, 78, 83	0
37	BQ	141/141 (100%)	0.76	2 (1%) 75 71	37, 52, 68, 77	0
37	DQ	141/141 (100%)	1.22	27 (19%) 1 1	41, 58, 72, 79	0
38	BR	118/118 (100%)	0.42	0 100 100	22, 34, 50, 59	0
38	DR	118/118 (100%)	0.65	6 (5%) 29 22	38, 53, 64, 75	0
39	BS	110/112 (98%)	0.33	0 100 100	34, 50, 64, 70	0
39	DS	110/112 (98%)	1.42	29 (26%) 1 0	70, 79, 87, 91	0
40	BT	131/146 (89%)	0.38	0 100 100	38, 51, 73, 82	0
40	DT	131/146 (89%)	0.23	2 (1%) 74 69	40, 54, 75, 81	0
41	BU	116/118 (98%)	0.43	0 100 100	17, 30, 50, 63	0
41	DU	116/118 (98%)	0.53	5 (4%) 36 28	40, 59, 79, 85	0
42	BV	101/101 (100%)	0.28	0 100 100	16, 38, 58, 68	0
42	DV	101/101 (100%)	0.32	4 (3%) 39 31	44, 73, 81, 92	0
43	BW	112/113 (99%)	0.37	0 100 100	22, 30, 49, 83	0
43	DW	112/113 (99%)	0.71	4 (3%) 43 35	35, 50, 66, 86	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
44	BX	95/96 (98%)	0.64	0 100 100	31, 46, 67, 83	0
44	DX	95/96 (98%)	0.70	10 (10%) 7 4	36, 50, 68, 83	0
45	BY	107/110 (97%)	0.47	1 (0%) 84 81	42, 59, 73, 84	0
45	DY	107/110 (97%)	0.77	12 (11%) 6 3	47, 61, 75, 84	0
46	BZ	171/206 (83%)	0.96	30 (17%) 2 1	40, 66, 91, 95	0
46	DZ	174/206 (84%)	1.92	67 (38%) 0 0	69, 85, 94, 101	0
47	B0	83/85 (97%)	0.96	6 (7%) 16 12	34, 50, 67, 75	0
47	D0	83/85 (97%)	1.14	10 (12%) 5 3	40, 56, 71, 76	0
48	B1	97/98 (98%)	0.47	2 (2%) 64 58	31, 49, 72, 76	0
48	D1	97/98 (98%)	0.54	5 (5%) 28 21	34, 53, 73, 78	0
49	B2	70/72 (97%)	0.42	0 100 100	33, 49, 64, 82	0
49	D2	70/72 (97%)	0.39	1 (1%) 75 71	58, 69, 78, 82	0
50	B3	59/60 (98%)	0.22	0 100 100	24, 37, 63, 74	0
50	D3	59/60 (98%)	0.92	8 (13%) 3 2	52, 65, 79, 87	0
51	B4	69/71 (97%)	0.46	4 (5%) 24 18	49, 76, 89, 91	0
51	D4	69/71 (97%)	1.73	27 (39%) 0 0	74, 89, 95, 99	0
52	B5	59/60 (98%)	0.41	1 (1%) 70 65	16, 30, 46, 68	0
52	D5	59/60 (98%)	0.30	1 (1%) 70 65	35, 49, 65, 77	0
53	B6	53/54 (98%)	0.31	0 100 100	32, 44, 57, 72	0
53	D6	53/54 (98%)	0.70	3 (5%) 24 18	49, 64, 74, 79	0
54	B7	48/49 (97%)	0.76	3 (6%) 21 15	23, 32, 58, 70	0
54	D7	48/49 (97%)	0.98	5 (10%) 7 4	26, 35, 61, 70	0
55	B8	64/65 (98%)	0.62	0 100 100	34, 42, 50, 65	0
55	D8	64/65 (98%)	0.55	1 (1%) 72 67	37, 46, 54, 65	0
56	B9	37/37 (100%)	0.94	1 (2%) 55 48	36, 51, 65, 73	0
56	D9	37/37 (100%)	0.71	4 (10%) 6 4	43, 55, 68, 76	0
All	All	20895/21748 (96%)	0.54	1600 (7%) 14 10	16, 64, 89, 108	0

The worst 5 of 1600 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	CB	165	VAL	12.1
46	DZ	155	LEU	10.5

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Mol	Chain	Res	Type	RSRZ
13	CM	124	PRO	10.0
46	DZ	107	THR	9.1
46	DZ	171	ILE	8.7

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 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
23	PSU	AW	32	20/21	0.86	0.26	-	77,84,98,106	0
23	MIA	AW	37	29/30	0.93	0.25	-	56,65,80,82	0
23	MIA	CW	37	22/30	0.87	0.30	-	72,86,92,96	0
24	31H	AX	76	32/33	0.94	0.33	-	31,57,76,77	10
23	7MG	AW	46	24/25	0.80	0.21	-	80,97,112,135	0
25	7MG	AY	46	24/25	0.82	0.18	-	80,99,107,116	0
24	4SU	CX	8	20/21	0.80	0.13	-	84,92,105,111	0
25	PSU	CY	32	20/21	0.83	0.26	-	77,91,109,114	0
23	PSU	CW	32	20/21	0.87	0.48	-	77,86,95,106	0
23	PSU	AW	55	20/21	0.83	0.28	-	76,88,103,105	0
25	PSU	CY	55	20/21	0.75	0.41	-	86,100,107,118	0
25	PSU	AY	55	20/21	0.80	0.20	-	85,96,106,117	0
23	5MU	AW	54	21/22	0.91	0.21	-	66,80,87,93	0
24	5MC	AX	32	21/22	0.97	0.20	-	50,57,69,76	0
23	4SU	AW	8	20/21	0.84	0.17	-	83,89,107,110	0
23	PSU	AW	39	20/21	0.93	0.24	-	71,82,92,93	0
25	MIA	AY	37	22/30	0.86	0.22	-	79,89,101,116	0
24	5MU	CX	54	21/22	0.94	0.21	-	71,85,94,104	0
24	5MC	CX	32	21/22	0.95	0.18	-	63,77,85,87	0
23	F3N	CW	76	33/34	0.93	0.44	-	53,69,79,80	0
25	PSU	AY	32	20/21	0.83	0.26	-	76,92,107,110	0
24	PSU	CX	55	20/21	0.92	0.15	-	81,87,92,97	0
23	5MU	CW	54	21/22	0.86	0.23	-	76,87,97,99	0
23	PSU	CW	55	20/21	0.84	0.34	-	76,90,103,106	0
25	4SU	CY	8	20/21	0.79	0.16	-	88,102,112,128	0
23	F3N	AW	76	33/34	0.94	0.38	-	44,58,72,77	0
24	PSU	AX	55	20/21	0.94	0.16	-	52,69,77,77	0
25	4SU	AY	8	20/21	0.83	0.13	-	83,95,104,129	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
25	5MU	CY	54	21/22	0.74	0.49	-	89,99,105,136	0
23	4SU	CW	8	20/21	0.77	0.29	-	85,96,117,121	0
25	PSU	CY	39	20/21	0.81	0.27	-	86,91,104,110	0
25	MIA	CY	37	22/30	0.79	0.30	-	79,95,102,124	0
25	5MU	AY	54	21/22	0.85	0.20	-	81,89,99,128	0
24	4SU	AX	8	20/21	0.93	0.17	-	59,69,79,85	0
23	7MG	CW	46	24/25	0.73	0.33	-	81,97,101,125	0
25	7MG	CY	46	24/25	0.71	0.25	-	87,101,108,135	0
23	PSU	CW	39	20/21	0.89	0.42	-	76,85,92,95	0
24	5MU	AX	54	21/22	0.96	0.16	-	46,72,77,86	0
25	PSU	AY	39	20/21	0.86	0.25	-	84,90,102,107	0
24	31H	CX	76	32/33	0.90	0.35	-	48,68,88,99	0

### 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

### 6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 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( $\text{\AA}^2$ )	Q<0.9
57	MG	BA	3770	1/1	0.97	0.44	27.31	49,49,49,49	0
57	MG	BA	3710	1/1	0.66	0.79	26.21	65,65,65,65	0
57	MG	BA	3174	1/1	0.97	0.53	25.24	38,38,38,38	0
57	MG	BA	3135	1/1	0.94	0.45	23.76	56,56,56,56	0
57	MG	BA	3214	1/1	0.96	0.50	23.57	43,43,43,43	0
57	MG	DA	3027	1/1	0.97	0.53	23.22	43,43,43,43	0
57	MG	BA	3219	1/1	0.92	0.50	19.46	58,58,58,58	0
57	MG	DA	3029	1/1	0.96	0.57	18.76	45,45,45,45	0
57	MG	BA	3033	1/1	0.97	0.40	16.53	31,31,31,31	0
57	MG	BA	3136	1/1	0.97	0.36	15.91	49,49,49,49	0
57	MG	BA	3215	1/1	0.96	0.42	14.79	37,37,37,37	0
57	MG	CA	3130	1/1	0.74	0.28	14.39	64,64,64,64	0
57	MG	BA	3103	1/1	0.85	0.35	13.36	63,63,63,63	0
57	MG	BA	3591	1/1	0.98	0.39	13.31	41,41,41,41	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	BA	3204	1/1	0.96	0.27	12.92	67,67,67,67	0
57	MG	BA	3111	1/1	0.83	0.32	12.80	53,53,53,53	0
57	MG	BA	3018	1/1	0.86	0.40	12.66	39,39,39,39	0
57	MG	BA	3456	1/1	0.86	0.30	12.30	37,37,37,37	0
57	MG	BA	3775	1/1	0.93	0.33	12.06	39,39,39,39	0
57	MG	BA	3743	1/1	0.94	0.59	11.52	47,47,47,47	0
57	MG	DA	3602	1/1	0.94	0.26	11.41	62,62,62,62	0
57	MG	DA	3102	1/1	0.95	0.32	10.88	40,40,40,40	0
57	MG	BA	3182	1/1	0.98	0.67	10.80	52,52,52,52	0
57	MG	BA	3256	1/1	0.97	0.34	10.60	34,34,34,34	0
57	MG	DA	3026	1/1	0.93	0.72	10.57	50,50,50,50	0
57	MG	DA	3500	1/1	0.87	0.35	10.41	55,55,55,55	0
57	MG	AX	3002	1/1	0.94	0.30	10.37	71,71,71,71	0
57	MG	BA	3044	1/1	0.94	0.35	10.11	43,43,43,43	0
57	MG	BA	3083	1/1	0.97	0.34	10.02	60,60,60,60	0
57	MG	BA	3171	1/1	0.90	0.32	9.99	35,35,35,35	0
57	MG	BA	3142	1/1	0.96	0.31	9.64	46,46,46,46	0
57	MG	BX	3001	1/1	0.91	0.35	9.48	44,44,44,44	0
57	MG	DU	201	1/1	0.88	0.57	9.39	58,58,58,58	0
57	MG	BA	3070	1/1	0.94	0.24	9.36	41,41,41,41	0
57	MG	BA	3100	1/1	0.94	0.25	9.27	61,61,61,61	0
57	MG	DA	3192	1/1	0.87	0.32	9.26	34,34,34,34	0
57	MG	DE	3001	1/1	0.98	0.44	9.21	31,31,31,31	0
57	MG	BF	306	1/1	0.91	0.33	8.90	49,49,49,49	0
57	MG	BA	3061	1/1	0.95	0.30	8.78	25,25,25,25	0
57	MG	BD	3003	1/1	0.91	0.30	8.72	37,37,37,37	0
57	MG	BV	201	1/1	0.94	0.36	8.67	31,31,31,31	0
57	MG	BA	3424	1/1	0.97	0.29	8.49	31,31,31,31	0
57	MG	DA	3042	1/1	0.87	0.29	8.28	49,49,49,49	0
57	MG	AA	1756	1/1	0.90	0.33	8.24	45,45,45,45	0
57	MG	DA	3624	1/1	0.75	0.48	8.23	59,59,59,59	0
57	MG	DV	201	1/1	0.88	0.50	8.23	58,58,58,58	0
57	MG	BA	3035	1/1	0.96	0.27	8.05	49,49,49,49	0
57	MG	DA	3660	1/1	0.94	0.52	7.98	46,46,46,46	0
57	MG	BA	3041	1/1	0.71	0.29	7.83	63,63,63,63	0
57	MG	BA	3561	1/1	0.87	0.26	7.57	34,34,34,34	0
57	MG	CA	3167	1/1	0.97	0.30	7.56	57,57,57,57	0
57	MG	BA	3688	1/1	0.72	0.27	7.44	61,61,61,61	0
57	MG	DF	305	1/1	0.93	0.59	7.17	45,45,45,45	0
57	MG	AA	1702	1/1	0.98	0.27	7.07	47,47,47,47	0
57	MG	DA	3464	1/1	0.93	0.30	6.86	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
57	MG	DA	3621	1/1	0.94	0.49	6.55	52,52,52,52	0
57	MG	BA	3674	1/1	0.97	0.34	6.50	48,48,48,48	0
57	MG	BA	3369	1/1	0.78	0.28	6.38	62,62,62,62	0
57	MG	BA	3680	1/1	0.73	0.32	6.32	42,42,42,42	0
57	MG	BA	3608	1/1	0.83	0.29	6.28	58,58,58,58	0
57	MG	AX	3003	1/1	0.86	0.23	5.98	56,56,56,56	0
57	MG	DA	3422	1/1	0.89	0.24	5.91	62,62,62,62	0
57	MG	BA	3124	1/1	0.92	0.28	5.90	57,57,57,57	0
57	MG	DA	3617	1/1	0.86	0.25	5.89	51,51,51,51	0
57	MG	DB	3008	1/1	0.95	0.17	5.88	56,56,56,56	0
57	MG	DA	3169	1/1	0.97	0.28	5.81	41,41,41,41	0
57	MG	BA	3216	1/1	0.96	0.28	5.69	39,39,39,39	0
57	MG	AA	1757	1/1	0.95	0.25	5.60	68,68,68,68	0
57	MG	DQ	3003	1/1	0.73	0.64	5.55	62,62,62,62	0
57	MG	DA	3160	1/1	0.91	0.34	5.31	62,62,62,62	0
57	MG	CA	3067	1/1	0.98	0.24	5.29	46,46,46,46	0
57	MG	BA	3176	1/1	0.74	0.26	5.09	55,55,55,55	0
57	MG	BA	3814	1/1	0.91	0.28	5.07	39,39,39,39	0
57	MG	BF	304	1/1	0.96	0.39	5.06	41,41,41,41	0
57	MG	DA	3456	1/1	0.84	0.21	5.05	38,38,38,38	0
57	MG	DA	3119	1/1	0.92	0.26	4.99	50,50,50,50	0
57	MG	BA	3507	1/1	0.91	0.26	4.90	43,43,43,43	0
57	MG	BF	302	1/1	0.94	0.31	4.88	30,30,30,30	0
57	MG	BU	201	1/1	0.94	0.36	4.81	43,43,43,43	0
57	MG	DA	3220	1/1	0.94	0.32	4.79	50,50,50,50	0
57	MG	DA	3491	1/1	0.85	0.25	4.78	43,43,43,43	0
57	MG	DA	3060	1/1	0.94	0.28	4.65	60,60,60,60	0
57	MG	BU	204	1/1	0.98	0.31	4.59	47,47,47,47	0
57	MG	DF	301	1/1	0.92	0.31	4.59	48,48,48,48	0
57	MG	BA	3672	1/1	0.92	0.25	4.46	44,44,44,44	0
57	MG	BA	3085	1/1	0.99	0.29	4.45	31,31,31,31	0
57	MG	BA	3403	1/1	0.93	0.29	4.43	33,33,33,33	0
57	MG	BA	3186	1/1	0.97	0.27	4.12	41,41,41,41	0
57	MG	AA	1675	1/1	0.93	0.24	4.08	61,61,61,61	0
57	MG	BU	203	1/1	0.97	0.31	3.63	34,34,34,34	0
57	MG	BA	3121	1/1	0.75	0.29	3.57	42,42,42,42	0
57	MG	BD	3007	1/1	0.95	0.30	3.48	46,46,46,46	0
57	MG	AA	1687	1/1	0.91	0.21	3.47	46,46,46,46	0
57	MG	DA	3070	1/1	0.59	0.19	3.47	65,65,65,65	0
57	MG	BA	3526	1/1	0.90	0.26	3.29	41,41,41,41	0
59	ZN	B6	102	1/1	0.99	0.26	3.29	50,50,50,50	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	DA	3657	1/1	0.79	0.45	3.26	54,54,54,54	0
57	MG	BA	3520	1/1	0.95	0.25	3.18	29,29,29,29	0
57	MG	DA	3503	1/1	0.96	0.22	2.98	38,38,38,38	0
57	MG	BA	3530	1/1	0.86	0.25	2.91	33,33,33,33	0
57	MG	DA	3103	1/1	0.98	0.22	2.90	56,56,56,56	0
57	MG	DA	3323	1/1	0.97	0.21	2.89	49,49,49,49	0
57	MG	BA	3210	1/1	0.94	0.25	2.84	41,41,41,41	0
57	MG	BA	3700	1/1	0.80	0.24	2.80	36,36,36,36	0
57	MG	BA	3716	1/1	0.95	0.25	2.79	45,45,45,45	0
57	MG	BD	3008	1/1	0.98	0.30	2.74	45,45,45,45	0
57	MG	BA	3543	1/1	0.93	0.23	2.69	52,52,52,52	0
57	MG	DA	3325	1/1	0.95	0.23	2.69	45,45,45,45	0
57	MG	DA	3362	1/1	0.92	0.24	2.68	42,42,42,42	0
57	MG	BF	303	1/1	0.96	0.26	2.66	33,33,33,33	0
57	MG	CA	3168	1/1	0.95	0.20	2.66	41,41,41,41	0
57	MG	BA	3425	1/1	0.98	0.25	2.60	48,48,48,48	0
57	MG	AA	1730	1/1	0.98	0.25	2.59	27,27,27,27	0
57	MG	BA	3007	1/1	0.97	0.23	2.55	21,21,21,21	0
57	MG	DA	3191	1/1	0.79	0.30	2.52	54,54,54,54	0
57	MG	BA	3310	1/1	0.98	0.23	2.51	26,26,26,26	0
57	MG	BA	3648	1/1	0.96	0.22	2.49	58,58,58,58	0
57	MG	DA	3274	1/1	0.98	0.22	2.36	40,40,40,40	0
57	MG	BA	3529	1/1	0.89	0.25	2.32	24,24,24,24	0
57	MG	BA	3244	1/1	0.95	0.26	2.30	31,31,31,31	0
57	MG	BA	3037	1/1	0.95	0.28	2.29	42,42,42,42	0
57	MG	BA	3200	1/1	0.83	0.25	2.24	48,48,48,48	0
57	MG	AA	1725	1/1	0.96	0.22	2.24	51,51,51,51	0
57	MG	DA	3161	1/1	0.86	0.17	2.19	50,50,50,50	0
57	MG	BA	3807	1/1	0.82	0.24	2.19	66,66,66,66	0
57	MG	BA	3400	1/1	0.92	0.24	2.15	39,39,39,39	0
57	MG	BA	3795	1/1	0.96	0.25	2.10	19,19,19,19	0
57	MG	DA	3105	1/1	0.93	0.22	2.08	45,45,45,45	0
57	MG	DA	3090	1/1	0.92	0.31	2.03	50,50,50,50	0
57	MG	DA	3606	1/1	0.83	0.20	2.00	74,74,74,74	0
57	MG	DA	3213	1/1	0.97	0.18	1.97	37,37,37,37	0
57	MG	AA	1691	1/1	0.92	0.27	1.93	62,62,62,62	0
57	MG	BA	3172	1/1	0.96	0.26	1.90	40,40,40,40	0
57	MG	B7	103	1/1	0.91	0.30	1.89	40,40,40,40	0
57	MG	DA	3124	1/1	0.95	0.17	1.88	43,43,43,43	0
57	MG	DA	3167	1/1	0.94	0.21	1.88	40,40,40,40	0
57	MG	CA	3093	1/1	0.95	0.20	1.86	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
57	MG	DA	3089	1/1	0.80	0.18	1.85	52,52,52,52	0
57	MG	BA	3356	1/1	0.97	0.24	1.82	31,31,31,31	0
57	MG	B5	101	1/1	0.99	0.28	1.82	30,30,30,30	0
57	MG	CA	3050	1/1	0.82	0.19	1.80	73,73,73,73	0
57	MG	BA	3194	1/1	0.89	0.25	1.76	39,39,39,39	0
57	MG	DA	3134	1/1	0.94	0.21	1.72	52,52,52,52	0
57	MG	DA	3334	1/1	0.97	0.22	1.70	57,57,57,57	0
57	MG	BA	3133	1/1	0.97	0.27	1.68	37,37,37,37	0
57	MG	DA	3247	1/1	0.94	0.16	1.66	49,49,49,49	0
57	MG	BA	3179	1/1	0.93	0.23	1.66	43,43,43,43	0
57	MG	BV	202	1/1	0.95	0.25	1.64	32,32,32,32	0
57	MG	DA	3410	1/1	0.95	0.22	1.63	40,40,40,40	0
57	MG	BA	3409	1/1	0.96	0.23	1.51	22,22,22,22	0
57	MG	BA	3226	1/1	0.96	0.22	1.50	25,25,25,25	0
57	MG	DA	3003	1/1	0.95	0.23	1.47	36,36,36,36	0
57	MG	CA	3037	1/1	0.94	0.21	1.39	53,53,53,53	0
57	MG	DA	3156	1/1	0.92	0.16	1.35	52,52,52,52	0
57	MG	BA	3798	1/1	0.93	0.24	1.30	22,22,22,22	0
57	MG	AA	1685	1/1	0.96	0.21	1.26	62,62,62,62	0
57	MG	BA	3152	1/1	0.95	0.26	1.25	23,23,23,23	0
57	MG	DA	3223	1/1	0.94	0.19	1.21	39,39,39,39	0
57	MG	BA	3277	1/1	0.95	0.43	1.20	52,52,52,52	0
57	MG	DA	3190	1/1	0.87	0.19	1.17	63,63,63,63	0
57	MG	AA	1615	1/1	0.95	0.21	1.16	51,51,51,51	0
57	MG	DA	3463	1/1	0.60	0.19	1.15	44,44,44,44	0
57	MG	BQ	3001	1/1	0.97	0.26	1.12	37,37,37,37	0
57	MG	DA	3656	1/1	0.95	0.25	1.11	41,41,41,41	0
57	MG	BA	3713	1/1	0.80	0.28	1.10	33,33,33,33	0
57	MG	BA	3373	1/1	0.94	0.22	1.07	34,34,34,34	0
57	MG	AA	1753	1/1	0.91	0.20	1.05	55,55,55,55	0
57	MG	BA	3177	1/1	0.93	0.23	1.05	46,46,46,46	0
57	MG	B9	502	1/1	0.96	0.34	1.05	46,46,46,46	0
57	MG	BA	3802	1/1	0.91	0.23	1.03	46,46,46,46	0
57	MG	BA	3576	1/1	0.97	0.24	0.96	30,30,30,30	0
57	MG	BA	3506	1/1	0.88	0.22	0.89	61,61,61,61	0
57	MG	DA	3662	1/1	0.92	0.22	0.85	50,50,50,50	0
57	MG	BA	3038	1/1	0.94	0.23	0.85	20,20,20,20	0
57	MG	DA	3264	1/1	0.97	0.18	0.80	51,51,51,51	0
57	MG	DA	3316	1/1	0.97	0.19	0.77	57,57,57,57	0
57	MG	DA	3549	1/1	0.82	0.20	0.77	49,49,49,49	0
57	MG	CA	3071	1/1	0.93	0.19	0.75	56,56,56,56	0
59	ZN	B5	103	1/1	0.99	0.21	0.73	40,40,40,40	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	BA	3048	1/1	0.94	0.22	0.71	29,29,29,29	0
57	MG	BA	3567	1/1	0.95	0.25	0.68	32,32,32,32	0
57	MG	CA	3020	1/1	0.88	0.20	0.62	45,45,45,45	0
57	MG	DA	3194	1/1	0.88	0.16	0.60	48,48,48,48	0
57	MG	BA	3432	1/1	0.93	0.22	0.57	32,32,32,32	0
57	MG	DA	3441	1/1	0.93	0.20	0.57	58,58,58,58	0
57	MG	BA	3034	1/1	0.96	0.23	0.53	35,35,35,35	0
59	ZN	D5	501	1/1	0.99	0.19	0.53	57,57,57,57	0
57	MG	DA	3232	1/1	0.89	0.19	0.53	56,56,56,56	0
57	MG	DA	3443	1/1	0.95	0.19	0.50	51,51,51,51	0
57	MG	BD	3005	1/1	0.97	0.24	0.49	44,44,44,44	0
57	MG	BA	3239	1/1	0.87	0.22	0.48	47,47,47,47	0
57	MG	BA	3187	1/1	0.94	0.22	0.44	38,38,38,38	0
57	MG	BA	3051	1/1	0.92	0.23	0.44	37,37,37,37	0
57	MG	BA	3441	1/1	0.87	0.20	0.43	39,39,39,39	0
57	MG	DA	3654	1/1	0.97	0.19	0.40	35,35,35,35	0
57	MG	BA	3308	1/1	0.96	0.23	0.38	39,39,39,39	0
57	MG	AA	1693	1/1	0.89	0.20	0.36	76,76,76,76	0
57	MG	BD	3002	1/1	0.98	0.21	0.36	28,28,28,28	0
57	MG	CA	3057	1/1	0.95	0.14	0.34	84,84,84,84	0
57	MG	DW	3001	1/1	0.96	0.21	0.33	41,41,41,41	0
57	MG	BA	3622	1/1	0.89	0.21	0.32	43,43,43,43	0
57	MG	D3	3001	1/1	0.94	0.27	0.31	63,63,63,63	0
57	MG	BA	3251	1/1	0.95	0.25	0.27	43,43,43,43	0
57	MG	DA	3023	1/1	0.87	0.14	0.25	58,58,58,58	0
57	MG	DA	3616	1/1	0.94	0.20	0.20	63,63,63,63	0
57	MG	DA	3014	1/1	0.97	0.22	0.11	44,44,44,44	0
57	MG	DA	3542	1/1	0.79	0.17	0.11	60,60,60,60	0
57	MG	AA	1613	1/1	0.84	0.18	0.08	75,75,75,75	0
57	MG	DA	3068	1/1	0.89	0.19	0.07	53,53,53,53	0
57	MG	DA	3215	1/1	0.96	0.18	0.05	40,40,40,40	0
57	MG	DA	3557	1/1	0.91	0.19	0.04	57,57,57,57	0
57	MG	CA	3096	1/1	0.97	0.18	0.03	43,43,43,43	0
57	MG	AA	1813	1/1	0.96	0.21	-0.00	38,38,38,38	0
57	MG	DA	3219	1/1	0.89	0.16	0.00	50,50,50,50	0
57	MG	CA	3061	1/1	0.80	0.21	-0.02	66,66,66,66	0
57	MG	BD	3010	1/1	0.97	0.20	-0.05	46,46,46,46	0
57	MG	DA	3178	1/1	0.98	0.17	-0.06	40,40,40,40	0
57	MG	AA	1806	1/1	0.94	0.18	-0.06	74,74,74,74	0
57	MG	BA	3793	1/1	0.98	0.22	-0.13	11,11,11,11	0
57	MG	BA	3485	1/1	0.85	0.24	-0.15	26,26,26,26	0
57	MG	AA	1672	1/1	0.99	0.17	-0.16	45,45,45,45	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	BA	3343	1/1	0.82	0.18	-0.18	54,54,54,54	0
57	MG	CA	3046	1/1	0.94	0.18	-0.18	61,61,61,61	0
59	ZN	D6	501	1/1	0.97	0.18	-0.21	65,65,65,65	0
59	ZN	B9	501	1/1	1.00	0.23	-0.24	49,49,49,49	0
57	MG	CA	3086	1/1	0.48	0.13	-0.25	93,93,93,93	0
57	MG	BD	3004	1/1	0.97	0.20	-0.27	28,28,28,28	0
57	MG	BA	3811	1/1	0.98	0.21	-0.30	48,48,48,48	0
57	MG	DA	3579	1/1	0.93	0.16	-0.30	62,62,62,62	0
57	MG	BA	3221	1/1	0.97	0.21	-0.32	29,29,29,29	0
57	MG	BA	3054	1/1	0.97	0.22	-0.33	30,30,30,30	0
57	MG	BA	3614	1/1	0.86	0.17	-0.33	53,53,53,53	0
57	MG	BA	3708	1/1	0.95	0.21	-0.35	33,33,33,33	0
57	MG	DA	3453	1/1	0.98	0.17	-0.36	54,54,54,54	0
57	MG	DB	3004	1/1	0.94	0.21	-0.36	63,63,63,63	0
57	MG	CE	202	1/1	0.26	0.19	-0.36	95,95,95,95	0
57	MG	BA	3184	1/1	0.97	0.22	-0.37	42,42,42,42	0
57	MG	BA	3686	1/1	0.93	0.19	-0.37	27,27,27,27	0
57	MG	CA	3044	1/1	0.99	0.16	-0.38	47,47,47,47	0
57	MG	BA	3280	1/1	0.94	0.21	-0.39	25,25,25,25	0
57	MG	BA	3139	1/1	0.88	0.22	-0.40	44,44,44,44	0
59	ZN	BY	501	1/1	0.95	0.18	-0.43	68,68,68,68	0
57	MG	CA	3032	1/1	0.77	0.16	-0.43	53,53,53,53	0
57	MG	DA	3465	1/1	0.94	0.17	-0.44	42,42,42,42	0
57	MG	DA	3425	1/1	0.92	0.16	-0.44	51,51,51,51	0
57	MG	DA	3072	1/1	0.90	0.17	-0.46	47,47,47,47	0
57	MG	DA	3005	1/1	0.97	0.16	-0.49	54,54,54,54	0
57	MG	BA	3314	1/1	0.92	0.18	-0.55	39,39,39,39	0
57	MG	BA	3235	1/1	0.83	0.20	-0.57	44,44,44,44	0
57	MG	DA	3637	1/1	0.85	0.14	-0.57	72,72,72,72	0
57	MG	BV	203	1/1	0.97	0.21	-0.58	23,23,23,23	0
57	MG	D8	5001	1/1	0.85	0.22	-0.61	44,44,44,44	0
57	MG	AA	1692	1/1	0.92	0.15	-0.61	65,65,65,65	0
57	MG	CT	3001	1/1	0.92	0.17	-0.64	60,60,60,60	0
57	MG	AA	1749	1/1	0.94	0.19	-0.64	50,50,50,50	0
57	MG	DA	3106	1/1	0.87	0.14	-0.65	50,50,50,50	0
57	MG	BA	3299	1/1	0.89	0.21	-0.66	60,60,60,60	0
57	MG	BA	3518	1/1	0.90	0.20	-0.69	46,46,46,46	0
57	MG	DA	3653	1/1	0.86	0.17	-0.69	33,33,33,33	0
57	MG	AA	1794	1/1	0.95	0.16	-0.72	58,58,58,58	0
57	MG	BA	3240	1/1	0.83	0.18	-0.75	53,53,53,53	0
57	MG	B7	105	1/1	0.96	0.20	-0.80	28,28,28,28	0
57	MG	AA	1695	1/1	0.84	0.20	-0.80	59,59,59,59	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	BA	3189	1/1	0.98	0.22	-0.81	39,39,39,39	0
57	MG	CA	3042	1/1	0.91	0.13	-0.81	57,57,57,57	0
57	MG	AN	503	1/1	0.89	0.18	-0.83	52,52,52,52	0
57	MG	DA	3133	1/1	0.93	0.18	-0.83	60,60,60,60	0
57	MG	DE	3004	1/1	0.96	0.17	-0.84	31,31,31,31	0
57	MG	BA	3417	1/1	0.99	0.21	-0.84	24,24,24,24	0
57	MG	BA	3261	1/1	0.95	0.21	-0.85	18,18,18,18	0
57	MG	CE	201	1/1	0.83	0.18	-0.86	65,65,65,65	0
57	MG	DA	3663	1/1	0.88	0.15	-0.86	73,73,73,73	0
57	MG	DA	3183	1/1	0.96	0.17	-0.87	41,41,41,41	0
59	ZN	AN	501	1/1	0.97	0.16	-0.90	77,77,77,77	0
57	MG	DA	3085	1/1	0.98	0.18	-0.90	28,28,28,28	0
57	MG	DA	3291	1/1	0.89	0.16	-0.92	36,36,36,36	0
57	MG	BA	3402	1/1	0.96	0.18	-0.93	27,27,27,27	0
57	MG	DA	3333	1/1	0.86	0.17	-0.94	47,47,47,47	0
57	MG	CA	3113	1/1	0.92	0.16	-0.95	47,47,47,47	0
59	ZN	DY	501	1/1	0.97	0.11	-0.95	90,90,90,90	0
57	MG	AA	1641	1/1	0.93	0.17	-0.96	65,65,65,65	0
57	MG	DB	3007	1/1	0.79	0.12	-0.96	67,67,67,67	0
57	MG	BA	3377	1/1	0.86	0.21	-0.98	51,51,51,51	0
57	MG	BA	3435	1/1	0.91	0.22	-0.98	53,53,53,53	0
57	MG	CA	3169	1/1	0.94	0.18	-0.99	62,62,62,62	0
59	ZN	D9	501	1/1	0.97	0.12	-1.02	64,64,64,64	0
57	MG	BH	201	1/1	0.97	0.20	-1.05	56,56,56,56	0
57	MG	CA	3144	1/1	0.94	0.13	-1.07	82,82,82,82	0
57	MG	DE	3002	1/1	0.95	0.16	-1.07	33,33,33,33	0
57	MG	BA	3508	1/1	0.88	0.21	-1.09	20,20,20,20	0
57	MG	BA	3334	1/1	0.94	0.21	-1.09	56,56,56,56	0
57	MG	BA	3039	1/1	0.98	0.19	-1.10	36,36,36,36	0
57	MG	DA	3595	1/1	0.93	0.13	-1.13	57,57,57,57	0
57	MG	CA	3166	1/1	0.91	0.15	-1.14	55,55,55,55	0
57	MG	DA	3411	1/1	0.84	0.18	-1.14	37,37,37,37	0
57	MG	BA	3260	1/1	0.97	0.20	-1.16	19,19,19,19	0
57	MG	BE	301	1/1	0.82	0.20	-1.18	31,31,31,31	0
57	MG	BA	3559	1/1	0.97	0.22	-1.19	26,26,26,26	0
58	SF4	AD	501	8/8	0.98	0.15	-1.24	59,68,73,79	0
57	MG	BA	3573	1/1	0.90	0.19	-1.24	41,41,41,41	0
57	MG	BA	3389	1/1	0.89	0.21	-1.24	37,37,37,37	0
57	MG	AX	3005	1/1	0.84	0.11	-1.25	65,65,65,65	0
57	MG	DA	3577	1/1	0.88	0.07	-1.25	60,60,60,60	0
57	MG	CA	3036	1/1	0.92	0.16	-1.26	73,73,73,73	0
57	MG	AB	3001	1/1	0.94	0.13	-1.26	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
57	MG	BA	3313	1/1	0.88	0.19	-1.28	38,38,38,38	0
57	MG	BA	3020	1/1	0.98	0.21	-1.31	25,25,25,25	0
57	MG	DA	3228	1/1	0.96	0.15	-1.31	44,44,44,44	0
57	MG	DA	3442	1/1	0.87	0.15	-1.31	64,64,64,64	0
57	MG	BA	3566	1/1	0.97	0.21	-1.32	31,31,31,31	0
57	MG	DA	3001	1/1	0.92	0.14	-1.35	57,57,57,57	0
57	MG	DA	3258	1/1	0.96	0.16	-1.36	45,45,45,45	0
57	MG	BA	3114	1/1	0.98	0.20	-1.36	39,39,39,39	0
57	MG	DA	3040	1/1	0.97	0.14	-1.38	28,28,28,28	0
57	MG	BA	3671	1/1	0.95	0.19	-1.38	24,24,24,24	0
57	MG	DA	3528	1/1	0.92	0.14	-1.38	36,36,36,36	0
57	MG	BA	3188	1/1	0.95	0.19	-1.41	32,32,32,32	0
57	MG	AA	1814	1/1	0.91	0.15	-1.42	57,57,57,57	0
57	MG	BA	3009	1/1	0.94	0.17	-1.42	31,31,31,31	0
57	MG	BA	3487	1/1	0.74	0.13	-1.48	54,54,54,54	0
57	MG	DA	3477	1/1	0.98	0.11	-1.48	53,53,53,53	0
57	MG	BA	3704	1/1	0.90	0.18	-1.49	26,26,26,26	0
59	ZN	B4	501	1/1	0.94	0.10	-1.50	118,118,118,118	0
57	MG	CA	3142	1/1	0.95	0.18	-1.56	50,50,50,50	0
57	MG	BA	3191	1/1	0.91	0.19	-1.57	40,40,40,40	0
57	MG	DA	3216	1/1	0.96	0.15	-1.58	35,35,35,35	0
59	ZN	D4	501	1/1	0.33	0.12	-1.58	162,162,162,162	0
57	MG	BA	3541	1/1	0.92	0.20	-1.58	38,38,38,38	0
57	MG	BA	3082	1/1	0.96	0.18	-1.58	28,28,28,28	0
57	MG	DG	3001	1/1	0.86	0.14	-1.60	66,66,66,66	0
57	MG	DA	3433	1/1	0.93	0.17	-1.61	59,59,59,59	0
57	MG	BA	3382	1/1	0.98	0.12	-1.63	55,55,55,55	0
57	MG	DA	3560	1/1	0.82	0.15	-1.63	60,60,60,60	0
57	MG	CA	3094	1/1	0.81	0.08	-1.64	61,61,61,61	0
57	MG	AA	1611	1/1	0.97	0.19	-1.65	20,20,20,20	0
57	MG	BA	3045	1/1	0.97	0.17	-1.66	39,39,39,39	0
57	MG	AA	1723	1/1	0.84	0.15	-1.66	63,63,63,63	0
57	MG	CA	3110	1/1	0.87	0.12	-1.69	63,63,63,63	0
57	MG	BA	3621	1/1	0.97	0.19	-1.69	43,43,43,43	0
57	MG	DA	3340	1/1	0.97	0.14	-1.70	27,27,27,27	0
57	MG	DA	3393	1/1	0.89	0.16	-1.71	37,37,37,37	0
57	MG	AA	1740	1/1	0.98	0.17	-1.71	41,41,41,41	0
57	MG	BA	3341	1/1	0.97	0.20	-1.72	18,18,18,18	0
57	MG	DA	3371	1/1	0.93	0.17	-1.72	34,34,34,34	0
57	MG	DA	3499	1/1	0.93	0.14	-1.73	52,52,52,52	0
57	MG	AA	1747	1/1	0.88	0.15	-1.74	55,55,55,55	0
57	MG	DA	3429	1/1	0.95	0.15	-1.74	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
57	MG	DA	3087	1/1	0.84	0.18	-1.75	55,55,55,55	0
57	MG	CA	3048	1/1	0.97	0.12	-1.76	58,58,58,58	0
57	MG	BA	3387	1/1	0.97	0.20	-1.77	29,29,29,29	0
57	MG	DA	3311	1/1	0.88	0.14	-1.77	46,46,46,46	0
57	MG	AA	1779	1/1	0.96	0.14	-1.78	59,59,59,59	0
57	MG	CA	3051	1/1	0.87	0.11	-1.79	77,77,77,77	0
57	MG	CA	3099	1/1	0.90	0.09	-1.79	64,64,64,64	0
57	MG	AA	1680	1/1	0.87	0.17	-1.79	51,51,51,51	0
57	MG	BB	3007	1/1	0.97	0.17	-1.80	41,41,41,41	0
57	MG	AA	1795	1/1	0.98	0.12	-1.80	55,55,55,55	0
57	MG	DA	3322	1/1	0.95	0.16	-1.82	42,42,42,42	0
57	MG	BA	3393	1/1	0.97	0.20	-1.82	23,23,23,23	0
57	MG	DA	3630	1/1	0.92	0.14	-1.86	69,69,69,69	0
57	MG	DA	3349	1/1	0.96	0.16	-1.87	34,34,34,34	0
57	MG	BA	3110	1/1	0.90	0.18	-1.88	36,36,36,36	0
57	MG	DA	3659	1/1	0.94	0.14	-1.89	41,41,41,41	0
57	MG	B5	102	1/1	0.93	0.19	-1.90	43,43,43,43	0
57	MG	DA	3331	1/1	0.95	0.15	-1.92	47,47,47,47	0
57	MG	BA	3719	1/1	0.98	0.20	-1.93	41,41,41,41	0
57	MG	BW	3003	1/1	0.95	0.15	-1.96	35,35,35,35	0
57	MG	BA	3311	1/1	0.97	0.19	-1.99	56,56,56,56	0
58	SF4	CD	501	8/8	0.98	0.14	-1.99	64,67,74,91	0
57	MG	BA	3706	1/1	0.94	0.16	-2.00	47,47,47,47	0
57	MG	BA	3358	1/1	0.91	0.18	-2.02	52,52,52,52	0
57	MG	BA	3144	1/1	0.96	0.18	-2.02	41,41,41,41	0
57	MG	BA	3448	1/1	0.97	0.18	-2.03	17,17,17,17	0
57	MG	DA	3652	1/1	0.96	0.16	-2.05	31,31,31,31	0
57	MG	DB	3003	1/1	0.82	0.10	-2.06	78,78,78,78	0
57	MG	DA	3421	1/1	0.93	0.12	-2.08	56,56,56,56	0
57	MG	DA	3607	1/1	0.82	0.14	-2.08	64,64,64,64	0
57	MG	DA	3039	1/1	0.97	0.16	-2.11	38,38,38,38	0
57	MG	B7	102	1/1	0.97	0.17	-2.12	41,41,41,41	0
57	MG	BA	3779	1/1	0.98	0.19	-2.14	17,17,17,17	0
57	MG	DA	3296	1/1	0.90	0.10	-2.15	60,60,60,60	0
57	MG	DA	3319	1/1	0.97	0.14	-2.15	33,33,33,33	0
57	MG	CA	3009	1/1	0.84	0.12	-2.15	73,73,73,73	0
57	MG	DA	3238	1/1	0.84	0.15	-2.16	48,48,48,48	0
57	MG	CA	3040	1/1	0.95	0.12	-2.18	56,56,56,56	0
57	MG	BD	3009	1/1	0.98	0.16	-2.18	37,37,37,37	0
59	ZN	CN	501	1/1	0.91	0.06	-2.19	100,100,100,100	0
57	MG	DA	3459	1/1	0.90	0.14	-2.19	49,49,49,49	0
57	MG	BA	3615	1/1	0.91	0.13	-2.21	71,71,71,71	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	DA	3268	1/1	0.94	0.12	-2.23	41,41,41,41	0
57	MG	BA	3756	1/1	0.96	0.19	-2.25	18,18,18,18	0
57	MG	BA	3533	1/1	0.98	0.18	-2.25	23,23,23,23	0
57	MG	DA	3649	1/1	0.80	0.13	-2.26	71,71,71,71	0
57	MG	BA	3118	1/1	0.95	0.21	-2.26	35,35,35,35	0
57	MG	AA	1681	1/1	0.99	0.12	-2.29	38,38,38,38	0
57	MG	DQ	3001	1/1	0.92	0.08	-2.30	50,50,50,50	0
57	MG	AM	3001	1/1	0.94	0.09	-2.32	66,66,66,66	0
57	MG	CA	3106	1/1	0.94	0.13	-2.32	58,58,58,58	0
57	MG	BB	3003	1/1	0.94	0.18	-2.34	30,30,30,30	0
57	MG	BA	3131	1/1	0.88	0.19	-2.37	44,44,44,44	0
57	MG	DA	3028	1/1	0.92	0.13	-2.37	39,39,39,39	0
57	MG	BA	3806	1/1	0.92	0.17	-2.39	43,43,43,43	0
57	MG	BA	3796	1/1	0.91	0.17	-2.39	47,47,47,47	0
57	MG	DA	3420	1/1	0.80	0.11	-2.39	49,49,49,49	0
57	MG	BA	3023	1/1	0.95	0.17	-2.41	41,41,41,41	0
57	MG	BG	202	1/1	0.78	0.15	-2.43	52,52,52,52	0
57	MG	BA	3089	1/1	0.97	0.19	-2.43	36,36,36,36	0
57	MG	DA	3661	1/1	0.97	0.10	-2.44	62,62,62,62	0
57	MG	BA	3120	1/1	0.95	0.18	-2.44	45,45,45,45	0
57	MG	BA	3519	1/1	0.94	0.19	-2.45	45,45,45,45	0
57	MG	AA	1676	1/1	0.94	0.16	-2.52	58,58,58,58	0
57	MG	DA	3416	1/1	0.90	0.14	-2.52	52,52,52,52	0
57	MG	DA	3132	1/1	0.89	0.13	-2.52	43,43,43,43	0
57	MG	DA	3108	1/1	0.77	0.12	-2.55	50,50,50,50	0
57	MG	DA	3036	1/1	0.97	0.17	-2.57	35,35,35,35	0
57	MG	CA	3016	1/1	0.83	0.13	-2.57	48,48,48,48	0
57	MG	DR	3001	1/1	0.92	0.13	-2.58	49,49,49,49	0
57	MG	BA	3419	1/1	0.91	0.20	-2.59	25,25,25,25	0
57	MG	BA	3312	1/1	0.98	0.19	-2.59	31,31,31,31	0
57	MG	BA	3439	1/1	0.61	0.18	-2.60	36,36,36,36	0
57	MG	BA	3129	1/1	0.88	0.16	-2.60	54,54,54,54	0
57	MG	DD	304	1/1	0.97	0.09	-2.63	36,36,36,36	0
57	MG	DA	3186	1/1	0.92	0.15	-2.63	49,49,49,49	0
57	MG	AA	1621	1/1	0.88	0.14	-2.64	44,44,44,44	0
57	MG	DA	3619	1/1	0.82	0.15	-2.68	40,40,40,40	0
57	MG	BA	3644	1/1	0.81	0.18	-2.69	64,64,64,64	0
57	MG	BA	3315	1/1	0.97	0.18	-2.71	40,40,40,40	0
57	MG	BA	3407	1/1	0.89	0.17	-2.71	32,32,32,32	0
57	MG	BA	3694	1/1	0.90	0.19	-2.73	53,53,53,53	0
57	MG	BA	3323	1/1	0.90	0.19	-2.78	57,57,57,57	0
57	MG	BA	3762	1/1	0.96	0.18	-2.79	20,20,20,20	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	BE	303	1/1	0.94	0.15	-2.80	43,43,43,43	0
57	MG	BA	3231	1/1	0.79	0.17	-2.81	57,57,57,57	0
57	MG	BA	3577	1/1	0.86	0.17	-2.81	58,58,58,58	0
57	MG	DA	3605	1/1	0.94	0.12	-2.82	45,45,45,45	0
57	MG	DA	3321	1/1	0.97	0.15	-2.86	29,29,29,29	0
57	MG	BA	3206	1/1	0.94	0.16	-2.89	34,34,34,34	0
57	MG	BA	3388	1/1	0.91	0.20	-2.91	25,25,25,25	0
57	MG	DA	3523	1/1	0.90	0.14	-2.92	39,39,39,39	0
57	MG	DA	3347	1/1	0.88	0.14	-2.93	35,35,35,35	0
57	MG	BU	202	1/1	0.95	0.15	-2.94	40,40,40,40	0
57	MG	AA	1759	1/1	0.89	0.14	-2.95	55,55,55,55	0
57	MG	CA	3053	1/1	0.95	0.12	-2.96	41,41,41,41	0
57	MG	CA	3119	1/1	0.89	0.12	-2.97	59,59,59,59	0
57	MG	AT	3001	1/1	0.91	0.13	-2.99	63,63,63,63	0
57	MG	BN	3001	1/1	0.91	0.15	-3.00	48,48,48,48	0
57	MG	DA	3303	1/1	0.97	0.12	-3.01	43,43,43,43	0
57	MG	DF	304	1/1	0.97	0.07	-3.04	51,51,51,51	0
57	MG	AA	1776	1/1	0.95	0.16	-3.05	73,73,73,73	0
57	MG	BB	3021	1/1	0.97	0.18	-3.06	41,41,41,41	0
57	MG	AA	1631	1/1	0.78	0.14	-3.09	64,64,64,64	0
57	MG	DA	3343	1/1	0.96	0.15	-3.10	34,34,34,34	0
57	MG	BA	3395	1/1	0.94	0.20	-3.11	30,30,30,30	0
57	MG	AA	1765	1/1	0.93	0.13	-3.11	65,65,65,65	0
57	MG	DA	3418	1/1	0.86	0.07	-3.13	47,47,47,47	0
57	MG	DA	3664	1/1	0.96	0.09	-3.14	51,51,51,51	0
57	MG	BA	3012	1/1	0.94	0.17	-3.14	25,25,25,25	0
57	MG	DA	3300	1/1	0.98	0.10	-3.15	38,38,38,38	0
57	MG	DA	3327	1/1	0.91	0.15	-3.15	45,45,45,45	0
57	MG	BA	3366	1/1	0.93	0.16	-3.16	52,52,52,52	0
57	MG	DA	3229	1/1	0.97	0.12	-3.17	38,38,38,38	0
57	MG	BA	3333	1/1	0.90	0.14	-3.18	57,57,57,57	0
57	MG	BA	3509	1/1	0.94	0.18	-3.20	50,50,50,50	0
57	MG	BB	3017	1/1	0.91	0.16	-3.25	81,81,81,81	0
57	MG	DA	3625	1/1	0.81	0.10	-3.27	60,60,60,60	0
57	MG	BA	3185	1/1	0.97	0.15	-3.29	33,33,33,33	0
57	MG	BA	3253	1/1	0.86	0.20	-3.29	31,31,31,31	0
57	MG	BA	3540	1/1	0.93	0.16	-3.29	31,31,31,31	0
57	MG	BA	3158	1/1	0.95	0.17	-3.29	41,41,41,41	0
57	MG	DA	3139	1/1	0.94	0.11	-3.31	44,44,44,44	0
57	MG	DA	3552	1/1	0.89	0.13	-3.33	34,34,34,34	0
57	MG	BA	3043	1/1	0.95	0.17	-3.33	31,31,31,31	0
57	MG	DA	3109	1/1	0.96	0.13	-3.35	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
57	MG	DA	3064	1/1	0.89	0.11	-3.35	46,46,46,46	0
57	MG	DA	3013	1/1	0.98	0.13	-3.36	39,39,39,39	0
57	MG	DA	3266	1/1	0.95	0.12	-3.39	37,37,37,37	0
57	MG	BA	3348	1/1	0.92	0.18	-3.40	37,37,37,37	0
57	MG	BA	3799	1/1	0.94	0.18	-3.41	42,42,42,42	0
57	MG	DA	3037	1/1	0.97	0.12	-3.41	26,26,26,26	0
57	MG	BA	3309	1/1	0.92	0.17	-3.42	65,65,65,65	0
57	MG	DA	3449	1/1	0.93	0.13	-3.43	34,34,34,34	0
57	MG	AA	1627	1/1	0.97	0.14	-3.46	54,54,54,54	0
57	MG	BA	3812	1/1	0.95	0.12	-3.46	42,42,42,42	0
57	MG	CA	3081	1/1	0.91	0.16	-3.46	44,44,44,44	0
57	MG	BA	3223	1/1	0.95	0.17	-3.46	41,41,41,41	0
57	MG	DA	3314	1/1	0.78	0.12	-3.51	43,43,43,43	0
57	MG	DA	3458	1/1	0.92	0.10	-3.52	41,41,41,41	0
57	MG	BA	3399	1/1	0.94	0.20	-3.54	41,41,41,41	0
57	MG	BA	3376	1/1	0.96	0.18	-3.54	29,29,29,29	0
57	MG	DA	3341	1/1	0.88	0.12	-3.56	55,55,55,55	0
57	MG	DA	3164	1/1	0.94	0.14	-3.57	44,44,44,44	0
57	MG	D0	101	1/1	0.91	0.13	-3.57	71,71,71,71	0
57	MG	BA	3220	1/1	0.93	0.15	-3.57	35,35,35,35	0
57	MG	AA	1644	1/1	0.82	0.12	-3.61	56,56,56,56	0
57	MG	DA	3010	1/1	0.87	0.10	-3.62	41,41,41,41	0
57	MG	BF	305	1/1	0.98	0.14	-3.62	36,36,36,36	0
57	MG	DA	3490	1/1	0.95	0.13	-3.63	33,33,33,33	0
57	MG	BD	3001	1/1	0.97	0.14	-3.65	34,34,34,34	0
57	MG	AM	3002	1/1	0.89	0.12	-3.65	68,68,68,68	0
57	MG	BA	3512	1/1	0.92	0.21	-3.66	23,23,23,23	0
57	MG	CA	3088	1/1	0.95	0.12	-3.74	43,43,43,43	0
57	MG	DA	3019	1/1	0.94	0.08	-3.79	42,42,42,42	0
57	MG	DA	3312	1/1	0.95	0.12	-3.85	42,42,42,42	0
57	MG	DA	3428	1/1	0.97	0.11	-3.88	38,38,38,38	0
57	MG	DA	3354	1/1	0.96	0.11	-3.93	41,41,41,41	0
57	MG	BA	3011	1/1	0.97	0.15	-3.93	30,30,30,30	0
57	MG	DA	3279	1/1	0.76	0.14	-3.94	36,36,36,36	0
57	MG	DA	3113	1/1	0.94	0.13	-3.95	35,35,35,35	0
57	MG	DA	3315	1/1	0.93	0.13	-3.95	44,44,44,44	0
57	MG	DA	3049	1/1	0.90	0.10	-4.00	47,47,47,47	0
57	MG	DA	3225	1/1	0.95	0.10	-4.00	55,55,55,55	0
57	MG	BA	3336	1/1	0.96	0.17	-4.03	20,20,20,20	0
57	MG	AA	1665	1/1	0.97	0.16	-4.04	55,55,55,55	0
57	MG	DA	3655	1/1	0.97	0.08	-4.05	38,38,38,38	0
57	MG	BA	3275	1/1	0.88	0.16	-4.06	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
57	MG	DA	3285	1/1	0.94	0.12	-4.08	50,50,50,50	0
57	MG	BA	3296	1/1	0.92	0.16	-4.08	55,55,55,55	0
57	MG	DA	3364	1/1	0.95	0.10	-4.09	45,45,45,45	0
57	MG	BA	3340	1/1	0.75	0.18	-4.12	27,27,27,27	0
57	MG	BA	3073	1/1	0.88	0.15	-4.12	32,32,32,32	0
57	MG	BA	3392	1/1	0.96	0.18	-4.14	26,26,26,26	0
57	MG	CA	3108	1/1	0.84	0.11	-4.14	72,72,72,72	0
57	MG	BA	3527	1/1	0.93	0.19	-4.16	24,24,24,24	0
57	MG	BD	3006	1/1	0.99	0.09	-4.17	34,34,34,34	0
57	MG	CA	3029	1/1	0.89	0.11	-4.27	50,50,50,50	0
57	MG	DA	3529	1/1	0.94	0.07	-4.28	76,76,76,76	0
57	MG	BF	309	1/1	0.96	0.18	-4.29	31,31,31,31	0
57	MG	BA	3723	1/1	0.86	0.18	-4.31	30,30,30,30	0
57	MG	DA	3561	1/1	0.92	0.16	-4.32	52,52,52,52	0
57	MG	BA	3607	1/1	0.95	0.17	-4.32	36,36,36,36	0
57	MG	BA	3544	1/1	0.97	0.18	-4.34	52,52,52,52	0
57	MG	DA	3440	1/1	0.97	0.13	-4.37	36,36,36,36	0
57	MG	BA	3050	1/1	0.96	0.15	-4.37	32,32,32,32	0
57	MG	DA	3147	1/1	0.95	0.14	-4.39	44,44,44,44	0
57	MG	DA	3100	1/1	0.92	0.09	-4.41	47,47,47,47	0
57	MG	AA	1742	1/1	0.95	0.14	-4.41	52,52,52,52	0
57	MG	BA	3689	1/1	0.89	0.19	-4.43	59,59,59,59	0
57	MG	BP	3001	1/1	0.96	0.14	-4.45	34,34,34,34	0
57	MG	CA	3023	1/1	0.89	0.10	-4.45	39,39,39,39	0
57	MG	BA	3794	1/1	0.88	0.13	-4.46	37,37,37,37	0
57	MG	DA	3426	1/1	0.84	0.12	-4.48	49,49,49,49	0
57	MG	DA	3434	1/1	0.95	0.07	-4.49	60,60,60,60	0
57	MG	DA	3414	1/1	0.93	0.15	-4.51	42,42,42,42	0
57	MG	BA	3289	1/1	0.93	0.17	-4.55	49,49,49,49	0
57	MG	DE	3007	1/1	0.96	0.11	-4.59	58,58,58,58	0
57	MG	DA	3267	1/1	0.97	0.12	-4.59	44,44,44,44	0
57	MG	BA	3397	1/1	0.96	0.15	-4.61	28,28,28,28	0
57	MG	DA	3562	1/1	0.98	0.12	-4.65	31,31,31,31	0
57	MG	CA	3114	1/1	0.94	0.14	-4.65	71,71,71,71	0
57	MG	DA	3310	1/1	0.92	0.13	-4.67	35,35,35,35	0
57	MG	BA	3412	1/1	0.97	0.17	-4.67	30,30,30,30	0
57	MG	BA	3473	1/1	0.97	0.19	-4.67	28,28,28,28	0
57	MG	BR	5002	1/1	0.94	0.14	-4.75	50,50,50,50	0
57	MG	BA	3725	1/1	0.97	0.17	-4.78	31,31,31,31	0
57	MG	BA	3742	1/1	0.98	0.21	-4.78	48,48,48,48	0
57	MG	BA	3254	1/1	0.88	0.16	-4.79	33,33,33,33	0
57	MG	BA	3813	1/1	0.98	0.13	-4.80	29,29,29,29	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	DD	302	1/1	0.87	0.14	-4.90	49,49,49,49	0
57	MG	AA	1684	1/1	0.75	0.13	-4.91	54,54,54,54	0
57	MG	BA	3486	1/1	0.96	0.13	-4.94	41,41,41,41	0
57	MG	BB	3020	1/1	0.75	0.16	-4.97	65,65,65,65	0
57	MG	DA	3522	1/1	0.88	0.11	-5.02	51,51,51,51	0
57	MG	BG	201	1/1	0.96	0.14	-5.03	39,39,39,39	0
57	MG	DA	3359	1/1	0.95	0.16	-5.10	40,40,40,40	0
57	MG	DA	3246	1/1	0.96	0.06	-5.11	46,46,46,46	0
57	MG	AA	1630	1/1	0.87	0.14	-5.18	53,53,53,53	0
57	MG	BA	3380	1/1	0.96	0.15	-5.18	40,40,40,40	0
57	MG	DA	3384	1/1	0.88	0.10	-5.19	38,38,38,38	0
57	MG	DA	3318	1/1	0.62	0.10	-5.19	45,45,45,45	0
57	MG	AA	1697	1/1	0.81	0.11	-5.23	65,65,65,65	0
57	MG	DA	3439	1/1	0.90	0.12	-5.28	40,40,40,40	0
57	MG	DA	3034	1/1	0.91	0.10	-5.32	42,42,42,42	0
57	MG	DA	3526	1/1	0.94	0.12	-5.33	52,52,52,52	0
57	MG	AA	1617	1/1	0.94	0.10	-5.36	58,58,58,58	0
57	MG	AA	1619	1/1	0.90	0.11	-5.46	64,64,64,64	0
57	MG	BA	3503	1/1	0.96	0.10	-5.46	51,51,51,51	0
57	MG	BA	3737	1/1	0.91	0.16	-5.51	34,34,34,34	0
57	MG	BA	3606	1/1	0.97	0.16	-5.51	36,36,36,36	0
57	MG	BA	3585	1/1	0.96	0.16	-5.52	29,29,29,29	0
57	MG	BA	3383	1/1	0.88	0.16	-5.53	37,37,37,37	0
57	MG	DA	3581	1/1	0.98	0.07	-5.53	44,44,44,44	0
57	MG	BA	3300	1/1	0.92	0.17	-5.56	53,53,53,53	0
57	MG	BA	3665	1/1	0.98	0.17	-5.56	42,42,42,42	0
57	MG	BA	3515	1/1	0.88	0.17	-5.57	27,27,27,27	0
57	MG	BA	3327	1/1	0.47	0.17	-5.60	39,39,39,39	0
57	MG	DA	3307	1/1	0.97	0.12	-5.61	51,51,51,51	0
57	MG	BA	3805	1/1	0.87	0.13	-5.61	48,48,48,48	0
57	MG	AA	1607	1/1	0.93	0.13	-5.62	55,55,55,55	0
57	MG	DA	3489	1/1	0.97	0.09	-5.72	48,48,48,48	0
57	MG	AA	1737	1/1	0.93	0.09	-5.72	60,60,60,60	0
57	MG	AA	1735	1/1	0.97	0.12	-5.73	45,45,45,45	0
57	MG	CA	3004	1/1	0.83	0.09	-5.75	69,69,69,69	0
57	MG	DA	3397	1/1	0.83	0.15	-5.75	42,42,42,42	0
57	MG	DA	3277	1/1	0.94	0.13	-5.79	50,50,50,50	0
57	MG	AA	1655	1/1	0.79	0.12	-5.83	53,53,53,53	0
57	MG	DA	3365	1/1	0.96	0.14	-5.87	19,19,19,19	0
57	MG	BA	3548	1/1	0.97	0.13	-5.93	35,35,35,35	0
57	MG	AA	1815	1/1	0.92	0.14	-5.93	47,47,47,47	0
57	MG	BE	306	1/1	0.94	0.10	-6.00	38,38,38,38	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	BB	3014	1/1	0.95	0.12	-6.01	67,67,67,67	0
57	MG	CA	3065	1/1	0.89	0.14	-6.04	59,59,59,59	0
57	MG	BA	3623	1/1	0.92	0.17	-6.05	43,43,43,43	0
57	MG	BA	3469	1/1	0.95	0.16	-6.07	61,61,61,61	0
57	MG	DA	3361	1/1	0.91	0.08	-6.08	33,33,33,33	0
57	MG	BA	3536	1/1	0.89	0.14	-6.09	32,32,32,32	0
57	MG	AA	1686	1/1	0.76	0.14	-6.09	61,61,61,61	0
57	MG	BA	3413	1/1	0.97	0.16	-6.18	37,37,37,37	0
57	MG	BV	205	1/1	0.99	0.12	-6.21	34,34,34,34	0
57	MG	BA	3494	1/1	0.97	0.11	-6.27	38,38,38,38	0
57	MG	CF	3001	1/1	0.96	0.12	-6.28	51,51,51,51	0
57	MG	DA	3532	1/1	0.90	0.13	-6.29	48,48,48,48	0
57	MG	DA	3338	1/1	0.87	0.07	-6.31	44,44,44,44	0
57	MG	BA	3736	1/1	0.97	0.16	-6.32	22,22,22,22	0
57	MG	AA	1770	1/1	0.99	0.13	-6.34	51,51,51,51	0
57	MG	BA	3365	1/1	0.87	0.13	-6.34	51,51,51,51	0
57	MG	BB	3016	1/1	0.90	0.14	-6.45	34,34,34,34	0
57	MG	BA	3234	1/1	0.96	0.12	-6.50	52,52,52,52	0
57	MG	DA	3363	1/1	0.92	0.09	-6.50	50,50,50,50	0
57	MG	BA	3371	1/1	0.98	0.10	-6.53	49,49,49,49	0
57	MG	BA	3752	1/1	0.95	0.12	-6.57	34,34,34,34	0
57	MG	DA	3214	1/1	0.96	0.08	-6.63	51,51,51,51	0
57	MG	DA	3492	1/1	0.97	0.07	-6.73	48,48,48,48	0
57	MG	BA	3036	1/1	0.91	0.12	-6.73	56,56,56,56	0
57	MG	DA	3385	1/1	0.95	0.07	-6.99	60,60,60,60	0
57	MG	BA	3225	1/1	0.85	0.13	-6.99	46,46,46,46	0
57	MG	DA	3521	1/1	0.98	0.09	-7.03	57,57,57,57	0
57	MG	BA	3346	1/1	0.86	0.10	-7.03	39,39,39,39	0
57	MG	DA	3292	1/1	0.91	0.11	-7.06	29,29,29,29	0
57	MG	B7	101	1/1	0.95	0.12	-7.21	41,41,41,41	0
57	MG	BA	3618	1/1	0.91	0.15	-7.25	35,35,35,35	0
57	MG	AA	1616	1/1	0.82	0.09	-7.33	73,73,73,73	0
57	MG	DA	3020	1/1	0.98	0.11	-7.35	26,26,26,26	0
57	MG	DA	3018	1/1	0.94	0.10	-7.35	31,31,31,31	0
57	MG	AA	1628	1/1	0.86	0.10	-7.39	65,65,65,65	0
57	MG	BF	307	1/1	0.92	0.13	-7.40	34,34,34,34	0
57	MG	DA	3282	1/1	0.93	0.10	-7.41	55,55,55,55	0
57	MG	AA	1787	1/1	0.85	0.15	-7.43	49,49,49,49	0
57	MG	BA	3714	1/1	0.94	0.12	-7.45	46,46,46,46	0
57	MG	DA	3454	1/1	0.92	0.12	-7.48	43,43,43,43	0
57	MG	BA	3410	1/1	0.90	0.16	-7.51	55,55,55,55	0
57	MG	CA	3085	1/1	0.99	0.15	-7.51	41,41,41,41	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	DA	3593	1/1	0.91	0.08	-7.64	60,60,60,60	0
57	MG	DA	3599	1/1	0.98	0.09	-7.70	48,48,48,48	0
57	MG	BA	3804	1/1	0.94	0.16	-7.70	36,36,36,36	0
57	MG	BA	3113	1/1	0.94	0.14	-7.71	50,50,50,50	0
57	MG	BA	3643	1/1	0.96	0.12	-7.86	52,52,52,52	0
57	MG	BA	3624	1/1	0.93	0.13	-7.97	38,38,38,38	0
57	MG	BA	3217	1/1	0.90	0.11	-7.99	50,50,50,50	0
57	MG	DA	3544	1/1	0.97	0.12	-8.06	53,53,53,53	0
57	MG	DA	3573	1/1	0.96	0.05	-8.08	61,61,61,61	0
57	MG	BA	3477	1/1	0.85	0.16	-8.10	68,68,68,68	0
57	MG	BA	3386	1/1	0.94	0.14	-8.30	28,28,28,28	0
57	MG	BA	3808	1/1	0.96	0.15	-8.39	38,38,38,38	0
57	MG	DA	3598	1/1	0.96	0.10	-8.47	55,55,55,55	0
57	MG	BA	3657	1/1	0.93	0.11	-8.52	38,38,38,38	0
57	MG	DA	3352	1/1	0.92	0.09	-8.56	34,34,34,34	0
57	MG	AA	1788	1/1	0.87	0.09	-8.59	75,75,75,75	0
57	MG	AA	1713	1/1	0.69	0.11	-8.61	67,67,67,67	0
57	MG	BA	3558	1/1	0.89	0.13	-8.63	51,51,51,51	0
57	MG	DA	3337	1/1	0.95	0.06	-8.64	48,48,48,48	0
57	MG	BA	3582	1/1	0.99	0.12	-8.71	31,31,31,31	0
57	MG	DA	3469	1/1	0.98	0.07	-8.77	50,50,50,50	0
57	MG	BA	3598	1/1	0.84	0.15	-8.78	33,33,33,33	0
57	MG	BA	3355	1/1	0.95	0.15	-9.20	35,35,35,35	0
57	MG	BA	3384	1/1	0.94	0.11	-9.21	45,45,45,45	0
57	MG	BA	3022	1/1	0.96	0.11	-9.23	25,25,25,25	0
57	MG	BF	308	1/1	0.96	0.08	-9.24	43,43,43,43	0
57	MG	BA	3459	1/1	0.95	0.15	-9.64	31,31,31,31	0
57	MG	DA	3280	1/1	0.85	0.09	-9.69	48,48,48,48	0
57	MG	DA	3170	1/1	0.86	0.10	-9.88	35,35,35,35	0
57	MG	BA	3583	1/1	0.99	0.15	-10.21	33,33,33,33	0
57	MG	BA	3635	1/1	0.97	0.12	-10.42	42,42,42,42	0
57	MG	BA	3330	1/1	0.92	0.15	-10.70	27,27,27,27	0
57	MG	DA	3373	1/1	0.98	0.09	-10.76	31,31,31,31	0
57	MG	DA	3283	1/1	0.94	0.07	-11.10	27,27,27,27	0
57	MG	DA	3586	1/1	0.95	0.08	-11.30	50,50,50,50	0
57	MG	BA	3021	1/1	0.98	0.12	-11.43	43,43,43,43	0
57	MG	BA	3046	1/1	0.96	0.15	-11.62	43,43,43,43	0
57	MG	BA	3059	1/1	0.94	0.14	-12.46	36,36,36,36	0
57	MG	BA	3741	1/1	0.92	0.11	-12.56	57,57,57,57	0
57	MG	BA	3587	1/1	0.92	0.11	-13.06	46,46,46,46	0
57	MG	BA	3625	1/1	0.90	0.14	-13.12	33,33,33,33	0
57	MG	BA	3525	1/1	0.86	0.16	-13.24	43,43,43,43	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	BA	3780	1/1	0.95	0.13	-13.48	42,42,42,42	0
57	MG	BA	3434	1/1	0.97	0.11	-13.99	19,19,19,19	0
57	MG	BA	3772	1/1	0.98	0.15	-14.06	36,36,36,36	0
57	MG	DA	3252	1/1	0.95	0.07	-14.13	50,50,50,50	0
57	MG	BA	3499	1/1	0.99	0.13	-14.31	39,39,39,39	0
57	MG	DA	3011	1/1	0.96	0.07	-15.38	35,35,35,35	0
57	MG	BA	3321	1/1	0.93	0.13	-16.04	53,53,53,53	0
57	MG	AA	1663	1/1	0.85	0.12	-21.27	50,50,50,50	0
57	MG	BA	3777	1/1	0.97	0.10	-22.29	41,41,41,41	0
57	MG	BA	3619	1/1	0.90	0.14	-29.83	28,28,28,28	0
57	MG	BA	3488	1/1	0.98	0.13	-35.95	20,20,20,20	0
57	MG	CA	3147	1/1	0.94	0.10	-41.86	70,70,70,70	0
57	MG	DA	3401	1/1	0.94	0.06	-	69,69,69,69	0
57	MG	DA	3497	1/1	0.82	0.19	-	58,58,58,58	0
57	MG	BA	3079	1/1	0.89	0.36	-	58,58,58,58	0
57	MG	BA	3653	1/1	0.87	0.21	-	57,57,57,57	0
57	MG	BA	3560	1/1	0.97	0.14	-	63,63,63,63	0
57	MG	BA	3247	1/1	0.93	0.17	-	29,29,29,29	0
57	MG	BE	305	1/1	0.95	0.07	-	48,48,48,48	0
57	MG	DA	3265	1/1	0.96	0.16	-	57,57,57,57	0
57	MG	CA	3137	1/1	0.89	0.15	-	78,78,78,78	0
57	MG	BA	3584	1/1	0.94	0.12	-	55,55,55,55	0
57	MG	AA	1603	1/1	0.88	0.15	-	64,64,64,64	0
57	MG	DA	3620	1/1	0.85	0.12	-	53,53,53,53	0
57	MG	BA	3760	1/1	0.97	0.17	-	50,50,50,50	0
57	MG	CA	3019	1/1	0.79	0.16	-	68,68,68,68	0
57	MG	DA	3400	1/1	0.76	0.14	-	62,62,62,62	0
57	MG	CA	3069	1/1	0.94	0.22	-	58,58,58,58	0
57	MG	DA	3498	1/1	0.95	0.17	-	35,35,35,35	0
57	MG	AX	3012	1/1	0.85	0.18	-	52,52,52,52	0
57	MG	BA	3052	1/1	0.86	0.27	-	50,50,50,50	0
57	MG	BZ	301	1/1	0.82	0.18	-	49,49,49,49	0
57	MG	BA	3224	1/1	0.77	0.30	-	59,59,59,59	0
57	MG	AA	1775	1/1	0.95	0.11	-	73,73,73,73	0
57	MG	DA	3399	1/1	0.90	0.15	-	59,59,59,59	0
57	MG	BA	3586	1/1	0.97	0.11	-	55,55,55,55	0
57	MG	DA	3121	1/1	0.96	0.10	-	40,40,40,40	0
57	MG	DA	3514	1/1	0.82	0.14	-	47,47,47,47	0
57	MG	CA	3031	1/1	0.83	0.14	-	58,58,58,58	0
57	MG	BB	3013	1/1	0.91	0.21	-	39,39,39,39	0
57	MG	BE	302	1/1	0.96	0.16	-	35,35,35,35	0
57	MG	BA	3155	1/1	0.84	0.19	-	40,40,40,40	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	BB	3009	1/1	0.90	0.09	-	57,57,57,57	0
57	MG	BA	3266	1/1	0.89	0.10	-	44,44,44,44	0
57	MG	DE	3005	1/1	0.92	0.14	-	35,35,35,35	0
57	MG	DA	3197	1/1	0.91	0.20	-	59,59,59,59	0
57	MG	BA	3553	1/1	0.91	0.19	-	45,45,45,45	0
57	MG	BA	3782	1/1	0.98	0.16	-	38,38,38,38	0
57	MG	DA	3022	1/1	0.92	0.45	-	60,60,60,60	0
57	MG	DA	3487	1/1	0.68	0.12	-	55,55,55,55	0
57	MG	AA	1637	1/1	0.96	0.10	-	61,61,61,61	0
57	MG	AX	3006	1/1	0.95	0.15	-	68,68,68,68	0
57	MG	DA	3479	1/1	0.91	0.10	-	42,42,42,42	0
57	MG	BA	3427	1/1	0.94	0.17	-	33,33,33,33	0
57	MG	DA	3231	1/1	0.96	0.18	-	61,61,61,61	0
57	MG	BA	3278	1/1	0.96	0.78	-	54,54,54,54	0
57	MG	DA	3572	1/1	0.90	0.19	-	65,65,65,65	0
57	MG	DA	3531	1/1	0.94	0.07	-	48,48,48,48	0
57	MG	DA	3211	1/1	0.90	0.21	-	51,51,51,51	0
57	MG	BA	3502	1/1	0.96	0.19	-	30,30,30,30	0
57	MG	AA	1653	1/1	0.97	0.23	-	54,54,54,54	0
57	MG	DA	3470	1/1	0.92	0.08	-	61,61,61,61	0
57	MG	BV	204	1/1	0.89	0.26	-	39,39,39,39	0
57	MG	DA	3097	1/1	0.74	0.14	-	47,47,47,47	0
57	MG	DA	3548	1/1	0.94	0.10	-	66,66,66,66	0
57	MG	CA	3043	1/1	0.97	0.17	-	44,44,44,44	0
57	MG	BA	3738	1/1	0.83	0.13	-	41,41,41,41	0
57	MG	AA	1704	1/1	0.88	0.13	-	57,57,57,57	0
57	MG	BA	3709	1/1	0.95	0.34	-	48,48,48,48	0
57	MG	DA	3302	1/1	0.97	0.23	-	53,53,53,53	0
57	MG	DA	3571	1/1	0.93	0.28	-	45,45,45,45	0
57	MG	CA	3052	1/1	0.86	0.12	-	71,71,71,71	0
57	MG	BA	3452	1/1	0.91	0.15	-	56,56,56,56	0
57	MG	AA	1703	1/1	0.97	0.29	-	43,43,43,43	0
57	MG	DA	3501	1/1	0.97	0.10	-	49,49,49,49	0
57	MG	DA	3587	1/1	0.93	0.12	-	51,51,51,51	0
57	MG	BA	3264	1/1	0.90	0.23	-	51,51,51,51	0
57	MG	DA	3448	1/1	0.90	0.10	-	55,55,55,55	0
57	MG	BA	3326	1/1	0.98	0.15	-	24,24,24,24	0
57	MG	DA	3395	1/1	0.81	0.17	-	58,58,58,58	0
57	MG	CA	3066	1/1	0.96	0.14	-	48,48,48,48	0
57	MG	CA	3030	1/1	0.88	0.07	-	74,74,74,74	0
57	MG	DA	3173	1/1	0.85	0.15	-	62,62,62,62	0
57	MG	AA	1722	1/1	0.98	0.18	-	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
57	MG	CA	3013	1/1	0.80	0.14	-	67,67,67,67	0
57	MG	BA	3414	1/1	0.90	0.20	-	54,54,54,54	0
57	MG	BA	3396	1/1	0.96	0.23	-	25,25,25,25	0
57	MG	DA	3370	1/1	0.97	0.13	-	59,59,59,59	0
57	MG	BA	3069	1/1	0.94	0.34	-	48,48,48,48	0
57	MG	AA	1645	1/1	0.93	0.15	-	61,61,61,61	0
57	MG	DA	3510	1/1	0.95	0.26	-	64,64,64,64	0
57	MG	DA	3380	1/1	0.96	0.05	-	66,66,66,66	0
57	MG	DA	3237	1/1	0.89	0.12	-	59,59,59,59	0
57	MG	BA	3015	1/1	0.77	0.18	-	47,47,47,47	0
57	MG	DA	3261	1/1	0.91	0.16	-	39,39,39,39	0
57	MG	CA	3079	1/1	0.98	0.12	-	49,49,49,49	0
57	MG	DA	3589	1/1	0.95	0.08	-	29,29,29,29	0
57	MG	BA	3196	1/1	0.96	0.23	-	56,56,56,56	0
57	MG	AA	1808	1/1	0.94	0.14	-	49,49,49,49	0
57	MG	BA	3683	1/1	0.97	0.21	-	62,62,62,62	0
57	MG	DA	3626	1/1	0.87	0.11	-	81,81,81,81	0
57	MG	BA	3027	1/1	0.94	0.41	-	64,64,64,64	0
57	MG	DA	3294	1/1	0.97	0.12	-	40,40,40,40	0
57	MG	BA	3193	1/1	0.94	0.13	-	37,37,37,37	0
57	MG	BA	3062	1/1	0.85	0.30	-	59,59,59,59	0
57	MG	DA	3324	1/1	0.88	0.10	-	54,54,54,54	0
57	MG	BA	3282	1/1	0.93	0.24	-	57,57,57,57	0
57	MG	BA	3102	1/1	0.86	0.31	-	57,57,57,57	0
57	MG	DA	3209	1/1	0.99	0.09	-	49,49,49,49	0
57	MG	BA	3097	1/1	0.94	0.12	-	41,41,41,41	0
57	MG	DA	3050	1/1	0.98	0.25	-	44,44,44,44	0
57	MG	BA	3727	1/1	0.71	0.24	-	53,53,53,53	0
57	MG	BA	3667	1/1	0.72	0.24	-	58,58,58,58	0
57	MG	DA	3651	1/1	0.90	0.12	-	48,48,48,48	0
57	MG	DA	3032	1/1	0.76	0.21	-	57,57,57,57	0
57	MG	DA	3506	1/1	0.92	0.08	-	55,55,55,55	0
57	MG	BA	3391	1/1	0.97	0.15	-	41,41,41,41	0
57	MG	BA	3199	1/1	0.95	0.30	-	64,64,64,64	0
57	MG	BA	3733	1/1	0.94	0.15	-	42,42,42,42	0
57	MG	BA	3273	1/1	0.90	0.21	-	45,45,45,45	0
57	MG	AA	1772	1/1	0.99	0.20	-	47,47,47,47	0
57	MG	DA	3092	1/1	0.85	0.16	-	57,57,57,57	0
57	MG	BA	3504	1/1	0.87	0.20	-	56,56,56,56	0
57	MG	BA	3731	1/1	0.99	0.14	-	32,32,32,32	0
57	MG	CW	3001	1/1	0.89	0.19	-	66,66,66,66	0
57	MG	CA	3091	1/1	0.80	0.15	-	69,69,69,69	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	BA	3233	1/1	0.83	0.28	-	40,40,40,40	0
57	MG	BA	3649	1/1	0.93	0.14	-	55,55,55,55	0
57	MG	DA	3435	1/1	0.86	0.12	-	44,44,44,44	0
57	MG	BA	3319	1/1	0.96	0.22	-	23,23,23,23	0
57	MG	CA	3041	1/1	0.85	0.11	-	57,57,57,57	0
57	MG	BA	3761	1/1	0.90	0.10	-	36,36,36,36	0
57	MG	BA	3789	1/1	0.92	0.14	-	47,47,47,47	0
57	MG	DA	3375	1/1	0.88	0.10	-	57,57,57,57	0
57	MG	AA	1710	1/1	0.81	0.15	-	64,64,64,64	0
57	MG	DA	3505	1/1	0.90	0.08	-	51,51,51,51	0
57	MG	BA	3149	1/1	0.87	0.19	-	42,42,42,42	0
57	MG	DA	3271	1/1	0.88	0.16	-	30,30,30,30	0
57	MG	DA	3075	1/1	0.92	0.14	-	55,55,55,55	0
57	MG	AA	1652	1/1	0.89	0.23	-	62,62,62,62	0
57	MG	AA	1707	1/1	0.88	0.12	-	57,57,57,57	0
57	MG	BA	3547	1/1	0.97	0.16	-	45,45,45,45	0
57	MG	DA	3185	1/1	0.95	0.15	-	51,51,51,51	0
57	MG	AA	1719	1/1	0.96	0.16	-	63,63,63,63	0
57	MG	BA	3198	1/1	0.94	0.16	-	44,44,44,44	0
57	MG	DA	3099	1/1	0.69	0.18	-	63,63,63,63	0
57	MG	DA	3212	1/1	0.89	0.23	-	62,62,62,62	0
57	MG	BA	3768	1/1	0.92	0.13	-	57,57,57,57	0
57	MG	DA	3568	1/1	0.84	0.14	-	43,43,43,43	0
57	MG	BA	3603	1/1	0.97	0.28	-	42,42,42,42	0
57	MG	AU	101	1/1	0.97	0.12	-	56,56,56,56	0
57	MG	DA	3485	1/1	0.90	0.09	-	56,56,56,56	0
57	MG	BA	3684	1/1	0.93	0.22	-	51,51,51,51	0
57	MG	BA	3699	1/1	0.93	0.20	-	67,67,67,67	0
57	MG	DA	3650	1/1	0.80	0.14	-	61,61,61,61	0
57	MG	DA	3578	1/1	0.88	0.14	-	43,43,43,43	0
57	MG	BA	3522	1/1	0.89	0.16	-	44,44,44,44	0
57	MG	CA	3141	1/1	0.90	0.14	-	62,62,62,62	0
57	MG	CA	3126	1/1	0.90	0.09	-	45,45,45,45	0
57	MG	BA	3588	1/1	0.87	0.09	-	43,43,43,43	0
57	MG	BA	3127	1/1	0.87	0.30	-	45,45,45,45	0
57	MG	BF	310	1/1	0.82	0.23	-	56,56,56,56	0
57	MG	DN	5001	1/1	0.95	0.11	-	63,63,63,63	0
57	MG	DA	3642	1/1	0.94	0.21	-	62,62,62,62	0
57	MG	BA	3500	1/1	0.92	0.20	-	57,57,57,57	0
57	MG	BA	3803	1/1	0.90	0.34	-	55,55,55,55	0
57	MG	BB	3011	1/1	0.97	0.20	-	47,47,47,47	0
57	MG	BA	3668	1/1	0.86	0.15	-	75,75,75,75	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	DA	3461	1/1	0.93	0.13	-	51,51,51,51	0
57	MG	BA	3363	1/1	0.95	0.17	-	52,52,52,52	0
57	MG	BA	3580	1/1	0.95	0.15	-	48,48,48,48	0
57	MG	BA	3138	1/1	0.89	0.15	-	43,43,43,43	0
57	MG	AA	1688	1/1	0.92	0.20	-	66,66,66,66	0
57	MG	DA	3530	1/1	0.82	0.14	-	55,55,55,55	0
57	MG	DA	3486	1/1	0.89	0.13	-	57,57,57,57	0
57	MG	AA	1639	1/1	0.91	0.07	-	54,54,54,54	0
57	MG	BA	3415	1/1	0.93	0.23	-	35,35,35,35	0
57	MG	CA	3060	1/1	0.94	0.08	-	71,71,71,71	0
57	MG	AA	1677	1/1	0.98	0.21	-	43,43,43,43	0
57	MG	BA	3693	1/1	0.64	0.16	-	77,77,77,77	0
57	MG	BA	3331	1/1	0.97	0.20	-	53,53,53,53	0
57	MG	BA	3378	1/1	0.91	0.24	-	39,39,39,39	0
57	MG	DA	3520	1/1	0.79	0.11	-	57,57,57,57	0
57	MG	DA	3431	1/1	0.92	0.23	-	42,42,42,42	0
57	MG	BA	3593	1/1	0.83	0.20	-	55,55,55,55	0
57	MG	AA	1656	1/1	0.93	0.16	-	63,63,63,63	0
57	MG	BA	3230	1/1	0.87	0.33	-	58,58,58,58	0
57	MG	DA	3527	1/1	0.95	0.13	-	52,52,52,52	0
57	MG	AA	1636	1/1	0.94	0.31	-	52,52,52,52	0
57	MG	DA	3069	1/1	0.91	0.08	-	43,43,43,43	0
57	MG	BA	3774	1/1	0.95	0.32	-	27,27,27,27	0
57	MG	DA	3152	1/1	0.96	0.17	-	45,45,45,45	0
57	MG	BA	3101	1/1	0.93	0.25	-	37,37,37,37	0
57	MG	DA	3304	1/1	0.97	0.14	-	42,42,42,42	0
57	MG	DA	3144	1/1	0.97	0.23	-	41,41,41,41	0
57	MG	BA	3437	1/1	0.94	0.23	-	62,62,62,62	0
57	MG	BA	3080	1/1	0.95	0.14	-	31,31,31,31	0
57	MG	AA	1699	1/1	0.85	0.32	-	58,58,58,58	0
57	MG	DA	3195	1/1	0.98	0.13	-	42,42,42,42	0
57	MG	BA	3086	1/1	0.92	0.33	-	42,42,42,42	0
57	MG	DA	3639	1/1	0.91	0.18	-	59,59,59,59	0
57	MG	DA	3377	1/1	0.89	0.11	-	50,50,50,50	0
57	MG	CA	3165	1/1	0.93	0.09	-	42,42,42,42	0
57	MG	AA	1659	1/1	0.94	0.19	-	65,65,65,65	0
57	MG	BA	3597	1/1	0.87	0.20	-	55,55,55,55	0
57	MG	DA	3107	1/1	0.91	0.11	-	61,61,61,61	0
57	MG	DA	3002	1/1	0.79	0.14	-	64,64,64,64	0
57	MG	DA	3576	1/1	0.92	0.16	-	67,67,67,67	0
57	MG	BA	3778	1/1	0.84	0.08	-	40,40,40,40	0
57	MG	DA	3585	1/1	0.94	0.26	-	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
57	MG	DA	3142	1/1	0.94	0.13	-	51,51,51,51	0
57	MG	BA	3564	1/1	0.87	0.09	-	44,44,44,44	0
57	MG	DA	3004	1/1	0.94	0.20	-	53,53,53,53	0
57	MG	AA	1712	1/1	0.89	0.21	-	69,69,69,69	0
57	MG	BA	3016	1/1	0.75	0.27	-	67,67,67,67	0
57	MG	BA	3611	1/1	0.78	0.18	-	59,59,59,59	0
57	MG	BA	3236	1/1	0.94	0.13	-	52,52,52,52	0
57	MG	CA	3135	1/1	0.90	0.06	-	59,59,59,59	0
57	MG	DA	3297	1/1	0.98	0.18	-	51,51,51,51	0
57	MG	CA	3005	1/1	0.76	0.20	-	73,73,73,73	0
57	MG	AA	1606	1/1	0.86	0.14	-	54,54,54,54	0
57	MG	BA	3325	1/1	0.89	0.15	-	45,45,45,45	0
57	MG	DA	3584	1/1	0.98	0.09	-	31,31,31,31	0
57	MG	AA	1714	1/1	0.91	0.20	-	56,56,56,56	0
57	MG	DB	3005	1/1	0.88	0.12	-	68,68,68,68	0
57	MG	DA	3451	1/1	0.89	0.08	-	55,55,55,55	0
57	MG	AA	1760	1/1	0.96	0.15	-	65,65,65,65	0
57	MG	BA	3538	1/1	0.74	0.12	-	68,68,68,68	0
57	MG	CA	3120	1/1	0.93	0.12	-	68,68,68,68	0
57	MG	BA	3599	1/1	0.93	0.16	-	60,60,60,60	0
57	MG	CA	3068	1/1	0.85	0.16	-	58,58,58,58	0
57	MG	BA	3471	1/1	0.95	0.18	-	27,27,27,27	0
57	MG	DA	3541	1/1	0.88	0.10	-	59,59,59,59	0
57	MG	AA	1690	1/1	0.93	0.42	-	52,52,52,52	0
57	MG	DA	3054	1/1	0.98	0.10	-	27,27,27,27	0
57	MG	DA	3550	1/1	0.91	0.04	-	60,60,60,60	0
57	MG	BA	3352	1/1	0.96	0.16	-	68,68,68,68	0
57	MG	DA	3383	1/1	0.99	0.13	-	28,28,28,28	0
57	MG	BA	3679	1/1	0.94	0.22	-	52,52,52,52	0
57	MG	BA	3227	1/1	0.97	0.17	-	33,33,33,33	0
57	MG	BZ	302	1/1	0.92	0.17	-	60,60,60,60	0
57	MG	DA	3407	1/1	0.92	0.08	-	58,58,58,58	0
57	MG	BA	3212	1/1	0.87	0.21	-	57,57,57,57	0
57	MG	AA	1667	1/1	0.85	0.19	-	55,55,55,55	0
57	MG	AA	1657	1/1	0.93	0.12	-	64,64,64,64	0
57	MG	DA	3484	1/1	0.96	0.07	-	46,46,46,46	0
57	MG	DA	3419	1/1	0.94	0.14	-	50,50,50,50	0
57	MG	BA	3446	1/1	0.91	0.09	-	59,59,59,59	0
57	MG	BA	3258	1/1	0.95	0.35	-	44,44,44,44	0
57	MG	DA	3041	1/1	0.78	0.18	-	60,60,60,60	0
57	MG	BA	3262	1/1	0.96	0.27	-	31,31,31,31	0
57	MG	BA	3474	1/1	0.94	0.27	-	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
57	MG	DA	3345	1/1	0.98	0.15	-	58,58,58,58	0
57	MG	BA	3663	1/1	0.92	0.20	-	50,50,50,50	0
57	MG	DA	3242	1/1	0.92	0.09	-	52,52,52,52	0
57	MG	DA	3567	1/1	0.94	0.26	-	44,44,44,44	0
57	MG	B0	3002	1/1	0.88	0.21	-	63,63,63,63	0
57	MG	DA	3061	1/1	0.76	0.22	-	60,60,60,60	0
57	MG	BA	3013	1/1	0.96	0.20	-	28,28,28,28	0
57	MG	AX	3010	1/1	0.88	0.40	-	68,68,68,68	0
57	MG	BA	3218	1/1	0.93	0.15	-	45,45,45,45	0
57	MG	DA	3472	1/1	0.99	0.14	-	25,25,25,25	0
57	MG	DA	3631	1/1	0.94	0.12	-	49,49,49,49	0
57	MG	DA	3269	1/1	0.95	0.11	-	50,50,50,50	0
57	MG	AA	1786	1/1	0.95	0.14	-	69,69,69,69	0
57	MG	BA	3354	1/1	0.95	0.12	-	47,47,47,47	0
57	MG	AA	1609	1/1	0.91	0.13	-	63,63,63,63	0
57	MG	DA	3104	1/1	0.92	0.11	-	57,57,57,57	0
57	MG	DA	3157	1/1	0.96	0.13	-	34,34,34,34	0
57	MG	BA	3228	1/1	0.95	0.10	-	65,65,65,65	0
57	MG	BA	3453	1/1	0.81	0.28	-	50,50,50,50	0
57	MG	AA	1648	1/1	0.92	0.19	-	56,56,56,56	0
57	MG	DA	3339	1/1	0.92	0.20	-	52,52,52,52	0
57	MG	AA	1709	1/1	0.95	0.26	-	55,55,55,55	0
57	MG	BA	3166	1/1	0.90	0.18	-	33,33,33,33	0
57	MG	BA	3068	1/1	0.71	0.17	-	49,49,49,49	0
57	MG	AA	1664	1/1	0.83	0.22	-	62,62,62,62	0
57	MG	BA	3243	1/1	0.86	0.67	-	44,44,44,44	0
57	MG	BA	3596	1/1	0.94	0.17	-	59,59,59,59	0
57	MG	DB	3006	1/1	0.94	0.14	-	55,55,55,55	0
57	MG	BA	3381	1/1	0.88	0.11	-	49,49,49,49	0
57	MG	DA	3326	1/1	0.97	0.10	-	46,46,46,46	0
57	MG	CA	3102	1/1	0.82	0.16	-	71,71,71,71	0
57	MG	AA	1642	1/1	0.97	0.23	-	59,59,59,59	0
57	MG	DA	3204	1/1	0.60	0.21	-	68,68,68,68	0
57	MG	BA	3317	1/1	0.94	0.20	-	43,43,43,43	0
57	MG	DA	3244	1/1	0.90	0.27	-	55,55,55,55	0
57	MG	AA	1668	1/1	0.97	0.10	-	63,63,63,63	0
57	MG	CA	3133	1/1	0.97	0.17	-	82,82,82,82	0
57	MG	DA	3117	1/1	0.96	0.09	-	56,56,56,56	0
57	MG	BA	3542	1/1	0.92	0.16	-	44,44,44,44	0
57	MG	BA	3005	1/1	0.86	0.19	-	44,44,44,44	0
57	MG	CA	3115	1/1	0.58	0.34	-	82,82,82,82	0
57	MG	BP	3002	1/1	0.89	0.14	-	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
57	MG	DA	3390	1/1	0.86	0.10	-	58,58,58,58	0
57	MG	BA	3010	1/1	0.92	0.18	-	53,53,53,53	0
57	MG	BA	3791	1/1	0.96	0.38	-	49,49,49,49	0
57	MG	BA	3274	1/1	0.90	0.27	-	66,66,66,66	0
57	MG	BA	3740	1/1	0.91	0.19	-	65,65,65,65	0
57	MG	AA	1602	1/1	0.85	0.10	-	68,68,68,68	0
57	MG	BA	3429	1/1	0.90	0.26	-	50,50,50,50	0
57	MG	BA	3551	1/1	0.99	0.15	-	44,44,44,44	0
57	MG	DA	3582	1/1	0.92	0.05	-	53,53,53,53	0
57	MG	DA	3289	1/1	0.88	0.16	-	52,52,52,52	0
57	MG	BA	3106	1/1	0.87	0.25	-	52,52,52,52	0
57	MG	BA	3339	1/1	0.98	0.21	-	43,43,43,43	0
57	MG	BA	3298	1/1	0.94	0.15	-	27,27,27,27	0
57	MG	BA	3209	1/1	0.91	0.24	-	48,48,48,48	0
57	MG	BA	3265	1/1	0.74	0.29	-	72,72,72,72	0
57	MG	CA	3028	1/1	0.96	0.27	-	48,48,48,48	0
57	MG	DA	3600	1/1	0.87	0.13	-	72,72,72,72	0
57	MG	DA	3379	1/1	0.84	0.09	-	46,46,46,46	0
57	MG	DA	3112	1/1	0.86	0.13	-	56,56,56,56	0
57	MG	BA	3720	1/1	0.96	0.12	-	38,38,38,38	0
57	MG	DA	3330	1/1	0.86	0.17	-	36,36,36,36	0
57	MG	DA	3008	1/1	0.85	0.12	-	45,45,45,45	0
57	MG	BA	3729	1/1	0.92	0.14	-	46,46,46,46	0
57	MG	AA	1816	1/1	0.90	0.20	-	59,59,59,59	0
57	MG	BA	3431	1/1	0.92	0.28	-	57,57,57,57	0
57	MG	AA	1732	1/1	0.98	0.20	-	63,63,63,63	0
57	MG	DA	3171	1/1	0.95	0.17	-	40,40,40,40	0
57	MG	BA	3641	1/1	0.92	0.18	-	68,68,68,68	0
57	MG	DA	3015	1/1	0.78	0.23	-	60,60,60,60	0
57	MG	DB	3009	1/1	0.94	0.14	-	58,58,58,58	0
57	MG	AA	1614	1/1	0.87	0.19	-	75,75,75,75	0
57	MG	DA	3281	1/1	0.85	0.11	-	36,36,36,36	0
57	MG	BA	3285	1/1	0.96	0.15	-	58,58,58,58	0
57	MG	BA	3480	1/1	0.94	0.18	-	47,47,47,47	0
57	MG	DA	3180	1/1	0.97	0.21	-	48,48,48,48	0
57	MG	B8	5001	1/1	0.94	0.20	-	42,42,42,42	0
57	MG	BA	3290	1/1	0.92	0.21	-	57,57,57,57	0
57	MG	DA	3408	1/1	0.98	0.23	-	55,55,55,55	0
57	MG	DA	3622	1/1	0.93	0.10	-	49,49,49,49	0
57	MG	DA	3025	1/1	0.98	0.45	-	47,47,47,47	0
57	MG	BA	3322	1/1	0.93	0.16	-	38,38,38,38	0
57	MG	DA	3614	1/1	0.91	0.14	-	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
57	MG	DA	3058	1/1	0.96	0.08	-	61,61,61,61	0
57	MG	BA	3428	1/1	0.93	0.16	-	51,51,51,51	0
57	MG	DA	3640	1/1	0.97	0.10	-	62,62,62,62	0
57	MG	BA	3205	1/1	0.96	0.43	-	57,57,57,57	0
57	MG	BA	3047	1/1	0.93	0.22	-	43,43,43,43	0
57	MG	AA	1780	1/1	0.94	0.11	-	69,69,69,69	0
57	MG	CA	3010	1/1	0.99	0.10	-	49,49,49,49	0
57	MG	BA	3259	1/1	0.98	0.18	-	25,25,25,25	0
57	MG	BA	3267	1/1	0.98	0.30	-	61,61,61,61	0
57	MG	BA	3531	1/1	0.91	0.14	-	60,60,60,60	0
57	MG	BA	3677	1/1	0.94	0.10	-	44,44,44,44	0
57	MG	BA	3613	1/1	0.91	0.23	-	53,53,53,53	0
57	MG	BA	3654	1/1	0.96	0.11	-	59,59,59,59	0
57	MG	DA	3468	1/1	0.82	0.14	-	62,62,62,62	0
57	MG	DA	3369	1/1	0.83	0.12	-	55,55,55,55	0
57	MG	DA	3374	1/1	0.92	0.22	-	62,62,62,62	0
57	MG	CA	3025	1/1	0.93	0.24	-	53,53,53,53	0
57	MG	AA	1792	1/1	0.98	0.12	-	47,47,47,47	0
57	MG	DA	3166	1/1	0.94	0.16	-	55,55,55,55	0
57	MG	CA	3021	1/1	0.91	0.10	-	61,61,61,61	0
57	MG	BA	3385	1/1	0.97	0.23	-	30,30,30,30	0
57	MG	BA	3472	1/1	0.98	0.20	-	24,24,24,24	0
57	MG	BA	3019	1/1	0.91	0.28	-	54,54,54,54	0
57	MG	AA	1784	1/1	0.34	0.29	-	72,72,72,72	0
57	MG	DA	3329	1/1	0.95	0.10	-	47,47,47,47	0
57	MG	AA	1728	1/1	0.94	0.25	-	49,49,49,49	0
57	MG	DA	3555	1/1	0.95	0.21	-	46,46,46,46	0
57	MG	AA	1612	1/1	0.85	0.16	-	63,63,63,63	0
57	MG	DA	3566	1/1	0.92	0.18	-	37,37,37,37	0
57	MG	BA	3025	1/1	0.92	0.18	-	43,43,43,43	0
57	MG	AA	1783	1/1	0.95	0.17	-	35,35,35,35	0
57	MG	BA	3620	1/1	0.94	0.14	-	29,29,29,29	0
57	MG	BB	3019	1/1	0.83	0.20	-	70,70,70,70	0
57	MG	DA	3306	1/1	0.88	0.28	-	65,65,65,65	0
57	MG	CA	3157	1/1	0.86	0.12	-	60,60,60,60	0
57	MG	DA	3051	1/1	0.88	0.13	-	44,44,44,44	0
57	MG	BA	3145	1/1	0.84	0.25	-	48,48,48,48	0
57	MG	BA	3301	1/1	0.93	0.18	-	62,62,62,62	0
57	MG	DA	3067	1/1	0.87	0.14	-	63,63,63,63	0
57	MG	AA	1802	1/1	0.93	0.10	-	54,54,54,54	0
57	MG	BA	3049	1/1	0.84	0.19	-	46,46,46,46	0
57	MG	CA	3007	1/1	0.88	0.12	-	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
57	MG	BA	3201	1/1	0.96	0.21	-	48,48,48,48	0
57	MG	DA	3235	1/1	0.86	0.13	-	48,48,48,48	0
57	MG	DA	3403	1/1	0.91	0.09	-	49,49,49,49	0
57	MG	BA	3651	1/1	0.93	0.14	-	66,66,66,66	0
57	MG	BA	3241	1/1	0.94	0.16	-	56,56,56,56	0
57	MG	BA	3479	1/1	0.95	0.06	-	53,53,53,53	0
57	MG	DA	3643	1/1	0.92	0.07	-	54,54,54,54	0
57	MG	AA	1796	1/1	0.97	0.07	-	64,64,64,64	0
57	MG	DA	3646	1/1	0.93	0.15	-	56,56,56,56	0
57	MG	DA	3017	1/1	0.88	0.12	-	59,59,59,59	0
57	MG	BA	3404	1/1	0.90	0.34	-	59,59,59,59	0
57	MG	DA	3603	1/1	0.87	0.06	-	65,65,65,65	0
57	MG	DA	3066	1/1	0.77	0.10	-	58,58,58,58	0
57	MG	BA	3722	1/1	0.94	0.19	-	64,64,64,64	0
57	MG	CA	3022	1/1	0.88	0.23	-	76,76,76,76	0
57	MG	BA	3563	1/1	0.92	0.12	-	50,50,50,50	0
57	MG	DA	3615	1/1	0.98	0.09	-	62,62,62,62	0
57	MG	BA	3669	1/1	0.97	0.20	-	28,28,28,28	0
57	MG	CA	3014	1/1	0.76	0.15	-	62,62,62,62	0
57	MG	DA	3251	1/1	0.94	0.15	-	40,40,40,40	0
57	MG	DA	3127	1/1	0.91	0.10	-	52,52,52,52	0
57	MG	AA	1689	1/1	0.77	0.29	-	71,71,71,71	0
57	MG	DA	3098	1/1	0.96	0.10	-	66,66,66,66	0
57	MG	BA	3718	1/1	0.99	0.17	-	47,47,47,47	0
57	MG	CA	3055	1/1	0.91	0.18	-	63,63,63,63	0
57	MG	DA	3569	1/1	0.92	0.24	-	45,45,45,45	0
57	MG	BA	3292	1/1	0.94	0.24	-	26,26,26,26	0
57	MG	CA	3105	1/1	0.97	0.12	-	75,75,75,75	0
57	MG	BA	3208	1/1	0.95	0.10	-	43,43,43,43	0
57	MG	BA	3661	1/1	0.93	0.24	-	25,25,25,25	0
57	MG	AA	1643	1/1	0.91	0.20	-	58,58,58,58	0
57	MG	AA	1807	1/1	0.95	0.07	-	68,68,68,68	0
57	MG	DA	3276	1/1	0.96	0.16	-	28,28,28,28	0
57	MG	CA	3138	1/1	0.96	0.10	-	65,65,65,65	0
57	MG	BA	3074	1/1	0.78	0.23	-	69,69,69,69	0
57	MG	DA	3016	1/1	0.79	0.09	-	66,66,66,66	0
57	MG	AA	1618	1/1	0.55	0.18	-	68,68,68,68	0
57	MG	BA	3303	1/1	0.93	0.23	-	26,26,26,26	0
57	MG	DA	3227	1/1	0.83	0.20	-	56,56,56,56	0
57	MG	DB	3010	1/1	0.83	0.13	-	75,75,75,75	0
57	MG	BA	3705	1/1	0.89	0.14	-	59,59,59,59	0
57	MG	DA	3084	1/1	0.91	0.17	-	44,44,44,44	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	AA	1626	1/1	0.89	0.21	-	59,59,59,59	0
57	MG	BA	3670	1/1	0.81	0.18	-	54,54,54,54	0
57	MG	AA	1778	1/1	0.92	0.09	-	51,51,51,51	0
57	MG	DA	3071	1/1	0.73	0.23	-	47,47,47,47	0
57	MG	BA	3192	1/1	0.94	0.20	-	19,19,19,19	0
57	MG	BA	3238	1/1	0.95	0.48	-	44,44,44,44	0
57	MG	DA	3317	1/1	0.85	0.10	-	54,54,54,54	0
57	MG	BA	3338	1/1	0.86	0.18	-	55,55,55,55	0
57	MG	AA	1736	1/1	0.96	0.10	-	49,49,49,49	0
57	MG	DA	3366	1/1	0.92	0.12	-	44,44,44,44	0
57	MG	AA	1638	1/1	0.93	0.23	-	60,60,60,60	0
57	MG	BB	3002	1/1	0.98	0.28	-	55,55,55,55	0
57	MG	BA	3126	1/1	0.91	0.23	-	36,36,36,36	0
57	MG	AA	1698	1/1	0.94	0.23	-	58,58,58,58	0
57	MG	DA	3287	1/1	0.95	0.21	-	52,52,52,52	0
57	MG	DA	3076	1/1	0.95	0.18	-	52,52,52,52	0
57	MG	DA	3415	1/1	0.85	0.18	-	43,43,43,43	0
57	MG	DA	3101	1/1	0.82	0.13	-	56,56,56,56	0
57	MG	CA	3128	1/1	0.97	0.13	-	52,52,52,52	0
57	MG	DA	3336	1/1	0.90	0.09	-	49,49,49,49	0
57	MG	BA	3178	1/1	0.95	0.17	-	32,32,32,32	0
57	MG	AA	1700	1/1	0.95	0.07	-	71,71,71,71	0
57	MG	DA	3122	1/1	0.70	0.19	-	60,60,60,60	0
57	MG	BA	3095	1/1	0.94	0.23	-	53,53,53,53	0
57	MG	DA	3021	1/1	0.89	0.17	-	50,50,50,50	0
57	MG	BA	3569	1/1	0.69	0.22	-	56,56,56,56	0
57	MG	DA	3502	1/1	0.75	0.24	-	48,48,48,48	0
57	MG	AA	1790	1/1	0.93	0.08	-	81,81,81,81	0
57	MG	DA	3446	1/1	0.90	0.14	-	50,50,50,50	0
57	MG	DA	3202	1/1	0.94	0.20	-	62,62,62,62	0
57	MG	DA	3168	1/1	0.98	0.12	-	44,44,44,44	0
57	MG	DP	201	1/1	0.87	0.21	-	69,69,69,69	0
57	MG	CA	3001	1/1	0.84	0.14	-	59,59,59,59	0
57	MG	BF	311	1/1	0.92	0.12	-	52,52,52,52	0
57	MG	DA	3335	1/1	0.93	0.25	-	49,49,49,49	0
57	MG	AA	1708	1/1	0.89	0.19	-	60,60,60,60	0
57	MG	DA	3299	1/1	0.95	0.09	-	46,46,46,46	0
57	MG	BA	3786	1/1	0.90	0.16	-	51,51,51,51	0
57	MG	AX	3008	1/1	0.88	0.15	-	76,76,76,76	0
57	MG	BA	3627	1/1	0.97	0.20	-	56,56,56,56	0
57	MG	DA	3136	1/1	0.86	0.18	-	48,48,48,48	0
57	MG	CA	3084	1/1	0.97	0.14	-	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
57	MG	BA	3128	1/1	0.91	0.19	-	42,42,42,42	0
57	MG	BA	3134	1/1	0.92	0.18	-	40,40,40,40	0
57	MG	BA	3125	1/1	0.89	0.25	-	38,38,38,38	0
57	MG	DA	3535	1/1	0.94	0.18	-	44,44,44,44	0
57	MG	DA	3024	1/1	0.80	0.41	-	61,61,61,61	0
57	MG	BA	3489	1/1	0.94	0.25	-	50,50,50,50	0
57	MG	AE	3001	1/1	0.96	0.07	-	63,63,63,63	0
57	MG	BA	3604	1/1	0.87	0.19	-	43,43,43,43	0
57	MG	DA	3088	1/1	0.86	0.25	-	50,50,50,50	0
57	MG	BA	3465	1/1	0.95	0.09	-	48,48,48,48	0
57	MG	CA	3152	1/1	0.91	0.10	-	71,71,71,71	0
57	MG	DA	3205	1/1	0.82	0.16	-	62,62,62,62	0
57	MG	BA	3466	1/1	0.96	0.17	-	51,51,51,51	0
57	MG	BA	3108	1/1	0.96	0.21	-	42,42,42,42	0
57	MG	CA	3107	1/1	0.85	0.12	-	68,68,68,68	0
57	MG	DE	3003	1/1	0.94	0.12	-	43,43,43,43	0
57	MG	BA	3293	1/1	0.95	0.11	-	58,58,58,58	0
57	MG	DA	3199	1/1	0.69	0.24	-	62,62,62,62	0
57	MG	DA	3165	1/1	0.95	0.20	-	55,55,55,55	0
57	MG	AA	1716	1/1	0.96	0.17	-	50,50,50,50	0
57	MG	BA	3394	1/1	0.94	0.28	-	40,40,40,40	0
57	MG	BA	3662	1/1	0.92	0.22	-	62,62,62,62	0
57	MG	BA	3436	1/1	0.92	0.15	-	57,57,57,57	0
57	MG	BA	3014	1/1	0.88	0.14	-	35,35,35,35	0
57	MG	BA	3590	1/1	0.96	0.15	-	33,33,33,33	0
57	MG	B5	104	1/1	0.97	0.09	-	58,58,58,58	0
57	MG	BA	3601	1/1	0.94	0.31	-	40,40,40,40	0
57	MG	BA	3305	1/1	0.92	0.15	-	46,46,46,46	0
57	MG	BA	3666	1/1	0.88	0.26	-	74,74,74,74	0
57	MG	CA	3008	1/1	0.89	0.31	-	47,47,47,47	0
57	MG	CA	3150	1/1	0.93	0.15	-	65,65,65,65	0
57	MG	DA	3376	1/1	0.74	0.11	-	51,51,51,51	0
57	MG	DA	3293	1/1	0.96	0.15	-	61,61,61,61	0
57	MG	BA	3316	1/1	0.97	0.20	-	54,54,54,54	0
57	MG	BB	3015	1/1	0.96	0.26	-	45,45,45,45	0
57	MG	BA	3555	1/1	0.94	0.19	-	50,50,50,50	0
57	MG	DA	3218	1/1	0.88	0.17	-	52,52,52,52	0
57	MG	AA	1705	1/1	0.91	0.23	-	70,70,70,70	0
57	MG	CA	3127	1/1	0.93	0.08	-	59,59,59,59	0
57	MG	BA	3257	1/1	0.81	0.18	-	43,43,43,43	0
57	MG	BA	3495	1/1	0.95	0.16	-	43,43,43,43	0
57	MG	BA	3721	1/1	0.80	0.10	-	47,47,47,47	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	DA	3082	1/1	0.95	0.22	-	47,47,47,47	0
57	MG	BA	3658	1/1	0.90	0.12	-	61,61,61,61	0
57	MG	BA	3284	1/1	0.95	0.10	-	57,57,57,57	0
57	MG	BA	3320	1/1	0.94	0.16	-	55,55,55,55	0
57	MG	DA	3618	1/1	0.83	0.10	-	46,46,46,46	0
57	MG	DA	3044	1/1	0.96	0.18	-	53,53,53,53	0
57	MG	AA	1634	1/1	0.87	0.15	-	64,64,64,64	0
57	MG	BA	3250	1/1	0.86	0.21	-	68,68,68,68	0
57	MG	DA	3546	1/1	0.98	0.04	-	47,47,47,47	0
57	MG	BA	3087	1/1	0.90	0.38	-	43,43,43,43	0
57	MG	BA	3734	1/1	0.57	0.14	-	65,65,65,65	0
57	MG	BA	3675	1/1	0.94	0.26	-	56,56,56,56	0
57	MG	BA	3279	1/1	0.93	0.32	-	52,52,52,52	0
57	MG	DA	3273	1/1	0.93	0.12	-	62,62,62,62	0
57	MG	DA	3405	1/1	0.92	0.07	-	47,47,47,47	0
57	MG	DA	3208	1/1	0.88	0.16	-	54,54,54,54	0
57	MG	DA	3462	1/1	0.85	0.22	-	50,50,50,50	0
57	MG	BA	3726	1/1	0.86	0.20	-	31,31,31,31	0
57	MG	B2	3001	1/1	0.87	0.25	-	53,53,53,53	0
57	MG	BA	3351	1/1	0.94	0.19	-	45,45,45,45	0
57	MG	BA	3245	1/1	0.87	0.32	-	59,59,59,59	0
57	MG	BA	3150	1/1	0.93	0.17	-	39,39,39,39	0
57	MG	DA	3445	1/1	0.88	0.13	-	52,52,52,52	0
57	MG	BA	3455	1/1	0.95	0.14	-	52,52,52,52	0
57	MG	DA	3047	1/1	0.94	0.16	-	45,45,45,45	0
57	MG	CA	3080	1/1	0.98	0.10	-	49,49,49,49	0
57	MG	BE	304	1/1	0.93	0.23	-	23,23,23,23	0
57	MG	DA	3378	1/1	0.95	0.14	-	52,52,52,52	0
57	MG	DA	3222	1/1	0.93	0.23	-	58,58,58,58	0
57	MG	DA	3224	1/1	0.95	0.08	-	39,39,39,39	0
57	MG	BA	3130	1/1	0.96	0.46	-	48,48,48,48	0
57	MG	AA	1651	1/1	0.87	0.25	-	58,58,58,58	0
57	MG	BA	3763	1/1	0.88	0.15	-	44,44,44,44	0
57	MG	DA	3609	1/1	0.94	0.10	-	61,61,61,61	0
57	MG	CA	3129	1/1	0.88	0.13	-	69,69,69,69	0
57	MG	BA	3691	1/1	0.95	0.11	-	43,43,43,43	0
57	MG	DA	3110	1/1	0.90	0.10	-	49,49,49,49	0
57	MG	BA	3809	1/1	0.84	0.37	-	61,61,61,61	0
57	MG	BA	3521	1/1	0.96	0.22	-	40,40,40,40	0
57	MG	DA	3079	1/1	0.77	0.11	-	72,72,72,72	0
57	MG	DA	3249	1/1	0.93	0.08	-	65,65,65,65	0
57	MG	CA	3058	1/1	0.72	0.19	-	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
57	MG	AA	1605	1/1	0.88	0.15	-	50,50,50,50	0
57	MG	BB	3022	1/1	0.92	0.20	-	60,60,60,60	0
57	MG	DA	3030	1/1	0.91	0.17	-	44,44,44,44	0
57	MG	BA	3562	1/1	0.94	0.16	-	55,55,55,55	0
57	MG	BA	3638	1/1	0.88	0.17	-	65,65,65,65	0
57	MG	DA	3254	1/1	0.43	0.15	-	68,68,68,68	0
57	MG	DA	3257	1/1	0.82	0.20	-	44,44,44,44	0
57	MG	DA	3406	1/1	0.90	0.17	-	70,70,70,70	0
57	MG	BA	3421	1/1	0.95	0.26	-	62,62,62,62	0
57	MG	DY	502	1/1	0.93	0.17	-	55,55,55,55	0
57	MG	DA	3575	1/1	0.92	0.08	-	56,56,56,56	0
57	MG	DA	3344	1/1	0.91	0.14	-	38,38,38,38	0
57	MG	DA	3475	1/1	0.94	0.17	-	56,56,56,56	0
57	MG	BA	3077	1/1	0.97	0.20	-	15,15,15,15	0
57	MG	BA	3655	1/1	0.69	0.13	-	55,55,55,55	0
57	MG	DA	3270	1/1	0.96	0.09	-	42,42,42,42	0
57	MG	DA	3172	1/1	0.86	0.21	-	61,61,61,61	0
57	MG	BA	3517	1/1	0.91	0.23	-	33,33,33,33	0
57	MG	DA	3033	1/1	0.60	0.49	-	68,68,68,68	0
57	MG	BA	3042	1/1	0.95	0.13	-	37,37,37,37	0
57	MG	CA	3148	1/1	0.89	0.15	-	68,68,68,68	0
57	MG	AA	1810	1/1	0.82	0.09	-	86,86,86,86	0
57	MG	AA	1661	1/1	0.97	0.37	-	54,54,54,54	0
57	MG	BA	3367	1/1	0.89	0.22	-	52,52,52,52	0
57	MG	BA	3104	1/1	0.99	0.19	-	24,24,24,24	0
57	MG	BA	3703	1/1	0.94	0.33	-	28,28,28,28	0
57	MG	BA	3066	1/1	0.93	0.24	-	58,58,58,58	0
57	MG	AA	1654	1/1	0.93	0.23	-	65,65,65,65	0
57	MG	DA	3396	1/1	0.93	0.17	-	46,46,46,46	0
57	MG	BA	3157	1/1	0.97	0.20	-	46,46,46,46	0
57	MG	BA	3165	1/1	0.95	0.31	-	52,52,52,52	0
57	MG	DA	3138	1/1	0.94	0.14	-	54,54,54,54	0
57	MG	BA	3785	1/1	0.93	0.14	-	56,56,56,56	0
57	MG	DA	3081	1/1	0.91	0.11	-	51,51,51,51	0
57	MG	BA	3463	1/1	0.97	0.21	-	56,56,56,56	0
57	MG	DA	3145	1/1	0.95	0.32	-	48,48,48,48	0
57	MG	DA	3055	1/1	0.90	0.14	-	53,53,53,53	0
57	MG	BA	3478	1/1	0.95	0.15	-	54,54,54,54	0
57	MG	DB	3012	1/1	0.88	0.24	-	66,66,66,66	0
57	MG	BA	3659	1/1	0.93	0.11	-	47,47,47,47	0
57	MG	AA	1799	1/1	0.92	0.11	-	78,78,78,78	0
57	MG	BA	3707	1/1	0.99	0.19	-	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
57	MG	BA	3501	1/1	0.89	0.14	-	42,42,42,42	0
57	MG	BA	3084	1/1	0.94	0.18	-	42,42,42,42	0
57	MG	DA	3540	1/1	0.94	0.06	-	50,50,50,50	0
57	MG	AA	1610	1/1	0.79	0.18	-	81,81,81,81	0
57	MG	BA	3287	1/1	0.97	0.17	-	27,27,27,27	0
57	MG	DA	3508	1/1	0.88	0.18	-	57,57,57,57	0
57	MG	DA	3177	1/1	0.93	0.13	-	58,58,58,58	0
57	MG	DA	3125	1/1	0.89	0.14	-	56,56,56,56	0
57	MG	DA	3495	1/1	0.97	0.05	-	50,50,50,50	0
57	MG	DA	3062	1/1	0.97	0.11	-	53,53,53,53	0
57	MG	BA	3170	1/1	0.92	0.17	-	38,38,38,38	0
57	MG	BA	3535	1/1	0.91	0.20	-	39,39,39,39	0
57	MG	DA	3348	1/1	0.97	0.20	-	53,53,53,53	0
57	MG	BB	3018	1/1	0.95	0.06	-	54,54,54,54	0
57	MG	DA	3221	1/1	0.96	0.10	-	41,41,41,41	0
57	MG	BA	3361	1/1	0.96	0.08	-	56,56,56,56	0
57	MG	BA	3612	1/1	0.97	0.10	-	60,60,60,60	0
57	MG	BA	3449	1/1	0.93	0.23	-	62,62,62,62	0
57	MG	BA	3058	1/1	0.82	0.19	-	54,54,54,54	0
57	MG	DA	3150	1/1	0.87	0.16	-	50,50,50,50	0
57	MG	AA	1646	1/1	0.94	0.23	-	58,58,58,58	0
57	MG	BA	3753	1/1	0.95	0.19	-	68,68,68,68	0
57	MG	DA	3423	1/1	0.95	0.20	-	37,37,37,37	0
57	MG	DA	3248	1/1	0.97	0.11	-	58,58,58,58	0
57	MG	AA	1715	1/1	0.94	0.23	-	45,45,45,45	0
57	MG	DA	3628	1/1	0.57	0.19	-	77,77,77,77	0
57	MG	AA	1734	1/1	0.96	0.13	-	43,43,43,43	0
57	MG	AA	1696	1/1	0.84	0.10	-	83,83,83,83	0
57	MG	DA	3038	1/1	0.95	0.14	-	56,56,56,56	0
57	MG	BA	3594	1/1	0.88	0.14	-	45,45,45,45	0
57	MG	DA	3496	1/1	0.95	0.17	-	56,56,56,56	0
57	MG	CA	3139	1/1	0.86	0.36	-	81,81,81,81	0
57	MG	DA	3517	1/1	0.94	0.12	-	48,48,48,48	0
57	MG	BA	3357	1/1	0.97	0.07	-	34,34,34,34	0
57	MG	BA	3660	1/1	0.87	0.19	-	60,60,60,60	0
57	MG	DA	3563	1/1	0.93	0.10	-	70,70,70,70	0
57	MG	AA	1711	1/1	0.79	0.13	-	51,51,51,51	0
57	MG	BA	3801	1/1	0.95	0.16	-	71,71,71,71	0
57	MG	DA	3647	1/1	0.96	0.11	-	52,52,52,52	0
57	MG	AA	1803	1/1	0.97	0.12	-	46,46,46,46	0
57	MG	BA	3631	1/1	0.90	0.26	-	46,46,46,46	0
57	MG	CA	3064	1/1	0.92	0.21	-	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
57	MG	AA	1623	1/1	0.81	0.24	-	65,65,65,65	0
57	MG	BA	3757	1/1	0.93	0.18	-	43,43,43,43	0
57	MG	DA	3131	1/1	0.93	0.25	-	49,49,49,49	0
57	MG	BA	3481	1/1	0.95	0.12	-	54,54,54,54	0
57	MG	BA	3173	1/1	0.98	0.28	-	32,32,32,32	0
57	MG	BA	3568	1/1	0.96	0.23	-	24,24,24,24	0
57	MG	DA	3592	1/1	0.82	0.14	-	67,67,67,67	0
57	MG	AA	1718	1/1	0.98	0.11	-	66,66,66,66	0
57	MG	BA	3539	1/1	0.98	0.14	-	42,42,42,42	0
57	MG	CA	3145	1/1	0.98	0.12	-	65,65,65,65	0
57	MG	DA	3200	1/1	0.88	0.16	-	41,41,41,41	0
57	MG	BA	3360	1/1	0.86	0.23	-	37,37,37,37	0
57	MG	DA	3295	1/1	0.95	0.20	-	67,67,67,67	0
57	MG	BA	3491	1/1	0.89	0.22	-	56,56,56,56	0
57	MG	AA	1781	1/1	0.91	0.10	-	59,59,59,59	0
57	MG	CA	3034	1/1	0.89	0.23	-	66,66,66,66	0
57	MG	BA	3213	1/1	0.95	0.15	-	43,43,43,43	0
57	MG	DA	3537	1/1	0.97	0.16	-	45,45,45,45	0
57	MG	BA	3673	1/1	0.93	0.28	-	61,61,61,61	0
57	MG	BA	3304	1/1	0.93	0.18	-	39,39,39,39	0
57	MG	DA	3243	1/1	0.90	0.12	-	48,48,48,48	0
57	MG	BW	3004	1/1	0.91	0.19	-	45,45,45,45	0
57	MG	DA	3153	1/1	0.86	0.15	-	44,44,44,44	0
57	MG	DA	3007	1/1	0.97	0.13	-	30,30,30,30	0
57	MG	DA	3638	1/1	0.96	0.09	-	47,47,47,47	0
57	MG	BA	3146	1/1	0.98	0.17	-	41,41,41,41	0
57	MG	BA	3758	1/1	0.94	0.12	-	41,41,41,41	0
57	MG	AX	3016	1/1	0.82	0.61	-	86,86,86,86	0
57	MG	AA	1733	1/1	0.94	0.12	-	50,50,50,50	0
57	MG	BA	3162	1/1	0.97	0.29	-	41,41,41,41	0
57	MG	B6	103	1/1	0.93	0.15	-	52,52,52,52	0
57	MG	BA	3800	1/1	0.99	0.18	-	29,29,29,29	0
57	MG	AX	3014	1/1	0.93	0.24	-	61,61,61,61	0
57	MG	DA	3518	1/1	0.97	0.10	-	56,56,56,56	0
57	MG	BA	3160	1/1	0.80	0.20	-	49,49,49,49	0
57	MG	DA	3263	1/1	0.96	0.13	-	65,65,65,65	0
57	MG	CA	3033	1/1	0.95	0.10	-	54,54,54,54	0
57	MG	DA	3543	1/1	0.92	0.14	-	64,64,64,64	0
57	MG	BA	3717	1/1	0.82	0.15	-	72,72,72,72	0
57	MG	DA	3203	1/1	0.97	0.18	-	53,53,53,53	0
57	MG	BA	3557	1/1	0.80	0.17	-	53,53,53,53	0
57	MG	DA	3328	1/1	0.91	0.21	-	42,42,42,42	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	BW	3002	1/1	0.95	0.27	-	58,58,58,58	0
57	MG	DA	3648	1/1	0.81	0.07	-	62,62,62,62	0
57	MG	DA	3313	1/1	0.70	0.11	-	39,39,39,39	0
57	MG	AA	1738	1/1	0.86	0.22	-	68,68,68,68	0
57	MG	DA	3594	1/1	0.95	0.09	-	58,58,58,58	0
57	MG	BA	3450	1/1	0.94	0.25	-	54,54,54,54	0
57	MG	BA	3642	1/1	0.88	0.18	-	64,64,64,64	0
57	MG	DA	3613	1/1	0.93	0.11	-	56,56,56,56	0
57	MG	BA	3056	1/1	0.85	0.31	-	46,46,46,46	0
57	MG	BA	3784	1/1	0.94	0.18	-	52,52,52,52	0
57	MG	DA	3163	1/1	0.98	0.21	-	34,34,34,34	0
57	MG	DA	3391	1/1	0.93	0.16	-	45,45,45,45	0
57	MG	BA	3690	1/1	0.93	0.13	-	39,39,39,39	0
57	MG	AA	1741	1/1	0.81	0.12	-	86,86,86,86	0
57	MG	DA	3120	1/1	0.97	0.33	-	56,56,56,56	0
57	MG	DA	3078	1/1	0.90	0.09	-	47,47,47,47	0
57	MG	DA	3392	1/1	0.99	0.19	-	53,53,53,53	0
57	MG	AA	1743	1/1	0.67	0.17	-	66,66,66,66	0
57	MG	CA	3153	1/1	0.88	0.11	-	69,69,69,69	0
57	MG	DA	3604	1/1	0.84	0.15	-	61,61,61,61	0
57	MG	DA	3597	1/1	0.98	0.15	-	48,48,48,48	0
57	MG	BA	3248	1/1	0.89	0.15	-	67,67,67,67	0
57	MG	DA	3381	1/1	0.98	0.15	-	40,40,40,40	0
57	MG	DA	3187	1/1	0.88	0.20	-	47,47,47,47	0
57	MG	BA	3443	1/1	0.89	0.18	-	59,59,59,59	0
57	MG	BA	3288	1/1	0.70	0.18	-	44,44,44,44	0
57	MG	BA	3783	1/1	0.96	0.15	-	37,37,37,37	0
57	MG	DQ	3002	1/1	0.90	0.16	-	47,47,47,47	0
57	MG	DA	3358	1/1	0.89	0.18	-	50,50,50,50	0
57	MG	BA	3008	1/1	0.91	0.14	-	28,28,28,28	0
57	MG	BA	3117	1/1	0.90	0.64	-	38,38,38,38	0
57	MG	BA	3438	1/1	0.96	0.20	-	35,35,35,35	0
57	MG	BA	3524	1/1	0.91	0.21	-	33,33,33,33	0
57	MG	CA	3124	1/1	0.93	0.22	-	69,69,69,69	0
57	MG	BA	3634	1/1	0.97	0.14	-	55,55,55,55	0
57	MG	BA	3306	1/1	0.96	0.17	-	15,15,15,15	0
57	MG	DA	3355	1/1	0.99	0.11	-	43,43,43,43	0
57	MG	AA	1727	1/1	0.97	0.14	-	50,50,50,50	0
57	MG	BA	3600	1/1	0.83	0.28	-	44,44,44,44	0
57	MG	BA	3272	1/1	0.66	0.26	-	64,64,64,64	0
57	MG	DA	3175	1/1	0.95	0.14	-	41,41,41,41	0
57	MG	AA	1662	1/1	0.89	0.20	-	58,58,58,58	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	BA	3246	1/1	0.94	0.31	-	55,55,55,55	0
57	MG	AA	1650	1/1	0.83	0.15	-	74,74,74,74	0
57	MG	AA	1777	1/1	0.86	0.09	-	71,71,71,71	0
57	MG	B4	502	1/1	0.92	0.09	-	70,70,70,70	0
57	MG	CA	3109	1/1	0.86	0.15	-	74,74,74,74	0
57	MG	CA	3070	1/1	0.83	0.15	-	69,69,69,69	0
57	MG	BA	3650	1/1	0.98	0.17	-	45,45,45,45	0
57	MG	CA	3002	1/1	0.83	0.14	-	77,77,77,77	0
57	MG	AA	1762	1/1	0.98	0.21	-	66,66,66,66	0
57	MG	DA	3512	1/1	0.86	0.12	-	37,37,37,37	0
57	MG	BA	3161	1/1	0.93	0.29	-	44,44,44,44	0
57	MG	DA	3308	1/1	0.91	0.21	-	62,62,62,62	0
57	MG	BA	3493	1/1	0.96	0.21	-	38,38,38,38	0
57	MG	DA	3612	1/1	0.80	0.08	-	58,58,58,58	0
57	MG	DA	3320	1/1	0.79	0.09	-	49,49,49,49	0
57	MG	DA	3290	1/1	0.97	0.14	-	33,33,33,33	0
57	MG	AA	1604	1/1	0.80	0.12	-	58,58,58,58	0
57	MG	BA	3423	1/1	0.83	0.16	-	69,69,69,69	0
57	MG	DA	3210	1/1	0.93	0.08	-	52,52,52,52	0
57	MG	DA	3256	1/1	0.92	0.16	-	51,51,51,51	0
57	MG	DA	3351	1/1	0.81	0.08	-	56,56,56,56	0
57	MG	BA	3232	1/1	0.86	0.24	-	49,49,49,49	0
57	MG	DA	3148	1/1	0.94	0.21	-	49,49,49,49	0
57	MG	AA	1751	1/1	0.93	0.23	-	53,53,53,53	0
57	MG	BA	3445	1/1	0.94	0.23	-	54,54,54,54	0
57	MG	BA	3203	1/1	0.88	0.34	-	61,61,61,61	0
57	MG	DA	3539	1/1	0.93	0.08	-	55,55,55,55	0
57	MG	BA	3484	1/1	0.87	0.13	-	40,40,40,40	0
57	MG	BA	3263	1/1	0.85	0.28	-	60,60,60,60	0
57	MG	AA	1801	1/1	0.91	0.09	-	71,71,71,71	0
57	MG	BA	3295	1/1	0.89	0.22	-	23,23,23,23	0
57	MG	DA	3644	1/1	0.94	0.24	-	58,58,58,58	0
57	MG	BA	3711	1/1	0.96	0.25	-	44,44,44,44	0
57	MG	CA	3090	1/1	0.83	0.17	-	76,76,76,76	0
57	MG	DA	3601	1/1	0.89	0.10	-	55,55,55,55	0
57	MG	BA	3735	1/1	0.89	0.23	-	50,50,50,50	0
57	MG	DA	3052	1/1	0.79	0.10	-	49,49,49,49	0
57	MG	AA	1798	1/1	0.91	0.11	-	62,62,62,62	0
57	MG	BA	3749	1/1	0.97	0.16	-	52,52,52,52	0
57	MG	CA	3163	1/1	0.98	0.19	-	62,62,62,62	0
57	MG	CA	3077	1/1	0.89	0.20	-	60,60,60,60	0
57	MG	DA	3634	1/1	0.73	0.14	-	68,68,68,68	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	CA	3100	1/1	0.91	0.15	-	59,59,59,59	0
57	MG	DA	3207	1/1	0.93	0.14	-	48,48,48,48	0
57	MG	CA	3075	1/1	0.94	0.24	-	65,65,65,65	0
57	MG	AA	1789	1/1	0.85	0.15	-	60,60,60,60	0
57	MG	CA	3017	1/1	0.83	0.15	-	54,54,54,54	0
57	MG	DA	3558	1/1	0.90	0.11	-	48,48,48,48	0
57	MG	CA	3161	1/1	0.84	0.13	-	76,76,76,76	0
57	MG	DA	3236	1/1	0.92	0.13	-	55,55,55,55	0
57	MG	BA	3153	1/1	0.95	0.15	-	45,45,45,45	0
57	MG	BA	3159	1/1	0.96	0.18	-	27,27,27,27	0
57	MG	DA	3206	1/1	0.94	0.08	-	50,50,50,50	0
57	MG	DA	3478	1/1	0.92	0.17	-	58,58,58,58	0
57	MG	BA	3460	1/1	0.92	0.11	-	52,52,52,52	0
57	MG	BA	3370	1/1	0.97	0.24	-	50,50,50,50	0
57	MG	DA	3255	1/1	0.94	0.24	-	47,47,47,47	0
57	MG	AF	3001	1/1	0.88	0.18	-	50,50,50,50	0
57	MG	BA	3747	1/1	0.85	0.24	-	55,55,55,55	0
57	MG	DA	3623	1/1	0.87	0.10	-	45,45,45,45	0
57	MG	BA	3552	1/1	0.93	0.15	-	55,55,55,55	0
57	MG	CA	3158	1/1	0.97	0.19	-	55,55,55,55	0
57	MG	BA	3116	1/1	0.95	0.35	-	46,46,46,46	0
57	MG	AA	1625	1/1	0.79	0.17	-	73,73,73,73	0
57	MG	BA	3746	1/1	0.93	0.14	-	78,78,78,78	0
57	MG	DA	3641	1/1	0.95	0.07	-	46,46,46,46	0
57	MG	DA	3346	1/1	0.95	0.14	-	49,49,49,49	0
57	MG	BA	3570	1/1	0.85	0.21	-	31,31,31,31	0
57	MG	BA	3063	1/1	0.90	0.33	-	47,47,47,47	0
57	MG	BA	3626	1/1	0.92	0.19	-	50,50,50,50	0
57	MG	BA	3759	1/1	0.79	0.13	-	70,70,70,70	0
57	MG	DA	3457	1/1	0.96	0.18	-	44,44,44,44	0
57	MG	CA	3104	1/1	0.98	0.23	-	37,37,37,37	0
57	MG	BA	3353	1/1	0.94	0.12	-	55,55,55,55	0
57	MG	BA	3788	1/1	0.94	0.24	-	44,44,44,44	0
57	MG	AA	1720	1/1	0.98	0.19	-	55,55,55,55	0
57	MG	BA	3093	1/1	0.95	0.24	-	41,41,41,41	0
57	MG	DA	3368	1/1	0.91	0.09	-	67,67,67,67	0
57	MG	DA	3387	1/1	0.96	0.10	-	59,59,59,59	0
57	MG	AA	1809	1/1	0.97	0.17	-	42,42,42,42	0
57	MG	AA	1721	1/1	0.90	0.16	-	57,57,57,57	0
57	MG	BA	3405	1/1	0.96	0.16	-	52,52,52,52	0
57	MG	DA	3413	1/1	0.90	0.20	-	62,62,62,62	0
57	MG	DA	3632	1/1	0.98	0.17	-	52,52,52,52	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	AA	1724	1/1	0.98	0.17	-	39,39,39,39	0
57	MG	AA	1731	1/1	0.94	0.18	-	56,56,56,56	0
57	MG	BA	3697	1/1	0.93	0.18	-	41,41,41,41	0
57	MG	DA	3253	1/1	0.75	0.13	-	54,54,54,54	0
57	MG	DA	3149	1/1	0.95	0.08	-	46,46,46,46	0
57	MG	DA	3536	1/1	0.93	0.08	-	52,52,52,52	0
57	MG	BA	3664	1/1	0.95	0.21	-	69,69,69,69	0
57	MG	BA	3702	1/1	0.49	0.12	-	39,39,39,39	0
57	MG	DA	3188	1/1	0.98	0.24	-	35,35,35,35	0
57	MG	DA	3126	1/1	0.94	0.15	-	59,59,59,59	0
57	MG	DA	3455	1/1	0.88	0.09	-	64,64,64,64	0
57	MG	AA	1673	1/1	0.94	0.13	-	48,48,48,48	0
57	MG	AA	1771	1/1	0.87	0.15	-	75,75,75,75	0
57	MG	DA	3350	1/1	0.96	0.18	-	31,31,31,31	0
57	MG	DA	3332	1/1	0.73	0.18	-	46,46,46,46	0
57	MG	DA	3570	1/1	0.90	0.16	-	43,43,43,43	0
57	MG	BA	3676	1/1	0.78	0.17	-	70,70,70,70	0
57	MG	AA	1746	1/1	0.95	0.10	-	56,56,56,56	0
57	MG	CA	3122	1/1	0.76	0.13	-	69,69,69,69	0
57	MG	DA	3080	1/1	0.92	0.10	-	49,49,49,49	0
57	MG	AA	1601	1/1	0.85	0.12	-	81,81,81,81	0
57	MG	BA	3475	1/1	0.81	0.09	-	49,49,49,49	0
57	MG	BA	3163	1/1	0.91	0.49	-	55,55,55,55	0
57	MG	DA	3524	1/1	0.90	0.17	-	52,52,52,52	0
57	MG	BA	3181	1/1	0.93	0.10	-	40,40,40,40	0
57	MG	BA	3375	1/1	0.92	0.22	-	39,39,39,39	0
57	MG	DA	3412	1/1	0.99	0.14	-	41,41,41,41	0
57	MG	AA	1805	1/1	0.94	0.07	-	48,48,48,48	0
57	MG	DA	3559	1/1	0.92	0.15	-	67,67,67,67	0
57	MG	DA	3241	1/1	0.91	0.13	-	55,55,55,55	0
57	MG	DA	3095	1/1	0.89	0.16	-	60,60,60,60	0
57	MG	AA	1793	1/1	0.96	0.17	-	63,63,63,63	0
57	MG	DA	3093	1/1	0.98	0.13	-	47,47,47,47	0
57	MG	DA	3201	1/1	0.88	0.10	-	52,52,52,52	0
57	MG	BA	3792	1/1	0.87	0.19	-	52,52,52,52	0
57	MG	BA	3739	1/1	0.98	0.11	-	21,21,21,21	0
57	MG	BA	3078	1/1	0.85	0.32	-	54,54,54,54	0
57	MG	BA	3692	1/1	0.90	0.12	-	58,58,58,58	0
57	MG	AA	1666	1/1	0.87	0.33	-	63,63,63,63	0
57	MG	BA	3379	1/1	0.89	0.18	-	35,35,35,35	0
57	MG	BA	3140	1/1	0.87	0.12	-	58,58,58,58	0
57	MG	BA	3532	1/1	0.90	0.14	-	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
57	MG	BA	3024	1/1	0.87	0.23	-	58,58,58,58	0
57	MG	BA	3687	1/1	0.84	0.18	-	64,64,64,64	0
57	MG	DA	3554	1/1	0.91	0.09	-	50,50,50,50	0
57	MG	AA	1679	1/1	0.69	0.19	-	51,51,51,51	0
57	MG	BA	3610	1/1	0.96	0.09	-	61,61,61,61	0
57	MG	DA	3473	1/1	0.96	0.22	-	50,50,50,50	0
57	MG	BA	3088	1/1	0.88	0.17	-	43,43,43,43	0
57	MG	CX	3002	1/1	0.90	0.14	-	67,67,67,67	0
57	MG	CA	3003	1/1	0.64	0.16	-	58,58,58,58	0
57	MG	AA	1726	1/1	0.92	0.16	-	58,58,58,58	0
57	MG	BA	3324	1/1	0.95	0.15	-	60,60,60,60	0
57	MG	BA	3156	1/1	0.92	0.23	-	35,35,35,35	0
57	MG	DA	3141	1/1	0.86	0.13	-	51,51,51,51	0
57	MG	BA	3105	1/1	0.94	0.12	-	46,46,46,46	0
57	MG	BA	3426	1/1	0.92	0.15	-	46,46,46,46	0
57	MG	CA	3082	1/1	0.91	0.13	-	66,66,66,66	0
57	MG	DF	302	1/1	0.84	0.14	-	53,53,53,53	0
57	MG	DA	3367	1/1	0.93	0.17	-	49,49,49,49	0
57	MG	BA	3090	1/1	0.96	0.26	-	38,38,38,38	0
57	MG	DA	3360	1/1	0.96	0.09	-	31,31,31,31	0
57	MG	BA	3810	1/1	0.97	0.21	-	35,35,35,35	0
57	MG	AA	1774	1/1	0.95	0.17	-	51,51,51,51	0
57	MG	DO	201	1/1	0.98	0.12	-	49,49,49,49	0
57	MG	BA	3057	1/1	0.85	0.18	-	48,48,48,48	0
57	MG	AN	502	1/1	0.97	0.29	-	62,62,62,62	0
57	MG	DA	3545	1/1	0.70	0.12	-	62,62,62,62	0
57	MG	BA	3467	1/1	0.98	0.13	-	46,46,46,46	0
57	MG	DO	202	1/1	0.91	0.12	-	60,60,60,60	0
57	MG	AA	1633	1/1	0.88	0.27	-	59,59,59,59	0
57	MG	BA	3332	1/1	0.94	0.14	-	54,54,54,54	0
57	MG	DA	3275	1/1	0.86	0.14	-	65,65,65,65	0
57	MG	CA	3039	1/1	0.84	0.15	-	64,64,64,64	0
57	MG	BA	3682	1/1	0.92	0.14	-	60,60,60,60	0
57	MG	AX	3013	1/1	0.85	0.20	-	70,70,70,70	0
57	MG	AA	1758	1/1	0.99	0.09	-	37,37,37,37	0
57	MG	CA	3121	1/1	0.90	0.13	-	67,67,67,67	0
57	MG	BA	3773	1/1	0.92	0.21	-	32,32,32,32	0
57	MG	AY	3003	1/1	0.89	0.15	-	79,79,79,79	0
57	MG	DA	3288	1/1	0.94	0.16	-	39,39,39,39	0
57	MG	CA	3123	1/1	0.90	0.32	-	61,61,61,61	0
57	MG	BA	3637	1/1	0.77	0.14	-	38,38,38,38	0
57	MG	AL	201	1/1	0.72	0.13	-	63,63,63,63	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	BA	3098	1/1	0.94	0.22	-	23,23,23,23	0
57	MG	DA	3629	1/1	0.97	0.12	-	57,57,57,57	0
57	MG	DA	3494	1/1	0.88	0.12	-	45,45,45,45	0
57	MG	AA	1658	1/1	0.86	0.14	-	64,64,64,64	0
57	MG	DA	3278	1/1	0.95	0.10	-	39,39,39,39	0
57	MG	BB	3006	1/1	0.88	0.14	-	62,62,62,62	0
57	MG	DA	3424	1/1	0.86	0.18	-	41,41,41,41	0
57	MG	BA	3345	1/1	0.98	0.19	-	51,51,51,51	0
57	MG	BN	3003	1/1	0.93	0.21	-	38,38,38,38	0
57	MG	BA	3003	1/1	0.99	0.17	-	33,33,33,33	0
57	MG	CA	3149	1/1	0.96	0.12	-	54,54,54,54	0
57	MG	DA	3298	1/1	0.92	0.20	-	55,55,55,55	0
57	MG	BA	3797	1/1	0.96	0.31	-	51,51,51,51	0
57	MG	AA	1745	1/1	0.92	0.16	-	36,36,36,36	0
57	MG	DA	3515	1/1	0.89	0.13	-	55,55,55,55	0
57	MG	AX	3009	1/1	0.95	0.37	-	65,65,65,65	0
57	MG	BA	3440	1/1	0.96	0.20	-	35,35,35,35	0
57	MG	DA	3636	1/1	0.85	0.15	-	62,62,62,62	0
57	MG	BA	3143	1/1	0.95	0.10	-	41,41,41,41	0
57	MG	BA	3430	1/1	0.96	0.24	-	34,34,34,34	0
57	MG	BA	3470	1/1	0.91	0.11	-	57,57,57,57	0
57	MG	BF	301	1/1	0.94	0.25	-	40,40,40,40	0
57	MG	CA	3059	1/1	0.73	0.16	-	75,75,75,75	0
57	MG	DE	3006	1/1	0.97	0.21	-	38,38,38,38	0
57	MG	DA	3447	1/1	0.98	0.16	-	59,59,59,59	0
57	MG	BA	3646	1/1	0.89	0.17	-	50,50,50,50	0
57	MG	BA	3754	1/1	0.92	0.14	-	42,42,42,42	0
57	MG	AA	1682	1/1	0.85	0.26	-	59,59,59,59	0
57	MG	AA	1635	1/1	0.90	0.15	-	65,65,65,65	0
57	MG	DA	3065	1/1	0.84	0.10	-	56,56,56,56	0
57	MG	CA	3146	1/1	0.82	0.18	-	72,72,72,72	0
57	MG	AX	3004	1/1	0.91	0.13	-	61,61,61,61	0
57	MG	DA	3094	1/1	0.92	0.06	-	39,39,39,39	0
57	MG	DA	3309	1/1	0.96	0.12	-	48,48,48,48	0
57	MG	BA	3004	1/1	0.97	0.22	-	36,36,36,36	0
57	MG	DA	3151	1/1	0.92	0.13	-	37,37,37,37	0
57	MG	BA	3115	1/1	0.90	0.23	-	33,33,33,33	0
57	MG	BA	3411	1/1	0.81	0.24	-	50,50,50,50	0
57	MG	BA	3636	1/1	0.90	0.19	-	66,66,66,66	0
57	MG	DA	3564	1/1	0.94	0.16	-	53,53,53,53	0
57	MG	BA	3374	1/1	0.96	0.19	-	50,50,50,50	0
57	MG	DA	3372	1/1	0.94	0.13	-	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
57	MG	AA	1640	1/1	0.88	0.22	-	54,54,54,54	0
57	MG	BA	3329	1/1	0.89	0.10	-	60,60,60,60	0
57	MG	DA	3035	1/1	0.83	0.12	-	37,37,37,37	0
57	MG	BA	3141	1/1	0.92	0.32	-	38,38,38,38	0
57	MG	BA	3109	1/1	0.86	0.13	-	56,56,56,56	0
57	MG	BA	3168	1/1	0.95	0.24	-	45,45,45,45	0
57	MG	BA	3647	1/1	0.91	0.08	-	53,53,53,53	0
57	MG	BA	3001	1/1	0.92	0.15	-	43,43,43,43	0
57	MG	DA	3590	1/1	0.90	0.22	-	51,51,51,51	0
57	MG	BA	3513	1/1	0.89	0.34	-	50,50,50,50	0
57	MG	DA	3608	1/1	0.94	0.09	-	57,57,57,57	0
57	MG	DA	3466	1/1	0.93	0.11	-	48,48,48,48	0
57	MG	CA	3132	1/1	0.97	0.14	-	64,64,64,64	0
57	MG	AA	1660	1/1	0.82	0.24	-	51,51,51,51	0
57	MG	DB	3011	1/1	0.89	0.26	-	67,67,67,67	0
57	MG	CA	3112	1/1	0.84	0.10	-	72,72,72,72	0
57	MG	CA	3078	1/1	0.93	0.16	-	65,65,65,65	0
57	MG	BA	3764	1/1	0.96	0.20	-	66,66,66,66	0
57	MG	AA	1797	1/1	0.92	0.17	-	59,59,59,59	0
57	MG	AA	1678	1/1	0.99	0.25	-	47,47,47,47	0
57	MG	BA	3681	1/1	0.86	0.23	-	61,61,61,61	0
57	MG	DA	3645	1/1	0.89	0.11	-	64,64,64,64	0
57	MG	BA	3765	1/1	0.90	0.24	-	49,49,49,49	0
57	MG	BA	3579	1/1	0.76	0.11	-	63,63,63,63	0
57	MG	DA	3043	1/1	0.95	0.19	-	53,53,53,53	0
57	MG	DA	3565	1/1	0.91	0.04	-	52,52,52,52	0
57	MG	BA	3064	1/1	0.94	0.22	-	45,45,45,45	0
57	MG	AA	1701	1/1	0.72	0.27	-	73,73,73,73	0
57	MG	CA	3083	1/1	0.96	0.16	-	50,50,50,50	0
57	MG	BA	3545	1/1	0.91	0.18	-	28,28,28,28	0
57	MG	DA	3128	1/1	0.94	0.28	-	56,56,56,56	0
57	MG	BA	3072	1/1	0.97	0.24	-	49,49,49,49	0
57	MG	BA	3283	1/1	0.85	0.40	-	57,57,57,57	0
57	MG	DA	3432	1/1	0.96	0.17	-	52,52,52,52	0
57	MG	BA	3523	1/1	0.86	0.21	-	41,41,41,41	0
57	MG	AA	1694	1/1	0.92	0.08	-	47,47,47,47	0
57	MG	BA	3270	1/1	0.81	0.22	-	56,56,56,56	0
57	MG	BA	3457	1/1	0.98	0.19	-	48,48,48,48	0
57	MG	BA	3724	1/1	0.96	0.18	-	20,20,20,20	0
57	MG	BA	3511	1/1	0.95	0.18	-	50,50,50,50	0
57	MG	BA	3055	1/1	0.93	0.23	-	37,37,37,37	0
57	MG	BA	3071	1/1	0.95	0.31	-	59,59,59,59	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	BA	3031	1/1	0.96	0.27	-	36,36,36,36	0
57	MG	BR	5001	1/1	0.93	0.20	-	50,50,50,50	0
57	MG	AA	1782	1/1	0.93	0.14	-	54,54,54,54	0
57	MG	DA	3143	1/1	0.82	0.14	-	62,62,62,62	0
57	MG	AA	1683	1/1	0.94	0.13	-	62,62,62,62	0
57	MG	B0	3001	1/1	0.93	0.19	-	47,47,47,47	0
57	MG	BA	3652	1/1	0.69	0.09	-	58,58,58,58	0
57	MG	CA	3056	1/1	0.94	0.10	-	64,64,64,64	0
57	MG	CA	3111	1/1	0.87	0.15	-	72,72,72,72	0
57	MG	DA	3009	1/1	0.94	0.17	-	61,61,61,61	0
57	MG	DA	3077	1/1	0.92	0.14	-	38,38,38,38	0
57	MG	DA	3551	1/1	0.94	0.17	-	49,49,49,49	0
57	MG	B7	104	1/1	0.84	0.27	-	62,62,62,62	0
57	MG	BB	3010	1/1	0.94	0.18	-	53,53,53,53	0
57	MG	DA	3427	1/1	0.88	0.16	-	47,47,47,47	0
57	MG	AA	1669	1/1	0.72	0.18	-	69,69,69,69	0
57	MG	AA	1752	1/1	0.93	0.14	-	48,48,48,48	0
57	MG	DA	3430	1/1	0.96	0.13	-	47,47,47,47	0
57	MG	BA	3169	1/1	0.95	0.24	-	50,50,50,50	0
57	MG	DA	3096	1/1	0.93	0.19	-	68,68,68,68	0
57	MG	AA	1769	1/1	0.95	0.19	-	50,50,50,50	0
57	MG	DA	3074	1/1	0.94	0.08	-	59,59,59,59	0
57	MG	AA	1729	1/1	0.91	0.15	-	35,35,35,35	0
57	MG	BA	3581	1/1	0.94	0.12	-	59,59,59,59	0
57	MG	BA	3698	1/1	0.97	0.11	-	47,47,47,47	0
57	MG	BA	3151	1/1	0.96	0.17	-	36,36,36,36	0
57	MG	CA	3049	1/1	0.81	0.21	-	65,65,65,65	0
57	MG	BA	3092	1/1	0.93	0.29	-	40,40,40,40	0
57	MG	BA	3482	1/1	0.96	0.16	-	51,51,51,51	0
57	MG	BA	3715	1/1	0.79	0.17	-	52,52,52,52	0
57	MG	BA	3732	1/1	0.87	0.24	-	33,33,33,33	0
57	MG	BA	3390	1/1	0.89	0.10	-	31,31,31,31	0
57	MG	BA	3537	1/1	0.95	0.08	-	43,43,43,43	0
57	MG	BA	3344	1/1	0.97	0.10	-	71,71,71,71	0
57	MG	DA	3198	1/1	0.97	0.16	-	52,52,52,52	0
57	MG	BA	3119	1/1	0.96	0.15	-	46,46,46,46	0
57	MG	DA	3174	1/1	0.76	0.19	-	52,52,52,52	0
57	MG	BA	3006	1/1	0.79	0.24	-	54,54,54,54	0
57	MG	BA	3401	1/1	0.95	0.26	-	26,26,26,26	0
57	MG	BA	3255	1/1	0.88	0.20	-	55,55,55,55	0
57	MG	AA	1785	1/1	0.94	0.11	-	72,72,72,72	0
57	MG	BA	3268	1/1	0.92	0.22	-	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
57	MG	DA	3053	1/1	0.92	0.13	-	47,47,47,47	0
57	MG	AA	1608	1/1	0.96	0.22	-	43,43,43,43	0
57	MG	BA	3190	1/1	0.97	0.28	-	54,54,54,54	0
57	MG	BA	3444	1/1	0.95	0.15	-	48,48,48,48	0
57	MG	DA	3389	1/1	0.95	0.19	-	59,59,59,59	0
57	MG	DA	3193	1/1	0.95	0.15	-	47,47,47,47	0
57	MG	BA	3335	1/1	0.95	0.15	-	40,40,40,40	0
57	MG	AA	1773	1/1	0.96	0.10	-	61,61,61,61	0
57	MG	DA	3059	1/1	0.96	0.10	-	50,50,50,50	0
57	MG	AA	1767	1/1	0.96	0.11	-	67,67,67,67	0
57	MG	DA	3574	1/1	0.85	0.07	-	61,61,61,61	0
57	MG	CA	3089	1/1	0.90	0.23	-	74,74,74,74	0
57	MG	DA	3137	1/1	0.96	0.17	-	52,52,52,52	0
57	MG	DA	3450	1/1	0.96	0.06	-	50,50,50,50	0
57	MG	BB	3001	1/1	0.82	0.29	-	68,68,68,68	0
57	MG	DA	3556	1/1	0.90	0.13	-	55,55,55,55	0
57	MG	DA	3525	1/1	0.96	0.15	-	28,28,28,28	0
57	MG	DA	3116	1/1	0.67	0.16	-	53,53,53,53	0
57	MG	CA	3117	1/1	0.93	0.09	-	63,63,63,63	0
57	MG	BA	3318	1/1	0.86	0.16	-	54,54,54,54	0
57	MG	BA	3528	1/1	0.92	0.20	-	36,36,36,36	0
57	MG	BA	3040	1/1	0.94	0.27	-	33,33,33,33	0
57	MG	BA	3252	1/1	0.91	0.19	-	36,36,36,36	0
57	MG	B8	5002	1/1	0.86	0.30	-	53,53,53,53	0
57	MG	AA	1755	1/1	0.87	0.09	-	80,80,80,80	0
57	MG	CA	3006	1/1	0.71	0.11	-	68,68,68,68	0
57	MG	CA	3045	1/1	0.87	0.22	-	62,62,62,62	0
57	MG	BN	3002	1/1	0.82	0.20	-	51,51,51,51	0
57	MG	CA	3024	1/1	0.94	0.16	-	67,67,67,67	0
57	MG	BA	3408	1/1	0.90	0.17	-	51,51,51,51	0
57	MG	AA	1804	1/1	0.95	0.12	-	70,70,70,70	0
57	MG	CA	3074	1/1	0.95	0.14	-	60,60,60,60	0
57	MG	BA	3249	1/1	0.96	0.23	-	53,53,53,53	0
57	MG	DA	3234	1/1	0.85	0.15	-	54,54,54,54	0
57	MG	BA	3398	1/1	0.96	0.22	-	32,32,32,32	0
57	MG	CA	3026	1/1	0.90	0.21	-	66,66,66,66	0
57	MG	DB	3001	1/1	0.83	0.17	-	63,63,63,63	0
57	MG	DA	3045	1/1	0.97	0.22	-	51,51,51,51	0
57	MG	BA	3766	1/1	0.89	0.16	-	47,47,47,47	0
57	MG	BA	3294	1/1	0.94	0.16	-	43,43,43,43	0
57	MG	BA	3728	1/1	0.91	0.16	-	52,52,52,52	0
57	MG	BA	3454	1/1	0.96	0.17	-	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
57	MG	BA	3755	1/1	0.83	0.24	-	43,43,43,43	0
57	MG	BA	3589	1/1	0.94	0.22	-	59,59,59,59	0
57	MG	BA	3628	1/1	0.97	0.28	-	52,52,52,52	0
57	MG	BA	3514	1/1	0.96	0.19	-	43,43,43,43	0
57	MG	CX	3001	1/1	0.95	0.18	-	57,57,57,57	0
57	MG	BA	3359	1/1	0.88	0.06	-	60,60,60,60	0
57	MG	BA	3605	1/1	0.96	0.18	-	47,47,47,47	0
57	MG	BA	3350	1/1	0.95	0.12	-	34,34,34,34	0
57	MG	DA	3272	1/1	0.94	0.19	-	49,49,49,49	0
57	MG	DA	3159	1/1	0.91	0.11	-	62,62,62,62	0
57	MG	DA	3012	1/1	0.94	0.11	-	43,43,43,43	0
57	MG	BA	3574	1/1	0.89	0.15	-	42,42,42,42	0
57	MG	BA	3091	1/1	0.92	0.40	-	42,42,42,42	0
57	MG	DD	303	1/1	0.93	0.34	-	51,51,51,51	0
57	MG	DA	3179	1/1	0.91	0.06	-	59,59,59,59	0
57	MG	BA	3505	1/1	0.84	0.22	-	53,53,53,53	0
57	MG	BB	3005	1/1	0.93	0.28	-	51,51,51,51	0
57	MG	AY	3001	1/1	0.88	0.32	-	63,63,63,63	0
57	MG	B6	101	1/1	0.93	0.32	-	60,60,60,60	0
57	MG	CA	3134	1/1	0.95	0.11	-	64,64,64,64	0
57	MG	DA	3357	1/1	0.92	0.13	-	33,33,33,33	0
57	MG	DA	3111	1/1	0.85	0.13	-	56,56,56,56	0
57	MG	BA	3678	1/1	0.80	0.10	-	67,67,67,67	0
57	MG	DA	3509	1/1	0.95	0.06	-	49,49,49,49	0
57	MG	BA	3730	1/1	0.78	0.17	-	68,68,68,68	0
57	MG	BA	3595	1/1	0.97	0.09	-	61,61,61,61	0
57	MG	BA	3242	1/1	0.94	0.69	-	55,55,55,55	0
57	MG	AA	1811	1/1	0.96	0.21	-	49,49,49,49	0
57	MG	CA	3151	1/1	0.91	0.10	-	64,64,64,64	0
57	MG	AX	3015	1/1	0.89	0.29	-	51,51,51,51	0
57	MG	BA	3616	1/1	0.94	0.20	-	59,59,59,59	0
57	MG	DP	202	1/1	0.89	0.09	-	49,49,49,49	0
57	MG	BA	3685	1/1	0.91	0.20	-	61,61,61,61	0
57	MG	BA	3546	1/1	0.90	0.14	-	68,68,68,68	0
57	MG	DA	3130	1/1	0.86	0.15	-	52,52,52,52	0
57	MG	AA	1744	1/1	0.96	0.17	-	44,44,44,44	0
57	MG	CA	3038	1/1	0.96	0.09	-	57,57,57,57	0
57	MG	BA	3776	1/1	0.97	0.22	-	60,60,60,60	0
57	MG	DA	3583	1/1	0.95	0.12	-	52,52,52,52	0
57	MG	BA	3645	1/1	0.91	0.18	-	47,47,47,47	0
57	MG	AA	1748	1/1	0.96	0.16	-	64,64,64,64	0
57	MG	BA	3468	1/1	0.96	0.19	-	45,45,45,45	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	AA	1624	1/1	0.97	0.25	-	66,66,66,66	0
57	MG	BB	3023	1/1	0.97	0.16	-	47,47,47,47	0
57	MG	DA	3507	1/1	0.96	0.07	-	59,59,59,59	0
57	MG	DA	3154	1/1	0.91	0.08	-	51,51,51,51	0
57	MG	BA	3701	1/1	0.98	0.23	-	39,39,39,39	0
57	MG	BA	3060	1/1	0.83	0.22	-	51,51,51,51	0
57	MG	AA	1649	1/1	0.94	0.18	-	28,28,28,28	0
57	MG	CA	3154	1/1	0.76	0.18	-	68,68,68,68	0
57	MG	DA	3056	1/1	0.81	0.12	-	49,49,49,49	0
57	MG	AA	1754	1/1	0.92	0.15	-	58,58,58,58	0
57	MG	BA	3148	1/1	0.93	0.28	-	38,38,38,38	0
57	MG	CA	3027	1/1	0.90	0.18	-	65,65,65,65	0
57	MG	DA	3474	1/1	0.95	0.09	-	53,53,53,53	0
57	MG	CA	3156	1/1	0.96	0.08	-	59,59,59,59	0
57	MG	BA	3291	1/1	0.96	0.26	-	53,53,53,53	0
57	MG	DA	3129	1/1	0.89	0.20	-	56,56,56,56	0
57	MG	BA	3418	1/1	0.88	0.21	-	38,38,38,38	0
57	MG	CA	3072	1/1	0.94	0.14	-	62,62,62,62	0
57	MG	BA	3029	1/1	0.86	0.27	-	36,36,36,36	0
57	MG	DA	3063	1/1	0.90	0.11	-	47,47,47,47	0
57	MG	DA	3226	1/1	0.94	0.18	-	57,57,57,57	0
57	MG	CA	3103	1/1	0.91	0.15	-	73,73,73,73	0
57	MG	DA	3260	1/1	0.91	0.17	-	39,39,39,39	0
57	MG	BA	3337	1/1	0.93	0.25	-	44,44,44,44	0
57	MG	DA	3480	1/1	0.89	0.12	-	58,58,58,58	0
57	MG	DA	3476	1/1	0.90	0.08	-	45,45,45,45	0
57	MG	DA	3031	1/1	0.91	0.14	-	42,42,42,42	0
57	MG	DD	301	1/1	0.95	0.22	-	44,44,44,44	0
57	MG	BA	3447	1/1	0.96	0.32	-	52,52,52,52	0
57	MG	AA	1800	1/1	0.93	0.13	-	59,59,59,59	0
57	MG	BA	3053	1/1	0.97	0.27	-	23,23,23,23	0
57	MG	BA	3451	1/1	0.95	0.25	-	44,44,44,44	0
57	MG	CA	3076	1/1	0.91	0.20	-	77,77,77,77	0
60	K	AX	3001	1/1	0.87	0.13	-	77,77,77,77	0
57	MG	DA	3382	1/1	0.95	0.12	-	41,41,41,41	0
57	MG	DA	3301	1/1	0.81	0.11	-	63,63,63,63	0
57	MG	CA	3092	1/1	0.99	0.24	-	51,51,51,51	0
57	MG	DB	3013	1/1	0.99	0.11	-	66,66,66,66	0
57	MG	CA	3143	1/1	0.83	0.20	-	74,74,74,74	0
57	MG	BO	5001	1/1	0.94	0.13	-	61,61,61,61	0
57	MG	DA	3547	1/1	0.98	0.08	-	48,48,48,48	0
57	MG	DA	3006	1/1	0.93	0.11	-	41,41,41,41	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	DA	3610	1/1	0.95	0.09	-	47,47,47,47	0
57	MG	DA	3452	1/1	0.88	0.11	-	45,45,45,45	0
57	MG	DA	3239	1/1	0.89	0.14	-	49,49,49,49	0
57	MG	BA	3572	1/1	0.95	0.26	-	39,39,39,39	0
57	MG	DA	3627	1/1	0.82	0.14	-	57,57,57,57	0
57	MG	AX	3007	1/1	0.63	0.30	-	68,68,68,68	0
57	MG	DA	3437	1/1	0.96	0.18	-	48,48,48,48	0
57	MG	BA	3222	1/1	0.89	0.14	-	42,42,42,42	0
57	MG	DA	3240	1/1	0.94	0.10	-	52,52,52,52	0
57	MG	BA	3745	1/1	0.87	0.24	-	61,61,61,61	0
57	MG	CA	3063	1/1	0.89	0.23	-	65,65,65,65	0
57	MG	BA	3639	1/1	0.97	0.18	-	49,49,49,49	0
57	MG	CA	3015	1/1	0.93	0.19	-	64,64,64,64	0
57	MG	BA	3771	1/1	0.94	0.11	-	41,41,41,41	0
57	MG	BA	3458	1/1	0.81	0.20	-	59,59,59,59	0
57	MG	BA	3347	1/1	0.82	0.19	-	38,38,38,38	0
57	MG	DA	3417	1/1	0.86	0.13	-	52,52,52,52	0
57	MG	BA	3406	1/1	0.89	0.10	-	56,56,56,56	0
57	MG	BA	3420	1/1	0.91	0.18	-	25,25,25,25	0
57	MG	CA	3140	1/1	0.96	0.16	-	57,57,57,57	0
57	MG	BA	3630	1/1	0.97	0.25	-	39,39,39,39	0
57	MG	DA	3534	1/1	0.94	0.10	-	46,46,46,46	0
57	MG	AA	1766	1/1	0.83	0.19	-	71,71,71,71	0
57	MG	BA	3229	1/1	0.79	0.24	-	52,52,52,52	0
57	MG	AA	1761	1/1	0.98	0.20	-	70,70,70,70	0
57	MG	DA	3633	1/1	0.88	0.10	-	58,58,58,58	0
57	MG	BA	3696	1/1	0.80	0.10	-	46,46,46,46	0
57	MG	DA	3118	1/1	0.86	0.16	-	39,39,39,39	0
57	MG	BA	3067	1/1	0.98	0.21	-	43,43,43,43	0
57	MG	BA	3602	1/1	0.96	0.11	-	47,47,47,47	0
57	MG	BA	3372	1/1	0.90	0.12	-	40,40,40,40	0
57	MG	BA	3342	1/1	0.97	0.29	-	67,67,67,67	0
57	MG	AA	1632	1/1	0.87	0.11	-	48,48,48,48	0
57	MG	BA	3107	1/1	0.86	0.33	-	57,57,57,57	0
57	MG	BQ	3002	1/1	0.95	0.28	-	46,46,46,46	0
57	MG	BA	3464	1/1	0.96	0.13	-	44,44,44,44	0
57	MG	DA	3123	1/1	0.84	0.16	-	54,54,54,54	0
57	MG	DA	3342	1/1	0.93	0.10	-	53,53,53,53	0
57	MG	AW	3002	1/1	0.92	0.14	-	79,79,79,79	0
57	MG	BA	3787	1/1	0.96	0.14	-	45,45,45,45	0
57	MG	DA	3471	1/1	0.89	0.32	-	54,54,54,54	0
57	MG	CA	3095	1/1	0.91	0.13	-	71,71,71,71	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	BA	3617	1/1	0.95	0.10	-	42,42,42,42	0
57	MG	AA	1768	1/1	0.90	0.11	-	53,53,53,53	0
57	MG	DA	3086	1/1	0.76	0.11	-	47,47,47,47	0
57	MG	DA	3504	1/1	0.93	0.09	-	52,52,52,52	0
57	MG	AA	1670	1/1	0.95	0.17	-	67,67,67,67	0
57	MG	BA	3099	1/1	0.86	0.24	-	61,61,61,61	0
57	MG	DA	3146	1/1	0.92	0.14	-	54,54,54,54	0
57	MG	BA	3422	1/1	0.94	0.16	-	36,36,36,36	0
57	MG	CA	3073	1/1	0.93	0.20	-	55,55,55,55	0
57	MG	DA	3184	1/1	0.95	0.12	-	52,52,52,52	0
57	MG	DA	3162	1/1	0.96	0.14	-	57,57,57,57	0
57	MG	AW	3001	1/1	0.84	0.11	-	59,59,59,59	0
57	MG	AA	1791	1/1	0.93	0.08	-	54,54,54,54	0
57	MG	DA	3482	1/1	0.90	0.15	-	60,60,60,60	0
57	MG	DA	3083	1/1	0.93	0.26	-	41,41,41,41	0
57	MG	BA	3571	1/1	0.85	0.24	-	28,28,28,28	0
57	MG	CA	3062	1/1	0.92	0.11	-	64,64,64,64	0
57	MG	DA	3460	1/1	0.94	0.18	-	37,37,37,37	0
57	MG	CA	3160	1/1	0.91	0.14	-	73,73,73,73	0
57	MG	BA	3002	1/1	0.83	0.28	-	53,53,53,53	0
57	MG	BA	3195	1/1	0.93	0.18	-	36,36,36,36	0
57	MG	AA	1763	1/1	0.86	0.07	-	79,79,79,79	0
57	MG	BA	3017	1/1	0.95	0.28	-	65,65,65,65	0
57	MG	DA	3057	1/1	0.63	0.20	-	44,44,44,44	0
57	MG	BA	3364	1/1	0.92	0.15	-	47,47,47,47	0
57	MG	AX	3011	1/1	0.93	0.13	-	60,60,60,60	0
57	MG	BA	3302	1/1	0.93	0.15	-	49,49,49,49	0
57	MG	DA	3404	1/1	0.95	0.08	-	43,43,43,43	0
57	MG	DA	3305	1/1	0.93	0.13	-	53,53,53,53	0
57	MG	DA	3250	1/1	0.88	0.08	-	50,50,50,50	0
57	MG	BA	3211	1/1	0.94	0.18	-	43,43,43,43	0
57	MG	BA	3656	1/1	0.85	0.17	-	45,45,45,45	0
57	MG	DA	3483	1/1	0.94	0.09	-	53,53,53,53	0
57	MG	BW	3001	1/1	0.86	0.35	-	44,44,44,44	0
57	MG	DA	3386	1/1	0.97	0.10	-	44,44,44,44	0
57	MG	DA	3481	1/1	0.92	0.13	-	40,40,40,40	0
57	MG	BA	3167	1/1	0.96	0.18	-	45,45,45,45	0
57	MG	BA	3094	1/1	0.86	0.19	-	52,52,52,52	0
57	MG	AA	1750	1/1	0.95	0.14	-	49,49,49,49	0
57	MG	BA	3175	1/1	0.85	0.29	-	57,57,57,57	0
57	MG	BA	3075	1/1	0.98	0.20	-	24,24,24,24	0
57	MG	DA	3538	1/1	0.86	0.12	-	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
57	MG	AA	1739	1/1	0.89	0.22	-	72,72,72,72	0
57	MG	CA	3035	1/1	0.92	0.11	-	53,53,53,53	0
57	MG	BA	3751	1/1	0.98	0.23	-	37,37,37,37	0
57	MG	BB	3012	1/1	0.94	0.19	-	56,56,56,56	0
57	MG	CA	3155	1/1	0.96	0.15	-	57,57,57,57	0
57	MG	DA	3091	1/1	0.90	0.20	-	54,54,54,54	0
57	MG	DF	303	1/1	0.84	0.15	-	42,42,42,42	0
57	MG	AK	3101	1/1	0.93	0.17	-	69,69,69,69	0
57	MG	DA	3048	1/1	0.93	0.12	-	59,59,59,59	0
57	MG	CA	3097	1/1	0.95	0.27	-	60,60,60,60	0
57	MG	AA	1717	1/1	0.91	0.16	-	75,75,75,75	0
57	MG	BA	3575	1/1	0.95	0.12	-	50,50,50,50	0
57	MG	DA	3245	1/1	0.98	0.08	-	58,58,58,58	0
57	MG	CA	3162	1/1	0.82	0.07	-	79,79,79,79	0
57	MG	DA	3115	1/1	0.95	0.29	-	55,55,55,55	0
57	MG	DA	3516	1/1	0.65	0.22	-	67,67,67,67	0
57	MG	CA	3131	1/1	0.90	0.24	-	69,69,69,69	0
57	MG	DA	3181	1/1	0.91	0.12	-	49,49,49,49	0
57	MG	BA	3609	1/1	0.89	0.20	-	56,56,56,56	0
57	MG	DA	3189	1/1	0.93	0.23	-	47,47,47,47	0
57	MG	BA	3462	1/1	0.93	0.11	-	53,53,53,53	0
57	MG	DA	3356	1/1	0.80	0.16	-	39,39,39,39	0
57	MG	BA	3712	1/1	0.71	0.22	-	51,51,51,51	0
57	MG	BY	502	1/1	0.91	0.24	-	46,46,46,46	0
57	MG	BA	3328	1/1	0.95	0.19	-	27,27,27,27	0
57	MG	BA	3549	1/1	0.87	0.11	-	66,66,66,66	0
57	MG	BA	3695	1/1	0.94	0.15	-	40,40,40,40	0
57	MG	BA	3183	1/1	0.82	0.48	-	49,49,49,49	0
57	MG	BA	3122	1/1	0.91	0.15	-	35,35,35,35	0
57	MG	DA	3176	1/1	0.94	0.24	-	38,38,38,38	0
57	MG	BA	3498	1/1	0.79	0.21	-	45,45,45,45	0
57	MG	AA	1706	1/1	0.96	0.22	-	60,60,60,60	0
57	MG	BA	3490	1/1	0.97	0.17	-	43,43,43,43	0
57	MG	DA	3444	1/1	0.88	0.21	-	44,44,44,44	0
57	MG	AA	1674	1/1	0.90	0.20	-	58,58,58,58	0
57	MG	AL	202	1/1	0.92	0.26	-	56,56,56,56	0
57	MG	BB	3008	1/1	0.95	0.36	-	59,59,59,59	0
57	MG	CA	3047	1/1	0.97	0.17	-	50,50,50,50	0
57	MG	DA	3658	1/1	0.90	0.49	-	62,62,62,62	0
57	MG	BA	3578	1/1	0.95	0.35	-	39,39,39,39	0
57	MG	DA	3135	1/1	0.49	0.18	-	63,63,63,63	0
57	MG	DA	3140	1/1	0.84	0.10	-	64,64,64,64	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	BA	3065	1/1	0.88	0.31	-	50,50,50,50	0
57	MG	BA	3629	1/1	0.95	0.25	-	58,58,58,58	0
57	MG	BA	3269	1/1	0.93	0.25	-	45,45,45,45	0
57	MG	BA	3461	1/1	0.97	0.11	-	45,45,45,45	0
57	MG	BA	3123	1/1	0.93	0.09	-	43,43,43,43	0
57	MG	BA	3416	1/1	0.86	0.26	-	60,60,60,60	0
57	MG	BA	3112	1/1	0.94	0.26	-	41,41,41,41	0
57	MG	DA	3611	1/1	0.86	0.10	-	53,53,53,53	0
57	MG	AA	1671	1/1	0.89	0.10	-	60,60,60,60	0
57	MG	AA	1764	1/1	0.85	0.10	-	66,66,66,66	0
57	MG	DA	3409	1/1	0.91	0.12	-	54,54,54,54	0
57	MG	BA	3368	1/1	0.98	0.24	-	32,32,32,32	0
57	MG	DA	3511	1/1	0.91	0.10	-	44,44,44,44	0
57	MG	DA	3388	1/1	0.90	0.14	-	47,47,47,47	0
57	MG	BA	3565	1/1	0.96	0.14	-	61,61,61,61	0
57	MG	BA	3744	1/1	0.94	0.18	-	55,55,55,55	0
57	MG	BA	3180	1/1	0.97	0.27	-	46,46,46,46	0
57	MG	BA	3633	1/1	0.86	0.18	-	57,57,57,57	0
57	MG	DA	3513	1/1	0.81	0.14	-	69,69,69,69	0
57	MG	DA	3394	1/1	0.83	0.05	-	60,60,60,60	0
57	MG	AA	1629	1/1	0.87	0.35	-	68,68,68,68	0
57	MG	BA	3032	1/1	0.95	0.21	-	33,33,33,33	0
57	MG	CA	3125	1/1	0.85	0.21	-	64,64,64,64	0
57	MG	DA	3438	1/1	0.94	0.08	-	42,42,42,42	0
57	MG	CA	3164	1/1	0.85	0.33	-	76,76,76,76	0
57	MG	AY	3002	1/1	0.93	0.31	-	52,52,52,52	0
57	MG	BA	3147	1/1	0.90	0.20	-	36,36,36,36	0
57	MG	BA	3632	1/1	0.85	0.26	-	55,55,55,55	0
57	MG	DA	3467	1/1	0.94	0.24	-	52,52,52,52	0
57	MG	BA	3271	1/1	0.86	0.18	-	60,60,60,60	0
57	MG	BA	3137	1/1	0.92	0.25	-	52,52,52,52	0
57	MG	DA	3073	1/1	0.97	0.08	-	33,33,33,33	0
57	MG	BA	3748	1/1	0.95	0.17	-	61,61,61,61	0
57	MG	DA	3519	1/1	0.86	0.14	-	58,58,58,58	0
57	MG	AA	1622	1/1	0.80	0.21	-	69,69,69,69	0
57	MG	AA	1647	1/1	0.96	0.22	-	44,44,44,44	0
57	MG	BA	3767	1/1	0.88	0.23	-	45,45,45,45	0
57	MG	DA	3635	1/1	0.94	0.11	-	43,43,43,43	0
57	MG	CA	3159	1/1	0.93	0.13	-	62,62,62,62	0
57	MG	DA	3286	1/1	0.86	0.09	-	55,55,55,55	0
57	MG	DA	3259	1/1	0.91	0.10	-	42,42,42,42	0
57	MG	BA	3592	1/1	0.86	0.09	-	65,65,65,65	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	CD	502	1/1	0.95	0.27	-	53,53,53,53	0
57	MG	BA	3433	1/1	0.95	0.20	-	27,27,27,27	0
57	MG	DA	3155	1/1	0.92	0.24	-	53,53,53,53	0
57	MG	CK	5001	1/1	0.96	0.05	-	61,61,61,61	0
57	MG	BA	3483	1/1	0.92	0.17	-	44,44,44,44	0
57	MG	BA	3030	1/1	0.94	0.24	-	39,39,39,39	0
57	MG	DA	3217	1/1	0.98	0.24	-	57,57,57,57	0
57	MG	BA	3276	1/1	0.95	0.40	-	44,44,44,44	0
57	MG	BA	3442	1/1	0.81	0.19	-	65,65,65,65	0
57	MG	BA	3307	1/1	0.96	0.19	-	28,28,28,28	0
57	MG	BA	3081	1/1	0.93	0.29	-	48,48,48,48	0
57	MG	DA	3553	1/1	0.92	0.07	-	72,72,72,72	0
57	MG	DA	3114	1/1	0.78	0.12	-	51,51,51,51	0
57	MG	CA	3118	1/1	0.97	0.18	-	60,60,60,60	0
57	MG	BA	3790	1/1	0.92	0.54	-	66,66,66,66	0
57	MG	BA	3750	1/1	0.98	0.22	-	46,46,46,46	0
57	MG	DA	3230	1/1	0.94	0.13	-	46,46,46,46	0
57	MG	DA	3436	1/1	0.97	0.11	-	35,35,35,35	0
57	MG	DA	3402	1/1	0.94	0.09	-	48,48,48,48	0
57	MG	BA	3028	1/1	0.94	0.20	-	37,37,37,37	0
57	MG	BA	3349	1/1	0.92	0.18	-	34,34,34,34	0
57	MG	DA	3046	1/1	0.85	0.14	-	56,56,56,56	0
57	MG	BB	3004	1/1	0.74	0.20	-	69,69,69,69	0
57	MG	BA	3096	1/1	0.90	0.18	-	60,60,60,60	0
57	MG	DA	3284	1/1	0.78	0.14	-	58,58,58,58	0
57	MG	BA	3197	1/1	0.81	0.25	-	58,58,58,58	0
57	MG	AA	1620	1/1	0.78	0.14	-	59,59,59,59	0
57	MG	BA	3554	1/1	0.89	0.09	-	51,51,51,51	0
57	MG	BA	3026	1/1	0.78	0.15	-	60,60,60,60	0
57	MG	BA	3237	1/1	0.93	0.17	-	44,44,44,44	0
57	MG	BA	3640	1/1	0.92	0.17	-	57,57,57,57	0
57	MG	BA	3154	1/1	0.63	0.21	-	52,52,52,52	0
57	MG	BA	3510	1/1	0.87	0.16	-	45,45,45,45	0
57	MG	DA	3158	1/1	0.90	0.39	-	56,56,56,56	0
57	MG	BA	3534	1/1	0.98	0.23	-	26,26,26,26	0
57	MG	CA	3087	1/1	0.87	0.07	-	57,57,57,57	0
57	MG	DA	3196	1/1	0.85	0.16	-	54,54,54,54	0
57	MG	CA	3098	1/1	0.93	0.11	-	54,54,54,54	0
57	MG	BA	3202	1/1	0.94	0.15	-	62,62,62,62	0
57	MG	BA	3076	1/1	0.96	0.38	-	42,42,42,42	0
57	MG	DA	3493	1/1	0.87	0.08	-	51,51,51,51	0
57	MG	BA	3297	1/1	0.95	0.22	-	42,42,42,42	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	CA	3054	1/1	0.93	0.33	-	69,69,69,69	0
57	MG	BA	3281	1/1	0.81	0.28	-	50,50,50,50	0
57	MG	CA	3136	1/1	0.94	0.14	-	48,48,48,48	0
57	MG	BA	3496	1/1	0.97	0.12	-	51,51,51,51	0
57	MG	BA	3550	1/1	0.95	0.16	-	50,50,50,50	0
57	MG	CA	3011	1/1	0.85	0.25	-	66,66,66,66	0
57	MG	BA	3164	1/1	0.77	0.22	-	46,46,46,46	0
57	MG	DA	3398	1/1	0.99	0.08	-	40,40,40,40	0
57	MG	CA	3018	1/1	0.94	0.13	-	63,63,63,63	0
57	MG	CA	3012	1/1	0.83	0.32	-	64,64,64,64	0
57	MG	BA	3476	1/1	0.99	0.16	-	48,48,48,48	0
57	MG	CA	3116	1/1	0.95	0.20	-	57,57,57,57	0
57	MG	CA	3101	1/1	0.93	0.11	-	65,65,65,65	0
57	MG	DA	3182	1/1	0.97	0.21	-	52,52,52,52	0
57	MG	DB	3002	1/1	0.94	0.26	-	63,63,63,63	0
57	MG	DA	3533	1/1	0.90	0.14	-	56,56,56,56	0
57	MG	BA	3132	1/1	0.91	0.18	-	50,50,50,50	0
57	MG	BA	3769	1/1	0.90	0.20	-	47,47,47,47	0
57	MG	DA	3596	1/1	0.73	0.19	-	69,69,69,69	0
57	MG	BA	3207	1/1	0.91	0.18	-	36,36,36,36	0
57	MG	DA	3353	1/1	0.97	0.13	-	47,47,47,47	0
57	MG	BA	3286	1/1	0.86	0.17	-	44,44,44,44	0
57	MG	BA	3781	1/1	0.91	0.16	-	56,56,56,56	0
57	MG	DA	3233	1/1	0.82	0.13	-	65,65,65,65	0
57	MG	DA	3591	1/1	0.81	0.06	-	66,66,66,66	0
57	MG	DA	3488	1/1	0.86	0.10	-	53,53,53,53	0
57	MG	BA	3556	1/1	0.94	0.07	-	46,46,46,46	0
57	MG	AA	1812	1/1	0.86	0.13	-	63,63,63,63	0
57	MG	CJ	5001	1/1	0.90	0.17	-	77,77,77,77	0
57	MG	BA	3516	1/1	0.91	0.24	-	46,46,46,46	0
57	MG	DA	3588	1/1	0.95	0.15	-	59,59,59,59	0
57	MG	BA	3492	1/1	0.96	0.12	-	38,38,38,38	0
57	MG	BA	3497	1/1	0.90	0.17	-	50,50,50,50	0
57	MG	DA	3580	1/1	0.88	0.21	-	62,62,62,62	0
57	MG	DA	3262	1/1	0.97	0.13	-	20,20,20,20	0
57	MG	BA	3362	1/1	0.97	0.22	-	47,47,47,47	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.