



wwPDB X-ray Structure Validation Summary Report ⓘ

Jan 31, 2016 – 11:42 PM GMT

PDB ID : 1VY6
Title : Crystal structure of the *Thermus thermophilus* 70S ribosome in the pre-attack state of peptide bond formation containing short substrate-mimic Cytidine-Puromycin in the A site and acylated tRNA in the P site.
Authors : Polikanov, Y.S.; Steitz, T.A.; Innis, C.A.
Deposited on : 2014-05-13
Resolution : 2.90 Å(reported)

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

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

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

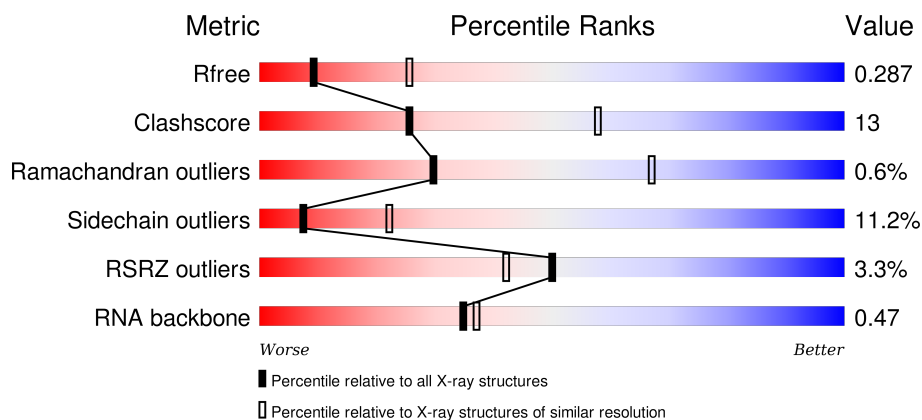
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	1451 (2.90-2.90)
Clashscore	102246	1668 (2.90-2.90)
Ramachandran outliers	100387	1630 (2.90-2.90)
Sidechain outliers	100360	1632 (2.90-2.90)
RSRZ outliers	91569	1456 (2.90-2.90)
RNA backbone	2183	1093 (3.30-2.50)

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

Mol	Chain	Length	Quality of chain
1	AA	1521	
1	CA	1521	
2	AB	256	
2	CB	256	





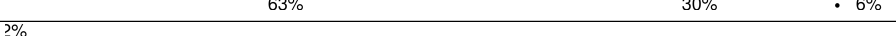
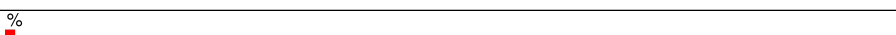

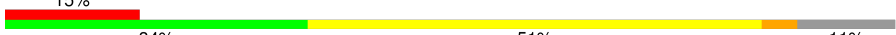







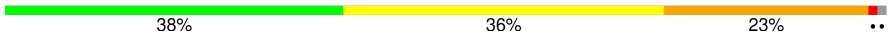



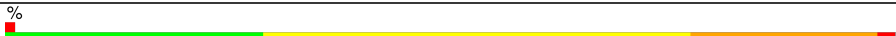





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Mol	Chain	Length	Quality of chain
3	AC	239	
3	CC	239	
4	AD	209	
4	CD	209	
5	AE	162	
5	CE	162	
6	AF	101	
6	CF	101	
7	AG	156	
7	CG	156	
8	AH	138	
8	CH	138	
9	AI	128	
9	CI	128	
10	AJ	105	
10	CJ	105	
11	AK	129	
11	CK	129	
12	AL	132	
12	CL	132	
13	AM	126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














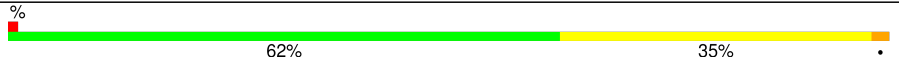
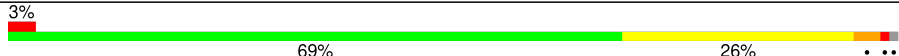

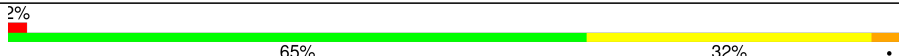
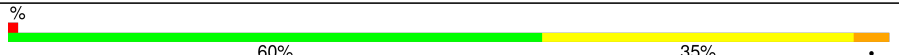
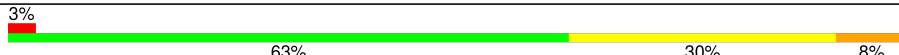
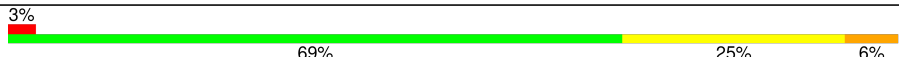
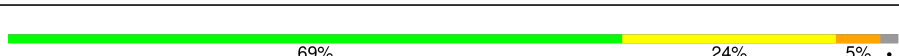



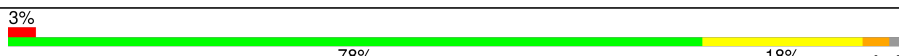
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Mol	Chain	Length	Quality of chain
15	CO	89	
16	AP	88	
16	CP	88	
17	AQ	105	
17	CQ	105	
18	AR	88	
18	CR	88	
19	AS	93	
19	CS	93	
20	AT	106	
20	CT	106	
21	AU	27	
21	CU	27	
22	AV	24	
22	CV	24	
23	AW	2	
23	CW	2	
24	AX	77	
24	CX	77	
25	BA	2915	
25	DA	2915	
26	BB	121	
26	DB	121	
27	BD	276	
27	DD	276	

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

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Mol	Chain	Length	Quality of chain
40	DU	118	
41	BV	101	
41	DV	101	
42	BW	113	
42	DW	113	
43	BX	96	
43	DX	96	
44	BY	110	
44	DY	110	
45	BZ	206	
45	DZ	206	
46	B0	85	
46	D0	85	
47	B1	98	
47	D1	98	
48	B2	72	
48	D2	72	
49	B3	60	
49	D3	60	
50	B4	71	
50	D4	71	
51	B5	60	
51	D5	60	
52	B6	54	
52	D6	54	

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Mol	Chain	Length	Quality of chain
53	B7	49	
53	D7	49	
54	B8	65	
54	D8	65	
55	B9	37	
55	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
56	MG	AA	3006	-	-	-	X
56	MG	AA	3008	-	-	-	X
56	MG	AA	3019	-	-	-	X
56	MG	AA	3054	-	-	-	X
56	MG	AA	3057	-	-	-	X
56	MG	AA	3107	-	-	-	X
56	MG	AA	3132	-	-	-	X
56	MG	AA	3134	-	-	-	X
56	MG	B7	3001	-	-	-	X
56	MG	BA	3014	-	-	-	X
56	MG	BA	3030	-	-	-	X
56	MG	BA	3031	-	-	-	X
56	MG	BA	3032	-	-	-	X
56	MG	BA	3094	-	-	-	X
56	MG	BA	3112	-	-	-	X
56	MG	BA	3117	-	-	-	X
56	MG	BA	3121	-	-	-	X
56	MG	BA	3144	-	-	-	X
56	MG	BA	3153	-	-	-	X
56	MG	BA	3154	-	-	-	X
56	MG	BA	3178	-	-	-	X
56	MG	BA	3210	-	-	-	X
56	MG	BA	3216	-	-	-	X
56	MG	BA	3221	-	-	-	X
56	MG	BA	3230	-	-	-	X
56	MG	BA	3244	-	-	-	X
56	MG	BA	3256	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
56	MG	BA	3268	-	-	-	X
56	MG	BA	3288	-	-	-	X
56	MG	BA	3295	-	-	-	X
56	MG	BA	3488	-	-	-	X
56	MG	BA	3495	-	-	-	X
56	MG	BA	3519	-	-	-	X
56	MG	BA	3553	-	-	-	X
56	MG	BA	3624	-	-	-	X
56	MG	BA	3634	-	-	-	X
56	MG	BA	3640	-	-	-	X
56	MG	BA	3667	-	-	-	X
56	MG	BA	3670	-	-	-	X
56	MG	BA	3671	-	-	-	X
56	MG	BD	302	-	-	-	X
56	MG	BD	303	-	-	-	X
56	MG	BE	302	-	-	-	X
56	MG	BF	303	-	-	-	X
56	MG	BP	201	-	-	-	X
56	MG	BP	202	-	-	-	X
56	MG	BU	203	-	-	-	X
56	MG	BV	201	-	-	-	X
56	MG	CA	3048	-	-	-	X
56	MG	D3	3001	-	-	-	X
56	MG	D5	502	-	-	-	X
56	MG	D7	101	-	-	-	X
56	MG	DA	3020	-	-	-	X
56	MG	DA	3092	-	-	-	X
56	MG	DA	3095	-	-	-	X
56	MG	DA	3125	-	-	-	X
56	MG	DA	3150	-	-	-	X
56	MG	DA	3152	-	-	-	X
56	MG	DA	3163	-	-	-	X
56	MG	DA	3214	-	-	-	X
56	MG	DA	3237	-	-	-	X
56	MG	DA	3246	-	-	-	X
56	MG	DA	3327	-	-	-	X
56	MG	DA	3381	-	-	-	X
56	MG	DA	3426	-	-	-	X
56	MG	DA	3435	-	-	-	X
56	MG	DA	3495	-	-	-	X
56	MG	DA	3521	-	-	-	X
56	MG	DA	3592	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
56	MG	DA	3593	-	-	-	X
56	MG	DA	3596	-	-	-	X
56	MG	DP	3001	-	-	-	X

2 Entry composition

There are 60 unique types of molecules in this entry. The entry contains 289646 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	AD	208	Total	C	N	O	S	0	0	0
			1659	1040	326	286	7			
4	CD	208	Total	C	N	O	S	0	0	0
			1670	1047	332	284	7			

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

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

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

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

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

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

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

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

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

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

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

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

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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		
			829	516	155	155	3	0	0
11	CK	114	Total	C	N	O	S		
			833	519	156	155	3	0	0

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

- Molecule 22 is a RNA chain called mRNA.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	AW	2	Total	C	N	O	P	0	0	0
			54	31	10	12	1			
23	CW	2	Total	C	N	O	P	0	0	0
			54	31	10	12	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 23S Ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
25	BA	2819	Total	C	N	O	P	0	0	0
			60729	27026	11370	19515	2818			
25	DA	2800	Total	C	N	O	P	0	0	0
			60311	26840	11284	19388	2799			

- Molecule 26 is a RNA chain called 5S Ribosomal RNA.

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

- Molecule 55 is a protein called 50S ribosomal protein L36.

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

- Molecule 56 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	B4	1	Total	Mg	0	0
			1	1		
56	BA	675	Total	Mg	0	0
			675	675		
56	AK	1	Total	Mg	0	0
			1	1		
56	DQ	3	Total	Mg	0	0
			3	3		
56	D3	1	Total	Mg	0	0
			1	1		
56	DF	3	Total	Mg	0	0
			3	3		
56	B8	1	Total	Mg	0	0
			1	1		
56	BE	6	Total	Mg	0	0
			6	6		
56	DU	1	Total	Mg	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	AN	1	Total 1	Mg 1	0	0
56	BP	4	Total 4	Mg 4	0	0
56	AX	7	Total 7	Mg 7	0	0
56	DN	1	Total 1	Mg 1	0	0
56	CA	154	Total 154	Mg 154	0	0
56	B5	2	Total 2	Mg 2	0	0
56	BB	18	Total 18	Mg 18	0	0
56	AE	2	Total 2	Mg 2	0	0
56	DG	1	Total 1	Mg 1	0	0
56	CF	1	Total 1	Mg 1	0	0
56	B9	1	Total 1	Mg 1	0	0
56	BF	5	Total 5	Mg 5	0	0
56	BX	3	Total 3	Mg 3	0	0
56	D8	2	Total 2	Mg 2	0	0
56	AA	187	Total 187	Mg 187	0	0
56	BQ	3	Total 3	Mg 3	0	0
56	D7	1	Total 1	Mg 1	0	0
56	CX	1	Total 1	Mg 1	0	0
56	DV	2	Total 2	Mg 2	0	0
56	AM	1	Total 1	Mg 1	0	0
56	BU	5	Total 5	Mg 5	0	0

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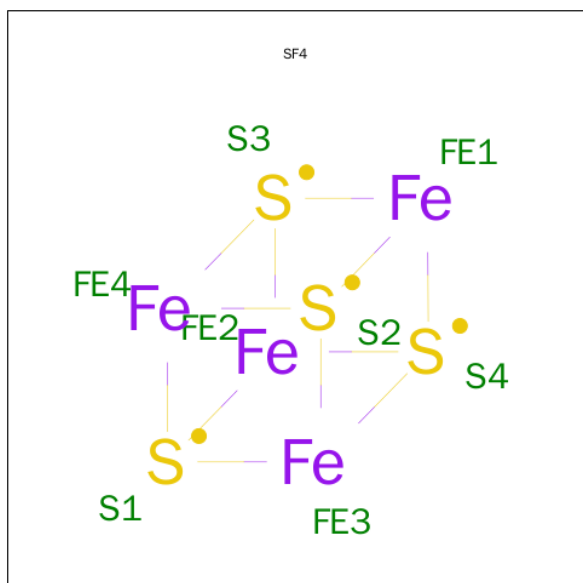
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	DR	2	Total 2	Mg 2	0	0
56	AD	1	Total 1	Mg 1	0	0
56	BN	2	Total 2	Mg 2	0	0
56	CT	1	Total 1	Mg 1	0	0
56	D0	1	Total 1	Mg 1	0	0
56	BG	3	Total 3	Mg 3	0	0
56	BY	2	Total 2	Mg 2	0	0
56	DE	5	Total 5	Mg 5	0	0
56	B3	2	Total 2	Mg 2	0	0
56	CJ	1	Total 1	Mg 1	0	0
56	BR	3	Total 3	Mg 3	0	0
56	DA	595	Total 595	Mg 595	0	0
56	DP	1	Total 1	Mg 1	0	0
56	DW	2	Total 2	Mg 2	0	0
56	B7	4	Total 4	Mg 4	0	0
56	AL	1	Total 1	Mg 1	0	0
56	BV	3	Total 3	Mg 3	0	0
56	BO	1	Total 1	Mg 1	0	0
56	BZ	1	Total 1	Mg 1	0	0
56	DY	1	Total 1	Mg 1	0	0
56	D5	1	Total 1	Mg 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	BD	8	Total 8	Mg 8	0	0
56	DT	1	Total 1	Mg 1	0	0
56	B0	5	Total 5	Mg 5	0	0
56	CE	2	Total 2	Mg 2	0	0
56	BW	4	Total 4	Mg 4	0	0
56	DB	12	Total 12	Mg 12	0	0
56	DD	2	Total 2	Mg 2	0	0
56	CK	1	Total 1	Mg 1	0	0
56	AF	1	Total 1	Mg 1	0	0
56	BH	1	Total 1	Mg 1	0	0

- Molecule 57 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe₄S₄).



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

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

- Molecule 58 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 59 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
59	AX	1	Total	K	0	0
			1	1		
59	DA	1	Total	K	0	0
			1	1		

- Molecule 60 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
60	AA	165	Total 165	O 165	0	0
60	AJ	1	Total 1	O 1	0	0
60	AL	3	Total 3	O 3	0	0
60	AP	1	Total 1	O 1	0	0
60	AU	1	Total 1	O 1	0	0
60	AV	2	Total 2	O 2	0	0
60	AW	3	Total 3	O 3	0	0
60	BA	924	Total 924	O 924	0	0
60	BB	27	Total 27	O 27	0	0
60	BD	6	Total 6	O 6	0	0
60	BE	8	Total 8	O 8	0	0
60	BF	6	Total 6	O 6	0	0
60	BG	1	Total 1	O 1	0	0
60	BH	1	Total 1	O 1	0	0
60	BN	3	Total 3	O 3	0	0
60	BO	1	Total 1	O 1	0	0
60	BP	14	Total 14	O 14	0	0
60	BQ	2	Total 2	O 2	0	0
60	BS	1	Total 1	O 1	0	0
60	BT	4	Total 4	O 4	0	0
60	BU	2	Total 2	O 2	0	0
60	BV	5	Total 5	O 5	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
60	BW	1	Total 1	O 1	0	0
60	BX	2	Total 2	O 2	0	0
60	BZ	1	Total 1	O 1	0	0
60	B0	4	Total 4	O 4	0	0
60	B1	2	Total 2	O 2	0	0
60	B2	1	Total 1	O 1	0	0
60	B3	1	Total 1	O 1	0	0
60	B5	2	Total 2	O 2	0	0
60	B7	2	Total 2	O 2	0	0
60	B8	8	Total 8	O 8	0	0
60	CA	113	Total 113	O 113	0	0
60	CE	2	Total 2	O 2	0	0
60	CJ	2	Total 2	O 2	0	0
60	CL	1	Total 1	O 1	0	0
60	CO	1	Total 1	O 1	0	0
60	CW	1	Total 1	O 1	0	0
60	CX	1	Total 1	O 1	0	0
60	DA	689	Total 689	O 689	0	0
60	DB	9	Total 9	O 9	0	0
60	DD	11	Total 11	O 11	0	0
60	DE	5	Total 5	O 5	0	0

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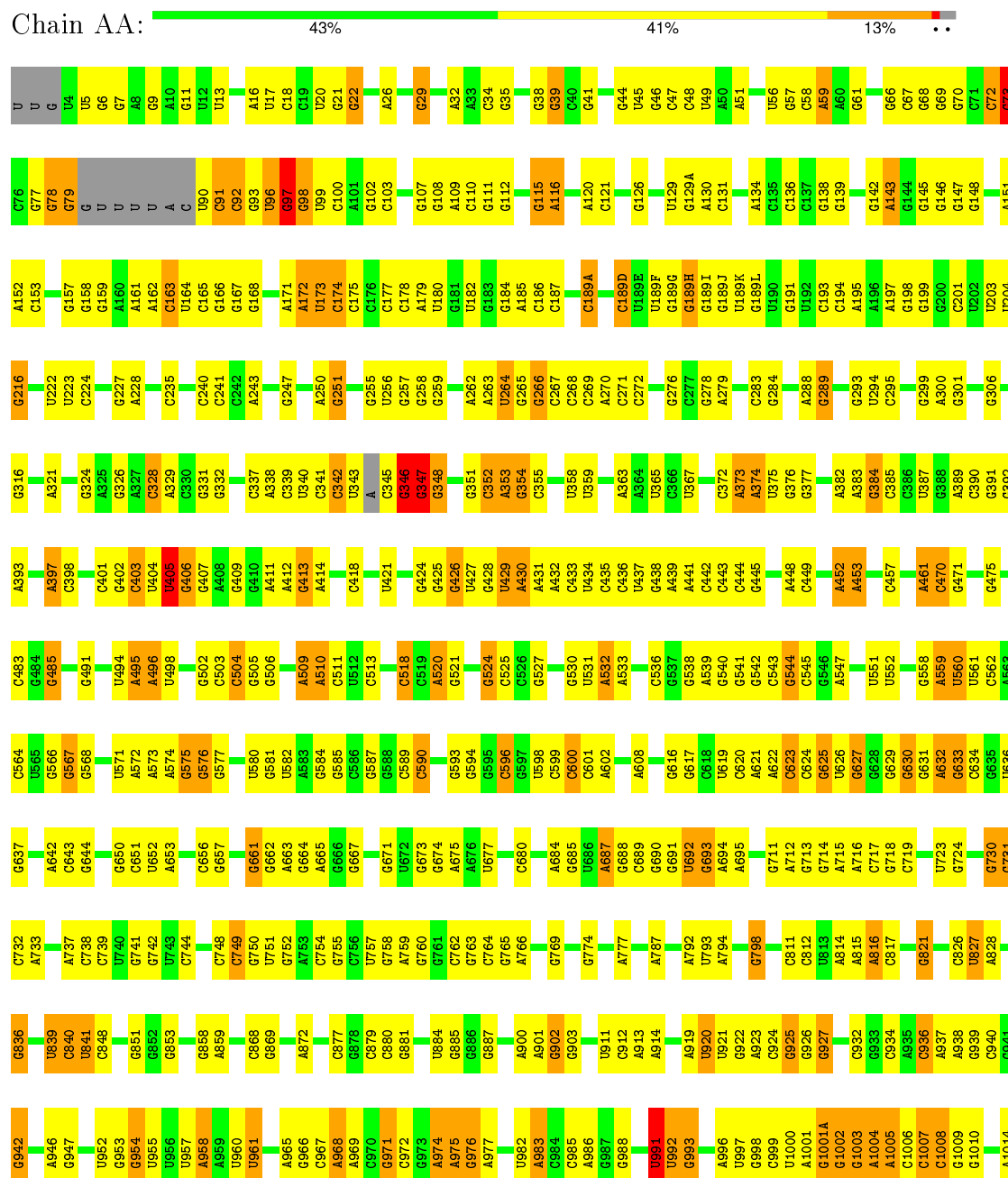
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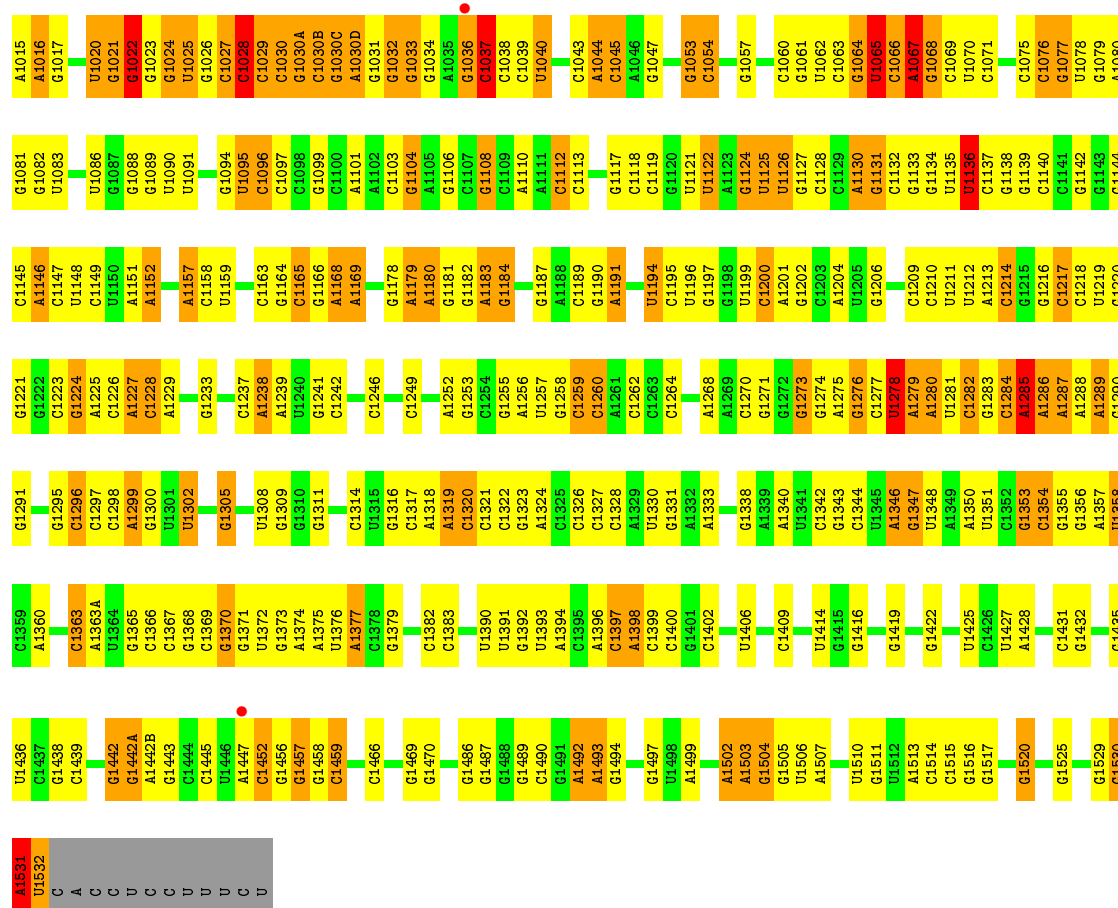
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60	DO	1	Total 1	O 1	0	0
60	DP	6	Total 6	O 6	0	0
60	DU	3	Total 3	O 3	0	0
60	DV	1	Total 1	O 1	0	0
60	DW	1	Total 1	O 1	0	0
60	DX	3	Total 3	O 3	0	0
60	D0	5	Total 5	O 5	0	0
60	D1	1	Total 1	O 1	0	0
60	D3	1	Total 1	O 1	0	0
60	D8	3	Total 3	O 3	0	0

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

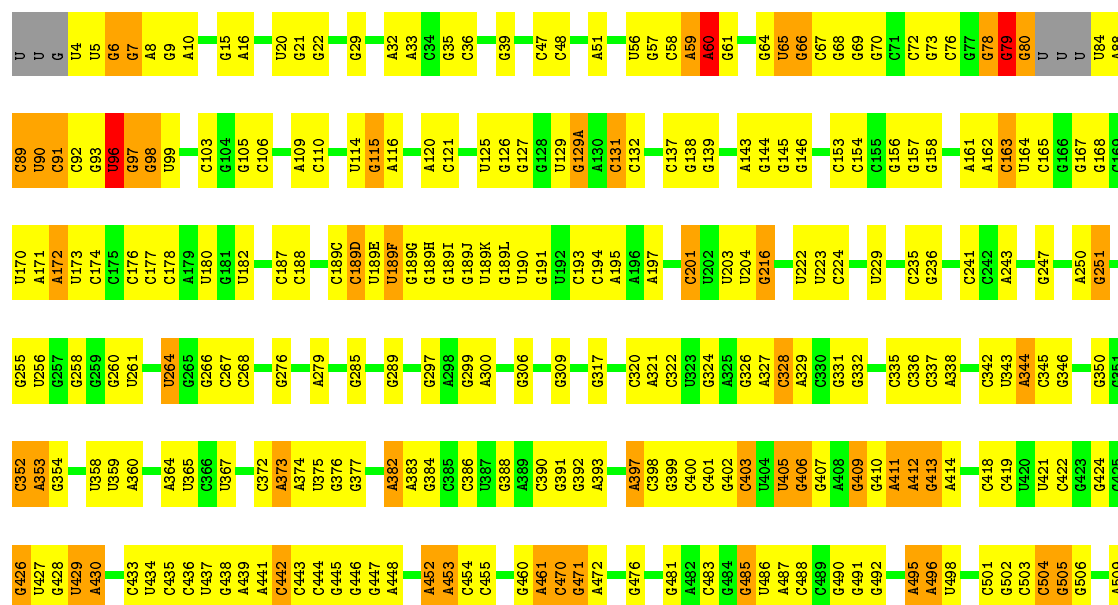
- Molecule 1: 16S Ribosomal RNA

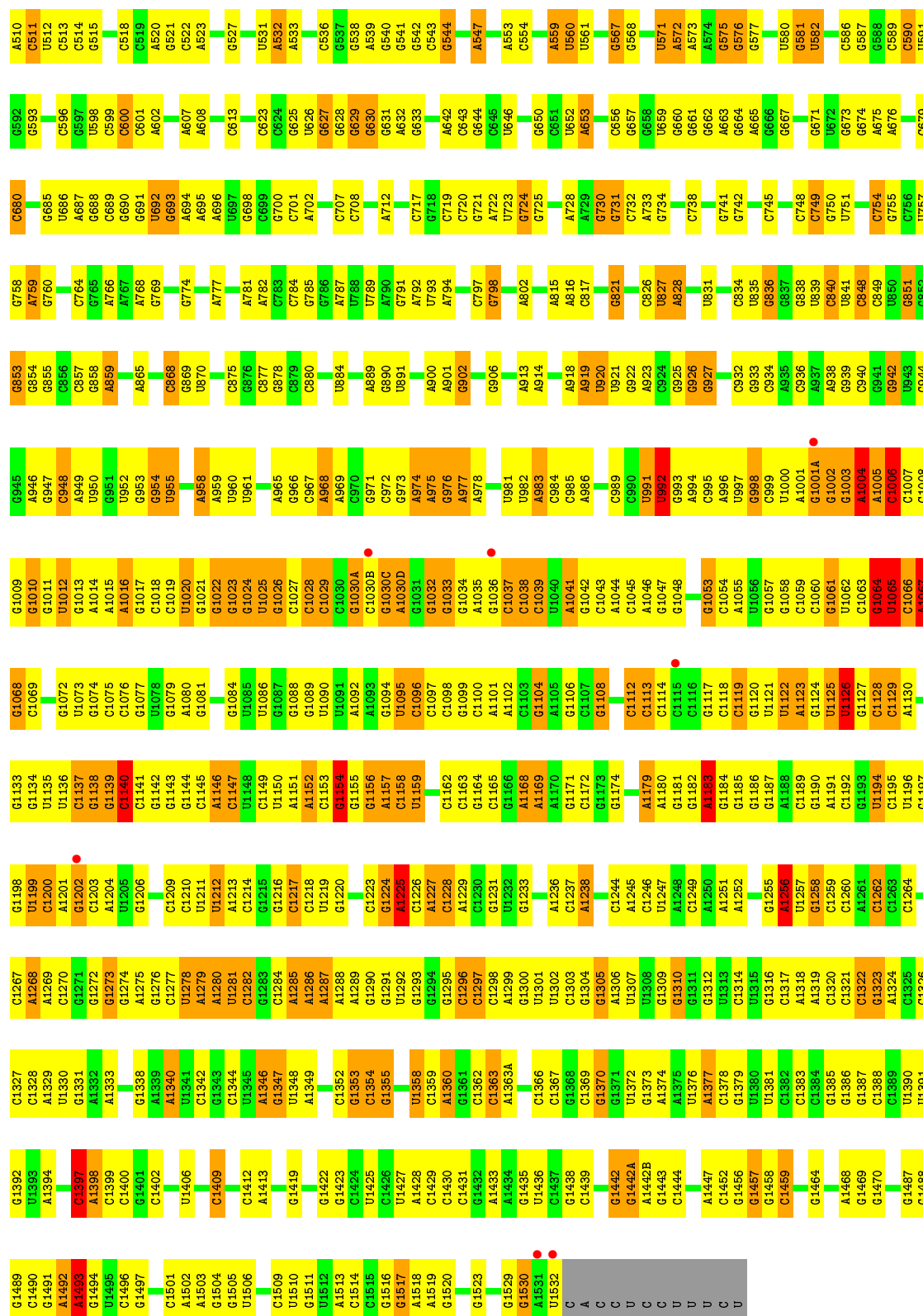




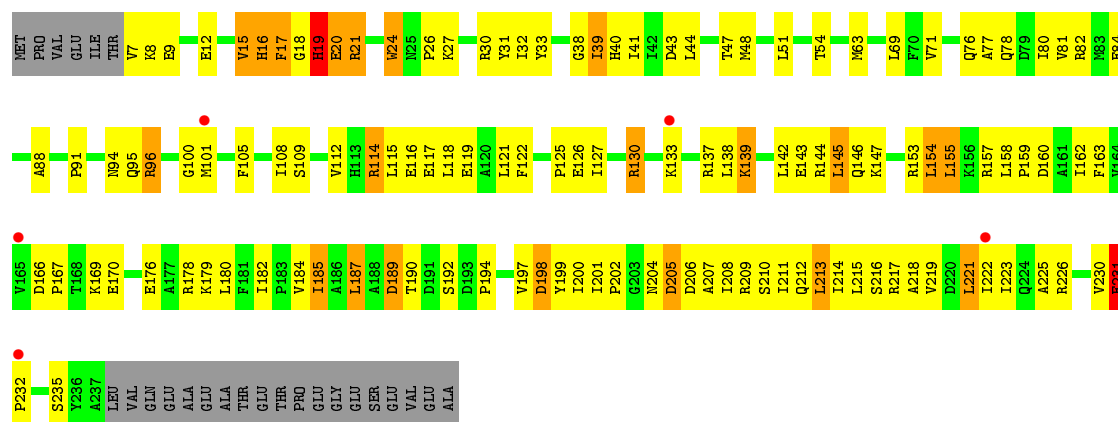
● Molecule 1: 16S Ribosomal RNA

Chain CA: 40% 44% 14% ..

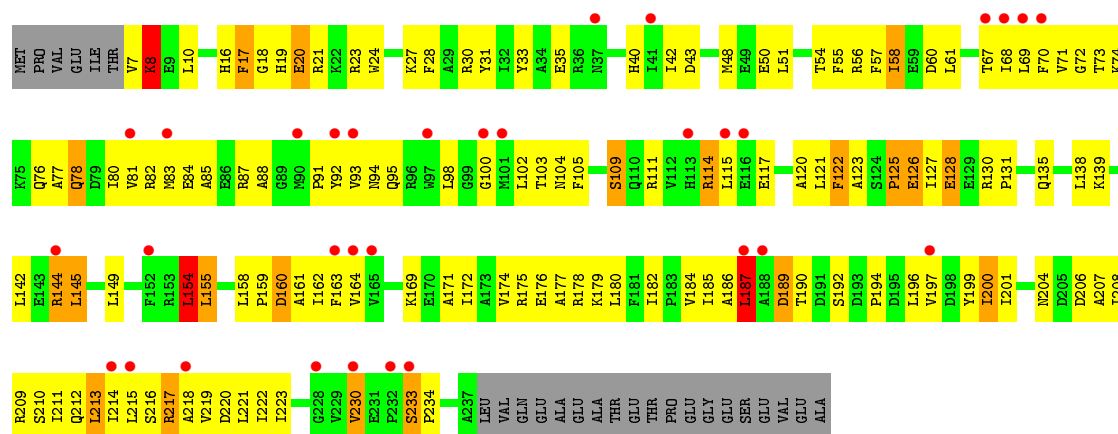




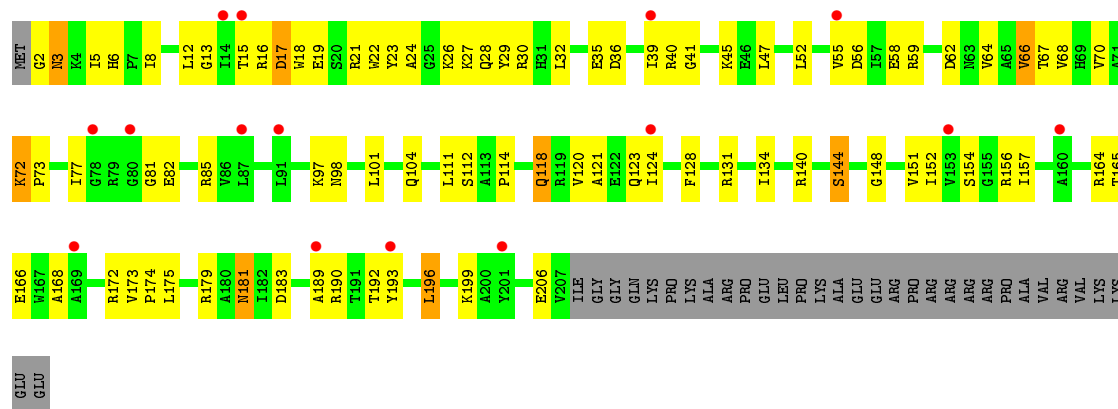
• Molecule 2: 30S ribosomal protein S2



• Molecule 2: 30S ribosomal protein S2

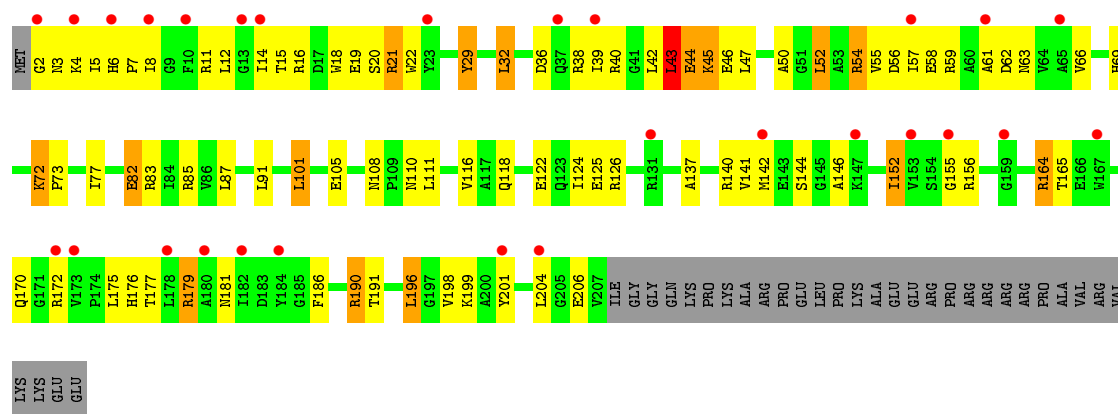


• Molecule 3: 30S ribosomal protein S3

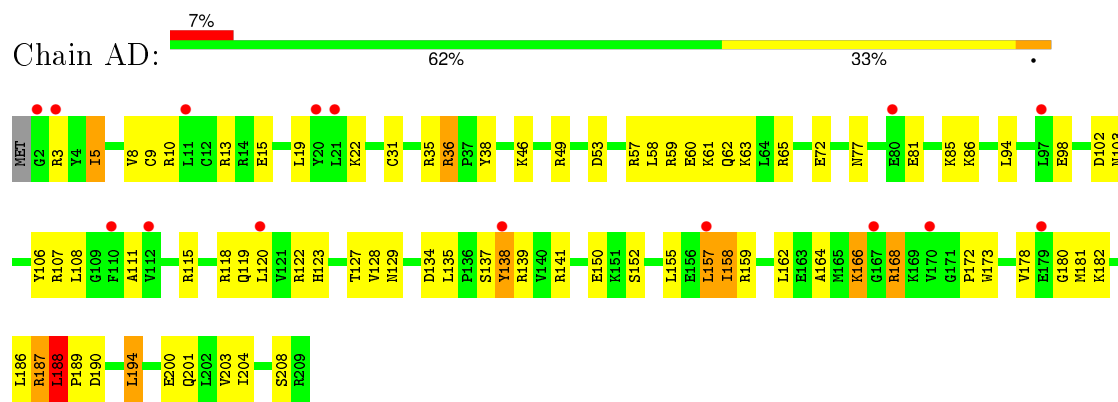


• Molecule 3: 30S ribosomal protein S3

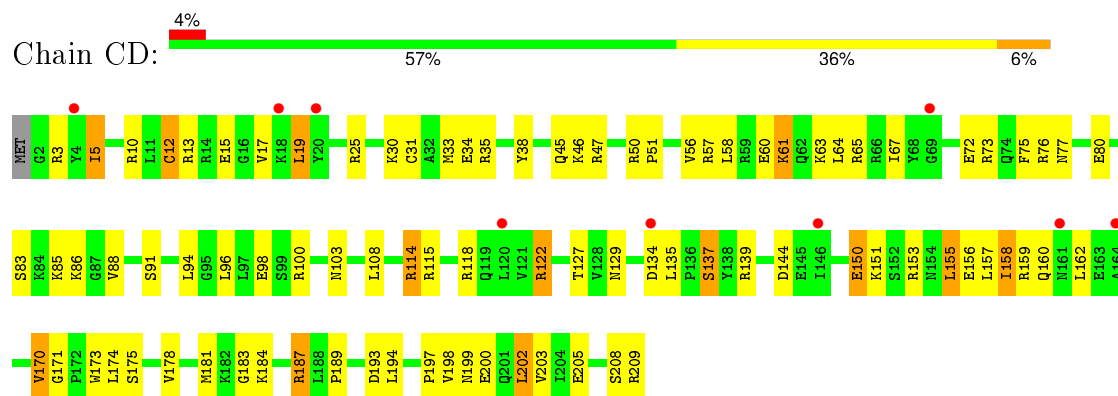




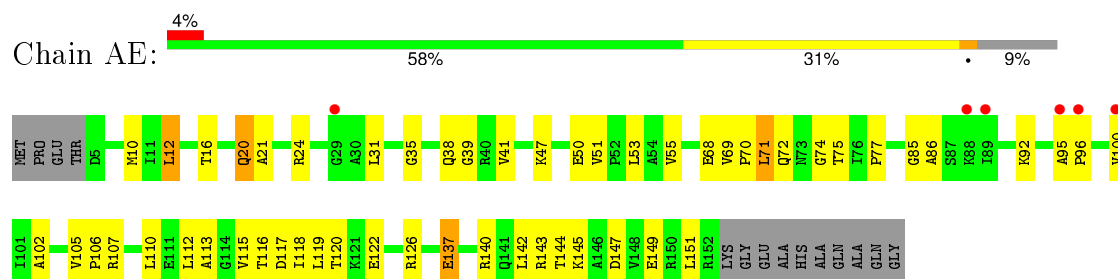
• Molecule 4: 30S ribosomal protein S4



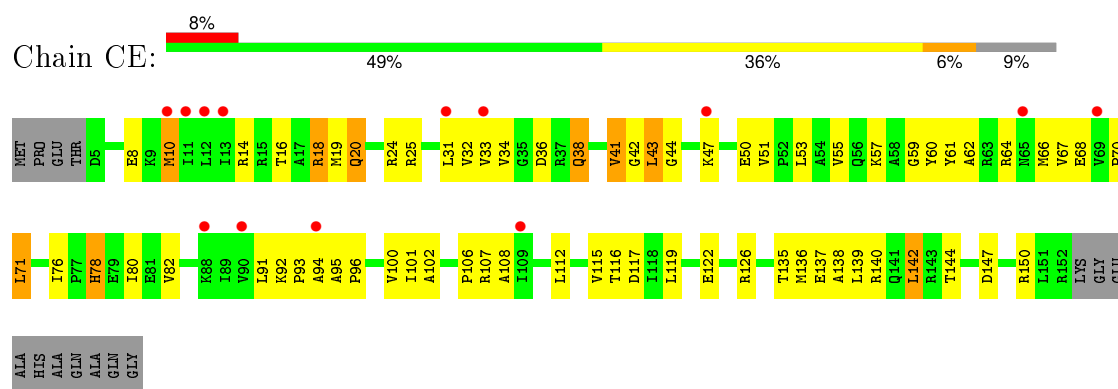
• Molecule 4: 30S ribosomal protein S4



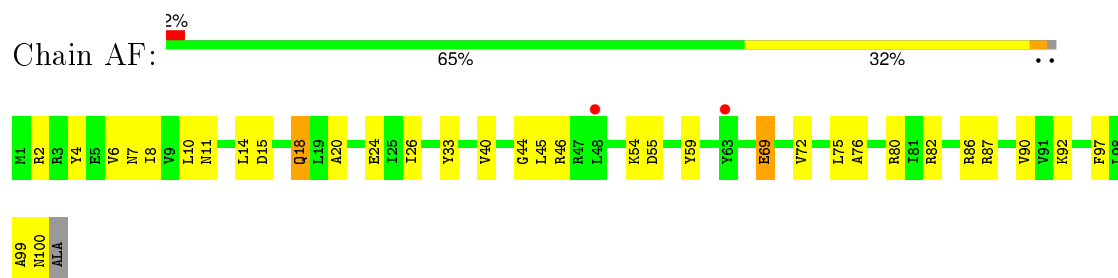
• Molecule 5: 30S ribosomal protein S5



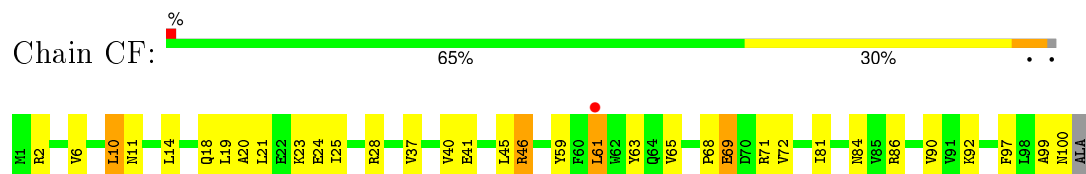
• Molecule 5: 30S ribosomal protein S5



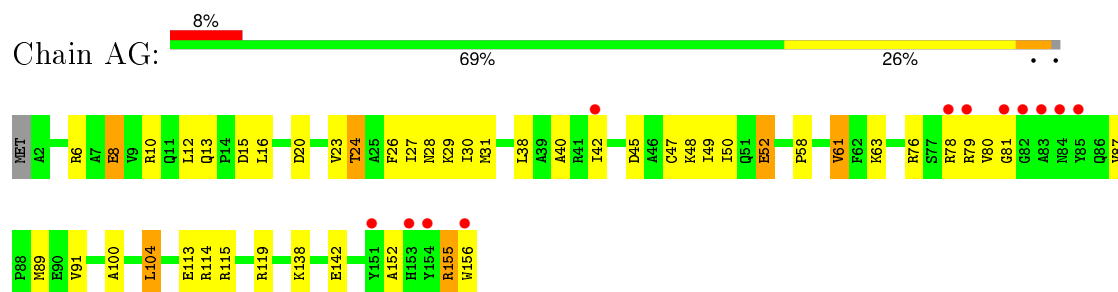
- Molecule 6: 30S ribosomal protein S6



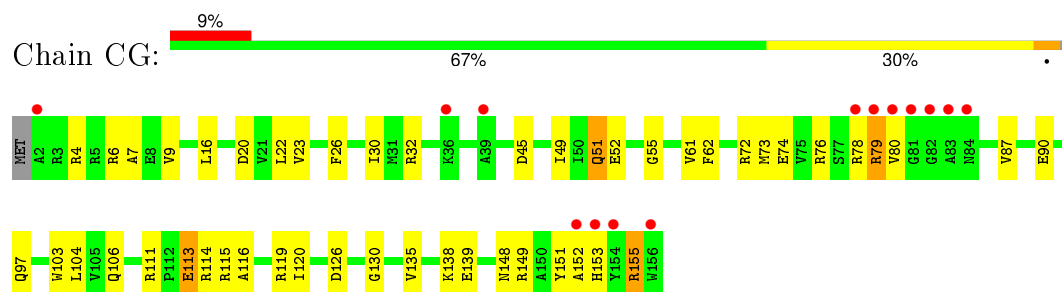
- Molecule 6: 30S ribosomal protein S6



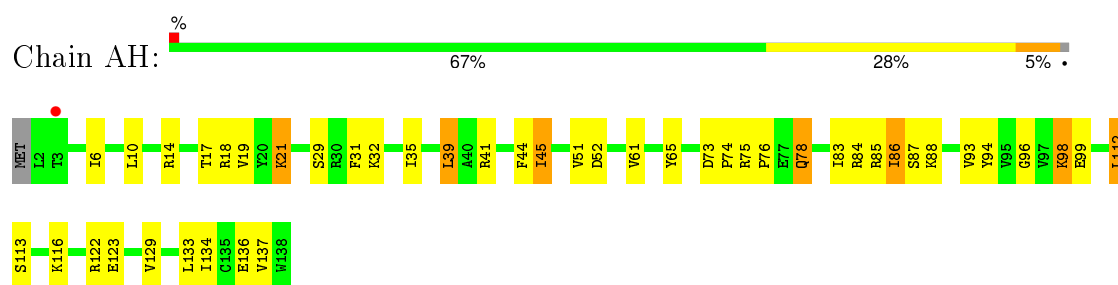
- Molecule 7: 30S ribosomal protein S7



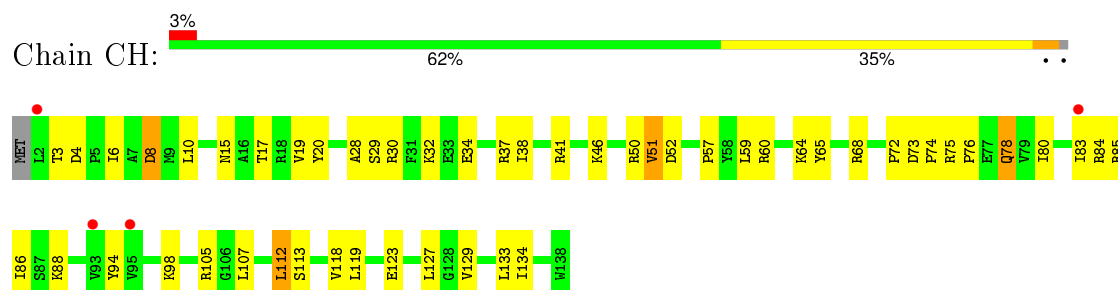
- Molecule 7: 30S ribosomal protein S7



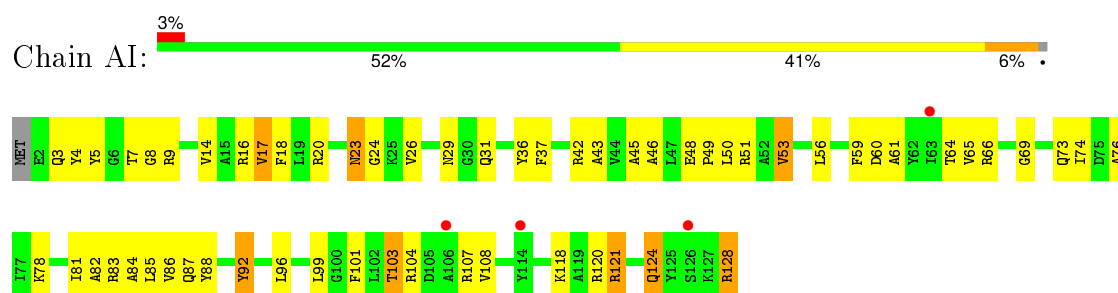
- Molecule 8: 30S ribosomal protein S8



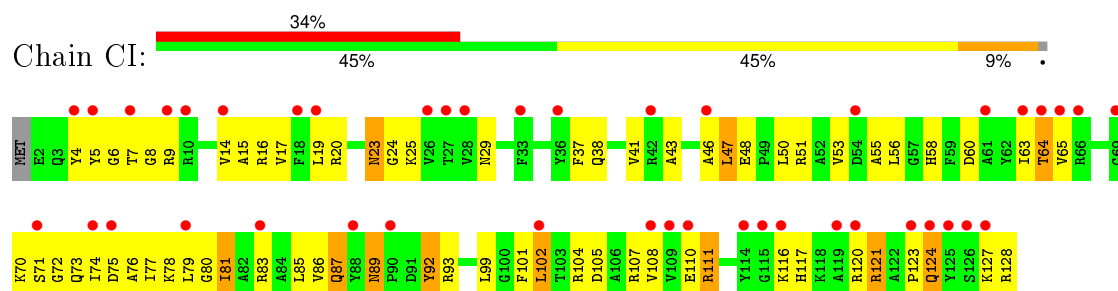
• Molecule 8: 30S ribosomal protein S8



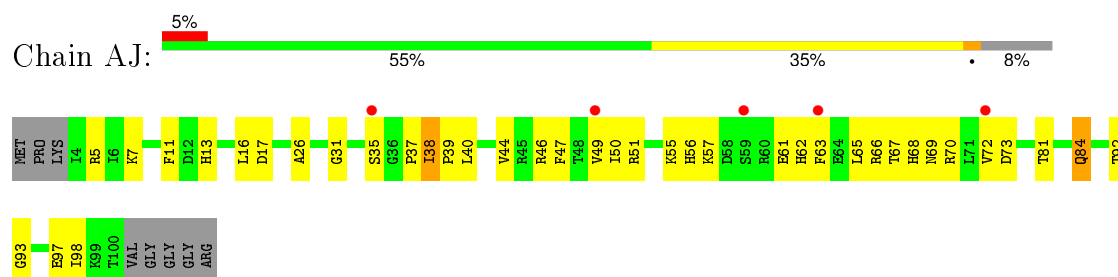
• Molecule 9: 30S ribosomal protein S9



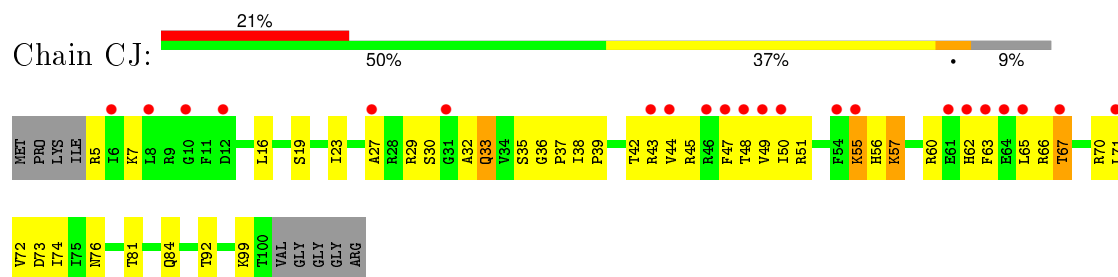
• Molecule 9: 30S ribosomal protein S9



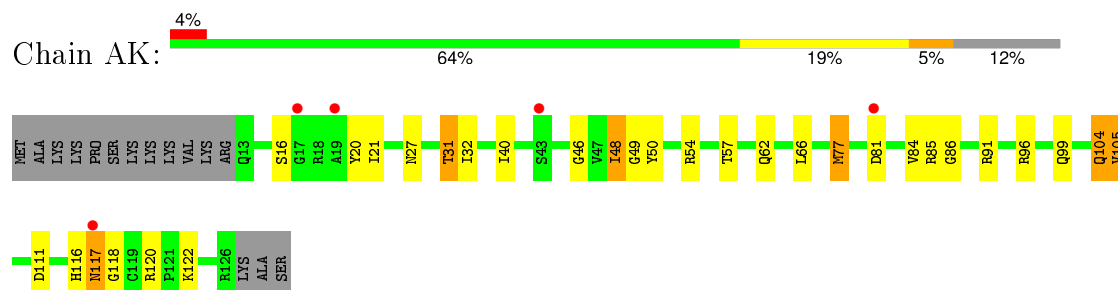
• Molecule 10: 30S ribosomal protein S10



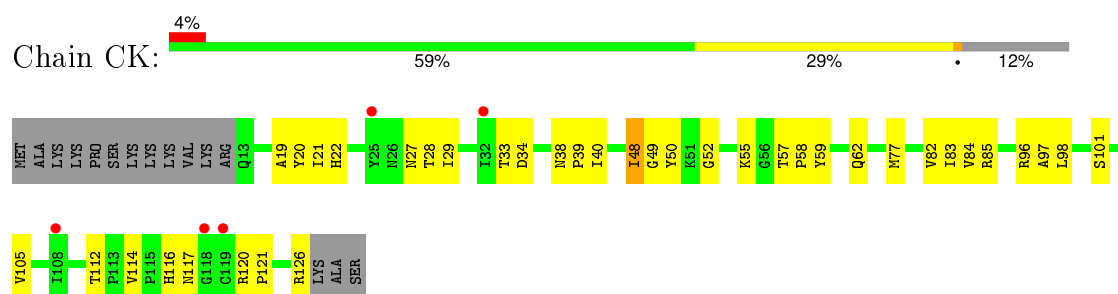
- Molecule 10: 30S ribosomal protein S10



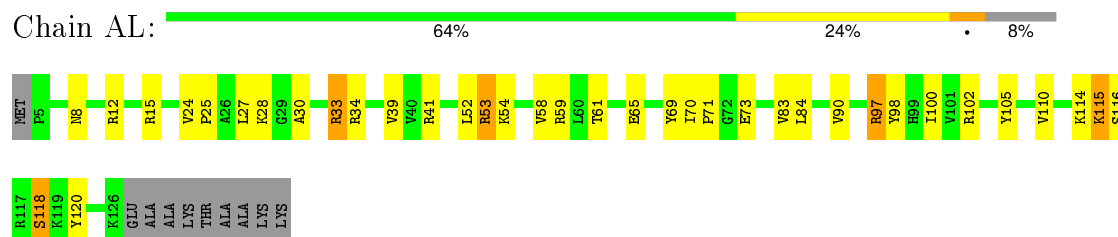
- Molecule 11: 30S ribosomal protein S11



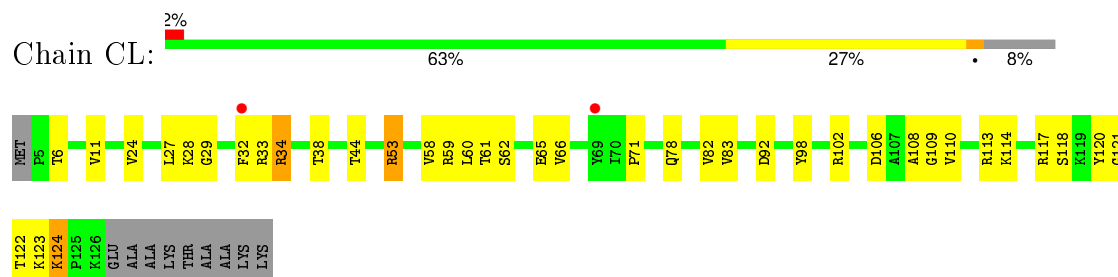
- Molecule 11: 30S ribosomal protein S11



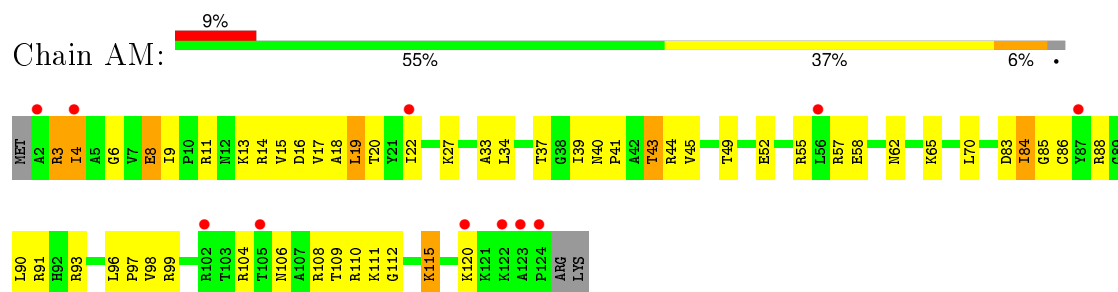
- Molecule 12: 30S ribosomal protein S12



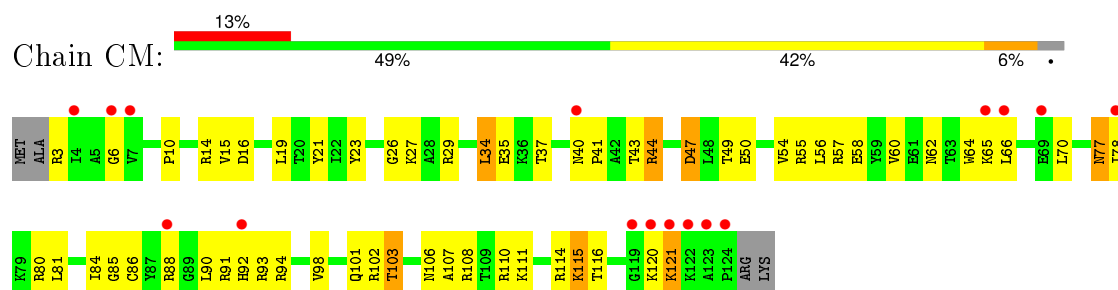
- Molecule 12: 30S ribosomal protein S12



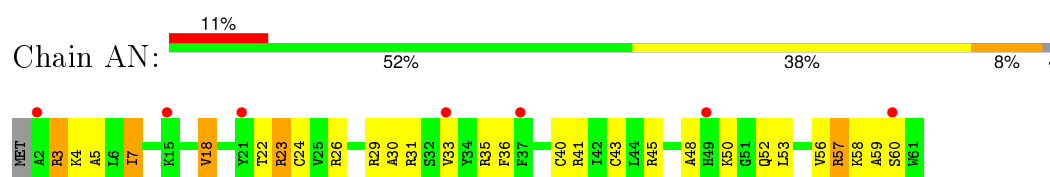
- Molecule 13: 30S ribosomal protein S13



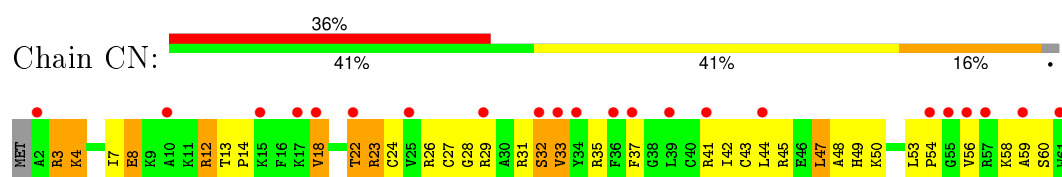
- Molecule 13: 30S ribosomal protein S13



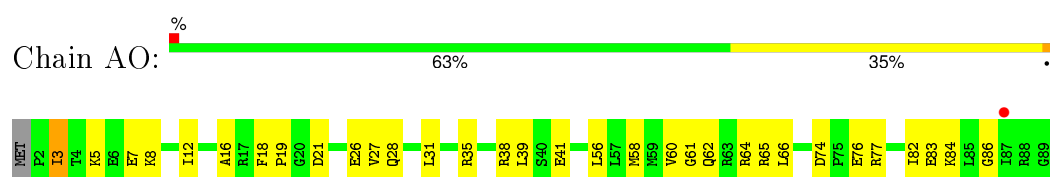
- Molecule 14: 30S ribosomal protein S14 type Z



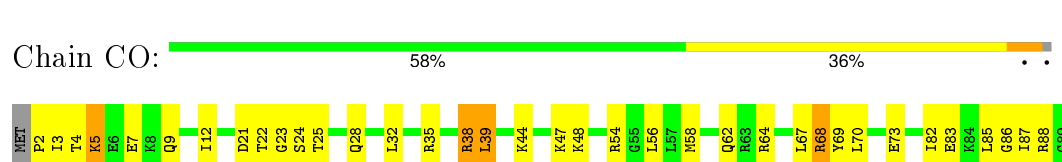
- Molecule 14: 30S ribosomal protein S14 type Z



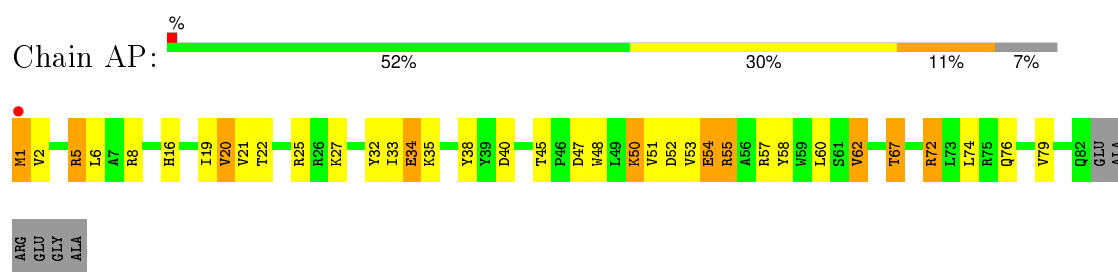
- Molecule 15: 30S ribosomal protein S15



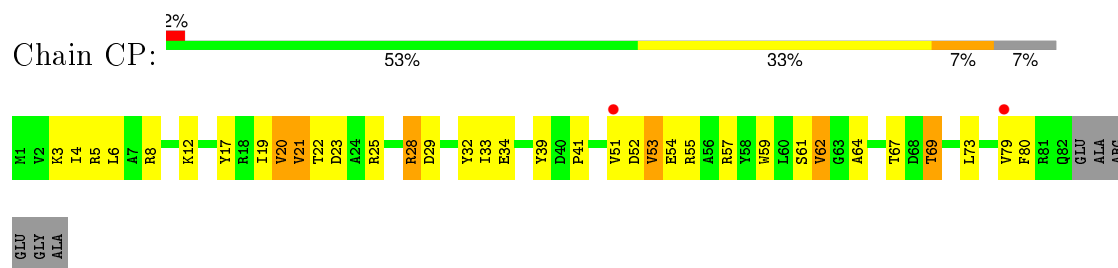
- Molecule 15: 30S ribosomal protein S15



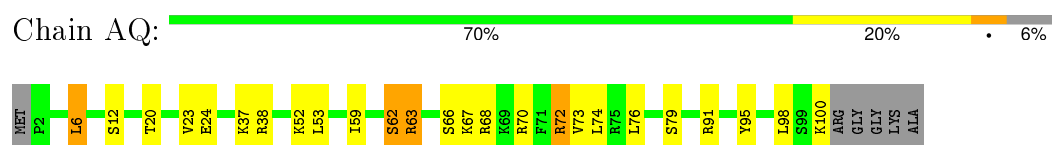
- Molecule 16: 30S ribosomal protein S16



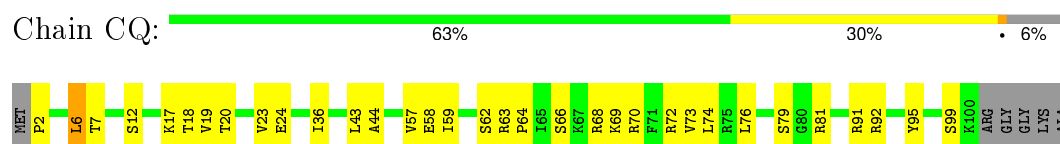
- Molecule 16: 30S ribosomal protein S16



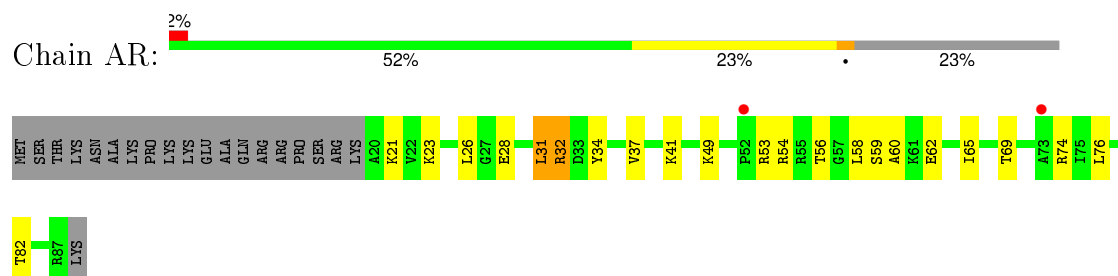
- Molecule 17: 30S ribosomal protein S17



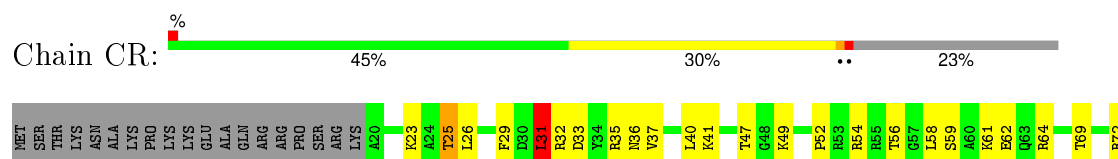
- Molecule 17: 30S ribosomal protein S17

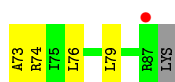


- Molecule 18: 30S ribosomal protein S18



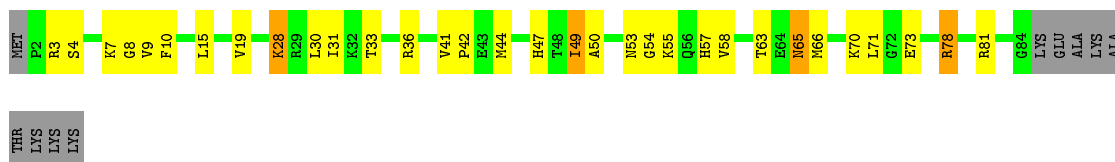
- Molecule 18: 30S ribosomal protein S18





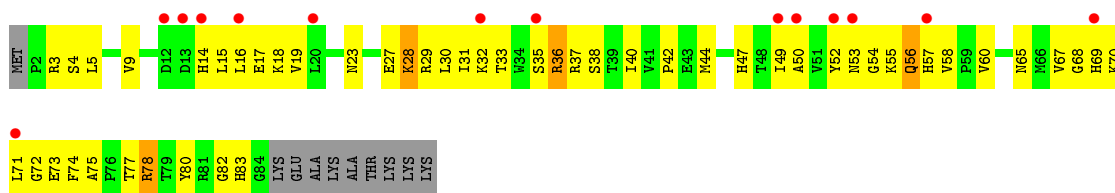
- Molecule 19: 30S ribosomal protein S19

Chain AS:



- Molecule 19: 30S ribosomal protein S19

Chain CS:



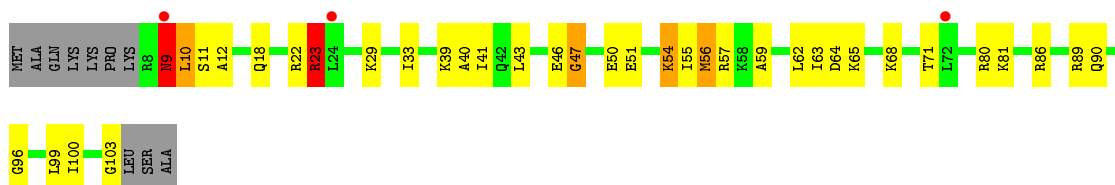
- Molecule 20: 30S ribosomal protein S20

Chain AT:



- Molecule 20: 30S ribosomal protein S20

Chain CT:

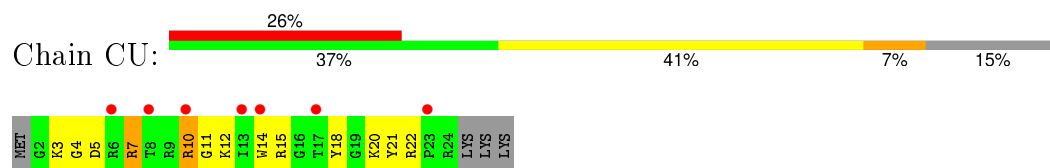


- Molecule 21: 30S ribosomal protein Thx

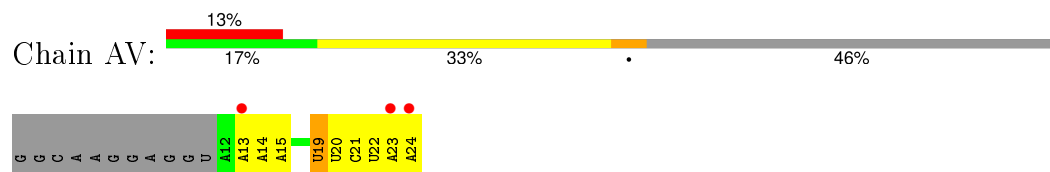
Chain AU:



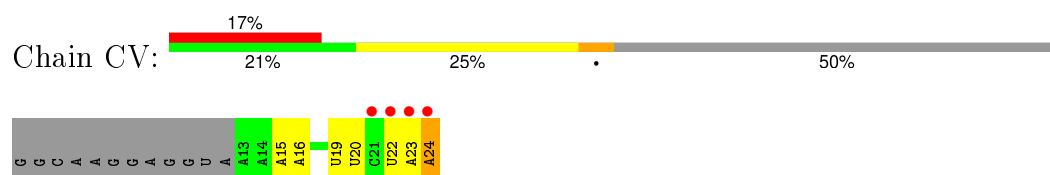
- Molecule 21: 30S ribosomal protein Thx



- Molecule 22: mRNA



- Molecule 22: mRNA



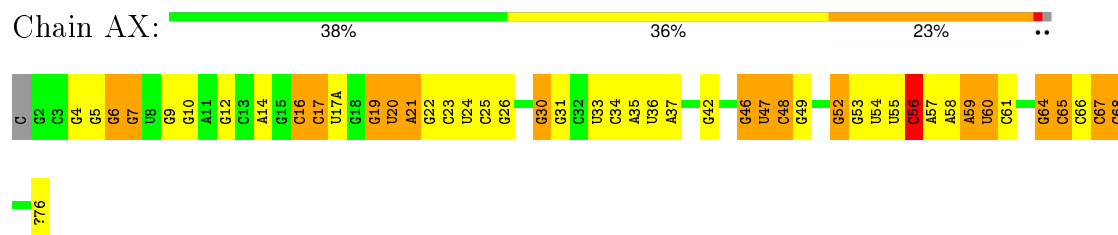
- Molecule 23: Cytidine-Puromycin



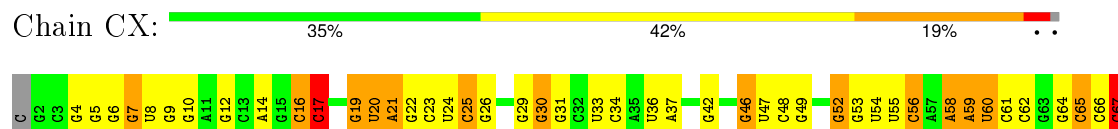
- Molecule 23: Cytidine-Puromycin

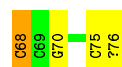


- Molecule 24: P-site tRNA

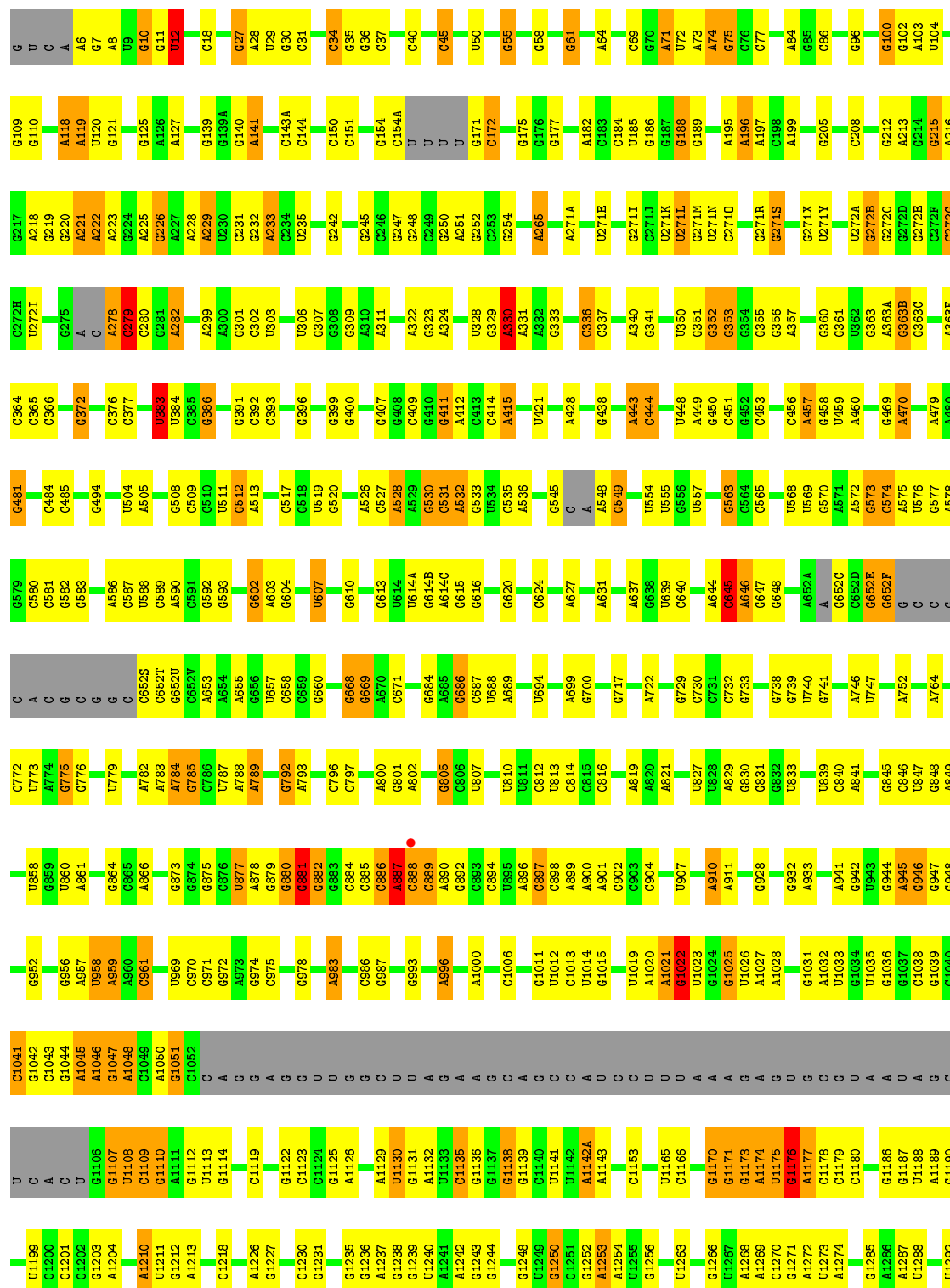


- Molecule 24: P-site tRNA



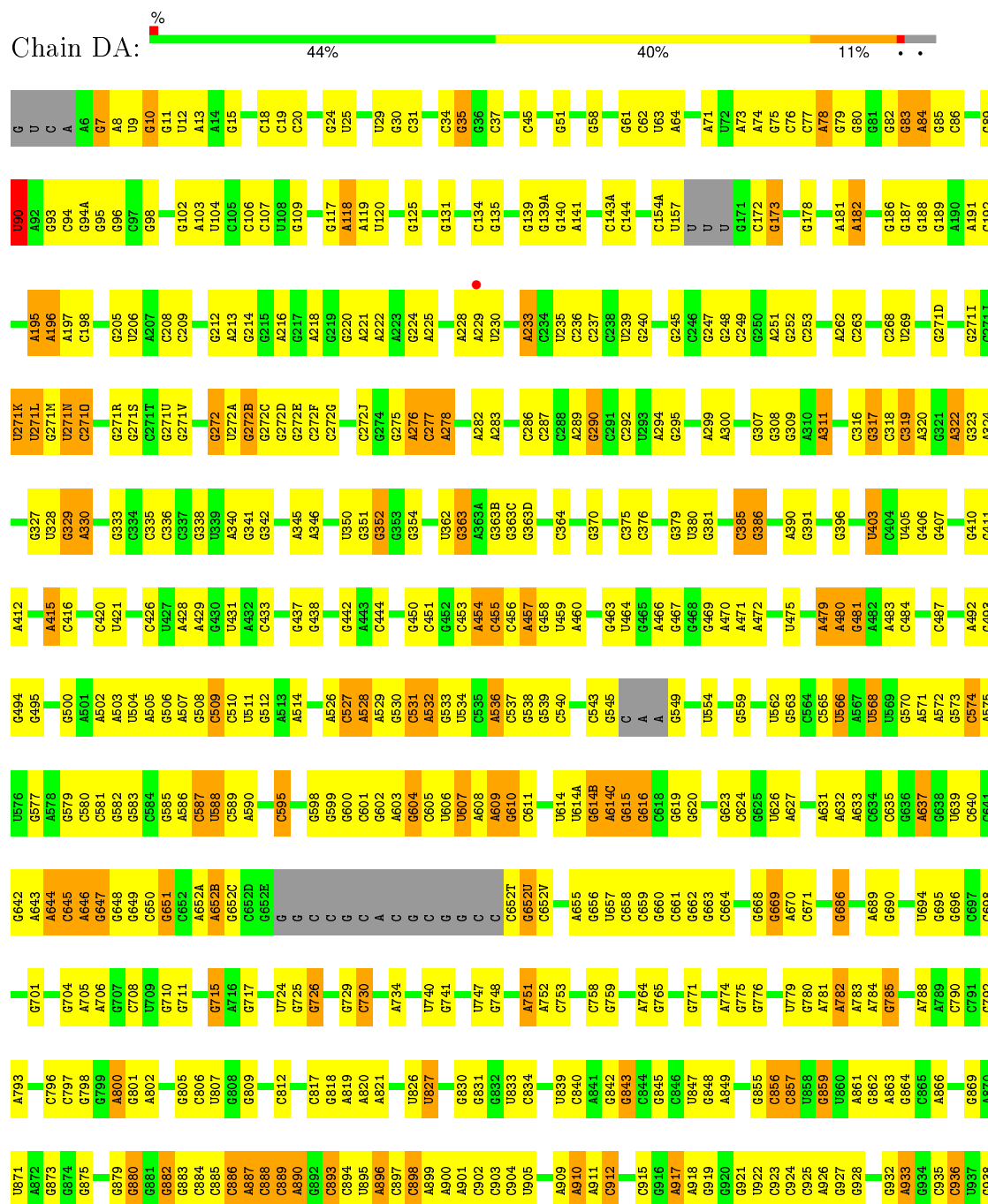


• Molecule 25: 23S Ribosomal RNA

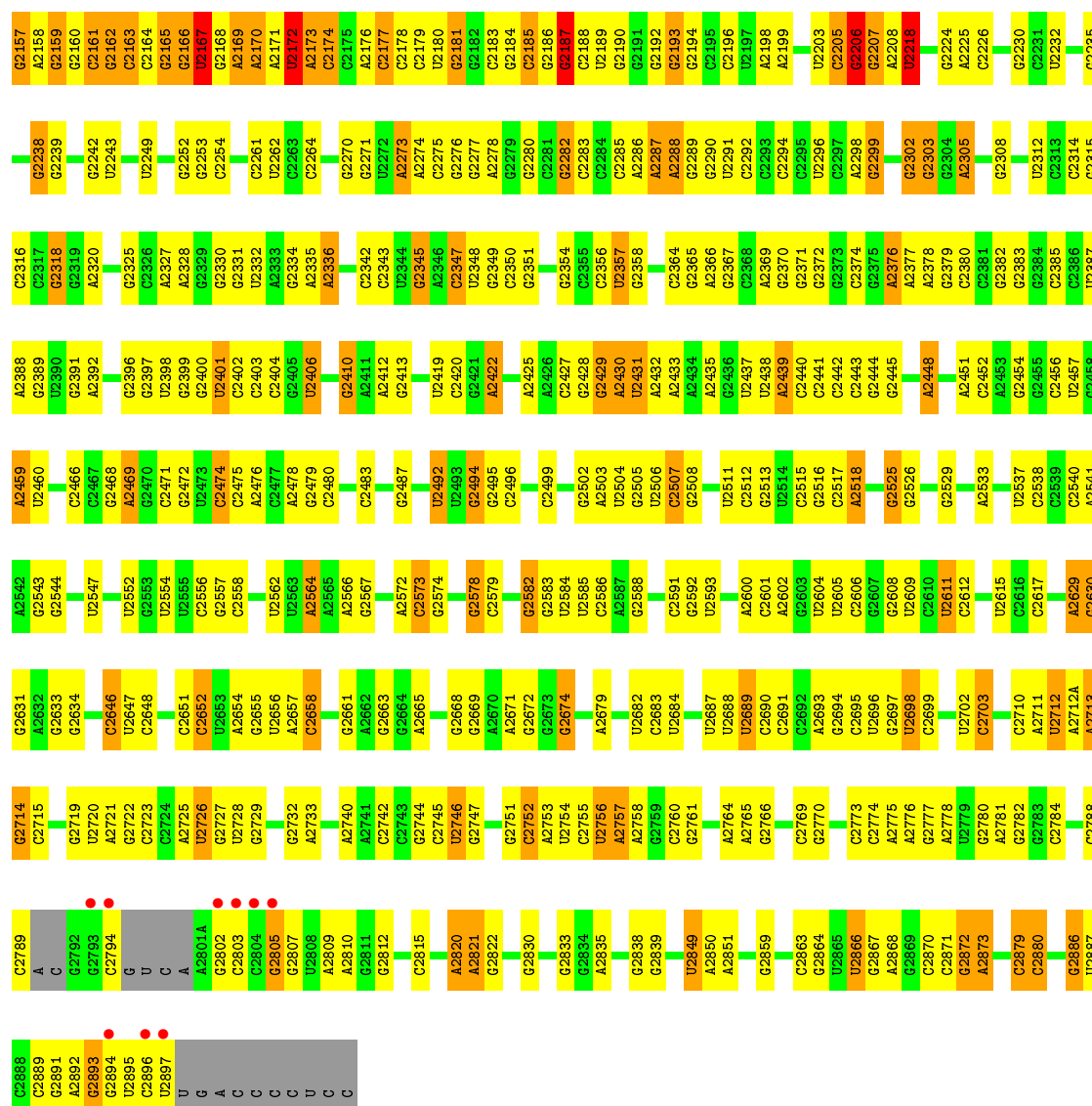


WORLDWIDE
PDB
PROTEIN DATA BANK

- Molecule 25: 23S Ribosomal RNA

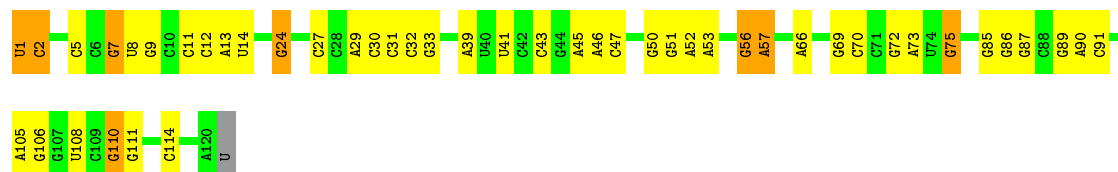


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A2019	A2019	C1914	G1801	G1623	C1550	G1479	A1395	C1221A	U1142	A	U1014	A941
C2021	C2021	U1915	A1802	G1624	C1551	G1480	G1395	C1224	A1142A	U	U1015	A945
U2022	U2022	A1916	A1803	C1625	A1554	U1481	U1405	G1225	G1144	C	G1016	A945
G2023	G2023	U1917	C1806	G1626	A1554	U1482	U1406	A1226	C1145	U	G1017	G947
							C1407	G1227	C1146	U	U1018	G947
							C1408	G1228		U	U1019	G948
							C1409	G1229	G1149	A	A1020	G952
							G1410	C1230	A1143	A	U1021	A953
							C1411	G1231	G1151	A	G1022	G954
							A1412	G1232	G1152	G	U1023	G955
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							G1416	U1234	G1154	G	G1025	G957
							C1417	G1235	A1155	U	U1026	A957
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							U1420	G1239	G1160	C	A1028	A959
							G1421	U1240	G1161	C	A1029	A960
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							G1426	G1243	G1164	A	A1032	U963
							A1427	G1245	U1165	U	G1033	
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							G1429	G1248	U1168	C	G974	G974
							U1430	U1249	G1169	U	C1038	C975
							U1431	G1250	G1170	C	G1039	
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							G1437	A1263	U	U	A980	A980
							G1443	G1261	A	G		A983
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							C1463	C1270	G1193	U		C995
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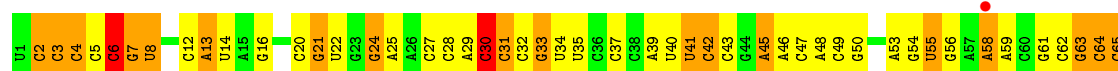
• Molecule 26: 5S Ribosomal RNA

Chain BB: 60% 32% 7% .



• Molecule 26: 5S Ribosomal RNA

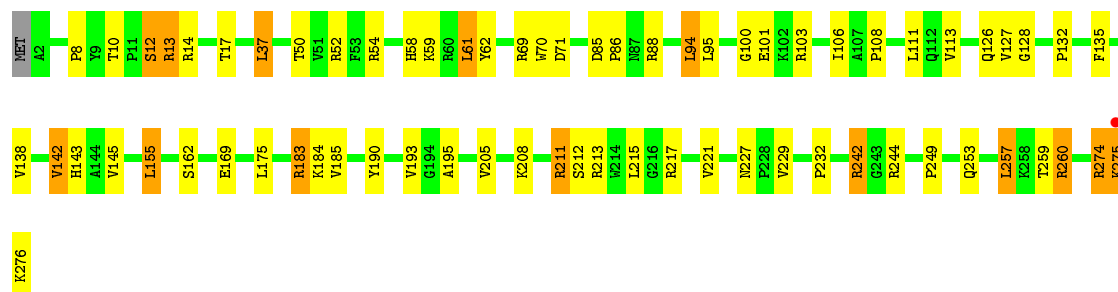
Chain DB: 29% 48% 21% . .





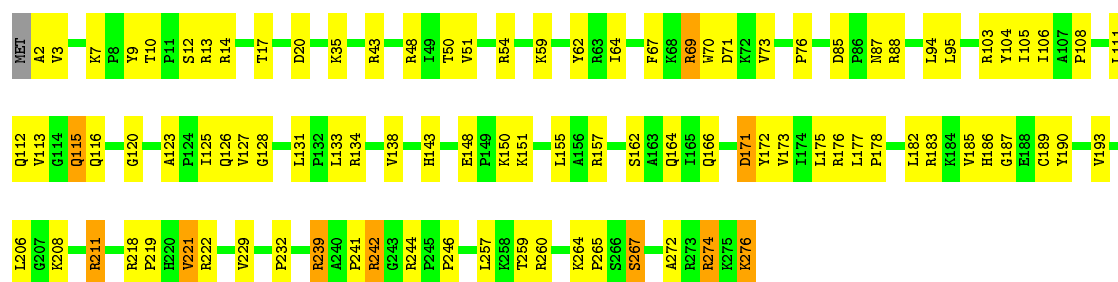
• Molecule 27: 50S ribosomal protein L2

Chain BD: 75% 20% 5%



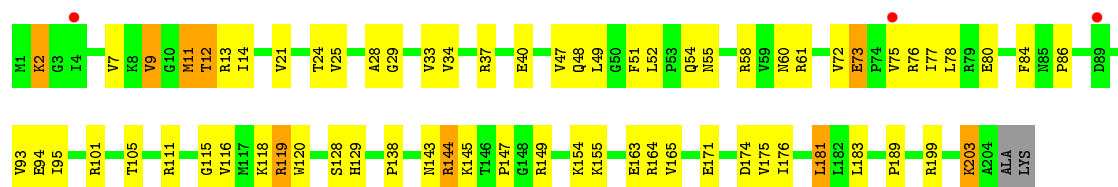
• Molecule 27: 50S ribosomal protein L2

Chain DD: 64% 32% .



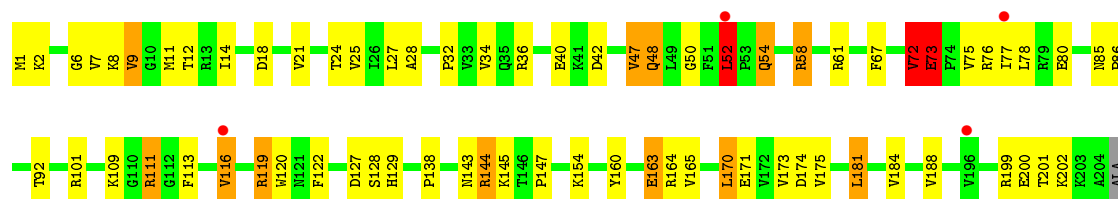
• Molecule 28: 50S ribosomal protein L3

Chain BE: 66% 29% . .



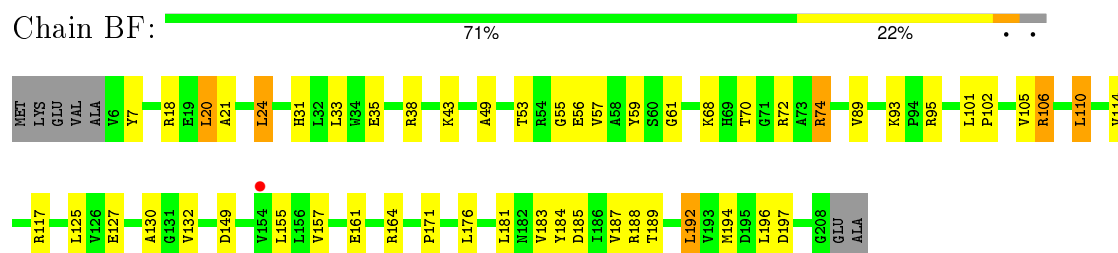
• Molecule 28: 50S ribosomal protein L3

Chain DE: 65% 27% 6% . .

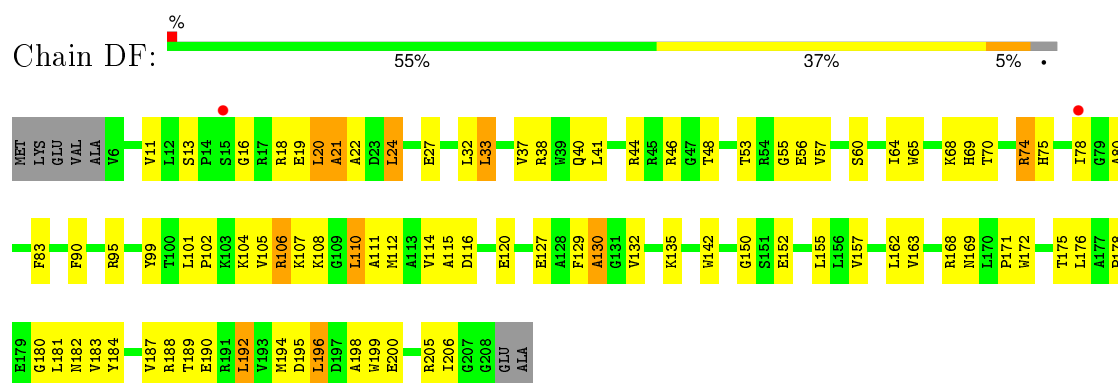


LYS

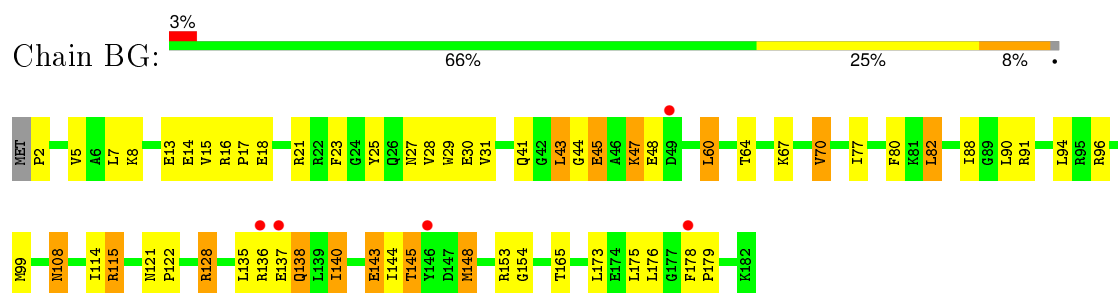
- Molecule 29: 50S ribosomal protein L4



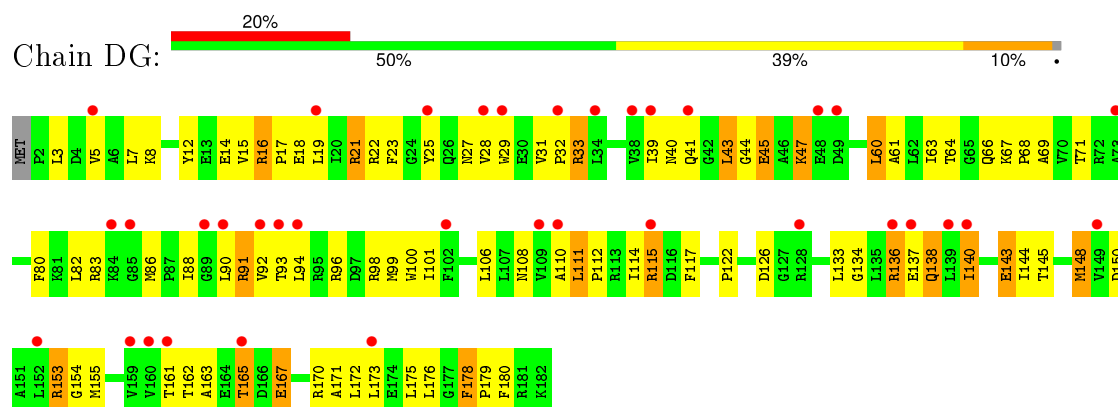
- Molecule 29: 50S ribosomal protein L4



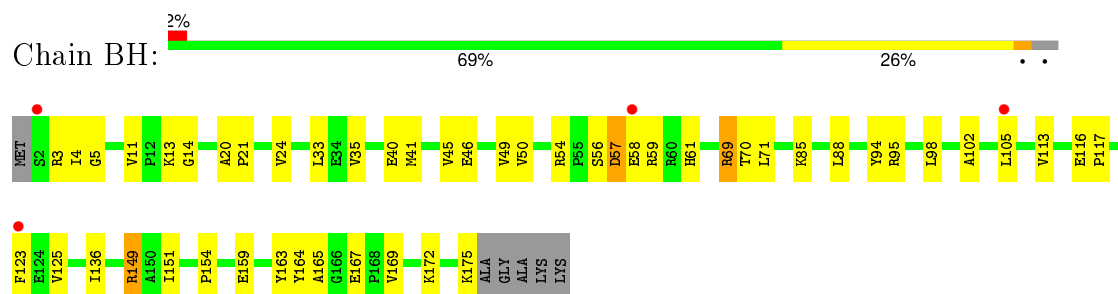
- Molecule 30: 50S ribosomal protein L5



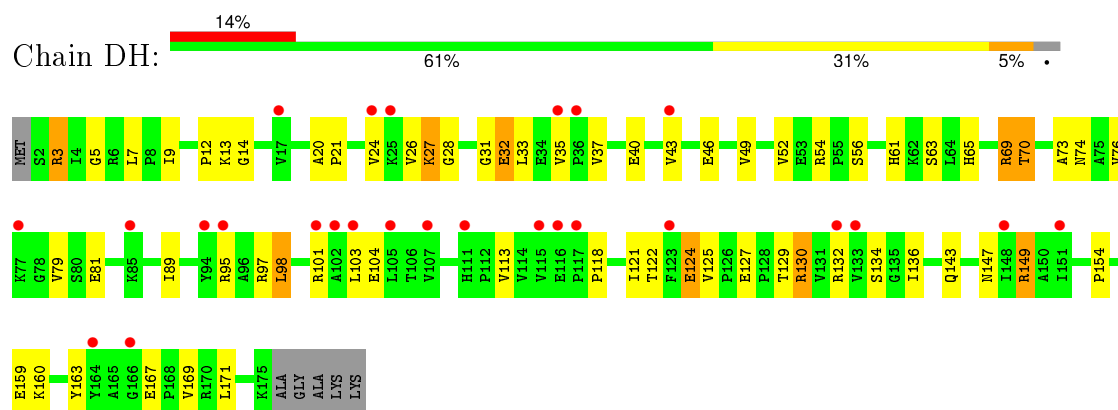
- Molecule 30: 50S ribosomal protein L5



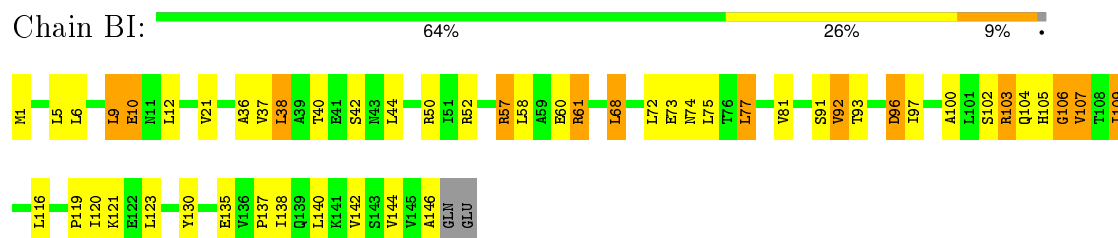
- Molecule 31: 50S ribosomal protein L6



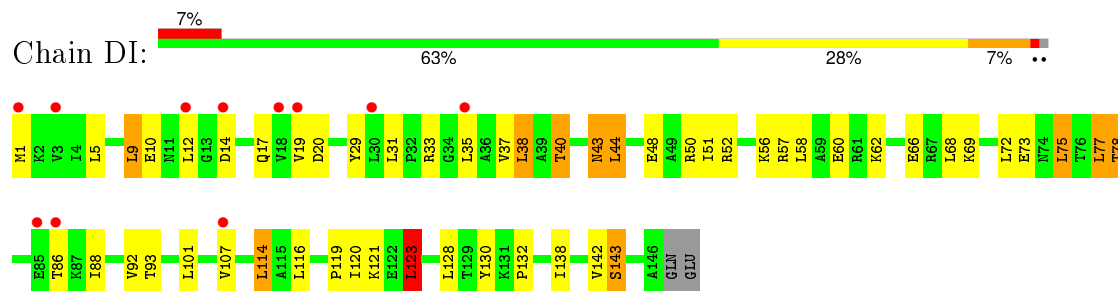
- Molecule 31: 50S ribosomal protein L6



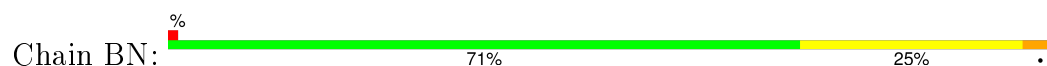
- Molecule 32: 50S ribosomal protein L9

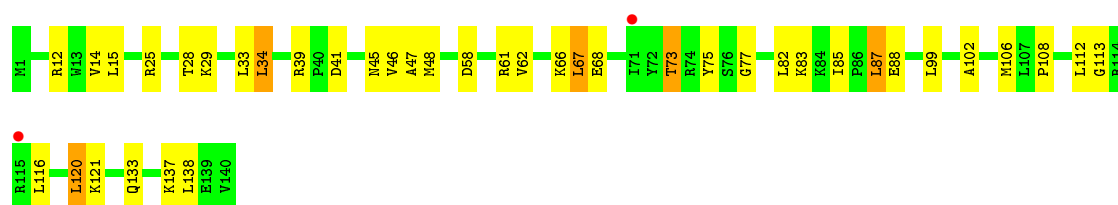


- Molecule 32: 50S ribosomal protein L9

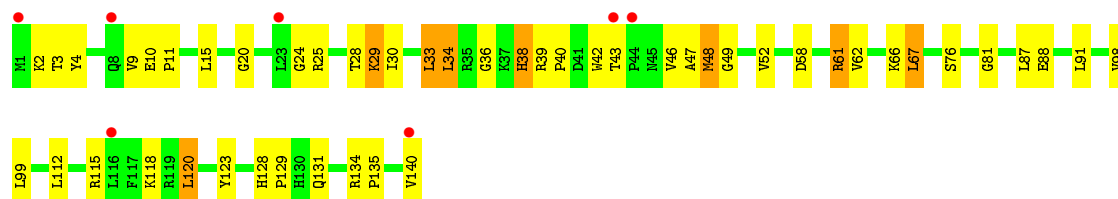


- Molecule 33: 50S ribosomal protein L13

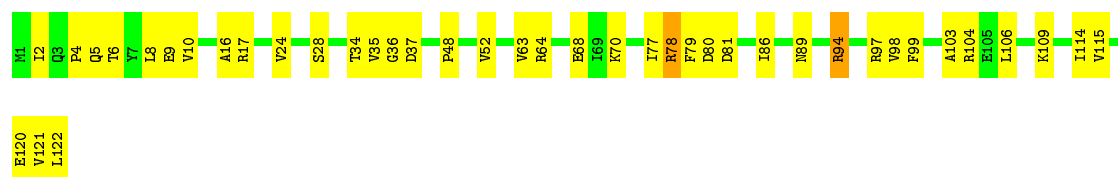




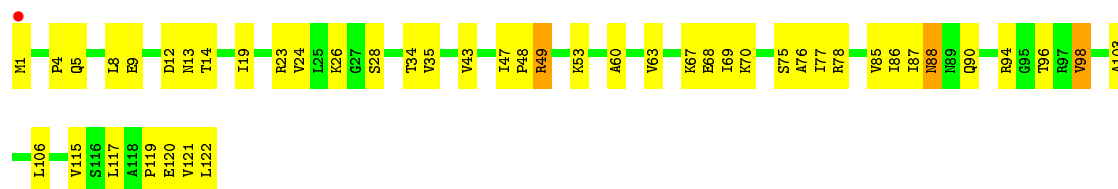
- Molecule 33: 50S ribosomal protein L13



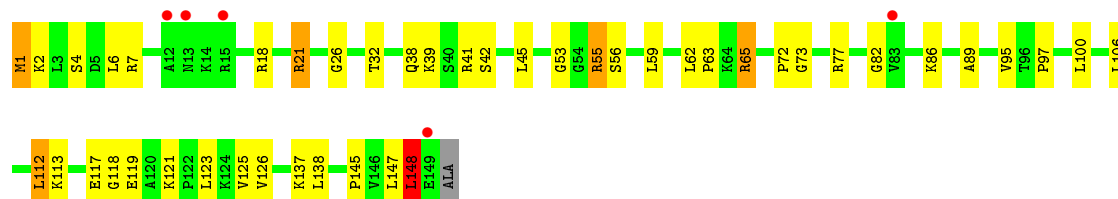
- Molecule 34: 50S ribosomal protein L14



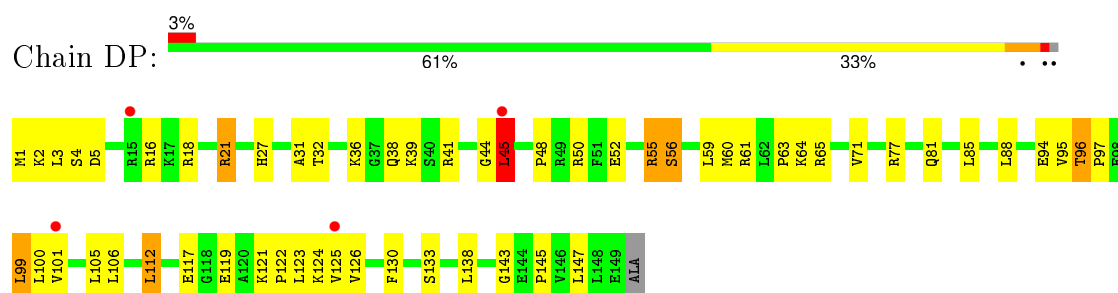
- Molecule 34: 50S ribosomal protein L14



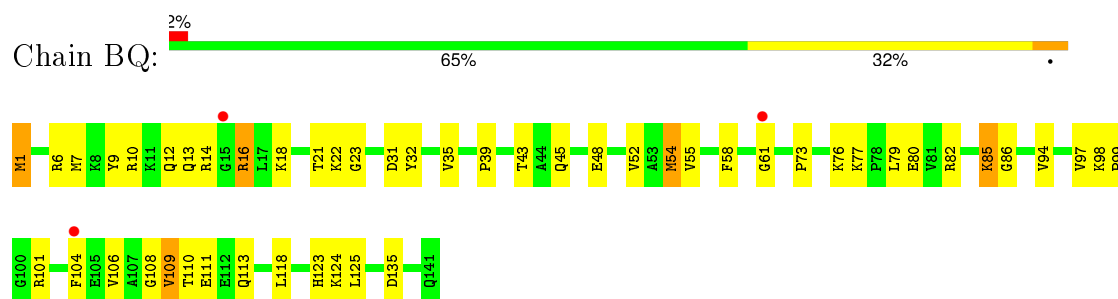
- Molecule 35: 50S ribosomal protein L15



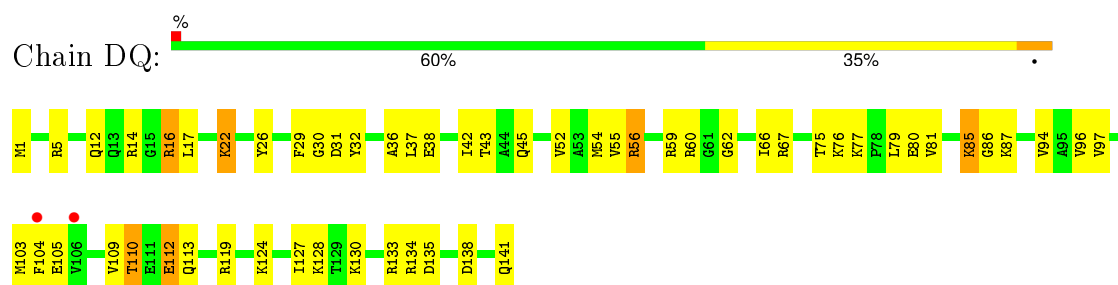
- Molecule 35: 50S ribosomal protein L15



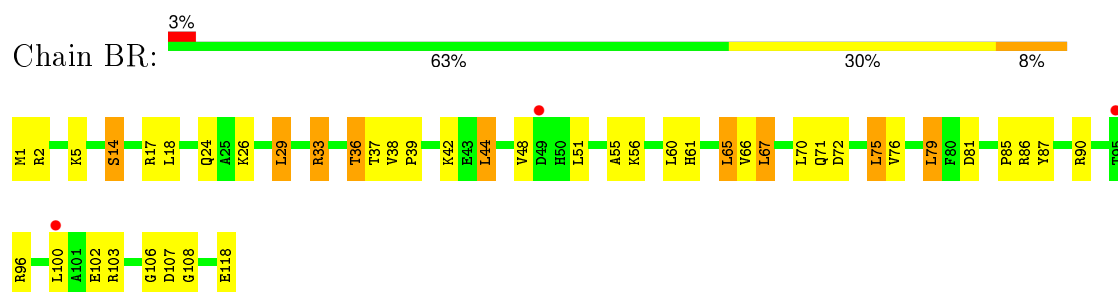
- Molecule 36: 50S ribosomal protein L16



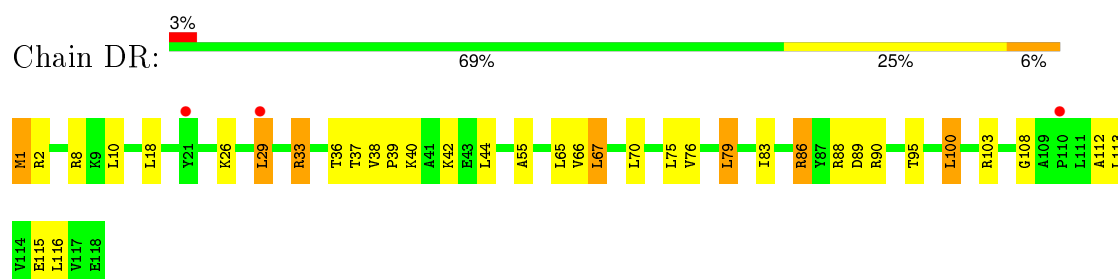
- Molecule 36: 50S ribosomal protein L16



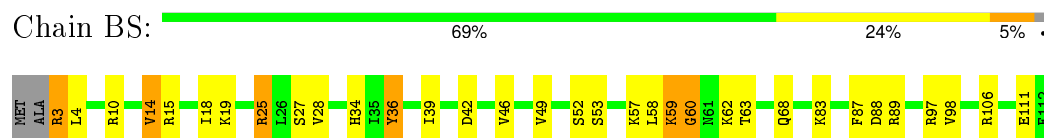
- Molecule 37: 50S ribosomal protein L17



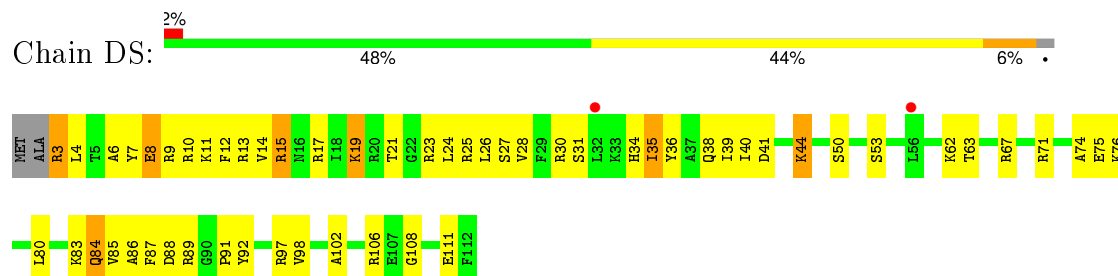
- Molecule 37: 50S ribosomal protein L17



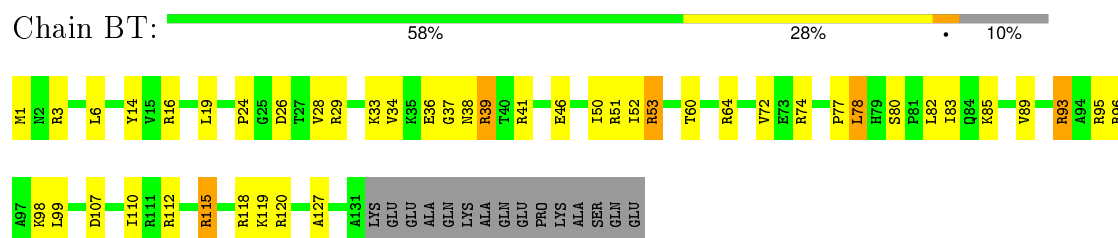
- Molecule 38: 50S ribosomal protein L18



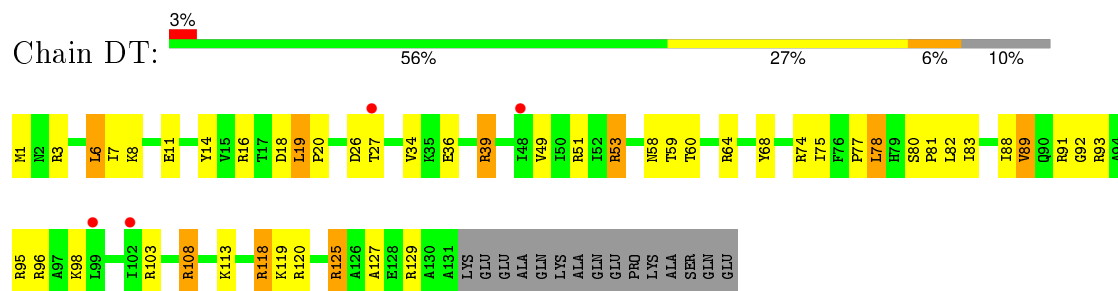
- Molecule 38: 50S ribosomal protein L18



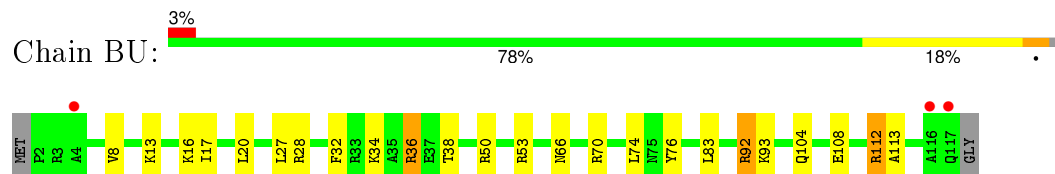
- Molecule 39: 50S ribosomal protein L19



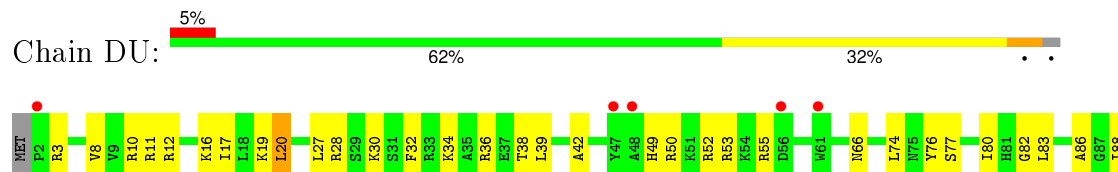
- Molecule 39: 50S ribosomal protein L19



- Molecule 40: 50S ribosomal protein L20

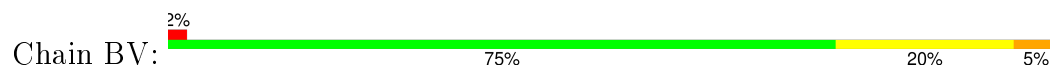


- Molecule 40: 50S ribosomal protein L20

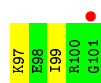




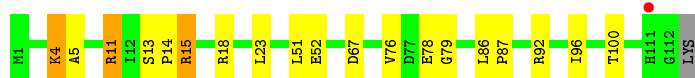
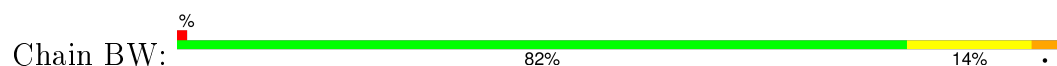
- Molecule 41: 50S ribosomal protein L21



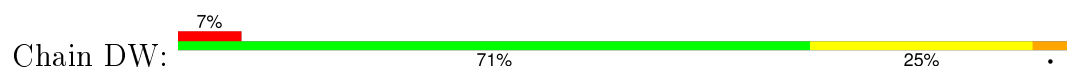
- Molecule 41: 50S ribosomal protein L21



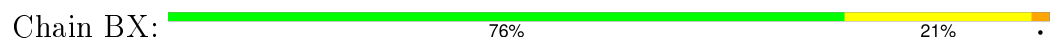
- Molecule 42: 50S ribosomal protein L22



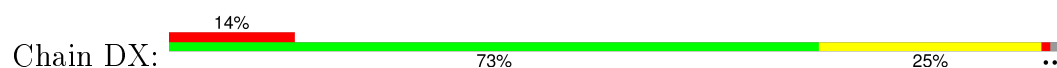
- Molecule 42: 50S ribosomal protein L22

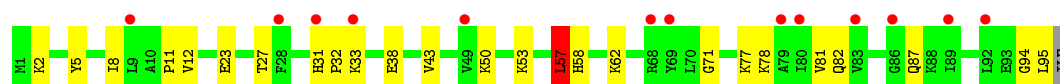


- Molecule 43: 50S ribosomal protein L23

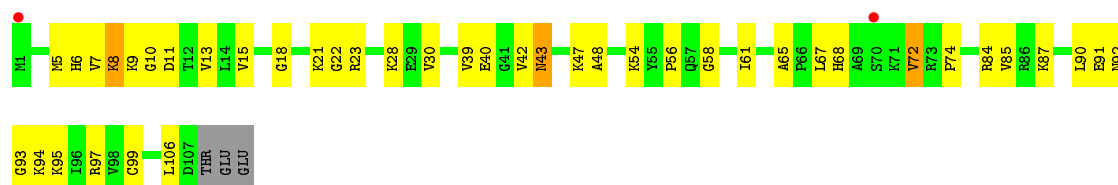


- Molecule 43: 50S ribosomal protein L23

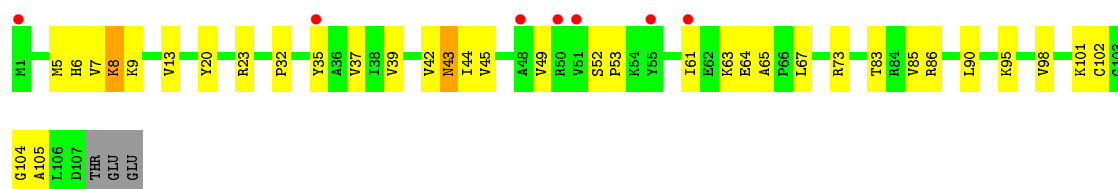




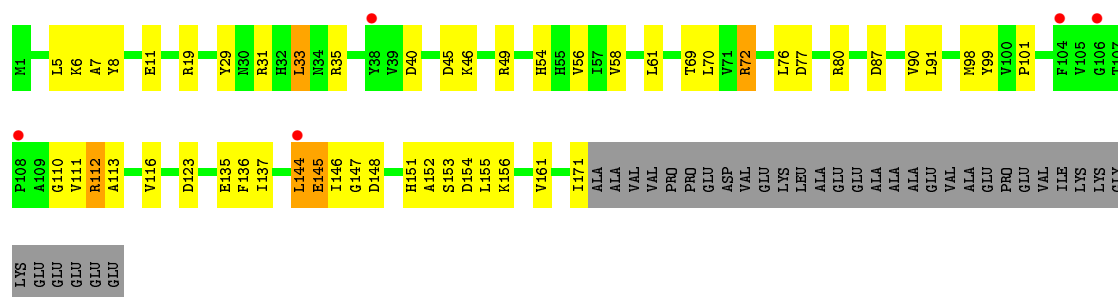
- Molecule 44: 50S ribosomal protein L24



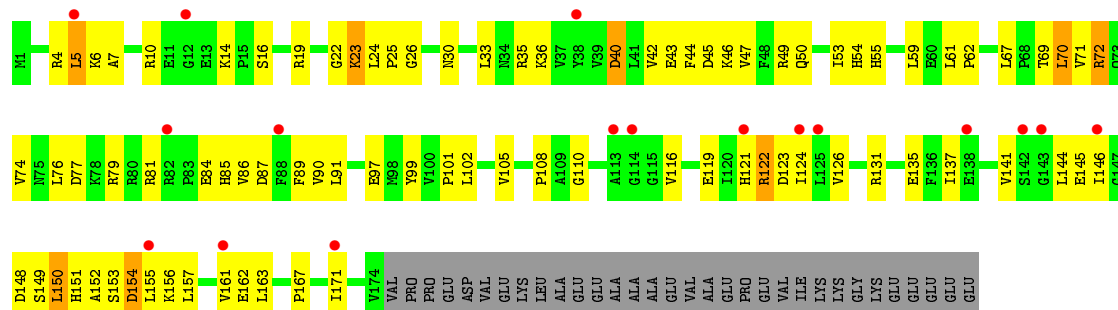
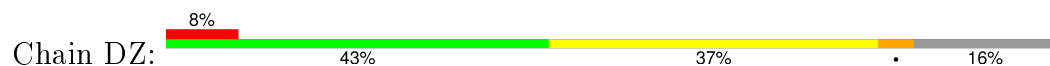
- Molecule 44: 50S ribosomal protein L24



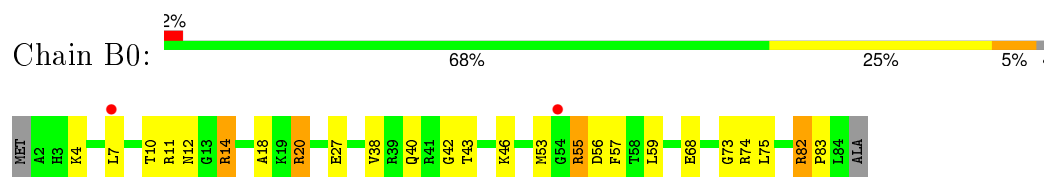
- Molecule 45: 50S ribosomal protein L25



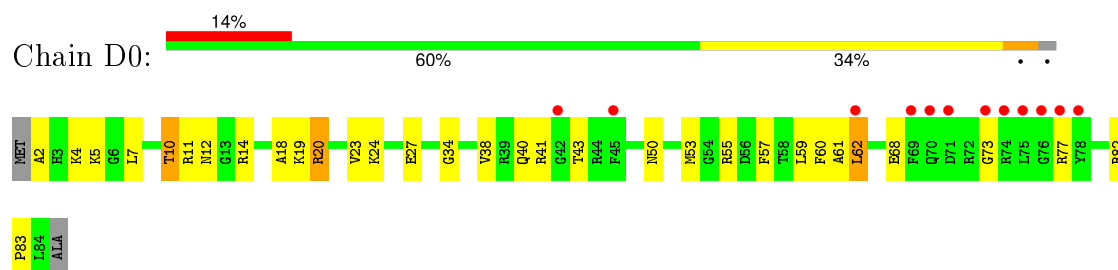
- Molecule 45: 50S ribosomal protein L25



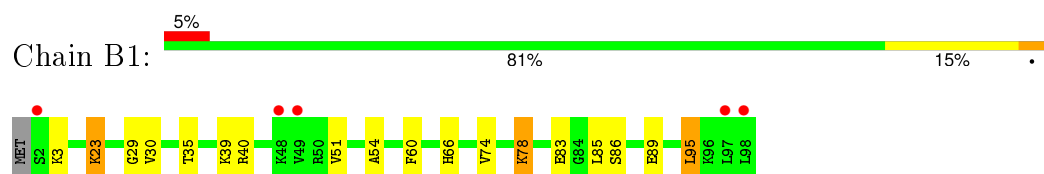
- Molecule 46: 50S ribosomal protein L27



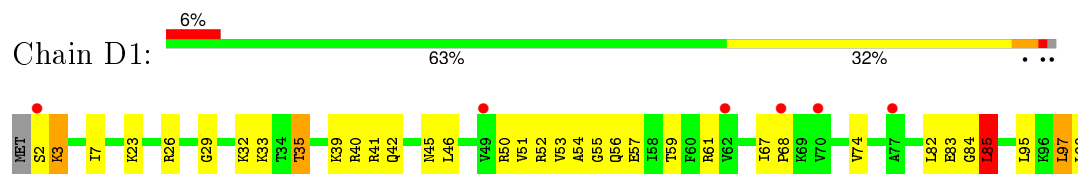
- Molecule 46: 50S ribosomal protein L27



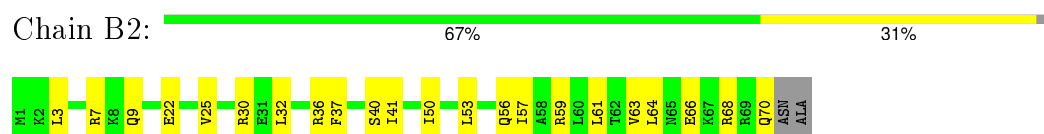
- Molecule 47: 50S ribosomal protein L28



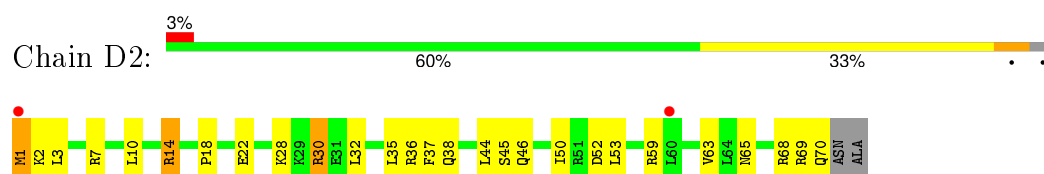
- Molecule 47: 50S ribosomal protein L28



- Molecule 48: 50S ribosomal protein L29

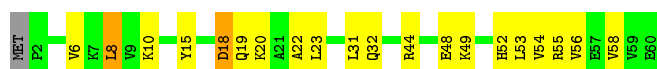


- Molecule 48: 50S ribosomal protein L29

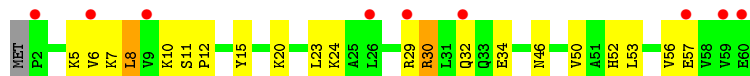


- Molecule 49: 50S ribosomal protein L30

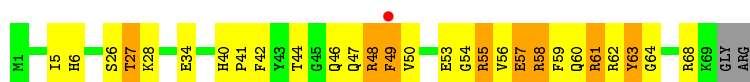




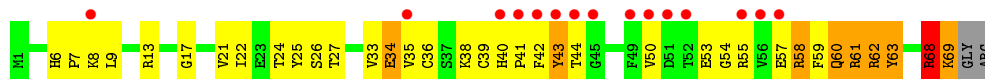
- Molecule 49: 50S ribosomal protein L30



- Molecule 50: 50S ribosomal protein L31



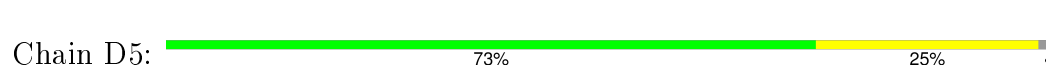
- Molecule 50: 50S ribosomal protein L31



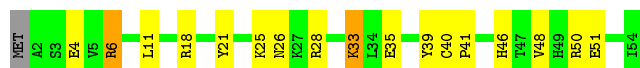
- Molecule 51: 50S ribosomal protein L32



- Molecule 51: 50S ribosomal protein L32

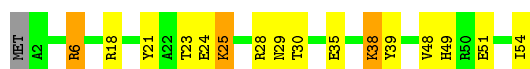


- Molecule 52: 50S ribosomal protein L33

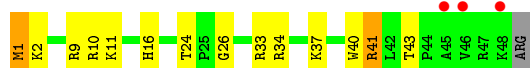


- Molecule 52: 50S ribosomal protein L33





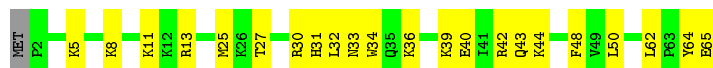
- Molecule 53: 50S ribosomal protein L34



- Molecule 53: 50S ribosomal protein L34



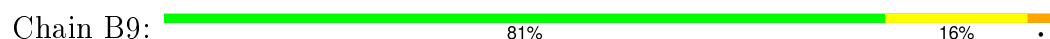
- Molecule 54: 50S ribosomal protein L35



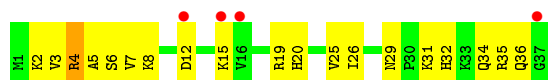
- Molecule 54: 50S ribosomal protein L35



- Molecule 55: 50S ribosomal protein L36



- Molecule 55: 50S ribosomal protein L36



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	209.25Å 448.46Å 618.08Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	362.98 – 2.90 362.98 – 2.90	Depositor EDS
% Data completeness (in resolution range)	96.9 (362.98-2.90) 96.9 (362.98-2.90)	Depositor EDS
R_{merge}	0.18	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.31 (at 2.91Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.2_1309)	Depositor
R, R_{free}	0.231 , 0.286 0.234 , 0.287	Depositor DCC
R_{free} test set	61606 reflections (5.28%)	DCC
Wilson B-factor (Å ²)	54.8	Xtriage
Anisotropy	0.140	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 72.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.37$, $\langle L^2 \rangle = 0.19$	Xtriage
Outliers	0 of 1229139 reflections	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	289646	wwPDB-VP
Average B, all atoms (Å ²)	61.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.87% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	AA	0.39	0/36049	0.94	50/56261 (0.1%)
1	CA	0.41	6/36170 (0.0%)	1.02	84/56452 (0.1%)
2	AB	0.31	0/1881	0.63	0/2542
2	CB	0.32	0/1860	0.65	3/2518 (0.1%)
3	AC	0.30	0/1576	0.51	0/2130
3	CC	0.31	0/1566	0.61	2/2119 (0.1%)
4	AD	0.31	0/1689	0.59	1/2267 (0.0%)
4	CD	0.30	0/1700	0.54	0/2280
5	AE	0.29	0/1145	0.56	0/1543
5	CE	0.32	0/1149	0.59	0/1548
6	AF	0.30	0/819	0.51	0/1111
6	CF	0.30	0/829	0.50	0/1123
7	AG	0.28	0/1250	0.51	0/1679
7	CG	0.30	0/1254	0.54	0/1683
8	AH	0.29	0/1108	0.51	0/1494
8	CH	0.28	0/1108	0.55	0/1494
9	AI	0.31	0/1002	0.59	0/1346
9	CI	0.32	0/997	0.56	0/1343
10	AJ	0.28	0/722	0.57	0/982
10	CJ	0.30	0/727	0.56	0/988
11	AK	0.28	0/844	0.51	0/1145
11	CK	0.29	0/848	0.51	0/1149
12	AL	0.31	0/946	0.51	0/1274
12	CL	0.31	0/946	0.57	0/1274
13	AM	0.28	0/969	0.63	0/1302
13	CM	0.32	0/961	0.61	0/1291
14	AN	0.32	0/501	0.54	0/664
14	CN	0.31	0/501	0.60	0/664
15	AO	0.29	0/739	0.50	0/985
15	CO	0.28	0/739	0.52	0/985
16	AP	0.30	0/697	0.54	0/939
16	CP	0.29	0/693	0.52	0/935

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	AQ	0.30	0/836	0.54	0/1117
17	CQ	0.29	0/836	0.52	0/1117
18	AR	0.29	0/560	0.54	0/746
18	CR	0.29	0/560	0.57	1/746 (0.1%)
19	AS	0.28	0/667	0.53	0/900
19	CS	0.32	0/661	0.67	0/893
20	AT	0.31	0/730	0.60	0/965
20	CT	0.29	0/729	0.63	1/965 (0.1%)
21	AU	0.28	0/203	0.49	0/266
21	CU	0.33	0/203	0.47	0/266
22	AV	0.42	0/310	0.95	0/480
22	CV	0.45	0/282	0.97	0/437
23	AW	0.35	0/18	0.66	0/26
23	CW	0.27	0/18	0.91	0/26
24	AX	0.52	0/1700	1.21	18/2650 (0.7%)
24	CX	0.55	3/1700 (0.2%)	1.24	16/2650 (0.6%)
25	BA	0.48	1/68013 (0.0%)	0.94	53/106165 (0.0%)
25	DA	0.42	0/67542	0.95	80/105428 (0.1%)
26	BB	0.42	0/2878	0.93	0/4490
26	DB	0.45	0/2878	1.00	3/4490 (0.1%)
27	BD	0.37	0/2186	0.57	0/2944
27	DD	0.33	0/2186	0.56	0/2944
28	BE	0.35	0/1592	0.55	0/2149
28	DE	0.33	0/1592	0.58	1/2149 (0.0%)
29	BF	0.34	0/1619	0.54	0/2193
29	DF	0.32	0/1615	0.57	0/2188
30	BG	0.30	0/1450	0.57	0/1959
30	DG	0.35	0/1449	0.61	0/1958
31	BH	0.32	0/1356	0.53	0/1834
31	DH	0.29	0/1356	0.55	0/1834
32	BI	0.29	0/1100	0.58	0/1501
32	DI	0.30	0/1076	0.60	1/1471 (0.1%)
33	BN	0.32	0/1144	0.52	0/1543
33	DN	0.31	0/1144	0.54	0/1543
34	BO	0.37	0/943	0.59	0/1269
34	DO	0.33	0/943	0.55	0/1269
35	BP	0.34	0/1152	0.58	1/1533 (0.1%)
35	DP	0.32	0/1152	0.60	0/1533
36	BQ	0.35	0/1143	0.53	0/1527
36	DQ	0.33	0/1143	0.55	0/1527
37	BR	0.34	0/982	0.55	0/1312
37	DR	0.30	0/982	0.53	0/1312
38	BS	0.33	0/887	0.56	0/1180

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
38	DS	0.30	0/880	0.59	0/1172
39	BT	0.33	0/1105	0.56	0/1477
39	DT	0.30	0/1097	0.54	0/1468
40	BU	0.36	0/977	0.53	0/1301
40	DU	0.31	0/977	0.55	0/1301
41	BV	0.36	0/782	0.54	0/1049
41	DV	0.32	0/782	0.57	0/1049
42	BW	0.35	0/897	0.54	0/1205
42	DW	0.31	0/897	0.52	0/1205
43	BX	0.38	0/764	0.58	1/1025 (0.1%)
43	DX	0.32	0/764	0.56	1/1025 (0.1%)
44	BY	0.35	0/819	0.56	0/1095
44	DY	0.31	0/819	0.56	0/1095
45	BZ	0.33	0/1379	0.61	0/1873
45	DZ	0.30	0/1390	0.55	0/1890
46	B0	0.35	0/662	0.59	0/881
46	D0	0.31	0/662	0.50	0/881
47	B1	0.34	0/762	0.56	0/1014
47	D1	0.33	0/762	0.57	1/1014 (0.1%)
48	B2	0.32	0/590	0.57	0/781
48	D2	0.30	0/590	0.49	0/781
49	B3	0.35	0/474	0.55	0/635
49	D3	0.30	0/469	0.53	0/630
50	B4	0.36	0/565	0.71	0/761
50	D4	0.35	0/545	0.69	0/737
51	B5	0.33	0/469	0.55	0/635
51	D5	0.32	0/469	0.54	0/635
52	B6	0.39	0/460	0.53	0/613
52	D6	0.33	0/456	0.53	0/608
53	B7	0.37	0/426	0.56	0/561
53	D7	0.34	0/426	0.48	0/561
54	B8	0.37	0/519	0.55	0/684
54	D8	0.31	0/525	0.52	0/691
55	B9	0.35	0/310	0.50	0/407
55	D9	0.34	0/310	0.54	0/407
All	All	0.40	10/310281 (0.0%)	0.87	318/464152 (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
7	AG	0	1
20	CT	0	1
27	BD	0	1
38	BS	0	1
All	All	0	6

The worst 5 of 10 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	CA	1154	G	C6-N1	-12.01	1.31	1.39
1	CA	1154	G	N1-C2	-11.43	1.28	1.37
1	CA	1119	C	N3-C4	-10.12	1.26	1.33
1	CA	1154	G	N7-C5	-6.67	1.35	1.39
24	CX	14	A	N7-C5	-5.86	1.35	1.39

The worst 5 of 318 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	CA	1119	C	N1-C2-O2	29.84	136.81	118.90
1	CA	1154	G	C5-C6-O6	27.03	144.82	128.60
1	CA	1154	G	N3-C2-N2	25.60	137.82	119.90
1	CA	1154	G	N1-C2-N2	-23.27	95.25	116.20
1	CA	1119	C	C2-N3-C4	19.75	129.77	119.90

There are no chirality outliers.

5 of 6 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	AB	231	GLU	Peptide
2	AB	9	GLU	Peptide
7	AG	79	ARG	Peptide
27	BD	274	ARG	Peptide
38	BS	58	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	32205	0	16254	640	0
1	CA	32312	0	16307	729	0
2	AB	1846	0	1867	85	0
2	CB	1825	0	1828	97	0
3	AC	1552	0	1546	67	0
3	CC	1542	0	1517	73	0
4	AD	1659	0	1676	65	0
4	CD	1670	0	1703	68	0
5	AE	1129	0	1185	30	0
5	CE	1133	0	1191	53	0
6	AF	806	0	793	28	0
6	CF	816	0	808	22	0
7	AG	1231	0	1238	28	0
7	CG	1235	0	1249	30	0
8	AH	1088	0	1126	25	0
8	CH	1088	0	1126	38	0
9	AI	983	0	986	53	0
9	CI	978	0	966	55	0
10	AJ	709	0	650	34	0
10	CJ	714	0	672	35	0
11	AK	829	0	825	18	0
11	CK	833	0	836	23	0
12	AL	930	0	979	31	0
12	CL	930	0	980	33	0
13	AM	958	0	1002	39	0
13	CM	950	0	988	56	0
14	AN	492	0	529	25	0
14	CN	492	0	529	36	0
15	AO	728	0	760	22	0
15	CO	728	0	760	30	0
16	AP	681	0	697	31	0
16	CP	677	0	686	26	0
17	AQ	823	0	891	24	0
17	CQ	823	0	891	21	0
18	AR	555	0	618	13	0
18	CR	555	0	618	21	0
19	AS	652	0	662	28	0
19	CS	646	0	644	52	0
20	AT	728	0	798	26	0
20	CT	727	0	796	28	0
21	AU	199	0	208	8	0
21	CU	199	0	208	12	0
22	AV	277	0	140	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
22	CV	252	0	130	8	0
23	AW	54	0	40	5	0
23	CW	54	0	40	7	0
24	AX	1635	0	838	34	0
24	CX	1635	0	838	40	0
25	BA	60729	0	30621	812	0
25	DA	60311	0	30408	1066	0
26	BB	2573	0	1306	29	0
26	DB	2573	0	1306	91	0
27	BD	2136	0	2218	58	0
27	DD	2136	0	2217	68	0
28	BE	1559	0	1618	52	0
28	DE	1559	0	1618	56	0
29	BF	1584	0	1625	36	0
29	DF	1580	0	1619	68	0
30	BG	1425	0	1443	45	0
30	DG	1424	0	1434	77	0
31	BH	1330	0	1407	29	0
31	DH	1330	0	1407	42	0
32	BI	1085	0	1114	39	0
32	DI	1061	0	1080	34	0
33	BN	1117	0	1184	24	0
33	DN	1117	0	1184	33	0
34	BO	933	0	996	26	0
34	DO	933	0	996	34	0
35	BP	1135	0	1212	34	0
35	DP	1135	0	1211	50	0
36	BQ	1122	0	1179	35	0
36	DQ	1122	0	1179	43	0
37	BR	968	0	1033	28	0
37	DR	968	0	1033	27	0
38	BS	877	0	938	22	0
38	DS	870	0	923	53	0
39	BT	1091	0	1151	30	0
39	DT	1083	0	1136	37	0
40	BU	959	0	1019	18	0
40	DU	959	0	1019	33	0
41	BV	771	0	830	14	0
41	DV	771	0	830	26	0
42	BW	886	0	940	9	0
42	DW	886	0	940	18	0
43	BX	750	0	814	13	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
43	DX	750	0	814	17	0
44	BY	806	0	881	31	0
44	DY	806	0	881	26	0
45	BZ	1349	0	1355	30	0
45	DZ	1360	0	1363	64	0
46	B0	653	0	674	26	0
46	D0	653	0	674	25	0
47	B1	755	0	826	12	0
47	D1	755	0	826	26	0
48	B2	588	0	643	12	0
48	D2	588	0	643	17	0
49	B3	469	0	518	9	0
49	D3	464	0	514	17	0
50	B4	552	0	533	25	0
50	D4	532	0	503	30	0
51	B5	455	0	465	12	0
51	D5	455	0	465	13	0
52	B6	453	0	473	9	0
52	D6	449	0	469	13	0
53	B7	418	0	467	13	0
53	D7	418	0	467	14	0
54	B8	511	0	571	18	0
54	D8	517	0	582	33	0
55	B9	307	0	335	4	0
55	D9	307	0	335	13	0
56	AA	187	0	0	0	0
56	AD	1	0	0	0	0
56	AE	2	0	0	0	0
56	AF	1	0	0	0	0
56	AK	1	0	0	0	0
56	AL	1	0	0	0	0
56	AM	1	0	0	0	0
56	AN	1	0	0	0	0
56	AX	7	0	0	0	0
56	B0	5	0	0	0	0
56	B3	2	0	0	0	0
56	B4	1	0	0	0	0
56	B5	2	0	0	0	0
56	B7	4	0	0	0	0
56	B8	1	0	0	0	0
56	B9	1	0	0	0	0
56	BA	675	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
56	BB	18	0	0	0	0
56	BD	8	0	0	0	0
56	BE	6	0	0	0	0
56	BF	5	0	0	0	0
56	BG	3	0	0	0	0
56	BH	1	0	0	0	0
56	BN	2	0	0	0	0
56	BO	1	0	0	0	0
56	BP	4	0	0	0	0
56	BQ	3	0	0	0	0
56	BR	3	0	0	0	0
56	BU	5	0	0	0	0
56	BV	3	0	0	0	0
56	BW	4	0	0	0	0
56	BX	3	0	0	0	0
56	BY	2	0	0	0	0
56	BZ	1	0	0	0	0
56	CA	154	0	0	0	0
56	CE	2	0	0	0	0
56	CF	1	0	0	0	0
56	CJ	1	0	0	0	0
56	CK	1	0	0	0	0
56	CT	1	0	0	0	0
56	CX	1	0	0	0	0
56	D0	1	0	0	0	0
56	D3	1	0	0	0	0
56	D5	1	0	0	0	0
56	D7	1	0	0	0	0
56	D8	2	0	0	0	0
56	DA	595	0	0	0	0
56	DB	12	0	0	0	0
56	DD	2	0	0	0	0
56	DE	5	0	0	0	0
56	DF	3	0	0	0	0
56	DG	1	0	0	0	0
56	DN	1	0	0	0	0
56	DP	1	0	0	0	0
56	DQ	3	0	0	0	0
56	DR	2	0	0	0	0
56	DT	1	0	0	0	0
56	DU	1	0	0	0	0
56	DV	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
56	DW	2	0	0	0	0
56	DY	1	0	0	0	0
57	AD	8	0	0	0	0
57	CD	8	0	0	0	0
58	AN	1	0	0	0	0
58	B4	1	0	0	0	0
58	B5	1	0	0	0	0
58	B6	1	0	0	0	0
58	B9	1	0	0	0	0
58	BY	1	0	0	0	0
58	CN	1	0	0	0	0
58	D4	1	0	0	0	0
58	D5	1	0	0	0	0
58	D6	1	0	0	0	0
58	D9	1	0	0	0	0
58	DY	1	0	0	0	0
59	AX	1	0	0	0	0
59	DA	1	0	0	0	0
60	AA	165	0	0	12	0
60	AJ	1	0	0	0	0
60	AL	3	0	0	2	0
60	AP	1	0	0	0	0
60	AU	1	0	0	0	0
60	AV	2	0	0	0	0
60	AW	3	0	0	0	0
60	B0	4	0	0	0	0
60	B1	2	0	0	0	0
60	B2	1	0	0	0	0
60	B3	1	0	0	0	0
60	B5	2	0	0	0	0
60	B7	2	0	0	1	0
60	B8	8	0	0	2	0
60	BA	924	0	0	62	0
60	BB	27	0	0	0	0
60	BD	6	0	0	2	0
60	BE	8	0	0	0	0
60	BF	6	0	0	1	0
60	BG	1	0	0	0	0
60	BH	1	0	0	1	0
60	BN	3	0	0	0	0
60	BO	1	0	0	0	0
60	BP	14	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
60	BQ	2	0	0	0	0
60	BS	1	0	0	0	0
60	BT	4	0	0	1	0
60	BU	2	0	0	0	0
60	BV	5	0	0	0	0
60	BW	1	0	0	0	0
60	BX	2	0	0	0	0
60	BZ	1	0	0	0	0
60	CA	113	0	0	5	0
60	CE	2	0	0	0	0
60	CJ	2	0	0	1	0
60	CL	1	0	0	1	0
60	CO	1	0	0	0	0
60	CW	1	0	0	1	0
60	CX	1	0	0	1	0
60	D0	5	0	0	0	0
60	D1	1	0	0	0	0
60	D3	1	0	0	3	0
60	D8	3	0	0	0	0
60	DA	689	0	0	58	0
60	DB	9	0	0	0	0
60	DD	11	0	0	2	0
60	DE	5	0	0	1	0
60	DF	6	0	0	0	0
60	DO	1	0	0	0	0
60	DP	6	0	0	0	0
60	DU	3	0	0	0	0
60	DV	1	0	0	0	0
60	DW	1	0	0	0	0
60	DX	3	0	0	0	0
All	All	289646	0	193084	5717	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 13.

The worst 5 of 5717 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)
25:DA:2121:G:H1	25:DA:2177:C:N4	1.35	1.23
19:CS:42:PRO:HG3	50:D4:61:ARG:HG2	1.39	1.04
1:AA:1028:C:N4	1:AA:1033:G:H1	1.56	1.01

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:DA:2128:C:H42	25:DA:2160:G:H1	1.08	1.00
25:DA:2137:C:H42	25:DA:2154:G:H1	1.05	0.99

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%)	18 (8%)	3 (1%)	15	46
2	CB	229/256 (90%)	206 (90%)	17 (7%)	6 (3%)	7	26
3	AC	204/239 (85%)	193 (95%)	10 (5%)	1 (0%)	34	71
3	CC	204/239 (85%)	187 (92%)	15 (7%)	2 (1%)	19	54
4	AD	206/209 (99%)	195 (95%)	9 (4%)	2 (1%)	19	54
4	CD	206/209 (99%)	194 (94%)	11 (5%)	1 (0%)	34	71
5	AE	146/162 (90%)	140 (96%)	4 (3%)	2 (1%)	14	44
5	CE	146/162 (90%)	142 (97%)	4 (3%)	0	100	100
6	AF	98/101 (97%)	96 (98%)	2 (2%)	0	100	100
6	CF	98/101 (97%)	96 (98%)	2 (2%)	0	100	100
7	AG	153/156 (98%)	148 (97%)	2 (1%)	3 (2%)	9	33
7	CG	153/156 (98%)	151 (99%)	1 (1%)	1 (1%)	26	63
8	AH	135/138 (98%)	133 (98%)	2 (2%)	0	100	100
8	CH	135/138 (98%)	132 (98%)	3 (2%)	0	100	100
9	AI	125/128 (98%)	118 (94%)	7 (6%)	0	100	100
9	CI	125/128 (98%)	120 (96%)	5 (4%)	0	100	100
10	AJ	95/105 (90%)	87 (92%)	7 (7%)	1 (1%)	17	51
10	CJ	94/105 (90%)	87 (93%)	5 (5%)	2 (2%)	9	32

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
11	AK	112/129 (87%)	104 (93%)	5 (4%)	3 (3%)	6	25
11	CK	112/129 (87%)	103 (92%)	7 (6%)	2 (2%)	11	37
12	AL	120/132 (91%)	115 (96%)	5 (4%)	0	100	100
12	CL	120/132 (91%)	113 (94%)	7 (6%)	0	100	100
13	AM	121/126 (96%)	113 (93%)	8 (7%)	0	100	100
13	CM	120/126 (95%)	114 (95%)	5 (4%)	1 (1%)	24	60
14	AN	58/61 (95%)	55 (95%)	3 (5%)	0	100	100
14	CN	58/61 (95%)	55 (95%)	3 (5%)	0	100	100
15	AO	86/89 (97%)	83 (96%)	3 (4%)	0	100	100
15	CO	86/89 (97%)	81 (94%)	5 (6%)	0	100	100
16	AP	80/88 (91%)	77 (96%)	3 (4%)	0	100	100
16	CP	80/88 (91%)	77 (96%)	2 (2%)	1 (1%)	15	46
17	AQ	97/105 (92%)	92 (95%)	4 (4%)	1 (1%)	19	54
17	CQ	97/105 (92%)	94 (97%)	3 (3%)	0	100	100
18	AR	66/88 (75%)	65 (98%)	1 (2%)	0	100	100
18	CR	66/88 (75%)	65 (98%)	1 (2%)	0	100	100
19	AS	81/93 (87%)	76 (94%)	5 (6%)	0	100	100
19	CS	81/93 (87%)	75 (93%)	6 (7%)	0	100	100
20	AT	94/106 (89%)	87 (93%)	6 (6%)	1 (1%)	17	51
20	CT	94/106 (89%)	86 (92%)	5 (5%)	3 (3%)	5	20
21	AU	21/27 (78%)	21 (100%)	0	0	100	100
21	CU	21/27 (78%)	21 (100%)	0	0	100	100
27	BD	273/276 (99%)	263 (96%)	9 (3%)	1 (0%)	39	74
27	DD	273/276 (99%)	262 (96%)	9 (3%)	2 (1%)	26	63
28	BE	202/206 (98%)	195 (96%)	6 (3%)	1 (0%)	34	71
28	DE	202/206 (98%)	193 (96%)	7 (4%)	2 (1%)	19	54
29	BF	201/210 (96%)	197 (98%)	3 (2%)	1 (0%)	34	71
29	DF	201/210 (96%)	197 (98%)	2 (1%)	2 (1%)	19	54
30	BG	179/182 (98%)	171 (96%)	7 (4%)	1 (1%)	30	67
30	DG	179/182 (98%)	167 (93%)	11 (6%)	1 (1%)	30	67
31	BH	172/180 (96%)	169 (98%)	3 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
31	DH	172/180 (96%)	168 (98%)	4 (2%)	0	100	100
32	BI	144/148 (97%)	130 (90%)	10 (7%)	4 (3%)	6	24
32	DI	144/148 (97%)	137 (95%)	6 (4%)	1 (1%)	26	63
33	BN	138/140 (99%)	137 (99%)	1 (1%)	0	100	100
33	DN	138/140 (99%)	135 (98%)	2 (1%)	1 (1%)	26	63
34	BO	120/122 (98%)	113 (94%)	7 (6%)	0	100	100
34	DO	120/122 (98%)	113 (94%)	7 (6%)	0	100	100
35	BP	147/150 (98%)	141 (96%)	6 (4%)	0	100	100
35	DP	147/150 (98%)	140 (95%)	5 (3%)	2 (1%)	14	44
36	BQ	139/141 (99%)	134 (96%)	5 (4%)	0	100	100
36	DQ	139/141 (99%)	133 (96%)	6 (4%)	0	100	100
37	BR	116/118 (98%)	112 (97%)	4 (3%)	0	100	100
37	DR	116/118 (98%)	111 (96%)	5 (4%)	0	100	100
38	BS	108/112 (96%)	103 (95%)	4 (4%)	1 (1%)	21	57
38	DS	108/112 (96%)	105 (97%)	2 (2%)	1 (1%)	21	57
39	BT	129/146 (88%)	123 (95%)	4 (3%)	2 (2%)	12	40
39	DT	129/146 (88%)	125 (97%)	3 (2%)	1 (1%)	24	60
40	BU	114/118 (97%)	114 (100%)	0	0	100	100
40	DU	114/118 (97%)	114 (100%)	0	0	100	100
41	BV	99/101 (98%)	93 (94%)	6 (6%)	0	100	100
41	DV	99/101 (98%)	95 (96%)	4 (4%)	0	100	100
42	BW	110/113 (97%)	110 (100%)	0	0	100	100
42	DW	110/113 (97%)	110 (100%)	0	0	100	100
43	BX	93/96 (97%)	89 (96%)	4 (4%)	0	100	100
43	DX	93/96 (97%)	90 (97%)	3 (3%)	0	100	100
44	BY	105/110 (96%)	99 (94%)	6 (6%)	0	100	100
44	DY	105/110 (96%)	102 (97%)	3 (3%)	0	100	100
45	BZ	169/206 (82%)	152 (90%)	16 (10%)	1 (1%)	30	67
45	DZ	172/206 (84%)	158 (92%)	14 (8%)	0	100	100
46	B0	81/85 (95%)	81 (100%)	0	0	100	100
46	D0	81/85 (95%)	79 (98%)	1 (1%)	1 (1%)	16	48

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
47	B1	95/98 (97%)	94 (99%)	1 (1%)	0	100	100
47	D1	95/98 (97%)	93 (98%)	1 (1%)	1 (1%)	17	51
48	B2	68/72 (94%)	67 (98%)	1 (2%)	0	100	100
48	D2	68/72 (94%)	67 (98%)	1 (2%)	0	100	100
49	B3	57/60 (95%)	57 (100%)	0	0	100	100
49	D3	57/60 (95%)	56 (98%)	1 (2%)	0	100	100
50	B4	67/71 (94%)	56 (84%)	9 (13%)	2 (3%)	5	22
50	D4	67/71 (94%)	54 (81%)	8 (12%)	5 (8%)	1	3
51	B5	57/60 (95%)	57 (100%)	0	0	100	100
51	D5	57/60 (95%)	56 (98%)	1 (2%)	0	100	100
52	B6	51/54 (94%)	50 (98%)	1 (2%)	0	100	100
52	D6	51/54 (94%)	49 (96%)	2 (4%)	0	100	100
53	B7	46/49 (94%)	46 (100%)	0	0	100	100
53	D7	46/49 (94%)	45 (98%)	0	1 (2%)	8	31
54	B8	62/65 (95%)	62 (100%)	0	0	100	100
54	D8	62/65 (95%)	62 (100%)	0	0	100	100
55	B9	35/37 (95%)	35 (100%)	0	0	100	100
55	D9	35/37 (95%)	35 (100%)	0	0	100	100
All	All	11409/12128 (94%)	10906 (96%)	432 (4%)	71 (1%)	30	67

5 of 71 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	AB	19	HIS
2	AB	231	GLU
4	AD	166	LYS
7	AG	80	VAL
27	BD	275	LYS

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%)	151 (79%)	41 (21%)	1	4
2	CB	187/220 (85%)	154 (82%)	33 (18%)	2	7
3	AC	143/188 (76%)	125 (87%)	18 (13%)	5	16
3	CC	140/188 (74%)	121 (86%)	19 (14%)	5	13
4	AD	170/181 (94%)	146 (86%)	24 (14%)	4	12
4	CD	172/181 (95%)	145 (84%)	27 (16%)	3	9
5	AE	113/123 (92%)	103 (91%)	10 (9%)	12	35
5	CE	114/123 (93%)	98 (86%)	16 (14%)	4	12
6	AF	83/90 (92%)	78 (94%)	5 (6%)	24	57
6	CF	85/90 (94%)	77 (91%)	8 (9%)	11	32
7	AG	119/127 (94%)	108 (91%)	11 (9%)	11	33
7	CG	120/127 (94%)	109 (91%)	11 (9%)	11	33
8	AH	114/119 (96%)	103 (90%)	11 (10%)	10	31
8	CH	114/119 (96%)	104 (91%)	10 (9%)	12	35
9	AI	90/99 (91%)	76 (84%)	14 (16%)	3	10
9	CI	89/99 (90%)	70 (79%)	19 (21%)	1	4
10	AJ	66/92 (72%)	63 (96%)	3 (4%)	34	70
10	CJ	69/92 (75%)	64 (93%)	5 (7%)	18	46
11	AK	82/99 (83%)	75 (92%)	7 (8%)	13	37
11	CK	83/99 (84%)	79 (95%)	4 (5%)	31	67
12	AL	97/109 (89%)	89 (92%)	8 (8%)	14	39
12	CL	97/109 (89%)	88 (91%)	9 (9%)	11	32
13	AM	93/101 (92%)	79 (85%)	14 (15%)	3	11
13	CM	92/101 (91%)	77 (84%)	15 (16%)	3	8
14	AN	49/50 (98%)	42 (86%)	7 (14%)	4	12
14	CN	49/50 (98%)	39 (80%)	10 (20%)	1	4
15	AO	78/80 (98%)	70 (90%)	8 (10%)	9	26
15	CO	78/80 (98%)	71 (91%)	7 (9%)	12	34
16	AP	69/74 (93%)	54 (78%)	15 (22%)	1	3
16	CP	68/74 (92%)	59 (87%)	9 (13%)	5	14
17	AQ	94/97 (97%)	87 (93%)	7 (7%)	17	44

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
17	CQ	94/97 (97%)	88 (94%)	6 (6%)	22	53
18	AR	59/77 (77%)	52 (88%)	7 (12%)	6	19
18	CR	59/77 (77%)	52 (88%)	7 (12%)	6	19
19	AS	69/80 (86%)	63 (91%)	6 (9%)	13	36
19	CS	67/80 (84%)	59 (88%)	8 (12%)	6	19
20	AT	70/82 (85%)	61 (87%)	9 (13%)	5	16
20	CT	70/82 (85%)	59 (84%)	11 (16%)	3	9
21	AU	18/22 (82%)	15 (83%)	3 (17%)	3	8
21	CU	18/22 (82%)	15 (83%)	3 (17%)	3	8
27	BD	215/218 (99%)	196 (91%)	19 (9%)	12	35
27	DD	215/218 (99%)	194 (90%)	21 (10%)	10	30
28	BE	164/166 (99%)	144 (88%)	20 (12%)	6	18
28	DE	164/166 (99%)	143 (87%)	21 (13%)	5	16
29	BF	160/166 (96%)	146 (91%)	14 (9%)	12	35
29	DF	159/166 (96%)	144 (91%)	15 (9%)	11	32
30	BG	143/156 (92%)	123 (86%)	20 (14%)	4	12
30	DG	142/156 (91%)	118 (83%)	24 (17%)	2	8
31	BH	144/148 (97%)	136 (94%)	8 (6%)	26	60
31	DH	144/148 (97%)	131 (91%)	13 (9%)	12	34
32	BI	110/124 (89%)	93 (84%)	17 (16%)	3	10
32	DI	104/124 (84%)	87 (84%)	17 (16%)	3	8
33	BN	118/119 (99%)	104 (88%)	14 (12%)	6	19
33	DN	118/119 (99%)	104 (88%)	14 (12%)	6	19
34	BO	100/100 (100%)	92 (92%)	8 (8%)	15	40
34	DO	100/100 (100%)	90 (90%)	10 (10%)	9	28
35	BP	115/116 (99%)	102 (89%)	13 (11%)	7	22
35	DP	115/116 (99%)	103 (90%)	12 (10%)	9	26
36	BQ	111/111 (100%)	100 (90%)	11 (10%)	10	29
36	DQ	111/111 (100%)	98 (88%)	13 (12%)	7	19
37	BR	101/101 (100%)	86 (85%)	15 (15%)	4	11
37	DR	101/101 (100%)	90 (89%)	11 (11%)	8	23

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
38	BS	87/88 (99%)	80 (92%)	7 (8%)	15	40
38	DS	85/88 (97%)	76 (89%)	9 (11%)	8	25
39	BT	115/127 (91%)	104 (90%)	11 (10%)	10	31
39	DT	113/127 (89%)	98 (87%)	15 (13%)	5	14
40	BU	93/94 (99%)	85 (91%)	8 (9%)	13	36
40	DU	93/94 (99%)	85 (91%)	8 (9%)	13	36
41	BV	80/82 (98%)	72 (90%)	8 (10%)	9	28
41	DV	80/82 (98%)	75 (94%)	5 (6%)	22	54
42	BW	90/92 (98%)	82 (91%)	8 (9%)	12	35
42	DW	90/92 (98%)	84 (93%)	6 (7%)	20	50
43	BX	77/78 (99%)	73 (95%)	4 (5%)	29	64
43	DX	77/78 (99%)	75 (97%)	2 (3%)	54	85
44	BY	85/91 (93%)	77 (91%)	8 (9%)	11	32
44	DY	85/91 (93%)	81 (95%)	4 (5%)	32	68
45	BZ	145/179 (81%)	126 (87%)	19 (13%)	5	15
45	DZ	145/179 (81%)	128 (88%)	17 (12%)	7	19
46	B0	65/67 (97%)	61 (94%)	4 (6%)	23	55
46	D0	65/67 (97%)	61 (94%)	4 (6%)	23	55
47	B1	80/83 (96%)	75 (94%)	5 (6%)	22	54
47	D1	80/83 (96%)	73 (91%)	7 (9%)	12	35
48	B2	65/67 (97%)	61 (94%)	4 (6%)	23	55
48	D2	65/67 (97%)	57 (88%)	8 (12%)	6	17
49	B3	51/52 (98%)	45 (88%)	6 (12%)	6	19
49	D3	50/52 (96%)	46 (92%)	4 (8%)	15	40
50	B4	59/63 (94%)	50 (85%)	9 (15%)	3	10
50	D4	53/63 (84%)	40 (76%)	13 (24%)	1	2
51	B5	50/52 (96%)	44 (88%)	6 (12%)	6	18
51	D5	50/52 (96%)	46 (92%)	4 (8%)	15	40
52	B6	51/52 (98%)	45 (88%)	6 (12%)	6	19
52	D6	50/52 (96%)	45 (90%)	5 (10%)	9	28
53	B7	41/42 (98%)	37 (90%)	4 (10%)	10	30

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
53	D7	41/42 (98%)	37 (90%)	4 (10%)	10	30
54	B8	53/55 (96%)	49 (92%)	4 (8%)	17	44
54	D8	54/55 (98%)	50 (93%)	4 (7%)	17	44
55	B9	34/34 (100%)	32 (94%)	2 (6%)	24	58
55	D9	34/34 (100%)	30 (88%)	4 (12%)	6	19
All	All	9318/10066 (93%)	8277 (89%)	1041 (11%)	7	22

5 of 1041 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
48	B2	32	LEU
4	CD	170	VAL
43	DX	57	LEU
50	B4	58	ARG
2	CB	144	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 128 such sidechains are listed below:

Mol	Chain	Res	Type
49	B3	32	GLN
4	CD	77	ASN
39	DT	123	GLN
52	B6	20	ASN
2	CB	224	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	AA	1495/1521 (98%)	387 (25%)	22 (1%)
1	CA	1501/1521 (98%)	391 (26%)	24 (1%)
22	AV	12/24 (50%)	4 (33%)	0
22	CV	11/24 (45%)	4 (36%)	0
23	AW	0/2	-	-
23	CW	0/2	-	-
24	AX	74/77 (96%)	25 (33%)	1 (1%)
24	CX	74/77 (96%)	26 (35%)	1 (1%)
25	BA	2811/2915 (96%)	537 (19%)	24 (0%)
25	DA	2791/2915 (95%)	622 (22%)	29 (1%)

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
26	BB	120/121 (99%)	19 (15%)	3 (2%)
26	DB	119/121 (98%)	36 (30%)	0
All	All	9008/9320 (96%)	2051 (22%)	104 (1%)

5 of 2051 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	AA	5	U
1	AA	6	G
1	AA	7	G
1	AA	9	G
1	AA	22	G

5 of 104 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
26	BB	1	U
1	CA	560	U
25	DA	2169	A
26	BB	52	A
1	CA	65	U

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
23	PPU	AW	76	25,23	30,40,41	0.98	1 (3%)	37,57,60	2.15	10 (27%)
24	5MC	AX	32	24	13,22,23	1.38	1 (7%)	15,32,35	0.92	1 (6%)
24	5MU	AX	54	24,56	12,22,23	0.28	0	14,32,35	2.36	2 (14%)
24	PSU	AX	55	24	13,21,22	1.42	2 (15%)	18,30,33	3.43	6 (33%)
24	31H	AX	76	24,56	25,34,35	1.10	2 (8%)	26,47,50	3.10	6 (23%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
24	4SU	AX	8	24	11,21,22	1.21	1 (9%)	13,30,33	1.56	1 (7%)
23	PPU	CW	76	23	30,40,41	0.91	1 (3%)	37,57,60	2.07	8 (21%)
24	5MC	CX	32	24	13,22,23	1.32	1 (7%)	15,32,35	1.00	1 (6%)
24	5MU	CX	54	24	12,22,23	0.35	0	14,32,35	2.28	2 (14%)
24	PSU	CX	55	24	13,21,22	1.40	1 (7%)	18,30,33	3.39	6 (33%)
24	31H	CX	76	24	25,34,35	1.13	3 (12%)	26,47,50	3.02	7 (26%)
24	4SU	CX	8	24	11,21,22	1.12	1 (9%)	13,30,33	1.86	1 (7%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	PPU	AW	76	25,23	-	0/21/43/44	0/4/4/4
24	5MC	AX	32	24	-	0/3/25/26	0/2/2/2
24	5MU	AX	54	24,56	-	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	24,56	-	1/18/40/41	0/3/3/3
24	4SU	AX	8	24	-	0/3/25/26	0/2/2/2
23	PPU	CW	76	23	-	0/21/43/44	0/4/4/4
24	5MC	CX	32	24	-	0/3/25/26	0/2/2/2
24	5MU	CX	54	24	-	0/3/25/26	0/2/2/2
24	PSU	CX	55	24	-	0/7/25/26	0/2/2/2
24	31H	CX	76	24	-	1/18/40/41	0/3/3/3
24	4SU	CX	8	24	-	0/3/25/26	0/2/2/2

The worst 5 of 14 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	CX	55	PSU	C5-C1'	-4.56	1.48	1.52
24	AX	55	PSU	C5-C1'	-4.50	1.48	1.52
24	AX	8	4SU	C4-S4	-3.79	1.60	1.67
24	CX	8	4SU	C4-S4	-3.60	1.60	1.67
24	AX	76	31H	C5-C4	-3.55	1.32	1.40

The worst 5 of 51 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	AX	76	31H	N3-C2-N1	-12.15	119.59	128.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	CX	76	31H	N3-C2-N1	-11.53	120.06	128.89
24	CX	55	PSU	N1-C2-N3	-10.35	121.73	128.33
24	AX	55	PSU	N1-C2-N3	-10.22	121.81	128.33
23	CW	76	PPU	N3-C2-N1	-6.64	123.81	128.89

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.

9 monomers are involved in 22 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
23	AW	76	PPU	5	0
24	AX	54	5MU	1	0
24	AX	55	PSU	1	0
24	AX	76	31H	3	0
23	CW	76	PPU	7	0
24	CX	54	5MU	2	0
24	CX	55	PSU	1	0
24	CX	76	31H	4	0
24	CX	8	4SU	1	0

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 1780 ligands modelled in this entry, 1778 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
57	SF4	AD	501	4	0,12,12	0.00	-	0,24,24	0.00	-
57	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
57	SF4	AD	501	4	-	0/0/48/48	0/6/5/5
57	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.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	AA	1498/1521 (98%)	0.10	2 (0%) 95 96	39, 74, 94, 105	0
1	CA	1503/1521 (98%)	0.04	7 (0%) 91 90	41, 75, 94, 105	0
2	AB	231/256 (90%)	0.30	5 (2%) 65 60	65, 82, 90, 96	0
2	CB	231/256 (90%)	0.86	32 (13%) 4 2	67, 83, 92, 96	0
3	AC	206/239 (86%)	0.55	15 (7%) 18 12	67, 78, 86, 94	0
3	CC	206/239 (86%)	0.78	28 (13%) 4 2	69, 80, 87, 92	0
4	AD	208/209 (99%)	0.57	15 (7%) 18 12	57, 72, 82, 86	0
4	CD	208/209 (99%)	0.47	9 (4%) 39 32	57, 73, 82, 87	0
5	AE	148/162 (91%)	0.47	6 (4%) 41 34	55, 71, 81, 86	0
5	CE	148/162 (91%)	0.70	13 (8%) 12 8	58, 73, 82, 89	0
6	AF	100/101 (99%)	0.23	2 (2%) 68 64	55, 71, 80, 82	0
6	CF	100/101 (99%)	0.07	1 (1%) 84 82	58, 73, 80, 82	0
7	AG	155/156 (99%)	0.41	12 (7%) 16 11	67, 76, 85, 94	0
7	CG	155/156 (99%)	0.56	14 (9%) 12 7	68, 78, 86, 96	0
8	AH	137/138 (99%)	0.21	1 (0%) 89 88	62, 72, 78, 86	0
8	CH	137/138 (99%)	0.44	4 (2%) 55 49	62, 73, 80, 88	0
9	AI	127/128 (99%)	0.27	4 (3%) 52 45	64, 82, 87, 90	0
9	CI	127/128 (99%)	1.58	43 (33%) 0 0	67, 83, 89, 91	0
10	AJ	97/105 (92%)	0.21	5 (5%) 31 24	63, 80, 89, 95	0
10	CJ	96/105 (91%)	1.12	22 (22%) 1 0	70, 86, 93, 100	0
11	AK	114/129 (88%)	0.49	5 (4%) 38 32	54, 72, 81, 83	0
11	CK	114/129 (88%)	0.39	5 (4%) 38 32	56, 72, 80, 83	0
12	AL	122/132 (92%)	0.30	0 100 100	55, 65, 75, 78	0
12	CL	122/132 (92%)	0.32	2 (1%) 74 72	57, 67, 75, 80	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	AM	123/126 (97%)	0.54	11 (8%) 12 7	64, 78, 86, 91	0
13	CM	122/126 (96%)	0.82	16 (13%) 5 3	68, 80, 88, 93	0
14	AN	60/61 (98%)	0.87	7 (11%) 6 4	65, 76, 83, 86	0
14	CN	60/61 (98%)	1.80	22 (36%) 0 0	69, 79, 84, 88	0
15	AO	88/89 (98%)	0.14	1 (1%) 82 80	56, 69, 80, 90	0
15	CO	88/89 (98%)	0.28	0 100 100	56, 70, 80, 90	0
16	AP	82/88 (93%)	0.36	1 (1%) 81 78	58, 73, 83, 85	0
16	CP	82/88 (93%)	0.48	2 (2%) 62 57	58, 72, 82, 85	0
17	AQ	99/105 (94%)	0.28	0 100 100	60, 70, 81, 85	0
17	CQ	99/105 (94%)	0.28	0 100 100	57, 70, 80, 84	0
18	AR	68/88 (77%)	0.39	2 (2%) 55 49	60, 70, 81, 85	0
18	CR	68/88 (77%)	0.34	1 (1%) 76 74	61, 72, 82, 86	0
19	AS	83/93 (89%)	0.29	0 100 100	67, 81, 88, 96	0
19	CS	83/93 (89%)	0.99	14 (16%) 2 1	71, 83, 91, 97	0
20	AT	96/106 (90%)	0.60	8 (8%) 14 9	58, 72, 82, 89	0
20	CT	96/106 (90%)	0.33	3 (3%) 52 45	59, 72, 82, 88	0
21	AU	23/27 (85%)	0.66	0 100 100	65, 75, 80, 86	0
21	CU	23/27 (85%)	1.44	7 (30%) 1 0	66, 76, 83, 87	0
22	AV	13/24 (54%)	1.34	3 (23%) 1 0	60, 92, 100, 100	0
22	CV	12/24 (50%)	1.76	4 (33%) 0 0	63, 93, 99, 99	0
23	AW	1/2 (50%)	0.77	0 100 100	42, 42, 42, 42	0
23	CW	1/2 (50%)	1.15	0 100 100	59, 59, 59, 59	0
24	AX	71/77 (92%)	0.14	0 100 100	37, 72, 84, 92	0
24	CX	71/77 (92%)	0.06	0 100 100	39, 73, 86, 92	0
25	BA	2819/2915 (96%)	0.35	30 (1%) 82 80	23, 46, 89, 107	0
25	DA	2800/2915 (96%)	0.06	21 (0%) 87 86	26, 50, 90, 107	0
26	BB	120/121 (99%)	0.26	0 100 100	40, 65, 76, 91	0
26	DB	120/121 (99%)	0.09	1 (0%) 87 86	44, 70, 81, 93	0
27	BD	275/276 (99%)	0.28	1 (0%) 93 92	24, 45, 61, 77	0
27	DD	275/276 (99%)	0.29	0 100 100	27, 47, 63, 78	0
28	BE	204/206 (99%)	0.41	3 (1%) 76 74	18, 44, 66, 80	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
28	DE	204/206 (99%)	0.32	4 (1%) 68 64	32, 57, 72, 86	0
29	BF	203/210 (96%)	0.43	1 (0%) 91 90	26, 55, 74, 84	0
29	DF	203/210 (96%)	0.12	2 (0%) 84 82	26, 58, 75, 85	0
30	BG	181/182 (99%)	0.40	5 (2%) 56 50	56, 70, 82, 91	0
30	DG	181/182 (99%)	0.90	36 (19%) 1 1	61, 73, 85, 91	0
31	BH	174/180 (96%)	0.39	4 (2%) 64 59	51, 66, 76, 82	0
31	DH	174/180 (96%)	0.87	26 (14%) 3 2	55, 69, 80, 85	0
32	BI	146/148 (98%)	0.17	0 100 100	46, 74, 85, 87	0
32	DI	146/148 (98%)	0.29	11 (7%) 17 11	50, 75, 84, 87	0
33	BN	140/140 (100%)	0.42	2 (1%) 78 76	33, 53, 72, 80	0
33	DN	140/140 (100%)	0.61	7 (5%) 32 26	36, 56, 72, 81	0
34	BO	122/122 (100%)	0.16	0 100 100	25, 43, 60, 76	0
34	DO	122/122 (100%)	0.19	1 (0%) 87 86	42, 59, 73, 77	0
35	BP	149/150 (99%)	0.47	5 (3%) 49 41	27, 57, 73, 87	0
35	DP	149/150 (99%)	0.42	4 (2%) 58 52	29, 59, 76, 86	0
36	BQ	141/141 (100%)	0.45	3 (2%) 67 62	35, 53, 64, 71	0
36	DQ	141/141 (100%)	0.48	2 (1%) 78 76	38, 56, 68, 76	0
37	BR	118/118 (100%)	0.34	3 (2%) 61 55	25, 37, 56, 66	0
37	DR	118/118 (100%)	0.46	3 (2%) 61 55	40, 54, 66, 76	0
38	BS	110/112 (98%)	0.17	0 100 100	40, 52, 63, 68	0
38	DS	110/112 (98%)	0.40	2 (1%) 71 68	57, 76, 86, 92	0
39	BT	131/146 (89%)	0.04	0 100 100	32, 50, 74, 86	0
39	DT	131/146 (89%)	0.35	4 (3%) 52 45	44, 60, 75, 85	0
40	BU	116/118 (98%)	0.43	3 (2%) 59 54	23, 35, 55, 76	0
40	DU	116/118 (98%)	0.76	6 (5%) 31 24	41, 61, 77, 87	0
41	BV	101/101 (100%)	0.26	2 (1%) 68 64	19, 43, 64, 76	0
41	DV	101/101 (100%)	0.59	8 (7%) 15 10	44, 71, 80, 88	0
42	BW	112/113 (99%)	0.43	1 (0%) 85 84	21, 38, 53, 75	0
42	DW	112/113 (99%)	0.73	8 (7%) 19 13	31, 51, 69, 85	0
43	BX	95/96 (98%)	0.37	0 100 100	25, 43, 64, 82	0
43	DX	95/96 (98%)	0.87	13 (13%) 4 2	43, 62, 78, 91	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
44	BY	107/110 (97%)	0.39	2 (1%) 70 66	36, 51, 69, 80	0
44	DY	107/110 (97%)	0.65	7 (6%) 22 16	55, 72, 81, 89	0
45	BZ	171/206 (83%)	0.36	5 (2%) 55 49	42, 63, 77, 92	0
45	DZ	174/206 (84%)	0.76	17 (9%) 10 6	61, 80, 90, 100	0
46	B0	83/85 (97%)	0.28	2 (2%) 62 57	16, 43, 56, 67	0
46	D0	83/85 (97%)	0.87	12 (14%) 3 2	44, 65, 74, 80	0
47	B1	97/98 (98%)	0.26	5 (5%) 31 24	27, 49, 70, 77	0
47	D1	97/98 (98%)	0.45	6 (6%) 24 17	38, 59, 75, 78	0
48	B2	70/72 (97%)	0.28	0 100 100	37, 50, 66, 72	0
48	D2	70/72 (97%)	0.40	2 (2%) 55 49	58, 70, 79, 85	0
49	B3	59/60 (98%)	0.26	0 100 100	26, 41, 61, 72	0
49	D3	59/60 (98%)	0.95	9 (15%) 3 1	44, 64, 77, 80	0
50	B4	69/71 (97%)	0.15	1 (1%) 78 76	57, 76, 91, 94	0
50	D4	69/71 (97%)	0.96	15 (21%) 1 0	77, 87, 97, 104	0
51	B5	59/60 (98%)	0.41	2 (3%) 49 41	19, 38, 57, 78	0
51	D5	59/60 (98%)	0.37	0 100 100	31, 52, 69, 76	0
52	B6	53/54 (98%)	0.06	0 100 100	29, 43, 60, 71	0
52	D6	53/54 (98%)	0.14	0 100 100	50, 63, 75, 83	0
53	B7	48/49 (97%)	0.49	3 (6%) 23 17	20, 30, 53, 72	0
53	D7	48/49 (97%)	0.56	5 (10%) 8 5	35, 46, 71, 76	0
54	B8	64/65 (98%)	0.41	0 100 100	27, 36, 47, 55	0
54	D8	64/65 (98%)	0.62	3 (4%) 35 29	44, 58, 67, 75	0
55	B9	37/37 (100%)	0.59	0 100 100	31, 52, 64, 69	0
55	D9	37/37 (100%)	0.70	4 (10%) 8 4	44, 58, 67, 73	0
All	All	20634/21448 (96%)	0.34	676 (3%) 50 42	16, 64, 87, 107	0

The worst 5 of 676 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
13	CM	124	PRO	11.3
14	CN	25	VAL	7.1
13	CM	123	ALA	6.3
31	DH	115	VAL	6.2
9	CI	26	VAL	6.1

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
24	PSU	CX	55	20/21	0.92	0.14	-	59,68,84,85	0
24	5MC	CX	32	21/22	0.96	0.15	-	52,69,78,83	0
23	PPU	CW	76	37/38	0.96	0.27	-	31,50,63,70	0
24	5MU	CX	54	21/22	0.92	0.20	-	66,78,87,98	0
24	4SU	AX	8	20/21	0.95	0.17	-	50,63,78,79	0
24	5MU	AX	54	21/22	0.96	0.15	-	55,69,75,82	0
24	4SU	CX	8	20/21	0.92	0.15	-	65,84,90,94	0
24	5MC	AX	32	21/22	0.97	0.17	-	46,61,70,75	0
24	31H	AX	76	32/33	0.97	0.27	-	27,44,76,98	0
23	PPU	AW	76	37/38	0.97	0.23	-	25,33,43,45	0
24	PSU	AX	55	20/21	0.95	0.14	-	57,66,78,79	0
24	31H	CX	76	32/33	0.94	0.30	-	33,54,78,89	0

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
56	MG	AA	3008	1/1	0.92	0.62	36.80	55,55,55,55	0
56	MG	BA	3031	1/1	0.98	0.47	22.90	46,46,46,46	0
56	MG	DA	3020	1/1	0.92	0.44	14.74	50,50,50,50	0
56	MG	BE	302	1/1	0.98	0.77	14.59	36,36,36,36	0
56	MG	BP	201	1/1	0.93	0.49	11.89	36,36,36,36	0
56	MG	DA	3095	1/1	0.98	0.33	11.86	47,47,47,47	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	BA	3117	1/1	0.97	0.39	10.83	40,40,40,40	0
56	MG	BA	3030	1/1	0.95	0.62	10.33	43,43,43,43	0
56	MG	AA	3132	1/1	0.98	0.25	10.25	50,50,50,50	0
56	MG	BA	3288	1/1	0.96	0.32	9.86	48,48,48,48	0
56	MG	BA	3244	1/1	0.85	0.56	9.18	46,46,46,46	0
56	MG	DA	3592	1/1	0.94	0.63	9.01	52,52,52,52	0
56	MG	BA	3553	1/1	0.95	0.67	8.37	48,48,48,48	0
56	MG	D3	3001	1/1	0.95	0.69	8.30	70,70,70,70	0
56	MG	BA	3634	1/1	0.86	0.30	8.12	41,41,41,41	0
56	MG	AA	3019	1/1	0.84	0.22	8.08	62,62,62,62	0
56	MG	BV	201	1/1	0.96	0.44	7.42	36,36,36,36	0
56	MG	BA	3671	1/1	0.97	0.28	7.11	48,48,48,48	0
56	MG	BA	3121	1/1	0.97	0.48	6.64	43,43,43,43	0
56	MG	DA	3150	1/1	0.81	0.70	6.55	55,55,55,55	0
56	MG	BA	3519	1/1	0.98	0.25	6.49	53,53,53,53	0
56	MG	BA	3153	1/1	0.92	0.29	6.49	39,39,39,39	0
56	MG	BA	3495	1/1	0.91	0.33	6.45	48,48,48,48	0
56	MG	AA	3107	1/1	0.98	0.24	6.38	36,36,36,36	0
56	MG	DA	3495	1/1	0.97	0.28	6.26	45,45,45,45	0
56	MG	DA	3435	1/1	0.94	0.20	6.19	33,33,33,33	0
56	MG	BA	3221	1/1	1.00	0.24	6.19	41,41,41,41	0
56	MG	DA	3246	1/1	0.98	0.36	6.13	38,38,38,38	0
56	MG	BA	3667	1/1	0.96	0.49	6.08	38,38,38,38	0
56	MG	BA	3670	1/1	0.99	0.31	6.04	34,34,34,34	0
56	MG	AA	3134	1/1	0.95	0.24	5.86	52,52,52,52	0
56	MG	BA	3268	1/1	0.90	0.26	5.66	39,39,39,39	0
56	MG	DA	3381	1/1	0.90	0.23	5.50	56,56,56,56	0
56	MG	BA	3295	1/1	0.94	0.30	5.43	61,61,61,61	0
56	MG	DA	3214	1/1	0.98	0.21	5.18	30,30,30,30	0
56	MG	BA	3154	1/1	0.93	0.30	5.14	40,40,40,40	0
56	MG	D7	101	1/1	0.93	0.75	4.99	51,51,51,51	0
56	MG	BA	3112	1/1	0.85	0.26	4.62	40,40,40,40	0
56	MG	BA	3210	1/1	0.95	0.23	4.40	24,24,24,24	0
56	MG	BA	3256	1/1	0.95	0.22	4.36	41,41,41,41	0
56	MG	BA	3094	1/1	0.88	0.20	4.34	45,45,45,45	0
56	MG	AA	3006	1/1	0.93	0.28	4.28	67,67,67,67	0
56	MG	BD	303	1/1	0.98	0.42	4.28	37,37,37,37	0
56	MG	DA	3163	1/1	0.94	0.26	4.08	31,31,31,31	0
56	MG	BP	202	1/1	0.96	0.47	4.06	31,31,31,31	0
56	MG	DA	3125	1/1	0.90	0.35	4.04	47,47,47,47	0
56	MG	BA	3032	1/1	0.97	0.24	3.82	40,40,40,40	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	BA	3640	1/1	0.96	0.25	3.78	33,33,33,33	0
56	MG	BA	3014	1/1	0.97	0.29	3.70	35,35,35,35	0
56	MG	AA	3054	1/1	0.92	0.18	3.68	65,65,65,65	0
56	MG	BA	3230	1/1	0.87	0.21	3.63	40,40,40,40	0
56	MG	BA	3488	1/1	0.92	0.27	3.59	36,36,36,36	0
56	MG	BA	3178	1/1	0.98	0.24	3.51	26,26,26,26	0
56	MG	BF	303	1/1	0.95	0.28	3.42	20,20,20,20	0
56	MG	AA	3057	1/1	0.95	0.23	3.35	67,67,67,67	0
56	MG	BD	302	1/1	0.92	0.33	3.17	45,45,45,45	0
56	MG	BA	3144	1/1	0.97	0.33	3.08	44,44,44,44	0
56	MG	BU	203	1/1	0.97	0.37	2.93	32,32,32,32	0
56	MG	DA	3152	1/1	0.90	0.17	2.68	34,34,34,34	0
56	MG	BA	3624	1/1	0.86	0.29	2.67	49,49,49,49	0
56	MG	BA	3216	1/1	0.99	0.24	2.64	33,33,33,33	0
56	MG	DA	3593	1/1	0.94	0.32	2.52	51,51,51,51	0
56	MG	D5	502	1/1	0.99	0.35	2.49	36,36,36,36	0
56	MG	DA	3327	1/1	0.96	0.18	2.42	34,34,34,34	0
56	MG	DA	3521	1/1	0.97	0.19	2.41	51,51,51,51	0
56	MG	DP	3001	1/1	0.92	0.30	2.40	44,44,44,44	0
56	MG	DA	3092	1/1	0.94	0.18	2.37	45,45,45,45	0
56	MG	DA	3596	1/1	0.98	0.28	2.28	54,54,54,54	0
56	MG	DA	3426	1/1	0.95	0.22	2.23	35,35,35,35	0
56	MG	DA	3237	1/1	0.96	0.29	2.19	39,39,39,39	0
56	MG	B7	3001	1/1	0.96	0.25	2.10	45,45,45,45	0
56	MG	CA	3048	1/1	0.94	0.30	2.03	52,52,52,52	0
56	MG	BA	3155	1/1	0.97	0.29	1.99	27,27,27,27	0
56	MG	DA	3067	1/1	0.90	0.17	1.93	53,53,53,53	0
56	MG	DA	3080	1/1	0.98	0.21	1.90	29,29,29,29	0
56	MG	BA	3172	1/1	0.97	0.15	1.89	54,54,54,54	0
56	MG	B5	502	1/1	0.98	0.32	1.87	34,34,34,34	0
56	MG	BB	3005	1/1	0.91	0.20	1.80	30,30,30,30	0
56	MG	BU	201	1/1	0.98	0.31	1.75	32,32,32,32	0
56	MG	BF	304	1/1	0.97	0.25	1.74	37,37,37,37	0
56	MG	DA	3442	1/1	0.96	0.19	1.71	42,42,42,42	0
56	MG	DA	3342	1/1	0.98	0.21	1.71	37,37,37,37	0
56	MG	CA	3039	1/1	0.98	0.18	1.66	50,50,50,50	0
56	MG	BQ	203	1/1	0.98	0.34	1.60	33,33,33,33	0
56	MG	BA	3641	1/1	0.96	0.21	1.56	33,33,33,33	0
56	MG	DA	3013	1/1	0.94	0.20	1.52	37,37,37,37	0
56	MG	DA	3412	1/1	0.89	0.20	1.51	53,53,53,53	0
56	MG	DA	3264	1/1	0.80	0.17	1.50	47,47,47,47	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	CA	3123	1/1	0.90	0.19	1.47	66,66,66,66	0
56	MG	BA	3024	1/1	0.97	0.31	1.45	32,32,32,32	0
56	MG	DW	3001	1/1	0.97	0.31	1.41	38,38,38,38	0
56	MG	DA	3084	1/1	0.99	0.30	1.38	39,39,39,39	0
56	MG	BA	3123	1/1	0.97	0.21	1.35	36,36,36,36	0
56	MG	BA	3208	1/1	0.98	0.24	1.32	25,25,25,25	0
56	MG	BA	3662	1/1	0.96	0.24	1.32	36,36,36,36	0
56	MG	DA	3094	1/1	0.90	0.23	1.27	35,35,35,35	0
56	MG	DV	3001	1/1	0.93	0.34	1.20	45,45,45,45	0
56	MG	DA	3149	1/1	0.98	0.23	1.18	41,41,41,41	0
56	MG	BA	3147	1/1	0.96	0.24	1.08	35,35,35,35	0
56	MG	DA	3487	1/1	0.86	0.18	1.05	50,50,50,50	0
56	MG	BA	3319	1/1	0.95	0.21	1.05	39,39,39,39	0
56	MG	CA	3149	1/1	0.92	0.23	1.05	66,66,66,66	0
56	MG	CA	3110	1/1	0.90	0.17	1.04	64,64,64,64	0
56	MG	CA	3060	1/1	0.96	0.19	1.01	50,50,50,50	0
56	MG	BA	3248	1/1	0.95	0.21	0.99	21,21,21,21	0
56	MG	DF	301	1/1	0.93	0.31	0.95	44,44,44,44	0
56	MG	BA	3035	1/1	0.97	0.20	0.90	21,21,21,21	0
56	MG	BX	102	1/1	0.96	0.28	0.89	38,38,38,38	0
56	MG	B3	101	1/1	0.94	0.26	0.86	35,35,35,35	0
56	MG	BB	3006	1/1	0.94	0.18	0.83	49,49,49,49	0
56	MG	CA	3066	1/1	0.93	0.20	0.75	43,43,43,43	0
56	MG	DA	3557	1/1	0.90	0.16	0.75	62,62,62,62	0
56	MG	CA	3011	1/1	0.76	0.17	0.73	66,66,66,66	0
56	MG	BA	3666	1/1	0.95	0.29	0.73	35,35,35,35	0
56	MG	AA	3096	1/1	0.98	0.18	0.72	53,53,53,53	0
56	MG	AA	3090	1/1	0.96	0.18	0.71	28,28,28,28	0
56	MG	DR	201	1/1	0.97	0.24	0.69	36,36,36,36	0
56	MG	BA	3240	1/1	0.91	0.21	0.64	43,43,43,43	0
56	MG	DA	3552	1/1	0.94	0.17	0.60	49,49,49,49	0
56	MG	DU	201	1/1	0.94	0.29	0.59	41,41,41,41	0
56	MG	BH	3001	1/1	0.89	0.20	0.57	56,56,56,56	0
56	MG	AA	3075	1/1	0.96	0.16	0.50	39,39,39,39	0
56	MG	B7	3002	1/1	0.97	0.23	0.46	35,35,35,35	0
56	MG	DB	3006	1/1	0.96	0.15	0.42	55,55,55,55	0
56	MG	DA	3075	1/1	0.95	0.18	0.40	41,41,41,41	0
56	MG	BA	3363	1/1	0.96	0.20	0.37	29,29,29,29	0
56	MG	CA	3071	1/1	0.82	0.18	0.37	51,51,51,51	0
56	MG	CA	3075	1/1	0.98	0.15	0.33	53,53,53,53	0
56	MG	B7	3003	1/1	0.97	0.21	0.32	28,28,28,28	0
56	MG	BA	3439	1/1	0.97	0.20	0.26	30,30,30,30	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	BA	3386	1/1	0.97	0.22	0.23	32,32,32,32	0
58	ZN	D6	501	1/1	0.97	0.19	0.22	68,68,68,68	0
56	MG	DA	3111	1/1	0.92	0.21	0.20	39,39,39,39	0
56	MG	BV	202	1/1	0.93	0.23	0.20	36,36,36,36	0
56	MG	DA	3004	1/1	0.92	0.15	0.19	51,51,51,51	0
56	MG	BA	3179	1/1	0.99	0.20	0.17	27,27,27,27	0
56	MG	DF	302	1/1	0.97	0.18	0.14	41,41,41,41	0
56	MG	BA	3326	1/1	0.98	0.20	0.10	28,28,28,28	0
56	MG	CA	3109	1/1	0.95	0.17	0.08	50,50,50,50	0
56	MG	BA	3237	1/1	0.84	0.19	0.07	57,57,57,57	0
56	MG	B3	102	1/1	0.99	0.23	0.07	22,22,22,22	0
56	MG	DA	3384	1/1	0.97	0.17	0.04	52,52,52,52	0
56	MG	DD	302	1/1	0.90	0.26	0.02	39,39,39,39	0
56	MG	DA	3419	1/1	0.93	0.22	0.01	59,59,59,59	0
56	MG	BA	3183	1/1	0.93	0.21	-0.01	35,35,35,35	0
56	MG	BA	3618	1/1	0.94	0.19	-0.01	54,54,54,54	0
56	MG	CA	3104	1/1	0.85	0.17	-0.05	74,74,74,74	0
56	MG	DA	3191	1/1	0.91	0.14	-0.06	53,53,53,53	0
56	MG	BA	3474	1/1	0.96	0.18	-0.06	53,53,53,53	0
56	MG	DA	3198	1/1	0.97	0.16	-0.11	54,54,54,54	0
56	MG	BA	3579	1/1	0.86	0.18	-0.13	46,46,46,46	0
56	MG	BD	304	1/1	0.88	0.20	-0.14	28,28,28,28	0
56	MG	BX	101	1/1	0.98	0.22	-0.14	46,46,46,46	0
56	MG	BA	3259	1/1	0.97	0.17	-0.15	35,35,35,35	0
58	ZN	D5	501	1/1	0.99	0.16	-0.15	67,67,67,67	0
58	ZN	B6	501	1/1	0.99	0.16	-0.16	45,45,45,45	0
56	MG	DA	3202	1/1	0.98	0.17	-0.17	24,24,24,24	0
56	MG	DE	3002	1/1	0.91	0.23	-0.17	35,35,35,35	0
56	MG	AN	502	1/1	0.98	0.20	-0.30	53,53,53,53	0
56	MG	DA	3578	1/1	0.91	0.18	-0.32	47,47,47,47	0
56	MG	AA	3136	1/1	0.94	0.17	-0.34	56,56,56,56	0
56	MG	DA	3009	1/1	0.91	0.19	-0.35	42,42,42,42	0
56	MG	DG	3001	1/1	0.35	0.26	-0.36	81,81,81,81	0
56	MG	BA	3200	1/1	0.95	0.18	-0.40	25,25,25,25	0
56	MG	CA	3055	1/1	0.88	0.14	-0.40	62,62,62,62	0
56	MG	AA	3070	1/1	0.97	0.17	-0.40	33,33,33,33	0
56	MG	AA	3151	1/1	0.94	0.18	-0.40	45,45,45,45	0
56	MG	BD	307	1/1	0.97	0.20	-0.40	27,27,27,27	0
56	MG	BA	3152	1/1	0.97	0.20	-0.43	39,39,39,39	0
56	MG	DA	3584	1/1	0.96	0.17	-0.44	61,61,61,61	0
56	MG	AA	3144	1/1	0.98	0.19	-0.44	42,42,42,42	0
56	MG	AA	3184	1/1	0.77	0.17	-0.46	74,74,74,74	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	CA	3051	1/1	0.98	0.13	-0.50	66,66,66,66	0
56	MG	DA	3159	1/1	0.97	0.17	-0.53	31,31,31,31	0
56	MG	DA	3333	1/1	0.95	0.18	-0.58	38,38,38,38	0
56	MG	DA	3494	1/1	0.96	0.17	-0.60	49,49,49,49	0
56	MG	DA	3187	1/1	0.78	0.13	-0.61	46,46,46,46	0
56	MG	BD	306	1/1	0.95	0.18	-0.69	36,36,36,36	0
56	MG	DA	3336	1/1	0.97	0.18	-0.69	22,22,22,22	0
56	MG	AK	3001	1/1	0.93	0.17	-0.69	43,43,43,43	0
56	MG	BA	3605	1/1	0.88	0.17	-0.70	46,46,46,46	0
58	ZN	B5	501	1/1	0.99	0.16	-0.71	42,42,42,42	0
56	MG	CA	3018	1/1	0.96	0.14	-0.73	43,43,43,43	0
58	ZN	B9	501	1/1	0.99	0.18	-0.74	45,45,45,45	0
56	MG	B9	502	1/1	0.94	0.21	-0.74	41,41,41,41	0
56	MG	DA	3236	1/1	0.93	0.14	-0.76	47,47,47,47	0
56	MG	BY	502	1/1	0.96	0.17	-0.76	35,35,35,35	0
56	MG	DA	3589	1/1	0.96	0.17	-0.76	33,33,33,33	0
56	MG	AA	3125	1/1	0.96	0.19	-0.76	41,41,41,41	0
56	MG	BA	3082	1/1	0.83	0.20	-0.78	47,47,47,47	0
56	MG	DA	3158	1/1	0.91	0.16	-0.79	36,36,36,36	0
57	SF4	AD	501	8/8	0.99	0.16	-0.83	50,63,78,83	0
56	MG	BA	3504	1/1	0.97	0.18	-0.83	39,39,39,39	0
56	MG	DA	3500	1/1	0.94	0.17	-0.83	46,46,46,46	0
56	MG	DA	3461	1/1	0.94	0.16	-0.84	33,33,33,33	0
56	MG	BA	3033	1/1	0.95	0.18	-0.84	33,33,33,33	0
56	MG	BA	3367	1/1	0.96	0.17	-0.84	49,49,49,49	0
56	MG	AA	3098	1/1	0.91	0.18	-0.86	48,48,48,48	0
56	MG	DA	3011	1/1	0.97	0.15	-0.86	38,38,38,38	0
56	MG	BA	3156	1/1	0.94	0.18	-0.86	48,48,48,48	0
56	MG	BE	303	1/1	0.84	0.19	-0.90	41,41,41,41	0
56	MG	AA	3087	1/1	0.88	0.21	-0.92	62,62,62,62	0
56	MG	DA	3486	1/1	0.89	0.17	-0.93	37,37,37,37	0
56	MG	DA	3565	1/1	0.93	0.16	-0.95	51,51,51,51	0
56	MG	BA	3065	1/1	0.97	0.15	-0.96	29,29,29,29	0
56	MG	CK	3001	1/1	0.93	0.14	-0.97	50,50,50,50	0
56	MG	BA	3369	1/1	0.97	0.16	-0.97	33,33,33,33	0
56	MG	BA	3372	1/1	0.98	0.19	-0.97	29,29,29,29	0
56	MG	DA	3160	1/1	0.98	0.15	-0.98	44,44,44,44	0
56	MG	DA	3588	1/1	0.94	0.16	-1.03	21,21,21,21	0
56	MG	CA	3095	1/1	0.93	0.16	-1.04	56,56,56,56	0
56	MG	BA	3209	1/1	0.99	0.20	-1.04	26,26,26,26	0
57	SF4	CD	501	8/8	0.99	0.14	-1.05	58,71,82,82	0
56	MG	DA	3316	1/1	0.96	0.15	-1.05	57,57,57,57	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	BA	3394	1/1	0.92	0.18	-1.05	35,35,35,35	0
58	ZN	CN	501	1/1	0.97	0.11	-1.08	82,82,82,82	0
56	MG	AA	3153	1/1	0.88	0.16	-1.10	50,50,50,50	0
56	MG	DA	3035	1/1	0.97	0.14	-1.10	46,46,46,46	0
56	MG	DA	3421	1/1	0.98	0.15	-1.10	52,52,52,52	0
56	MG	DA	3008	1/1	0.93	0.14	-1.11	38,38,38,38	0
56	MG	BW	3002	1/1	0.87	0.19	-1.13	57,57,57,57	0
56	MG	DA	3440	1/1	0.96	0.16	-1.13	52,52,52,52	0
56	MG	DA	3463	1/1	0.98	0.13	-1.14	28,28,28,28	0
56	MG	DA	3211	1/1	0.97	0.15	-1.17	35,35,35,35	0
56	MG	CA	3153	1/1	0.98	0.13	-1.18	37,37,37,37	0
56	MG	BA	3181	1/1	0.98	0.16	-1.22	37,37,37,37	0
56	MG	CA	3093	1/1	0.93	0.10	-1.23	72,72,72,72	0
56	MG	AA	3056	1/1	0.89	0.15	-1.24	69,69,69,69	0
58	ZN	DY	501	1/1	0.97	0.12	-1.25	92,92,92,92	0
56	MG	DA	3124	1/1	0.99	0.15	-1.26	29,29,29,29	0
56	MG	BA	3162	1/1	0.96	0.18	-1.26	39,39,39,39	0
56	MG	DA	3371	1/1	0.93	0.11	-1.26	46,46,46,46	0
56	MG	DA	3305	1/1	0.97	0.16	-1.28	30,30,30,30	0
56	MG	BA	3245	1/1	0.98	0.17	-1.29	27,27,27,27	0
56	MG	DA	3241	1/1	0.96	0.15	-1.30	36,36,36,36	0
56	MG	DA	3566	1/1	0.90	0.14	-1.30	61,61,61,61	0
56	MG	CA	3031	1/1	0.97	0.13	-1.32	52,52,52,52	0
56	MG	BA	3207	1/1	0.97	0.16	-1.32	36,36,36,36	0
56	MG	DD	301	1/1	0.94	0.15	-1.33	43,43,43,43	0
56	MG	BA	3377	1/1	0.99	0.17	-1.34	31,31,31,31	0
56	MG	CA	3061	1/1	0.98	0.13	-1.34	45,45,45,45	0
56	MG	BA	3352	1/1	0.98	0.14	-1.34	32,32,32,32	0
56	MG	BA	3188	1/1	0.91	0.17	-1.34	39,39,39,39	0
56	MG	BA	3023	1/1	0.92	0.17	-1.36	40,40,40,40	0
56	MG	CA	3143	1/1	0.96	0.15	-1.38	42,42,42,42	0
56	MG	DA	3529	1/1	0.94	0.16	-1.39	41,41,41,41	0
56	MG	DA	3064	1/1	0.93	0.13	-1.39	48,48,48,48	0
56	MG	BA	3673	1/1	0.97	0.10	-1.40	37,37,37,37	0
56	MG	AM	3001	1/1	0.97	0.13	-1.41	54,54,54,54	0
58	ZN	AN	501	1/1	0.99	0.14	-1.41	67,67,67,67	0
56	MG	CA	3154	1/1	0.76	0.14	-1.41	62,62,62,62	0
56	MG	AA	3085	1/1	0.93	0.11	-1.42	63,63,63,63	0
56	MG	BD	308	1/1	0.97	0.17	-1.42	35,35,35,35	0
56	MG	BA	3404	1/1	0.98	0.17	-1.43	38,38,38,38	0
56	MG	BA	3081	1/1	0.86	0.19	-1.44	42,42,42,42	0
56	MG	CA	3036	1/1	0.80	0.11	-1.44	56,56,56,56	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	DA	3517	1/1	0.99	0.15	-1.45	47,47,47,47	0
56	MG	BA	3550	1/1	0.84	0.17	-1.46	44,44,44,44	0
56	MG	DF	303	1/1	0.92	0.13	-1.48	57,57,57,57	0
56	MG	BA	3249	1/1	0.96	0.15	-1.49	48,48,48,48	0
56	MG	DA	3535	1/1	0.93	0.15	-1.50	22,22,22,22	0
56	MG	DA	3002	1/1	0.96	0.13	-1.51	33,33,33,33	0
56	MG	BA	3034	1/1	0.99	0.18	-1.52	24,24,24,24	0
56	MG	DA	3276	1/1	0.98	0.17	-1.52	50,50,50,50	0
58	ZN	D9	501	1/1	0.97	0.10	-1.53	54,54,54,54	0
56	MG	BB	3001	1/1	0.95	0.15	-1.54	36,36,36,36	0
56	MG	AA	3186	1/1	0.98	0.13	-1.54	55,55,55,55	0
56	MG	BA	3310	1/1	0.99	0.18	-1.54	35,35,35,35	0
56	MG	CA	3152	1/1	0.85	0.16	-1.55	75,75,75,75	0
56	MG	DA	3378	1/1	0.96	0.15	-1.59	31,31,31,31	0
56	MG	BA	3120	1/1	0.95	0.18	-1.61	44,44,44,44	0
56	MG	BA	3110	1/1	0.94	0.18	-1.61	31,31,31,31	0
56	MG	BA	3494	1/1	0.96	0.17	-1.62	34,34,34,34	0
56	MG	CA	3092	1/1	0.96	0.12	-1.63	54,54,54,54	0
56	MG	AA	3118	1/1	0.98	0.15	-1.64	36,36,36,36	0
56	MG	BA	3668	1/1	0.95	0.17	-1.64	26,26,26,26	0
56	MG	DA	3452	1/1	0.96	0.14	-1.65	56,56,56,56	0
56	MG	DA	3238	1/1	0.94	0.15	-1.66	42,42,42,42	0
56	MG	DA	3344	1/1	0.95	0.16	-1.66	31,31,31,31	0
58	ZN	D4	501	1/1	0.96	0.05	-1.67	141,141,141,141	0
56	MG	AA	3005	1/1	0.96	0.18	-1.68	37,37,37,37	0
56	MG	DA	3079	1/1	0.99	0.12	-1.68	54,54,54,54	0
56	MG	DA	3032	1/1	0.93	0.13	-1.68	42,42,42,42	0
56	MG	BA	3452	1/1	0.97	0.17	-1.70	38,38,38,38	0
56	MG	BA	3497	1/1	0.92	0.14	-1.70	34,34,34,34	0
56	MG	BA	3416	1/1	0.90	0.17	-1.71	64,64,64,64	0
56	MG	DA	3449	1/1	0.96	0.14	-1.71	29,29,29,29	0
56	MG	BA	3038	1/1	0.99	0.13	-1.72	30,30,30,30	0
56	MG	BA	3043	1/1	0.95	0.17	-1.72	36,36,36,36	0
56	MG	CT	3001	1/1	0.88	0.09	-1.75	50,50,50,50	0
56	MG	DA	3350	1/1	0.98	0.12	-1.79	36,36,36,36	0
56	MG	BB	3008	1/1	0.97	0.15	-1.80	21,21,21,21	0
56	MG	DA	3574	1/1	0.87	0.12	-1.80	56,56,56,56	0
56	MG	BF	301	1/1	0.92	0.14	-1.81	56,56,56,56	0
56	MG	BA	3560	1/1	0.97	0.18	-1.81	55,55,55,55	0
56	MG	DA	3030	1/1	0.90	0.14	-1.81	30,30,30,30	0
56	MG	BA	3300	1/1	0.96	0.15	-1.82	39,39,39,39	0
56	MG	BA	3564	1/1	0.98	0.16	-1.82	29,29,29,29	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	DA	3556	1/1	0.98	0.15	-1.82	36,36,36,36	0
56	MG	BA	3159	1/1	0.98	0.17	-1.85	27,27,27,27	0
56	MG	AA	3077	1/1	0.98	0.14	-1.85	39,39,39,39	0
56	MG	AA	3045	1/1	0.91	0.13	-1.85	60,60,60,60	0
56	MG	DQ	3001	1/1	0.97	0.13	-1.86	48,48,48,48	0
56	MG	BA	3246	1/1	0.90	0.18	-1.88	56,56,56,56	0
56	MG	AA	3102	1/1	0.92	0.13	-1.89	60,60,60,60	0
56	MG	DA	3575	1/1	0.93	0.11	-1.92	49,49,49,49	0
56	MG	DA	3492	1/1	0.90	0.09	-1.92	44,44,44,44	0
56	MG	DA	3110	1/1	0.96	0.14	-1.93	42,42,42,42	0
58	ZN	BY	501	1/1	0.98	0.15	-1.93	51,51,51,51	0
56	MG	AA	3017	1/1	0.94	0.13	-1.93	63,63,63,63	0
56	MG	CE	201	1/1	0.92	0.14	-1.94	52,52,52,52	0
56	MG	DA	3297	1/1	0.99	0.15	-1.95	38,38,38,38	0
56	MG	BA	3318	1/1	0.94	0.16	-1.96	44,44,44,44	0
56	MG	DA	3190	1/1	0.94	0.14	-1.99	34,34,34,34	0
58	ZN	B4	501	1/1	0.93	0.07	-2.00	106,106,106,106	0
56	MG	BA	3196	1/1	0.98	0.18	-2.01	17,17,17,17	0
56	MG	BA	3417	1/1	0.95	0.17	-2.02	24,24,24,24	0
56	MG	DA	3338	1/1	0.92	0.13	-2.02	36,36,36,36	0
56	MG	DA	3047	1/1	0.91	0.13	-2.03	41,41,41,41	0
56	MG	DA	3322	1/1	0.98	0.17	-2.03	23,23,23,23	0
56	MG	DA	3555	1/1	0.95	0.13	-2.03	51,51,51,51	0
56	MG	DA	3012	1/1	0.99	0.12	-2.04	30,30,30,30	0
56	MG	BA	3511	1/1	0.96	0.14	-2.06	38,38,38,38	0
56	MG	DA	3180	1/1	0.96	0.11	-2.06	30,30,30,30	0
56	MG	DA	3177	1/1	0.99	0.11	-2.08	52,52,52,52	0
56	MG	DA	3154	1/1	0.99	0.13	-2.12	24,24,24,24	0
56	MG	DA	3216	1/1	0.94	0.12	-2.13	37,37,37,37	0
56	MG	DA	3045	1/1	0.94	0.12	-2.14	48,48,48,48	0
56	MG	DA	3099	1/1	0.91	0.14	-2.15	37,37,37,37	0
56	MG	BA	3468	1/1	0.94	0.15	-2.17	32,32,32,32	0
56	MG	DA	3053	1/1	0.99	0.13	-2.18	41,41,41,41	0
56	MG	BA	3228	1/1	0.92	0.14	-2.18	40,40,40,40	0
56	MG	BU	204	1/1	0.99	0.16	-2.19	29,29,29,29	0
56	MG	BA	3411	1/1	0.97	0.16	-2.20	25,25,25,25	0
56	MG	BA	3036	1/1	0.90	0.11	-2.21	56,56,56,56	0
56	MG	BW	3003	1/1	0.99	0.15	-2.21	27,27,27,27	0
56	MG	BA	3362	1/1	0.91	0.15	-2.22	30,30,30,30	0
56	MG	BA	3234	1/1	0.92	0.15	-2.25	57,57,57,57	0
56	MG	DA	3359	1/1	0.85	0.13	-2.25	43,43,43,43	0
56	MG	DA	3594	1/1	0.95	0.12	-2.28	48,48,48,48	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	DB	3002	1/1	0.90	0.13	-2.30	50,50,50,50	0
56	MG	BA	3317	1/1	0.92	0.16	-2.30	35,35,35,35	0
56	MG	BG	3003	1/1	0.94	0.10	-2.32	41,41,41,41	0
56	MG	DA	3209	1/1	0.89	0.11	-2.35	38,38,38,38	0
56	MG	BA	3071	1/1	0.96	0.13	-2.36	32,32,32,32	0
56	MG	DA	3456	1/1	0.96	0.13	-2.36	34,34,34,34	0
56	MG	BA	3515	1/1	0.91	0.16	-2.36	25,25,25,25	0
56	MG	CA	3119	1/1	0.90	0.09	-2.38	48,48,48,48	0
56	MG	BA	3323	1/1	0.96	0.07	-2.38	61,61,61,61	0
56	MG	BA	3343	1/1	0.97	0.16	-2.39	27,27,27,27	0
56	MG	BA	3185	1/1	0.89	0.13	-2.40	43,43,43,43	0
56	MG	BA	3085	1/1	0.97	0.16	-2.40	27,27,27,27	0
56	MG	DA	3018	1/1	0.97	0.12	-2.41	39,39,39,39	0
56	MG	DA	3405	1/1	0.94	0.12	-2.41	45,45,45,45	0
56	MG	DA	3200	1/1	0.95	0.12	-2.44	28,28,28,28	0
56	MG	BA	3540	1/1	0.96	0.16	-2.46	46,46,46,46	0
56	MG	DA	3587	1/1	0.93	0.11	-2.46	53,53,53,53	0
56	MG	BA	3657	1/1	0.94	0.13	-2.46	24,24,24,24	0
56	MG	BA	3005	1/1	0.96	0.16	-2.49	29,29,29,29	0
56	MG	DA	3284	1/1	0.98	0.10	-2.49	23,23,23,23	0
56	MG	DA	3145	1/1	0.89	0.14	-2.51	31,31,31,31	0
56	MG	DA	3348	1/1	0.94	0.13	-2.51	25,25,25,25	0
56	MG	CA	3053	1/1	0.97	0.15	-2.51	44,44,44,44	0
56	MG	DA	3410	1/1	0.98	0.14	-2.52	64,64,64,64	0
56	MG	DA	3132	1/1	0.94	0.10	-2.52	35,35,35,35	0
56	MG	DA	3225	1/1	0.93	0.14	-2.52	33,33,33,33	0
56	MG	DA	3188	1/1	0.96	0.14	-2.52	25,25,25,25	0
56	MG	AA	3026	1/1	0.94	0.14	-2.52	40,40,40,40	0
56	MG	CA	3139	1/1	0.93	0.10	-2.54	67,67,67,67	0
56	MG	DA	3026	1/1	0.98	0.11	-2.54	34,34,34,34	0
56	MG	DA	3457	1/1	0.96	0.12	-2.54	38,38,38,38	0
56	MG	DA	3558	1/1	0.96	0.09	-2.55	39,39,39,39	0
56	MG	AA	3076	1/1	0.98	0.10	-2.56	52,52,52,52	0
56	MG	BA	3516	1/1	0.95	0.14	-2.57	43,43,43,43	0
56	MG	DA	3311	1/1	0.94	0.13	-2.57	43,43,43,43	0
56	MG	BA	3020	1/1	0.95	0.15	-2.57	33,33,33,33	0
56	MG	BG	3002	1/1	0.92	0.10	-2.58	27,27,27,27	0
56	MG	BA	3621	1/1	0.95	0.15	-2.58	30,30,30,30	0
56	MG	CA	3062	1/1	0.92	0.08	-2.59	57,57,57,57	0
56	MG	DA	3197	1/1	0.94	0.14	-2.59	38,38,38,38	0
56	MG	DA	3201	1/1	0.98	0.11	-2.61	51,51,51,51	0
56	MG	BA	3078	1/1	0.89	0.13	-2.61	53,53,53,53	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	CA	3088	1/1	0.94	0.09	-2.61	41,41,41,41	0
56	MG	CA	3044	1/1	0.94	0.09	-2.62	56,56,56,56	0
56	MG	CA	3080	1/1	0.93	0.13	-2.62	41,41,41,41	0
56	MG	BD	305	1/1	0.97	0.15	-2.67	38,38,38,38	0
56	MG	BA	3541	1/1	0.97	0.11	-2.67	26,26,26,26	0
56	MG	DA	3285	1/1	0.97	0.13	-2.67	52,52,52,52	0
56	MG	BA	3371	1/1	0.84	0.18	-2.68	25,25,25,25	0
56	MG	DA	3210	1/1	0.97	0.10	-2.68	37,37,37,37	0
56	MG	AA	3164	1/1	0.88	0.14	-2.69	61,61,61,61	0
56	MG	CA	3014	1/1	0.94	0.10	-2.71	39,39,39,39	0
56	MG	BA	3469	1/1	0.92	0.16	-2.71	28,28,28,28	0
56	MG	CA	3068	1/1	0.89	0.09	-2.72	74,74,74,74	0
56	MG	DA	3218	1/1	0.91	0.12	-2.72	33,33,33,33	0
56	MG	DA	3301	1/1	0.88	0.13	-2.74	56,56,56,56	0
56	MG	BA	3191	1/1	0.93	0.16	-2.74	33,33,33,33	0
56	MG	BA	3459	1/1	0.93	0.15	-2.79	42,42,42,42	0
56	MG	DA	3038	1/1	0.98	0.11	-2.82	30,30,30,30	0
56	MG	BA	3199	1/1	0.97	0.17	-2.85	32,32,32,32	0
56	MG	DA	3335	1/1	0.97	0.15	-2.85	36,36,36,36	0
56	MG	DA	3562	1/1	0.97	0.13	-2.88	42,42,42,42	0
56	MG	DA	3056	1/1	0.88	0.09	-2.89	36,36,36,36	0
56	MG	DA	3083	1/1	0.94	0.09	-2.90	48,48,48,48	0
56	MG	BA	3329	1/1	0.92	0.11	-2.90	30,30,30,30	0
56	MG	DA	3370	1/1	0.97	0.11	-2.91	44,44,44,44	0
56	MG	DA	3550	1/1	0.94	0.14	-2.92	46,46,46,46	0
56	MG	BA	3299	1/1	0.96	0.13	-2.92	36,36,36,36	0
56	MG	DA	3416	1/1	0.91	0.16	-2.94	44,44,44,44	0
56	MG	BA	3132	1/1	0.98	0.16	-2.95	25,25,25,25	0
56	MG	BO	5001	1/1	0.93	0.12	-2.95	62,62,62,62	0
56	MG	BA	3101	1/1	0.96	0.14	-2.97	30,30,30,30	0
56	MG	BA	3659	1/1	0.98	0.14	-2.97	28,28,28,28	0
56	MG	BA	3182	1/1	0.95	0.18	-3.01	30,30,30,30	0
56	MG	AA	3012	1/1	0.91	0.10	-3.06	64,64,64,64	0
56	MG	DA	3114	1/1	0.97	0.10	-3.06	37,37,37,37	0
56	MG	DE	3003	1/1	0.93	0.11	-3.07	40,40,40,40	0
56	MG	DA	3330	1/1	0.95	0.12	-3.09	42,42,42,42	0
56	MG	BA	3158	1/1	0.92	0.13	-3.11	33,33,33,33	0
56	MG	BQ	201	1/1	0.94	0.09	-3.12	52,52,52,52	0
56	MG	BN	3001	1/1	0.97	0.12	-3.13	57,57,57,57	0
56	MG	DA	3176	1/1	0.94	0.11	-3.14	29,29,29,29	0
56	MG	BA	3151	1/1	0.97	0.12	-3.14	34,34,34,34	0
56	MG	BA	3409	1/1	0.99	0.16	-3.14	28,28,28,28	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	BA	3324	1/1	0.93	0.12	-3.14	53,53,53,53	0
56	MG	DA	3215	1/1	0.96	0.13	-3.16	31,31,31,31	0
56	MG	BA	3456	1/1	0.97	0.13	-3.16	33,33,33,33	0
56	MG	BA	3212	1/1	0.98	0.16	-3.18	28,28,28,28	0
56	MG	DA	3401	1/1	0.93	0.12	-3.18	55,55,55,55	0
56	MG	CA	3025	1/1	0.90	0.09	-3.19	48,48,48,48	0
56	MG	BA	3080	1/1	0.95	0.14	-3.20	29,29,29,29	0
56	MG	BA	3042	1/1	0.95	0.17	-3.23	33,33,33,33	0
56	MG	BA	3419	1/1	0.97	0.12	-3.24	20,20,20,20	0
56	MG	DA	3278	1/1	0.91	0.14	-3.25	50,50,50,50	0
56	MG	CA	3017	1/1	0.94	0.10	-3.30	41,41,41,41	0
56	MG	BA	3009	1/1	0.94	0.14	-3.30	34,34,34,34	0
56	MG	BA	3227	1/1	0.94	0.17	-3.30	32,32,32,32	0
56	MG	BF	302	1/1	0.98	0.08	-3.31	45,45,45,45	0
56	MG	DA	3397	1/1	0.93	0.14	-3.36	18,18,18,18	0
56	MG	DA	3183	1/1	0.93	0.09	-3.38	37,37,37,37	0
56	MG	BA	3055	1/1	0.96	0.16	-3.39	13,13,13,13	0
56	MG	BA	3652	1/1	0.97	0.14	-3.40	49,49,49,49	0
56	MG	BA	3502	1/1	0.98	0.16	-3.42	33,33,33,33	0
56	MG	BA	3289	1/1	0.99	0.15	-3.42	28,28,28,28	0
56	MG	AA	3067	1/1	0.94	0.13	-3.42	42,42,42,42	0
56	MG	DA	3027	1/1	0.95	0.12	-3.44	30,30,30,30	0
56	MG	DA	3434	1/1	0.95	0.13	-3.45	41,41,41,41	0
56	MG	DA	3465	1/1	0.95	0.13	-3.49	38,38,38,38	0
56	MG	BA	3040	1/1	0.94	0.13	-3.50	43,43,43,43	0
56	MG	BA	3622	1/1	0.97	0.13	-3.51	45,45,45,45	0
56	MG	AA	3081	1/1	0.87	0.11	-3.52	44,44,44,44	0
56	MG	BA	3011	1/1	0.97	0.10	-3.54	30,30,30,30	0
56	MG	BA	3508	1/1	0.98	0.13	-3.58	25,25,25,25	0
56	MG	BB	3009	1/1	0.84	0.12	-3.61	67,67,67,67	0
56	MG	DA	3542	1/1	0.98	0.12	-3.62	30,30,30,30	0
56	MG	DA	3298	1/1	0.94	0.09	-3.64	32,32,32,32	0
56	MG	BA	3203	1/1	0.96	0.14	-3.64	35,35,35,35	0
56	MG	AL	201	1/1	0.97	0.08	-3.65	63,63,63,63	0
56	MG	DA	3104	1/1	0.98	0.11	-3.66	35,35,35,35	0
56	MG	DA	3282	1/1	0.97	0.12	-3.68	30,30,30,30	0
56	MG	BA	3044	1/1	0.95	0.15	-3.70	30,30,30,30	0
56	MG	AA	3082	1/1	0.97	0.10	-3.73	57,57,57,57	0
56	MG	DA	3146	1/1	0.94	0.12	-3.78	34,34,34,34	0
56	MG	DA	3511	1/1	0.96	0.08	-3.80	53,53,53,53	0
56	MG	DA	3299	1/1	0.95	0.12	-3.81	50,50,50,50	0
56	MG	BA	3533	1/1	0.89	0.11	-3.82	45,45,45,45	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	CA	3086	1/1	0.74	0.09	-3.84	68,68,68,68	0
56	MG	DA	3331	1/1	0.92	0.07	-3.86	41,41,41,41	0
56	MG	AX	3008	1/1	0.97	0.15	-3.86	23,23,23,23	0
56	MG	DA	3462	1/1	0.97	0.12	-3.90	35,35,35,35	0
56	MG	BA	3292	1/1	0.96	0.12	-3.91	43,43,43,43	0
56	MG	DA	3334	1/1	0.99	0.11	-3.91	24,24,24,24	0
56	MG	AA	3140	1/1	0.96	0.12	-3.91	31,31,31,31	0
56	MG	DA	3019	1/1	0.96	0.13	-3.93	40,40,40,40	0
56	MG	DA	3363	1/1	0.97	0.09	-3.93	36,36,36,36	0
56	MG	BA	3501	1/1	0.98	0.13	-3.94	44,44,44,44	0
56	MG	BB	3007	1/1	0.96	0.15	-3.94	35,35,35,35	0
56	MG	DA	3485	1/1	0.77	0.12	-3.94	60,60,60,60	0
56	MG	AA	3042	1/1	0.91	0.13	-3.95	54,54,54,54	0
56	MG	BA	3664	1/1	0.97	0.16	-3.96	30,30,30,30	0
56	MG	BB	3015	1/1	0.92	0.14	-3.97	48,48,48,48	0
56	MG	BA	3391	1/1	0.96	0.10	-4.02	37,37,37,37	0
56	MG	DA	3169	1/1	0.98	0.10	-4.02	38,38,38,38	0
56	MG	BA	3578	1/1	0.94	0.14	-4.06	59,59,59,59	0
56	MG	BA	3098	1/1	0.98	0.12	-4.07	56,56,56,56	0
56	MG	DA	3199	1/1	0.92	0.09	-4.09	52,52,52,52	0
56	MG	BA	3656	1/1	0.98	0.09	-4.09	12,12,12,12	0
56	MG	BA	3380	1/1	0.93	0.16	-4.09	17,17,17,17	0
56	MG	AA	3129	1/1	0.94	0.10	-4.13	35,35,35,35	0
56	MG	BA	3052	1/1	0.96	0.14	-4.13	27,27,27,27	0
56	MG	DA	3181	1/1	0.96	0.10	-4.13	40,40,40,40	0
56	MG	DA	3217	1/1	0.95	0.12	-4.15	39,39,39,39	0
56	MG	CA	3001	1/1	0.95	0.07	-4.15	72,72,72,72	0
56	MG	BA	3382	1/1	0.98	0.14	-4.17	27,27,27,27	0
56	MG	BA	3499	1/1	0.95	0.16	-4.26	35,35,35,35	0
56	MG	DA	3029	1/1	0.94	0.11	-4.28	40,40,40,40	0
56	MG	BA	3220	1/1	0.92	0.14	-4.28	31,31,31,31	0
56	MG	BA	3109	1/1	0.98	0.09	-4.33	36,36,36,36	0
56	MG	DA	3369	1/1	0.95	0.11	-4.34	45,45,45,45	0
56	MG	BA	3482	1/1	0.98	0.12	-4.37	23,23,23,23	0
56	MG	AA	3022	1/1	0.96	0.10	-4.38	39,39,39,39	0
56	MG	BA	3192	1/1	0.94	0.13	-4.44	58,58,58,58	0
56	MG	BA	3287	1/1	0.98	0.13	-4.51	46,46,46,46	0
56	MG	AA	3097	1/1	0.91	0.11	-4.55	49,49,49,49	0
56	MG	DA	3353	1/1	0.94	0.13	-4.57	32,32,32,32	0
56	MG	AA	3185	1/1	0.90	0.05	-4.60	64,64,64,64	0
56	MG	DA	3453	1/1	0.98	0.13	-4.65	31,31,31,31	0
56	MG	DA	3131	1/1	0.89	0.12	-4.66	46,46,46,46	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	AX	3006	1/1	0.88	0.09	-4.67	54,54,54,54	0
56	MG	BA	3534	1/1	0.98	0.14	-4.69	20,20,20,20	0
56	MG	DA	3060	1/1	0.91	0.10	-4.74	45,45,45,45	0
56	MG	DA	3357	1/1	0.87	0.11	-4.74	33,33,33,33	0
56	MG	BA	3290	1/1	0.99	0.15	-4.75	36,36,36,36	0
56	MG	DA	3591	1/1	0.95	0.07	-4.75	42,42,42,42	0
56	MG	DA	3493	1/1	0.99	0.06	-4.76	45,45,45,45	0
56	MG	BA	3568	1/1	0.97	0.12	-4.80	42,42,42,42	0
56	MG	AA	3135	1/1	0.98	0.09	-4.84	46,46,46,46	0
56	MG	BA	3357	1/1	0.96	0.13	-4.85	30,30,30,30	0
56	MG	BA	3527	1/1	0.89	0.12	-4.86	40,40,40,40	0
56	MG	CA	3105	1/1	0.90	0.08	-4.89	84,84,84,84	0
56	MG	BA	3296	1/1	0.96	0.08	-4.91	25,25,25,25	0
56	MG	DA	3082	1/1	0.94	0.13	-4.92	58,58,58,58	0
56	MG	BA	3486	1/1	0.95	0.17	-4.95	21,21,21,21	0
56	MG	CA	3046	1/1	0.96	0.09	-4.96	41,41,41,41	0
56	MG	BA	3013	1/1	0.89	0.16	-5.00	35,35,35,35	0
56	MG	DA	3168	1/1	0.98	0.14	-5.08	39,39,39,39	0
56	MG	BA	3398	1/1	0.96	0.15	-5.09	41,41,41,41	0
56	MG	BA	3549	1/1	0.97	0.12	-5.10	57,57,57,57	0
56	MG	BA	3379	1/1	0.98	0.14	-5.13	31,31,31,31	0
56	MG	BA	3022	1/1	0.98	0.14	-5.13	26,26,26,26	0
56	MG	AA	3030	1/1	0.93	0.10	-5.18	47,47,47,47	0
56	MG	DA	3157	1/1	0.98	0.10	-5.18	40,40,40,40	0
56	MG	DA	3232	1/1	0.93	0.13	-5.25	38,38,38,38	0
56	MG	BA	3257	1/1	0.97	0.08	-5.32	29,29,29,29	0
56	MG	DA	3567	1/1	0.96	0.10	-5.33	41,41,41,41	0
56	MG	BA	3284	1/1	0.96	0.10	-5.35	41,41,41,41	0
56	MG	DA	3380	1/1	0.97	0.10	-5.38	33,33,33,33	0
56	MG	BA	3279	1/1	0.97	0.10	-5.39	38,38,38,38	0
56	MG	BA	3665	1/1	0.96	0.11	-5.39	30,30,30,30	0
56	MG	DA	3347	1/1	0.86	0.14	-5.41	41,41,41,41	0
56	MG	BA	3384	1/1	0.98	0.11	-5.45	28,28,28,28	0
56	MG	BA	3655	1/1	0.92	0.13	-5.47	18,18,18,18	0
56	MG	BA	3298	1/1	0.95	0.11	-5.52	28,28,28,28	0
56	MG	BA	3401	1/1	0.90	0.14	-5.52	32,32,32,32	0
56	MG	DA	3516	1/1	0.88	0.08	-5.59	61,61,61,61	0
56	MG	BA	3442	1/1	0.98	0.15	-5.67	20,20,20,20	0
56	MG	DA	3049	1/1	0.97	0.06	-5.68	40,40,40,40	0
56	MG	AA	3104	1/1	0.96	0.07	-5.69	56,56,56,56	0
56	MG	BA	3609	1/1	0.95	0.11	-5.78	44,44,44,44	0
56	MG	BA	3378	1/1	0.97	0.16	-5.82	16,16,16,16	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	BA	3397	1/1	0.96	0.11	-5.87	30,30,30,30	0
56	MG	BA	3361	1/1	0.98	0.10	-5.88	45,45,45,45	0
56	MG	AA	3091	1/1	0.95	0.11	-5.93	36,36,36,36	0
56	MG	DA	3140	1/1	0.96	0.10	-5.93	37,37,37,37	0
56	MG	DA	3096	1/1	0.91	0.12	-5.98	29,29,29,29	0
56	MG	BA	3487	1/1	0.92	0.15	-5.98	17,17,17,17	0
56	MG	AA	3050	1/1	0.97	0.12	-5.99	24,24,24,24	0
56	MG	BE	306	1/1	0.97	0.08	-6.16	32,32,32,32	0
56	MG	DA	3361	1/1	0.92	0.13	-6.17	38,38,38,38	0
56	MG	DA	3372	1/1	0.97	0.10	-6.17	21,21,21,21	0
56	MG	BA	3301	1/1	0.94	0.13	-6.26	46,46,46,46	0
56	MG	BA	3037	1/1	0.99	0.13	-6.27	24,24,24,24	0
56	MG	BA	3334	1/1	0.88	0.10	-6.29	32,32,32,32	0
56	MG	DA	3526	1/1	0.98	0.07	-6.29	64,64,64,64	0
56	MG	DA	3243	1/1	0.89	0.09	-6.32	50,50,50,50	0
56	MG	DA	3390	1/1	0.96	0.07	-6.34	41,41,41,41	0
56	MG	DA	3367	1/1	0.93	0.12	-6.39	47,47,47,47	0
56	MG	BA	3491	1/1	0.97	0.11	-6.45	39,39,39,39	0
56	MG	BB	3003	1/1	0.81	0.10	-6.53	61,61,61,61	0
56	MG	BA	3286	1/1	0.96	0.12	-6.57	32,32,32,32	0
56	MG	BA	3473	1/1	0.98	0.10	-6.66	37,37,37,37	0
56	MG	BA	3045	1/1	0.97	0.13	-6.68	34,34,34,34	0
56	MG	BA	3591	1/1	0.98	0.09	-6.69	36,36,36,36	0
56	MG	AX	3002	1/1	0.95	0.08	-6.71	56,56,56,56	0
56	MG	BA	3650	1/1	0.99	0.08	-6.80	31,31,31,31	0
56	MG	DA	3326	1/1	0.90	0.12	-6.89	41,41,41,41	0
56	MG	DA	3014	1/1	0.98	0.10	-6.90	33,33,33,33	0
56	MG	DA	3267	1/1	0.98	0.07	-7.04	47,47,47,47	0
56	MG	BA	3581	1/1	0.96	0.10	-7.29	34,34,34,34	0
56	MG	BA	3003	1/1	0.97	0.10	-7.30	49,49,49,49	0
56	MG	DA	3480	1/1	0.95	0.08	-7.41	32,32,32,32	0
56	MG	DA	3025	1/1	0.99	0.09	-7.49	41,41,41,41	0
56	MG	BA	3559	1/1	0.90	0.13	-7.60	52,52,52,52	0
56	MG	DA	3389	1/1	0.91	0.08	-7.62	42,42,42,42	0
56	MG	BA	3467	1/1	0.98	0.17	-8.12	20,20,20,20	0
56	MG	DA	3514	1/1	0.95	0.07	-8.28	40,40,40,40	0
56	MG	BA	3351	1/1	0.97	0.06	-8.57	33,33,33,33	0
56	MG	BA	3434	1/1	0.97	0.12	-8.82	43,43,43,43	0
56	MG	AA	3029	1/1	0.93	0.11	-8.93	52,52,52,52	0
56	MG	DA	3182	1/1	0.94	0.09	-8.94	38,38,38,38	0
56	MG	CA	3023	1/1	0.95	0.09	-9.16	38,38,38,38	0
56	MG	BA	3261	1/1	0.94	0.10	-9.36	53,53,53,53	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	BA	3548	1/1	0.97	0.11	-9.59	30,30,30,30	0
56	MG	BA	3647	1/1	0.98	0.10	-9.75	30,30,30,30	0
56	MG	AA	3148	1/1	0.88	0.06	-9.87	56,56,56,56	0
56	MG	BA	3366	1/1	0.97	0.07	-9.99	34,34,34,34	0
56	MG	AA	3165	1/1	0.95	0.07	-10.05	43,43,43,43	0
56	MG	BA	3068	1/1	0.97	0.09	-10.25	39,39,39,39	0
56	MG	BA	3342	1/1	0.96	0.15	-10.61	35,35,35,35	0
56	MG	BA	3430	1/1	0.95	0.12	-10.77	29,29,29,29	0
56	MG	BA	3420	1/1	0.96	0.10	-10.84	24,24,24,24	0
56	MG	AA	3083	1/1	0.93	0.07	-11.05	59,59,59,59	0
56	MG	BA	3477	1/1	0.96	0.10	-11.11	50,50,50,50	0
56	MG	DA	3286	1/1	0.96	0.07	-11.32	35,35,35,35	0
56	MG	DA	3296	1/1	0.94	0.09	-11.67	28,28,28,28	0
56	MG	AA	3011	1/1	0.97	0.08	-12.46	24,24,24,24	0
56	MG	BA	3523	1/1	0.89	0.10	-12.78	50,50,50,50	0
56	MG	AA	3163	1/1	0.96	0.06	-12.80	49,49,49,49	0
56	MG	BA	3616	1/1	0.84	0.13	-13.59	34,34,34,34	0
56	MG	BA	3174	1/1	0.94	0.08	-19.37	29,29,29,29	0
56	MG	BA	3273	1/1	0.96	0.09	-19.80	29,29,29,29	0
56	MG	AA	3105	1/1	0.96	0.15	-	44,44,44,44	0
56	MG	BA	3164	1/1	0.90	0.11	-	37,37,37,37	0
56	MG	BA	3472	1/1	0.98	0.11	-	34,34,34,34	0
56	MG	BA	3428	1/1	0.92	0.08	-	58,58,58,58	0
56	MG	DA	3580	1/1	0.94	0.13	-	58,58,58,58	0
56	MG	DA	3345	1/1	0.96	0.16	-	33,33,33,33	0
56	MG	BA	3139	1/1	0.97	0.19	-	31,31,31,31	0
56	MG	BA	3470	1/1	0.94	0.15	-	48,48,48,48	0
56	MG	B5	503	1/1	0.98	0.21	-	47,47,47,47	0
56	MG	DA	3085	1/1	0.94	0.12	-	40,40,40,40	0
56	MG	BA	3341	1/1	0.92	0.11	-	32,32,32,32	0
56	MG	B8	5001	1/1	0.84	0.15	-	36,36,36,36	0
56	MG	DA	3117	1/1	0.92	0.19	-	43,43,43,43	0
56	MG	BA	3506	1/1	0.98	0.09	-	39,39,39,39	0
56	MG	BA	3536	1/1	0.93	0.15	-	53,53,53,53	0
56	MG	DA	3439	1/1	0.99	0.13	-	28,28,28,28	0
56	MG	BA	3224	1/1	0.91	0.17	-	45,45,45,45	0
56	MG	BA	3669	1/1	0.97	0.17	-	29,29,29,29	0
56	MG	DA	3450	1/1	0.95	0.07	-	37,37,37,37	0
56	MG	CA	3098	1/1	0.94	0.17	-	42,42,42,42	0
56	MG	BA	3612	1/1	0.96	0.19	-	51,51,51,51	0
56	MG	CA	3026	1/1	0.97	0.22	-	44,44,44,44	0
56	MG	BA	3142	1/1	0.94	0.11	-	40,40,40,40	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	CA	3140	1/1	0.94	0.19	-	61,61,61,61	0
56	MG	BA	3148	1/1	0.96	0.19	-	25,25,25,25	0
56	MG	DA	3408	1/1	0.95	0.16	-	28,28,28,28	0
56	MG	DA	3036	1/1	0.95	0.09	-	38,38,38,38	0
56	MG	BA	3218	1/1	0.94	0.18	-	38,38,38,38	0
56	MG	BA	3316	1/1	0.92	0.09	-	61,61,61,61	0
56	MG	BA	3021	1/1	0.96	0.10	-	37,37,37,37	0
56	MG	CA	3016	1/1	0.67	0.14	-	68,68,68,68	0
56	MG	BA	3105	1/1	0.96	0.13	-	32,32,32,32	0
56	MG	AA	3173	1/1	0.95	0.15	-	32,32,32,32	0
56	MG	BE	304	1/1	0.96	0.15	-	13,13,13,13	0
56	MG	BA	3561	1/1	0.94	0.10	-	55,55,55,55	0
56	MG	DA	3307	1/1	0.89	0.21	-	53,53,53,53	0
56	MG	DA	3569	1/1	0.95	0.25	-	55,55,55,55	0
56	MG	DA	3046	1/1	0.93	0.23	-	34,34,34,34	0
56	MG	DA	3234	1/1	0.93	0.14	-	45,45,45,45	0
56	MG	AA	3016	1/1	0.93	0.19	-	49,49,49,49	0
56	MG	BA	3265	1/1	0.96	0.29	-	47,47,47,47	0
56	MG	CA	3057	1/1	0.97	0.14	-	41,41,41,41	0
56	MG	AA	3149	1/1	0.88	0.12	-	68,68,68,68	0
56	MG	BA	3331	1/1	0.86	0.15	-	59,59,59,59	0
56	MG	DA	3070	1/1	0.95	0.20	-	49,49,49,49	0
56	MG	BA	3060	1/1	0.92	0.14	-	42,42,42,42	0
56	MG	BA	3586	1/1	0.96	0.17	-	45,45,45,45	0
56	MG	DN	5001	1/1	0.91	0.14	-	65,65,65,65	0
56	MG	BA	3312	1/1	0.97	0.13	-	18,18,18,18	0
56	MG	BA	3565	1/1	0.93	0.12	-	51,51,51,51	0
56	MG	CA	3081	1/1	0.84	0.16	-	56,56,56,56	0
56	MG	AA	3047	1/1	0.94	0.13	-	45,45,45,45	0
56	MG	B0	101	1/1	0.94	0.14	-	71,71,71,71	0
56	MG	BA	3447	1/1	0.95	0.12	-	55,55,55,55	0
56	MG	CA	3002	1/1	0.96	0.09	-	43,43,43,43	0
56	MG	BA	3471	1/1	0.94	0.18	-	35,35,35,35	0
56	MG	DA	3317	1/1	0.98	0.09	-	53,53,53,53	0
56	MG	BA	3276	1/1	0.98	0.12	-	42,42,42,42	0
56	MG	BA	3562	1/1	0.91	0.09	-	46,46,46,46	0
56	MG	DA	3532	1/1	0.99	0.06	-	51,51,51,51	0
56	MG	DA	3510	1/1	0.98	0.09	-	53,53,53,53	0
56	MG	BA	3213	1/1	0.95	0.23	-	21,21,21,21	0
56	MG	DA	3582	1/1	0.86	0.17	-	38,38,38,38	0
56	MG	DA	3136	1/1	0.93	0.16	-	36,36,36,36	0
56	MG	BA	3007	1/1	0.96	0.12	-	32,32,32,32	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	CA	3121	1/1	0.79	0.13	-	61,61,61,61	0
56	MG	D0	5001	1/1	0.98	0.06	-	39,39,39,39	0
56	MG	BA	3445	1/1	0.98	0.09	-	22,22,22,22	0
56	MG	DA	3206	1/1	0.91	0.15	-	50,50,50,50	0
56	MG	AA	3041	1/1	0.97	0.20	-	52,52,52,52	0
56	MG	BA	3254	1/1	0.91	0.17	-	45,45,45,45	0
56	MG	BA	3047	1/1	0.95	0.22	-	41,41,41,41	0
56	MG	CA	3094	1/1	0.96	0.10	-	67,67,67,67	0
56	MG	AA	3051	1/1	0.96	0.14	-	49,49,49,49	0
56	MG	BA	3389	1/1	0.99	0.19	-	35,35,35,35	0
56	MG	AA	3014	1/1	0.93	0.14	-	49,49,49,49	0
56	MG	BA	3026	1/1	0.99	0.22	-	46,46,46,46	0
56	MG	BA	3061	1/1	0.90	0.21	-	44,44,44,44	0
56	MG	BA	3054	1/1	0.91	0.14	-	42,42,42,42	0
56	MG	DA	3123	1/1	0.92	0.13	-	51,51,51,51	0
56	MG	CA	3147	1/1	0.97	0.17	-	52,52,52,52	0
56	MG	BA	3490	1/1	0.96	0.11	-	38,38,38,38	0
56	MG	BA	3484	1/1	0.93	0.12	-	46,46,46,46	0
56	MG	DA	3273	1/1	0.95	0.19	-	31,31,31,31	0
56	MG	DA	3266	1/1	0.95	0.10	-	46,46,46,46	0
56	MG	BA	3496	1/1	0.92	0.19	-	31,31,31,31	0
56	MG	AA	3108	1/1	0.94	0.14	-	54,54,54,54	0
56	MG	AA	3166	1/1	0.92	0.14	-	53,53,53,53	0
56	MG	DA	3351	1/1	0.92	0.15	-	46,46,46,46	0
56	MG	DA	3328	1/1	0.94	0.14	-	48,48,48,48	0
56	MG	BA	3400	1/1	0.93	0.28	-	45,45,45,45	0
56	MG	DA	3135	1/1	0.87	0.16	-	47,47,47,47	0
56	MG	DA	3572	1/1	0.92	0.08	-	51,51,51,51	0
56	MG	BA	3529	1/1	0.96	0.18	-	33,33,33,33	0
56	MG	CA	3130	1/1	0.95	0.12	-	57,57,57,57	0
56	MG	DA	3156	1/1	0.91	0.08	-	38,38,38,38	0
56	MG	CA	3079	1/1	0.94	0.17	-	55,55,55,55	0
56	MG	CA	3052	1/1	0.94	0.11	-	39,39,39,39	0
56	MG	BA	3056	1/1	0.80	0.13	-	46,46,46,46	0
56	MG	BA	3252	1/1	0.94	0.37	-	51,51,51,51	0
56	MG	BA	3017	1/1	0.94	0.15	-	40,40,40,40	0
56	MG	BA	3593	1/1	0.93	0.23	-	39,39,39,39	0
56	MG	BU	202	1/1	0.95	0.09	-	40,40,40,40	0
56	MG	DA	3337	1/1	0.96	0.09	-	42,42,42,42	0
56	MG	B0	105	1/1	0.96	0.10	-	43,43,43,43	0
56	MG	DA	3548	1/1	0.97	0.20	-	40,40,40,40	0
56	MG	DA	3573	1/1	0.95	0.14	-	45,45,45,45	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	BA	3637	1/1	0.98	0.21	-	24,24,24,24	0
56	MG	BA	3304	1/1	0.96	0.08	-	43,43,43,43	0
56	MG	DA	3379	1/1	0.96	0.08	-	26,26,26,26	0
56	MG	DA	3142	1/1	0.92	0.16	-	37,37,37,37	0
56	MG	CA	3032	1/1	0.90	0.16	-	68,68,68,68	0
56	MG	DA	3252	1/1	0.95	0.15	-	53,53,53,53	0
56	MG	BA	3651	1/1	0.96	0.14	-	42,42,42,42	0
56	MG	BA	3202	1/1	0.95	0.14	-	30,30,30,30	0
56	MG	BA	3539	1/1	0.94	0.16	-	58,58,58,58	0
56	MG	DA	3062	1/1	0.94	0.22	-	42,42,42,42	0
56	MG	AX	3007	1/1	0.89	0.11	-	60,60,60,60	0
56	MG	BA	3161	1/1	0.95	0.10	-	39,39,39,39	0
56	MG	DB	3011	1/1	0.98	0.09	-	29,29,29,29	0
56	MG	BA	3039	1/1	0.99	0.08	-	31,31,31,31	0
56	MG	BP	204	1/1	0.98	0.16	-	31,31,31,31	0
56	MG	BA	3270	1/1	0.97	0.16	-	21,21,21,21	0
56	MG	BA	3214	1/1	0.98	0.22	-	28,28,28,28	0
56	MG	CA	3133	1/1	0.96	0.11	-	68,68,68,68	0
56	MG	BA	3517	1/1	0.97	0.12	-	40,40,40,40	0
56	MG	AA	3126	1/1	0.95	0.12	-	54,54,54,54	0
56	MG	AA	3156	1/1	0.96	0.15	-	61,61,61,61	0
56	MG	BR	3003	1/1	0.97	0.15	-	39,39,39,39	0
56	MG	BA	3332	1/1	0.97	0.07	-	61,61,61,61	0
56	MG	BA	3631	1/1	0.88	0.12	-	41,41,41,41	0
56	MG	CA	3020	1/1	0.96	0.27	-	46,46,46,46	0
56	MG	AA	3137	1/1	0.94	0.07	-	79,79,79,79	0
56	MG	DA	3164	1/1	0.94	0.15	-	36,36,36,36	0
56	MG	DA	3055	1/1	0.97	0.09	-	34,34,34,34	0
56	MG	BA	3645	1/1	0.96	0.10	-	66,66,66,66	0
56	MG	CA	3087	1/1	0.95	0.12	-	33,33,33,33	0
56	MG	DA	3247	1/1	0.89	0.13	-	49,49,49,49	0
56	MG	AA	3116	1/1	0.96	0.12	-	51,51,51,51	0
56	MG	BA	3423	1/1	0.94	0.14	-	47,47,47,47	0
56	MG	BA	3125	1/1	0.81	0.19	-	51,51,51,51	0
56	MG	AA	3078	1/1	0.99	0.12	-	34,34,34,34	0
56	MG	DA	3245	1/1	0.93	0.13	-	46,46,46,46	0
56	MG	BA	3016	1/1	0.96	0.15	-	50,50,50,50	0
56	MG	DA	3395	1/1	0.97	0.10	-	41,41,41,41	0
56	MG	AA	3146	1/1	0.96	0.14	-	41,41,41,41	0
56	MG	BA	3283	1/1	0.97	0.11	-	57,57,57,57	0
56	MG	BA	3387	1/1	0.92	0.23	-	49,49,49,49	0
56	MG	DA	3174	1/1	0.96	0.10	-	44,44,44,44	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	BA	3466	1/1	0.89	0.22	-	49,49,49,49	0
56	MG	BA	3554	1/1	0.93	0.07	-	47,47,47,47	0
56	MG	DA	3109	1/1	0.90	0.13	-	50,50,50,50	0
56	MG	DA	3137	1/1	0.95	0.10	-	37,37,37,37	0
56	MG	DA	3059	1/1	0.93	0.11	-	33,33,33,33	0
56	MG	BA	3067	1/1	0.94	0.16	-	34,34,34,34	0
56	MG	BA	3393	1/1	0.94	0.12	-	49,49,49,49	0
56	MG	AA	3039	1/1	0.95	0.13	-	45,45,45,45	0
56	MG	AA	3003	1/1	0.94	0.15	-	57,57,57,57	0
56	MG	BA	3458	1/1	0.93	0.07	-	60,60,60,60	0
56	MG	AA	3112	1/1	0.91	0.18	-	94,94,94,94	0
56	MG	AA	3037	1/1	0.95	0.14	-	51,51,51,51	0
56	MG	DA	3033	1/1	0.92	0.17	-	37,37,37,37	0
56	MG	DA	3409	1/1	0.97	0.17	-	53,53,53,53	0
56	MG	DA	3475	1/1	0.89	0.20	-	41,41,41,41	0
56	MG	AA	3117	1/1	0.94	0.09	-	47,47,47,47	0
56	MG	BA	3140	1/1	0.95	0.16	-	33,33,33,33	0
56	MG	BA	3282	1/1	0.97	0.23	-	31,31,31,31	0
56	MG	DA	3496	1/1	0.90	0.05	-	46,46,46,46	0
56	MG	DA	3074	1/1	0.94	0.14	-	29,29,29,29	0
56	MG	BA	3446	1/1	0.84	0.20	-	61,61,61,61	0
56	MG	BA	3330	1/1	0.94	0.23	-	44,44,44,44	0
56	MG	BA	3236	1/1	0.94	0.19	-	42,42,42,42	0
56	MG	DA	3358	1/1	0.98	0.23	-	45,45,45,45	0
56	MG	DA	3153	1/1	0.97	0.14	-	42,42,42,42	0
56	MG	DA	3097	1/1	0.91	0.14	-	46,46,46,46	0
56	MG	AA	3138	1/1	0.97	0.15	-	50,50,50,50	0
59	K	AX	3001	1/1	0.94	0.07	-	48,48,48,48	0
56	MG	BA	3537	1/1	0.96	0.10	-	58,58,58,58	0
56	MG	BA	3104	1/1	0.94	0.20	-	42,42,42,42	0
56	MG	DA	3404	1/1	0.98	0.10	-	46,46,46,46	0
56	MG	DA	3048	1/1	0.96	0.16	-	41,41,41,41	0
56	MG	CA	3128	1/1	0.96	0.09	-	39,39,39,39	0
56	MG	DA	3391	1/1	0.95	0.06	-	42,42,42,42	0
56	MG	DA	3291	1/1	0.96	0.07	-	38,38,38,38	0
56	MG	BA	3285	1/1	0.97	0.10	-	48,48,48,48	0
56	MG	BA	3204	1/1	0.96	0.16	-	35,35,35,35	0
56	MG	AA	3013	1/1	0.94	0.09	-	58,58,58,58	0
56	MG	BA	3211	1/1	0.95	0.27	-	29,29,29,29	0
56	MG	AA	3143	1/1	0.99	0.10	-	32,32,32,32	0
56	MG	BA	3114	1/1	0.98	0.21	-	34,34,34,34	0
56	MG	AA	3175	1/1	0.96	0.12	-	53,53,53,53	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	BA	3599	1/1	0.91	0.15	-	46,46,46,46	0
56	MG	BA	3235	1/1	0.84	0.22	-	51,51,51,51	0
56	MG	CA	3106	1/1	0.99	0.15	-	40,40,40,40	0
56	MG	DA	3076	1/1	0.88	0.11	-	43,43,43,43	0
56	MG	CA	3089	1/1	0.94	0.13	-	40,40,40,40	0
56	MG	BA	3217	1/1	0.96	0.28	-	29,29,29,29	0
56	MG	BA	3195	1/1	0.95	0.13	-	47,47,47,47	0
56	MG	CA	3054	1/1	0.97	0.09	-	44,44,44,44	0
56	MG	DA	3289	1/1	0.99	0.16	-	26,26,26,26	0
56	MG	DA	3443	1/1	0.87	0.08	-	49,49,49,49	0
56	MG	AA	3021	1/1	0.96	0.09	-	41,41,41,41	0
56	MG	CA	3137	1/1	0.98	0.13	-	66,66,66,66	0
56	MG	DA	3165	1/1	0.94	0.13	-	34,34,34,34	0
56	MG	CA	3056	1/1	0.93	0.21	-	40,40,40,40	0
56	MG	CA	3019	1/1	0.85	0.20	-	71,71,71,71	0
56	MG	DB	3007	1/1	0.81	0.14	-	38,38,38,38	0
56	MG	BA	3646	1/1	0.96	0.15	-	23,23,23,23	0
56	MG	AA	3036	1/1	0.96	0.07	-	41,41,41,41	0
56	MG	DA	3102	1/1	0.91	0.17	-	51,51,51,51	0
56	MG	DA	3280	1/1	0.95	0.12	-	50,50,50,50	0
56	MG	BA	3485	1/1	0.95	0.14	-	64,64,64,64	0
56	MG	BA	3571	1/1	0.96	0.14	-	50,50,50,50	0
56	MG	CA	3047	1/1	0.91	0.17	-	51,51,51,51	0
56	MG	BA	3092	1/1	0.90	0.23	-	44,44,44,44	0
56	MG	BA	3512	1/1	0.95	0.14	-	45,45,45,45	0
56	MG	BA	3267	1/1	0.88	0.17	-	40,40,40,40	0
56	MG	BA	3492	1/1	0.95	0.15	-	42,42,42,42	0
56	MG	BA	3029	1/1	0.97	0.15	-	12,12,12,12	0
56	MG	BA	3424	1/1	0.99	0.20	-	38,38,38,38	0
56	MG	AA	3035	1/1	0.89	0.19	-	65,65,65,65	0
56	MG	DA	3329	1/1	0.90	0.07	-	48,48,48,48	0
56	MG	DA	3571	1/1	0.94	0.16	-	48,48,48,48	0
56	MG	AA	3046	1/1	0.95	0.11	-	42,42,42,42	0
56	MG	BA	3305	1/1	0.95	0.15	-	28,28,28,28	0
56	MG	DA	3383	1/1	0.95	0.08	-	47,47,47,47	0
56	MG	AA	3121	1/1	0.97	0.09	-	40,40,40,40	0
56	MG	AA	3174	1/1	0.97	0.09	-	55,55,55,55	0
56	MG	DA	3272	1/1	0.95	0.08	-	57,57,57,57	0
56	MG	AA	3101	1/1	0.96	0.13	-	53,53,53,53	0
56	MG	DA	3519	1/1	0.95	0.08	-	42,42,42,42	0
56	MG	BA	3395	1/1	0.88	0.23	-	54,54,54,54	0
56	MG	BA	3510	1/1	0.95	0.22	-	25,25,25,25	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	AA	3154	1/1	0.98	0.18	-	51,51,51,51	0
56	MG	AA	3020	1/1	0.91	0.18	-	49,49,49,49	0
56	MG	DA	3523	1/1	0.97	0.14	-	40,40,40,40	0
56	MG	AA	3131	1/1	0.95	0.12	-	55,55,55,55	0
56	MG	BA	3585	1/1	0.83	0.16	-	50,50,50,50	0
56	MG	BA	3643	1/1	0.94	0.12	-	42,42,42,42	0
56	MG	AA	3111	1/1	0.95	0.21	-	45,45,45,45	0
56	MG	DV	3002	1/1	0.92	0.16	-	43,43,43,43	0
56	MG	BA	3141	1/1	0.92	0.10	-	45,45,45,45	0
56	MG	DA	3365	1/1	0.93	0.10	-	29,29,29,29	0
56	MG	DA	3579	1/1	0.96	0.08	-	54,54,54,54	0
56	MG	BA	3552	1/1	0.96	0.08	-	31,31,31,31	0
56	MG	AA	3060	1/1	0.93	0.14	-	55,55,55,55	0
56	MG	DA	3320	1/1	0.98	0.08	-	46,46,46,46	0
56	MG	BA	3335	1/1	0.94	0.11	-	40,40,40,40	0
56	MG	DA	3308	1/1	0.96	0.13	-	29,29,29,29	0
56	MG	DA	3549	1/1	0.91	0.09	-	41,41,41,41	0
56	MG	BY	503	1/1	0.89	0.12	-	42,42,42,42	0
56	MG	BA	3157	1/1	0.93	0.19	-	34,34,34,34	0
56	MG	BB	3004	1/1	0.91	0.11	-	49,49,49,49	0
56	MG	BA	3241	1/1	0.99	0.29	-	26,26,26,26	0
56	MG	BA	3604	1/1	0.94	0.10	-	28,28,28,28	0
56	MG	BA	3461	1/1	0.97	0.24	-	52,52,52,52	0
56	MG	CA	3150	1/1	0.97	0.15	-	62,62,62,62	0
56	MG	DA	3356	1/1	0.95	0.09	-	31,31,31,31	0
56	MG	BB	3014	1/1	0.97	0.17	-	35,35,35,35	0
56	MG	CA	3059	1/1	0.94	0.15	-	58,58,58,58	0
56	MG	BA	3462	1/1	0.98	0.08	-	44,44,44,44	0
56	MG	DA	3466	1/1	0.97	0.12	-	38,38,38,38	0
56	MG	DA	3413	1/1	0.99	0.17	-	24,24,24,24	0
56	MG	BA	3058	1/1	0.89	0.15	-	43,43,43,43	0
56	MG	BW	3001	1/1	0.96	0.15	-	25,25,25,25	0
56	MG	BR	3002	1/1	0.96	0.13	-	23,23,23,23	0
56	MG	CA	3108	1/1	0.95	0.12	-	59,59,59,59	0
56	MG	BA	3606	1/1	0.97	0.15	-	32,32,32,32	0
56	MG	BA	3600	1/1	0.97	0.13	-	68,68,68,68	0
56	MG	DA	3423	1/1	0.96	0.15	-	40,40,40,40	0
56	MG	BA	3556	1/1	0.97	0.07	-	41,41,41,41	0
56	MG	BA	3383	1/1	0.97	0.11	-	33,33,33,33	0
56	MG	CA	3135	1/1	0.94	0.09	-	62,62,62,62	0
56	MG	DA	3061	1/1	0.97	0.08	-	35,35,35,35	0
56	MG	AA	3179	1/1	0.91	0.18	-	63,63,63,63	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	DA	3366	1/1	0.91	0.17	-	43,43,43,43	0
56	MG	BA	3638	1/1	0.95	0.10	-	32,32,32,32	0
56	MG	CA	3100	1/1	0.96	0.14	-	56,56,56,56	0
56	MG	DA	3314	1/1	0.96	0.14	-	54,54,54,54	0
56	MG	BA	3309	1/1	0.84	0.14	-	32,32,32,32	0
56	MG	BA	3479	1/1	0.98	0.15	-	45,45,45,45	0
56	MG	BA	3435	1/1	0.97	0.17	-	36,36,36,36	0
56	MG	BA	3088	1/1	0.95	0.11	-	42,42,42,42	0
56	MG	AA	3127	1/1	0.96	0.05	-	68,68,68,68	0
56	MG	DA	3128	1/1	0.96	0.21	-	42,42,42,42	0
56	MG	DA	3422	1/1	0.95	0.07	-	63,63,63,63	0
56	MG	DA	3454	1/1	0.96	0.08	-	64,64,64,64	0
56	MG	BA	3126	1/1	0.88	0.12	-	45,45,45,45	0
56	MG	DA	3101	1/1	0.94	0.10	-	46,46,46,46	0
56	MG	DA	3281	1/1	0.90	0.14	-	56,56,56,56	0
56	MG	DA	3122	1/1	0.90	0.17	-	45,45,45,45	0
56	MG	BA	3422	1/1	0.94	0.11	-	46,46,46,46	0
56	MG	DA	3303	1/1	0.99	0.07	-	43,43,43,43	0
56	MG	AA	3114	1/1	0.96	0.14	-	56,56,56,56	0
56	MG	BA	3526	1/1	0.99	0.23	-	25,25,25,25	0
56	MG	DA	3071	1/1	0.94	0.17	-	36,36,36,36	0
56	MG	DA	3170	1/1	0.97	0.14	-	38,38,38,38	0
56	MG	DA	3525	1/1	0.95	0.08	-	44,44,44,44	0
56	MG	DA	3240	1/1	0.95	0.09	-	54,54,54,54	0
56	MG	BA	3457	1/1	0.98	0.14	-	29,29,29,29	0
56	MG	DA	3489	1/1	0.96	0.16	-	49,49,49,49	0
56	MG	BN	3002	1/1	0.94	0.13	-	27,27,27,27	0
56	MG	BA	3051	1/1	0.94	0.19	-	41,41,41,41	0
56	MG	DA	3173	1/1	0.90	0.12	-	54,54,54,54	0
56	MG	AA	3065	1/1	0.94	0.13	-	48,48,48,48	0
56	MG	DA	3258	1/1	0.96	0.18	-	49,49,49,49	0
56	MG	DA	3476	1/1	0.98	0.06	-	32,32,32,32	0
56	MG	DA	3352	1/1	0.95	0.12	-	45,45,45,45	0
56	MG	DA	3471	1/1	0.93	0.16	-	50,50,50,50	0
56	MG	BA	3577	1/1	0.97	0.08	-	57,57,57,57	0
56	MG	DA	3545	1/1	0.93	0.07	-	58,58,58,58	0
56	MG	BA	3654	1/1	0.98	0.10	-	64,64,64,64	0
56	MG	BA	3463	1/1	0.93	0.12	-	43,43,43,43	0
56	MG	CA	3005	1/1	0.91	0.10	-	42,42,42,42	0
56	MG	DA	3005	1/1	0.94	0.11	-	26,26,26,26	0
56	MG	DA	3255	1/1	0.97	0.20	-	32,32,32,32	0
56	MG	BA	3364	1/1	0.98	0.18	-	29,29,29,29	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	DA	3253	1/1	0.90	0.12	-	26,26,26,26	0
56	MG	AA	3178	1/1	0.94	0.22	-	62,62,62,62	0
56	MG	DA	3162	1/1	0.89	0.11	-	57,57,57,57	0
56	MG	BE	305	1/1	0.88	0.25	-	51,51,51,51	0
56	MG	BA	3322	1/1	0.99	0.13	-	40,40,40,40	0
56	MG	BA	3138	1/1	0.96	0.19	-	35,35,35,35	0
56	MG	DA	3113	1/1	0.91	0.12	-	41,41,41,41	0
56	MG	BA	3345	1/1	0.90	0.18	-	41,41,41,41	0
56	MG	BA	3197	1/1	0.96	0.16	-	19,19,19,19	0
56	MG	BA	3356	1/1	0.95	0.10	-	46,46,46,46	0
56	MG	BA	3569	1/1	0.80	0.18	-	55,55,55,55	0
56	MG	BA	3165	1/1	0.91	0.25	-	43,43,43,43	0
56	MG	DA	3444	1/1	0.99	0.19	-	53,53,53,53	0
56	MG	DA	3254	1/1	0.96	0.07	-	46,46,46,46	0
56	MG	DA	3436	1/1	0.98	0.10	-	27,27,27,27	0
56	MG	BA	3405	1/1	0.93	0.14	-	26,26,26,26	0
56	MG	DA	3407	1/1	0.99	0.05	-	40,40,40,40	0
56	MG	DA	3148	1/1	0.90	0.10	-	47,47,47,47	0
56	MG	AA	3128	1/1	0.96	0.10	-	57,57,57,57	0
56	MG	DA	3319	1/1	0.98	0.20	-	38,38,38,38	0
56	MG	DA	3294	1/1	0.97	0.13	-	37,37,37,37	0
56	MG	DA	3428	1/1	0.91	0.18	-	33,33,33,33	0
56	MG	DA	3269	1/1	0.96	0.21	-	43,43,43,43	0
56	MG	DA	3042	1/1	0.99	0.10	-	32,32,32,32	0
56	MG	AA	3043	1/1	0.93	0.08	-	53,53,53,53	0
56	MG	BA	3131	1/1	0.95	0.22	-	36,36,36,36	0
56	MG	DA	3230	1/1	0.95	0.12	-	41,41,41,41	0
56	MG	DA	3229	1/1	0.92	0.18	-	38,38,38,38	0
56	MG	BA	3598	1/1	0.97	0.16	-	48,48,48,48	0
56	MG	CA	3037	1/1	0.98	0.09	-	45,45,45,45	0
56	MG	DR	202	1/1	0.97	0.14	-	32,32,32,32	0
56	MG	BA	3551	1/1	0.96	0.09	-	48,48,48,48	0
56	MG	BA	3097	1/1	0.95	0.13	-	53,53,53,53	0
56	MG	CA	3116	1/1	0.94	0.08	-	59,59,59,59	0
56	MG	DA	3560	1/1	0.94	0.12	-	51,51,51,51	0
56	MG	BP	203	1/1	0.85	0.14	-	47,47,47,47	0
56	MG	DA	3208	1/1	0.96	0.10	-	43,43,43,43	0
56	MG	BA	3608	1/1	0.97	0.13	-	45,45,45,45	0
56	MG	AA	3139	1/1	0.95	0.09	-	36,36,36,36	0
56	MG	DA	3147	1/1	0.95	0.18	-	47,47,47,47	0
56	MG	BA	3368	1/1	0.98	0.09	-	42,42,42,42	0
56	MG	BA	3297	1/1	0.93	0.12	-	39,39,39,39	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	DA	3553	1/1	0.97	0.12	-	46,46,46,46	0
56	MG	DA	3388	1/1	0.97	0.05	-	35,35,35,35	0
56	MG	CA	3072	1/1	0.91	0.14	-	57,57,57,57	0
56	MG	DA	3185	1/1	0.97	0.22	-	32,32,32,32	0
56	MG	AA	3124	1/1	0.90	0.19	-	30,30,30,30	0
56	MG	BA	3129	1/1	0.86	0.17	-	42,42,42,42	0
56	MG	AA	3074	1/1	0.96	0.15	-	38,38,38,38	0
56	MG	BA	3627	1/1	0.98	0.10	-	54,54,54,54	0
56	MG	BA	3100	1/1	0.98	0.11	-	29,29,29,29	0
56	MG	BG	3001	1/1	0.98	0.12	-	71,71,71,71	0
56	MG	BA	3438	1/1	0.98	0.12	-	33,33,33,33	0
56	MG	BA	3588	1/1	0.97	0.10	-	51,51,51,51	0
56	MG	DA	3144	1/1	0.94	0.14	-	38,38,38,38	0
56	MG	DA	3537	1/1	0.97	0.12	-	47,47,47,47	0
56	MG	DA	3581	1/1	0.94	0.19	-	53,53,53,53	0
56	MG	DA	3538	1/1	0.88	0.10	-	39,39,39,39	0
56	MG	B0	102	1/1	0.94	0.23	-	42,42,42,42	0
56	MG	AA	3159	1/1	0.93	0.08	-	56,56,56,56	0
56	MG	AA	3031	1/1	0.98	0.12	-	60,60,60,60	0
56	MG	BA	3374	1/1	0.95	0.11	-	29,29,29,29	0
56	MG	CA	3082	1/1	0.94	0.17	-	62,62,62,62	0
56	MG	CA	3120	1/1	0.96	0.13	-	51,51,51,51	0
56	MG	BA	3108	1/1	0.92	0.12	-	38,38,38,38	0
56	MG	DA	3065	1/1	0.89	0.15	-	49,49,49,49	0
56	MG	B7	3004	1/1	0.94	0.09	-	34,34,34,34	0
56	MG	DA	3418	1/1	0.95	0.13	-	29,29,29,29	0
56	MG	D8	5002	1/1	0.91	0.23	-	64,64,64,64	0
56	MG	BA	3453	1/1	0.99	0.09	-	27,27,27,27	0
56	MG	DA	3195	1/1	0.96	0.14	-	38,38,38,38	0
56	MG	DA	3543	1/1	0.94	0.08	-	63,63,63,63	0
56	MG	DA	3431	1/1	0.94	0.11	-	61,61,61,61	0
56	MG	AA	3071	1/1	0.84	0.12	-	36,36,36,36	0
56	MG	CA	3035	1/1	0.84	0.14	-	66,66,66,66	0
56	MG	DA	3224	1/1	0.97	0.15	-	22,22,22,22	0
56	MG	BA	3167	1/1	0.96	0.12	-	46,46,46,46	0
56	MG	CA	3030	1/1	0.94	0.10	-	41,41,41,41	0
56	MG	AD	502	1/1	0.94	0.21	-	55,55,55,55	0
56	MG	BA	3566	1/1	0.91	0.17	-	46,46,46,46	0
56	MG	BA	3460	1/1	0.95	0.14	-	57,57,57,57	0
56	MG	BA	3590	1/1	0.95	0.13	-	55,55,55,55	0
56	MG	BD	301	1/1	0.99	0.16	-	30,30,30,30	0
56	MG	CA	3029	1/1	0.92	0.14	-	48,48,48,48	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	BA	3633	1/1	0.89	0.14	-	57,57,57,57	0
56	MG	DA	3213	1/1	0.97	0.11	-	34,34,34,34	0
56	MG	CA	3148	1/1	0.95	0.10	-	57,57,57,57	0
56	MG	CA	3145	1/1	0.92	0.09	-	59,59,59,59	0
56	MG	DA	3586	1/1	0.97	0.09	-	47,47,47,47	0
56	MG	BA	3062	1/1	0.94	0.16	-	46,46,46,46	0
56	MG	DA	3559	1/1	0.98	0.09	-	55,55,55,55	0
56	MG	DA	3432	1/1	0.97	0.18	-	33,33,33,33	0
56	MG	DA	3368	1/1	0.92	0.07	-	25,25,25,25	0
56	MG	AA	3064	1/1	0.92	0.15	-	45,45,45,45	0
56	MG	BA	3171	1/1	0.86	0.14	-	44,44,44,44	0
56	MG	DA	3501	1/1	0.95	0.09	-	55,55,55,55	0
56	MG	BA	3619	1/1	0.75	0.16	-	30,30,30,30	0
56	MG	DA	3515	1/1	0.91	0.09	-	64,64,64,64	0
56	MG	BA	3455	1/1	0.99	0.11	-	21,21,21,21	0
56	MG	AA	3113	1/1	0.98	0.18	-	53,53,53,53	0
56	MG	BA	3355	1/1	0.99	0.09	-	31,31,31,31	0
56	MG	BA	3219	1/1	0.96	0.10	-	20,20,20,20	0
56	MG	BA	3070	1/1	0.94	0.11	-	30,30,30,30	0
56	MG	AA	3152	1/1	0.98	0.12	-	57,57,57,57	0
56	MG	CA	3125	1/1	0.94	0.22	-	71,71,71,71	0
56	MG	BA	3303	1/1	0.96	0.13	-	31,31,31,31	0
56	MG	BA	3542	1/1	0.98	0.05	-	51,51,51,51	0
56	MG	DA	3037	1/1	0.89	0.10	-	40,40,40,40	0
56	MG	DA	3129	1/1	0.94	0.14	-	54,54,54,54	0
56	MG	DA	3118	1/1	0.95	0.20	-	49,49,49,49	0
56	MG	CA	3127	1/1	0.97	0.08	-	49,49,49,49	0
56	MG	DA	3227	1/1	0.96	0.15	-	49,49,49,49	0
56	MG	DA	3472	1/1	0.91	0.16	-	53,53,53,53	0
56	MG	BA	3580	1/1	0.83	0.13	-	62,62,62,62	0
56	MG	BA	3663	1/1	0.98	0.08	-	20,20,20,20	0
56	MG	AF	3001	1/1	0.83	0.15	-	52,52,52,52	0
56	MG	CA	3114	1/1	0.97	0.09	-	80,80,80,80	0
56	MG	DA	3126	1/1	0.93	0.18	-	42,42,42,42	0
56	MG	BA	3091	1/1	0.99	0.14	-	19,19,19,19	0
56	MG	DA	3116	1/1	0.94	0.14	-	29,29,29,29	0
56	MG	DA	3505	1/1	0.98	0.10	-	44,44,44,44	0
56	MG	BA	3370	1/1	0.97	0.15	-	29,29,29,29	0
56	MG	AA	3002	1/1	0.91	0.17	-	43,43,43,43	0
56	MG	DA	3023	1/1	0.98	0.14	-	37,37,37,37	0
56	MG	CA	3138	1/1	0.87	0.15	-	58,58,58,58	0
56	MG	BA	3448	1/1	0.97	0.12	-	42,42,42,42	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	BA	3205	1/1	0.94	0.16	-	40,40,40,40	0
56	MG	BA	3115	1/1	0.92	0.13	-	34,34,34,34	0
56	MG	DA	3192	1/1	0.90	0.09	-	51,51,51,51	0
56	MG	BA	3260	1/1	0.88	0.22	-	49,49,49,49	0
56	MG	BA	3611	1/1	0.93	0.40	-	59,59,59,59	0
56	MG	CA	3132	1/1	0.91	0.18	-	73,73,73,73	0
56	MG	CA	3022	1/1	0.97	0.14	-	34,34,34,34	0
56	MG	DA	3256	1/1	0.84	0.15	-	45,45,45,45	0
56	MG	DA	3362	1/1	0.98	0.08	-	43,43,43,43	0
56	MG	BA	3396	1/1	0.93	0.22	-	38,38,38,38	0
56	MG	CA	3076	1/1	0.97	0.23	-	48,48,48,48	0
56	MG	DA	3239	1/1	0.89	0.20	-	56,56,56,56	0
56	MG	DA	3445	1/1	0.95	0.13	-	48,48,48,48	0
56	MG	BA	3545	1/1	0.93	0.08	-	54,54,54,54	0
56	MG	CA	3007	1/1	0.94	0.09	-	50,50,50,50	0
56	MG	AA	3048	1/1	0.96	0.21	-	42,42,42,42	0
56	MG	DA	3052	1/1	0.89	0.15	-	49,49,49,49	0
56	MG	DA	3590	1/1	0.97	0.35	-	38,38,38,38	0
56	MG	DA	3425	1/1	0.89	0.14	-	37,37,37,37	0
56	MG	DA	3504	1/1	0.87	0.12	-	49,49,49,49	0
56	MG	DE	3001	1/1	0.90	0.20	-	43,43,43,43	0
56	MG	DA	3112	1/1	0.96	0.14	-	24,24,24,24	0
56	MG	AA	3066	1/1	0.92	0.18	-	46,46,46,46	0
56	MG	CA	3006	1/1	0.98	0.28	-	37,37,37,37	0
56	MG	BA	3427	1/1	0.93	0.21	-	49,49,49,49	0
56	MG	DA	3415	1/1	0.96	0.17	-	40,40,40,40	0
56	MG	AA	3145	1/1	0.94	0.12	-	35,35,35,35	0
56	MG	AA	3095	1/1	0.97	0.16	-	55,55,55,55	0
56	MG	BA	3127	1/1	0.79	0.25	-	45,45,45,45	0
56	MG	BA	3242	1/1	0.96	0.26	-	46,46,46,46	0
56	MG	AA	3122	1/1	0.91	0.11	-	58,58,58,58	0
56	MG	BA	3169	1/1	0.86	0.13	-	39,39,39,39	0
56	MG	BA	3099	1/1	0.98	0.19	-	32,32,32,32	0
56	MG	DA	3547	1/1	0.93	0.17	-	41,41,41,41	0
56	MG	BA	3500	1/1	0.97	0.11	-	35,35,35,35	0
56	MG	DA	3346	1/1	0.92	0.11	-	33,33,33,33	0
56	MG	AA	3161	1/1	0.96	0.10	-	66,66,66,66	0
56	MG	BA	3015	1/1	0.96	0.13	-	27,27,27,27	0
56	MG	AA	3133	1/1	0.98	0.08	-	38,38,38,38	0
56	MG	DA	3138	1/1	0.97	0.12	-	33,33,33,33	0
56	MG	DB	3010	1/1	0.92	0.20	-	60,60,60,60	0
56	MG	CA	3049	1/1	0.86	0.17	-	51,51,51,51	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	DB	3008	1/1	0.93	0.13	-	35,35,35,35	0
56	MG	DA	3394	1/1	0.95	0.09	-	41,41,41,41	0
56	MG	BA	3563	1/1	0.96	0.17	-	47,47,47,47	0
56	MG	CA	3129	1/1	0.87	0.14	-	55,55,55,55	0
56	MG	DA	3424	1/1	0.92	0.18	-	30,30,30,30	0
56	MG	DA	3105	1/1	0.91	0.09	-	36,36,36,36	0
56	MG	D8	5001	1/1	0.97	0.13	-	50,50,50,50	0
56	MG	AA	3052	1/1	0.94	0.19	-	60,60,60,60	0
56	MG	BA	3280	1/1	0.95	0.10	-	48,48,48,48	0
56	MG	DA	3089	1/1	0.94	0.34	-	33,33,33,33	0
56	MG	DT	5001	1/1	0.97	0.07	-	42,42,42,42	0
56	MG	BA	3189	1/1	0.91	0.22	-	26,26,26,26	0
56	MG	BA	3522	1/1	0.98	0.10	-	52,52,52,52	0
56	MG	BA	3010	1/1	0.91	0.14	-	33,33,33,33	0
56	MG	BA	3576	1/1	0.83	0.17	-	48,48,48,48	0
56	MG	BA	3385	1/1	0.99	0.09	-	20,20,20,20	0
56	MG	BA	3180	1/1	0.91	0.32	-	33,33,33,33	0
56	MG	BA	3592	1/1	0.92	0.20	-	52,52,52,52	0
56	MG	AA	3157	1/1	0.96	0.09	-	55,55,55,55	0
56	MG	BA	3143	1/1	0.97	0.33	-	36,36,36,36	0
56	MG	BA	3613	1/1	0.98	0.15	-	45,45,45,45	0
56	MG	AA	3171	1/1	0.95	0.10	-	62,62,62,62	0
56	MG	BA	3344	1/1	0.94	0.14	-	35,35,35,35	0
56	MG	BA	3509	1/1	0.97	0.16	-	23,23,23,23	0
56	MG	AA	3092	1/1	0.88	0.17	-	61,61,61,61	0
56	MG	DA	3349	1/1	0.99	0.15	-	46,46,46,46	0
56	MG	DA	3271	1/1	0.90	0.09	-	55,55,55,55	0
56	MG	DA	3373	1/1	0.87	0.13	-	42,42,42,42	0
56	MG	DA	3115	1/1	0.91	0.14	-	36,36,36,36	0
56	MG	DA	3277	1/1	0.97	0.10	-	48,48,48,48	0
56	MG	DA	3304	1/1	0.93	0.18	-	32,32,32,32	0
56	MG	BA	3173	1/1	0.98	0.19	-	45,45,45,45	0
56	MG	DA	3133	1/1	0.97	0.11	-	53,53,53,53	0
56	MG	DA	3313	1/1	0.98	0.09	-	40,40,40,40	0
56	MG	DA	3106	1/1	0.93	0.06	-	43,43,43,43	0
56	MG	BA	3130	1/1	0.95	0.28	-	40,40,40,40	0
56	MG	DA	3533	1/1	0.91	0.08	-	60,60,60,60	0
56	MG	BA	3375	1/1	0.96	0.21	-	51,51,51,51	0
56	MG	DA	3205	1/1	0.95	0.16	-	32,32,32,32	0
56	MG	BA	3444	1/1	0.97	0.11	-	34,34,34,34	0
56	MG	CA	3028	1/1	0.89	0.12	-	52,52,52,52	0
56	MG	DA	3507	1/1	0.94	0.08	-	54,54,54,54	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	DA	3478	1/1	0.86	0.14	-	53,53,53,53	0
56	MG	BA	3538	1/1	0.94	0.14	-	55,55,55,55	0
56	MG	DA	3518	1/1	0.89	0.19	-	53,53,53,53	0
56	MG	DA	3524	1/1	0.96	0.08	-	51,51,51,51	0
56	MG	DA	3171	1/1	0.94	0.24	-	51,51,51,51	0
56	MG	DA	3483	1/1	0.95	0.13	-	54,54,54,54	0
56	MG	DA	3119	1/1	0.89	0.20	-	37,37,37,37	0
56	MG	AX	3004	1/1	0.96	0.17	-	39,39,39,39	0
56	MG	AA	3176	1/1	0.90	0.12	-	60,60,60,60	0
56	MG	CA	3038	1/1	0.97	0.12	-	44,44,44,44	0
56	MG	BA	3531	1/1	0.88	0.09	-	41,41,41,41	0
56	MG	DA	3121	1/1	0.75	0.44	-	50,50,50,50	0
56	MG	BA	3584	1/1	0.92	0.19	-	44,44,44,44	0
56	MG	DA	3167	1/1	0.93	0.09	-	51,51,51,51	0
56	MG	CA	3041	1/1	0.89	0.13	-	67,67,67,67	0
56	MG	BA	3048	1/1	0.88	0.15	-	47,47,47,47	0
56	MG	DA	3323	1/1	0.92	0.12	-	35,35,35,35	0
56	MG	AA	3094	1/1	0.92	0.20	-	49,49,49,49	0
56	MG	BA	3353	1/1	0.95	0.13	-	39,39,39,39	0
56	MG	BA	3525	1/1	0.93	0.09	-	46,46,46,46	0
56	MG	AA	3093	1/1	0.88	0.18	-	45,45,45,45	0
56	MG	DA	3497	1/1	0.98	0.08	-	45,45,45,45	0
56	MG	BA	3337	1/1	0.98	0.12	-	37,37,37,37	0
56	MG	BA	3476	1/1	0.95	0.07	-	51,51,51,51	0
56	MG	BA	3079	1/1	0.92	0.12	-	46,46,46,46	0
56	MG	DA	3460	1/1	0.96	0.18	-	50,50,50,50	0
56	MG	AA	3015	1/1	0.96	0.13	-	56,56,56,56	0
56	MG	DA	3477	1/1	0.87	0.13	-	42,42,42,42	0
56	MG	BA	3291	1/1	0.97	0.14	-	14,14,14,14	0
56	MG	DA	3024	1/1	0.93	0.16	-	36,36,36,36	0
56	MG	DA	3398	1/1	0.81	0.13	-	51,51,51,51	0
56	MG	AA	3123	1/1	0.96	0.16	-	38,38,38,38	0
56	MG	DA	3458	1/1	0.98	0.13	-	34,34,34,34	0
56	MG	CA	3042	1/1	0.96	0.12	-	56,56,56,56	0
56	MG	BA	3306	1/1	0.92	0.13	-	54,54,54,54	0
56	MG	BA	3333	1/1	0.98	0.19	-	35,35,35,35	0
56	MG	BA	3046	1/1	0.95	0.21	-	29,29,29,29	0
56	MG	BA	3338	1/1	0.93	0.11	-	48,48,48,48	0
56	MG	BA	3543	1/1	0.93	0.10	-	47,47,47,47	0
56	MG	DA	3244	1/1	0.93	0.14	-	48,48,48,48	0
56	MG	DA	3528	1/1	0.95	0.06	-	37,37,37,37	0
56	MG	DA	3261	1/1	0.92	0.15	-	49,49,49,49	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	DA	3120	1/1	0.95	0.22	-	33,33,33,33	0
56	MG	BA	3314	1/1	0.97	0.18	-	36,36,36,36	0
56	MG	BA	3247	1/1	0.93	0.19	-	48,48,48,48	0
56	MG	BA	3582	1/1	0.96	0.11	-	31,31,31,31	0
56	MG	CA	3013	1/1	0.88	0.16	-	53,53,53,53	0
56	MG	BA	3083	1/1	0.92	0.17	-	34,34,34,34	0
56	MG	DA	3570	1/1	0.96	0.14	-	52,52,52,52	0
56	MG	BA	3075	1/1	0.83	0.28	-	58,58,58,58	0
56	MG	CA	3040	1/1	0.96	0.25	-	52,52,52,52	0
56	MG	BA	3481	1/1	0.97	0.15	-	31,31,31,31	0
56	MG	CA	3069	1/1	0.93	0.12	-	34,34,34,34	0
56	MG	CA	3091	1/1	0.97	0.15	-	66,66,66,66	0
56	MG	BA	3443	1/1	0.95	0.11	-	44,44,44,44	0
56	MG	CA	3099	1/1	0.97	0.14	-	57,57,57,57	0
56	MG	BA	3320	1/1	0.98	0.13	-	44,44,44,44	0
56	MG	DQ	3002	1/1	0.92	0.21	-	38,38,38,38	0
56	MG	DA	3003	1/1	0.93	0.20	-	47,47,47,47	0
56	MG	CA	3009	1/1	0.92	0.13	-	55,55,55,55	0
56	MG	BA	3521	1/1	0.85	0.11	-	54,54,54,54	0
56	MG	BA	3089	1/1	0.97	0.14	-	37,37,37,37	0
56	MG	DA	3103	1/1	0.96	0.07	-	56,56,56,56	0
56	MG	DA	3021	1/1	0.84	0.15	-	55,55,55,55	0
56	MG	DA	3010	1/1	0.93	0.16	-	36,36,36,36	0
56	MG	DA	3219	1/1	0.98	0.12	-	33,33,33,33	0
56	MG	BA	3583	1/1	0.94	0.10	-	37,37,37,37	0
56	MG	BA	3076	1/1	0.94	0.08	-	29,29,29,29	0
56	MG	CA	3142	1/1	0.96	0.12	-	42,42,42,42	0
56	MG	BA	3464	1/1	0.96	0.08	-	41,41,41,41	0
56	MG	DA	3490	1/1	0.98	0.15	-	34,34,34,34	0
56	MG	BA	3163	1/1	0.93	0.12	-	31,31,31,31	0
56	MG	BB	3002	1/1	0.93	0.20	-	41,41,41,41	0
56	MG	DA	3360	1/1	0.95	0.09	-	39,39,39,39	0
56	MG	DA	3161	1/1	0.91	0.16	-	24,24,24,24	0
56	MG	DA	3459	1/1	0.97	0.24	-	38,38,38,38	0
56	MG	BA	3441	1/1	0.87	0.12	-	44,44,44,44	0
56	MG	CA	3003	1/1	0.93	0.10	-	65,65,65,65	0
56	MG	DA	3057	1/1	0.93	0.12	-	30,30,30,30	0
56	MG	DA	3536	1/1	0.98	0.11	-	56,56,56,56	0
56	MG	DA	3194	1/1	0.91	0.09	-	47,47,47,47	0
56	MG	AA	3109	1/1	0.86	0.18	-	44,44,44,44	0
56	MG	DA	3073	1/1	0.87	0.14	-	51,51,51,51	0
56	MG	BA	3223	1/1	0.96	0.16	-	51,51,51,51	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	DB	3005	1/1	0.77	0.21	-	56,56,56,56	0
56	MG	BA	3614	1/1	0.98	0.05	-	55,55,55,55	0
56	MG	BA	3187	1/1	0.90	0.13	-	37,37,37,37	0
56	MG	DA	3249	1/1	0.95	0.09	-	34,34,34,34	0
56	MG	AA	3053	1/1	0.94	0.07	-	50,50,50,50	0
56	MG	AA	3119	1/1	0.93	0.11	-	57,57,57,57	0
56	MG	BA	3090	1/1	0.78	0.20	-	44,44,44,44	0
56	MG	CA	3077	1/1	0.98	0.14	-	44,44,44,44	0
56	MG	DA	3257	1/1	0.94	0.17	-	55,55,55,55	0
56	MG	DA	3482	1/1	0.95	0.10	-	46,46,46,46	0
56	MG	BW	3004	1/1	0.88	0.23	-	30,30,30,30	0
56	MG	BA	3415	1/1	0.95	0.21	-	54,54,54,54	0
56	MG	BB	3016	1/1	0.94	0.11	-	24,24,24,24	0
56	MG	BA	3480	1/1	0.95	0.21	-	43,43,43,43	0
56	MG	AA	3028	1/1	0.93	0.18	-	39,39,39,39	0
56	MG	BA	3450	1/1	0.96	0.15	-	45,45,45,45	0
56	MG	AA	3142	1/1	0.94	0.15	-	60,60,60,60	0
56	MG	CA	3067	1/1	0.94	0.07	-	63,63,63,63	0
56	MG	BA	3587	1/1	0.97	0.14	-	42,42,42,42	0
56	MG	CA	3083	1/1	0.79	0.20	-	66,66,66,66	0
56	MG	BA	3514	1/1	0.99	0.08	-	32,32,32,32	0
56	MG	DA	3143	1/1	0.97	0.21	-	27,27,27,27	0
56	MG	BA	3327	1/1	0.96	0.14	-	44,44,44,44	0
56	MG	BA	3336	1/1	0.97	0.09	-	43,43,43,43	0
59	K	DA	3001	1/1	0.94	0.10	-	48,48,48,48	0
56	MG	CF	3001	1/1	0.91	0.13	-	45,45,45,45	0
56	MG	DA	3300	1/1	0.93	0.18	-	58,58,58,58	0
56	MG	BA	3555	1/1	0.96	0.20	-	42,42,42,42	0
56	MG	BA	3630	1/1	0.95	0.12	-	47,47,47,47	0
56	MG	BA	3002	1/1	0.90	0.14	-	39,39,39,39	0
56	MG	BE	301	1/1	0.99	0.08	-	45,45,45,45	0
56	MG	CA	3107	1/1	0.93	0.15	-	56,56,56,56	0
56	MG	BA	3225	1/1	0.94	0.11	-	31,31,31,31	0
56	MG	BA	3119	1/1	0.90	0.09	-	29,29,29,29	0
56	MG	BA	3399	1/1	0.94	0.12	-	42,42,42,42	0
56	MG	AA	3072	1/1	0.92	0.10	-	39,39,39,39	0
56	MG	BA	3359	1/1	0.92	0.13	-	54,54,54,54	0
56	MG	BA	3206	1/1	0.88	0.20	-	41,41,41,41	0
56	MG	DA	3207	1/1	0.96	0.13	-	39,39,39,39	0
56	MG	DA	3078	1/1	0.92	0.09	-	46,46,46,46	0
56	MG	BA	3134	1/1	0.96	0.28	-	40,40,40,40	0
56	MG	BA	3321	1/1	0.98	0.07	-	53,53,53,53	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	AX	3003	1/1	0.92	0.23	-	50,50,50,50	0
56	MG	BA	3170	1/1	0.98	0.12	-	34,34,34,34	0
56	MG	DA	3539	1/1	0.94	0.12	-	52,52,52,52	0
56	MG	DA	3583	1/1	0.93	0.10	-	43,43,43,43	0
56	MG	BA	3493	1/1	0.96	0.14	-	40,40,40,40	0
56	MG	CA	3124	1/1	0.93	0.12	-	52,52,52,52	0
56	MG	DA	3585	1/1	0.97	0.08	-	37,37,37,37	0
56	MG	AA	3167	1/1	0.89	0.14	-	73,73,73,73	0
56	MG	CA	3078	1/1	0.90	0.07	-	66,66,66,66	0
56	MG	CE	202	1/1	0.94	0.12	-	68,68,68,68	0
56	MG	DA	3068	1/1	0.91	0.14	-	35,35,35,35	0
56	MG	BA	3231	1/1	0.96	0.22	-	41,41,41,41	0
56	MG	DA	3377	1/1	0.98	0.14	-	37,37,37,37	0
56	MG	BA	3431	1/1	0.96	0.10	-	44,44,44,44	0
56	MG	BA	3232	1/1	0.92	0.18	-	41,41,41,41	0
56	MG	BA	3623	1/1	0.90	0.10	-	48,48,48,48	0
56	MG	CA	3021	1/1	0.91	0.21	-	52,52,52,52	0
56	MG	BA	3410	1/1	0.96	0.14	-	43,43,43,43	0
56	MG	BA	3145	1/1	0.94	0.22	-	30,30,30,30	0
56	MG	BA	3275	1/1	0.99	0.18	-	39,39,39,39	0
56	MG	DA	3479	1/1	0.75	0.12	-	63,63,63,63	0
56	MG	DA	3502	1/1	0.99	0.12	-	39,39,39,39	0
56	MG	BA	3049	1/1	0.91	0.14	-	43,43,43,43	0
56	MG	BA	3573	1/1	0.94	0.18	-	44,44,44,44	0
56	MG	AA	3183	1/1	0.83	0.19	-	55,55,55,55	0
56	MG	DA	3544	1/1	0.85	0.18	-	51,51,51,51	0
56	MG	BA	3059	1/1	0.99	0.11	-	27,27,27,27	0
56	MG	CA	3144	1/1	0.97	0.12	-	56,56,56,56	0
56	MG	BA	3607	1/1	0.94	0.14	-	51,51,51,51	0
56	MG	BA	3602	1/1	0.93	0.16	-	31,31,31,31	0
56	MG	BA	3086	1/1	0.91	0.18	-	39,39,39,39	0
56	MG	DA	3270	1/1	0.97	0.08	-	37,37,37,37	0
56	MG	AA	3033	1/1	0.93	0.29	-	48,48,48,48	0
56	MG	DA	3400	1/1	0.97	0.17	-	38,38,38,38	0
56	MG	AA	3177	1/1	0.94	0.15	-	32,32,32,32	0
56	MG	DA	3108	1/1	0.87	0.10	-	46,46,46,46	0
56	MG	DA	3448	1/1	0.97	0.20	-	29,29,29,29	0
56	MG	DA	3235	1/1	0.98	0.18	-	42,42,42,42	0
56	MG	BA	3403	1/1	0.93	0.14	-	18,18,18,18	0
56	MG	BA	3489	1/1	0.99	0.25	-	41,41,41,41	0
56	MG	AA	3032	1/1	0.95	0.15	-	42,42,42,42	0
56	MG	BA	3365	1/1	0.95	0.11	-	41,41,41,41	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	BA	3012	1/1	0.84	0.14	-	39,39,39,39	0
56	MG	DA	3287	1/1	0.96	0.11	-	38,38,38,38	0
56	MG	BA	3620	1/1	0.99	0.16	-	41,41,41,41	0
56	MG	BA	3675	1/1	0.93	0.39	-	33,33,33,33	0
56	MG	BA	3346	1/1	0.97	0.08	-	43,43,43,43	0
56	MG	DA	3054	1/1	0.85	0.23	-	45,45,45,45	0
56	MG	DA	3469	1/1	0.90	0.18	-	33,33,33,33	0
56	MG	BB	3013	1/1	0.98	0.16	-	57,57,57,57	0
56	MG	DA	3470	1/1	0.93	0.19	-	52,52,52,52	0
56	MG	DA	3186	1/1	0.90	0.14	-	41,41,41,41	0
56	MG	BA	3215	1/1	0.97	0.14	-	32,32,32,32	0
56	MG	AA	3040	1/1	0.97	0.16	-	27,27,27,27	0
56	MG	DA	3058	1/1	0.93	0.22	-	45,45,45,45	0
56	MG	DA	3295	1/1	0.97	0.25	-	61,61,61,61	0
56	MG	AA	3084	1/1	0.93	0.10	-	43,43,43,43	0
56	MG	BA	3176	1/1	0.98	0.10	-	47,47,47,47	0
56	MG	DW	3002	1/1	0.84	0.19	-	60,60,60,60	0
56	MG	DA	3503	1/1	0.96	0.07	-	38,38,38,38	0
56	MG	BA	3074	1/1	0.93	0.14	-	45,45,45,45	0
56	MG	BA	3425	1/1	0.93	0.23	-	53,53,53,53	0
56	MG	DA	3196	1/1	0.93	0.14	-	33,33,33,33	0
56	MG	DA	3265	1/1	0.91	0.28	-	51,51,51,51	0
56	MG	CA	3084	1/1	0.84	0.10	-	72,72,72,72	0
56	MG	DA	3288	1/1	0.98	0.11	-	64,64,64,64	0
56	MG	CA	3136	1/1	0.81	0.12	-	53,53,53,53	0
56	MG	BA	3354	1/1	0.98	0.11	-	42,42,42,42	0
56	MG	DA	3248	1/1	0.96	0.28	-	52,52,52,52	0
56	MG	AA	3010	1/1	0.81	0.15	-	60,60,60,60	0
56	MG	DA	3151	1/1	0.87	0.14	-	34,34,34,34	0
56	MG	DA	3315	1/1	0.97	0.16	-	43,43,43,43	0
56	MG	BA	3166	1/1	0.97	0.12	-	35,35,35,35	0
56	MG	CA	3102	1/1	0.98	0.19	-	30,30,30,30	0
56	MG	BA	3594	1/1	0.92	0.13	-	37,37,37,37	0
56	MG	DA	3263	1/1	0.95	0.11	-	39,39,39,39	0
56	MG	BA	3175	1/1	0.96	0.14	-	33,33,33,33	0
56	MG	DA	3341	1/1	0.95	0.13	-	25,25,25,25	0
56	MG	BA	3406	1/1	0.98	0.22	-	39,39,39,39	0
56	MG	CA	3141	1/1	0.93	0.17	-	54,54,54,54	0
56	MG	BA	3632	1/1	0.97	0.14	-	54,54,54,54	0
56	MG	DA	3339	1/1	0.95	0.14	-	32,32,32,32	0
56	MG	BA	3250	1/1	0.96	0.18	-	33,33,33,33	0
56	MG	BA	3053	1/1	0.95	0.18	-	31,31,31,31	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	DA	3251	1/1	0.68	0.18	-	62,62,62,62	0
56	MG	DA	3429	1/1	0.91	0.12	-	35,35,35,35	0
56	MG	DA	3387	1/1	0.98	0.07	-	53,53,53,53	0
56	MG	DA	3130	1/1	0.97	0.26	-	47,47,47,47	0
56	MG	BA	3201	1/1	0.94	0.11	-	41,41,41,41	0
56	MG	BB	3012	1/1	0.97	0.14	-	44,44,44,44	0
56	MG	BA	3087	1/1	0.90	0.18	-	36,36,36,36	0
56	MG	AA	3061	1/1	0.87	0.13	-	62,62,62,62	0
56	MG	BA	3027	1/1	0.97	0.21	-	28,28,28,28	0
56	MG	BA	3597	1/1	0.95	0.15	-	43,43,43,43	0
56	MG	BA	3281	1/1	0.98	0.22	-	51,51,51,51	0
56	MG	BB	3017	1/1	0.94	0.11	-	40,40,40,40	0
56	MG	CA	3015	1/1	0.95	0.15	-	43,43,43,43	0
56	MG	AA	3162	1/1	0.98	0.12	-	40,40,40,40	0
56	MG	DA	3166	1/1	0.97	0.15	-	35,35,35,35	0
56	MG	BA	3413	1/1	0.98	0.16	-	26,26,26,26	0
56	MG	DA	3193	1/1	0.96	0.23	-	49,49,49,49	0
56	MG	BA	3629	1/1	0.93	0.08	-	60,60,60,60	0
56	MG	BA	3272	1/1	0.98	0.10	-	37,37,37,37	0
56	MG	CA	3122	1/1	0.94	0.21	-	54,54,54,54	0
56	MG	BA	3063	1/1	0.96	0.09	-	47,47,47,47	0
56	MG	AX	3005	1/1	0.96	0.26	-	42,42,42,42	0
56	MG	BA	3066	1/1	0.92	0.18	-	48,48,48,48	0
56	MG	BA	3610	1/1	0.96	0.17	-	47,47,47,47	0
56	MG	BA	3547	1/1	0.97	0.06	-	60,60,60,60	0
56	MG	AA	3158	1/1	0.95	0.09	-	54,54,54,54	0
56	MG	BA	3160	1/1	0.96	0.15	-	29,29,29,29	0
56	MG	CA	3027	1/1	0.94	0.15	-	64,64,64,64	0
56	MG	BA	3390	1/1	0.95	0.09	-	47,47,47,47	0
56	MG	DA	3274	1/1	0.90	0.10	-	56,56,56,56	0
56	MG	BA	3073	1/1	0.95	0.18	-	14,14,14,14	0
56	MG	DA	3433	1/1	0.98	0.16	-	33,33,33,33	0
56	MG	BA	3238	1/1	0.95	0.21	-	47,47,47,47	0
56	MG	BA	3421	1/1	0.98	0.18	-	36,36,36,36	0
56	MG	DA	3090	1/1	0.85	0.10	-	54,54,54,54	0
56	MG	BA	3347	1/1	0.85	0.11	-	53,53,53,53	0
56	MG	CA	3074	1/1	0.94	0.19	-	48,48,48,48	0
56	MG	DA	3385	1/1	0.93	0.08	-	45,45,45,45	0
56	MG	BA	3574	1/1	0.97	0.12	-	55,55,55,55	0
56	MG	BA	3436	1/1	0.97	0.10	-	35,35,35,35	0
56	MG	BA	3674	1/1	0.96	0.23	-	54,54,54,54	0
56	MG	DA	3312	1/1	0.99	0.04	-	47,47,47,47	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	BA	3358	1/1	0.98	0.17	-	39,39,39,39	0
56	MG	AA	3169	1/1	0.95	0.12	-	71,71,71,71	0
56	MG	BA	3483	1/1	0.92	0.13	-	47,47,47,47	0
56	MG	CA	3070	1/1	0.97	0.08	-	39,39,39,39	0
56	MG	BA	3118	1/1	0.91	0.31	-	45,45,45,45	0
56	MG	CX	101	1/1	0.93	0.19	-	48,48,48,48	0
56	MG	DA	3325	1/1	0.90	0.13	-	54,54,54,54	0
56	MG	BA	3025	1/1	0.95	0.14	-	37,37,37,37	0
56	MG	AA	3089	1/1	0.89	0.14	-	36,36,36,36	0
56	MG	DA	3139	1/1	0.94	0.22	-	39,39,39,39	0
56	MG	BA	3277	1/1	0.95	0.22	-	32,32,32,32	0
56	MG	BA	3628	1/1	0.97	0.12	-	38,38,38,38	0
56	MG	BA	3262	1/1	0.98	0.17	-	24,24,24,24	0
56	MG	CA	3085	1/1	0.89	0.12	-	52,52,52,52	0
56	MG	BA	3293	1/1	0.96	0.13	-	17,17,17,17	0
56	MG	BA	3028	1/1	0.80	0.16	-	41,41,41,41	0
56	MG	DB	3012	1/1	0.92	0.14	-	53,53,53,53	0
56	MG	BA	3498	1/1	0.94	0.19	-	37,37,37,37	0
56	MG	BA	3239	1/1	0.94	0.14	-	52,52,52,52	0
56	MG	DA	3420	1/1	0.94	0.17	-	46,46,46,46	0
56	MG	BA	3233	1/1	0.94	0.12	-	41,41,41,41	0
56	MG	BA	3376	1/1	0.94	0.12	-	39,39,39,39	0
56	MG	BA	3528	1/1	0.96	0.19	-	38,38,38,38	0
56	MG	BA	3137	1/1	0.95	0.22	-	30,30,30,30	0
56	MG	CA	3024	1/1	0.97	0.08	-	64,64,64,64	0
56	MG	DB	3001	1/1	0.98	0.17	-	40,40,40,40	0
56	MG	DA	3306	1/1	0.95	0.11	-	38,38,38,38	0
56	MG	CA	3045	1/1	0.92	0.16	-	52,52,52,52	0
56	MG	DA	3310	1/1	0.96	0.09	-	41,41,41,41	0
56	MG	BA	3146	1/1	0.98	0.18	-	31,31,31,31	0
56	MG	AA	3130	1/1	0.97	0.11	-	50,50,50,50	0
56	MG	BA	3535	1/1	0.99	0.10	-	47,47,47,47	0
56	MG	AA	3038	1/1	0.90	0.14	-	53,53,53,53	0
56	MG	BA	3465	1/1	0.96	0.10	-	37,37,37,37	0
56	MG	AA	3187	1/1	0.96	0.14	-	33,33,33,33	0
56	MG	BA	3426	1/1	0.93	0.12	-	43,43,43,43	0
56	MG	AA	3079	1/1	0.97	0.33	-	49,49,49,49	0
56	MG	DA	3093	1/1	0.92	0.22	-	46,46,46,46	0
56	MG	BA	3360	1/1	0.98	0.15	-	21,21,21,21	0
56	MG	BA	3392	1/1	0.95	0.17	-	41,41,41,41	0
56	MG	DA	3006	1/1	0.98	0.15	-	33,33,33,33	0
56	MG	DA	3541	1/1	0.97	0.15	-	57,57,57,57	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	BA	3311	1/1	0.96	0.11	-	39,39,39,39	0
56	MG	BA	3402	1/1	0.97	0.23	-	28,28,28,28	0
56	MG	DA	3279	1/1	0.97	0.12	-	27,27,27,27	0
56	MG	DA	3260	1/1	0.97	0.20	-	36,36,36,36	0
56	MG	DA	3031	1/1	0.98	0.13	-	21,21,21,21	0
56	MG	BA	3636	1/1	0.95	0.11	-	32,32,32,32	0
56	MG	AA	3009	1/1	0.95	0.11	-	54,54,54,54	0
56	MG	BA	3348	1/1	0.96	0.13	-	31,31,31,31	0
56	MG	CA	3103	1/1	0.92	0.11	-	52,52,52,52	0
56	MG	DA	3072	1/1	0.97	0.10	-	33,33,33,33	0
56	MG	BA	3184	1/1	0.97	0.10	-	37,37,37,37	0
56	MG	CA	3010	1/1	0.95	0.14	-	53,53,53,53	0
56	MG	BA	3617	1/1	0.89	0.26	-	66,66,66,66	0
56	MG	DA	3283	1/1	0.97	0.11	-	38,38,38,38	0
56	MG	DA	3563	1/1	0.92	0.17	-	60,60,60,60	0
56	MG	BA	3186	1/1	0.93	0.15	-	39,39,39,39	0
56	MG	BA	3258	1/1	0.95	0.23	-	30,30,30,30	0
56	MG	DY	502	1/1	0.94	0.15	-	51,51,51,51	0
56	MG	BA	3412	1/1	0.96	0.17	-	48,48,48,48	0
56	MG	DA	3107	1/1	0.94	0.17	-	46,46,46,46	0
56	MG	DA	3467	1/1	0.95	0.12	-	47,47,47,47	0
56	MG	DA	3551	1/1	0.95	0.17	-	52,52,52,52	0
56	MG	AA	3004	1/1	0.97	0.15	-	67,67,67,67	0
56	MG	BA	3546	1/1	0.86	0.10	-	57,57,57,57	0
56	MG	DA	3039	1/1	0.94	0.28	-	51,51,51,51	0
56	MG	BA	3226	1/1	0.94	0.45	-	32,32,32,32	0
56	MG	BA	3520	1/1	0.98	0.14	-	24,24,24,24	0
56	MG	BA	3626	1/1	0.91	0.17	-	50,50,50,50	0
56	MG	DA	3340	1/1	0.91	0.10	-	47,47,47,47	0
56	MG	DA	3343	1/1	0.95	0.17	-	56,56,56,56	0
56	MG	CA	3146	1/1	0.94	0.05	-	42,42,42,42	0
56	MG	BA	3128	1/1	0.93	0.18	-	29,29,29,29	0
56	MG	AA	3024	1/1	0.81	0.18	-	60,60,60,60	0
56	MG	DA	3324	1/1	0.98	0.12	-	52,52,52,52	0
56	MG	BA	3505	1/1	0.92	0.18	-	46,46,46,46	0
56	MG	AA	3180	1/1	0.83	0.11	-	56,56,56,56	0
56	MG	CJ	5001	1/1	0.89	0.09	-	60,60,60,60	0
56	MG	BA	3518	1/1	0.92	0.19	-	41,41,41,41	0
56	MG	DA	3554	1/1	0.90	0.09	-	68,68,68,68	0
56	MG	AA	3141	1/1	0.97	0.07	-	47,47,47,47	0
56	MG	BQ	202	1/1	0.97	0.08	-	14,14,14,14	0
56	MG	BA	3328	1/1	0.95	0.13	-	39,39,39,39	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	DA	3546	1/1	0.96	0.07	-	40,40,40,40	0
56	MG	BA	3603	1/1	0.98	0.05	-	49,49,49,49	0
56	MG	DA	3141	1/1	0.89	0.07	-	42,42,42,42	0
56	MG	DA	3184	1/1	0.95	0.19	-	30,30,30,30	0
56	MG	BA	3642	1/1	0.93	0.19	-	47,47,47,47	0
56	MG	BA	3429	1/1	0.96	0.18	-	41,41,41,41	0
56	MG	DA	3468	1/1	0.95	0.24	-	55,55,55,55	0
56	MG	DA	3513	1/1	0.99	0.12	-	32,32,32,32	0
56	MG	DA	3427	1/1	0.97	0.15	-	25,25,25,25	0
56	MG	DA	3302	1/1	0.90	0.10	-	43,43,43,43	0
56	MG	DA	3293	1/1	0.96	0.13	-	34,34,34,34	0
56	MG	DA	3212	1/1	0.88	0.17	-	39,39,39,39	0
56	MG	DA	3376	1/1	0.96	0.05	-	38,38,38,38	0
56	MG	AA	3027	1/1	0.83	0.16	-	71,71,71,71	0
56	MG	DA	3262	1/1	0.98	0.12	-	39,39,39,39	0
56	MG	AA	3058	1/1	0.86	0.13	-	62,62,62,62	0
56	MG	BA	3302	1/1	0.95	0.12	-	55,55,55,55	0
56	MG	BA	3069	1/1	0.93	0.10	-	47,47,47,47	0
56	MG	BA	3243	1/1	0.90	0.17	-	45,45,45,45	0
56	MG	DA	3406	1/1	0.94	0.10	-	50,50,50,50	0
56	MG	CA	3073	1/1	0.93	0.13	-	57,57,57,57	0
56	MG	DA	3481	1/1	0.97	0.09	-	41,41,41,41	0
56	MG	CA	3033	1/1	0.91	0.13	-	52,52,52,52	0
56	MG	DA	3374	1/1	0.95	0.12	-	35,35,35,35	0
56	MG	CA	3096	1/1	0.93	0.13	-	61,61,61,61	0
56	MG	BA	3653	1/1	0.90	0.14	-	33,33,33,33	0
56	MG	DB	3004	1/1	0.92	0.13	-	36,36,36,36	0
56	MG	DA	3474	1/1	0.82	0.11	-	62,62,62,62	0
56	MG	DA	3022	1/1	0.83	0.13	-	39,39,39,39	0
56	MG	DA	3396	1/1	0.95	0.10	-	45,45,45,45	0
56	MG	BB	3018	1/1	0.98	0.16	-	30,30,30,30	0
56	MG	BA	3388	1/1	0.96	0.06	-	54,54,54,54	0
56	MG	DA	3488	1/1	0.93	0.12	-	41,41,41,41	0
56	MG	BA	3050	1/1	0.96	0.17	-	44,44,44,44	0
56	MG	BA	3077	1/1	0.94	0.17	-	37,37,37,37	0
56	MG	BA	3008	1/1	0.96	0.09	-	27,27,27,27	0
56	MG	AA	3099	1/1	0.95	0.26	-	33,33,33,33	0
56	MG	DA	3540	1/1	0.97	0.11	-	46,46,46,46	0
56	MG	CA	3064	1/1	0.92	0.08	-	60,60,60,60	0
56	MG	BA	3503	1/1	0.97	0.13	-	30,30,30,30	0
56	MG	BA	3567	1/1	0.89	0.18	-	53,53,53,53	0
56	MG	BA	3407	1/1	0.94	0.12	-	43,43,43,43	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	DA	3534	1/1	0.90	0.14	-	54,54,54,54	0
56	MG	DA	3577	1/1	0.96	0.17	-	35,35,35,35	0
56	MG	DA	3332	1/1	0.94	0.07	-	43,43,43,43	0
56	MG	BA	3595	1/1	0.92	0.12	-	47,47,47,47	0
56	MG	DA	3034	1/1	0.94	0.18	-	46,46,46,46	0
56	MG	AA	3182	1/1	0.96	0.14	-	57,57,57,57	0
56	MG	DA	3226	1/1	0.94	0.10	-	27,27,27,27	0
56	MG	BA	3006	1/1	0.96	0.41	-	36,36,36,36	0
56	MG	BB	3010	1/1	0.74	0.14	-	77,77,77,77	0
56	MG	DB	3009	1/1	0.95	0.14	-	60,60,60,60	0
56	MG	DA	3179	1/1	0.92	0.14	-	20,20,20,20	0
56	MG	AA	3055	1/1	0.95	0.14	-	72,72,72,72	0
56	MG	DA	3127	1/1	0.97	0.13	-	41,41,41,41	0
56	MG	BA	3660	1/1	0.95	0.08	-	49,49,49,49	0
56	MG	AA	3100	1/1	0.94	0.11	-	35,35,35,35	0
56	MG	DA	3464	1/1	0.97	0.11	-	46,46,46,46	0
56	MG	B4	502	1/1	0.89	0.16	-	61,61,61,61	0
56	MG	BA	3635	1/1	0.96	0.19	-	63,63,63,63	0
56	MG	BA	3558	1/1	0.96	0.12	-	59,59,59,59	0
56	MG	CA	3101	1/1	0.97	0.13	-	53,53,53,53	0
56	MG	DA	3204	1/1	0.97	0.07	-	37,37,37,37	0
56	MG	CA	3118	1/1	0.84	0.10	-	78,78,78,78	0
56	MG	DA	3531	1/1	0.87	0.12	-	69,69,69,69	0
56	MG	DA	3393	1/1	0.93	0.09	-	48,48,48,48	0
56	MG	DA	3411	1/1	0.95	0.08	-	36,36,36,36	0
56	MG	AA	3086	1/1	0.96	0.25	-	61,61,61,61	0
56	MG	AA	3147	1/1	0.77	0.08	-	67,67,67,67	0
56	MG	BA	3269	1/1	0.95	0.08	-	34,34,34,34	0
56	MG	BA	3136	1/1	0.84	0.18	-	44,44,44,44	0
56	MG	AA	3106	1/1	0.88	0.17	-	50,50,50,50	0
56	MG	AA	3115	1/1	0.99	0.07	-	35,35,35,35	0
56	MG	BB	3011	1/1	0.97	0.08	-	45,45,45,45	0
56	MG	DA	3318	1/1	0.91	0.12	-	43,43,43,43	0
56	MG	BA	3093	1/1	0.84	0.21	-	40,40,40,40	0
56	MG	BZ	3001	1/1	0.78	0.25	-	58,58,58,58	0
56	MG	DA	3043	1/1	0.95	0.10	-	30,30,30,30	0
56	MG	DA	3382	1/1	0.96	0.12	-	50,50,50,50	0
56	MG	AA	3155	1/1	0.98	0.09	-	61,61,61,61	0
56	MG	BA	3263	1/1	0.90	0.21	-	64,64,64,64	0
56	MG	BA	3625	1/1	0.99	0.12	-	25,25,25,25	0
56	MG	AA	3069	1/1	0.92	0.12	-	50,50,50,50	0
56	MG	DA	3077	1/1	0.95	0.14	-	34,34,34,34	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	BA	3544	1/1	0.98	0.19	-	25,25,25,25	0
56	MG	DA	3402	1/1	0.93	0.13	-	63,63,63,63	0
56	MG	AA	3150	1/1	0.97	0.19	-	51,51,51,51	0
56	MG	AA	3059	1/1	0.94	0.12	-	54,54,54,54	0
56	MG	AA	3080	1/1	0.99	0.24	-	39,39,39,39	0
56	MG	BA	3658	1/1	0.97	0.13	-	27,27,27,27	0
56	MG	DA	3250	1/1	0.96	0.17	-	37,37,37,37	0
56	MG	CA	3113	1/1	0.99	0.12	-	57,57,57,57	0
56	MG	BA	3106	1/1	0.98	0.14	-	40,40,40,40	0
56	MG	BA	3278	1/1	0.77	0.12	-	50,50,50,50	0
56	MG	BA	3672	1/1	0.89	0.10	-	46,46,46,46	0
56	MG	BA	3122	1/1	0.94	0.41	-	39,39,39,39	0
56	MG	DQ	3003	1/1	0.89	0.18	-	50,50,50,50	0
56	MG	DA	3414	1/1	0.98	0.05	-	42,42,42,42	0
56	MG	DA	3044	1/1	0.94	0.07	-	47,47,47,47	0
56	MG	BA	3150	1/1	0.96	0.13	-	32,32,32,32	0
56	MG	BA	3381	1/1	0.94	0.19	-	31,31,31,31	0
56	MG	DA	3447	1/1	0.96	0.08	-	33,33,33,33	0
56	MG	DA	3527	1/1	0.93	0.13	-	43,43,43,43	0
56	MG	BA	3308	1/1	0.94	0.17	-	52,52,52,52	0
56	MG	BA	3449	1/1	0.95	0.08	-	47,47,47,47	0
56	MG	BA	3644	1/1	0.95	0.08	-	41,41,41,41	0
56	MG	BA	3475	1/1	0.99	0.10	-	45,45,45,45	0
56	MG	AE	3001	1/1	0.98	0.09	-	71,71,71,71	0
56	MG	DA	3498	1/1	0.97	0.13	-	48,48,48,48	0
56	MG	DA	3041	1/1	0.97	0.08	-	35,35,35,35	0
56	MG	BA	3177	1/1	0.89	0.13	-	44,44,44,44	0
56	MG	DA	3189	1/1	0.97	0.27	-	31,31,31,31	0
56	MG	DA	3175	1/1	0.97	0.13	-	47,47,47,47	0
56	MG	BA	3589	1/1	0.97	0.13	-	27,27,27,27	0
56	MG	BA	3325	1/1	0.97	0.16	-	42,42,42,42	0
56	MG	AA	3023	1/1	0.75	0.20	-	71,71,71,71	0
56	MG	DA	3050	1/1	0.96	0.09	-	41,41,41,41	0
56	MG	DA	3203	1/1	0.96	0.16	-	21,21,21,21	0
56	MG	BV	203	1/1	0.96	0.09	-	24,24,24,24	0
56	MG	BA	3414	1/1	0.97	0.15	-	31,31,31,31	0
56	MG	DA	3172	1/1	0.87	0.11	-	35,35,35,35	0
56	MG	DA	3221	1/1	0.96	0.10	-	33,33,33,33	0
56	MG	BA	3102	1/1	0.96	0.06	-	49,49,49,49	0
56	MG	BA	3437	1/1	0.97	0.13	-	58,58,58,58	0
56	MG	DA	3015	1/1	0.99	0.26	-	41,41,41,41	0
56	MG	AA	3120	1/1	0.91	0.12	-	47,47,47,47	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	DA	3223	1/1	0.98	0.09	-	47,47,47,47	0
56	MG	BA	3307	1/1	0.92	0.07	-	63,63,63,63	0
56	MG	BA	3264	1/1	0.98	0.19	-	35,35,35,35	0
56	MG	DA	3354	1/1	0.80	0.19	-	51,51,51,51	0
56	MG	DA	3508	1/1	0.92	0.11	-	38,38,38,38	0
56	MG	DA	3364	1/1	0.98	0.06	-	37,37,37,37	0
56	MG	DA	3091	1/1	0.86	0.15	-	45,45,45,45	0
56	MG	CA	3034	1/1	0.95	0.12	-	67,67,67,67	0
56	MG	BA	3135	1/1	0.95	0.21	-	36,36,36,36	0
56	MG	BA	3107	1/1	0.95	0.16	-	21,21,21,21	0
56	MG	DA	3386	1/1	0.95	0.13	-	48,48,48,48	0
56	MG	BA	3190	1/1	0.94	0.26	-	31,31,31,31	0
56	MG	BA	3294	1/1	0.97	0.10	-	32,32,32,32	0
56	MG	DA	3509	1/1	0.97	0.08	-	36,36,36,36	0
56	MG	DA	3564	1/1	0.90	0.07	-	36,36,36,36	0
56	MG	BA	3001	1/1	0.93	0.14	-	35,35,35,35	0
56	MG	CA	3115	1/1	0.96	0.09	-	62,62,62,62	0
56	MG	DA	3576	1/1	0.93	0.15	-	36,36,36,36	0
56	MG	DA	3392	1/1	0.93	0.14	-	54,54,54,54	0
56	MG	DA	3268	1/1	0.95	0.13	-	38,38,38,38	0
56	MG	BA	3454	1/1	0.96	0.17	-	21,21,21,21	0
56	MG	DA	3275	1/1	0.71	0.10	-	45,45,45,45	0
56	MG	DA	3087	1/1	0.90	0.30	-	35,35,35,35	0
56	MG	DA	3233	1/1	0.98	0.41	-	36,36,36,36	0
56	MG	DA	3499	1/1	0.97	0.13	-	45,45,45,45	0
56	MG	BA	3649	1/1	0.70	0.14	-	50,50,50,50	0
56	MG	BA	3168	1/1	0.98	0.16	-	47,47,47,47	0
56	MG	CA	3090	1/1	0.88	0.16	-	66,66,66,66	0
56	MG	DA	3446	1/1	0.87	0.09	-	46,46,46,46	0
56	MG	CA	3065	1/1	0.91	0.07	-	55,55,55,55	0
56	MG	AA	3172	1/1	0.89	0.09	-	69,69,69,69	0
56	MG	DA	3430	1/1	0.87	0.19	-	30,30,30,30	0
56	MG	DA	3069	1/1	0.86	0.12	-	35,35,35,35	0
56	MG	CA	3126	1/1	0.78	0.23	-	73,73,73,73	0
56	MG	BX	103	1/1	0.96	0.21	-	25,25,25,25	0
56	MG	DA	3473	1/1	0.95	0.06	-	50,50,50,50	0
56	MG	BA	3194	1/1	0.98	0.15	-	23,23,23,23	0
56	MG	AA	3170	1/1	0.93	0.14	-	54,54,54,54	0
56	MG	DA	3100	1/1	0.94	0.11	-	34,34,34,34	0
56	MG	AA	3088	1/1	0.81	0.16	-	62,62,62,62	0
56	MG	DA	3530	1/1	0.89	0.10	-	60,60,60,60	0
56	MG	BA	3018	1/1	0.94	0.21	-	47,47,47,47	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	BU	205	1/1	0.95	0.24	-	53,53,53,53	0
56	MG	AA	3168	1/1	0.98	0.10	-	56,56,56,56	0
56	MG	BA	3251	1/1	0.96	0.28	-	37,37,37,37	0
56	MG	DA	3028	1/1	0.88	0.35	-	47,47,47,47	0
56	MG	BA	3440	1/1	0.98	0.06	-	38,38,38,38	0
56	MG	CA	3097	1/1	0.96	0.19	-	67,67,67,67	0
56	MG	DA	3522	1/1	0.97	0.10	-	44,44,44,44	0
56	MG	BA	3193	1/1	0.92	0.20	-	48,48,48,48	0
56	MG	BA	3601	1/1	0.84	0.14	-	50,50,50,50	0
56	MG	DA	3222	1/1	0.91	0.12	-	36,36,36,36	0
56	MG	DA	3259	1/1	0.96	0.19	-	42,42,42,42	0
56	MG	AA	3110	1/1	0.93	0.10	-	60,60,60,60	0
56	MG	BA	3350	1/1	0.79	0.17	-	59,59,59,59	0
56	MG	DA	3506	1/1	0.73	0.14	-	65,65,65,65	0
56	MG	BA	3349	1/1	0.95	0.08	-	46,46,46,46	0
56	MG	DA	3155	1/1	0.97	0.24	-	45,45,45,45	0
56	MG	AA	3062	1/1	0.77	0.18	-	58,58,58,58	0
56	MG	BA	3004	1/1	0.97	0.13	-	23,23,23,23	0
56	MG	DA	3231	1/1	0.94	0.12	-	37,37,37,37	0
56	MG	BA	3313	1/1	0.99	0.12	-	17,17,17,17	0
56	MG	DA	3098	1/1	0.93	0.10	-	46,46,46,46	0
56	MG	BA	3019	1/1	0.95	0.22	-	49,49,49,49	0
56	MG	BR	3001	1/1	0.96	0.12	-	31,31,31,31	0
56	MG	DA	3228	1/1	0.96	0.07	-	51,51,51,51	0
56	MG	DA	3081	1/1	0.92	0.10	-	44,44,44,44	0
56	MG	AA	3049	1/1	0.89	0.22	-	47,47,47,47	0
56	MG	DA	3375	1/1	0.92	0.14	-	49,49,49,49	0
56	MG	BA	3373	1/1	0.79	0.17	-	41,41,41,41	0
56	MG	DE	3005	1/1	0.98	0.12	-	20,20,20,20	0
56	MG	DA	3321	1/1	0.96	0.10	-	45,45,45,45	0
56	MG	DB	3003	1/1	0.97	0.11	-	29,29,29,29	0
56	MG	DA	3399	1/1	0.92	0.17	-	40,40,40,40	0
56	MG	BA	3340	1/1	0.88	0.13	-	42,42,42,42	0
56	MG	BA	3530	1/1	0.97	0.14	-	36,36,36,36	0
56	MG	BA	3615	1/1	0.96	0.12	-	42,42,42,42	0
56	MG	DA	3309	1/1	0.92	0.13	-	60,60,60,60	0
56	MG	BA	3111	1/1	0.97	0.14	-	27,27,27,27	0
56	MG	BA	3274	1/1	0.95	0.28	-	47,47,47,47	0
56	MG	BA	3271	1/1	0.94	0.10	-	49,49,49,49	0
56	MG	CA	3134	1/1	0.98	0.13	-	53,53,53,53	0
56	MG	BA	3084	1/1	0.98	0.23	-	34,34,34,34	0
56	MG	BF	305	1/1	0.92	0.39	-	61,61,61,61	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	CA	3012	1/1	0.94	0.11	-	52,52,52,52	0
56	MG	DA	3520	1/1	0.98	0.09	-	34,34,34,34	0
56	MG	B0	104	1/1	0.89	0.36	-	48,48,48,48	0
56	MG	BA	3072	1/1	0.97	0.16	-	24,24,24,24	0
56	MG	DA	3595	1/1	0.92	0.10	-	43,43,43,43	0
56	MG	CA	3131	1/1	0.83	0.08	-	65,65,65,65	0
56	MG	CA	3151	1/1	0.95	0.13	-	50,50,50,50	0
56	MG	BA	3222	1/1	0.91	0.20	-	45,45,45,45	0
56	MG	BA	3095	1/1	0.94	0.09	-	33,33,33,33	0
56	MG	DA	3355	1/1	0.93	0.07	-	36,36,36,36	0
56	MG	BA	3478	1/1	0.95	0.13	-	47,47,47,47	0
56	MG	CA	3008	1/1	0.95	0.30	-	31,31,31,31	0
56	MG	DA	3484	1/1	0.94	0.14	-	34,34,34,34	0
56	MG	AA	3160	1/1	0.85	0.09	-	71,71,71,71	0
56	MG	DA	3088	1/1	0.90	0.12	-	39,39,39,39	0
56	MG	BA	3124	1/1	0.93	0.17	-	58,58,58,58	0
56	MG	BA	3266	1/1	0.95	0.21	-	29,29,29,29	0
56	MG	BA	3661	1/1	0.94	0.22	-	38,38,38,38	0
56	MG	DA	3561	1/1	0.76	0.18	-	63,63,63,63	0
56	MG	BA	3575	1/1	0.93	0.15	-	55,55,55,55	0
56	MG	DA	3178	1/1	0.97	0.24	-	46,46,46,46	0
56	MG	BA	3096	1/1	0.93	0.10	-	44,44,44,44	0
56	MG	BA	3103	1/1	0.95	0.13	-	42,42,42,42	0
56	MG	BA	3253	1/1	0.87	0.38	-	47,47,47,47	0
56	MG	DA	3040	1/1	0.97	0.23	-	34,34,34,34	0
56	MG	AA	3001	1/1	0.91	0.19	-	57,57,57,57	0
56	MG	CA	3063	1/1	0.92	0.23	-	53,53,53,53	0
56	MG	DA	3242	1/1	0.96	0.14	-	60,60,60,60	0
56	MG	DA	3292	1/1	0.97	0.18	-	45,45,45,45	0
56	MG	AA	3007	1/1	0.97	0.14	-	30,30,30,30	0
56	MG	AA	3034	1/1	0.91	0.20	-	54,54,54,54	0
56	MG	AA	3103	1/1	0.97	0.13	-	51,51,51,51	0
56	MG	BA	3064	1/1	0.98	0.19	-	30,30,30,30	0
56	MG	BA	3116	1/1	0.96	0.19	-	50,50,50,50	0
56	MG	BA	3557	1/1	0.94	0.14	-	42,42,42,42	0
56	MG	DA	3417	1/1	0.98	0.15	-	40,40,40,40	0
56	MG	B0	103	1/1	0.95	0.12	-	33,33,33,33	0
56	MG	AE	3002	1/1	0.99	0.13	-	38,38,38,38	0
56	MG	BA	3432	1/1	0.98	0.11	-	37,37,37,37	0
56	MG	BA	3648	1/1	0.98	0.11	-	28,28,28,28	0
56	MG	AA	3018	1/1	0.96	0.13	-	50,50,50,50	0
56	MG	BA	3339	1/1	0.91	0.11	-	34,34,34,34	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	AA	3044	1/1	0.90	0.19	-	50,50,50,50	0
56	MG	AA	3181	1/1	0.70	0.17	-	53,53,53,53	0
56	MG	BA	3513	1/1	0.91	0.14	-	60,60,60,60	0
56	MG	CA	3111	1/1	0.97	0.12	-	43,43,43,43	0
56	MG	DA	3066	1/1	0.97	0.23	-	49,49,49,49	0
56	MG	AA	3025	1/1	0.97	0.16	-	37,37,37,37	0
56	MG	DA	3086	1/1	0.96	0.08	-	41,41,41,41	0
56	MG	DA	3438	1/1	0.94	0.10	-	38,38,38,38	0
56	MG	DA	3220	1/1	0.89	0.13	-	43,43,43,43	0
56	MG	AA	3068	1/1	0.89	0.20	-	31,31,31,31	0
56	MG	BA	3113	1/1	0.93	0.15	-	41,41,41,41	0
56	MG	DA	3512	1/1	0.98	0.11	-	36,36,36,36	0
56	MG	CA	3050	1/1	0.84	0.13	-	67,67,67,67	0
56	MG	CA	3117	1/1	0.94	0.22	-	42,42,42,42	0
56	MG	DA	3568	1/1	0.84	0.13	-	60,60,60,60	0
56	MG	BA	3057	1/1	0.97	0.16	-	38,38,38,38	0
56	MG	DA	3017	1/1	0.91	0.20	-	46,46,46,46	0
56	MG	BA	3255	1/1	0.96	0.21	-	32,32,32,32	0
56	MG	DA	3051	1/1	0.96	0.11	-	50,50,50,50	0
56	MG	CA	3112	1/1	0.94	0.14	-	55,55,55,55	0
56	MG	BA	3149	1/1	0.95	0.11	-	50,50,50,50	0
56	MG	BA	3507	1/1	0.95	0.12	-	53,53,53,53	0
56	MG	DA	3437	1/1	0.96	0.26	-	48,48,48,48	0
56	MG	AA	3073	1/1	0.90	0.19	-	50,50,50,50	0
56	MG	BA	3433	1/1	0.92	0.10	-	33,33,33,33	0
56	MG	DA	3403	1/1	0.96	0.08	-	39,39,39,39	0
56	MG	BA	3532	1/1	0.99	0.04	-	53,53,53,53	0
56	MG	BA	3229	1/1	0.92	0.21	-	54,54,54,54	0
56	MG	DA	3007	1/1	0.95	0.08	-	39,39,39,39	0
56	MG	DA	3491	1/1	0.90	0.13	-	40,40,40,40	0
56	MG	BA	3524	1/1	0.98	0.07	-	57,57,57,57	0
56	MG	BA	3315	1/1	0.99	0.17	-	31,31,31,31	0
56	MG	DE	3004	1/1	0.91	0.12	-	48,48,48,48	0
56	MG	CA	3004	1/1	0.82	0.13	-	51,51,51,51	0
56	MG	BA	3133	1/1	0.96	0.11	-	33,33,33,33	0
56	MG	BA	3418	1/1	0.96	0.12	-	46,46,46,46	0
56	MG	DA	3290	1/1	0.92	0.09	-	36,36,36,36	0
56	MG	BA	3639	1/1	0.78	0.19	-	64,64,64,64	0
56	MG	DA	3063	1/1	0.91	0.11	-	31,31,31,31	0
56	MG	BA	3451	1/1	0.93	0.08	-	48,48,48,48	0
56	MG	DA	3016	1/1	0.97	0.18	-	31,31,31,31	0
56	MG	BA	3408	1/1	0.97	0.13	-	56,56,56,56	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	DA	3455	1/1	0.98	0.16	-	45,45,45,45	0
56	MG	BA	3572	1/1	0.95	0.11	-	59,59,59,59	0
56	MG	BA	3041	1/1	0.94	0.12	-	42,42,42,42	0
56	MG	AA	3063	1/1	0.95	0.26	-	39,39,39,39	0
56	MG	DA	3451	1/1	0.99	0.11	-	30,30,30,30	0
56	MG	CA	3058	1/1	0.91	0.11	-	56,56,56,56	0
56	MG	BA	3596	1/1	0.90	0.14	-	56,56,56,56	0
56	MG	DA	3134	1/1	0.94	0.23	-	33,33,33,33	0
56	MG	BA	3570	1/1	0.97	0.07	-	36,36,36,36	0
56	MG	CA	3043	1/1	0.95	0.14	-	60,60,60,60	0
56	MG	DA	3441	1/1	0.98	0.12	-	45,45,45,45	0
56	MG	BA	3198	1/1	0.94	0.10	-	34,34,34,34	0

6.5 Other polymers [i](#)

There are no such residues in this entry.