



# wwPDB X-ray Structure Validation Summary Report ⓘ

May 17, 2020 – 04:43 am BST

PDB ID : 4WQY  
Title : Crystal structure of the *Thermus thermophilus* 70S ribosome in complex with elongation factor G in the post-translocational state (without fusitic acid)  
Authors : Lin, J.; Gagnon, M.G.; Steitz, T.A.  
Deposited on : 2014-10-22  
Resolution : 2.80 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

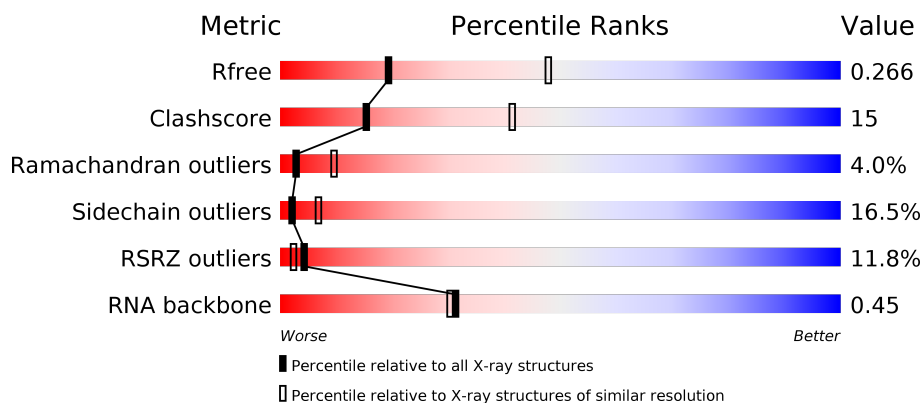
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.80 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)
RNA backbone	3102	1227 (3.10-2.50)

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. 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	2915	<div> <div>4%</div> <div>17% 47% 29% 5%</div> </div>
1	CA	2915	<div> <div>7%</div> <div>32% 44% 19%</div> </div>
2	AB	121	<div> <div>25% 47% 24%</div> </div>
2	CB	121	<div> <div>43% 46% 9%</div> </div>



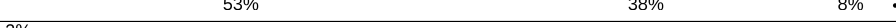

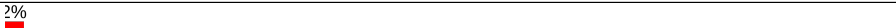
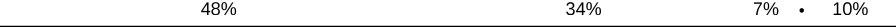
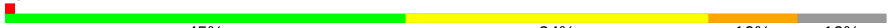
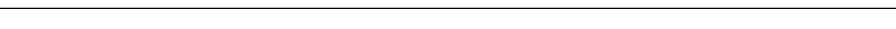

















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Mol	Chain	Length	Quality of chain
3	AC	228	
3	CC	228	
4	AD	276	
4	CD	276	
5	AE	206	
5	CE	206	
6	AF	210	
6	CF	210	
7	AG	182	
7	CG	182	
8	AH	180	
8	CH	180	
9	AK	173	
9	CK	173	
10	AL	147	
10	CL	147	
11	AN	140	
11	CN	140	
12	AO	122	
12	CO	122	
13	AP	150	
13	CP	150	
14	AQ	141	
14	CQ	141	
15	AR	118	

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Mol	Chain	Length	Quality of chain
15	CR	118	
16	AS	112	
16	CS	112	
17	AT	146	
17	CT	146	
18	AU	118	
18	CU	118	
19	AV	101	
19	CV	101	
20	AW	113	
20	CW	113	
21	AX	96	
21	CX	96	
22	AY	110	
22	CY	110	
23	AZ	206	
23	CZ	206	
24	A0	85	
24	C0	85	
25	A1	98	
25	C1	98	
26	A2	72	
26	C2	72	
27	A3	60	
27	C3	60	

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Mol	Chain	Length	Quality of chain
28	A4	71	
28	C4	71	
29	A5	60	
29	C5	60	
30	A6	54	
30	C6	54	
31	A7	49	
31	C7	49	
32	A8	65	
32	C8	65	
33	A9	37	
33	C9	37	
34	BA	1521	
34	DA	1521	
35	BB	256	
35	DB	256	
36	BC	239	
36	DC	239	
37	BD	209	
37	DD	209	
38	BE	162	
38	DE	162	
39	BF	101	
39	DF	101	
40	BG	156	

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Mol	Chain	Length	Quality of chain
40	DG	156	
41	BH	138	
41	DH	138	
42	BI	128	
42	DI	128	
43	BJ	105	
43	DJ	105	
44	BK	129	
44	DK	129	
45	BL	132	
45	DL	132	
46	BM	126	
46	DM	126	
47	BN	61	
47	DN	61	
48	BO	89	
48	DO	89	
49	BP	88	
49	DP	88	
50	BQ	105	
50	DQ	105	
51	BR	88	
51	DR	88	
52	BS	93	
52	DS	93	

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Mol	Chain	Length	Quality of chain
53	BT	106	
53	DT	106	
54	BU	27	
54	DU	27	
55	BV	24	
55	DV	24	
56	BX	77	
56	DX	77	
57	BZ	758	
57	DZ	758	

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
58	MG	AA	3018	-	-	-	X
58	MG	AA	3026	-	-	-	X
58	MG	AA	3088	-	-	-	X
58	MG	AA	3096	-	-	-	X
58	MG	AA	3109	-	-	-	X
58	MG	AA	3113	-	-	-	X
58	MG	AA	3122	-	-	-	X
58	MG	AA	3193	-	-	-	X
58	MG	AA	3641	-	-	-	X
58	MG	AA	3752	-	-	-	X
58	MG	AA	3784	-	-	-	X
58	MG	AB	3006	-	-	-	X
58	MG	AZ	301	-	-	-	X
58	MG	BA	3035	-	-	-	X
58	MG	BA	3088	-	-	-	X
58	MG	BA	3092	-	-	-	X
58	MG	BA	3106	-	-	-	X
58	MG	BA	3112	-	-	-	X
58	MG	BA	3169	-	-	-	X
58	MG	CA	3002	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
58	MG	CA	3042	-	-	-	X
58	MG	CA	3067	-	-	-	X
58	MG	CA	3074	-	-	-	X
58	MG	CA	3094	-	-	-	X
58	MG	CA	3124	-	-	-	X
58	MG	CA	3130	-	-	-	X
58	MG	CA	3135	-	-	-	X
58	MG	CA	3141	-	-	-	X
58	MG	CA	3181	-	-	-	X
58	MG	CA	3184	-	-	-	X
58	MG	CA	3195	-	-	-	X
58	MG	CA	3209	-	-	-	X
58	MG	CA	3225	-	-	-	X
58	MG	CA	3232	-	-	-	X
58	MG	CA	3238	-	-	-	X
58	MG	CA	3286	-	-	-	X
58	MG	CA	3292	-	-	-	X
58	MG	CA	3461	-	-	-	X
58	MG	CA	3494	-	-	-	X
58	MG	CE	304	-	-	-	X
58	MG	DA	1605	-	-	-	X
58	MG	DA	1635	-	-	-	X
58	MG	DA	1659	-	-	-	X
58	MG	DA	1677	-	-	-	X
58	MG	DA	1704	-	-	-	X
58	MG	DA	1753	-	-	-	X
58	MG	DE	202	-	-	-	X
58	MG	DZ	701	-	-	-	X



## 2 Entry composition

There are 63 unique types of molecules in this entry. The entry contains 305548 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 23S Ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	AA	2852	Total	C	N	O	P	0	0	0
			61426	27339	11489	19747	2851			
1	CA	2848	Total	C	N	O	P	0	0	0
			61337	27299	11470	19721	2847			

- Molecule 2 is a RNA chain called 5S Ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	AB	120	Total	C	N	O	P	0	0	0
			2573	1146	476	832	119			
2	CB	120	Total	C	N	O	P	0	0	0
			2573	1146	476	832	119			

- Molecule 3 is a protein called 50S ribosomal protein L1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	AC	137	Total	C	N	O	S	0	0	0
			1063	669	201	192	1			
3	CC	137	Total	C	N	O	S	0	0	0
			1063	669	201	192	1			

- Molecule 4 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	AD	275	Total	C	N	O	S	0	0	0
			2136	1349	423	361	3			
4	CD	275	Total	C	N	O	S	0	0	0
			2142	1352	426	361	3			

- Molecule 5 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	AE	204	Total	C	N	O	S	0	0	0
			1559	985	298	270	6			
5	CE	204	Total	C	N	O	S	0	0	0
			1559	985	298	270	6			

- Molecule 6 is a protein called 50S ribosomal protein L4.

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

- Molecule 7 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	AG	181	Total	C	N	O	S	0	0	0
			1425	914	256	251	4			
7	CG	181	Total	C	N	O	S	0	0	0
			1424	911	258	251	4			

- Molecule 8 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	AH	174	Total	C	N	O	S	0	0	0
			1330	845	248	236	1			
8	CH	174	Total	C	N	O	S	0	0	0
			1330	845	248	236	1			

- Molecule 9 is a protein called 50S ribosomal protein L10.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	AK	130	Total	C	N	O		0	0	0
			641	381	130	130				
9	CK	130	Total	C	N	O		0	0	0
			641	381	130	130				

- Molecule 10 is a protein called 50S ribosomal protein L11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	AL	139	Total	C	N	O	S	0	0	0
			1025	653	181	186	5			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	CL	139	Total	C	N	O	S	0	0	0
			1025	653	181	186	5			

- Molecule 11 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	AN	140	Total	C	N	O	S	0	0	0
			1117	719	207	187	4			
11	CN	140	Total	C	N	O	S	0	0	0
			1117	719	207	187	4			

- Molecule 12 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	AO	122	Total	C	N	O	S	0	0	0
			933	588	171	170	4			
12	CO	122	Total	C	N	O	S	0	0	0
			933	588	171	170	4			

- Molecule 13 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	AP	149	Total	C	N	O	S	0	0	0
			1139	709	231	196	3			
13	CP	149	Total	C	N	O	S	0	0	0
			1135	706	230	196	3			

- Molecule 14 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	AQ	141	Total	C	N	O	S	0	0	0
			1122	715	212	188	7			
14	CQ	141	Total	C	N	O	S	0	0	0
			1122	715	212	188	7			

- Molecule 15 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	AR	118	Total	C	N	O	S	0	0	0
			968	604	203	160	1			
15	CR	118	Total	C	N	O	S	0	0	0
			968	604	203	160	1			

- Molecule 16 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
16	AS	110	Total	C	N	O	0	0	0
			877	553	175	149			
16	CS	110	Total	C	N	O	0	0	0
			870	549	173	148			

- Molecule 17 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	AT	131	Total	C	N	O	S	0	0	0
			1091	680	225	185	1			
17	CT	131	Total	C	N	O	S	0	0	0
			1083	675	224	183	1			

- Molecule 18 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
18	AU	116	Total	C	N	O	S	0	0	0
			959	608	201	149	1			
18	CU	116	Total	C	N	O	S	0	0	0
			959	608	201	149	1			

- Molecule 19 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	AV	101	Total	C	N	O	S	0	0	0
			771	495	140	135	1			
19	CV	101	Total	C	N	O	S	0	0	0
			771	495	140	135	1			

- Molecule 20 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	AW	112	Total	C	N	O	S	0	0	0
			886	557	174	153	2			
20	CW	112	Total	C	N	O	S	0	0	0
			886	557	174	153	2			

- Molecule 21 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
21	AX	95	Total	C	N	O	S	0	0	0
			750	488	135	126	1			
21	CX	95	Total	C	N	O	S	0	0	0
			750	488	135	126	1			

- Molecule 22 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	AY	107	Total	C	N	O	S	0	0	0
			806	517	152	131	6			
22	CY	107	Total	C	N	O	S	0	0	0
			806	517	152	131	6			

- Molecule 23 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	AZ	185	Total	C	N	O	S	0	0	0
			1451	927	258	264	2			
23	CZ	185	Total	C	N	O	S	0	0	0
			1451	927	258	264	2			

- Molecule 24 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	A0	83	Total	C	N	O	S	0	0	0
			653	404	139	109	1			
24	C0	83	Total	C	N	O	S	0	0	0
			653	404	139	109	1			

- Molecule 25 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
25	A1	97	Total	C	N	O	S	0	0	0
			755	475	148	131	1			
25	C1	97	Total	C	N	O	S	0	0	0
			755	475	148	131	1			

- Molecule 26 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	A2	70	Total	C	N	O	S	0	0	0
			588	365	118	103	2			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	C2	70	Total	C	N	O	S	0	0	0
			588	365	118	103	2			

- Molecule 27 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
27	A3	59	Total	C	N	O		0	0	0
			469	298	90	81				
27	C3	59	Total	C	N	O		0	0	0
			464	296	90	78				

- Molecule 28 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
28	A4	69	Total	C	N	O	S	0	0	0
			558	352	102	99	5			
28	C4	69	Total	C	N	O	S	0	0	0
			532	339	97	91	5			

- Molecule 29 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
29	A5	59	Total	C	N	O	S	0	0	0
			455	285	89	76	5			
29	C5	59	Total	C	N	O	S	0	0	0
			455	285	89	76	5			

- Molecule 30 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
30	A6	53	Total	C	N	O	S	0	0	0
			453	281	91	77	4			
30	C6	53	Total	C	N	O	S	0	0	0
			449	279	91	75	4			

- Molecule 31 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
31	A7	48	Total	C	N	O	S	0	0	0
			418	257	104	55	2			
31	C7	48	Total	C	N	O	S	0	0	0
			418	257	104	55	2			

- Molecule 32 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
32	A8	64	Total	C	N	O	S	0	0	0
			517	331	102	82	2			
32	C8	64	Total	C	N	O	S	0	0	0
			517	331	102	82	2			

- Molecule 33 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
33	A9	37	Total	C	N	O	S	0	0	0
			307	188	68	47	4			
33	C9	37	Total	C	N	O	S	0	0	0
			307	188	68	47	4			

- Molecule 34 is a RNA chain called 16S Ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
34	BA	1495	Total	C	N	O	P	0	0	0
			32141	14304	5958	10384	1495			
34	DA	1501	Total	C	N	O	P	0	0	0
			32268	14361	5980	10426	1501			

- Molecule 35 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
35	BB	231	Total	C	N	O	S	0	0	0
			1846	1179	331	331	5			
35	DB	231	Total	C	N	O	S	0	0	0
			1825	1167	326	327	5			

- Molecule 36 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
36	BC	206	Total	C	N	O	S	0	0	0
			1552	976	302	273	1			
36	DC	206	Total	C	N	O	S	0	0	0
			1544	970	300	273	1			

- Molecule 37 is a protein called 30S ribosomal protein S4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
37	BD	208	Total	C	N	O	S	0	0	0
			1659	1040	326	286	7			
37	DD	208	Total	C	N	O	S	0	0	0
			1678	1052	333	286	7			

- Molecule 38 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
38	BE	148	Total	C	N	O	S	0	0	0
			1129	714	213	198	4			
38	DE	148	Total	C	N	O	S	0	0	0
			1133	716	214	199	4			

- Molecule 39 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
39	BF	100	Total	C	N	O	S	0	0	0
			812	514	146	149	3			
39	DF	100	Total	C	N	O	S	0	0	0
			820	518	147	152	3			

- Molecule 40 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
40	BG	155	Total	C	N	O	S	0	0	0
			1231	766	243	216	6			
40	DG	155	Total	C	N	O	S	0	0	0
			1235	769	244	216	6			

- Molecule 41 is a protein called 30S ribosomal protein S8.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
41	BH	137	Total	C	N	O	S	0	0	0
			1088	689	206	191	2			
41	DH	137	Total	C	N	O	S	0	0	0
			1088	689	206	191	2			

- Molecule 42 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
42	BI	127	Total	C	N	O		0	0	0
			986	626	193	167				

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
42	DI	127	Total	C	N	O	0	0	0
			978	619	190	169			

- Molecule 43 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
43	BJ	97	Total	C	N	O	0	0	0
			709	440	138	131			
43	DJ	96	Total	C	N	O	0	0	0
			714	445	138	131			

- Molecule 44 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
44	BK	114	Total	C	N	O	S	0	0	0
			833	519	156	155	3			
44	DK	114	Total	C	N	O	S	0	0	0
			833	519	156	155	3			

- Molecule 45 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
45	BL	122	Total	C	N	O	S	0	0	0
			930	585	185	159	1			
45	DL	122	Total	C	N	O	S	0	0	0
			930	585	185	159	1			

- Molecule 46 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
46	BM	117	Total	C	N	O	S	0	0	0
			923	570	191	160	2			
46	DM	122	Total	C	N	O	S	0	0	0
			950	586	197	165	2			

- Molecule 47 is a protein called 30S ribosomal protein S14 type Z.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
47	BN	60	Total	C	N	O	S	0	0	0
			492	312	104	72	4			
47	DN	60	Total	C	N	O	S	0	0	0
			492	312	104	72	4			

- Molecule 48 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
48	BO	88	Total	C	N	O	S	0	0	0
			728	456	144	126	2			
48	DO	88	Total	C	N	O	S	0	0	0
			728	456	144	126	2			

- Molecule 49 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
49	BP	82	Total	C	N	O	S	0	0	0
			681	433	134	113	1			
49	DP	82	Total	C	N	O	S	0	0	0
			677	430	133	113	1			

- Molecule 50 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
50	BQ	99	Total	C	N	O	S	0	0	0
			823	528	151	142	2			
50	DQ	99	Total	C	N	O	S	0	0	0
			823	528	151	142	2			

- Molecule 51 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
51	BR	68	Total	C	N	O	0	0	0
			555	355	108	92			
51	DR	68	Total	C	N	O	0	0	0
			555	355	108	92			

- Molecule 52 is a protein called 30S ribosomal protein S19.

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

- Molecule 53 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
53	BT	96	Total	C	N	O	S	0	0	0
			728	446	156	124	2			
53	DT	96	Total	C	N	O	S	0	0	0
			731	449	156	124	2			

- Molecule 54 is a protein called 30S ribosomal protein Thx.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
54	BU	23	Total	C	N	O		0	0	0
			199	122	48	29				
54	DU	23	Total	C	N	O		0	0	0
			199	122	48	29				

- Molecule 55 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
55	BV	13	Total	C	N	O	P	0	0	0
			277	125	51	88	13			
55	DV	6	Total	C	N	O	P	0	0	0
			128	59	27	37	5			

- Molecule 56 is a RNA chain called P-site tRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
56	BX	76	Total	C	N	O	P	0	0	0
			1625	725	294	529	76			
56	DX	76	Total	C	N	O	P	0	0	0
			1621	723	292	529	76			

- Molecule 57 is a protein called 50S ribosomal protein L9,Elongation factor G.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
57	BZ	730	Total	C	N	O	S	0	0	0
			4869	3031	886	942	10			
57	DZ	730	Total	C	N	O	S	0	0	0
			4867	3029	886	942	10			

- Molecule 58 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
58	AP	2	Total	Mg	0	0
			2	2		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
58	CR	1	Total 1	Mg 1	0	0
58	BA	212	Total 212	Mg 212	0	0
58	CA	666	Total 666	Mg 666	0	0
58	C8	1	Total 1	Mg 1	0	0
58	AB	23	Total 23	Mg 23	0	0
58	BL	4	Total 4	Mg 4	0	0
58	CV	2	Total 2	Mg 2	0	0
58	A6	2	Total 2	Mg 2	0	0
58	DL	2	Total 2	Mg 2	0	0
58	BE	1	Total 1	Mg 1	0	0
58	AW	4	Total 4	Mg 4	0	0
58	C1	1	Total 1	Mg 1	0	0
58	AN	3	Total 3	Mg 3	0	0
58	DZ	3	Total 3	Mg 3	0	0
58	AX	2	Total 2	Mg 2	0	0
58	CN	1	Total 1	Mg 1	0	0
58	A2	1	Total 1	Mg 1	0	0
58	CY	1	Total 1	Mg 1	0	0
58	DD	1	Total 1	Mg 1	0	0
58	BB	1	Total 1	Mg 1	0	0
58	BT	1	Total 1	Mg 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
58	AE	4	Total 4	Mg 4	0	0
58	CU	2	Total 2	Mg 2	0	0
58	BF	1	Total 1	Mg 1	0	0
58	AV	2	Total 2	Mg 2	0	0
58	BX	10	Total 10	Mg 10	0	0
58	DA	166	Total 166	Mg 166	0	0
58	CB	13	Total 13	Mg 13	0	0
58	C0	1	Total 1	Mg 1	0	0
58	AA	836	Total 836	Mg 836	0	0
58	CQ	4	Total 4	Mg 4	0	0
58	A5	2	Total 2	Mg 2	0	0
58	AR	1	Total 1	Mg 1	0	0
58	CG	1	Total 1	Mg 1	0	0
58	DK	1	Total 1	Mg 1	0	0
58	A1	1	Total 1	Mg 1	0	0
58	AD	10	Total 10	Mg 10	0	0
58	BN	2	Total 2	Mg 2	0	0
58	DJ	1	Total 1	Mg 1	0	0
58	DF	1	Total 1	Mg 1	0	0
58	C7	1	Total 1	Mg 1	0	0
58	C3	1	Total 1	Mg 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
58	AZ	2	Total 2	Mg 2	0	0
58	A4	1	Total 1	Mg 1	0	0
58	BK	1	Total 1	Mg 1	0	0
58	AU	3	Total 3	Mg 3	0	0
58	A9	1	Total 1	Mg 1	0	0
58	CF	4	Total 4	Mg 4	0	0
58	BV	1	Total 1	Mg 1	0	0
58	A0	4	Total 4	Mg 4	0	0
58	AG	2	Total 2	Mg 2	0	0
58	DE	2	Total 2	Mg 2	0	0
58	AQ	2	Total 2	Mg 2	0	0
58	CE	7	Total 7	Mg 7	0	0
58	AH	2	Total 2	Mg 2	0	0
58	BZ	1	Total 1	Mg 1	0	0
58	CO	2	Total 2	Mg 2	0	0
58	A7	1	Total 1	Mg 1	0	0
58	CD	3	Total 3	Mg 3	0	0
58	BD	1	Total 1	Mg 1	0	0
58	DT	1	Total 1	Mg 1	0	0
58	A8	2	Total 2	Mg 2	0	0
58	AO	1	Total 1	Mg 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
58	AF	5	Total	Mg	0	0
			5	5		

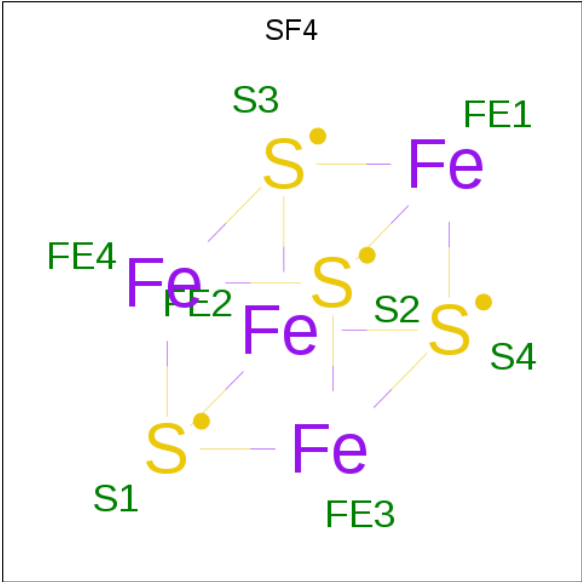
- Molecule 59 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
59	AA	1	Total	K	0	0
			1	1		

- Molecule 60 is ZINC ION (three-letter code: ZN) (formula: Zn).

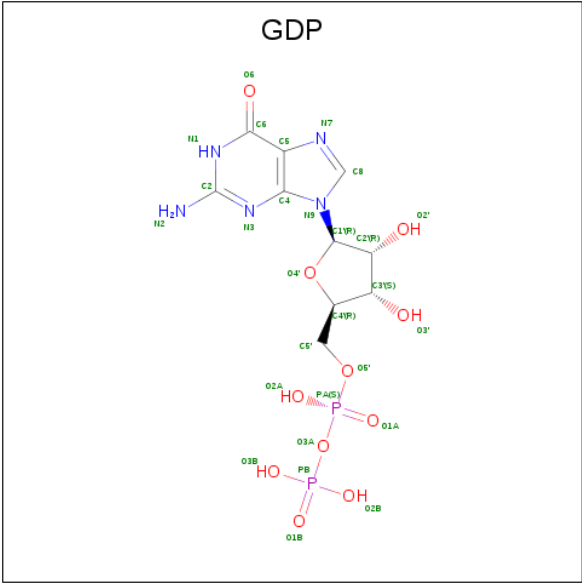
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
60	AY	1	Total	Zn	0	0
			1	1		
60	BN	1	Total	Zn	0	0
			1	1		
60	C4	1	Total	Zn	0	0
			1	1		
60	C5	1	Total	Zn	0	0
			1	1		
60	C6	1	Total	Zn	0	0
			1	1		
60	A6	1	Total	Zn	0	0
			1	1		
60	C9	1	Total	Zn	0	0
			1	1		
60	DN	1	Total	Zn	0	0
			1	1		
60	A4	1	Total	Zn	0	0
			1	1		
60	A5	1	Total	Zn	0	0
			1	1		
60	A9	1	Total	Zn	0	0
			1	1		
60	CY	1	Total	Zn	0	0
			1	1		

- Molecule 61 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe<sub>4</sub>S<sub>4</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
61	BD	1	Total	Fe	S	0	0
			8	4	4		
61	DD	1	Total	Fe	S	0	0
			8	4	4		

- Molecule 62 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula: C<sub>10</sub>H<sub>15</sub>N<sub>5</sub>O<sub>11</sub>P<sub>2</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
62	BZ	1	Total	C	N	O	P	0
			28	10	5	11	2	

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
62	DZ	1	Total	C	N	O	P	0	0
			28	10	5	11	2		

- Molecule 63 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
63	AA	1406	Total	O	0	0
			1406	1406		
63	AB	37	Total	O	0	0
			37	37		
63	AD	16	Total	O	0	0
			16	16		
63	AE	14	Total	O	0	0
			14	14		
63	AF	6	Total	O	0	0
			6	6		
63	AG	3	Total	O	0	0
			3	3		
63	AH	1	Total	O	0	0
			1	1		
63	AN	3	Total	O	0	0
			3	3		
63	AO	1	Total	O	0	0
			1	1		
63	AP	18	Total	O	0	0
			18	18		
63	AQ	5	Total	O	0	0
			5	5		
63	AR	2	Total	O	0	0
			2	2		
63	AS	1	Total	O	0	0
			1	1		
63	AT	3	Total	O	0	0
			3	3		
63	AU	4	Total	O	0	0
			4	4		
63	AV	1	Total	O	0	0
			1	1		
63	AW	1	Total	O	0	0
			1	1		
63	AX	4	Total	O	0	0
			4	4		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
63	AZ	1	Total	O	0	0
			1	1		
63	A0	9	Total	O	0	0
			9	9		
63	A1	2	Total	O	0	0
			2	2		
63	A2	1	Total	O	0	0
			1	1		
63	A3	2	Total	O	0	0
			2	2		
63	A5	4	Total	O	0	0
			4	4		
63	A7	4	Total	O	0	0
			4	4		
63	A8	9	Total	O	0	0
			9	9		
63	A9	1	Total	O	0	0
			1	1		
63	BA	203	Total	O	0	0
			203	203		
63	BD	3	Total	O	0	0
			3	3		
63	BE	2	Total	O	0	0
			2	2		
63	BG	1	Total	O	0	0
			1	1		
63	BJ	1	Total	O	0	0
			1	1		
63	BL	1	Total	O	0	0
			1	1		
63	BM	1	Total	O	0	0
			1	1		
63	BO	2	Total	O	0	0
			2	2		
63	BP	1	Total	O	0	0
			1	1		
63	BV	3	Total	O	0	0
			3	3		
63	BX	5	Total	O	0	0
			5	5		
63	BZ	2	Total	O	0	0
			2	2		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
63	CA	974	Total 974	O 974	0	0
63	CB	9	Total 9	O 9	0	0
63	CD	17	Total 17	O 17	0	0
63	CE	14	Total 14	O 14	0	0
63	CF	6	Total 6	O 6	0	0
63	CN	2	Total 2	O 2	0	0
63	CP	12	Total 12	O 12	0	0
63	CQ	2	Total 2	O 2	0	0
63	CT	3	Total 3	O 3	0	0
63	CU	2	Total 2	O 2	0	0
63	CV	2	Total 2	O 2	0	0
63	CW	1	Total 1	O 1	0	0
63	CX	2	Total 2	O 2	0	0
63	CY	2	Total 2	O 2	0	0
63	C0	5	Total 5	O 5	0	0
63	C1	1	Total 1	O 1	0	0
63	C3	2	Total 2	O 2	0	0
63	C6	1	Total 1	O 1	0	0
63	C7	1	Total 1	O 1	0	0
63	C8	3	Total 3	O 3	0	0
63	DA	154	Total 154	O 154	0	0

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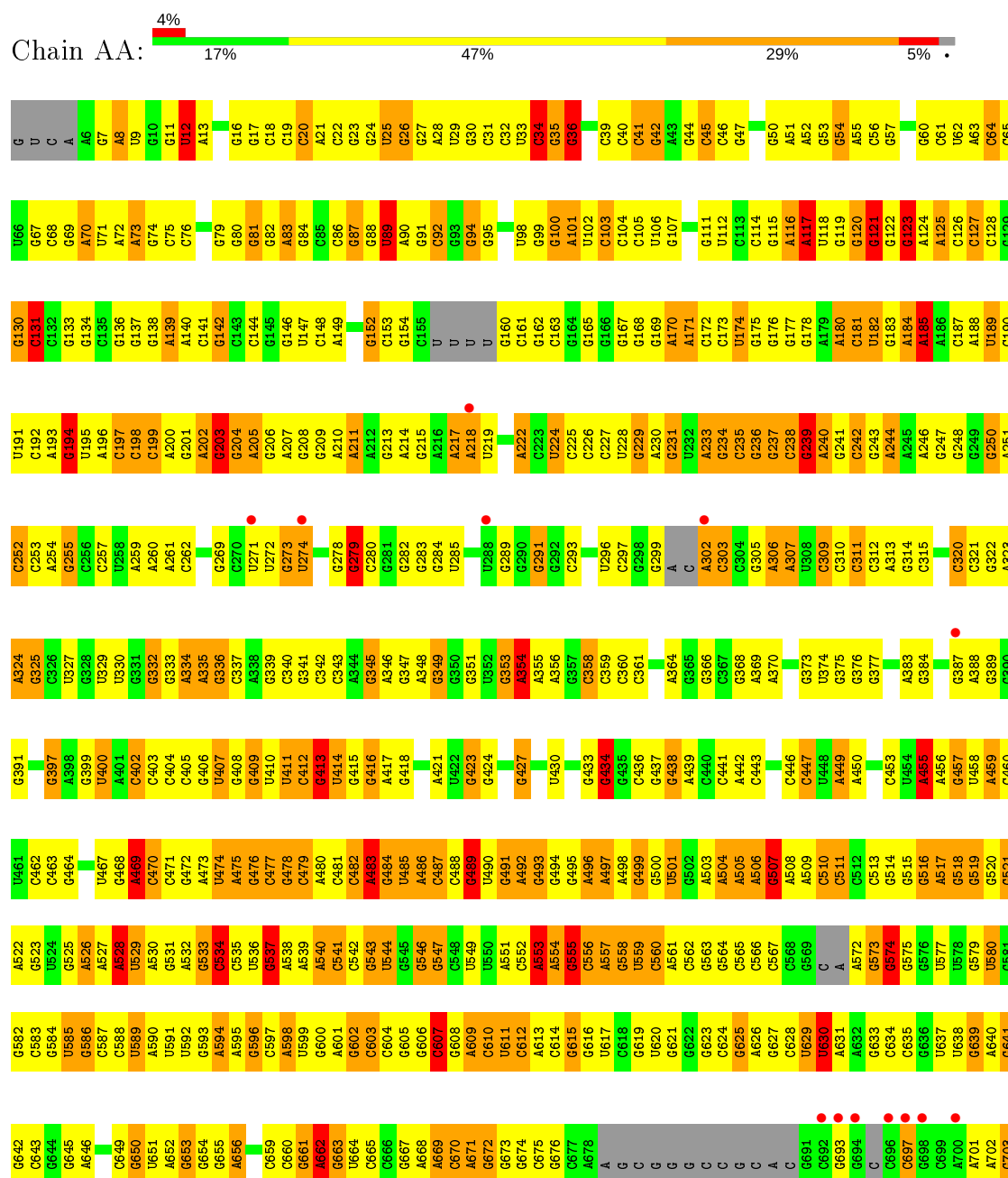
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
63	DE	3	Total	O	0	0
			3	3		
63	DH	1	Total	O	0	0
			1	1		
63	DJ	1	Total	O	0	0
			1	1		
63	DK	2	Total	O	0	0
			2	2		
63	DP	1	Total	O	0	0
			1	1		
63	DT	1	Total	O	0	0
			1	1		
63	DV	1	Total	O	0	0
			1	1		
63	DZ	1	Total	O	0	0
			1	1		

### 3 Residue-property plots

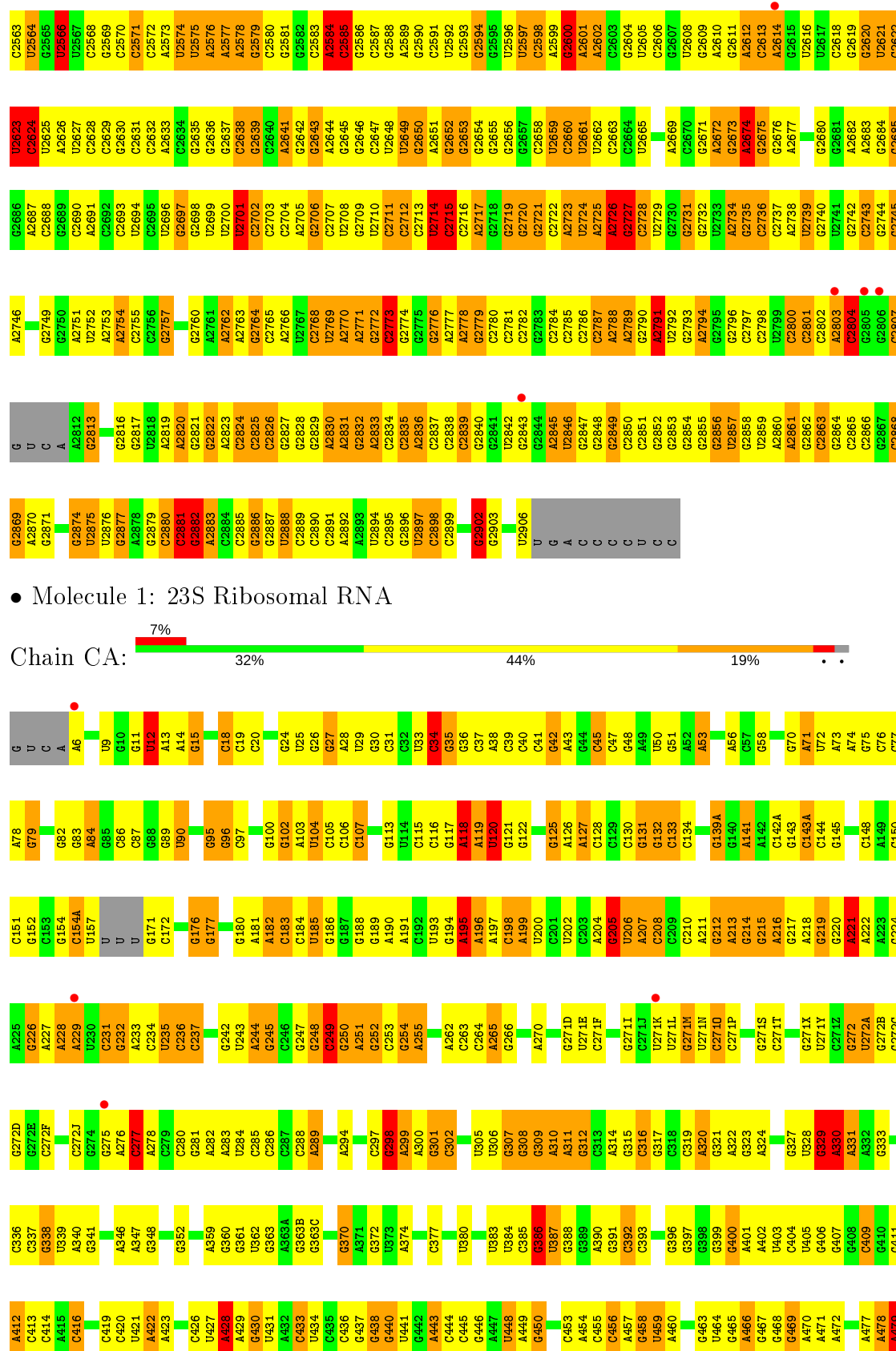
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are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

#### • Molecule 1: 23S Ribosomal RNA



A1574	A1575	A1576	A1577	C1578	C1579	G	U	A	C	G1584	G1585	G1586	G1587	A1588	A1589	A1590	G1599	A1600	G1602	C1603	G1604	A1605	A1606	G1606	G1607	G1608	A1609	G1610	G1611	G1612	A1613	A1614	G1615	A1616	A1617	A1618	A1619	G1620	G1621	G1622	G1623	G1624	G1625	G1626	G1627	G1628	G1629	A1630	G1631	A1632	A1633	G1634	G1635	G1636	G1637	G1638	G1639	A1640	G1641																																																																																			
G1512	G1513	C1514	G1517	G1518	A1519	A1520	C1521	G1522	G1523	A1524	G1525	G1526	G1529	G1530	G1531	A1532	G1533	A1534	G1535	G1536	G1537	G1538	C1539	A1540	A1541	A1542	A1543	C1544	C1545	G1546	C1547	G1548	U1549	C1550	C1551	G1552	A1553	A1554	C1555	A1556	G1557	G1558	G1559	U1560	C1561	U1562	G1563	G1565	G1566	G1567	G1568	U1569	G1570	G1571	G1572	G1573																																																																																						
C1449	C1450	U1451	C1452	C1453	C1454	C1455	G1456	G1457	G1458	A1459	A1460	G1461	G1462	G1463	U1466	G1467	G1468	G1469	G1470	G1471	G1472	A1473	C1474	G1475	G1476	A1477	G1478	U1479	A1480	G1481	G1482	C1483	U1484	A1485	G1486	A1487	G1488	G1489	A1490	A1491	C1492	C1493	A1496	G1497	C1498	C1499	A1500	U1501	A1502	G1503	U1504	A1505	A1506	G1507	G1508	C1509	G1510	C1511																																																																																				
A1388	G1389	G1390	G1391	G1392	G1393	G1394	A1395	G1396	G1397	U1398	A1399	A1400	G1401	G1402	U1403	G1404	A1405	A1406	G1407	A1408	C1409	G1410	A1411	A1412	A1413	A1414	G1415	A1416	G1417	U1418	A1419	G1420	G1421	C1422	G1423	A1424	A1425	G1426	G1427	G1428	A1429	G1430	A1431	G1432	C1433	U1436	U1437	A1438	A1439	U1440	A1441	U1442	U1443	G1444	G1445	G1446	G1447	G1448																																																																																				
U1328	G1329	A1330	G1331	A1332	A1333	U1334	C1335	C1336	C1337	U1338	C1339	U1340	G1341	G1342	C1343	C1344	G1345	U1346	A1347	A1348	G1349	C1350	C1351	C1352	A1353	A1354	G1355	G1356	G1357	U1358	U1359	C1360	C1361	U1362	A1363	C1364	G1365	C1366	A1367	U1368	U1369	G1370	G1371	U1372	C1373	G1374	U1375	A1376	G1377	G1378	G1379	G1380	U1381	A1382	G1383	G1384	G1385	G1386	U1387																																																																																			
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U1203	C1204	U1205	G1206	G1207	G1208	G1209	G1210	U1211	C1212	G1215	G1216	G1217	G1218	A1219	U1220	G1221	A1222	C1223	G1228	G1229	C1230	G1231	G1232	U1233	A1234	G1235	G1236	G1237	G1238	A1239	G1240	C1241	U1242	U1243	U1244	C1245	G1246	C1247	U1248	A1249	U1250	G1251	C1252	A1253	G1254	A1255	U1256	G1257	A1258	A1259	G1260	G1261	C1262	C1263	G1264	A1265	C1266																																																																																					
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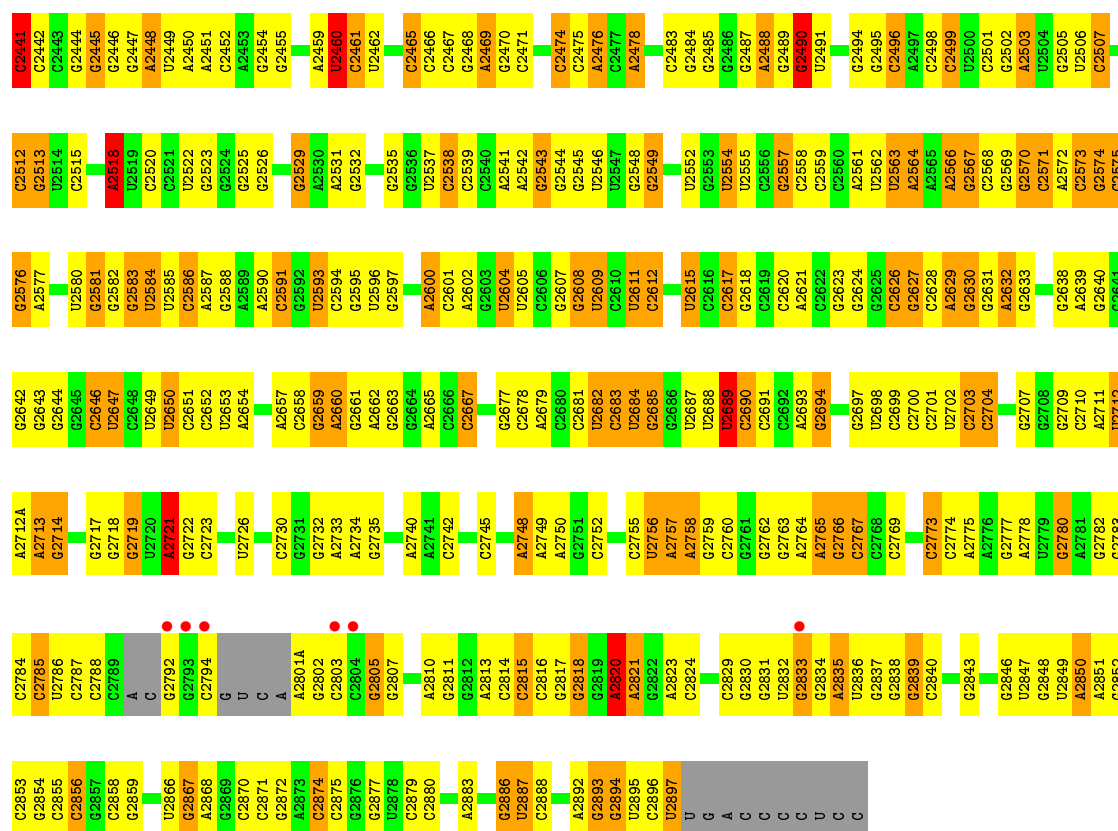
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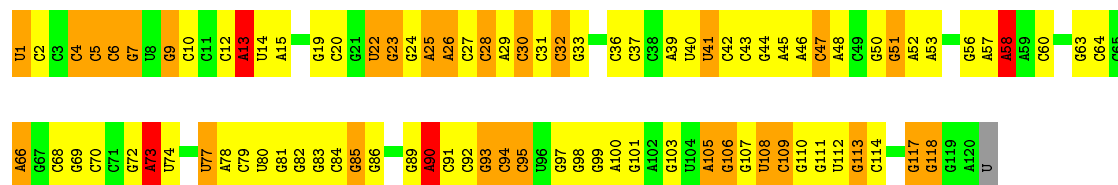


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C2363	C2296		C2229	C2153	G2088	C2025	C1959		A1810			C1582	U1503
C2364	U2296		G2230	G2154	C2088	C2026	A1960		G1811			A1583	C1504
G2365			U2233	G2155	C2095	C2027	C1961		A1812			C1584	C1505
	G2298		C2234	C2156	U2096	G2300	C1962		A1813			C1585	C1506
A2433	G2300		G2235	G2157	C2097	G2029	U1963		G1814			A1586	C1507
A2434	C2301		C2236	A2158	U2098	G2301	C1964		A1815			C1587	C1508
A2435			C2237	C2159	U2099	A2301	C1965		A1816			C1588	A1509
A2436			U2205										



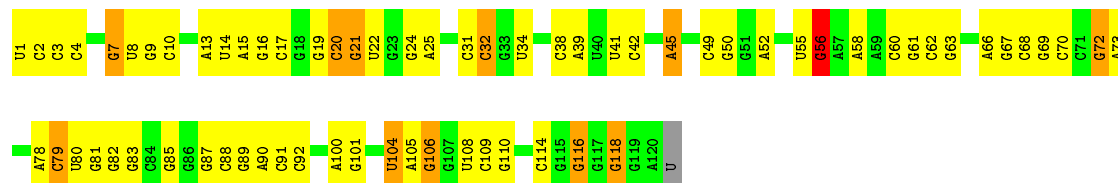
• Molecule 2: 5S Ribosomal RNA

Chain AB: 25% 47% 24% ..



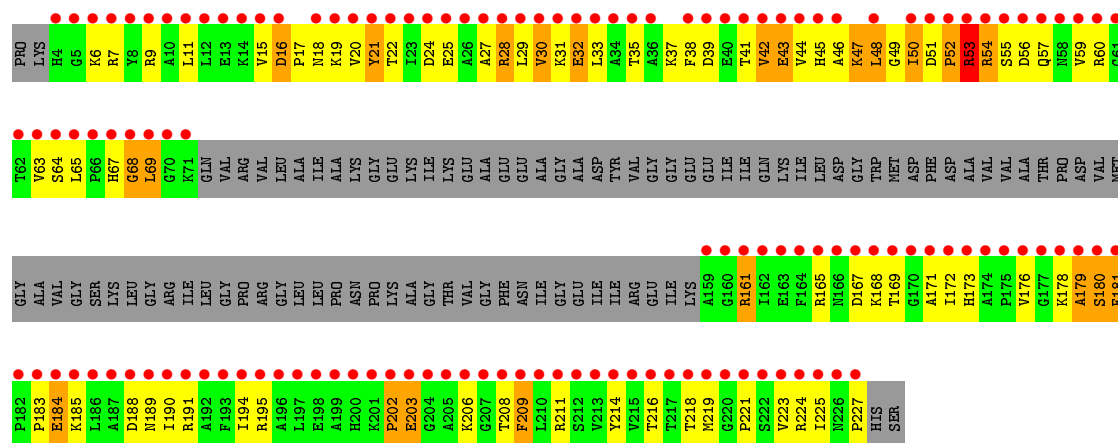
• Molecule 2: 5S Ribosomal RNA

Chain CB: 43% 46% 9% ..

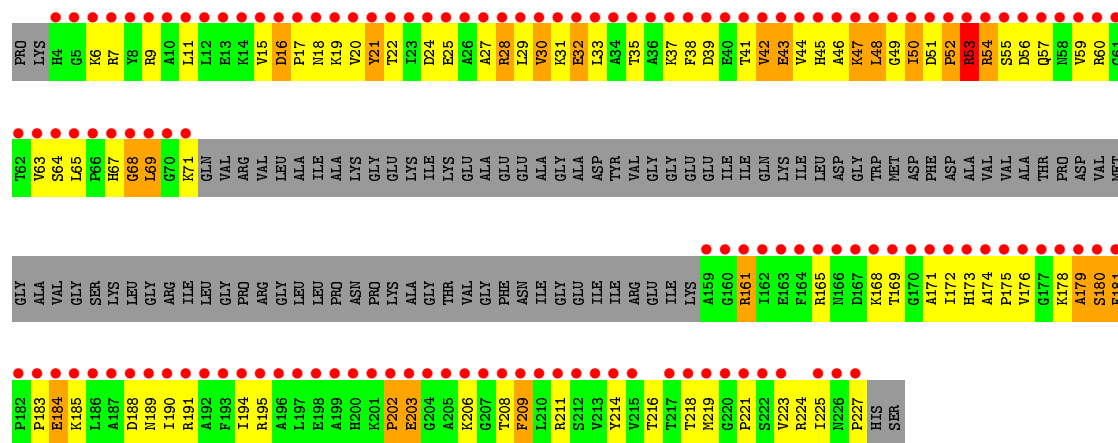


• Molecule 3: 50S ribosomal protein L1

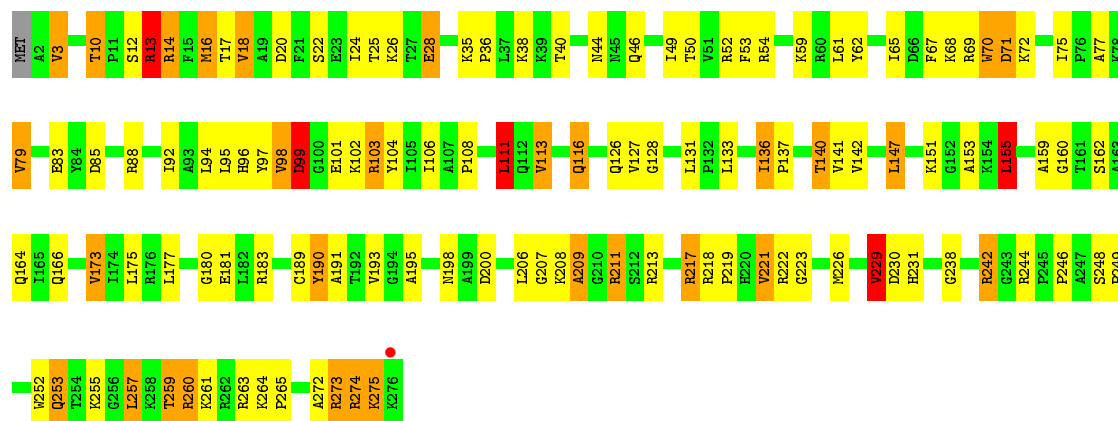
Chain AC: 22% 28% 10% 40% ..



• Molecule 3: 50S ribosomal protein L1

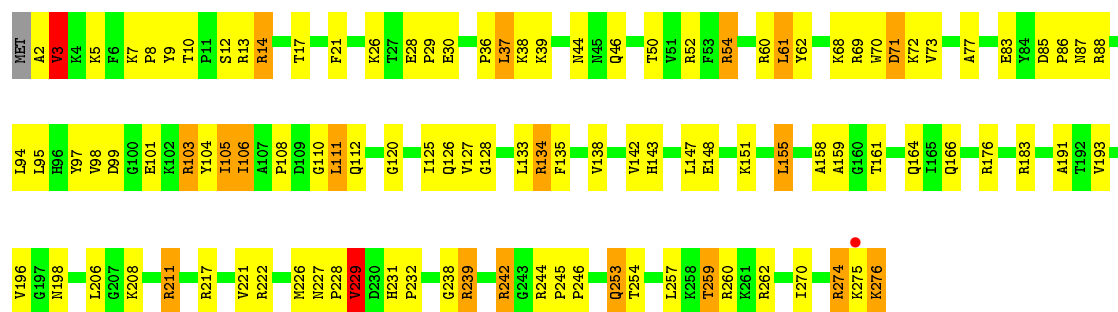


• Molecule 4: 50S ribosomal protein L2



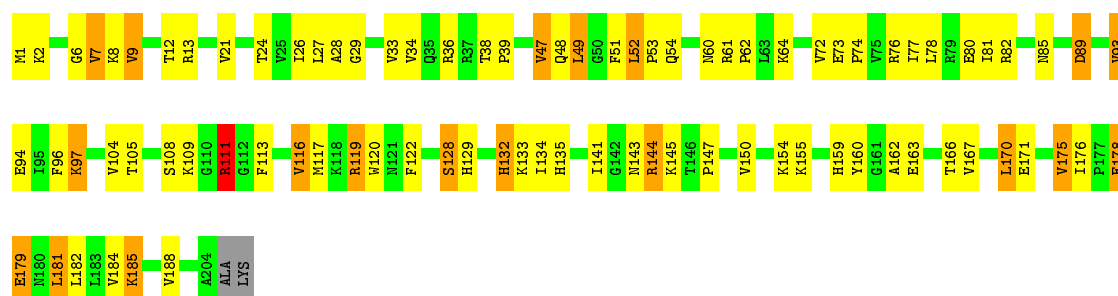
• Molecule 4: 50S ribosomal protein L2

Chain CD: 



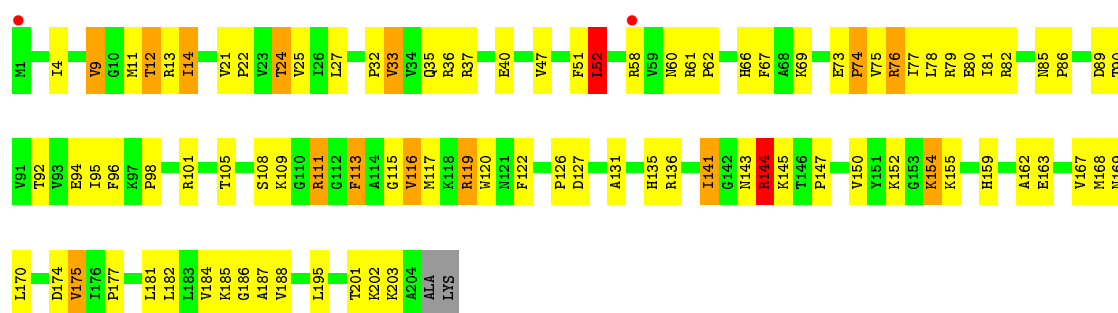
• Molecule 5: 50S ribosomal protein L3

Chain AE: 



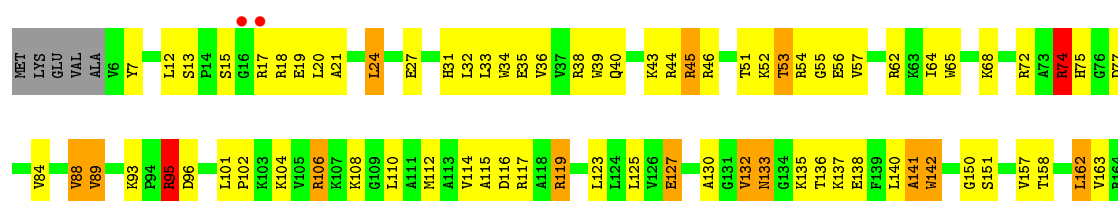
• Molecule 5: 50S ribosomal protein L3

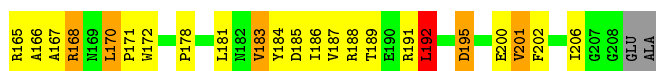
Chain CE: 



• Molecule 6: 50S ribosomal protein L4

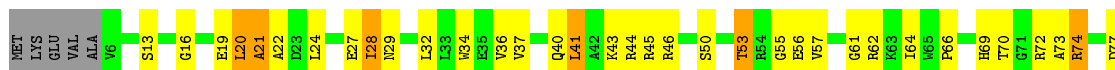
Chain AF: 





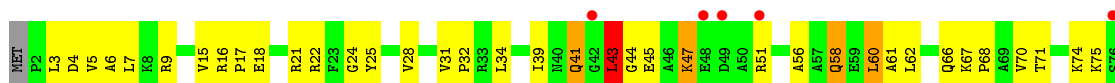
- Molecule 6: 50S ribosomal protein L4

Chain CF: 50% 39% 8%



- Molecule 7: 50S ribosomal protein L5

Chain AG: 4% 50% 38% 10%



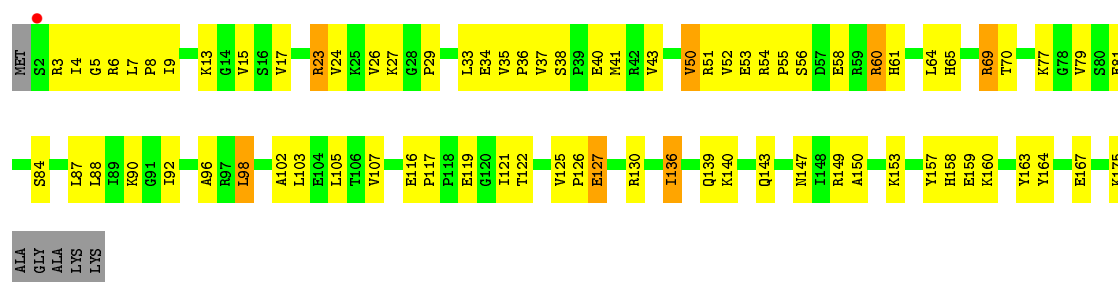
- Molecule 7: 50S ribosomal protein L5

Chain CG: 16% 48% 41% 9%

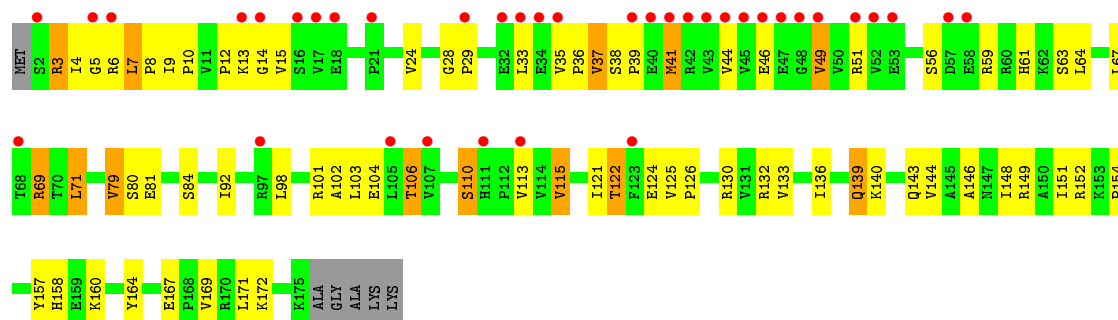


- Molecule 8: 50S ribosomal protein L6

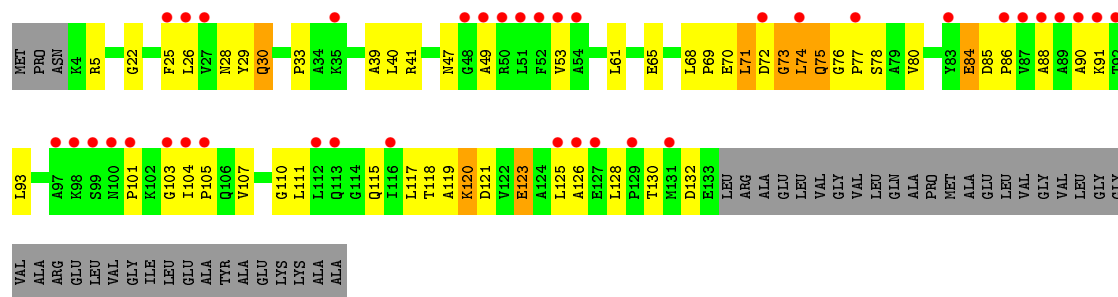
Chain AH: 54% 39% 7%



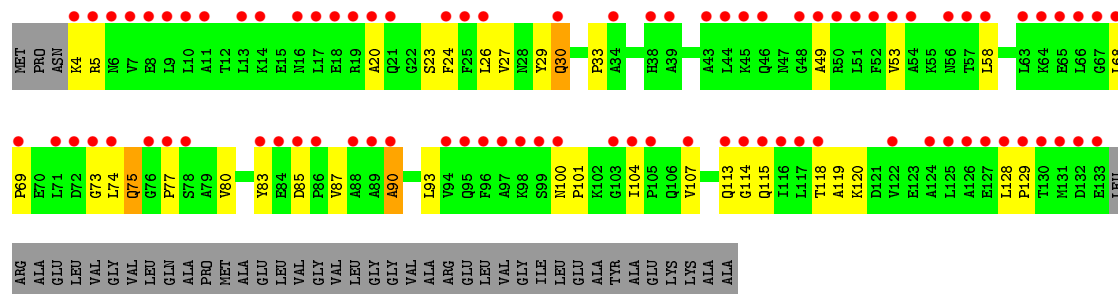
• Molecule 8: 50S ribosomal protein L6



• Molecule 9: 50S ribosomal protein L10

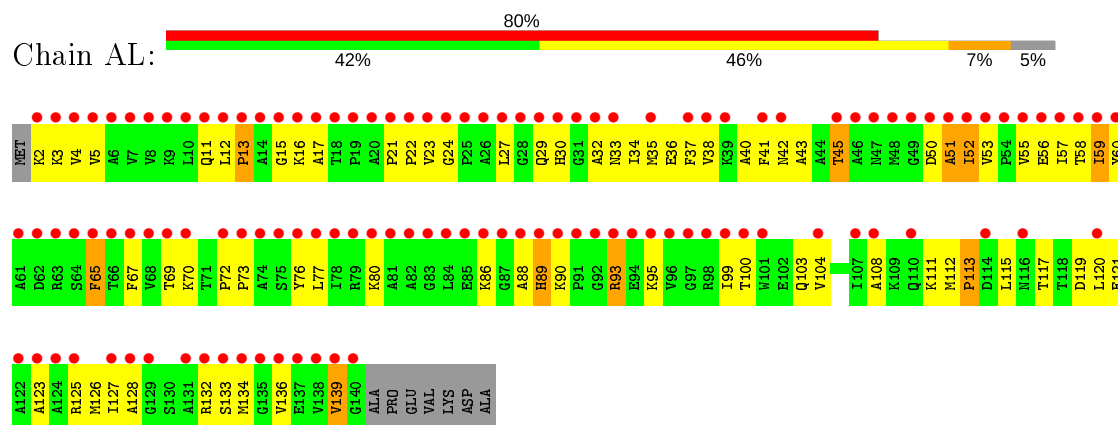


• Molecule 9: 50S ribosomal protein L10



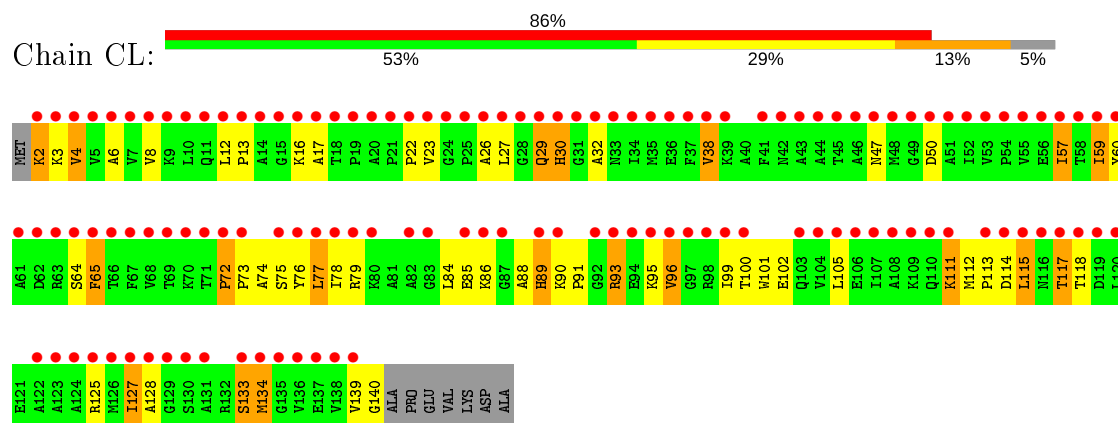
- Molecule 10: 50S ribosomal protein L11

Chain AL:



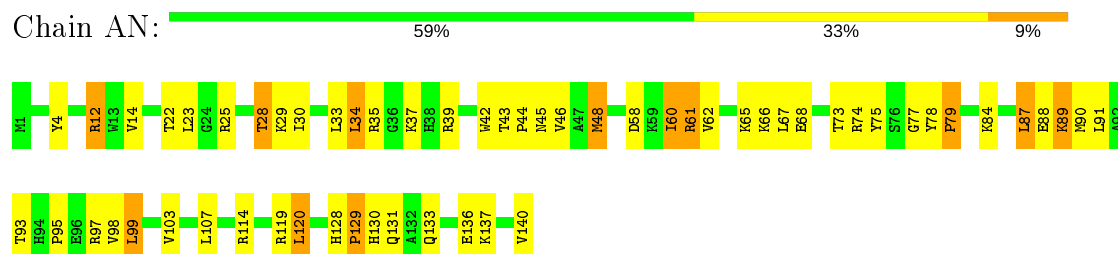
- Molecule 10: 50S ribosomal protein L11

Chain CL:



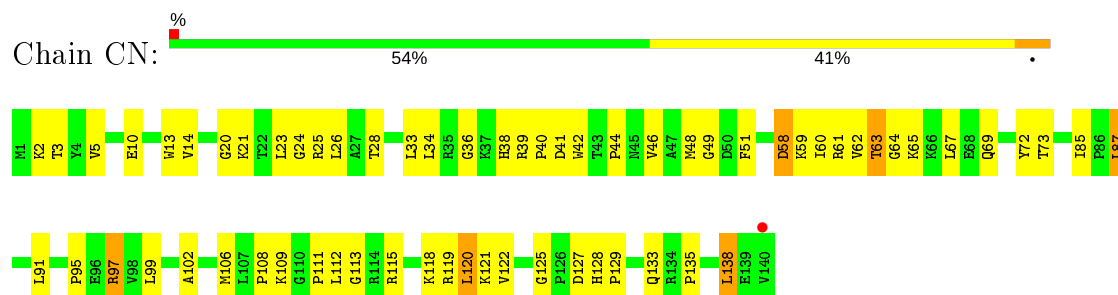
- Molecule 11: 50S ribosomal protein L13

Chain AN:



- Molecule 11: 50S ribosomal protein L13

Chain CN:

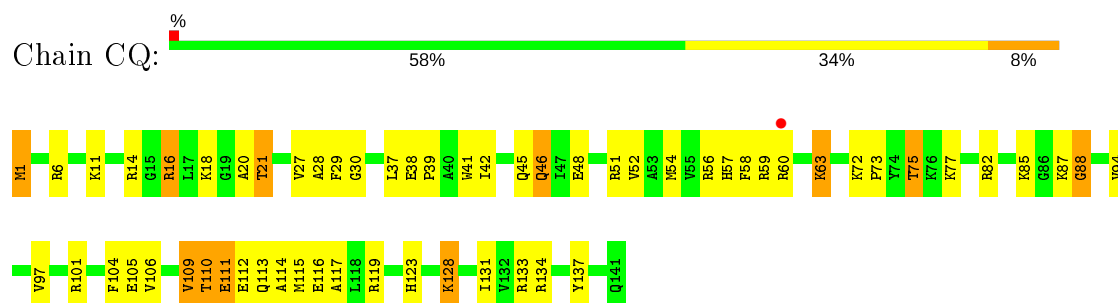


- Molecule 12: 50S ribosomal protein L14

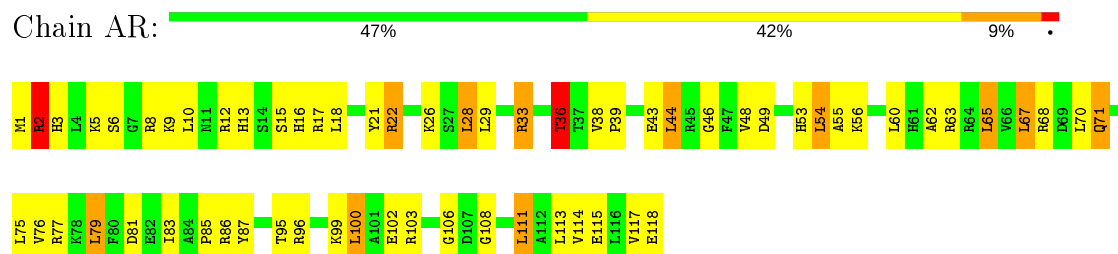




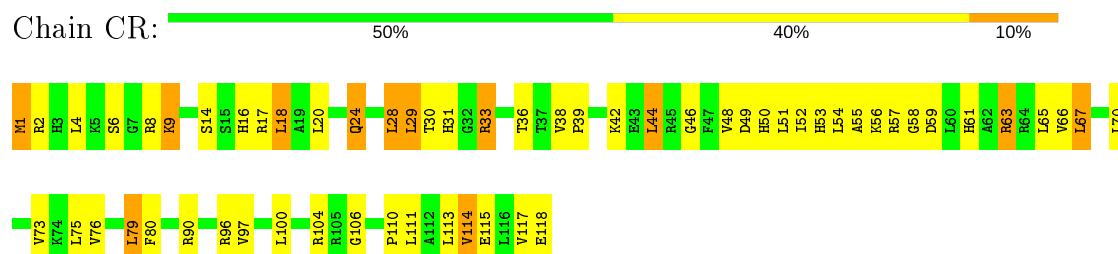
- Molecule 14: 50S ribosomal protein L16



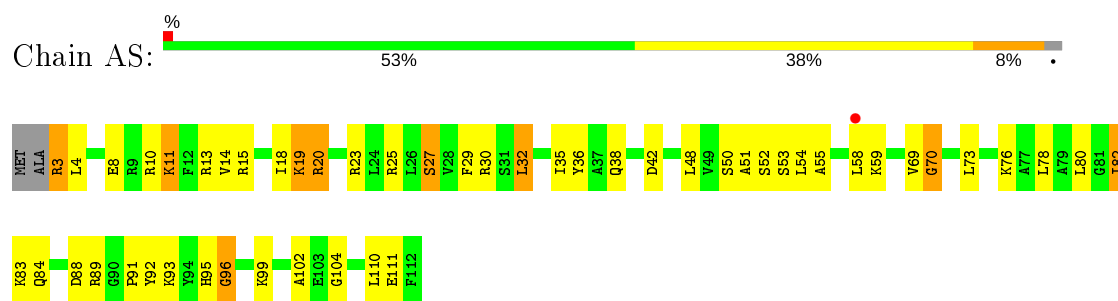
- Molecule 15: 50S ribosomal protein L17



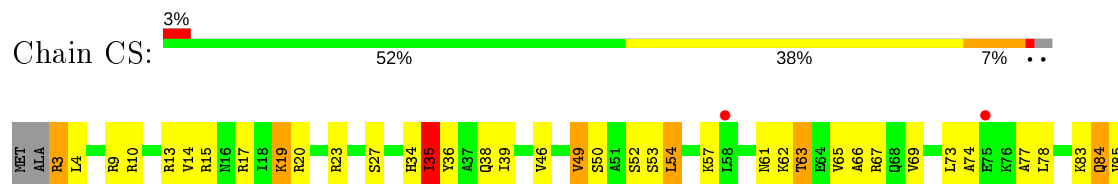
- Molecule 15: 50S ribosomal protein L17

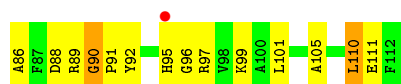


- Molecule 16: 50S ribosomal protein L18

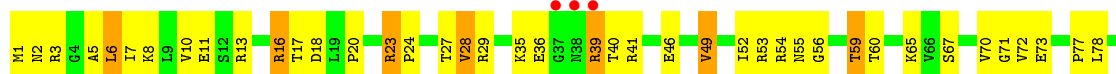


- Molecule 16: 50S ribosomal protein L18

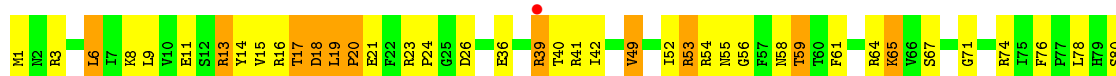




- Molecule 17: 50S ribosomal protein L19



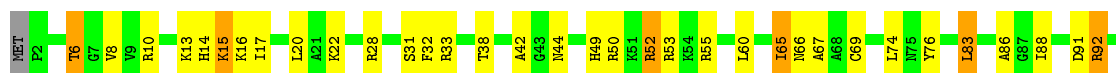
- Molecule 17: 50S ribosomal protein L19



- Molecule 18: 50S ribosomal protein L20

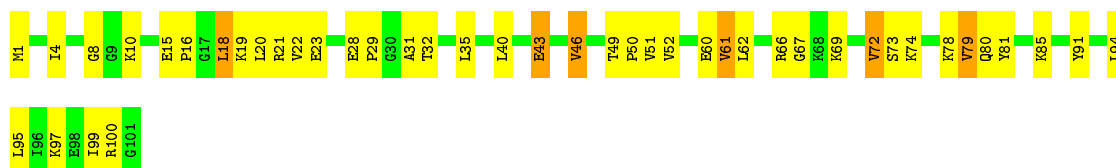


- Molecule 18: 50S ribosomal protein L20

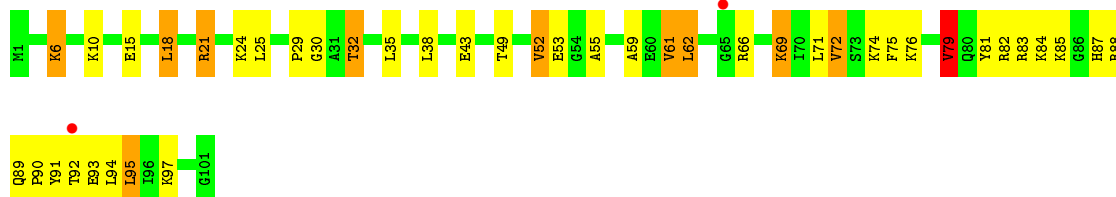


- Molecule 19: 50S ribosomal protein L21

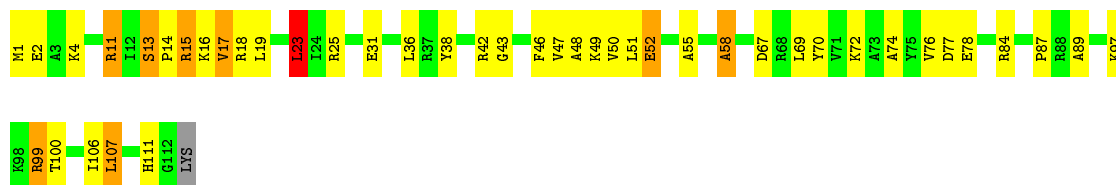




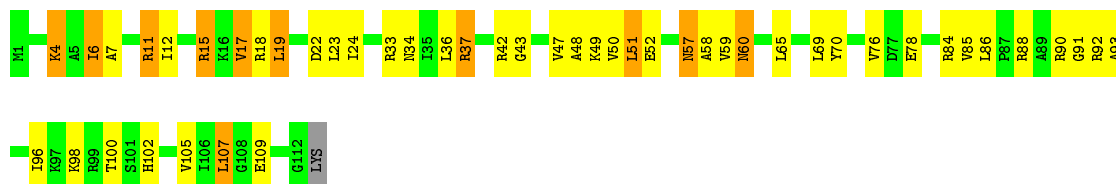
- Molecule 19: 50S ribosomal protein L21



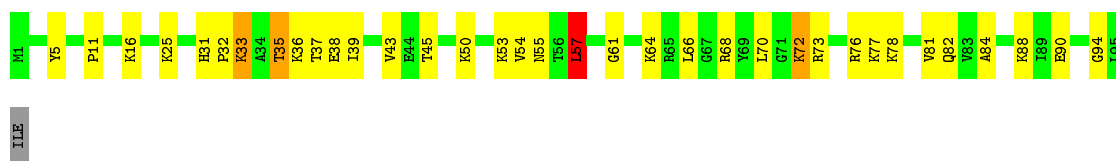
- Molecule 20: 50S ribosomal protein L22



- Molecule 20: 50S ribosomal protein L22

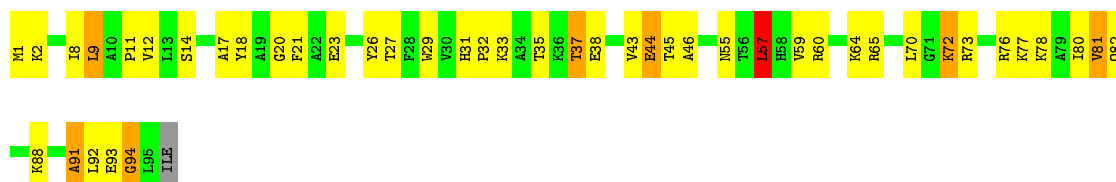


- Molecule 21: 50S ribosomal protein L23

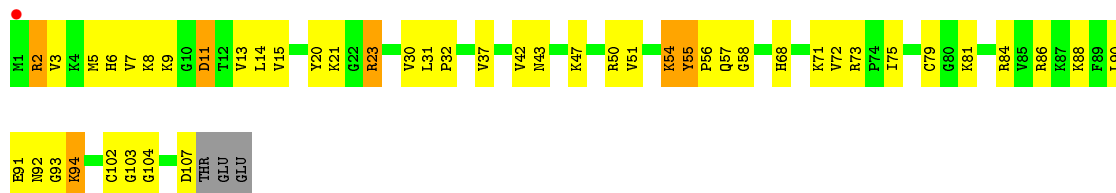


- Molecule 21: 50S ribosomal protein L23

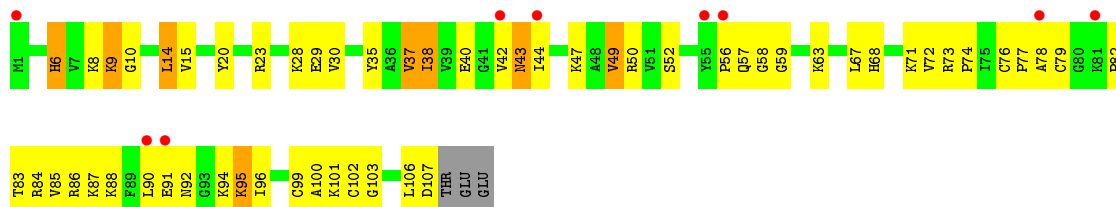




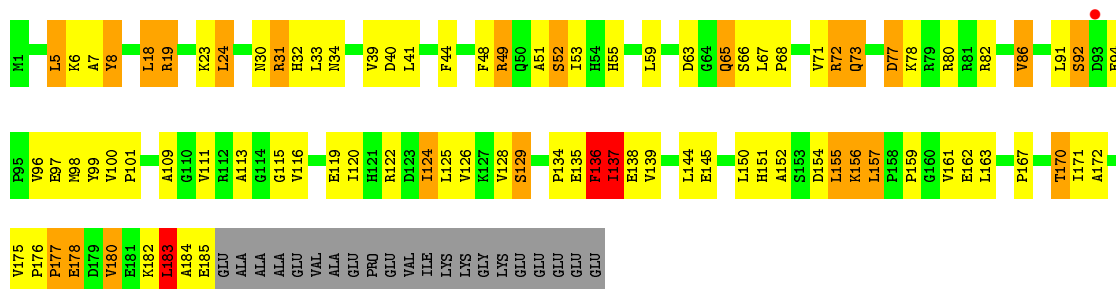
- Molecule 22: 50S ribosomal protein L24



- Molecule 22: 50S ribosomal protein L24

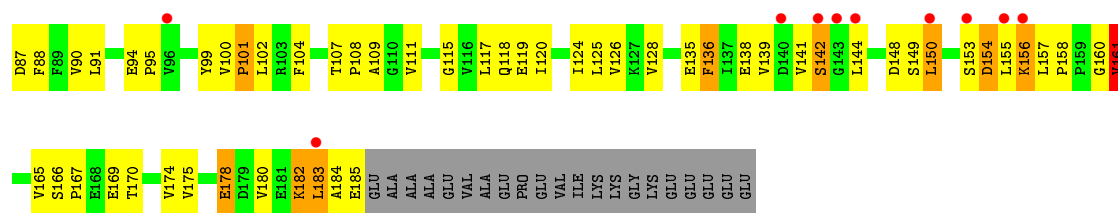


- Molecule 23: 50S ribosomal protein L25

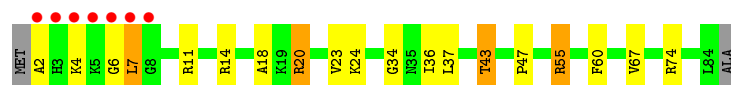
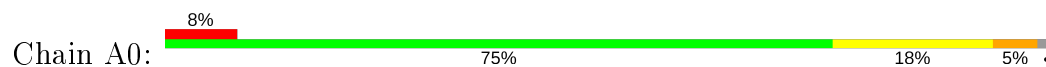


- Molecule 23: 50S ribosomal protein L25





• Molecule 24: 50S ribosomal protein L27



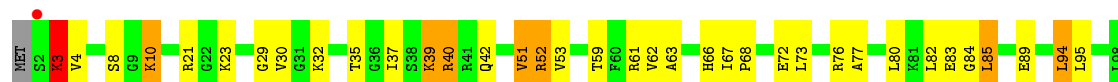
• Molecule 24: 50S ribosomal protein L27



• Molecule 25: 50S ribosomal protein L28



• Molecule 25: 50S ribosomal protein L28



• Molecule 26: 50S ribosomal protein L29



• Molecule 26: 50S ribosomal protein L29





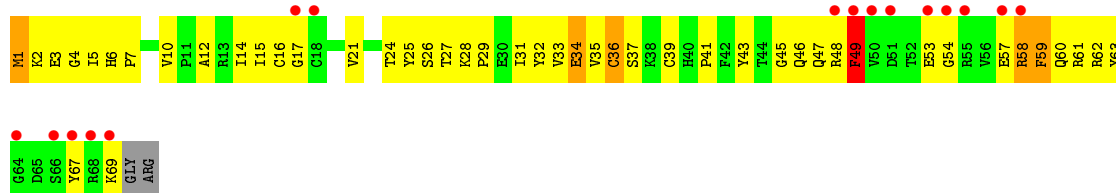
- Molecule 27: 50S ribosomal protein L30



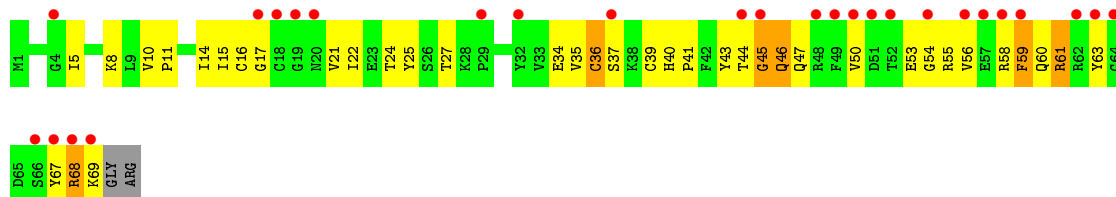
- Molecule 27: 50S ribosomal protein L30



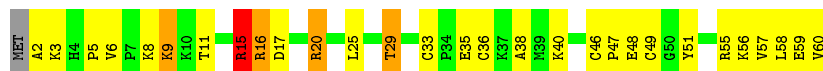
- Molecule 28: 50S ribosomal protein L31



- Molecule 28: 50S ribosomal protein L31



- Molecule 29: 50S ribosomal protein L32



- Molecule 29: 50S ribosomal protein L32

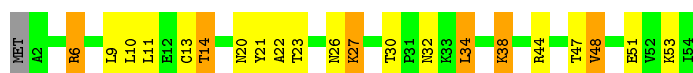




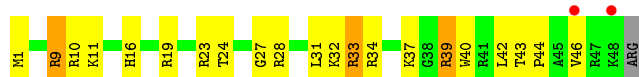
- Molecule 30: 50S ribosomal protein L33



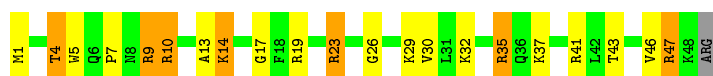
- Molecule 30: 50S ribosomal protein L33



- Molecule 31: 50S ribosomal protein L34



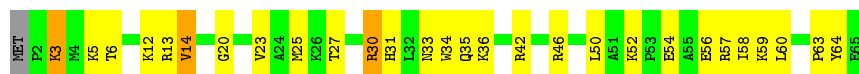
- Molecule 31: 50S ribosomal protein L34



- Molecule 32: 50S ribosomal protein L35



- Molecule 32: 50S ribosomal protein L35



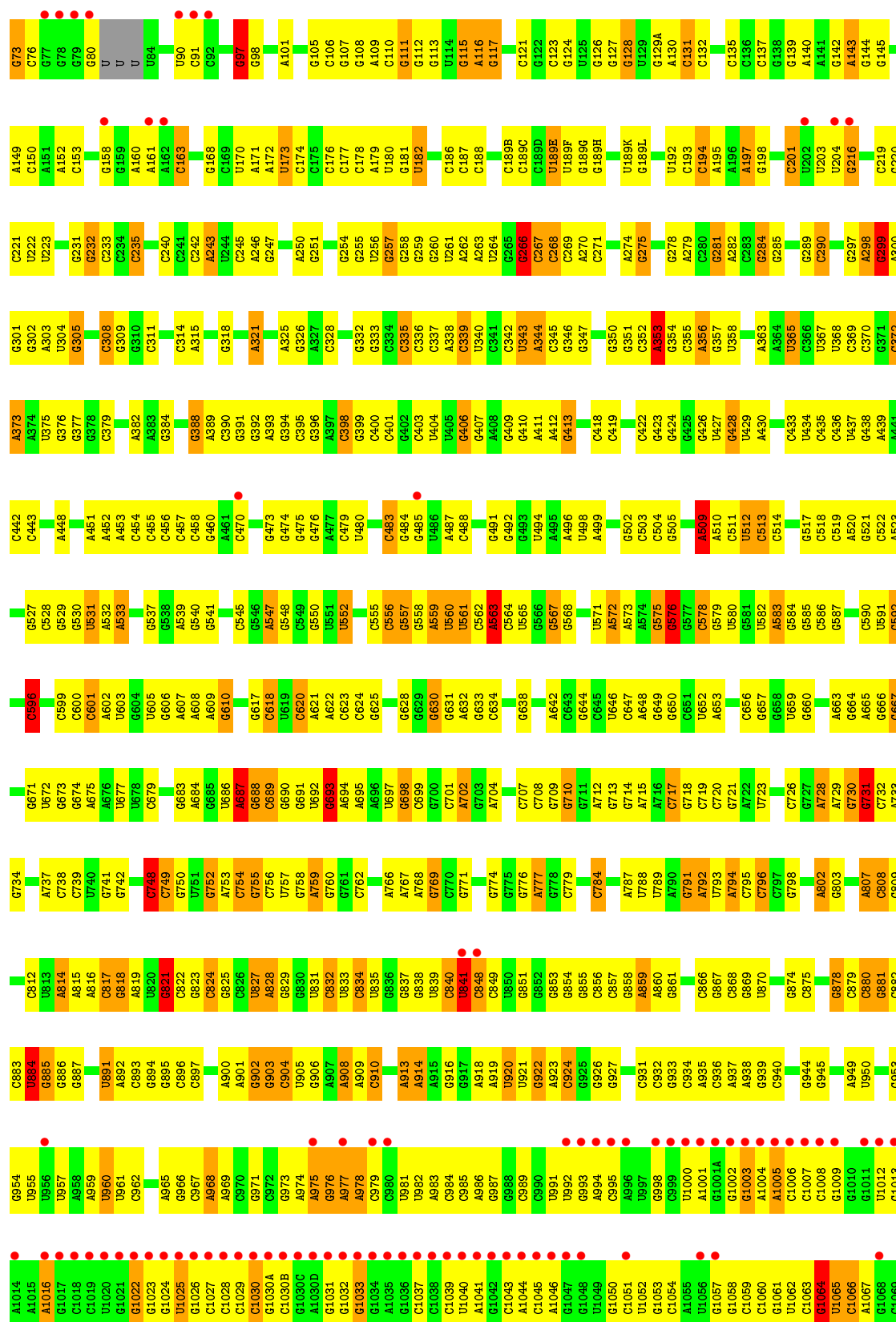
- Molecule 33: 50S ribosomal protein L36

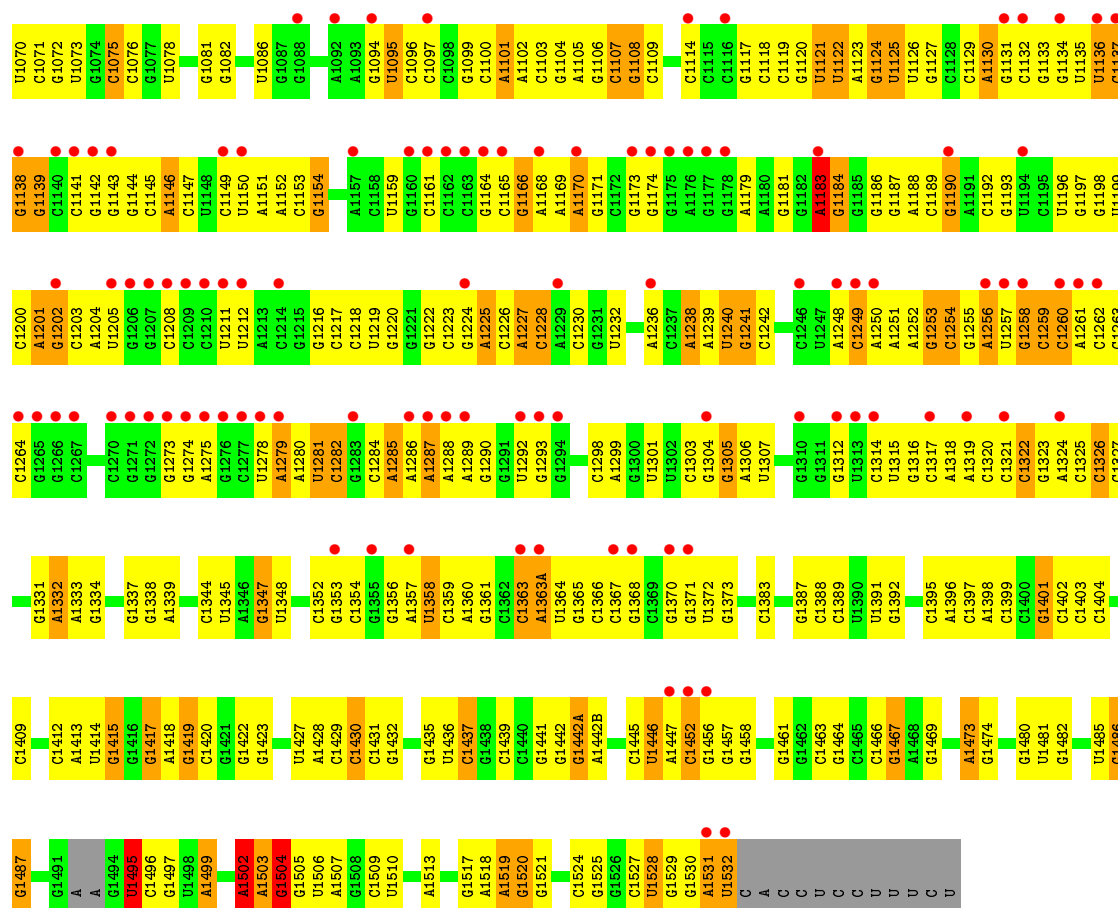




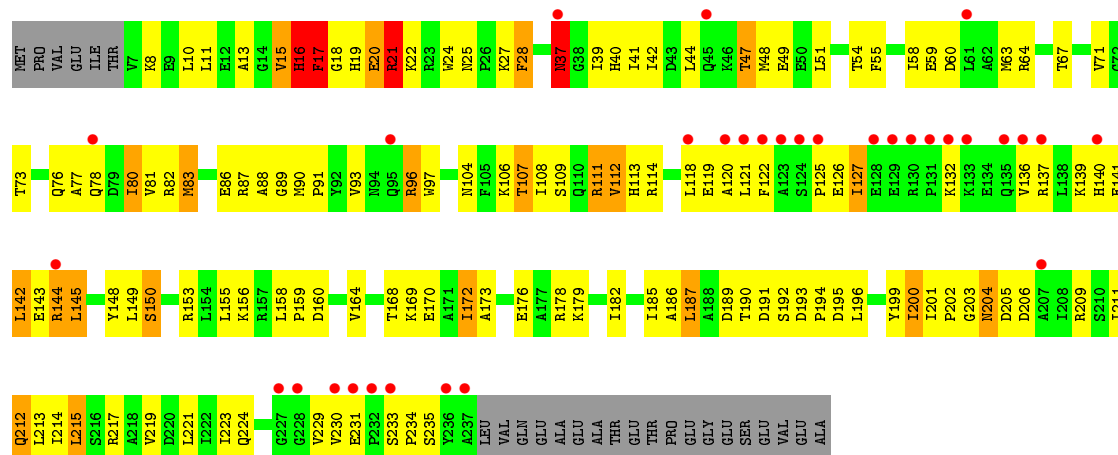






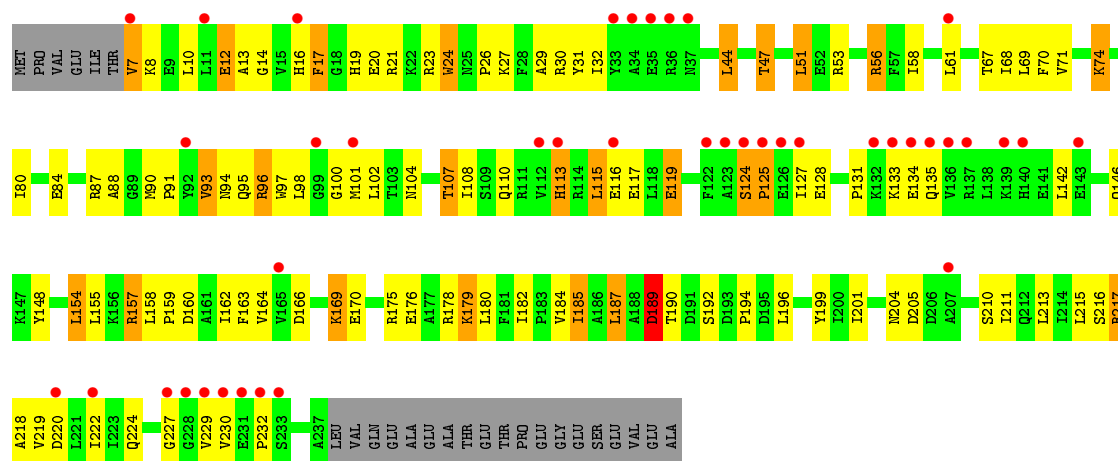


• Molecule 35: 30S ribosomal protein S2



• Molecule 35: 30S ribosomal protein S2





• Molecule 36: 30S ribosomal protein S3

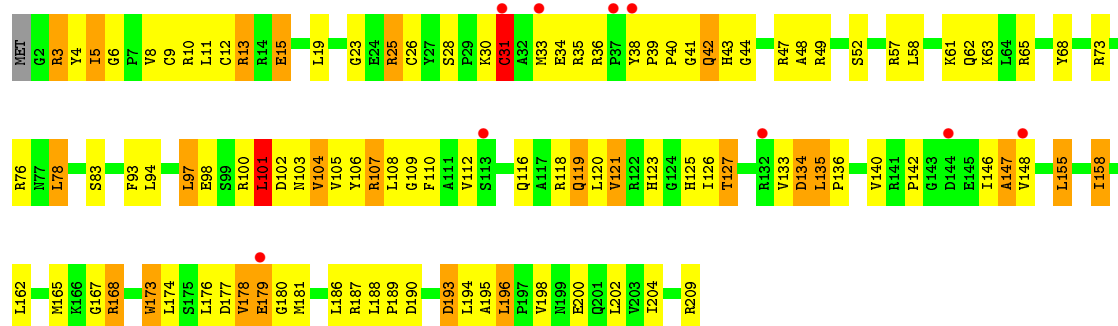


• Molecule 36: 30S ribosomal protein S3



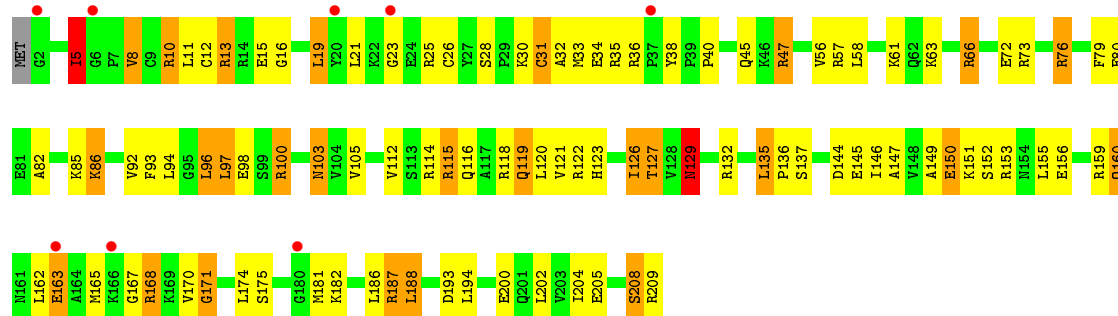
• Molecule 37: 30S ribosomal protein S4

Chain BD: 



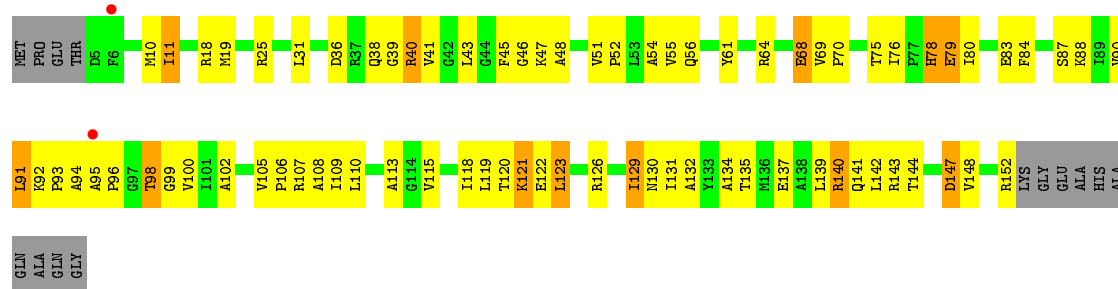
- Molecule 37: 30S ribosomal protein S4

Chain DD: 



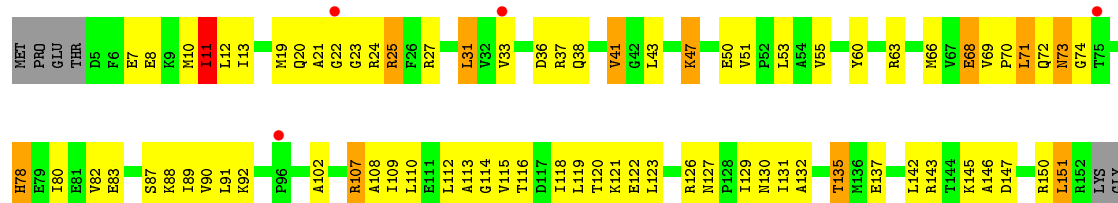
- Molecule 38: 30S ribosomal protein S5

Chain BE: 



- Molecule 38: 30S ribosomal protein S5

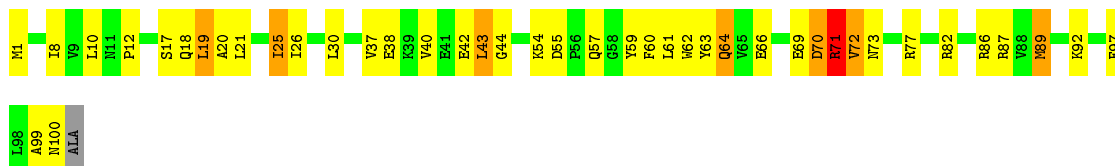
Chain DE: 



GLU  
ALA  
HIS  
ALA  
GLN  
ALA  
GLN  
GLY

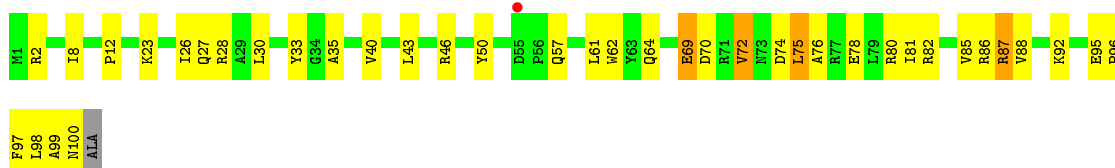
• Molecule 39: 30S ribosomal protein S6

Chain BF:  57% 34% 7% ..



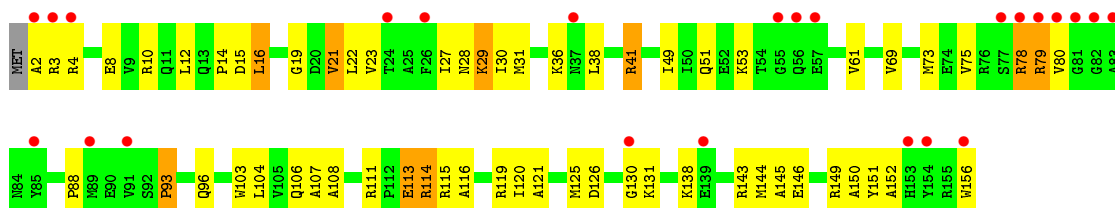
• Molecule 39: 30S ribosomal protein S6

Chain DF:  60% 35% . .




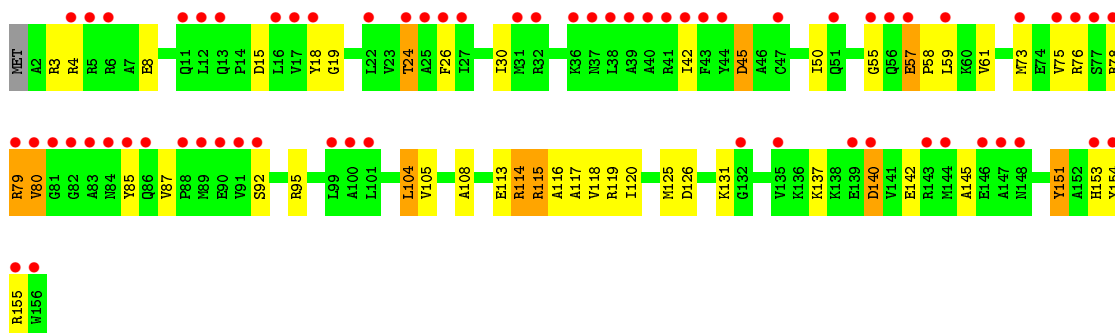
• Molecule 40: 30S ribosomal protein S7

Chain BG:  15% 60% 33% 6% .



• Molecule 40: 30S ribosomal protein S7

Chain DG:  42% 68% 25% 6% .



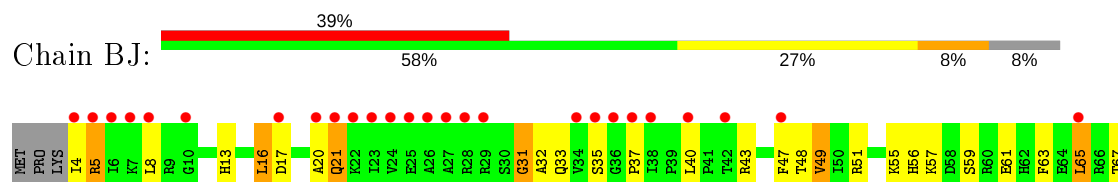
• Molecule 41: 30S ribosomal protein S8

- Molecule 41: 30S ribosomal protein S8

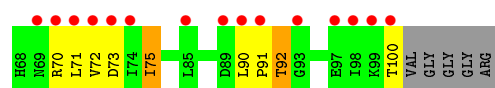
- Molecule 42: 30S ribosomal protein S9

- Molecule 42: 30S ribosomal protein S9

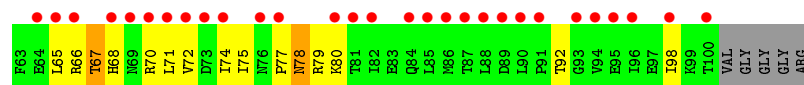
- Molecule 43: 30S ribosomal protein S10



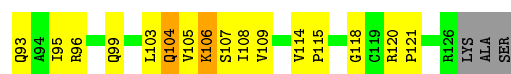




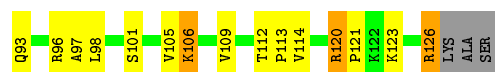
- Molecule 43: 30S ribosomal protein S10



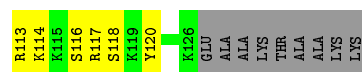
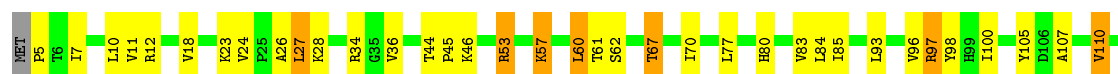
- Molecule 44: 30S ribosomal protein S11



- Molecule 44: 30S ribosomal protein S11

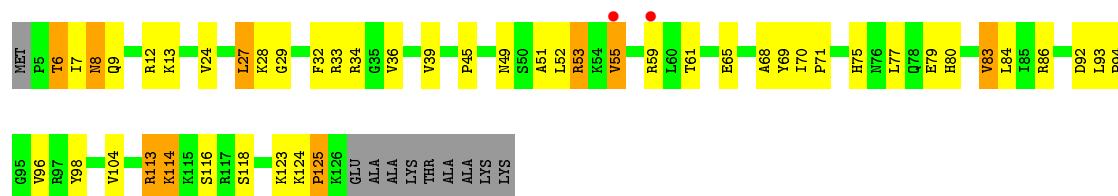


- Molecule 45: 30S ribosomal protein S12

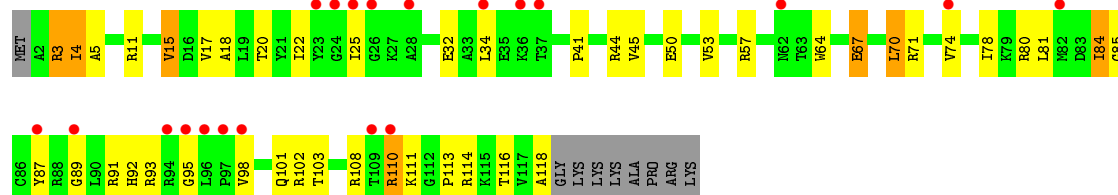


- Molecule 45: 30S ribosomal protein S12

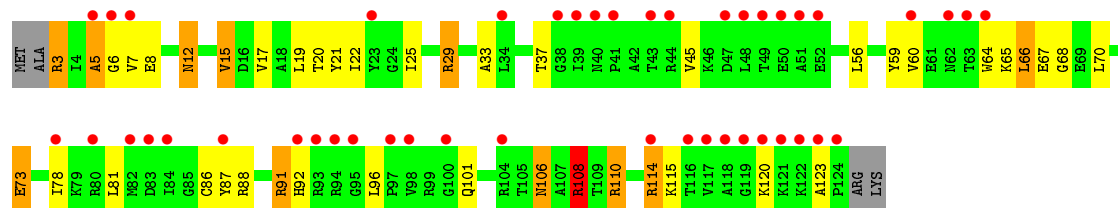




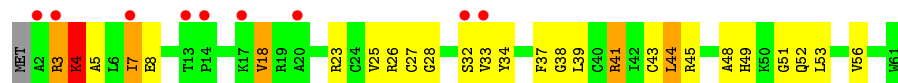
- Molecule 46: 30S ribosomal protein S13



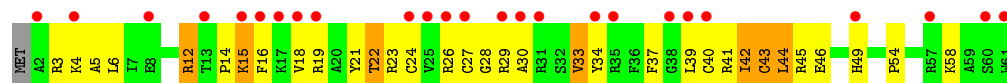
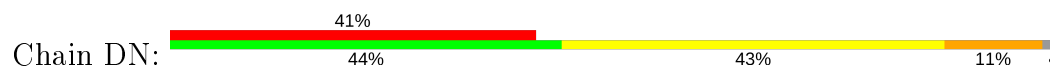
- Molecule 46: 30S ribosomal protein S13



- Molecule 47: 30S ribosomal protein S14 type Z



- Molecule 47: 30S ribosomal protein S14 type Z



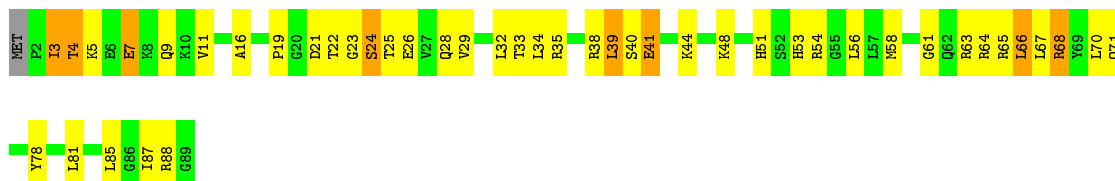
- Molecule 48: 30S ribosomal protein S15





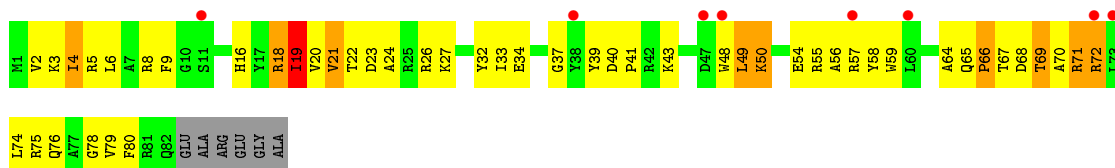
- Molecule 48: 30S ribosomal protein S15

Chain DO: 48% 42% 9%



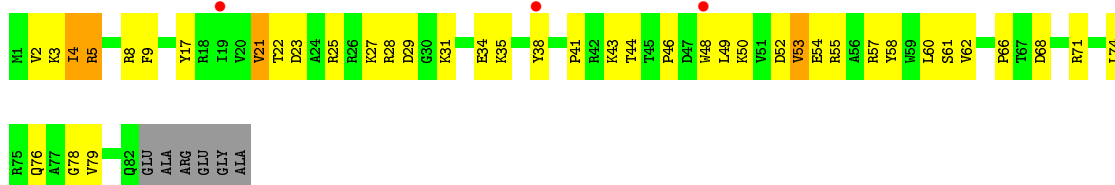
- Molecule 49: 30S ribosomal protein S16

Chain BP: 9% 38% 44% 10% 7%



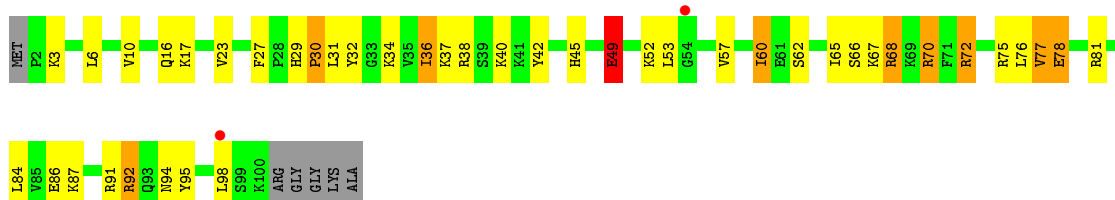
- Molecule 49: 30S ribosomal protein S16

Chain DP: 3% 47% 42% 5% 7%



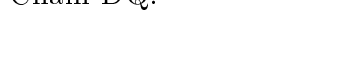
- Molecule 50: 30S ribosomal protein S17

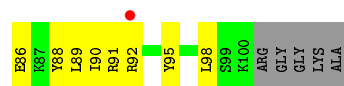
Chain BQ: 2% 53% 31% 9% 6%



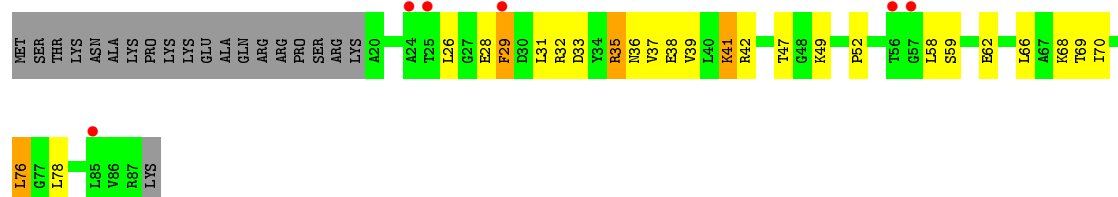
- Molecule 50: 30S ribosomal protein S17

Chain DQ: 53% 37% 6%

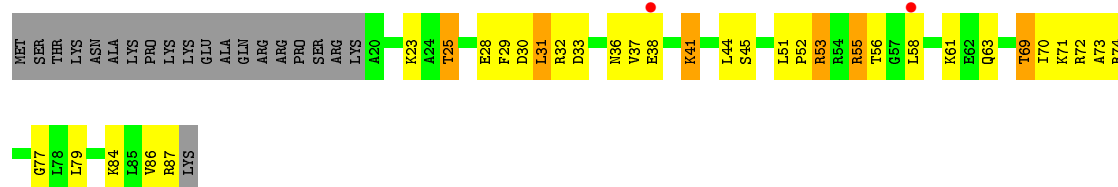




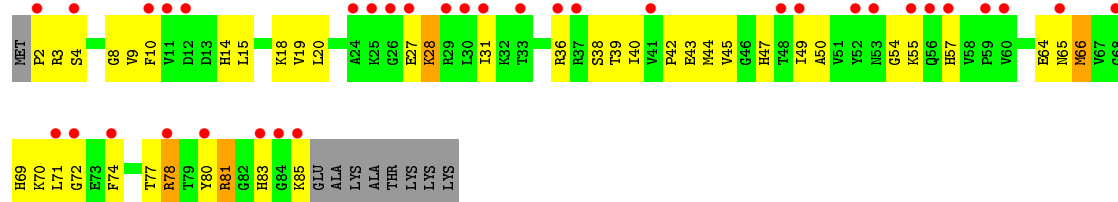
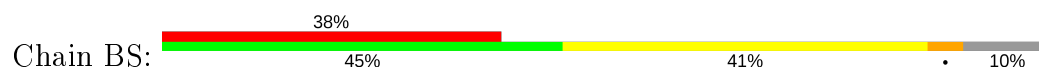
• Molecule 51: 30S ribosomal protein S18



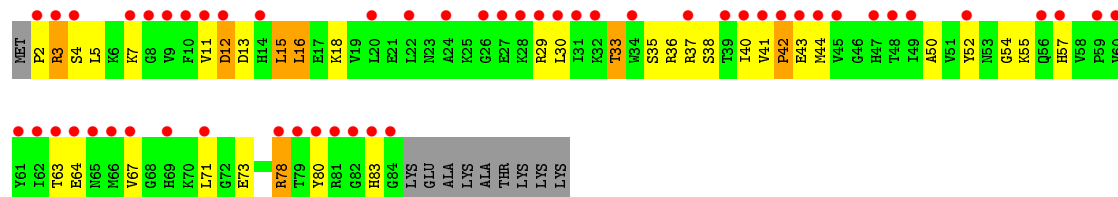
• Molecule 51: 30S ribosomal protein S18



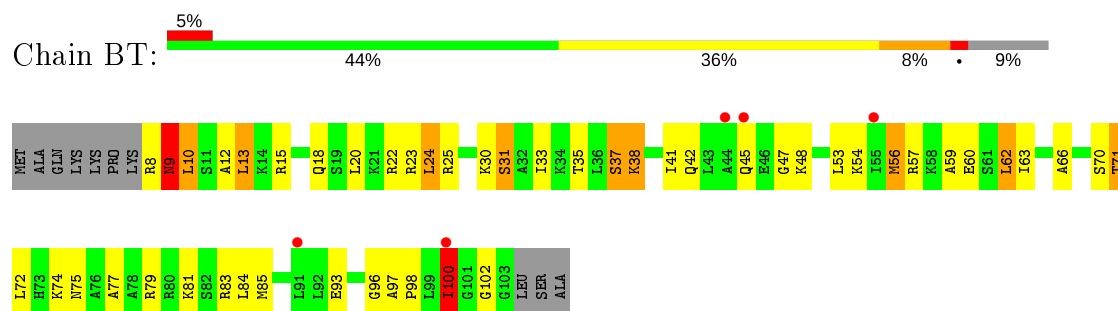
• Molecule 52: 30S ribosomal protein S19



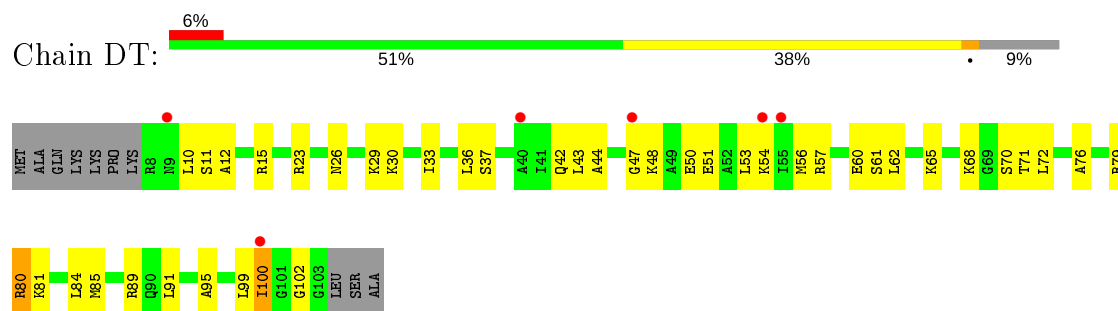
• Molecule 52: 30S ribosomal protein S19



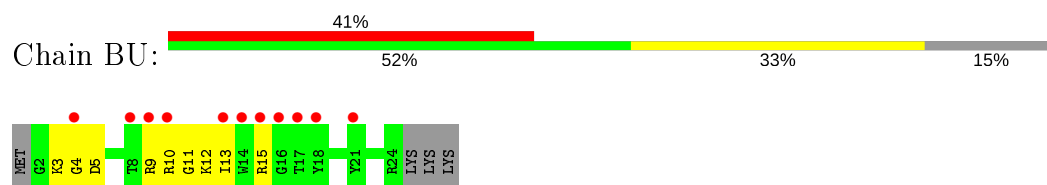
- Molecule 53: 30S ribosomal protein S20



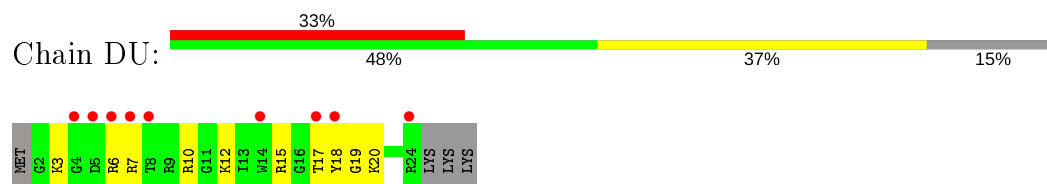
- Molecule 53: 30S ribosomal protein S20



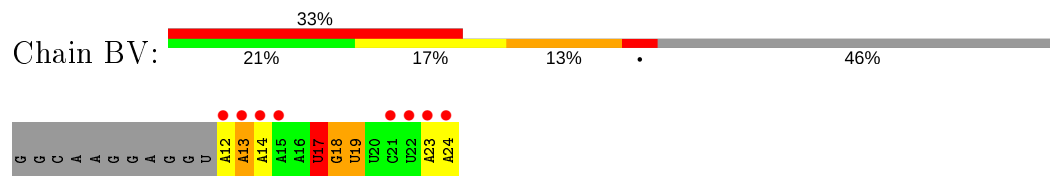
- Molecule 54: 30S ribosomal protein Thx



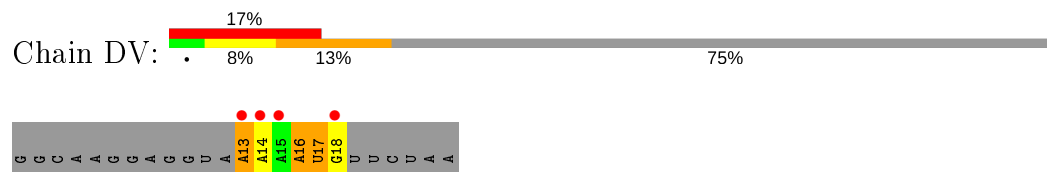
- Molecule 54: 30S ribosomal protein Thx



- Molecule 55: mRNA



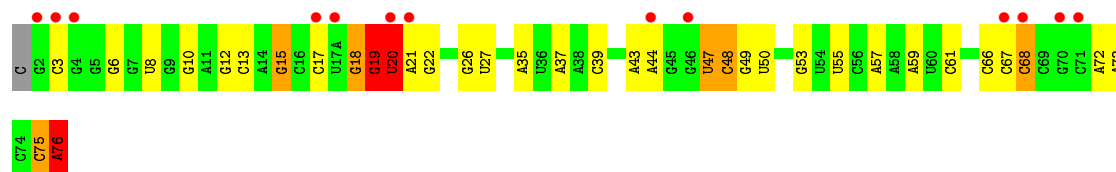
- Molecule 55: mRNA



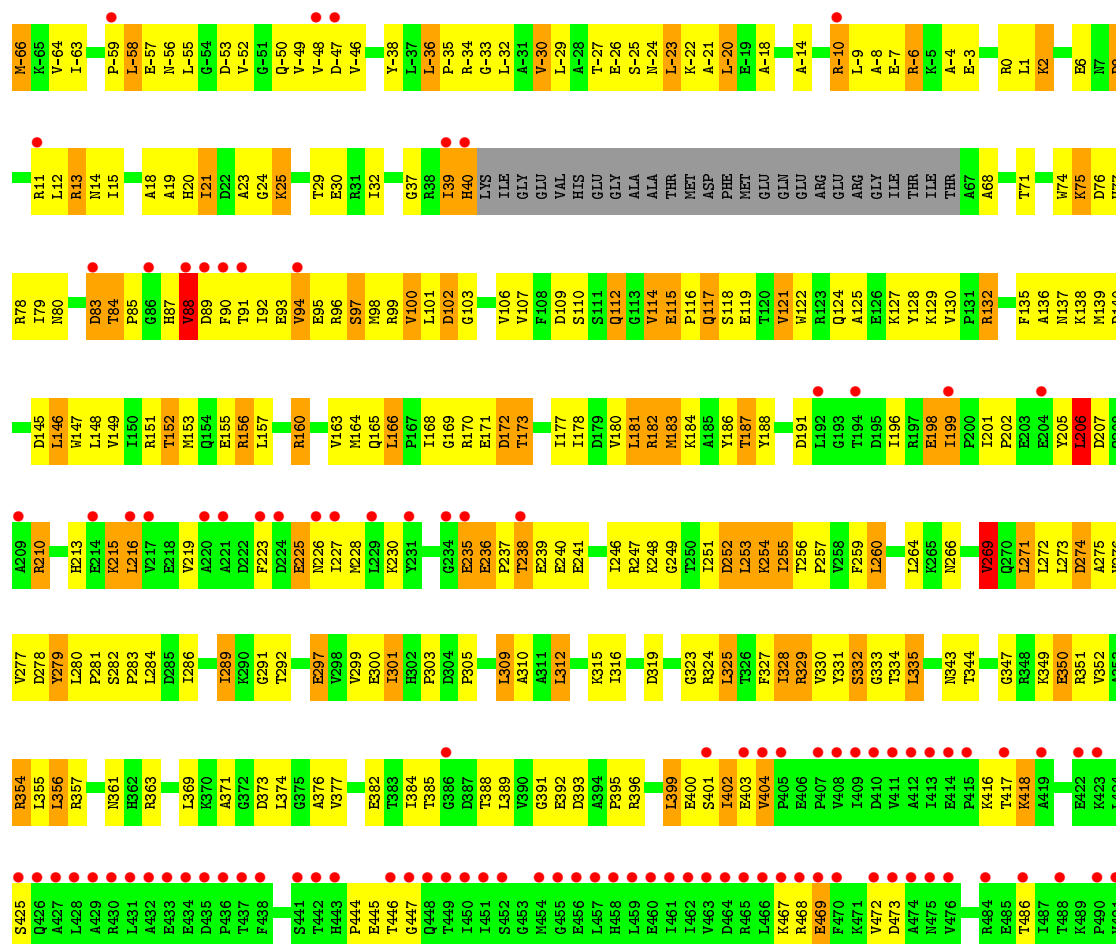
## ● Molecule 56: P-site tRNA

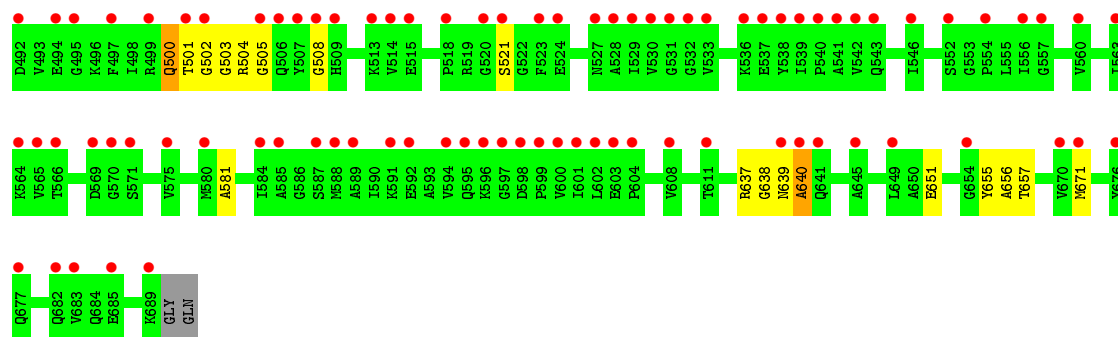


## ● Molecule 56: P-site tRNA

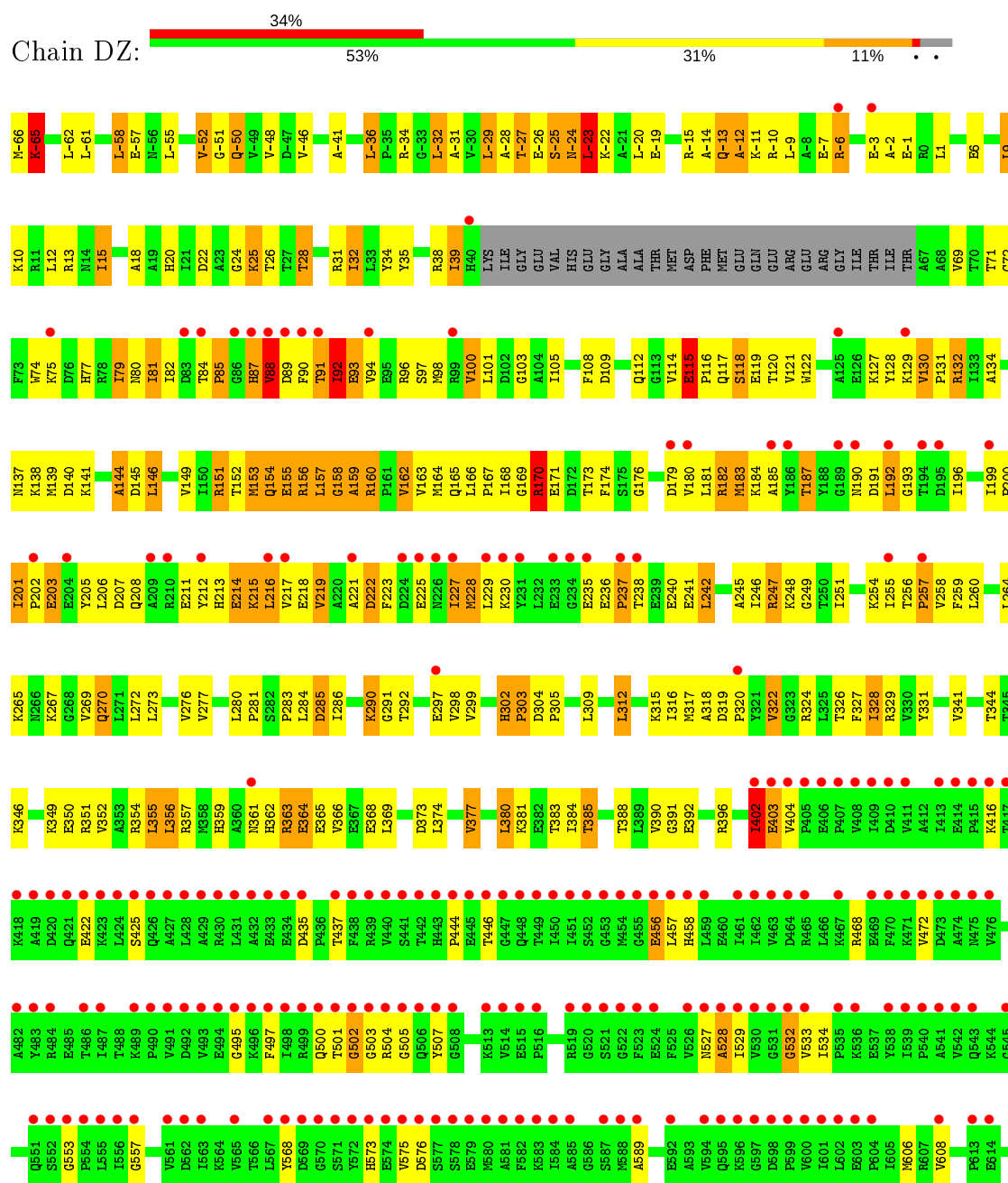


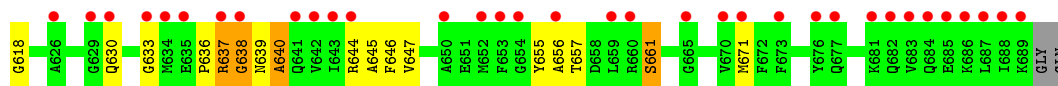
## ● Molecule 57: 50S ribosomal protein L9,Elongation factor G





- Molecule 57: 50S ribosomal protein L9, Elongation factor G







## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	209.48 Å   448.89 Å   622.84 Å 90.00°   90.00°   90.00°	Depositor
Resolution (Å)	49.31 – 2.80 49.71 – 2.80	Depositor EDS
% Data completeness (in resolution range)	96.8 (49.31-2.80) 96.8 (49.71-2.80)	Depositor EDS
$R_{merge}$	0.16	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.37 (at 2.81 Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE: 1.8.2_1309)	Depositor
R, $R_{free}$	0.221 , 0.266 0.221 , 0.266	Depositor DCC
$R_{free}$ test set	69082 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	47.2	Xtriage
Anisotropy	0.111	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.26 , 71.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.38$ , $\langle L^2 \rangle = 0.20$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.89	EDS
Total number of atoms	305548	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	78.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.88% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	AA	1.44	524/68792 (0.8%)	2.20	4798/107377 (4.5%)
1	CA	1.00	54/68691 (0.1%)	1.63	1529/107219 (1.4%)
2	AB	1.20	7/2878 (0.2%)	2.00	147/4490 (3.3%)
2	CB	0.69	0/2878	1.28	12/4490 (0.3%)
3	AC	0.34	0/1083	0.65	0/1460
3	CC	0.34	0/1083	0.65	0/1460
4	AD	0.91	1/2186 (0.0%)	1.09	10/2944 (0.3%)
4	CD	0.75	0/2192	0.94	2/2951 (0.1%)
5	AE	0.99	0/1592	1.10	1/2149 (0.0%)
5	CE	0.65	0/1592	0.87	1/2149 (0.0%)
6	AF	0.92	1/1619 (0.1%)	1.06	11/2193 (0.5%)
6	CF	0.67	0/1615	0.84	1/2188 (0.0%)
7	AG	0.60	0/1450	0.80	0/1959
7	CG	0.41	0/1449	0.65	0/1958
8	AH	0.82	0/1356	0.95	0/1834
8	CH	0.40	0/1356	0.61	0/1834
9	AK	0.40	0/640	0.75	0/889
9	CK	0.31	0/640	0.64	0/889
10	AL	0.38	0/1044	0.58	0/1416
10	CL	0.39	0/1044	0.59	0/1416
11	AN	1.06	0/1144	1.09	4/1543 (0.3%)
11	CN	0.54	0/1144	0.74	0/1543
12	AO	0.91	2/943 (0.2%)	1.07	3/1269 (0.2%)
12	CO	0.71	0/943	0.81	0/1269
13	AP	0.87	0/1156	1.10	4/1537 (0.3%)
13	CP	0.60	0/1152	0.85	1/1533 (0.1%)
14	AQ	0.99	0/1143	1.05	2/1527 (0.1%)
14	CQ	0.64	0/1143	0.79	0/1527
15	AR	1.00	0/982	1.14	3/1312 (0.2%)
15	CR	0.62	0/982	0.85	0/1312
16	AS	0.77	0/887	0.90	0/1180
16	CS	0.53	0/880	0.76	0/1172

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
17	AT	0.89	0/1105	1.08	3/1477 (0.2%)
17	CT	0.64	0/1097	0.88	0/1468
18	AU	1.17	1/977 (0.1%)	1.18	5/1301 (0.4%)
18	CU	0.65	0/977	0.78	0/1301
19	AV	1.13	0/782	1.15	1/1049 (0.1%)
19	CV	0.54	0/782	0.76	0/1049
20	AW	1.16	1/897 (0.1%)	1.23	8/1205 (0.7%)
20	CW	0.78	0/897	0.89	0/1205
21	AX	0.96	0/764	1.09	2/1025 (0.2%)
21	CX	0.68	0/764	0.88	1/1025 (0.1%)
22	AY	0.86	0/819	1.01	0/1095
22	CY	0.59	0/819	0.78	0/1095
23	AZ	0.74	0/1483	0.96	3/2017 (0.1%)
23	CZ	0.44	0/1483	0.71	0/2017
24	A0	0.92	0/662	1.01	0/881
24	C0	0.61	0/662	0.75	0/881
25	A1	0.84	0/762	1.00	1/1014 (0.1%)
25	C1	0.69	0/762	0.86	0/1014
26	A2	0.89	1/590 (0.2%)	0.96	0/781
26	C2	0.58	0/590	0.79	0/781
27	A3	0.97	0/474	1.17	0/635
27	C3	0.57	0/469	0.77	1/630 (0.2%)
28	A4	0.47	0/571	0.72	0/768
28	C4	0.36	0/545	0.57	0/737
29	A5	1.16	2/469 (0.4%)	1.21	3/635 (0.5%)
29	C5	0.73	0/469	0.93	2/635 (0.3%)
30	A6	0.93	0/460	1.01	2/613 (0.3%)
30	C6	0.68	0/456	0.86	0/608
31	A7	1.07	2/426 (0.5%)	1.21	3/561 (0.5%)
31	C7	0.79	0/426	0.92	2/561 (0.4%)
32	A8	0.99	0/525	1.07	1/691 (0.1%)
32	C8	0.68	0/525	0.85	0/691
33	A9	0.94	0/310	1.05	0/407
33	C9	0.59	0/310	0.78	0/407
34	BA	0.78	9/35976 (0.0%)	1.40	403/56145 (0.7%)
34	DA	0.70	5/36119 (0.0%)	1.30	246/56370 (0.4%)
35	BB	0.45	0/1881	0.72	0/2542
35	DB	0.39	0/1860	0.65	0/2518
36	BC	0.40	0/1576	0.58	0/2130
36	DC	0.37	0/1568	0.57	0/2122
37	BD	0.51	0/1689	0.74	0/2267
37	DD	0.49	0/1708	0.73	0/2289
38	BE	0.59	0/1145	0.81	1/1543 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
38	DE	0.54	0/1149	0.79	0/1548
39	BF	0.52	0/825	0.73	1/1118 (0.1%)
39	DF	0.56	0/833	0.74	1/1128 (0.1%)
40	BG	0.44	0/1250	0.57	0/1679
40	DG	0.35	0/1254	0.55	0/1683
41	BH	0.59	0/1108	0.80	0/1494
41	DH	0.50	0/1108	0.72	0/1494
42	BI	0.41	0/1005	0.63	0/1350
42	DI	0.37	0/997	0.55	0/1343
43	BJ	0.36	0/722	0.62	0/982
43	DJ	0.37	0/727	0.59	0/988
44	BK	0.50	0/848	0.71	0/1149
44	DK	0.52	0/848	0.68	0/1149
45	BL	0.68	0/946	0.82	0/1274
45	DL	0.56	0/946	0.78	0/1274
46	BM	0.36	0/933	0.61	0/1253
46	DM	0.33	0/961	0.56	0/1291
47	BN	0.44	0/501	0.70	1/664 (0.2%)
47	DN	0.39	0/501	0.56	1/664 (0.2%)
48	BO	0.58	0/739	0.81	0/985
48	DO	0.56	0/739	0.77	0/985
49	BP	0.55	0/697	0.79	0/939
49	DP	0.47	0/693	0.70	0/935
50	BQ	0.61	0/836	0.79	0/1117
50	DQ	0.57	0/836	0.72	0/1117
51	BR	0.53	0/560	0.77	0/746
51	DR	0.56	0/560	0.65	0/746
52	BS	0.33	0/676	0.56	0/911
52	DS	0.33	0/661	0.59	0/893
53	BT	0.52	0/730	0.75	0/965
53	DT	0.48	0/733	0.74	0/969
54	BU	0.38	0/203	0.67	0/266
54	DU	0.33	0/203	0.56	0/266
55	BV	1.23	1/310 (0.3%)	1.38	3/480 (0.6%)
55	DV	0.94	0/144	1.64	5/223 (2.2%)
56	BX	0.90	2/1725 (0.1%)	1.50	30/2689 (1.1%)
56	DX	0.80	5/1719 (0.3%)	1.31	15/2677 (0.6%)
57	BZ	0.62	0/4927	0.84	2/6727 (0.0%)
57	DZ	0.54	0/4925	0.77	3/6724 (0.0%)
All	All	0.97	618/325388 (0.2%)	1.54	7279/485060 (1.5%)

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
4	AD	0	3
5	AE	0	1
8	AH	0	1
12	AO	0	2
21	CX	0	1
23	AZ	0	1
37	BD	0	1
53	BT	0	1
57	BZ	0	1
57	DZ	0	4
All	All	0	16

The worst 5 of 618 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	AA	990	A	N9-C4	-14.73	1.29	1.37
1	AA	1188	A	N9-C4	-13.98	1.29	1.37
1	AA	2065	C	N3-C4	-12.04	1.25	1.33
1	AA	354	A	N9-C4	-11.71	1.30	1.37
1	AA	2517	G	N3-C4	-11.66	1.27	1.35

The worst 5 of 7279 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	990	A	C5-N7-C8	-26.49	90.66	103.90
1	AA	990	A	N7-C8-N9	22.72	125.16	113.80
1	AA	990	A	N1-C6-N6	21.81	131.68	118.60
1	AA	991	G	O5'-P-OP1	-21.27	85.17	110.70
1	AA	990	A	C6-C5-N7	-21.06	117.56	132.30

There are no chirality outliers.

5 of 16 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	AD	141	VAL	Peptide
4	AD	70	TRP	Peptide
4	AD	98	VAL	Peptide
5	AE	132	HIS	Sidechain
8	AH	23	ARG	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	61426	0	30938	1072	0
1	CA	61337	0	30928	1179	0
2	AB	2573	0	1306	32	0
2	CB	2573	0	1306	43	0
3	AC	1063	0	1089	151	0
3	CC	1063	0	1091	214	0
4	AD	2136	0	2218	104	0
4	CD	2142	0	2229	84	0
5	AE	1559	0	1618	65	0
5	CE	1559	0	1618	59	0
6	AF	1584	0	1625	68	0
6	CF	1580	0	1619	78	0
7	AG	1425	0	1443	63	0
7	CG	1424	0	1434	61	0
8	AH	1330	0	1407	47	0
8	CH	1330	0	1407	48	0
9	AK	641	0	309	20	0
9	CK	641	0	309	11	0
10	AL	1025	0	1066	52	0
10	CL	1025	0	1066	46	0
11	AN	1117	0	1184	35	0
11	CN	1117	0	1184	40	0
12	AO	933	0	996	36	0
12	CO	933	0	996	26	0
13	AP	1139	0	1223	50	0
13	CP	1135	0	1212	53	0
14	AQ	1122	0	1179	57	0
14	CQ	1122	0	1179	52	0
15	AR	968	0	1033	49	0
15	CR	968	0	1033	48	0
16	AS	877	0	938	47	0
16	CS	870	0	923	36	0
17	AT	1091	0	1151	53	0
17	CT	1083	0	1136	45	0
18	AU	959	0	1019	37	0
18	CU	959	0	1018	31	0
19	AV	771	0	829	21	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
19	CV	771	0	830	30	0
20	AW	886	0	940	23	0
20	CW	886	0	940	35	0
21	AX	750	0	814	31	0
21	CX	750	0	814	36	0
22	AY	806	0	881	26	0
22	CY	806	0	881	33	0
23	AZ	1451	0	1457	61	0
23	CZ	1451	0	1457	50	0
24	A0	653	0	674	21	0
24	C0	653	0	674	25	0
25	A1	755	0	826	33	0
25	C1	755	0	826	25	0
26	A2	588	0	643	14	0
26	C2	588	0	643	18	0
27	A3	469	0	518	26	0
27	C3	464	0	514	12	0
28	A4	558	0	545	28	0
28	C4	532	0	504	19	0
29	A5	455	0	466	20	0
29	C5	455	0	465	12	0
30	A6	453	0	473	20	0
30	C6	449	0	469	15	0
31	A7	418	0	467	23	0
31	C7	418	0	467	20	0
32	A8	517	0	582	28	0
32	C8	517	0	582	26	0
33	A9	307	0	335	15	0
33	C9	307	0	335	15	0
34	BA	32141	0	16222	665	0
34	DA	32268	0	16287	692	0
35	BB	1846	0	1867	96	0
35	DB	1825	0	1828	89	0
36	BC	1552	0	1546	51	0
36	DC	1544	0	1524	52	0
37	BD	1659	0	1677	95	0
37	DD	1678	0	1719	68	0
38	BE	1129	0	1185	52	0
38	DE	1133	0	1191	61	0
39	BF	812	0	804	28	0
39	DF	820	0	814	29	0
40	BG	1231	0	1238	37	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
40	DG	1235	0	1249	23	0
41	BH	1088	0	1126	54	0
41	DH	1088	0	1126	46	0
42	BI	986	0	995	37	0
42	DI	978	0	966	42	0
43	BJ	709	0	650	31	0
43	DJ	714	0	672	38	0
44	BK	833	0	836	31	0
44	DK	833	0	836	25	0
45	BL	930	0	980	24	0
45	DL	930	0	980	42	0
46	BM	923	0	970	31	0
46	DM	950	0	988	31	0
47	BN	492	0	529	19	0
47	DN	492	0	531	34	0
48	BO	728	0	760	33	0
48	DO	728	0	760	32	0
49	BP	681	0	697	34	0
49	DP	677	0	686	28	0
50	BQ	823	0	891	27	0
50	DQ	823	0	891	37	0
51	BR	555	0	618	19	0
51	DR	555	0	618	25	0
52	BS	661	0	675	31	0
52	DS	646	0	644	27	0
53	BT	728	0	798	34	0
53	DT	731	0	807	29	0
54	BU	199	0	208	5	0
54	DU	199	0	208	7	0
55	BV	277	0	140	4	0
55	DV	128	0	67	5	0
56	BX	1625	0	829	24	0
56	DX	1621	0	826	21	0
57	BZ	4869	0	4164	253	0
57	DZ	4867	0	4166	237	0
58	A0	4	0	0	0	0
58	A1	1	0	0	0	0
58	A2	1	0	0	0	0
58	A4	1	0	0	0	0
58	A5	2	0	0	0	0
58	A6	2	0	0	0	0
58	A7	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
58	A8	2	0	0	0	0
58	A9	1	0	0	0	0
58	AA	836	0	0	0	0
58	AB	23	0	0	0	0
58	AD	10	0	0	0	0
58	AE	4	0	0	0	0
58	AF	5	0	0	0	0
58	AG	2	0	0	0	0
58	AH	2	0	0	0	0
58	AN	3	0	0	0	0
58	AO	1	0	0	0	0
58	AP	2	0	0	0	0
58	AQ	2	0	0	0	0
58	AR	1	0	0	0	0
58	AU	3	0	0	0	0
58	AV	2	0	0	0	0
58	AW	4	0	0	0	0
58	AX	2	0	0	0	0
58	AZ	2	0	0	0	0
58	BA	212	0	0	0	0
58	BB	1	0	0	0	0
58	BD	1	0	0	0	0
58	BE	1	0	0	0	0
58	BF	1	0	0	0	0
58	BK	1	0	0	0	0
58	BL	4	0	0	0	0
58	BN	2	0	0	0	0
58	BT	1	0	0	0	0
58	BV	1	0	0	0	0
58	BX	10	0	0	0	0
58	BZ	1	0	0	0	0
58	C0	1	0	0	0	0
58	C1	1	0	0	0	0
58	C3	1	0	0	0	0
58	C7	1	0	0	0	0
58	C8	1	0	0	0	0
58	CA	666	0	0	0	0
58	CB	13	0	0	0	0
58	CD	3	0	0	0	0
58	CE	7	0	0	0	0
58	CF	4	0	0	0	0
58	CG	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
58	CN	1	0	0	0	0
58	CO	2	0	0	0	0
58	CQ	4	0	0	0	0
58	CR	1	0	0	0	0
58	CU	2	0	0	0	0
58	CV	2	0	0	0	0
58	CY	1	0	0	0	0
58	DA	166	0	0	0	0
58	DD	1	0	0	0	0
58	DE	2	0	0	0	0
58	DF	1	0	0	0	0
58	DJ	1	0	0	0	0
58	DK	1	0	0	0	0
58	DL	2	0	0	0	0
58	DT	1	0	0	0	0
58	DZ	3	0	0	0	0
59	AA	1	0	0	0	0
60	A4	1	0	0	0	0
60	A5	1	0	0	0	0
60	A6	1	0	0	0	0
60	A9	1	0	0	0	0
60	AY	1	0	0	0	0
60	BN	1	0	0	0	0
60	C4	1	0	0	0	0
60	C5	1	0	0	0	0
60	C6	1	0	0	0	0
60	C9	1	0	0	0	0
60	CY	1	0	0	0	0
60	DN	1	0	0	0	0
61	BD	8	0	0	0	0
61	DD	8	0	0	0	0
62	BZ	28	0	12	4	0
62	DZ	28	0	12	7	0
63	A0	9	0	0	2	0
63	A1	2	0	0	1	0
63	A2	1	0	0	0	0
63	A3	2	0	0	0	0
63	A5	4	0	0	1	0
63	A7	4	0	0	2	0
63	A8	9	0	0	3	0
63	A9	1	0	0	0	0
63	AA	1406	0	0	76	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
63	AB	37	0	0	3	0
63	AD	16	0	0	0	0
63	AE	14	0	0	3	0
63	AF	6	0	0	2	0
63	AG	3	0	0	0	0
63	AH	1	0	0	0	0
63	AN	3	0	0	0	0
63	AO	1	0	0	0	0
63	AP	18	0	0	0	0
63	AQ	5	0	0	1	0
63	AR	2	0	0	0	0
63	AS	1	0	0	0	0
63	AT	3	0	0	0	0
63	AU	4	0	0	0	0
63	AV	1	0	0	0	0
63	AW	1	0	0	0	0
63	AX	4	0	0	0	0
63	AZ	1	0	0	0	0
63	BA	203	0	0	15	0
63	BD	3	0	0	0	0
63	BE	2	0	0	0	0
63	BG	1	0	0	0	0
63	BJ	1	0	0	0	0
63	BL	1	0	0	0	0
63	BM	1	0	0	0	0
63	BO	2	0	0	0	0
63	BP	1	0	0	0	0
63	BV	3	0	0	0	0
63	BX	5	0	0	0	0
63	BZ	2	0	0	0	0
63	C0	5	0	0	0	0
63	C1	1	0	0	0	0
63	C3	2	0	0	0	0
63	C6	1	0	0	1	0
63	C7	1	0	0	0	0
63	C8	3	0	0	0	0
63	CA	974	0	0	87	0
63	CB	9	0	0	0	0
63	CD	17	0	0	0	0
63	CE	14	0	0	3	0
63	CF	6	0	0	0	0
63	CN	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
63	CP	12	0	0	2	0
63	CQ	2	0	0	1	0
63	CT	3	0	0	0	0
63	CU	2	0	0	1	0
63	CV	2	0	0	0	0
63	CW	1	0	0	0	0
63	CX	2	0	0	0	0
63	CY	2	0	0	1	0
63	DA	154	0	0	11	0
63	DE	3	0	0	0	0
63	DH	1	0	0	0	0
63	DJ	1	0	0	0	0
63	DK	2	0	0	0	0
63	DP	1	0	0	0	0
63	DT	1	0	0	0	0
63	DV	1	0	0	0	0
63	DZ	1	0	0	0	0
All	All	305548	0	205094	7289	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 15.

The worst 5 of 7289 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:CA:2128:C:H5''	3:CC:219:MET:CE	1.49	1.42
1:CA:2132:U:O2	3:CC:6:LYS:CB	1.64	1.41
1:CA:2128:C:OP1	3:CC:219:MET:CE	1.71	1.39
1:CA:2176:A:H4'	3:CC:45:HIS:CD2	1.60	1.37
1:AA:2143:G:N2	3:AC:169:THR:OG1	1.58	1.36

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	
3	AC	133/228 (58%)	90 (68%)	25 (19%)	18 (14%)	0	0
3	CC	133/228 (58%)	90 (68%)	25 (19%)	18 (14%)	0	0
4	AD	273/276 (99%)	239 (88%)	28 (10%)	6 (2%)	6	22
4	CD	273/276 (99%)	234 (86%)	35 (13%)	4 (2%)	10	33
5	AE	202/206 (98%)	181 (90%)	19 (9%)	2 (1%)	15	44
5	CE	202/206 (98%)	178 (88%)	20 (10%)	4 (2%)	7	24
6	AF	201/210 (96%)	182 (90%)	15 (8%)	4 (2%)	7	24
6	CF	201/210 (96%)	181 (90%)	14 (7%)	6 (3%)	4	15
7	AG	179/182 (98%)	152 (85%)	19 (11%)	8 (4%)	2	8
7	CG	179/182 (98%)	148 (83%)	21 (12%)	10 (6%)	2	5
8	AH	172/180 (96%)	152 (88%)	17 (10%)	3 (2%)	9	29
8	CH	172/180 (96%)	149 (87%)	20 (12%)	3 (2%)	9	29
9	AK	128/173 (74%)	66 (52%)	31 (24%)	31 (24%)	0	0
9	CK	128/173 (74%)	77 (60%)	29 (23%)	22 (17%)	0	0
10	AL	137/147 (93%)	105 (77%)	24 (18%)	8 (6%)	1	4
10	CL	137/147 (93%)	97 (71%)	35 (26%)	5 (4%)	3	11
11	AN	138/140 (99%)	127 (92%)	10 (7%)	1 (1%)	22	53
11	CN	138/140 (99%)	127 (92%)	9 (6%)	2 (1%)	11	34
12	AO	120/122 (98%)	106 (88%)	13 (11%)	1 (1%)	19	49
12	CO	120/122 (98%)	108 (90%)	9 (8%)	3 (2%)	5	19
13	AP	147/150 (98%)	133 (90%)	10 (7%)	4 (3%)	5	17
13	CP	147/150 (98%)	124 (84%)	18 (12%)	5 (3%)	3	13
14	AQ	139/141 (99%)	126 (91%)	11 (8%)	2 (1%)	11	34
14	CQ	139/141 (99%)	124 (89%)	12 (9%)	3 (2%)	6	22
15	AR	116/118 (98%)	105 (90%)	9 (8%)	2 (2%)	9	29
15	CR	116/118 (98%)	100 (86%)	14 (12%)	2 (2%)	9	29
16	AS	108/112 (96%)	92 (85%)	12 (11%)	4 (4%)	3	11
16	CS	108/112 (96%)	91 (84%)	13 (12%)	4 (4%)	3	11
17	AT	129/146 (88%)	115 (89%)	13 (10%)	1 (1%)	19	49
17	CT	129/146 (88%)	118 (92%)	9 (7%)	2 (2%)	9	31

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
18	AU	114/118 (97%)	106 (93%)	6 (5%)	2 (2%)	8	28
18	CU	114/118 (97%)	102 (90%)	11 (10%)	1 (1%)	17	46
19	AV	99/101 (98%)	90 (91%)	6 (6%)	3 (3%)	4	15
19	CV	99/101 (98%)	85 (86%)	9 (9%)	5 (5%)	2	6
20	AW	110/113 (97%)	99 (90%)	9 (8%)	2 (2%)	8	28
20	CW	110/113 (97%)	97 (88%)	11 (10%)	2 (2%)	8	28
21	AX	93/96 (97%)	83 (89%)	9 (10%)	1 (1%)	14	41
21	CX	93/96 (97%)	75 (81%)	14 (15%)	4 (4%)	2	8
22	AY	105/110 (96%)	90 (86%)	11 (10%)	4 (4%)	3	10
22	CY	105/110 (96%)	82 (78%)	21 (20%)	2 (2%)	8	26
23	AZ	183/206 (89%)	147 (80%)	23 (13%)	13 (7%)	1	2
23	CZ	183/206 (89%)	147 (80%)	24 (13%)	12 (7%)	1	3
24	A0	81/85 (95%)	72 (89%)	7 (9%)	2 (2%)	5	19
24	C0	81/85 (95%)	73 (90%)	7 (9%)	1 (1%)	13	39
25	A1	95/98 (97%)	90 (95%)	3 (3%)	2 (2%)	7	23
25	C1	95/98 (97%)	88 (93%)	4 (4%)	3 (3%)	4	13
26	A2	68/72 (94%)	59 (87%)	9 (13%)	0	100	100
26	C2	68/72 (94%)	60 (88%)	7 (10%)	1 (2%)	10	33
27	A3	57/60 (95%)	55 (96%)	2 (4%)	0	100	100
27	C3	57/60 (95%)	54 (95%)	3 (5%)	0	100	100
28	A4	67/71 (94%)	45 (67%)	15 (22%)	7 (10%)	0	1
28	C4	67/71 (94%)	52 (78%)	10 (15%)	5 (8%)	1	2
29	A5	57/60 (95%)	53 (93%)	4 (7%)	0	100	100
29	C5	57/60 (95%)	51 (90%)	6 (10%)	0	100	100
30	A6	51/54 (94%)	47 (92%)	4 (8%)	0	100	100
30	C6	51/54 (94%)	44 (86%)	6 (12%)	1 (2%)	7	24
31	A7	46/49 (94%)	41 (89%)	5 (11%)	0	100	100
31	C7	46/49 (94%)	39 (85%)	6 (13%)	1 (2%)	6	22
32	A8	62/65 (95%)	54 (87%)	5 (8%)	3 (5%)	2	7
32	C8	62/65 (95%)	58 (94%)	4 (6%)	0	100	100
33	A9	35/37 (95%)	34 (97%)	0	1 (3%)	4	15

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
33	C9	35/37 (95%)	33 (94%)	2 (6%)	0	100	100
35	BB	229/256 (90%)	174 (76%)	42 (18%)	13 (6%)	1	5
35	DB	229/256 (90%)	176 (77%)	40 (18%)	13 (6%)	1	5
36	BC	204/239 (85%)	165 (81%)	32 (16%)	7 (3%)	3	13
36	DC	204/239 (85%)	172 (84%)	30 (15%)	2 (1%)	15	44
37	BD	206/209 (99%)	150 (73%)	42 (20%)	14 (7%)	1	3
37	DD	206/209 (99%)	165 (80%)	30 (15%)	11 (5%)	2	6
38	BE	146/162 (90%)	123 (84%)	17 (12%)	6 (4%)	3	9
38	DE	146/162 (90%)	122 (84%)	19 (13%)	5 (3%)	3	13
39	BF	98/101 (97%)	84 (86%)	10 (10%)	4 (4%)	3	9
39	DF	98/101 (97%)	86 (88%)	12 (12%)	0	100	100
40	BG	153/156 (98%)	127 (83%)	20 (13%)	6 (4%)	3	10
40	DG	153/156 (98%)	127 (83%)	19 (12%)	7 (5%)	2	7
41	BH	135/138 (98%)	111 (82%)	17 (13%)	7 (5%)	2	6
41	DH	135/138 (98%)	120 (89%)	13 (10%)	2 (2%)	10	33
42	BI	125/128 (98%)	105 (84%)	14 (11%)	6 (5%)	2	7
42	DI	125/128 (98%)	109 (87%)	15 (12%)	1 (1%)	19	49
43	BJ	95/105 (90%)	80 (84%)	12 (13%)	3 (3%)	4	13
43	DJ	94/105 (90%)	76 (81%)	9 (10%)	9 (10%)	0	1
44	BK	112/129 (87%)	94 (84%)	16 (14%)	2 (2%)	8	28
44	DK	112/129 (87%)	93 (83%)	15 (13%)	4 (4%)	3	11
45	BL	120/132 (91%)	108 (90%)	12 (10%)	0	100	100
45	DL	120/132 (91%)	109 (91%)	9 (8%)	2 (2%)	9	29
46	BM	115/126 (91%)	97 (84%)	15 (13%)	3 (3%)	5	18
46	DM	120/126 (95%)	96 (80%)	18 (15%)	6 (5%)	2	6
47	BN	58/61 (95%)	46 (79%)	10 (17%)	2 (3%)	3	13
47	DN	58/61 (95%)	56 (97%)	2 (3%)	0	100	100
48	BO	86/89 (97%)	71 (83%)	15 (17%)	0	100	100
48	DO	86/89 (97%)	72 (84%)	10 (12%)	4 (5%)	2	7
49	BP	80/88 (91%)	55 (69%)	19 (24%)	6 (8%)	1	2
49	DP	80/88 (91%)	67 (84%)	10 (12%)	3 (4%)	3	10

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
50	BQ	97/105 (92%)	87 (90%)	8 (8%)	2 (2%)	7	23
50	DQ	97/105 (92%)	88 (91%)	9 (9%)	0	100	100
51	BR	66/88 (75%)	57 (86%)	9 (14%)	0	100	100
51	DR	66/88 (75%)	56 (85%)	9 (14%)	1 (2%)	10	33
52	BS	82/93 (88%)	71 (87%)	10 (12%)	1 (1%)	13	39
52	DS	81/93 (87%)	69 (85%)	8 (10%)	4 (5%)	2	7
53	BT	94/106 (89%)	81 (86%)	5 (5%)	8 (8%)	1	1
53	DT	94/106 (89%)	80 (85%)	10 (11%)	4 (4%)	2	8
54	BU	21/27 (78%)	20 (95%)	1 (5%)	0	100	100
54	DU	21/27 (78%)	18 (86%)	2 (10%)	1 (5%)	2	7
57	BZ	726/758 (96%)	561 (77%)	115 (16%)	50 (7%)	1	3
57	DZ	726/758 (96%)	558 (77%)	113 (16%)	55 (8%)	1	2
All	All	13389/14444 (93%)	11204 (84%)	1645 (12%)	540 (4%)	3	9

5 of 540 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	AC	42	VAL
3	AC	47	LYS
3	AC	68	GLY
3	AC	180	SER
3	AC	181	PHE

### 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	
3	AC	111/180 (62%)	103 (93%)	8 (7%)	14	38
3	CC	111/180 (62%)	103 (93%)	8 (7%)	14	38
4	AD	215/218 (99%)	178 (83%)	37 (17%)	2	6
4	CD	216/218 (99%)	183 (85%)	33 (15%)	2	8

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	AE	164/166 (99%)	134 (82%)	30 (18%)	1	5
5	CE	164/166 (99%)	134 (82%)	30 (18%)	1	5
6	AF	160/166 (96%)	123 (77%)	37 (23%)	1	2
6	CF	159/166 (96%)	127 (80%)	32 (20%)	1	4
7	AG	143/156 (92%)	114 (80%)	29 (20%)	1	4
7	CG	142/156 (91%)	110 (78%)	32 (22%)	1	2
8	AH	144/148 (97%)	126 (88%)	18 (12%)	4	14
8	CH	144/148 (97%)	123 (85%)	21 (15%)	3	9
10	AL	104/111 (94%)	88 (85%)	16 (15%)	2	8
10	CL	104/111 (94%)	82 (79%)	22 (21%)	1	3
11	AN	118/119 (99%)	96 (81%)	22 (19%)	1	5
11	CN	118/119 (99%)	99 (84%)	19 (16%)	2	7
12	AO	100/100 (100%)	87 (87%)	13 (13%)	4	13
12	CO	100/100 (100%)	85 (85%)	15 (15%)	3	9
13	AP	116/116 (100%)	95 (82%)	21 (18%)	1	5
13	CP	115/116 (99%)	98 (85%)	17 (15%)	3	9
14	AQ	111/111 (100%)	92 (83%)	19 (17%)	2	6
14	CQ	111/111 (100%)	98 (88%)	13 (12%)	5	16
15	AR	101/101 (100%)	82 (81%)	19 (19%)	1	5
15	CR	101/101 (100%)	82 (81%)	19 (19%)	1	5
16	AS	87/88 (99%)	76 (87%)	11 (13%)	4	14
16	CS	85/88 (97%)	68 (80%)	17 (20%)	1	4
17	AT	115/127 (91%)	98 (85%)	17 (15%)	3	9
17	CT	113/127 (89%)	90 (80%)	23 (20%)	1	4
18	AU	93/94 (99%)	83 (89%)	10 (11%)	6	19
18	CU	93/94 (99%)	78 (84%)	15 (16%)	2	7
19	AV	80/82 (98%)	62 (78%)	18 (22%)	1	2
19	CV	80/82 (98%)	68 (85%)	12 (15%)	3	9
20	AW	90/92 (98%)	76 (84%)	14 (16%)	2	8
20	CW	90/92 (98%)	76 (84%)	14 (16%)	2	8
21	AX	77/78 (99%)	70 (91%)	7 (9%)	9	27

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
21	CX	77/78 (99%)	67 (87%)	10 (13%)	4	13
22	AY	85/91 (93%)	70 (82%)	15 (18%)	2	5
22	CY	85/91 (93%)	68 (80%)	17 (20%)	1	4
23	AZ	156/179 (87%)	126 (81%)	30 (19%)	1	4
23	CZ	156/179 (87%)	135 (86%)	21 (14%)	4	11
24	A0	65/67 (97%)	60 (92%)	5 (8%)	13	35
24	C0	65/67 (97%)	58 (89%)	7 (11%)	6	19
25	A1	80/83 (96%)	69 (86%)	11 (14%)	3	11
25	C1	80/83 (96%)	69 (86%)	11 (14%)	3	11
26	A2	65/67 (97%)	54 (83%)	11 (17%)	2	6
26	C2	65/67 (97%)	59 (91%)	6 (9%)	9	27
27	A3	51/52 (98%)	39 (76%)	12 (24%)	1	2
27	C3	50/52 (96%)	42 (84%)	8 (16%)	2	7
28	A4	60/63 (95%)	49 (82%)	11 (18%)	1	5
28	C4	53/63 (84%)	40 (76%)	13 (24%)	0	2
29	A5	50/52 (96%)	42 (84%)	8 (16%)	2	7
29	C5	50/52 (96%)	38 (76%)	12 (24%)	0	2
30	A6	51/52 (98%)	40 (78%)	11 (22%)	1	3
30	C6	50/52 (96%)	40 (80%)	10 (20%)	1	4
31	A7	41/42 (98%)	37 (90%)	4 (10%)	8	24
31	C7	41/42 (98%)	31 (76%)	10 (24%)	0	2
32	A8	54/55 (98%)	45 (83%)	9 (17%)	2	6
32	C8	54/55 (98%)	47 (87%)	7 (13%)	4	13
33	A9	34/34 (100%)	31 (91%)	3 (9%)	10	29
33	C9	34/34 (100%)	30 (88%)	4 (12%)	5	16
35	BB	192/220 (87%)	153 (80%)	39 (20%)	1	4
35	DB	187/220 (85%)	152 (81%)	35 (19%)	1	5
36	BC	143/188 (76%)	131 (92%)	12 (8%)	11	31
36	DC	141/188 (75%)	117 (83%)	24 (17%)	2	6
37	BD	170/181 (94%)	139 (82%)	31 (18%)	1	5
37	DD	174/181 (96%)	139 (80%)	35 (20%)	1	4

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
38	BE	113/123 (92%)	99 (88%)	14 (12%)	4	14
38	DE	114/123 (93%)	96 (84%)	18 (16%)	2	8
39	BF	84/90 (93%)	70 (83%)	14 (17%)	2	6
39	DF	86/90 (96%)	78 (91%)	8 (9%)	9	26
40	BG	119/127 (94%)	102 (86%)	17 (14%)	3	10
40	DG	120/127 (94%)	101 (84%)	19 (16%)	2	8
41	BH	114/119 (96%)	91 (80%)	23 (20%)	1	4
41	DH	114/119 (96%)	94 (82%)	20 (18%)	2	6
42	BI	91/99 (92%)	78 (86%)	13 (14%)	3	10
42	DI	89/99 (90%)	74 (83%)	15 (17%)	2	6
43	BJ	66/92 (72%)	60 (91%)	6 (9%)	9	27
43	DJ	69/92 (75%)	64 (93%)	5 (7%)	14	38
44	BK	83/99 (84%)	72 (87%)	11 (13%)	4	12
44	DK	83/99 (84%)	74 (89%)	9 (11%)	6	19
45	BL	97/109 (89%)	85 (88%)	12 (12%)	4	14
45	DL	97/109 (89%)	83 (86%)	14 (14%)	3	10
46	BM	91/101 (90%)	79 (87%)	12 (13%)	4	12
46	DM	92/101 (91%)	78 (85%)	14 (15%)	3	8
47	BN	49/50 (98%)	38 (78%)	11 (22%)	1	2
47	DN	49/50 (98%)	41 (84%)	8 (16%)	2	7
48	BO	78/80 (98%)	66 (85%)	12 (15%)	2	8
48	DO	78/80 (98%)	66 (85%)	12 (15%)	2	8
49	BP	69/74 (93%)	57 (83%)	12 (17%)	2	6
49	DP	68/74 (92%)	58 (85%)	10 (15%)	3	9
50	BQ	94/97 (97%)	80 (85%)	14 (15%)	3	9
50	DQ	94/97 (97%)	87 (93%)	7 (7%)	13	37
51	BR	59/77 (77%)	51 (86%)	8 (14%)	3	11
51	DR	59/77 (77%)	49 (83%)	10 (17%)	2	6
52	BS	70/80 (88%)	61 (87%)	9 (13%)	4	13
52	DS	67/80 (84%)	59 (88%)	8 (12%)	5	16
53	BT	70/82 (85%)	54 (77%)	16 (23%)	1	2

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
53	DT	71/82 (87%)	65 (92%)	6 (8%)	10	31
54	BU	18/22 (82%)	16 (89%)	2 (11%)	6	19
54	DU	18/22 (82%)	17 (94%)	1 (6%)	21	51
57	BZ	369/636 (58%)	280 (76%)	89 (24%)	0	2
57	DZ	370/636 (58%)	280 (76%)	90 (24%)	0	2
All	All	10306/11672 (88%)	8607 (84%)	1699 (16%)	2	7

5 of 1699 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
57	BZ	-49	VAL
6	CF	192	LEU
49	DP	8	ARG
57	BZ	97	SER
4	CD	12	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 164 such sidechains are listed below:

Mol	Chain	Res	Type
50	BQ	94	ASN
4	CD	116	GLN
45	DL	75	HIS
52	BS	69	HIS
57	BZ	80	ASN

### 5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	AA	2845/2915 (97%)	563 (19%)	43 (1%)
1	CA	2839/2915 (97%)	578 (20%)	33 (1%)
2	AB	119/121 (98%)	25 (21%)	1 (0%)
2	CB	119/121 (98%)	23 (19%)	0
34	BA	1491/1521 (98%)	299 (20%)	18 (1%)
34	DA	1498/1521 (98%)	296 (19%)	20 (1%)
55	BV	12/24 (50%)	7 (58%)	0
55	DV	5/24 (20%)	1 (20%)	0
56	BX	75/77 (97%)	15 (20%)	1 (1%)
56	DX	75/77 (97%)	11 (14%)	0

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
All	All	9078/9316 (97%)	1818 (20%)	116 (1%)

5 of 1818 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	AA	12	U
1	AA	13	A
1	AA	17	G
1	AA	34	C
1	AA	36	G

5 of 116 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
34	BA	793	U
1	CA	199	A
34	DA	913	A
34	BA	913	A
34	BA	1165	C

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

8 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
56	4SU	DX	8	56	14,21,22	1.27	1 (7%)	15,30,33	1.64	3 (20%)
56	4SU	BX	8	56	14,21,22	1.45	2 (14%)	15,30,33	1.28	2 (13%)
56	5MU	BX	54	56,58	15,22,23	1.27	1 (6%)	16,32,35	1.95	2 (12%)
56	PSU	BX	55	56	17,21,22	1.36	2 (11%)	20,30,33	3.08	6 (30%)
56	PSU	DX	55	56	17,21,22	1.63	2 (11%)	20,30,33	3.42	7 (35%)
56	5MC	BX	32	56	15,22,23	1.08	1 (6%)	19,32,35	1.65	3 (15%)
56	5MC	DX	32	56	15,22,23	1.59	1 (6%)	19,32,35	1.39	2 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
56	5MU	DX	54	56	15,22,23	1.06	1 (6%)	16,32,35	1.88	2 (12%)

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
56	4SU	DX	8	56	-	0/5/25/26	0/2/2/2
56	4SU	BX	8	56	-	0/5/25/26	0/2/2/2
56	5MU	BX	54	56,58	-	0/5/25/26	0/2/2/2
56	PSU	BX	55	56	-	0/7/25/26	0/2/2/2
56	PSU	DX	55	56	-	0/7/25/26	0/2/2/2
56	5MC	BX	32	56	-	0/5/25/26	0/2/2/2
56	5MC	DX	32	56	-	0/5/25/26	0/2/2/2
56	5MU	DX	54	56	-	0/5/25/26	0/2/2/2

The worst 5 of 11 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
56	DX	32	5MC	C5-C4	5.85	1.50	1.41
56	DX	55	PSU	C5-C1'	-4.31	1.48	1.52
56	BX	54	5MU	C4-C5	4.22	1.50	1.41
56	BX	8	4SU	C4-S4	-4.21	1.59	1.67
56	BX	32	5MC	C5-C4	3.85	1.47	1.41

The worst 5 of 27 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
56	DX	55	PSU	N1-C2-N3	-8.89	121.36	128.43
56	BX	55	PSU	N1-C2-N3	-8.45	121.71	128.43
56	DX	55	PSU	C4-N3-C2	7.29	121.29	115.14
56	BX	54	5MU	C4-N3-C2	7.13	121.17	115.14
56	DX	54	5MU	C4-N3-C2	6.65	120.76	115.14

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
56	DX	8	4SU	1	0
56	BX	8	4SU	1	0
56	DX	55	PSU	1	0
56	BX	32	5MC	4	0

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 2062 ligands modelled in this entry, 2058 are monoatomic - leaving 4 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$
61	SF4	BD	501	37	0,12,12	0.00	-	-		
61	SF4	DD	501	37	0,12,12	0.00	-	-		
62	GDP	DZ	704	58	24,30,30	1.21	3 (12%)	31,47,47	2.02	9 (29%)
62	GDP	BZ	801	58	24,30,30	1.24	2 (8%)	31,47,47	2.14	8 (25%)

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
61	SF4	BD	501	37	-	-	0/6/5/5
61	SF4	DD	501	37	-	-	0/6/5/5
62	GDP	DZ	704	58	-	5/12/32/32	0/3/3/3
62	GDP	BZ	801	58	-	5/12/32/32	0/3/3/3

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
62	BZ	801	GDP	C6-C5	4.73	1.49	1.41
62	DZ	704	GDP	C6-C5	4.06	1.48	1.41
62	DZ	704	GDP	C5-C4	2.24	1.46	1.40
62	BZ	801	GDP	C5-C4	2.11	1.46	1.40
62	DZ	704	GDP	C2'-C1'	-2.02	1.50	1.53

The worst 5 of 17 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
62	BZ	801	GDP	C2-N3-C4	4.82	120.86	115.36
62	BZ	801	GDP	PA-O3A-PB	-4.54	117.26	132.83
62	DZ	704	GDP	PA-O3A-PB	-4.48	117.47	132.83
62	DZ	704	GDP	C5-C6-N1	-4.47	117.32	123.43
62	BZ	801	GDP	C5-C6-N1	-4.24	117.63	123.43

There are no chirality outliers.

5 of 10 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
62	DZ	704	GDP	C5'-O5'-PA-O3A
62	BZ	801	GDP	C5'-O5'-PA-O3A
62	DZ	704	GDP	O4'-C4'-C5'-O5'
62	DZ	704	GDP	C3'-C4'-C5'-O5'
62	BZ	801	GDP	O4'-C4'-C5'-O5'

There are no ring outliers.

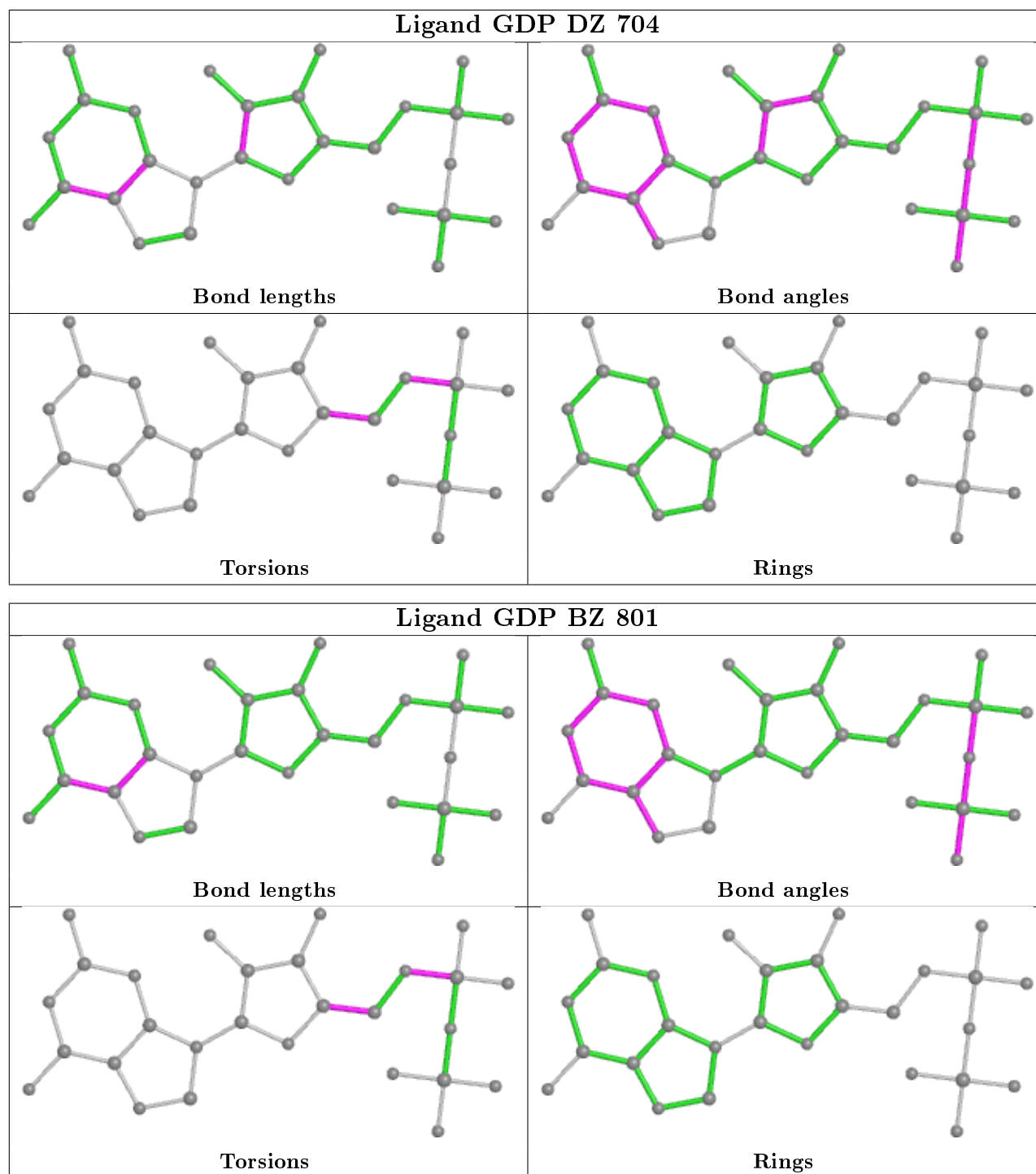
2 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
62	DZ	704	GDP	7	0
62	BZ	801	GDP	4	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient



equivalents in the CSD to analyse the geometry.



## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	AA	2852/2915 (97%)	0.37	131 (4%) 32 22	14, 34, 142, 356	0
1	CA	2848/2915 (97%)	0.56	198 (6%) 16 9	27, 58, 179, 348	0
2	AB	120/121 (99%)	-0.01	0 100 100	23, 51, 72, 109	0
2	CB	120/121 (99%)	0.34	0 100 100	66, 92, 119, 166	0
3	AC	137/228 (60%)	8.87	133 (97%) 0 0	132, 205, 251, 280	0
3	CC	137/228 (60%)	8.97	135 (98%) 0 0	144, 214, 251, 276	0
4	AD	275/276 (99%)	-0.27	1 (0%) 92 91	12, 35, 61, 136	0
4	CD	275/276 (99%)	-0.28	1 (0%) 92 91	24, 47, 74, 128	0
5	AE	204/206 (99%)	-0.33	0 100 100	6, 34, 58, 82	0
5	CE	204/206 (99%)	0.04	2 (0%) 82 77	20, 63, 107, 135	0
6	AF	203/210 (96%)	-0.23	2 (0%) 82 77	11, 35, 78, 173	0
6	CF	203/210 (96%)	-0.18	0 100 100	21, 63, 106, 155	0
7	AG	181/182 (99%)	0.26	8 (4%) 34 24	37, 77, 134, 208	0
7	CG	181/182 (99%)	0.97	30 (16%) 1 1	72, 111, 175, 201	0
8	AH	174/180 (96%)	-0.28	1 (0%) 89 86	25, 46, 70, 111	0
8	CH	174/180 (96%)	1.19	37 (21%) 0 0	64, 113, 162, 199	0
9	AK	130/173 (75%)	1.49	38 (29%) 0 0	47, 104, 172, 222	0
9	CK	130/173 (75%)	3.08	86 (66%) 0 0	75, 160, 200, 225	0
10	AL	139/147 (94%)	4.82	118 (84%) 0 0	96, 172, 230, 251	0
10	CL	139/147 (94%)	6.28	127 (91%) 0 0	128, 195, 248, 278	0
11	AN	140/140 (100%)	-0.43	0 100 100	14, 28, 59, 95	0
11	CN	140/140 (100%)	0.11	1 (0%) 87 84	33, 71, 108, 151	0
12	AO	122/122 (100%)	-0.38	0 100 100	19, 37, 61, 78	0
12	CO	122/122 (100%)	-0.13	0 100 100	36, 58, 85, 108	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
13	AP	149/150 (99%)	0.14	2 (1%) 77 72	12, 44, 81, 111	0
13	CP	149/150 (99%)	0.23	3 (2%) 65 56	31, 68, 116, 136	0
14	AQ	141/141 (100%)	-0.35	0 100 100	12, 34, 55, 84	0
14	CQ	141/141 (100%)	0.02	1 (0%) 87 84	38, 69, 100, 120	0
15	AR	118/118 (100%)	-0.33	0 100 100	16, 29, 47, 55	0
15	CR	118/118 (100%)	-0.07	0 100 100	34, 56, 91, 103	0
16	AS	110/112 (98%)	0.02	1 (0%) 84 80	31, 50, 81, 94	0
16	CS	110/112 (98%)	0.50	3 (2%) 54 44	47, 86, 120, 150	0
17	AT	131/146 (89%)	-0.18	3 (2%) 60 51	24, 40, 91, 169	0
17	CT	131/146 (89%)	-0.07	1 (0%) 86 81	43, 65, 107, 142	0
18	AU	116/118 (98%)	-0.31	0 100 100	10, 23, 39, 88	0
18	CU	116/118 (98%)	-0.03	0 100 100	28, 65, 92, 106	0
19	AV	101/101 (100%)	-0.38	0 100 100	9, 28, 51, 74	0
19	CV	101/101 (100%)	0.28	2 (1%) 65 56	36, 79, 113, 165	0
20	AW	112/113 (99%)	-0.35	0 100 100	13, 25, 43, 111	0
20	CW	112/113 (99%)	-0.18	0 100 100	29, 50, 80, 117	0
21	AX	95/96 (98%)	-0.22	0 100 100	16, 35, 69, 99	0
21	CX	95/96 (98%)	0.03	0 100 100	39, 61, 85, 105	0
22	AY	107/110 (97%)	-0.17	1 (0%) 84 80	23, 45, 84, 165	0
22	CY	107/110 (97%)	0.59	9 (8%) 11 5	45, 75, 115, 172	0
23	AZ	185/206 (89%)	-0.12	1 (0%) 91 88	28, 57, 92, 145	0
23	CZ	185/206 (89%)	0.69	17 (9%) 9 5	62, 105, 150, 210	0
24	A0	83/85 (97%)	0.06	7 (8%) 11 5	13, 35, 85, 220	0
24	C0	83/85 (97%)	0.69	8 (9%) 8 4	44, 66, 120, 224	0
25	A1	97/98 (98%)	-0.12	1 (1%) 82 77	20, 44, 79, 102	0
25	C1	97/98 (98%)	-0.11	1 (1%) 82 77	30, 52, 90, 127	0
26	A2	70/72 (97%)	-0.31	0 100 100	24, 44, 71, 121	0
26	C2	70/72 (97%)	0.16	0 100 100	48, 71, 102, 116	0
27	A3	59/60 (98%)	-0.37	0 100 100	15, 30, 55, 101	0
27	C3	59/60 (98%)	0.50	1 (1%) 70 63	46, 73, 112, 147	0
28	A4	69/71 (97%)	1.03	16 (23%) 0 0	61, 118, 203, 235	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
28	C4	69/71 (97%)	1.83	27 (39%) 0 0	81, 159, 204, 222	0
29	A5	59/60 (98%)	-0.34	0 100 100	9, 25, 41, 53	0
29	C5	59/60 (98%)	-0.07	1 (1%) 70 63	26, 52, 89, 105	0
30	A6	53/54 (98%)	-0.28	0 100 100	22, 41, 56, 76	0
30	C6	53/54 (98%)	0.02	0 100 100	41, 60, 80, 106	0
31	A7	48/49 (97%)	-0.10	2 (4%) 36 26	14, 25, 68, 134	0
31	C7	48/49 (97%)	-0.10	0 100 100	28, 39, 95, 119	0
32	A8	64/65 (98%)	-0.32	0 100 100	15, 28, 46, 67	0
32	C8	64/65 (98%)	-0.08	0 100 100	38, 52, 72, 87	0
33	A9	37/37 (100%)	-0.13	0 100 100	23, 36, 56, 67	0
33	C9	37/37 (100%)	0.35	1 (2%) 54 44	45, 78, 96, 127	0
34	BA	1495/1521 (98%)	0.63	106 (7%) 16 9	32, 84, 187, 330	0
34	DA	1501/1521 (98%)	0.80	189 (12%) 3 2	39, 89, 197, 334	0
35	BB	231/256 (90%)	0.77	32 (13%) 2 1	43, 105, 171, 220	0
35	DB	231/256 (90%)	1.03	41 (17%) 1 1	71, 124, 177, 210	0
36	BC	206/239 (86%)	1.17	39 (18%) 1 1	58, 118, 174, 198	0
36	DC	206/239 (86%)	1.61	60 (29%) 0 0	69, 136, 181, 210	0
37	BD	208/209 (99%)	0.40	9 (4%) 35 25	45, 87, 138, 188	0
37	DD	208/209 (99%)	0.25	8 (3%) 40 30	59, 86, 135, 200	0
38	BE	148/162 (91%)	0.09	2 (1%) 75 70	34, 73, 104, 127	0
38	DE	148/162 (91%)	0.38	4 (2%) 54 44	50, 79, 117, 179	0
39	BF	100/101 (99%)	0.12	0 100 100	57, 86, 116, 135	0
39	DF	100/101 (99%)	0.08	1 (1%) 82 77	49, 86, 117, 135	0
40	BG	155/156 (99%)	1.05	24 (15%) 2 1	68, 112, 181, 225	0
40	DG	155/156 (99%)	2.07	65 (41%) 0 0	71, 133, 192, 216	0
41	BH	137/138 (99%)	0.02	1 (0%) 87 84	47, 72, 100, 119	0
41	DH	137/138 (99%)	0.17	1 (0%) 87 84	57, 80, 110, 141	0
42	BI	127/128 (99%)	1.68	42 (33%) 0 0	64, 124, 167, 200	0
42	DI	127/128 (99%)	2.42	74 (58%) 0 0	88, 145, 191, 215	0
43	BJ	97/105 (92%)	2.05	41 (42%) 0 0	81, 130, 183, 212	0
43	DJ	96/105 (91%)	2.65	58 (60%) 0 0	90, 150, 197, 223	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
44	BK	114/129 (88%)	0.28	0 100 100	36, 78, 126, 148	0
44	DK	114/129 (88%)	0.36	1 (0%) 84 80	51, 89, 115, 172	0
45	BL	122/132 (92%)	-0.09	0 100 100	37, 59, 78, 112	0
45	DL	122/132 (92%)	0.14	2 (1%) 72 66	47, 70, 95, 116	0
46	BM	117/126 (92%)	1.07	20 (17%) 1 1	77, 135, 181, 203	0
46	DM	122/126 (96%)	2.08	45 (36%) 0 0	94, 151, 199, 268	0
47	BN	60/61 (98%)	1.09	9 (15%) 2 1	66, 112, 146, 172	0
47	DN	60/61 (98%)	2.12	25 (41%) 0 0	99, 139, 177, 195	0
48	BO	88/89 (98%)	0.17	1 (1%) 80 75	37, 70, 106, 120	0
48	DO	88/89 (98%)	0.25	0 100 100	46, 71, 106, 153	0
49	BP	82/88 (93%)	0.79	8 (9%) 7 4	50, 80, 119, 168	0
49	DP	82/88 (93%)	0.55	3 (3%) 41 31	54, 78, 112, 155	0
50	BQ	99/105 (94%)	0.09	2 (2%) 65 56	45, 72, 98, 125	0
50	DQ	99/105 (94%)	0.24	1 (1%) 82 77	44, 77, 104, 116	0
51	BR	68/88 (77%)	0.49	6 (8%) 10 5	41, 80, 122, 134	0
51	DR	68/88 (77%)	0.52	2 (2%) 51 41	52, 83, 128, 144	0
52	BS	84/93 (90%)	2.08	35 (41%) 0 0	96, 145, 196, 210	0
52	DS	83/93 (89%)	2.81	53 (63%) 0 0	92, 165, 213, 224	0
53	BT	96/106 (90%)	0.47	5 (5%) 27 18	61, 84, 123, 166	0
53	DT	96/106 (90%)	0.47	6 (6%) 20 12	57, 86, 134, 156	0
54	BU	23/27 (85%)	1.82	11 (47%) 0 0	64, 117, 156, 182	0
54	DU	23/27 (85%)	1.73	9 (39%) 0 0	90, 136, 172, 185	0
55	BV	13/24 (54%)	3.99	8 (61%) 0 0	49, 87, 172, 178	0
55	DV	6/24 (25%)	2.41	4 (66%) 0 0	63, 79, 171, 199	0
56	BX	72/77 (93%)	0.76	4 (5%) 24 16	34, 78, 124, 188	0
56	DX	72/77 (93%)	1.33	13 (18%) 1 1	41, 100, 148, 162	0
57	BZ	730/758 (96%)	1.17	186 (25%) 0 0	35, 78, 136, 188	0
57	DZ	730/758 (96%)	1.77	255 (34%) 0 0	37, 101, 167, 222	0
All	All	22704/23760 (95%)	0.71	2669 (11%) 4 2	6, 70, 180, 356	0

The worst 5 of 2669 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	CC	166	ASN	26.5
3	CC	4	HIS	23.3
3	AC	159	ALA	23.0
3	CC	35	THR	21.6
3	AC	176	VAL	19.0

## 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. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
56	PSU	DX	55	20/21	0.85	0.20	95,95,95,95	0
56	4SU	DX	8	20/21	0.89	0.22	96,96,96,96	0
56	PSU	BX	55	20/21	0.90	0.27	74,74,74,74	0
56	5MC	DX	32	21/22	0.90	0.22	86,86,86,86	0
56	5MU	DX	54	21/22	0.90	0.19	108,108,108,108	0
56	5MU	BX	54	21/22	0.92	0.26	85,85,85,85	0
56	4SU	BX	8	20/21	0.94	0.17	70,70,70,70	1
56	5MC	BX	32	21/22	0.96	0.17	65,65,65,65	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. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
58	MG	CA	3494	1/1	0.04	1.04	88,88,88,88	0
58	MG	DA	1753	1/1	0.04	0.87	83,83,83,83	0
58	MG	BA	3169	1/1	0.06	0.49	130,130,130,130	0
58	MG	DA	1704	1/1	0.20	0.47	128,128,128,128	0
58	MG	CA	3046	1/1	0.23	0.34	113,113,113,113	0
58	MG	AA	3784	1/1	0.26	0.64	73,73,73,73	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
58	MG	CA	3141	1/1	0.26	0.54	97,97,97,97	0
58	MG	CB	3013	1/1	0.28	0.24	96,96,96,96	0
58	MG	DA	1624	1/1	0.29	0.14	115,115,115,115	0
58	MG	CA	3296	1/1	0.29	0.37	80,80,80,80	0
58	MG	CA	3074	1/1	0.30	0.79	91,91,91,91	0
58	MG	DA	1714	1/1	0.34	0.30	78,78,78,78	0
58	MG	DZ	701	1/1	0.37	0.47	112,112,112,112	0
58	MG	CA	3067	1/1	0.38	0.98	83,83,83,83	0
58	MG	BA	3112	1/1	0.42	0.51	70,70,70,70	0
58	MG	CA	3114	1/1	0.46	0.29	94,94,94,94	0
58	MG	AA	3026	1/1	0.48	0.57	83,83,83,83	0
58	MG	DA	1690	1/1	0.50	0.29	85,85,85,85	0
58	MG	DA	1725	1/1	0.51	0.15	64,64,64,64	0
58	MG	CA	3466	1/1	0.52	0.23	65,65,65,65	0
58	MG	CA	3461	1/1	0.52	0.42	107,107,107,107	0
58	MG	CA	3553	1/1	0.52	0.38	88,88,88,88	0
58	MG	AA	3246	1/1	0.52	0.19	98,98,98,98	0
58	MG	CA	3002	1/1	0.53	0.59	112,112,112,112	0
58	MG	AZ	301	1/1	0.53	0.52	98,98,98,98	0
58	MG	AA	3113	1/1	0.54	1.10	97,97,97,97	0
58	MG	DE	202	1/1	0.54	0.49	93,93,93,93	0
58	MG	CA	3081	1/1	0.55	0.37	85,85,85,85	0
58	MG	BA	3110	1/1	0.55	0.23	103,103,103,103	0
58	MG	CA	3209	1/1	0.58	0.49	82,82,82,82	0
58	MG	CA	3124	1/1	0.58	1.55	87,87,87,87	0
58	MG	BA	3035	1/1	0.60	0.55	99,99,99,99	0
58	MG	AA	3109	1/1	0.60	0.49	124,124,124,124	0
58	MG	CA	3066	1/1	0.61	0.20	50,50,50,50	0
58	MG	AA	3538	1/1	0.61	0.24	91,91,91,91	0
58	MG	CA	3094	1/1	0.61	0.78	83,83,83,83	0
58	MG	BA	3119	1/1	0.62	0.27	79,79,79,79	0
58	MG	DA	1659	1/1	0.62	0.50	87,87,87,87	0
58	MG	AB	3006	1/1	0.63	0.42	70,70,70,70	0
58	MG	CA	3166	1/1	0.63	0.20	61,61,61,61	0
58	MG	AA	3193	1/1	0.63	0.57	72,72,72,72	0
58	MG	CA	3523	1/1	0.63	0.19	62,62,62,62	0
58	MG	CA	3070	1/1	0.64	0.32	82,82,82,82	0
58	MG	DA	1634	1/1	0.65	0.32	71,71,71,71	0
58	MG	CA	3537	1/1	0.65	0.28	67,67,67,67	0
58	MG	DK	5001	1/1	0.66	0.34	101,101,101,101	0
58	MG	AD	306	1/1	0.66	0.30	70,70,70,70	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
58	MG	AA	3756	1/1	0.66	0.21	61,61,61,61	0
58	MG	AN	3001	1/1	0.66	0.38	83,83,83,83	0
58	MG	BA	3106	1/1	0.66	0.52	93,93,93,93	0
58	MG	BA	3072	1/1	0.66	0.26	75,75,75,75	0
58	MG	AA	3752	1/1	0.66	0.41	64,64,64,64	1
58	MG	CA	3181	1/1	0.66	0.64	108,108,108,108	0
58	MG	BA	3140	1/1	0.66	0.14	91,91,91,91	0
58	MG	CA	3238	1/1	0.67	0.47	85,85,85,85	0
58	MG	BA	3209	1/1	0.67	0.20	79,79,79,79	0
58	MG	BA	3179	1/1	0.67	0.27	78,78,78,78	0
58	MG	CA	3153	1/1	0.67	0.34	55,55,55,55	0
58	MG	BA	3107	1/1	0.68	0.29	59,59,59,59	0
58	MG	BA	3069	1/1	0.68	0.32	82,82,82,82	0
58	MG	CA	3106	1/1	0.68	0.14	79,79,79,79	0
58	MG	CA	3195	1/1	0.68	0.45	69,69,69,69	0
58	MG	CA	3529	1/1	0.68	0.11	79,79,79,79	0
58	MG	BL	3001	1/1	0.68	0.23	80,80,80,80	0
58	MG	BA	3090	1/1	0.68	0.38	90,90,90,90	0
58	MG	DA	1635	1/1	0.69	0.43	89,89,89,89	0
58	MG	AA	3736	1/1	0.69	0.19	35,35,35,35	0
58	MG	CA	3119	1/1	0.69	0.23	55,55,55,55	0
58	MG	CA	3156	1/1	0.69	0.29	84,84,84,84	0
58	MG	CA	3060	1/1	0.69	0.36	60,60,60,60	0
58	MG	AA	3745	1/1	0.69	0.33	84,84,84,84	0
58	MG	AA	3767	1/1	0.69	0.28	66,66,66,66	0
58	MG	AA	3122	1/1	0.69	0.53	67,67,67,67	0
58	MG	BA	3163	1/1	0.70	0.18	52,52,52,52	0
58	MG	CA	3078	1/1	0.70	0.28	66,66,66,66	0
58	MG	BA	3103	1/1	0.70	0.26	85,85,85,85	0
58	MG	CA	3140	1/1	0.70	0.23	122,122,122,122	0
58	MG	CA	3118	1/1	0.71	0.19	67,67,67,67	0
58	MG	CA	3008	1/1	0.71	0.37	98,98,98,98	0
58	MG	AB	3020	1/1	0.71	0.16	53,53,53,53	0
58	MG	CA	3090	1/1	0.71	0.37	79,79,79,79	0
58	MG	A4	502	1/1	0.71	0.21	120,120,120,120	0
58	MG	CA	3108	1/1	0.71	0.22	106,106,106,106	0
58	MG	CA	3130	1/1	0.71	0.41	68,68,68,68	0
58	MG	AA	3353	1/1	0.71	0.14	75,75,75,75	0
58	MG	CA	3527	1/1	0.71	0.17	81,81,81,81	0
58	MG	CA	3275	1/1	0.71	0.32	67,67,67,67	0
58	MG	BA	3056	1/1	0.71	0.29	67,67,67,67	0
58	MG	CA	3149	1/1	0.71	0.36	63,63,63,63	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
58	MG	DA	1603	1/1	0.72	0.17	81,81,81,81	0
58	MG	CA	3351	1/1	0.72	0.11	83,83,83,83	0
58	MG	AA	3704	1/1	0.72	0.12	76,76,76,76	0
58	MG	CA	3611	1/1	0.72	0.35	58,58,58,58	0
58	MG	DA	1620	1/1	0.72	0.27	69,69,69,69	0
58	MG	BA	3088	1/1	0.72	0.45	68,68,68,68	0
58	MG	CA	3098	1/1	0.72	0.31	79,79,79,79	0
58	MG	CA	3184	1/1	0.73	0.64	85,85,85,85	0
58	MG	CA	3545	1/1	0.73	0.27	61,61,61,61	0
58	MG	BN	503	1/1	0.73	0.28	66,66,66,66	0
58	MG	AA	3641	1/1	0.73	0.60	76,76,76,76	0
58	MG	BX	104	1/1	0.73	0.28	69,69,69,69	0
58	MG	BA	3055	1/1	0.73	0.14	54,54,54,54	0
58	MG	BA	3092	1/1	0.73	0.48	86,86,86,86	0
58	MG	AA	3639	1/1	0.73	0.27	71,71,71,71	0
58	MG	CA	3216	1/1	0.73	0.09	74,74,74,74	0
58	MG	CE	304	1/1	0.73	0.55	65,65,65,65	0
58	MG	AB	3004	1/1	0.73	0.37	87,87,87,87	0
58	MG	BX	101	1/1	0.74	0.23	78,78,78,78	0
58	MG	CA	3173	1/1	0.74	0.33	81,81,81,81	0
58	MG	AA	3711	1/1	0.74	0.33	74,74,74,74	0
58	MG	CA	3587	1/1	0.74	0.31	81,81,81,81	0
58	MG	CA	3635	1/1	0.74	0.18	79,79,79,79	0
58	MG	BA	3205	1/1	0.74	0.14	68,68,68,68	0
58	MG	CA	3297	1/1	0.74	0.13	83,83,83,83	0
58	MG	DA	1740	1/1	0.74	0.36	79,79,79,79	0
58	MG	DA	1752	1/1	0.74	0.20	79,79,79,79	0
58	MG	AA	3806	1/1	0.74	0.21	60,60,60,60	0
58	MG	CA	3031	1/1	0.74	0.11	74,74,74,74	0
58	MG	CA	3582	1/1	0.75	0.12	96,96,96,96	0
58	MG	CA	3059	1/1	0.75	0.32	76,76,76,76	0
58	MG	CA	3656	1/1	0.75	0.33	96,96,96,96	0
58	MG	CA	3232	1/1	0.75	0.68	65,65,65,65	0
58	MG	AA	3598	1/1	0.75	0.13	61,61,61,61	0
58	MG	CA	3225	1/1	0.75	0.66	79,79,79,79	0
58	MG	AA	3018	1/1	0.75	0.86	75,75,75,75	0
58	MG	AG	202	1/1	0.75	0.09	73,73,73,73	0
58	MG	CA	3501	1/1	0.76	0.23	63,63,63,63	0
58	MG	CA	3604	1/1	0.76	0.10	74,74,74,74	0
58	MG	CA	3042	1/1	0.76	0.71	96,96,96,96	0
58	MG	BA	3052	1/1	0.76	0.25	102,102,102,102	0
58	MG	BA	3144	1/1	0.76	0.22	53,53,53,53	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
58	MG	AA	3821	1/1	0.76	0.33	46,46,46,46	0
58	MG	CA	3572	1/1	0.76	0.29	76,76,76,76	0
58	MG	CA	3035	1/1	0.76	0.36	58,58,58,58	0
58	MG	CA	3577	1/1	0.76	0.29	43,43,43,43	1
58	MG	AA	3675	1/1	0.76	0.10	40,40,40,40	0
58	MG	BA	3068	1/1	0.76	0.28	87,87,87,87	0
58	MG	AA	3195	1/1	0.76	0.26	43,43,43,43	0
58	MG	CA	3646	1/1	0.76	0.10	75,75,75,75	0
58	MG	AA	3277	1/1	0.77	0.30	78,78,78,78	0
58	MG	CA	3650	1/1	0.77	0.11	67,67,67,67	0
58	MG	CA	3565	1/1	0.77	0.09	90,90,90,90	0
58	MG	AA	3689	1/1	0.77	0.17	55,55,55,55	0
58	MG	BA	3108	1/1	0.77	0.26	49,49,49,49	0
58	MG	CA	3580	1/1	0.77	0.30	79,79,79,79	0
58	MG	AA	3765	1/1	0.77	0.33	61,61,61,61	0
58	MG	AA	3762	1/1	0.77	0.29	58,58,58,58	0
58	MG	BA	3025	1/1	0.77	0.18	88,88,88,88	0
58	MG	DA	1602	1/1	0.77	0.28	95,95,95,95	0
58	MG	BA	3067	1/1	0.77	0.35	73,73,73,73	0
58	MG	BA	3061	1/1	0.77	0.24	67,67,67,67	0
58	MG	DA	1749	1/1	0.77	0.16	80,80,80,80	0
58	MG	CA	3057	1/1	0.77	0.15	84,84,84,84	0
58	MG	CA	3606	1/1	0.77	0.20	51,51,51,51	0
58	MG	CB	3012	1/1	0.77	0.30	74,74,74,74	0
58	MG	CA	3530	1/1	0.77	0.32	78,78,78,78	0
58	MG	AA	3461	1/1	0.78	0.34	64,64,64,64	0
58	MG	AA	3444	1/1	0.78	0.20	73,73,73,73	0
58	MG	DA	1605	1/1	0.78	0.43	75,75,75,75	0
58	MG	DA	1631	1/1	0.78	0.22	59,59,59,59	0
58	MG	DA	1742	1/1	0.78	0.10	77,77,77,77	0
58	MG	CA	3379	1/1	0.78	0.17	86,86,86,86	0
58	MG	CA	3407	1/1	0.78	0.14	70,70,70,70	0
58	MG	DA	1677	1/1	0.78	0.45	80,80,80,80	0
58	MG	BA	3094	1/1	0.78	0.12	78,78,78,78	0
58	MG	CA	3013	1/1	0.78	0.22	61,61,61,61	0
58	MG	DA	1764	1/1	0.78	0.35	72,72,72,72	0
58	MG	BA	3098	1/1	0.78	0.35	78,78,78,78	0
58	MG	CG	3001	1/1	0.78	0.23	81,81,81,81	0
58	MG	CA	3509	1/1	0.78	0.17	96,96,96,96	0
58	MG	CA	3082	1/1	0.78	0.27	66,66,66,66	0
58	MG	AA	3088	1/1	0.78	0.47	73,73,73,73	0
58	MG	BA	3203	1/1	0.78	0.26	83,83,83,83	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
58	MG	BA	3152	1/1	0.78	0.11	58,58,58,58	0
58	MG	CA	3647	1/1	0.78	0.32	82,82,82,82	0
58	MG	BA	3015	1/1	0.78	0.25	87,87,87,87	0
58	MG	DA	1686	1/1	0.79	0.15	101,101,101,101	0
58	MG	CA	3135	1/1	0.79	0.96	84,84,84,84	0
58	MG	CO	201	1/1	0.79	0.17	61,61,61,61	0
58	MG	AA	3442	1/1	0.79	0.19	64,64,64,64	0
58	MG	CA	3292	1/1	0.79	0.45	75,75,75,75	0
58	MG	CA	3596	1/1	0.79	0.19	77,77,77,77	0
58	MG	AA	3269	1/1	0.79	0.18	84,84,84,84	0
58	MG	AA	3622	1/1	0.79	0.19	46,46,46,46	0
58	MG	DA	1672	1/1	0.79	0.38	100,100,100,100	0
58	MG	BV	101	1/1	0.79	0.30	110,110,110,110	0
58	MG	CA	3015	1/1	0.79	0.38	82,82,82,82	0
58	MG	AA	3580	1/1	0.79	0.10	39,39,39,39	0
58	MG	CA	3500	1/1	0.79	0.16	82,82,82,82	0
58	MG	CA	3644	1/1	0.79	0.24	66,66,66,66	0
58	MG	AA	3614	1/1	0.79	0.14	103,103,103,103	0
58	MG	CA	3583	1/1	0.79	0.17	78,78,78,78	0
58	MG	DA	1738	1/1	0.79	0.19	78,78,78,78	0
58	MG	AA	3441	1/1	0.79	0.20	46,46,46,46	0
58	MG	AA	3640	1/1	0.79	0.19	74,74,74,74	0
58	MG	BA	3093	1/1	0.79	0.19	65,65,65,65	0
58	MG	AA	3681	1/1	0.79	0.33	63,63,63,63	0
58	MG	DA	1628	1/1	0.79	0.15	69,69,69,69	0
58	MG	CA	3377	1/1	0.79	0.12	64,64,64,64	0
58	MG	AA	3266	1/1	0.79	0.31	74,74,74,74	0
58	MG	AA	3201	1/1	0.79	0.24	91,91,91,91	0
58	MG	DA	1622	1/1	0.79	0.15	42,42,42,42	0
58	MG	AA	3423	1/1	0.79	0.14	65,65,65,65	0
58	MG	AA	3665	1/1	0.80	0.24	83,83,83,83	0
58	MG	CA	3406	1/1	0.80	0.20	89,89,89,89	0
58	MG	CA	3412	1/1	0.80	0.27	58,58,58,58	0
58	MG	CA	3200	1/1	0.80	0.37	72,72,72,72	0
58	MG	AA	3071	1/1	0.80	0.27	59,59,59,59	0
58	MG	BA	3155	1/1	0.80	0.27	96,96,96,96	0
58	MG	AA	3096	1/1	0.80	0.51	81,81,81,81	0
58	MG	BA	3018	1/1	0.80	0.19	72,72,72,72	0
58	MG	AA	3579	1/1	0.80	0.34	53,53,53,53	0
58	MG	CA	3286	1/1	0.80	0.42	90,90,90,90	0
58	MG	BA	3100	1/1	0.80	0.21	74,74,74,74	0
58	MG	DA	1656	1/1	0.80	0.15	91,91,91,91	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
58	MG	AA	3100	1/1	0.80	0.10	60,60,60,60	0
58	MG	CA	3185	1/1	0.80	0.23	66,66,66,66	0
58	MG	CA	3154	1/1	0.80	0.14	77,77,77,77	0
58	MG	CA	3086	1/1	0.80	0.32	63,63,63,63	0
58	MG	AA	3546	1/1	0.80	0.12	53,53,53,53	1
58	MG	AA	3099	1/1	0.80	0.23	57,57,57,57	0
58	MG	BA	3167	1/1	0.80	0.20	85,85,85,85	0
58	MG	BA	3188	1/1	0.80	0.18	86,86,86,86	0
58	MG	CA	3349	1/1	0.80	0.20	54,54,54,54	0
58	MG	CA	3413	1/1	0.80	0.21	79,79,79,79	0
58	MG	CA	3484	1/1	0.80	0.34	67,67,67,67	0
58	MG	CA	3174	1/1	0.80	0.27	65,65,65,65	0
58	MG	CA	3638	1/1	0.80	0.25	78,78,78,78	0
58	MG	BA	3047	1/1	0.80	0.66	71,71,71,71	0
58	MG	CA	3505	1/1	0.80	0.09	60,60,60,60	0
58	MG	CA	3193	1/1	0.80	0.14	57,57,57,57	0
58	MG	BX	106	1/1	0.80	0.11	55,55,55,55	0
58	MG	CA	3555	1/1	0.80	0.17	80,80,80,80	0
58	MG	CA	3663	1/1	0.80	0.15	73,73,73,73	0
58	MG	CA	3628	1/1	0.80	0.66	76,76,76,76	0
58	MG	CA	3088	1/1	0.80	0.24	65,65,65,65	0
58	MG	AA	3801	1/1	0.80	0.07	89,89,89,89	0
58	MG	CA	3248	1/1	0.80	0.21	58,58,58,58	0
58	MG	CA	3203	1/1	0.81	0.70	76,76,76,76	0
58	MG	CA	3389	1/1	0.81	0.28	81,81,81,81	0
58	MG	AP	202	1/1	0.81	0.22	41,41,41,41	0
58	MG	CA	3390	1/1	0.81	0.28	74,74,74,74	0
58	MG	BA	3017	1/1	0.81	0.68	133,133,133,133	0
58	MG	CA	3243	1/1	0.81	0.41	110,110,110,110	0
58	MG	AF	301	1/1	0.81	0.15	41,41,41,41	0
58	MG	CA	3590	1/1	0.81	0.30	62,62,62,62	0
58	MG	CA	3623	1/1	0.81	0.16	69,69,69,69	0
58	MG	DA	1662	1/1	0.81	0.22	70,70,70,70	0
58	MG	CA	3571	1/1	0.81	0.32	77,77,77,77	0
58	MG	DA	1665	1/1	0.81	0.16	64,64,64,64	0
58	MG	BA	3033	1/1	0.81	0.19	52,52,52,52	0
58	MG	AA	3206	1/1	0.81	0.24	62,62,62,62	0
58	MG	BA	3074	1/1	0.81	0.15	66,66,66,66	0
58	MG	CA	3645	1/1	0.81	0.80	79,79,79,79	0
58	MG	CA	3255	1/1	0.81	0.09	95,95,95,95	0
58	MG	AA	3148	1/1	0.81	0.36	68,68,68,68	0
58	MG	BA	3099	1/1	0.81	0.23	70,70,70,70	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
58	MG	AA	3695	1/1	0.81	0.21	44,44,44,44	0
58	MG	CA	3100	1/1	0.81	0.17	90,90,90,90	0
58	MG	CA	3077	1/1	0.81	0.31	81,81,81,81	0
58	MG	DA	1651	1/1	0.81	0.17	70,70,70,70	0
58	MG	BA	3081	1/1	0.81	0.95	82,82,82,82	0
58	MG	BA	3186	1/1	0.81	0.15	67,67,67,67	0
58	MG	CA	3337	1/1	0.81	0.21	68,68,68,68	0
58	MG	BA	3028	1/1	0.81	0.47	90,90,90,90	0
58	MG	CA	3516	1/1	0.81	0.41	105,105,105,105	0
58	MG	CA	3585	1/1	0.81	0.23	80,80,80,80	0
58	MG	CA	3311	1/1	0.81	0.14	48,48,48,48	0
58	MG	BX	103	1/1	0.81	0.23	87,87,87,87	0
58	MG	DA	1734	1/1	0.81	0.12	78,78,78,78	0
58	MG	DA	1711	1/1	0.81	0.21	70,70,70,70	0
58	MG	AA	3119	1/1	0.81	0.36	62,62,62,62	0
58	MG	AA	3057	1/1	0.81	0.24	56,56,56,56	0
58	MG	CA	3043	1/1	0.82	0.69	101,101,101,101	0
58	MG	AA	3760	1/1	0.82	0.12	27,27,27,27	0
58	MG	BA	3046	1/1	0.82	0.81	60,60,60,60	0
58	MG	AA	3431	1/1	0.82	0.30	56,56,56,56	0
58	MG	AA	3452	1/1	0.82	0.18	67,67,67,67	0
58	MG	AA	3713	1/1	0.82	0.26	47,47,47,47	0
58	MG	CA	3069	1/1	0.82	0.23	56,56,56,56	0
58	MG	DA	1737	1/1	0.82	0.29	78,78,78,78	0
58	MG	CA	3541	1/1	0.82	0.35	71,71,71,71	0
58	MG	CA	3428	1/1	0.82	0.09	55,55,55,55	0
58	MG	DA	1710	1/1	0.82	0.18	79,79,79,79	0
58	MG	CB	3006	1/1	0.82	0.12	82,82,82,82	0
58	MG	BA	3023	1/1	0.82	0.96	75,75,75,75	0
58	MG	DA	1642	1/1	0.82	0.23	76,76,76,76	0
58	MG	CQ	203	1/1	0.82	0.31	59,59,59,59	0
58	MG	A8	5001	1/1	0.82	0.27	57,57,57,57	0
58	MG	AA	3616	1/1	0.82	0.20	37,37,37,37	1
58	MG	BA	3051	1/1	0.82	0.39	71,71,71,71	0
58	MG	CD	302	1/1	0.82	0.13	76,76,76,76	0
58	MG	DA	1613	1/1	0.82	0.33	70,70,70,70	0
58	MG	CA	3072	1/1	0.82	0.33	93,93,93,93	0
58	MG	CA	3210	1/1	0.82	0.44	93,93,93,93	0
58	MG	DA	1626	1/1	0.82	0.42	72,72,72,72	0
58	MG	CA	3397	1/1	0.82	0.22	59,59,59,59	0
58	MG	DA	1660	1/1	0.82	0.23	70,70,70,70	0
58	MG	BA	3210	1/1	0.82	0.20	68,68,68,68	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
58	MG	BA	3078	1/1	0.82	0.24	66,66,66,66	0
58	MG	BX	109	1/1	0.82	0.12	78,78,78,78	0
58	MG	CA	3637	1/1	0.82	0.28	79,79,79,79	0
58	MG	AA	3002	1/1	0.82	0.18	54,54,54,54	0
58	MG	CA	3139	1/1	0.82	0.10	63,63,63,63	0
58	MG	CA	3592	1/1	0.82	0.29	93,93,93,93	0
58	MG	BB	3001	1/1	0.82	0.26	76,76,76,76	0
58	MG	BA	3042	1/1	0.82	0.20	69,69,69,69	0
58	MG	CA	3250	1/1	0.82	0.38	76,76,76,76	0
58	MG	AA	3285	1/1	0.82	0.26	44,44,44,44	0
58	MG	AB	3014	1/1	0.82	0.15	67,67,67,67	0
59	K	AA	3818	1/1	0.83	0.36	87,87,87,87	0
58	MG	DA	1761	1/1	0.83	0.13	75,75,75,75	0
58	MG	BA	3029	1/1	0.83	0.30	54,54,54,54	0
58	MG	BA	3158	1/1	0.83	0.15	63,63,63,63	0
58	MG	AA	3440	1/1	0.83	0.21	51,51,51,51	0
58	MG	DA	1607	1/1	0.83	1.19	82,82,82,82	0
58	MG	AA	3651	1/1	0.83	0.27	49,49,49,49	0
58	MG	CA	3175	1/1	0.83	0.54	60,60,60,60	0
58	MG	BA	3013	1/1	0.83	0.20	75,75,75,75	0
58	MG	AA	3086	1/1	0.83	0.40	53,53,53,53	0
58	MG	CA	3136	1/1	0.83	0.29	64,64,64,64	0
58	MG	AA	3634	1/1	0.83	0.27	57,57,57,57	1
58	MG	BA	3154	1/1	0.83	0.13	94,94,94,94	0
58	MG	AA	3609	1/1	0.83	0.12	71,71,71,71	0
58	MG	AA	3625	1/1	0.83	0.27	63,63,63,63	0
58	MG	BA	3185	1/1	0.83	0.52	111,111,111,111	0
58	MG	CA	3056	1/1	0.83	0.43	61,61,61,61	0
58	MG	AA	3354	1/1	0.83	0.23	58,58,58,58	0
58	MG	CA	3206	1/1	0.83	0.65	104,104,104,104	0
58	MG	AA	3410	1/1	0.83	0.21	46,46,46,46	0
58	MG	CA	3511	1/1	0.83	0.15	74,74,74,74	0
58	MG	CA	3649	1/1	0.83	0.18	94,94,94,94	0
58	MG	BA	3190	1/1	0.83	0.28	89,89,89,89	0
58	MG	CA	3450	1/1	0.83	0.08	66,66,66,66	0
58	MG	CA	3197	1/1	0.83	0.56	63,63,63,63	0
58	MG	AA	3239	1/1	0.83	0.15	69,69,69,69	0
58	MG	AA	3060	1/1	0.83	0.48	64,64,64,64	0
58	MG	AA	3769	1/1	0.83	0.36	56,56,56,56	0
58	MG	AA	3483	1/1	0.83	0.11	44,44,44,44	0
58	MG	DA	1654	1/1	0.83	0.32	57,57,57,57	0
58	MG	AA	3649	1/1	0.83	0.29	90,90,90,90	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
58	MG	CA	3617	1/1	0.83	0.37	52,52,52,52	0
58	MG	AA	3264	1/1	0.83	0.51	77,77,77,77	0
58	MG	CA	3473	1/1	0.83	0.40	70,70,70,70	0
58	MG	AA	3247	1/1	0.83	0.78	68,68,68,68	0
58	MG	CA	3125	1/1	0.83	0.14	47,47,47,47	0
58	MG	DA	1687	1/1	0.83	0.17	66,66,66,66	0
58	MG	CA	3548	1/1	0.83	0.12	116,116,116,116	0
58	MG	CA	3214	1/1	0.83	0.24	43,43,43,43	0
58	MG	AA	3690	1/1	0.83	0.19	69,69,69,69	0
58	MG	CA	3486	1/1	0.83	0.33	81,81,81,81	0
58	MG	CA	3034	1/1	0.83	0.42	100,100,100,100	0
58	MG	CA	3190	1/1	0.83	0.19	68,68,68,68	0
58	MG	CA	3039	1/1	0.84	0.58	69,69,69,69	0
58	MG	DA	1683	1/1	0.84	0.45	70,70,70,70	0
58	MG	CA	3224	1/1	0.84	0.45	64,64,64,64	0
58	MG	AA	3766	1/1	0.84	0.20	70,70,70,70	0
58	MG	CA	3160	1/1	0.84	0.62	74,74,74,74	0
58	MG	CA	3211	1/1	0.84	0.37	72,72,72,72	0
58	MG	CA	3071	1/1	0.84	0.94	84,84,84,84	0
58	MG	CA	3205	1/1	0.84	0.25	71,71,71,71	0
58	MG	AA	3729	1/1	0.84	0.27	58,58,58,58	0
58	MG	AA	3017	1/1	0.84	0.17	78,78,78,78	0
58	MG	CA	3479	1/1	0.84	0.12	56,56,56,56	0
58	MG	AA	3116	1/1	0.84	0.43	75,75,75,75	0
58	MG	CA	3151	1/1	0.84	0.15	54,54,54,54	0
58	MG	BA	3160	1/1	0.84	0.22	61,61,61,61	0
58	MG	CA	3394	1/1	0.84	0.13	84,84,84,84	0
58	MG	DA	1723	1/1	0.84	0.08	68,68,68,68	0
58	MG	AA	3278	1/1	0.84	0.18	35,35,35,35	0
58	MG	CA	3576	1/1	0.84	0.29	71,71,71,71	0
58	MG	BA	3199	1/1	0.84	0.18	68,68,68,68	0
58	MG	DA	1729	1/1	0.84	0.60	79,79,79,79	0
58	MG	AA	3186	1/1	0.84	0.24	41,41,41,41	0
58	MG	AA	3591	1/1	0.84	0.21	66,66,66,66	0
58	MG	BA	3004	1/1	0.84	0.16	64,64,64,64	0
58	MG	CA	3191	1/1	0.84	0.17	84,84,84,84	0
58	MG	AA	3737	1/1	0.84	0.46	75,75,75,75	0
58	MG	AA	3443	1/1	0.84	0.12	61,61,61,61	0
58	MG	CA	3526	1/1	0.84	0.20	75,75,75,75	0
58	MG	CA	3084	1/1	0.84	0.47	86,86,86,86	0
58	MG	CA	3227	1/1	0.84	0.37	68,68,68,68	0
58	MG	CE	306	1/1	0.84	0.51	99,99,99,99	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
58	MG	DA	1629	1/1	0.84	0.21	73,73,73,73	0
58	MG	A6	101	1/1	0.84	0.28	58,58,58,58	0
58	MG	DA	1688	1/1	0.84	0.14	57,57,57,57	0
58	MG	AA	3728	1/1	0.84	0.14	48,48,48,48	0
58	MG	CA	3633	1/1	0.84	0.12	61,61,61,61	0
58	MG	AA	3807	1/1	0.84	0.26	65,65,65,65	0
58	MG	AA	3652	1/1	0.84	0.20	74,74,74,74	0
58	MG	AA	3759	1/1	0.84	0.28	63,63,63,63	0
58	MG	BA	3063	1/1	0.84	0.19	51,51,51,51	0
58	MG	AA	3364	1/1	0.85	0.33	79,79,79,79	0
58	MG	CA	3666	1/1	0.85	0.34	62,62,62,62	0
58	MG	CA	3464	1/1	0.85	0.23	47,47,47,47	0
58	MG	AA	3158	1/1	0.85	0.17	35,35,35,35	0
58	MG	AA	3126	1/1	0.85	0.36	26,26,26,26	0
58	MG	DD	502	1/1	0.85	0.40	61,61,61,61	0
58	MG	DT	3001	1/1	0.85	0.34	66,66,66,66	0
58	MG	CA	3102	1/1	0.85	0.16	76,76,76,76	0
58	MG	CA	3378	1/1	0.85	0.14	78,78,78,78	0
58	MG	AA	3761	1/1	0.85	0.25	48,48,48,48	0
58	MG	AA	3345	1/1	0.85	0.18	67,67,67,67	0
58	MG	AA	3082	1/1	0.85	0.20	38,38,38,38	0
58	MG	CA	3616	1/1	0.85	0.34	71,71,71,71	0
58	MG	CA	3083	1/1	0.85	0.26	70,70,70,70	0
58	MG	CA	3116	1/1	0.85	0.12	75,75,75,75	0
58	MG	CA	3455	1/1	0.85	0.18	78,78,78,78	0
58	MG	CA	3429	1/1	0.85	0.34	62,62,62,62	1
58	MG	AA	3087	1/1	0.85	0.38	49,49,49,49	0
58	MG	CA	3099	1/1	0.85	0.28	82,82,82,82	0
58	MG	CA	3619	1/1	0.85	0.58	79,79,79,79	0
58	MG	BA	3058	1/1	0.85	0.41	69,69,69,69	0
58	MG	DA	1655	1/1	0.85	0.29	73,73,73,73	0
58	MG	BA	3133	1/1	0.85	0.12	68,68,68,68	0
58	MG	DA	1675	1/1	0.85	0.15	77,77,77,77	0
58	MG	AA	3167	1/1	0.85	0.26	29,29,29,29	0
58	MG	CA	3535	1/1	0.85	0.13	79,79,79,79	0
58	MG	AA	3562	1/1	0.85	0.18	57,57,57,57	0
58	MG	CA	3538	1/1	0.85	0.10	69,69,69,69	0
58	MG	AA	3179	1/1	0.85	0.35	78,78,78,78	0
58	MG	AB	3018	1/1	0.85	0.18	81,81,81,81	0
58	MG	BA	3126	1/1	0.85	0.17	59,59,59,59	0
58	MG	CA	3374	1/1	0.85	0.28	56,56,56,56	0
58	MG	AA	3112	1/1	0.85	0.29	46,46,46,46	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
58	MG	CA	3148	1/1	0.85	0.37	77,77,77,77	0
58	MG	AA	3004	1/1	0.85	0.21	24,24,24,24	0
58	MG	CN	5001	1/1	0.85	0.14	76,76,76,76	0
58	MG	AA	3611	1/1	0.85	0.13	55,55,55,55	0
58	MG	AA	3727	1/1	0.85	0.18	66,66,66,66	0
58	MG	AA	3198	1/1	0.85	0.25	36,36,36,36	0
58	MG	CA	3624	1/1	0.85	0.33	72,72,72,72	0
58	MG	AA	3137	1/1	0.85	0.10	49,49,49,49	0
58	MG	AA	3597	1/1	0.85	0.20	40,40,40,40	0
58	MG	DA	1615	1/1	0.85	0.63	85,85,85,85	0
58	MG	CA	3107	1/1	0.85	0.37	54,54,54,54	0
58	MG	BA	3131	1/1	0.85	0.13	76,76,76,76	0
58	MG	BA	3101	1/1	0.85	0.20	60,60,60,60	0
58	MG	AA	3268	1/1	0.85	0.51	61,61,61,61	0
58	MG	BA	3157	1/1	0.86	0.32	67,67,67,67	0
58	MG	BA	3148	1/1	0.86	0.33	67,67,67,67	0
58	MG	DA	1648	1/1	0.86	0.54	90,90,90,90	0
58	MG	AA	3577	1/1	0.86	0.21	36,36,36,36	0
58	MG	CA	3539	1/1	0.86	0.45	77,77,77,77	0
58	MG	BA	3135	1/1	0.86	0.41	80,80,80,80	0
58	MG	AA	3836	1/1	0.86	0.32	48,48,48,48	0
58	MG	CA	3048	1/1	0.86	0.49	85,85,85,85	0
60	ZN	C4	501	1/1	0.86	0.07	192,192,192,192	0
58	MG	AA	3036	1/1	0.86	0.20	49,49,49,49	0
58	MG	DA	1717	1/1	0.86	0.15	74,74,74,74	0
58	MG	DA	1720	1/1	0.86	0.21	64,64,64,64	0
58	MG	CE	303	1/1	0.86	0.39	53,53,53,53	0
58	MG	CA	3472	1/1	0.86	0.15	45,45,45,45	0
58	MG	AA	3680	1/1	0.86	0.20	58,58,58,58	0
58	MG	DA	1744	1/1	0.86	0.41	90,90,90,90	0
58	MG	AA	3626	1/1	0.86	0.18	58,58,58,58	0
58	MG	AA	3249	1/1	0.86	0.25	62,62,62,62	0
58	MG	CA	3127	1/1	0.86	0.25	94,94,94,94	0
58	MG	CA	3245	1/1	0.86	0.32	77,77,77,77	0
58	MG	DA	1621	1/1	0.86	0.17	58,58,58,58	0
58	MG	BA	3062	1/1	0.86	1.07	81,81,81,81	0
58	MG	AA	3024	1/1	0.86	0.19	55,55,55,55	0
58	MG	DA	1709	1/1	0.86	0.14	44,44,44,44	0
58	MG	DA	1611	1/1	0.86	0.14	74,74,74,74	0
58	MG	CA	3657	1/1	0.86	0.29	62,62,62,62	0
58	MG	CA	3014	1/1	0.86	0.31	62,62,62,62	0
58	MG	CA	3241	1/1	0.86	0.23	74,74,74,74	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
58	MG	BA	3030	1/1	0.86	0.29	62,62,62,62	0
58	MG	AA	3014	1/1	0.86	0.15	44,44,44,44	0
58	MG	BT	3001	1/1	0.86	0.50	60,60,60,60	0
58	MG	AA	3813	1/1	0.86	0.23	57,57,57,57	0
58	MG	CA	3194	1/1	0.86	0.19	61,61,61,61	0
58	MG	AA	3330	1/1	0.86	0.14	66,66,66,66	0
58	MG	BA	3031	1/1	0.86	0.12	61,61,61,61	0
58	MG	DE	201	1/1	0.86	0.24	82,82,82,82	0
58	MG	AA	3304	1/1	0.86	0.23	30,30,30,30	0
58	MG	BA	3014	1/1	0.86	0.12	97,97,97,97	0
58	MG	AA	3238	1/1	0.86	0.26	55,55,55,55	0
58	MG	AA	3162	1/1	0.86	0.38	58,58,58,58	0
58	MG	AA	3115	1/1	0.86	0.17	15,15,15,15	0
58	MG	CA	3510	1/1	0.86	0.24	93,93,93,93	0
58	MG	CF	303	1/1	0.86	0.20	50,50,50,50	0
58	MG	CA	3514	1/1	0.86	0.39	63,63,63,63	0
58	MG	CA	3339	1/1	0.86	0.17	62,62,62,62	0
58	MG	CA	3575	1/1	0.86	0.19	78,78,78,78	0
58	MG	AA	3519	1/1	0.86	0.19	32,32,32,32	0
58	MG	CA	3485	1/1	0.86	0.18	74,74,74,74	0
58	MG	CA	3591	1/1	0.87	0.17	77,77,77,77	0
58	MG	DA	1733	1/1	0.87	0.53	81,81,81,81	0
58	MG	AA	3650	1/1	0.87	0.08	59,59,59,59	0
58	MG	AA	3492	1/1	0.87	0.37	61,61,61,61	0
58	MG	CA	3260	1/1	0.87	0.30	69,69,69,69	0
58	MG	BA	3070	1/1	0.87	0.17	72,72,72,72	0
58	MG	AA	3132	1/1	0.87	0.39	53,53,53,53	0
58	MG	AA	3192	1/1	0.87	0.16	41,41,41,41	0
58	MG	CA	3445	1/1	0.87	0.23	91,91,91,91	0
58	MG	CA	3095	1/1	0.87	0.35	86,86,86,86	0
58	MG	CA	3613	1/1	0.87	0.22	96,96,96,96	0
58	MG	CA	3076	1/1	0.87	0.68	69,69,69,69	0
58	MG	AA	3437	1/1	0.87	0.15	55,55,55,55	0
58	MG	AA	3802	1/1	0.87	0.25	54,54,54,54	0
58	MG	DA	1695	1/1	0.87	0.40	88,88,88,88	0
58	MG	BD	502	1/1	0.87	0.45	80,80,80,80	0
58	MG	AA	3373	1/1	0.87	0.19	57,57,57,57	0
58	MG	CA	3131	1/1	0.87	0.63	70,70,70,70	0
58	MG	AA	3783	1/1	0.87	0.15	52,52,52,52	0
58	MG	BA	3057	1/1	0.87	0.11	89,89,89,89	0
58	MG	CA	3010	1/1	0.87	0.15	40,40,40,40	0
58	MG	CA	3552	1/1	0.87	0.13	34,34,34,34	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
58	MG	DA	1646	1/1	0.87	0.27	57,57,57,57	0
58	MG	CA	3237	1/1	0.87	0.57	75,75,75,75	0
58	MG	CA	3134	1/1	0.87	0.28	69,69,69,69	0
58	MG	CA	3448	1/1	0.87	0.30	78,78,78,78	0
58	MG	BX	108	1/1	0.87	0.10	78,78,78,78	0
58	MG	AA	3683	1/1	0.87	0.38	65,65,65,65	0
58	MG	CA	3223	1/1	0.87	0.45	75,75,75,75	0
58	MG	CA	3543	1/1	0.87	0.21	70,70,70,70	0
58	MG	AA	3703	1/1	0.87	0.28	41,41,41,41	1
58	MG	AA	3273	1/1	0.87	0.24	52,52,52,52	0
58	MG	AA	3382	1/1	0.87	0.13	38,38,38,38	1
58	MG	AA	3006	1/1	0.87	0.42	52,52,52,52	0
58	MG	AA	3027	1/1	0.87	0.40	77,77,77,77	0
58	MG	AA	3572	1/1	0.87	0.13	49,49,49,49	0
58	MG	AA	3794	1/1	0.87	0.23	68,68,68,68	0
58	MG	AA	3589	1/1	0.87	0.16	38,38,38,38	0
58	MG	AE	301	1/1	0.87	0.40	68,68,68,68	0
58	MG	AA	3491	1/1	0.87	0.28	33,33,33,33	0
58	MG	DL	3001	1/1	0.87	0.43	57,57,57,57	0
58	MG	AA	3531	1/1	0.87	0.11	52,52,52,52	0
58	MG	BA	3071	1/1	0.87	0.29	93,93,93,93	0
58	MG	CA	3274	1/1	0.87	0.41	73,73,73,73	0
58	MG	BA	3045	1/1	0.87	0.29	75,75,75,75	0
58	MG	BA	3016	1/1	0.87	0.26	73,73,73,73	0
58	MG	AA	3165	1/1	0.87	0.16	56,56,56,56	0
58	MG	CA	3559	1/1	0.87	0.12	75,75,75,75	0
58	MG	AA	3232	1/1	0.87	0.45	79,79,79,79	0
58	MG	CA	3481	1/1	0.87	0.29	55,55,55,55	0
58	MG	CA	3239	1/1	0.87	0.23	74,74,74,74	0
58	MG	CA	3414	1/1	0.87	0.17	39,39,39,39	0
58	MG	AA	3042	1/1	0.87	0.27	36,36,36,36	0
58	MG	CA	3278	1/1	0.87	0.18	48,48,48,48	0
58	MG	CA	3651	1/1	0.87	0.34	51,51,51,51	0
58	MG	AF	304	1/1	0.88	0.29	61,61,61,61	0
58	MG	DA	1705	1/1	0.88	0.32	86,86,86,86	0
58	MG	AA	3587	1/1	0.88	0.15	59,59,59,59	0
58	MG	AA	3696	1/1	0.88	0.69	76,76,76,76	0
58	MG	BA	3043	1/1	0.88	0.22	65,65,65,65	0
58	MG	CA	3044	1/1	0.88	0.30	52,52,52,52	0
58	MG	AA	3606	1/1	0.88	0.14	64,64,64,64	0
58	MG	AA	3001	1/1	0.88	0.14	36,36,36,36	0
58	MG	AA	3235	1/1	0.88	0.27	54,54,54,54	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
58	MG	CA	3196	1/1	0.88	0.21	58,58,58,58	0
58	MG	CA	3579	1/1	0.88	0.20	83,83,83,83	0
58	MG	DA	1699	1/1	0.88	0.36	123,123,123,123	0
58	MG	CA	3138	1/1	0.88	0.35	70,70,70,70	0
58	MG	AB	3001	1/1	0.88	0.63	85,85,85,85	0
58	MG	CA	3187	1/1	0.88	0.43	67,67,67,67	0
58	MG	CA	3017	1/1	0.88	0.39	45,45,45,45	0
58	MG	BA	3177	1/1	0.88	0.17	73,73,73,73	0
58	MG	CA	3546	1/1	0.88	0.09	79,79,79,79	0
58	MG	BA	3019	1/1	0.88	0.34	55,55,55,55	0
58	MG	AA	3079	1/1	0.88	0.28	63,63,63,63	0
58	MG	AD	307	1/1	0.88	0.34	37,37,37,37	0
58	MG	BA	3059	1/1	0.88	0.56	76,76,76,76	0
58	MG	BA	3162	1/1	0.88	0.09	54,54,54,54	0
58	MG	AA	3253	1/1	0.88	0.37	65,65,65,65	0
58	MG	AA	3034	1/1	0.88	0.29	56,56,56,56	0
58	MG	CA	3038	1/1	0.88	0.20	46,46,46,46	0
58	MG	AA	3271	1/1	0.88	0.15	55,55,55,55	0
58	MG	BA	3077	1/1	0.88	0.43	86,86,86,86	0
58	MG	AA	3781	1/1	0.88	0.23	52,52,52,52	1
58	MG	CA	3636	1/1	0.88	0.25	65,65,65,65	0
58	MG	BA	3117	1/1	0.88	0.09	65,65,65,65	0
58	MG	CA	3659	1/1	0.88	0.33	104,104,104,104	0
58	MG	BA	3007	1/1	0.88	0.17	75,75,75,75	0
58	MG	CA	3463	1/1	0.88	0.09	50,50,50,50	0
58	MG	DA	1739	1/1	0.88	0.21	76,76,76,76	0
58	MG	BA	3104	1/1	0.88	0.41	76,76,76,76	0
58	MG	CA	3235	1/1	0.88	0.41	70,70,70,70	0
58	MG	CA	3128	1/1	0.88	0.32	60,60,60,60	0
60	ZN	A4	501	1/1	0.88	0.07	133,133,133,133	0
58	MG	AA	3563	1/1	0.88	0.19	49,49,49,49	1
58	MG	DA	1661	1/1	0.88	0.13	62,62,62,62	0
58	MG	AA	3490	1/1	0.88	0.11	50,50,50,50	0
58	MG	DA	1689	1/1	0.88	0.39	80,80,80,80	0
58	MG	CA	3300	1/1	0.88	0.28	66,66,66,66	0
58	MG	CA	3329	1/1	0.88	0.17	57,57,57,57	0
58	MG	CA	3376	1/1	0.88	0.46	70,70,70,70	0
58	MG	CA	3212	1/1	0.88	0.12	37,37,37,37	0
58	MG	DA	1630	1/1	0.88	0.30	56,56,56,56	0
58	MG	AA	3019	1/1	0.88	0.30	57,57,57,57	0
58	MG	CA	3189	1/1	0.88	0.59	58,58,58,58	0
58	MG	AA	3379	1/1	0.88	0.14	30,30,30,30	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
58	MG	AA	3633	1/1	0.88	0.27	75,75,75,75	0
58	MG	AA	3052	1/1	0.88	0.49	63,63,63,63	0
58	MG	CA	3634	1/1	0.88	0.16	75,75,75,75	0
58	MG	DA	1617	1/1	0.88	0.15	63,63,63,63	0
58	MG	C7	101	1/1	0.88	0.25	47,47,47,47	0
58	MG	CA	3476	1/1	0.88	0.25	54,54,54,54	0
58	MG	CA	3459	1/1	0.88	0.20	48,48,48,48	0
58	MG	CA	3437	1/1	0.88	0.14	74,74,74,74	0
58	MG	AA	3013	1/1	0.88	0.28	34,34,34,34	0
58	MG	BA	3173	1/1	0.88	0.62	113,113,113,113	0
58	MG	BA	3089	1/1	0.88	0.64	89,89,89,89	0
58	MG	DA	1640	1/1	0.88	0.15	74,74,74,74	0
58	MG	CA	3018	1/1	0.88	0.25	62,62,62,62	0
58	MG	AA	3170	1/1	0.88	0.23	39,39,39,39	0
58	MG	AA	3144	1/1	0.89	0.38	47,47,47,47	0
58	MG	BA	3065	1/1	0.89	0.28	57,57,57,57	0
58	MG	DA	1758	1/1	0.89	0.17	64,64,64,64	0
58	MG	CA	3458	1/1	0.89	0.26	46,46,46,46	0
58	MG	AA	3092	1/1	0.89	0.40	43,43,43,43	0
58	MG	AA	3229	1/1	0.89	0.26	54,54,54,54	0
58	MG	CQ	204	1/1	0.89	0.61	79,79,79,79	0
58	MG	CA	3400	1/1	0.89	0.12	73,73,73,73	0
58	MG	DA	1751	1/1	0.89	0.21	69,69,69,69	0
58	MG	AA	3574	1/1	0.89	0.12	47,47,47,47	0
58	MG	CA	3598	1/1	0.89	0.25	66,66,66,66	0
58	MG	AA	3808	1/1	0.89	0.24	33,33,33,33	1
58	MG	AA	3645	1/1	0.89	0.56	78,78,78,78	0
58	MG	BL	3002	1/1	0.89	0.17	49,49,49,49	0
58	MG	DA	1706	1/1	0.89	0.10	85,85,85,85	0
58	MG	CA	3221	1/1	0.89	0.18	76,76,76,76	0
58	MG	AA	3805	1/1	0.89	0.24	40,40,40,40	1
58	MG	AA	3062	1/1	0.89	0.53	66,66,66,66	0
58	MG	CA	3549	1/1	0.89	0.17	61,61,61,61	0
58	MG	BA	3097	1/1	0.89	0.40	66,66,66,66	0
58	MG	CQ	202	1/1	0.89	0.15	66,66,66,66	0
58	MG	AA	3267	1/1	0.89	0.31	49,49,49,49	0
58	MG	BA	3032	1/1	0.89	0.18	47,47,47,47	0
58	MG	CA	3271	1/1	0.89	0.22	84,84,84,84	0
58	MG	DA	1606	1/1	0.89	0.11	72,72,72,72	0
58	MG	CA	3512	1/1	0.89	0.11	64,64,64,64	0
58	MG	BA	3010	1/1	0.89	0.11	68,68,68,68	0
58	MG	CB	3010	1/1	0.89	0.14	53,53,53,53	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
58	MG	CA	3422	1/1	0.89	0.24	74,74,74,74	0
58	MG	CA	3513	1/1	0.89	0.19	66,66,66,66	0
58	MG	CA	3593	1/1	0.89	0.15	82,82,82,82	0
58	MG	AA	3248	1/1	0.89	0.49	72,72,72,72	0
58	MG	BA	3066	1/1	0.89	0.38	53,53,53,53	0
58	MG	CA	3603	1/1	0.89	0.16	48,48,48,48	0
58	MG	AA	3029	1/1	0.89	0.32	50,50,50,50	0
58	MG	AA	3184	1/1	0.89	0.20	36,36,36,36	0
58	MG	DJ	5001	1/1	0.89	0.26	105,105,105,105	0
58	MG	AA	3274	1/1	0.89	0.50	88,88,88,88	0
58	MG	AA	3789	1/1	0.89	0.22	52,52,52,52	0
58	MG	AA	3458	1/1	0.89	0.14	70,70,70,70	0
58	MG	AA	3539	1/1	0.89	0.37	63,63,63,63	0
58	MG	BA	3125	1/1	0.89	0.26	63,63,63,63	0
58	MG	BA	3121	1/1	0.89	0.15	59,59,59,59	0
58	MG	AA	3477	1/1	0.89	0.20	57,57,57,57	0
58	MG	DA	1641	1/1	0.89	0.17	79,79,79,79	0
58	MG	CA	3570	1/1	0.89	0.07	41,41,41,41	0
58	MG	CA	3404	1/1	0.89	0.06	86,86,86,86	0
58	MG	BA	3195	1/1	0.89	0.33	73,73,73,73	0
58	MG	AA	3544	1/1	0.89	0.17	52,52,52,52	0
58	MG	CA	3222	1/1	0.89	0.31	53,53,53,53	0
58	MG	BA	3006	1/1	0.89	0.14	71,71,71,71	0
58	MG	DA	1685	1/1	0.89	0.19	52,52,52,52	0
58	MG	CA	3233	1/1	0.89	0.15	56,56,56,56	0
58	MG	DA	1670	1/1	0.89	0.33	81,81,81,81	0
58	MG	AA	3056	1/1	0.89	0.24	61,61,61,61	0
58	MG	AA	3292	1/1	0.89	0.20	71,71,71,71	0
58	MG	AA	3106	1/1	0.89	0.12	80,80,80,80	0
58	MG	AA	3677	1/1	0.89	0.20	40,40,40,40	0
58	MG	AA	3730	1/1	0.89	0.08	38,38,38,38	0
58	MG	AB	3023	1/1	0.89	0.30	74,74,74,74	0
58	MG	AA	3107	1/1	0.89	0.32	48,48,48,48	0
58	MG	CA	3155	1/1	0.89	0.29	69,69,69,69	0
58	MG	BA	3083	1/1	0.89	0.34	68,68,68,68	0
58	MG	CA	3240	1/1	0.89	0.27	58,58,58,58	0
58	MG	CA	3204	1/1	0.89	0.12	58,58,58,58	0
58	MG	BA	3082	1/1	0.89	0.08	69,69,69,69	0
58	MG	AA	3129	1/1	0.89	0.36	57,57,57,57	0
58	MG	AF	303	1/1	0.89	0.45	48,48,48,48	0
58	MG	CA	3254	1/1	0.89	0.26	63,63,63,63	0
58	MG	CA	3308	1/1	0.89	0.23	50,50,50,50	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
58	MG	CA	3279	1/1	0.89	0.11	89,89,89,89	0
58	MG	CV	202	1/1	0.89	0.35	85,85,85,85	0
58	MG	CA	3242	1/1	0.89	0.21	63,63,63,63	0
58	MG	CA	3068	1/1	0.89	0.33	72,72,72,72	0
58	MG	BA	3073	1/1	0.89	0.83	74,74,74,74	0
58	MG	BA	3136	1/1	0.89	0.25	70,70,70,70	0
58	MG	AA	3302	1/1	0.89	0.23	56,56,56,56	0
58	MG	DA	1728	1/1	0.89	0.13	85,85,85,85	0
58	MG	BA	3176	1/1	0.89	0.22	61,61,61,61	0
58	MG	AA	3590	1/1	0.89	0.26	23,23,23,23	1
58	MG	AA	3391	1/1	0.89	0.13	42,42,42,42	0
58	MG	CA	3627	1/1	0.89	0.19	101,101,101,101	0
58	MG	AA	3754	1/1	0.89	0.12	40,40,40,40	0
58	MG	AA	3130	1/1	0.89	0.38	70,70,70,70	0
58	MG	CA	3080	1/1	0.89	0.20	56,56,56,56	0
58	MG	AA	3715	1/1	0.89	0.22	54,54,54,54	0
58	MG	CA	3142	1/1	0.89	0.32	54,54,54,54	0
58	MG	BA	3003	1/1	0.89	0.13	51,51,51,51	0
58	MG	DA	1623	1/1	0.89	0.49	77,77,77,77	0
58	MG	AA	3743	1/1	0.89	0.18	80,80,80,80	0
58	MG	DA	1668	1/1	0.89	0.34	82,82,82,82	0
58	MG	BA	3170	1/1	0.89	0.09	71,71,71,71	0
58	MG	BA	3048	1/1	0.89	0.15	75,75,75,75	0
58	MG	CA	3424	1/1	0.89	0.24	51,51,51,51	0
58	MG	AA	3792	1/1	0.89	0.22	27,27,27,27	0
58	MG	AA	3197	1/1	0.89	0.37	49,49,49,49	0
58	MG	AA	3816	1/1	0.89	0.25	91,91,91,91	0
58	MG	AA	3480	1/1	0.89	0.18	54,54,54,54	0
58	MG	CB	3008	1/1	0.89	0.14	58,58,58,58	0
58	MG	BF	3001	1/1	0.89	0.42	71,71,71,71	0
58	MG	AA	3498	1/1	0.89	0.07	45,45,45,45	0
58	MG	CA	3103	1/1	0.89	0.26	55,55,55,55	0
58	MG	AA	3275	1/1	0.90	0.25	56,56,56,56	0
58	MG	DA	1746	1/1	0.90	0.16	77,77,77,77	0
58	MG	DA	1763	1/1	0.90	0.31	94,94,94,94	0
58	MG	AA	3163	1/1	0.90	0.22	45,45,45,45	0
58	MG	CA	3431	1/1	0.90	0.33	51,51,51,51	0
58	MG	AA	3231	1/1	0.90	0.29	41,41,41,41	0
58	MG	DA	1676	1/1	0.90	0.18	75,75,75,75	0
58	MG	DZ	702	1/1	0.90	0.27	61,61,61,61	0
58	MG	CA	3129	1/1	0.90	0.27	69,69,69,69	0
58	MG	AB	3010	1/1	0.90	0.20	51,51,51,51	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
58	MG	A5	103	1/1	0.90	0.33	60,60,60,60	0
58	MG	AA	3138	1/1	0.90	0.22	54,54,54,54	0
58	MG	AA	3237	1/1	0.90	0.20	63,63,63,63	0
58	MG	DA	1760	1/1	0.90	0.05	71,71,71,71	0
58	MG	CA	3064	1/1	0.90	0.27	51,51,51,51	0
58	MG	BX	102	1/1	0.90	0.20	67,67,67,67	0
58	MG	AA	3481	1/1	0.90	0.11	50,50,50,50	0
58	MG	DA	1716	1/1	0.90	0.26	75,75,75,75	0
58	MG	DA	1671	1/1	0.90	0.41	72,72,72,72	0
58	MG	AA	3044	1/1	0.90	0.23	34,34,34,34	0
58	MG	CA	3342	1/1	0.90	0.20	69,69,69,69	0
58	MG	BA	3054	1/1	0.90	0.29	77,77,77,77	0
58	MG	AA	3272	1/1	0.90	0.23	69,69,69,69	0
58	MG	AA	3181	1/1	0.90	0.31	94,94,94,94	0
58	MG	BA	3012	1/1	0.90	0.14	29,29,29,29	0
58	MG	AA	3064	1/1	0.90	0.19	35,35,35,35	0
58	MG	DA	1718	1/1	0.90	0.23	72,72,72,72	0
58	MG	CA	3122	1/1	0.90	0.15	43,43,43,43	0
58	MG	AA	3283	1/1	0.90	0.42	59,59,59,59	0
58	MG	CA	3052	1/1	0.90	0.39	69,69,69,69	0
58	MG	CA	3432	1/1	0.90	0.31	96,96,96,96	0
58	MG	AA	3714	1/1	0.90	0.29	55,55,55,55	1
58	MG	CA	3199	1/1	0.90	0.16	36,36,36,36	0
58	MG	BA	3116	1/1	0.90	0.28	82,82,82,82	0
58	MG	AA	3362	1/1	0.90	0.36	67,67,67,67	0
58	MG	DA	1736	1/1	0.90	0.71	78,78,78,78	0
58	MG	BA	3091	1/1	0.90	0.41	72,72,72,72	0
58	MG	AA	3605	1/1	0.90	0.21	40,40,40,40	1
58	MG	CE	305	1/1	0.90	0.26	41,41,41,41	0
58	MG	AA	3422	1/1	0.90	0.10	23,23,23,23	0
58	MG	AA	3187	1/1	0.90	0.08	36,36,36,36	0
58	MG	DA	1682	1/1	0.90	0.28	52,52,52,52	0
58	MG	AA	3593	1/1	0.90	0.21	51,51,51,51	0
58	MG	CA	3477	1/1	0.90	0.22	54,54,54,54	0
58	MG	AA	3073	1/1	0.90	0.11	25,25,25,25	0
58	MG	CA	3262	1/1	0.90	0.20	64,64,64,64	0
58	MG	AH	3002	1/1	0.90	0.31	77,77,77,77	0
58	MG	CA	3491	1/1	0.90	0.18	65,65,65,65	0
58	MG	BA	3128	1/1	0.90	0.13	47,47,47,47	0
58	MG	AA	3257	1/1	0.90	0.25	26,26,26,26	0
58	MG	CA	3063	1/1	0.90	0.28	66,66,66,66	0
58	MG	AA	3039	1/1	0.90	0.20	44,44,44,44	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
58	MG	CA	3536	1/1	0.90	0.15	75,75,75,75	0
58	MG	AB	3017	1/1	0.90	0.21	76,76,76,76	0
58	MG	BA	3115	1/1	0.90	0.45	86,86,86,86	0
58	MG	DA	1703	1/1	0.90	0.09	68,68,68,68	0
58	MG	DA	1637	1/1	0.90	0.38	67,67,67,67	0
58	MG	BA	3168	1/1	0.90	0.06	57,57,57,57	0
58	MG	DA	1627	1/1	0.90	0.52	48,48,48,48	0
58	MG	CA	3493	1/1	0.90	0.74	105,105,105,105	0
58	MG	AD	309	1/1	0.90	0.22	55,55,55,55	0
58	MG	AA	3097	1/1	0.90	0.16	61,61,61,61	0
58	MG	CA	3315	1/1	0.90	0.60	76,76,76,76	0
58	MG	AA	3721	1/1	0.90	0.54	76,76,76,76	0
58	MG	CA	3050	1/1	0.90	0.10	43,43,43,43	0
58	MG	AA	3200	1/1	0.90	0.07	52,52,52,52	0
58	MG	CA	3054	1/1	0.90	0.24	68,68,68,68	0
58	MG	CA	3061	1/1	0.90	0.53	74,74,74,74	0
58	MG	CB	3002	1/1	0.90	0.18	64,64,64,64	0
58	MG	CA	3654	1/1	0.90	0.12	29,29,29,29	0
58	MG	CA	3410	1/1	0.90	0.20	40,40,40,40	0
58	MG	CA	3420	1/1	0.90	0.25	58,58,58,58	0
58	MG	AA	3757	1/1	0.90	0.17	43,43,43,43	0
58	MG	AA	3142	1/1	0.90	0.17	41,41,41,41	0
58	MG	CA	3602	1/1	0.90	0.13	78,78,78,78	0
58	MG	BA	3146	1/1	0.90	0.28	65,65,65,65	0
58	MG	AA	3089	1/1	0.90	0.29	33,33,33,33	0
58	MG	DA	1755	1/1	0.90	0.25	71,71,71,71	0
58	MG	CA	3147	1/1	0.90	0.29	58,58,58,58	0
58	MG	CA	3246	1/1	0.90	0.49	77,77,77,77	0
58	MG	AA	3488	1/1	0.90	0.17	23,23,23,23	0
58	MG	AA	3188	1/1	0.90	0.14	31,31,31,31	0
58	MG	AA	3547	1/1	0.90	0.21	30,30,30,30	0
58	MG	BA	3191	1/1	0.90	0.17	74,74,74,74	0
58	MG	BA	3194	1/1	0.90	0.15	60,60,60,60	0
58	MG	BA	3060	1/1	0.90	0.25	82,82,82,82	0
58	MG	AA	3270	1/1	0.90	0.20	80,80,80,80	0
58	MG	BL	3004	1/1	0.90	0.25	67,67,67,67	0
58	MG	AA	3172	1/1	0.90	0.64	32,32,32,32	0
58	MG	BA	3049	1/1	0.90	0.18	36,36,36,36	0
58	MG	CF	301	1/1	0.90	0.28	62,62,62,62	0
58	MG	AA	3381	1/1	0.90	0.14	26,26,26,26	0
58	MG	AA	3243	1/1	0.90	0.20	66,66,66,66	0
58	MG	CA	3363	1/1	0.90	0.19	42,42,42,42	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
58	MG	CA	3266	1/1	0.90	0.27	58,58,58,58	0
58	MG	DA	1645	1/1	0.90	0.20	61,61,61,61	0
58	MG	AA	3303	1/1	0.90	0.29	53,53,53,53	0
58	MG	CA	3033	1/1	0.90	0.60	88,88,88,88	0
58	MG	AA	3733	1/1	0.91	0.20	66,66,66,66	0
58	MG	AA	3159	1/1	0.91	0.30	97,97,97,97	0
58	MG	CA	3143	1/1	0.91	0.23	69,69,69,69	0
58	MG	DA	1754	1/1	0.91	0.20	66,66,66,66	0
58	MG	BA	3021	1/1	0.91	0.09	37,37,37,37	0
60	ZN	DN	501	1/1	0.91	0.07	127,127,127,127	0
58	MG	CA	3145	1/1	0.91	0.32	66,66,66,66	0
58	MG	AA	3125	1/1	0.91	0.23	63,63,63,63	0
58	MG	AA	3685	1/1	0.91	0.19	47,47,47,47	0
58	MG	AA	3691	1/1	0.91	0.18	87,87,87,87	0
58	MG	AA	3083	1/1	0.91	0.17	27,27,27,27	1
58	MG	CA	3047	1/1	0.91	0.16	60,60,60,60	0
58	MG	DA	1643	1/1	0.91	0.11	55,55,55,55	0
58	MG	AA	3234	1/1	0.91	0.40	77,77,77,77	0
58	MG	AA	3679	1/1	0.91	0.18	64,64,64,64	0
58	MG	AA	3455	1/1	0.91	0.19	56,56,56,56	0
58	MG	AA	3147	1/1	0.91	0.37	37,37,37,37	0
58	MG	AA	3205	1/1	0.91	0.33	56,56,56,56	0
58	MG	AA	3335	1/1	0.91	0.16	40,40,40,40	0
58	MG	CA	3006	1/1	0.91	0.22	65,65,65,65	0
58	MG	CA	3483	1/1	0.91	0.25	68,68,68,68	0
58	MG	AA	3653	1/1	0.91	0.08	67,67,67,67	0
58	MG	AA	3795	1/1	0.91	0.20	49,49,49,49	0
58	MG	AA	3825	1/1	0.91	0.28	43,43,43,43	0
58	MG	AA	3449	1/1	0.91	0.22	53,53,53,53	0
58	MG	CA	3247	1/1	0.91	0.24	55,55,55,55	0
58	MG	CA	3356	1/1	0.91	0.08	41,41,41,41	0
58	MG	BA	3159	1/1	0.91	0.07	55,55,55,55	0
58	MG	BA	3044	1/1	0.91	0.10	56,56,56,56	0
58	MG	BN	502	1/1	0.91	0.23	64,64,64,64	0
58	MG	BA	3139	1/1	0.91	0.18	54,54,54,54	0
58	MG	AA	3095	1/1	0.91	0.81	110,110,110,110	0
58	MG	CB	3009	1/1	0.91	0.18	64,64,64,64	0
58	MG	BA	3204	1/1	0.91	0.35	68,68,68,68	0
58	MG	AA	3007	1/1	0.91	0.17	20,20,20,20	0
58	MG	CA	3380	1/1	0.91	0.27	63,63,63,63	0
58	MG	CA	3290	1/1	0.91	0.22	53,53,53,53	0
58	MG	AA	3203	1/1	0.91	0.22	46,46,46,46	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
58	MG	AA	3601	1/1	0.91	0.31	59,59,59,59	0
58	MG	BA	3211	1/1	0.91	0.20	59,59,59,59	0
58	MG	BA	3161	1/1	0.91	0.28	87,87,87,87	0
58	MG	AA	3662	1/1	0.91	0.20	58,58,58,58	0
58	MG	AA	3043	1/1	0.91	0.28	32,32,32,32	0
58	MG	BA	3009	1/1	0.91	0.52	58,58,58,58	0
58	MG	CA	3573	1/1	0.91	0.19	64,64,64,64	0
58	MG	AA	3627	1/1	0.91	0.29	72,72,72,72	0
58	MG	CA	3192	1/1	0.91	0.23	65,65,65,65	0
58	MG	AA	3637	1/1	0.91	0.27	64,64,64,64	0
58	MG	AA	3758	1/1	0.91	0.43	81,81,81,81	0
58	MG	CA	3158	1/1	0.91	0.19	54,54,54,54	0
58	MG	AA	3091	1/1	0.91	0.34	34,34,34,34	0
58	MG	DA	1673	1/1	0.91	0.34	61,61,61,61	0
58	MG	AA	3411	1/1	0.91	0.21	41,41,41,41	0
58	MG	DA	1608	1/1	0.91	0.14	58,58,58,58	0
58	MG	AA	3173	1/1	0.91	0.37	71,71,71,71	0
58	MG	AA	3333	1/1	0.91	0.12	66,66,66,66	0
58	MG	CB	3004	1/1	0.91	0.12	67,67,67,67	0
58	MG	AA	3222	1/1	0.91	0.26	61,61,61,61	0
58	MG	A6	102	1/1	0.91	0.31	64,64,64,64	0
58	MG	DA	1700	1/1	0.91	0.20	62,62,62,62	0
58	MG	AA	3336	1/1	0.91	0.14	53,53,53,53	0
58	MG	CA	3439	1/1	0.91	0.09	46,46,46,46	0
58	MG	AA	3319	1/1	0.91	0.19	66,66,66,66	0
58	MG	CA	3282	1/1	0.91	0.11	31,31,31,31	0
58	MG	AA	3252	1/1	0.91	0.23	46,46,46,46	0
58	MG	CA	3159	1/1	0.91	0.40	68,68,68,68	0
58	MG	AA	3204	1/1	0.91	0.23	55,55,55,55	0
58	MG	AA	3402	1/1	0.91	0.11	27,27,27,27	0
58	MG	AA	3012	1/1	0.91	0.27	34,34,34,34	0
58	MG	CA	3001	1/1	0.91	0.33	71,71,71,71	0
58	MG	BA	3109	1/1	0.91	0.12	79,79,79,79	0
58	MG	AA	3778	1/1	0.91	0.43	55,55,55,55	0
58	MG	AA	3025	1/1	0.91	0.45	41,41,41,41	0
58	MG	DA	1726	1/1	0.91	0.08	61,61,61,61	0
58	MG	CA	3542	1/1	0.91	0.37	82,82,82,82	0
58	MG	AB	3021	1/1	0.91	0.23	60,60,60,60	0
58	MG	CA	3626	1/1	0.91	0.14	62,62,62,62	0
58	MG	AA	3183	1/1	0.91	0.16	75,75,75,75	0
58	MG	AA	3325	1/1	0.91	0.07	65,65,65,65	0
58	MG	AA	3543	1/1	0.91	0.17	62,62,62,62	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
58	MG	AA	3618	1/1	0.91	0.12	49,49,49,49	0
58	MG	A1	101	1/1	0.91	0.11	54,54,54,54	0
58	MG	CA	3169	1/1	0.91	0.45	55,55,55,55	0
58	MG	CA	3482	1/1	0.91	0.15	89,89,89,89	0
58	MG	AA	3414	1/1	0.91	0.12	55,55,55,55	0
58	MG	AA	3121	1/1	0.91	0.24	46,46,46,46	0
58	MG	AA	3350	1/1	0.91	0.22	32,32,32,32	0
58	MG	DA	1618	1/1	0.91	0.09	47,47,47,47	0
58	MG	AA	3718	1/1	0.91	0.24	47,47,47,47	0
58	MG	AA	3656	1/1	0.91	0.15	55,55,55,55	0
58	MG	DA	1766	1/1	0.91	0.19	53,53,53,53	0
58	MG	CA	3117	1/1	0.91	0.61	73,73,73,73	0
58	MG	BA	3181	1/1	0.91	0.14	47,47,47,47	0
58	MG	AA	3564	1/1	0.91	0.10	48,48,48,48	0
58	MG	CA	3289	1/1	0.91	0.22	51,51,51,51	0
58	MG	CA	3305	1/1	0.91	0.10	90,90,90,90	0
58	MG	BA	3208	1/1	0.91	0.12	81,81,81,81	0
58	MG	AA	3196	1/1	0.91	0.14	50,50,50,50	0
58	MG	AW	3001	1/1	0.91	0.28	50,50,50,50	0
58	MG	BA	3196	1/1	0.91	0.51	84,84,84,84	0
58	MG	AA	3041	1/1	0.91	0.30	75,75,75,75	0
58	MG	AA	3279	1/1	0.91	0.21	51,51,51,51	0
58	MG	AA	3090	1/1	0.91	0.24	50,50,50,50	0
58	MG	BA	3008	1/1	0.91	0.13	61,61,61,61	0
58	MG	CA	3226	1/1	0.91	0.44	64,64,64,64	0
58	MG	BA	3192	1/1	0.91	0.16	65,65,65,65	0
58	MG	AA	3360	1/1	0.91	0.17	111,111,111,111	0
58	MG	AW	3004	1/1	0.91	0.27	64,64,64,64	0
58	MG	AA	3811	1/1	0.91	0.22	53,53,53,53	0
58	MG	AA	3428	1/1	0.91	0.23	41,41,41,41	0
58	MG	CA	3259	1/1	0.92	0.42	56,56,56,56	0
58	MG	CA	3132	1/1	0.92	0.25	61,61,61,61	0
58	MG	A0	103	1/1	0.92	0.18	41,41,41,41	0
58	MG	AA	3021	1/1	0.92	0.20	39,39,39,39	0
58	MG	DA	1719	1/1	0.92	0.14	66,66,66,66	0
58	MG	AA	3048	1/1	0.92	0.33	33,33,33,33	0
58	MG	AA	3349	1/1	0.92	0.19	39,39,39,39	0
58	MG	AA	3610	1/1	0.92	0.13	51,51,51,51	0
58	MG	AA	3294	1/1	0.92	0.06	65,65,65,65	0
58	MG	AA	3028	1/1	0.92	0.30	55,55,55,55	0
58	MG	BA	3034	1/1	0.92	0.19	61,61,61,61	0
58	MG	DA	1701	1/1	0.92	0.33	64,64,64,64	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
58	MG	CA	3608	1/1	0.92	0.18	70,70,70,70	0
58	MG	AA	3495	1/1	0.92	0.24	50,50,50,50	0
58	MG	AA	3210	1/1	0.92	0.20	63,63,63,63	0
58	MG	CA	3188	1/1	0.92	0.17	36,36,36,36	0
58	MG	CA	3317	1/1	0.92	0.11	51,51,51,51	0
58	MG	CA	3229	1/1	0.92	0.40	61,61,61,61	0
58	MG	AA	3108	1/1	0.92	0.24	74,74,74,74	0
58	MG	AA	3493	1/1	0.92	0.35	44,44,44,44	0
58	MG	CA	3444	1/1	0.92	0.11	37,37,37,37	0
58	MG	CA	3451	1/1	0.92	0.12	47,47,47,47	0
58	MG	CA	3557	1/1	0.92	0.21	82,82,82,82	0
58	MG	AA	3701	1/1	0.92	0.23	33,33,33,33	0
58	MG	BA	3143	1/1	0.92	0.14	79,79,79,79	0
58	MG	AA	3466	1/1	0.92	0.10	59,59,59,59	0
58	MG	AA	3215	1/1	0.92	0.21	56,56,56,56	0
58	MG	CA	3020	1/1	0.92	0.16	61,61,61,61	0
58	MG	AA	3310	1/1	0.92	0.15	57,57,57,57	0
58	MG	CA	3393	1/1	0.92	0.22	35,35,35,35	0
58	MG	CA	3408	1/1	0.92	0.17	54,54,54,54	0
58	MG	BK	201	1/1	0.92	0.19	56,56,56,56	0
58	MG	CA	3137	1/1	0.92	0.12	51,51,51,51	0
58	MG	AA	3055	1/1	0.92	0.22	34,34,34,34	0
58	MG	CA	3179	1/1	0.92	0.17	55,55,55,55	0
58	MG	CA	3302	1/1	0.92	0.25	84,84,84,84	0
58	MG	CA	3234	1/1	0.92	0.13	58,58,58,58	0
58	MG	CA	3665	1/1	0.92	0.18	55,55,55,55	0
58	MG	AA	3560	1/1	0.92	0.20	39,39,39,39	0
58	MG	AA	3059	1/1	0.92	0.27	49,49,49,49	0
58	MG	CA	3215	1/1	0.92	0.22	39,39,39,39	0
58	MG	AA	3291	1/1	0.92	0.18	44,44,44,44	0
58	MG	AA	3819	1/1	0.92	0.12	44,44,44,44	0
58	MG	BA	3022	1/1	0.92	0.28	46,46,46,46	0
58	MG	AA	3317	1/1	0.92	0.21	57,57,57,57	0
58	MG	DA	1669	1/1	0.92	0.12	73,73,73,73	0
58	MG	CA	3344	1/1	0.92	0.11	36,36,36,36	0
58	MG	BA	3200	1/1	0.92	0.13	63,63,63,63	0
58	MG	CA	3396	1/1	0.92	0.38	64,64,64,64	0
58	MG	CE	307	1/1	0.92	0.10	65,65,65,65	0
58	MG	AD	310	1/1	0.92	0.55	58,58,58,58	0
58	MG	CA	3168	1/1	0.92	0.12	58,58,58,58	0
58	MG	CA	3294	1/1	0.92	0.12	71,71,71,71	0
58	MG	AA	3399	1/1	0.92	0.34	39,39,39,39	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
58	MG	AA	3035	1/1	0.92	0.35	59,59,59,59	0
58	MG	CB	3007	1/1	0.92	0.27	64,64,64,64	0
58	MG	AA	3510	1/1	0.92	0.17	47,47,47,47	0
58	MG	CF	302	1/1	0.92	0.51	63,63,63,63	0
58	MG	AA	3244	1/1	0.92	0.10	69,69,69,69	0
58	MG	BA	3096	1/1	0.92	0.13	64,64,64,64	0
58	MG	AA	3334	1/1	0.92	0.21	58,58,58,58	0
58	MG	DA	1619	1/1	0.92	0.35	62,62,62,62	0
58	MG	AA	3470	1/1	0.92	0.12	28,28,28,28	0
58	MG	AA	3258	1/1	0.92	0.24	13,13,13,13	0
58	MG	CB	3001	1/1	0.92	0.24	96,96,96,96	0
58	MG	AA	3742	1/1	0.92	0.22	39,39,39,39	1
58	MG	BA	3174	1/1	0.92	0.13	69,69,69,69	0
58	MG	CA	3228	1/1	0.92	0.17	51,51,51,51	0
58	MG	CA	3032	1/1	0.92	0.65	67,67,67,67	0
58	MG	CA	3357	1/1	0.92	0.21	57,57,57,57	0
58	MG	AA	3251	1/1	0.92	0.45	33,33,33,33	1
58	MG	CA	3471	1/1	0.92	0.24	69,69,69,69	0
58	MG	AA	3740	1/1	0.92	0.33	92,92,92,92	0
58	MG	BA	3037	1/1	0.92	0.22	64,64,64,64	0
58	MG	BA	3002	1/1	0.92	0.19	91,91,91,91	0
58	MG	CA	3595	1/1	0.92	0.11	69,69,69,69	0
58	MG	DA	1691	1/1	0.92	0.12	74,74,74,74	0
58	MG	CA	3343	1/1	0.92	0.15	46,46,46,46	0
58	MG	AA	3462	1/1	0.92	0.30	70,70,70,70	0
58	MG	AA	3827	1/1	0.92	0.56	51,51,51,51	0
58	MG	DA	1664	1/1	0.92	0.34	59,59,59,59	0
58	MG	CA	3320	1/1	0.92	0.14	66,66,66,66	0
58	MG	AA	3372	1/1	0.92	0.34	61,61,61,61	0
58	MG	DA	1601	1/1	0.92	0.20	59,59,59,59	0
58	MG	CA	3318	1/1	0.92	0.08	45,45,45,45	0
58	MG	AA	3716	1/1	0.92	0.13	63,63,63,63	0
58	MG	CA	3531	1/1	0.92	0.09	58,58,58,58	0
58	MG	DA	1609	1/1	0.92	0.14	45,45,45,45	0
58	MG	AA	3344	1/1	0.92	0.12	85,85,85,85	0
58	MG	CA	3438	1/1	0.92	0.14	49,49,49,49	0
58	MG	DA	1639	1/1	0.92	0.35	83,83,83,83	0
58	MG	AA	3502	1/1	0.92	0.08	24,24,24,24	0
58	MG	CD	301	1/1	0.92	0.28	79,79,79,79	0
58	MG	CA	3285	1/1	0.92	0.21	59,59,59,59	0
58	MG	AA	3045	1/1	0.92	0.60	43,43,43,43	0
58	MG	CD	303	1/1	0.92	0.28	35,35,35,35	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
58	MG	AA	3117	1/1	0.92	0.23	50,50,50,50	0
58	MG	AA	3744	1/1	0.92	0.24	77,77,77,77	0
58	MG	AA	3160	1/1	0.92	0.30	50,50,50,50	0
58	MG	AA	3070	1/1	0.92	0.21	33,33,33,33	0
58	MG	CA	3025	1/1	0.92	0.42	75,75,75,75	0
60	ZN	BN	501	1/1	0.92	0.06	121,121,121,121	0
58	MG	CA	3609	1/1	0.92	0.24	64,64,64,64	0
58	MG	BA	3075	1/1	0.92	0.18	56,56,56,56	0
58	MG	AA	3282	1/1	0.92	0.31	39,39,39,39	0
58	MG	CA	3392	1/1	0.92	0.08	63,63,63,63	0
58	MG	AA	3347	1/1	0.92	0.10	40,40,40,40	0
58	MG	AA	3460	1/1	0.92	0.19	71,71,71,71	0
58	MG	AA	3828	1/1	0.92	0.35	44,44,44,44	0
58	MG	AA	3647	1/1	0.92	0.21	71,71,71,71	0
58	MG	CU	3001	1/1	0.92	0.37	91,91,91,91	0
58	MG	BA	3138	1/1	0.92	0.28	62,62,62,62	0
58	MG	AA	3225	1/1	0.92	0.43	34,34,34,34	0
58	MG	BL	3003	1/1	0.92	0.18	79,79,79,79	0
58	MG	CA	3370	1/1	0.92	0.14	56,56,56,56	0
58	MG	AA	3700	1/1	0.92	0.25	48,48,48,48	0
58	MG	CA	3402	1/1	0.92	0.30	67,67,67,67	0
58	MG	AA	3815	1/1	0.92	0.54	53,53,53,53	0
58	MG	DA	1657	1/1	0.93	0.15	72,72,72,72	0
58	MG	AZ	302	1/1	0.93	0.23	66,66,66,66	0
58	MG	AA	3323	1/1	0.93	0.16	21,21,21,21	0
58	MG	AA	3226	1/1	0.93	0.29	73,73,73,73	0
58	MG	DA	1724	1/1	0.93	0.11	77,77,77,77	0
58	MG	AO	5001	1/1	0.93	0.20	53,53,53,53	0
58	MG	DA	1759	1/1	0.93	0.20	64,64,64,64	0
58	MG	AA	3717	1/1	0.93	0.16	56,56,56,56	0
58	MG	BA	3166	1/1	0.93	0.10	58,58,58,58	0
58	MG	CA	3488	1/1	0.93	0.10	69,69,69,69	0
58	MG	AA	3153	1/1	0.93	0.20	67,67,67,67	0
58	MG	CA	3281	1/1	0.93	0.14	34,34,34,34	0
58	MG	AA	3365	1/1	0.93	0.18	54,54,54,54	0
58	MG	AA	3566	1/1	0.93	0.24	28,28,28,28	0
58	MG	AA	3548	1/1	0.93	0.08	29,29,29,29	0
58	MG	AV	202	1/1	0.93	0.23	37,37,37,37	0
58	MG	AA	3261	1/1	0.93	0.39	69,69,69,69	0
58	MG	AA	3306	1/1	0.93	0.13	47,47,47,47	0
58	MG	CA	3534	1/1	0.93	0.20	79,79,79,79	0
58	MG	DA	1638	1/1	0.93	0.16	74,74,74,74	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
58	MG	CA	3348	1/1	0.93	0.14	58,58,58,58	0
58	MG	AA	3421	1/1	0.93	0.06	70,70,70,70	0
58	MG	AA	3832	1/1	0.93	0.23	43,43,43,43	1
58	MG	BA	3084	1/1	0.93	0.10	80,80,80,80	0
58	MG	AA	3404	1/1	0.93	0.37	43,43,43,43	0
58	MG	AA	3166	1/1	0.93	0.30	57,57,57,57	0
58	MG	CA	3520	1/1	0.93	0.34	83,83,83,83	0
58	MG	CA	3324	1/1	0.93	0.12	66,66,66,66	0
58	MG	AA	3674	1/1	0.93	0.20	74,74,74,74	0
58	MG	DA	1698	1/1	0.93	0.12	76,76,76,76	0
58	MG	AA	3635	1/1	0.93	0.45	60,60,60,60	0
58	MG	BA	3198	1/1	0.93	0.36	68,68,68,68	0
58	MG	CA	3053	1/1	0.93	0.56	57,57,57,57	0
58	MG	BA	3005	1/1	0.93	0.22	64,64,64,64	0
58	MG	BA	3105	1/1	0.93	0.36	60,60,60,60	0
58	MG	AA	3663	1/1	0.93	0.65	60,60,60,60	0
58	MG	DA	1650	1/1	0.93	0.29	57,57,57,57	0
58	MG	BA	3113	1/1	0.93	0.11	60,60,60,60	0
58	MG	BA	3164	1/1	0.93	0.10	60,60,60,60	0
58	MG	CA	3532	1/1	0.93	0.12	58,58,58,58	0
58	MG	BA	3129	1/1	0.93	0.17	52,52,52,52	0
58	MG	CA	3498	1/1	0.93	0.30	71,71,71,71	0
58	MG	CA	3452	1/1	0.93	0.12	62,62,62,62	0
58	MG	CA	3551	1/1	0.93	0.05	57,57,57,57	0
58	MG	CA	3198	1/1	0.93	0.35	62,62,62,62	0
58	MG	AA	3774	1/1	0.93	0.45	78,78,78,78	0
58	MG	DA	1633	1/1	0.93	0.38	60,60,60,60	0
58	MG	CA	3569	1/1	0.93	0.16	54,54,54,54	0
58	MG	AU	202	1/1	0.93	0.34	56,56,56,56	0
58	MG	AA	3456	1/1	0.93	0.11	32,32,32,32	0
58	MG	CA	3036	1/1	0.93	0.12	42,42,42,42	0
58	MG	AA	3435	1/1	0.93	0.24	37,37,37,37	0
58	MG	AA	3262	1/1	0.93	0.24	49,49,49,49	0
58	MG	BA	3187	1/1	0.93	0.08	59,59,59,59	0
58	MG	CA	3201	1/1	0.93	0.45	52,52,52,52	0
58	MG	AA	3020	1/1	0.93	0.15	23,23,23,23	0
58	MG	AA	3094	1/1	0.93	0.26	29,29,29,29	0
58	MG	AA	3817	1/1	0.93	0.46	57,57,57,57	0
58	MG	CA	3073	1/1	0.93	0.32	53,53,53,53	0
58	MG	AA	3202	1/1	0.93	0.15	63,63,63,63	0
58	MG	CA	3502	1/1	0.93	0.36	69,69,69,69	0
58	MG	CA	3620	1/1	0.93	0.12	34,34,34,34	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
58	MG	CA	3395	1/1	0.93	0.09	53,53,53,53	0
58	MG	CA	3556	1/1	0.93	0.24	66,66,66,66	0
58	MG	AA	3240	1/1	0.93	0.38	60,60,60,60	0
58	MG	DA	1604	1/1	0.93	0.15	72,72,72,72	0
58	MG	AA	3191	1/1	0.93	0.17	44,44,44,44	0
58	MG	AA	3615	1/1	0.93	0.12	55,55,55,55	0
58	MG	AA	3804	1/1	0.93	0.21	65,65,65,65	0
58	MG	AA	3670	1/1	0.93	0.16	31,31,31,31	0
58	MG	AA	3638	1/1	0.93	0.21	45,45,45,45	0
58	MG	BA	3124	1/1	0.93	0.22	71,71,71,71	0
58	MG	AE	304	1/1	0.93	0.16	29,29,29,29	0
58	MG	CA	3287	1/1	0.93	0.19	55,55,55,55	0
58	MG	DA	1730	1/1	0.93	0.27	75,75,75,75	0
58	MG	CA	3252	1/1	0.93	0.13	51,51,51,51	0
58	MG	AA	3321	1/1	0.93	0.22	69,69,69,69	0
58	MG	CA	3026	1/1	0.93	0.24	79,79,79,79	0
58	MG	AA	3324	1/1	0.93	0.09	32,32,32,32	0
58	MG	DA	1732	1/1	0.93	0.09	80,80,80,80	0
58	MG	CA	3055	1/1	0.93	0.51	37,37,37,37	0
58	MG	AA	3241	1/1	0.93	0.35	64,64,64,64	0
58	MG	AA	3453	1/1	0.93	0.22	54,54,54,54	0
58	MG	DA	1693	1/1	0.93	0.25	60,60,60,60	0
58	MG	CA	3058	1/1	0.93	0.12	48,48,48,48	0
58	MG	CA	3387	1/1	0.93	0.25	62,62,62,62	0
58	MG	A2	3001	1/1	0.93	0.24	50,50,50,50	0
58	MG	CA	3607	1/1	0.93	0.10	67,67,67,67	0
58	MG	CA	3309	1/1	0.93	0.11	40,40,40,40	0
58	MG	CA	3280	1/1	0.93	0.22	38,38,38,38	0
58	MG	BA	3079	1/1	0.93	0.12	35,35,35,35	0
58	MG	CA	3178	1/1	0.93	0.16	34,34,34,34	0
58	MG	DA	1762	1/1	0.93	0.10	53,53,53,53	0
58	MG	CA	3648	1/1	0.93	0.11	77,77,77,77	0
58	MG	DL	3002	1/1	0.93	0.33	74,74,74,74	0
58	MG	AA	3586	1/1	0.93	0.15	65,65,65,65	0
58	MG	A0	102	1/1	0.93	0.09	54,54,54,54	0
58	MG	AA	3407	1/1	0.93	0.11	19,19,19,19	0
58	MG	AA	3436	1/1	0.93	0.20	52,52,52,52	0
58	MG	AA	3359	1/1	0.93	0.14	49,49,49,49	0
58	MG	AA	3741	1/1	0.93	0.22	45,45,45,45	0
58	MG	CA	3544	1/1	0.93	0.26	66,66,66,66	0
58	MG	AA	3209	1/1	0.93	0.38	59,59,59,59	0
58	MG	CA	3386	1/1	0.93	0.30	63,63,63,63	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
58	MG	CA	3126	1/1	0.93	0.36	71,71,71,71	0
58	MG	AA	3764	1/1	0.93	0.19	54,54,54,54	0
58	MG	CA	3362	1/1	0.93	0.25	57,57,57,57	0
58	MG	AA	3280	1/1	0.93	0.28	46,46,46,46	0
58	MG	AA	3102	1/1	0.93	0.34	50,50,50,50	0
58	MG	BA	3156	1/1	0.93	0.14	36,36,36,36	0
58	MG	BA	3182	1/1	0.93	0.14	80,80,80,80	0
58	MG	AA	3401	1/1	0.93	0.24	33,33,33,33	0
58	MG	AD	303	1/1	0.93	0.27	64,64,64,64	0
58	MG	CA	3332	1/1	0.93	0.23	50,50,50,50	0
58	MG	CA	3385	1/1	0.93	0.26	70,70,70,70	0
58	MG	DA	1684	1/1	0.93	0.19	63,63,63,63	0
58	MG	BA	3011	1/1	0.93	0.10	76,76,76,76	0
58	MG	AA	3124	1/1	0.93	0.47	43,43,43,43	0
58	MG	CA	3467	1/1	0.93	0.35	54,54,54,54	0
58	MG	AA	3046	1/1	0.93	0.15	35,35,35,35	0
58	MG	CA	3207	1/1	0.93	0.47	55,55,55,55	0
58	MG	BA	3202	1/1	0.93	0.12	62,62,62,62	0
58	MG	CA	3258	1/1	0.93	0.14	40,40,40,40	0
58	MG	CA	3249	1/1	0.93	0.48	64,64,64,64	0
58	MG	CA	3264	1/1	0.93	0.12	60,60,60,60	0
58	MG	AA	3049	1/1	0.93	0.20	51,51,51,51	0
58	MG	AA	3375	1/1	0.93	0.21	57,57,57,57	0
58	MG	AA	3620	1/1	0.93	0.14	42,42,42,42	0
58	MG	AA	3133	1/1	0.93	0.30	30,30,30,30	0
58	MG	C8	5001	1/1	0.93	0.53	48,48,48,48	0
58	MG	AW	3002	1/1	0.93	0.20	52,52,52,52	0
58	MG	AA	3709	1/1	0.93	0.19	53,53,53,53	0
58	MG	AA	3093	1/1	0.93	0.25	52,52,52,52	0
58	MG	DA	1632	1/1	0.93	0.19	69,69,69,69	0
58	MG	CA	3478	1/1	0.93	0.12	73,73,73,73	0
58	MG	DA	1735	1/1	0.93	0.08	70,70,70,70	0
58	MG	CA	3469	1/1	0.93	0.13	61,61,61,61	0
58	MG	BA	3201	1/1	0.93	0.10	68,68,68,68	0
58	MG	AA	3061	1/1	0.93	0.20	26,26,26,26	0
58	MG	BA	3102	1/1	0.93	0.35	56,56,56,56	0
58	MG	AA	3753	1/1	0.93	0.51	72,72,72,72	0
58	MG	DA	1702	1/1	0.93	0.42	73,73,73,73	0
58	MG	AA	3010	1/1	0.93	0.39	66,66,66,66	0
58	MG	BX	107	1/1	0.93	0.49	67,67,67,67	0
58	MG	AA	3161	1/1	0.93	0.11	54,54,54,54	0
58	MG	CA	3347	1/1	0.93	0.12	33,33,33,33	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
58	MG	AA	3573	1/1	0.93	0.13	31,31,31,31	0
58	MG	AA	3698	1/1	0.93	0.16	62,62,62,62	0
58	MG	DA	1757	1/1	0.93	0.39	73,73,73,73	0
58	MG	AA	3505	1/1	0.93	0.14	55,55,55,55	0
58	MG	AA	3658	1/1	0.93	0.11	60,60,60,60	0
58	MG	AA	3080	1/1	0.93	0.20	33,33,33,33	0
58	MG	CA	3490	1/1	0.93	0.32	78,78,78,78	0
58	MG	AA	3063	1/1	0.93	0.46	66,66,66,66	0
58	MG	A8	5002	1/1	0.93	0.20	30,30,30,30	0
58	MG	AA	3415	1/1	0.93	0.17	30,30,30,30	0
58	MG	AA	3139	1/1	0.93	0.29	49,49,49,49	0
58	MG	AA	3185	1/1	0.93	0.22	65,65,65,65	0
58	MG	AA	3705	1/1	0.93	0.18	57,57,57,57	0
58	MG	CQ	201	1/1	0.93	0.51	63,63,63,63	0
58	MG	AA	3030	1/1	0.93	0.22	31,31,31,31	1
58	MG	CA	3495	1/1	0.94	0.33	62,62,62,62	0
58	MG	CA	3391	1/1	0.94	0.14	61,61,61,61	0
58	MG	AA	3657	1/1	0.94	0.19	51,51,51,51	1
58	MG	CA	3186	1/1	0.94	0.38	58,58,58,58	0
58	MG	AA	3297	1/1	0.94	0.20	20,20,20,20	0
58	MG	AA	3629	1/1	0.94	0.25	74,74,74,74	0
58	MG	AA	3451	1/1	0.94	0.17	53,53,53,53	1
58	MG	DA	1713	1/1	0.94	0.38	74,74,74,74	0
58	MG	CA	3496	1/1	0.94	0.19	64,64,64,64	0
58	MG	AA	3619	1/1	0.94	0.15	37,37,37,37	0
58	MG	CA	3322	1/1	0.94	0.06	32,32,32,32	0
58	MG	AA	3796	1/1	0.94	0.25	19,19,19,19	1
58	MG	CA	3584	1/1	0.94	0.17	43,43,43,43	0
58	MG	BA	3149	1/1	0.94	0.37	82,82,82,82	0
58	MG	AA	3078	1/1	0.94	0.27	49,49,49,49	0
58	MG	CA	3251	1/1	0.94	0.15	47,47,47,47	0
58	MG	CA	3499	1/1	0.94	0.46	65,65,65,65	0
58	MG	CA	3359	1/1	0.94	0.25	44,44,44,44	0
58	MG	CA	3163	1/1	0.94	0.24	45,45,45,45	0
58	MG	CA	3109	1/1	0.94	0.14	59,59,59,59	0
58	MG	AH	3001	1/1	0.94	0.34	50,50,50,50	0
58	MG	AA	3156	1/1	0.94	0.29	63,63,63,63	0
58	MG	CA	3299	1/1	0.94	0.30	54,54,54,54	0
58	MG	AA	3682	1/1	0.94	0.16	51,51,51,51	0
58	MG	CA	3588	1/1	0.94	0.17	68,68,68,68	0
58	MG	CA	3012	1/1	0.94	0.13	58,58,58,58	0
58	MG	CA	3489	1/1	0.94	0.15	53,53,53,53	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
58	MG	CA	3231	1/1	0.94	0.28	50,50,50,50	0
58	MG	AA	3289	1/1	0.94	0.12	26,26,26,26	0
58	MG	CA	3045	1/1	0.94	0.65	65,65,65,65	0
58	MG	AA	3567	1/1	0.94	0.20	26,26,26,26	0
58	MG	CA	3433	1/1	0.94	0.25	61,61,61,61	0
58	MG	AD	301	1/1	0.94	0.46	70,70,70,70	0
58	MG	CA	3574	1/1	0.94	0.13	53,53,53,53	0
58	MG	AA	3749	1/1	0.94	0.17	55,55,55,55	0
58	MG	CA	3355	1/1	0.94	0.21	59,59,59,59	0
58	MG	CA	3295	1/1	0.94	0.13	69,69,69,69	0
58	MG	BA	3036	1/1	0.94	0.17	72,72,72,72	0
58	MG	AA	3176	1/1	0.94	0.23	49,49,49,49	0
58	MG	CA	3652	1/1	0.94	0.19	84,84,84,84	0
58	MG	BA	3151	1/1	0.94	0.35	63,63,63,63	0
58	MG	AA	3509	1/1	0.94	0.19	48,48,48,48	0
58	MG	CA	3183	1/1	0.94	0.28	25,25,25,25	0
58	MG	CA	3664	1/1	0.94	0.29	55,55,55,55	0
58	MG	AA	3584	1/1	0.94	0.14	14,14,14,14	0
58	MG	CA	3515	1/1	0.94	0.34	73,73,73,73	0
58	MG	AA	3613	1/1	0.94	0.15	54,54,54,54	0
58	MG	CA	3091	1/1	0.94	0.36	63,63,63,63	0
58	MG	CA	3105	1/1	0.94	0.16	45,45,45,45	0
58	MG	AA	3582	1/1	0.94	0.17	37,37,37,37	0
58	MG	AA	3473	1/1	0.94	0.17	17,17,17,17	0
58	MG	BA	3132	1/1	0.94	0.07	61,61,61,61	0
58	MG	AA	3553	1/1	0.94	0.22	60,60,60,60	0
58	MG	AA	3786	1/1	0.94	0.23	57,57,57,57	0
58	MG	AA	3190	1/1	0.94	0.31	40,40,40,40	0
58	MG	AA	3671	1/1	0.94	0.11	57,57,57,57	0
58	MG	AA	3798	1/1	0.94	0.24	32,32,32,32	0
58	MG	C1	101	1/1	0.94	0.19	67,67,67,67	0
58	MG	CA	3599	1/1	0.94	0.14	69,69,69,69	0
58	MG	CA	3003	1/1	0.94	0.25	44,44,44,44	0
58	MG	CA	3269	1/1	0.94	0.12	54,54,54,54	0
58	MG	CA	3152	1/1	0.94	0.21	49,49,49,49	0
58	MG	CA	3096	1/1	0.94	0.30	63,63,63,63	0
58	MG	CA	3062	1/1	0.94	0.45	65,65,65,65	0
58	MG	CA	3024	1/1	0.94	0.52	87,87,87,87	0
58	MG	AA	3833	1/1	0.94	0.24	47,47,47,47	0
58	MG	CA	3293	1/1	0.94	0.15	26,26,26,26	0
58	MG	AX	102	1/1	0.94	0.29	72,72,72,72	0
58	MG	AB	3008	1/1	0.94	0.41	51,51,51,51	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
58	MG	CA	3089	1/1	0.94	0.26	73,73,73,73	0
58	MG	DA	1644	1/1	0.94	0.13	64,64,64,64	0
58	MG	AA	3242	1/1	0.94	0.21	28,28,28,28	0
58	MG	CA	3177	1/1	0.94	0.37	50,50,50,50	0
58	MG	AA	3387	1/1	0.94	0.22	24,24,24,24	0
58	MG	AA	3218	1/1	0.94	0.30	49,49,49,49	0
58	MG	CA	3273	1/1	0.94	0.26	54,54,54,54	0
58	MG	CA	3612	1/1	0.94	0.23	74,74,74,74	0
58	MG	BA	3053	1/1	0.94	0.16	69,69,69,69	0
58	MG	AA	3069	1/1	0.94	0.20	63,63,63,63	0
58	MG	AA	3596	1/1	0.94	0.13	54,54,54,54	0
58	MG	CA	3313	1/1	0.94	0.13	51,51,51,51	0
58	MG	AW	3003	1/1	0.94	0.26	55,55,55,55	0
58	MG	BA	3050	1/1	0.94	0.29	67,67,67,67	0
58	MG	CA	3508	1/1	0.94	0.13	57,57,57,57	0
58	MG	CA	3284	1/1	0.94	0.14	48,48,48,48	0
58	MG	CA	3468	1/1	0.94	0.54	80,80,80,80	0
58	MG	CA	3182	1/1	0.94	0.08	47,47,47,47	0
58	MG	CA	3354	1/1	0.94	0.15	46,46,46,46	0
58	MG	CA	3643	1/1	0.94	0.16	57,57,57,57	0
58	MG	BA	3137	1/1	0.94	0.10	73,73,73,73	0
58	MG	AA	3314	1/1	0.94	0.15	28,28,28,28	0
58	MG	AA	3281	1/1	0.94	0.32	60,60,60,60	0
58	MG	DA	1653	1/1	0.94	0.12	29,29,29,29	0
58	MG	CA	3283	1/1	0.94	0.18	49,49,49,49	0
58	MG	A0	101	1/1	0.94	0.05	43,43,43,43	0
58	MG	AA	3207	1/1	0.94	0.33	37,37,37,37	0
58	MG	DA	1652	1/1	0.94	0.14	58,58,58,58	0
58	MG	CA	3465	1/1	0.94	0.15	46,46,46,46	0
58	MG	CA	3517	1/1	0.94	0.15	77,77,77,77	0
58	MG	AA	3529	1/1	0.94	0.14	28,28,28,28	0
58	MG	AA	3515	1/1	0.94	0.18	18,18,18,18	0
58	MG	CA	3506	1/1	0.94	0.12	61,61,61,61	0
58	MG	AA	3536	1/1	0.94	0.13	15,15,15,15	0
58	MG	AA	3223	1/1	0.94	0.45	54,54,54,54	0
58	MG	DA	1674	1/1	0.94	0.19	72,72,72,72	0
58	MG	AA	3780	1/1	0.94	0.22	41,41,41,41	0
58	MG	AA	3550	1/1	0.94	0.07	52,52,52,52	0
58	MG	AA	3309	1/1	0.94	0.21	44,44,44,44	0
58	MG	AA	3693	1/1	0.94	0.20	60,60,60,60	0
58	MG	DA	1658	1/1	0.94	0.09	63,63,63,63	0
58	MG	AA	3667	1/1	0.94	0.24	29,29,29,29	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
58	MG	AA	3016	1/1	0.94	0.43	57,57,57,57	0
58	MG	AA	3311	1/1	0.94	0.12	34,34,34,34	0
58	MG	AA	3803	1/1	0.94	0.26	62,62,62,62	0
58	MG	CA	3217	1/1	0.94	0.30	66,66,66,66	0
58	MG	DA	1692	1/1	0.94	0.20	53,53,53,53	0
58	MG	CA	3009	1/1	0.94	0.57	67,67,67,67	0
58	MG	CA	3075	1/1	0.94	0.36	52,52,52,52	0
58	MG	AA	3213	1/1	0.94	0.48	50,50,50,50	1
58	MG	CA	3345	1/1	0.94	0.12	87,87,87,87	0
58	MG	CA	3049	1/1	0.94	0.39	78,78,78,78	0
58	MG	AA	3621	1/1	0.94	0.20	39,39,39,39	0
58	MG	AA	3478	1/1	0.94	0.15	40,40,40,40	0
58	MG	CA	3503	1/1	0.94	0.26	49,49,49,49	1
58	MG	CA	3375	1/1	0.94	0.36	74,74,74,74	0
58	MG	AA	3276	1/1	0.94	0.23	50,50,50,50	0
58	MG	AA	3367	1/1	0.94	0.21	50,50,50,50	0
58	MG	AA	3688	1/1	0.94	0.11	29,29,29,29	0
58	MG	DA	1745	1/1	0.94	0.12	69,69,69,69	0
58	MG	AA	3748	1/1	0.94	0.38	56,56,56,56	0
58	MG	AA	3259	1/1	0.94	0.33	20,20,20,20	0
58	MG	CA	3528	1/1	0.94	0.10	38,38,38,38	0
58	MG	CA	3218	1/1	0.94	0.19	50,50,50,50	0
58	MG	AA	3169	1/1	0.94	0.27	61,61,61,61	0
58	MG	AA	3520	1/1	0.94	0.17	23,23,23,23	0
58	MG	BA	3165	1/1	0.94	0.23	61,61,61,61	0
58	MG	CA	3405	1/1	0.94	0.14	53,53,53,53	0
58	MG	CA	3171	1/1	0.94	0.23	45,45,45,45	0
58	MG	CA	3328	1/1	0.94	0.27	52,52,52,52	0
58	MG	DA	1663	1/1	0.94	0.14	63,63,63,63	0
58	MG	CA	3521	1/1	0.94	0.27	77,77,77,77	0
58	MG	AA	3686	1/1	0.94	0.14	70,70,70,70	0
58	MG	AA	3554	1/1	0.94	0.22	40,40,40,40	0
58	MG	AA	3371	1/1	0.94	0.28	59,59,59,59	0
58	MG	AA	3793	1/1	0.94	0.12	60,60,60,60	0
58	MG	CA	3121	1/1	0.94	0.36	60,60,60,60	0
58	MG	AA	3383	1/1	0.94	0.07	34,34,34,34	0
58	MG	CA	3257	1/1	0.94	0.40	65,65,65,65	0
58	MG	AA	3171	1/1	0.94	0.34	53,53,53,53	0
58	MG	AA	3224	1/1	0.94	0.27	26,26,26,26	0
58	MG	AA	3630	1/1	0.94	0.12	58,58,58,58	0
58	MG	AA	3672	1/1	0.94	0.35	32,32,32,32	1
58	MG	C0	101	1/1	0.94	0.19	64,64,64,64	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
58	MG	AA	3555	1/1	0.94	0.08	49,49,49,49	0
58	MG	AA	3775	1/1	0.94	0.14	45,45,45,45	0
58	MG	DA	1666	1/1	0.94	0.38	47,47,47,47	0
58	MG	CA	3522	1/1	0.94	0.11	59,59,59,59	0
58	MG	CA	3037	1/1	0.94	0.12	57,57,57,57	0
58	MG	BA	3041	1/1	0.94	0.18	53,53,53,53	0
58	MG	DA	1722	1/1	0.94	0.22	58,58,58,58	0
58	MG	DA	1747	1/1	0.94	0.38	78,78,78,78	0
58	MG	AA	3098	1/1	0.94	0.28	24,24,24,24	0
58	MG	AA	3263	1/1	0.95	0.44	71,71,71,71	0
58	MG	AA	3479	1/1	0.95	0.28	53,53,53,53	0
58	MG	CA	3533	1/1	0.95	0.19	52,52,52,52	0
58	MG	AR	5001	1/1	0.95	0.19	32,32,32,32	0
58	MG	CA	3112	1/1	0.95	0.13	70,70,70,70	0
58	MG	AA	3164	1/1	0.95	0.41	37,37,37,37	0
58	MG	BA	3175	1/1	0.95	0.22	78,78,78,78	0
58	MG	AA	3592	1/1	0.95	0.09	63,63,63,63	0
58	MG	CA	3597	1/1	0.95	0.17	51,51,51,51	0
58	MG	CA	3366	1/1	0.95	0.12	47,47,47,47	0
62	GDP	DZ	704	28/28	0.95	0.14	80,80,80,80	0
58	MG	BA	3001	1/1	0.95	0.15	55,55,55,55	0
58	MG	AA	3250	1/1	0.95	0.26	62,62,62,62	0
58	MG	AA	3712	1/1	0.95	0.22	36,36,36,36	1
58	MG	CA	3011	1/1	0.95	0.11	46,46,46,46	0
58	MG	BA	3206	1/1	0.95	0.24	62,62,62,62	0
58	MG	DA	1625	1/1	0.95	0.09	42,42,42,42	0
58	MG	AA	3174	1/1	0.95	0.29	62,62,62,62	0
58	MG	CA	3164	1/1	0.95	0.25	38,38,38,38	0
58	MG	CA	3180	1/1	0.95	0.42	74,74,74,74	0
58	MG	AA	3385	1/1	0.95	0.16	28,28,28,28	0
58	MG	AA	3523	1/1	0.95	0.15	27,27,27,27	0
58	MG	AA	3578	1/1	0.95	0.09	34,34,34,34	0
58	MG	AA	3067	1/1	0.95	0.08	50,50,50,50	0
58	MG	AA	3556	1/1	0.95	0.13	37,37,37,37	0
58	MG	AA	3015	1/1	0.95	0.33	62,62,62,62	0
58	MG	CA	3144	1/1	0.95	0.57	56,56,56,56	0
58	MG	AD	305	1/1	0.95	0.24	56,56,56,56	0
58	MG	BA	3027	1/1	0.95	0.21	75,75,75,75	0
58	MG	AA	3154	1/1	0.95	0.33	56,56,56,56	0
58	MG	CA	3030	1/1	0.95	0.29	57,57,57,57	0
58	MG	BA	3141	1/1	0.95	0.19	49,49,49,49	0
58	MG	CA	3004	1/1	0.95	0.45	64,64,64,64	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
58	MG	CA	3622	1/1	0.95	0.30	51,51,51,51	0
58	MG	AA	3145	1/1	0.95	0.11	38,38,38,38	0
58	MG	AA	3624	1/1	0.95	0.22	70,70,70,70	0
58	MG	CA	3340	1/1	0.95	0.12	35,35,35,35	0
58	MG	AA	3595	1/1	0.95	0.22	42,42,42,42	0
58	MG	CA	3027	1/1	0.95	0.19	47,47,47,47	0
58	MG	BA	3120	1/1	0.95	0.28	78,78,78,78	0
58	MG	AA	3141	1/1	0.95	0.27	51,51,51,51	0
58	MG	AB	3003	1/1	0.95	0.26	50,50,50,50	0
58	MG	AD	308	1/1	0.95	0.39	44,44,44,44	0
58	MG	BA	3111	1/1	0.95	0.53	72,72,72,72	0
58	MG	AA	3474	1/1	0.95	0.22	50,50,50,50	0
58	MG	BA	3038	1/1	0.95	0.36	65,65,65,65	0
58	MG	CA	3110	1/1	0.95	0.19	51,51,51,51	0
58	MG	AA	3058	1/1	0.95	0.15	35,35,35,35	0
58	MG	CA	3330	1/1	0.95	0.15	29,29,29,29	0
58	MG	CB	3005	1/1	0.95	0.33	61,61,61,61	0
58	MG	AG	201	1/1	0.95	0.12	49,49,49,49	0
58	MG	AA	3111	1/1	0.95	0.34	79,79,79,79	0
58	MG	AA	3787	1/1	0.95	0.20	50,50,50,50	0
58	MG	AA	3822	1/1	0.95	0.17	19,19,19,19	0
58	MG	CA	3600	1/1	0.95	0.10	39,39,39,39	0
58	MG	AA	3447	1/1	0.95	0.08	75,75,75,75	0
58	MG	CA	3005	1/1	0.95	0.33	56,56,56,56	0
58	MG	AA	3076	1/1	0.95	0.12	8,8,8,8	0
58	MG	AA	3066	1/1	0.95	0.29	48,48,48,48	0
58	MG	CA	3150	1/1	0.95	0.14	63,63,63,63	0
58	MG	AA	3397	1/1	0.95	0.15	15,15,15,15	0
58	MG	AA	3676	1/1	0.95	0.22	64,64,64,64	0
58	MG	AA	3040	1/1	0.95	0.27	45,45,45,45	0
58	MG	AA	3518	1/1	0.95	0.12	19,19,19,19	0
58	MG	BA	3122	1/1	0.95	0.22	58,58,58,58	0
58	MG	DA	1731	1/1	0.95	0.11	82,82,82,82	0
58	MG	AA	3559	1/1	0.95	0.10	50,50,50,50	0
58	MG	CA	3563	1/1	0.95	0.09	92,92,92,92	0
58	MG	CA	3029	1/1	0.95	0.12	32,32,32,32	0
58	MG	AA	3194	1/1	0.95	0.22	60,60,60,60	0
58	MG	CA	3430	1/1	0.95	0.38	71,71,71,71	0
58	MG	AA	3482	1/1	0.95	0.10	64,64,64,64	0
58	MG	AA	3608	1/1	0.95	0.08	29,29,29,29	0
58	MG	AA	3799	1/1	0.95	0.21	48,48,48,48	0
58	MG	CA	3399	1/1	0.95	0.12	63,63,63,63	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
58	MG	BA	3147	1/1	0.95	0.08	84,84,84,84	0
58	MG	AA	3110	1/1	0.95	0.20	50,50,50,50	0
58	MG	AA	3475	1/1	0.95	0.12	60,60,60,60	0
58	MG	CA	3019	1/1	0.95	0.18	27,27,27,27	0
58	MG	CA	3364	1/1	0.95	0.17	65,65,65,65	0
58	MG	AA	3212	1/1	0.95	0.27	31,31,31,31	1
58	MG	DA	1715	1/1	0.95	0.21	49,49,49,49	0
58	MG	AA	3396	1/1	0.95	0.16	16,16,16,16	0
58	MG	AA	3189	1/1	0.95	0.17	11,11,11,11	0
58	MG	CA	3457	1/1	0.95	0.15	58,58,58,58	0
58	MG	AA	3660	1/1	0.95	0.23	68,68,68,68	0
58	MG	AA	3472	1/1	0.95	0.16	25,25,25,25	0
58	MG	AA	3569	1/1	0.95	0.15	15,15,15,15	0
58	MG	AA	3588	1/1	0.95	0.35	54,54,54,54	0
58	MG	AA	3342	1/1	0.95	0.15	4,4,4,4	0
58	MG	AA	3149	1/1	0.95	0.38	67,67,67,67	0
58	MG	AA	3284	1/1	0.95	0.31	43,43,43,43	0
58	MG	AF	305	1/1	0.95	0.19	55,55,55,55	0
58	MG	CA	3436	1/1	0.95	0.11	53,53,53,53	0
58	MG	AA	3068	1/1	0.95	0.36	53,53,53,53	0
58	MG	CA	3101	1/1	0.95	0.55	77,77,77,77	0
58	MG	CY	502	1/1	0.95	0.15	54,54,54,54	0
58	MG	CA	3085	1/1	0.95	0.28	62,62,62,62	0
58	MG	AA	3178	1/1	0.95	0.26	61,61,61,61	0
58	MG	BA	3197	1/1	0.95	0.11	75,75,75,75	0
58	MG	AA	3476	1/1	0.95	0.20	68,68,68,68	0
58	MG	AB	3009	1/1	0.95	0.16	55,55,55,55	0
58	MG	CA	3157	1/1	0.95	0.25	68,68,68,68	0
58	MG	CA	3487	1/1	0.95	0.27	68,68,68,68	0
58	MG	DA	1765	1/1	0.95	0.16	64,64,64,64	0
58	MG	AA	3425	1/1	0.95	0.16	49,49,49,49	0
58	MG	CA	3625	1/1	0.95	0.28	53,53,53,53	0
58	MG	CA	3352	1/1	0.95	0.14	46,46,46,46	0
58	MG	AA	3105	1/1	0.95	0.16	31,31,31,31	0
58	MG	CA	3381	1/1	0.95	0.18	68,68,68,68	0
58	MG	AA	3389	1/1	0.95	0.22	34,34,34,34	0
58	MG	AA	3809	1/1	0.95	0.35	60,60,60,60	0
58	MG	AA	3118	1/1	0.95	0.24	36,36,36,36	1
58	MG	BA	3130	1/1	0.95	0.15	49,49,49,49	0
58	MG	CU	3002	1/1	0.95	0.33	63,63,63,63	0
58	MG	CA	3133	1/1	0.95	0.20	29,29,29,29	0
58	MG	AA	3355	1/1	0.95	0.13	57,57,57,57	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
58	MG	AA	3527	1/1	0.95	0.12	21,21,21,21	0
58	MG	CA	3079	1/1	0.95	0.16	46,46,46,46	0
58	MG	AA	3408	1/1	0.95	0.15	44,44,44,44	0
58	MG	AA	3576	1/1	0.95	0.23	69,69,69,69	0
58	MG	AA	3751	1/1	0.95	0.12	26,26,26,26	0
58	MG	AA	3776	1/1	0.95	0.09	40,40,40,40	0
58	MG	DA	1616	1/1	0.95	0.38	51,51,51,51	0
58	MG	CA	3443	1/1	0.95	0.48	66,66,66,66	0
58	MG	AA	3720	1/1	0.95	0.14	59,59,59,59	0
58	MG	CA	3566	1/1	0.95	0.19	41,41,41,41	1
58	MG	AA	3308	1/1	0.95	0.14	28,28,28,28	0
58	MG	AA	3341	1/1	0.95	0.20	15,15,15,15	0
58	MG	AA	3424	1/1	0.95	0.18	17,17,17,17	0
58	MG	AA	3668	1/1	0.95	0.20	38,38,38,38	0
58	MG	CA	3427	1/1	0.95	0.23	53,53,53,53	0
58	MG	CA	3316	1/1	0.95	0.09	60,60,60,60	0
58	MG	CA	3087	1/1	0.95	0.33	35,35,35,35	0
58	MG	CA	3361	1/1	0.95	0.18	48,48,48,48	0
58	MG	AA	3254	1/1	0.95	0.21	35,35,35,35	0
58	MG	AA	3211	1/1	0.95	0.33	86,86,86,86	0
58	MG	BA	3087	1/1	0.95	0.41	70,70,70,70	0
58	MG	CA	3641	1/1	0.95	0.22	54,54,54,54	0
58	MG	CA	3401	1/1	0.95	0.29	60,60,60,60	0
58	MG	AA	3824	1/1	0.95	0.22	31,31,31,31	1
58	MG	BA	3189	1/1	0.95	0.18	66,66,66,66	0
58	MG	CR	201	1/1	0.95	0.32	51,51,51,51	0
58	MG	CA	3244	1/1	0.95	0.17	40,40,40,40	0
58	MG	CA	3314	1/1	0.95	0.24	50,50,50,50	0
58	MG	CA	3540	1/1	0.95	0.09	70,70,70,70	0
58	MG	CA	3123	1/1	0.95	0.22	66,66,66,66	0
58	MG	CA	3550	1/1	0.95	0.10	54,54,54,54	1
58	MG	CA	3601	1/1	0.95	0.09	73,73,73,73	0
58	MG	AA	3837	1/1	0.95	0.23	44,44,44,44	1
58	MG	AA	3445	1/1	0.95	0.18	59,59,59,59	0
58	MG	AA	3503	1/1	0.95	0.13	52,52,52,52	0
58	MG	AA	3581	1/1	0.95	0.13	27,27,27,27	0
58	MG	BA	3020	1/1	0.95	0.13	51,51,51,51	0
58	MG	AA	3081	1/1	0.95	0.19	56,56,56,56	0
58	MG	AA	3687	1/1	0.95	0.20	46,46,46,46	0
58	MG	AA	3400	1/1	0.95	0.21	33,33,33,33	0
58	MG	CA	3261	1/1	0.95	0.19	47,47,47,47	0
58	MG	BX	105	1/1	0.95	0.14	78,78,78,78	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
58	MG	CA	3041	1/1	0.95	0.28	31,31,31,31	0
58	MG	AA	3134	1/1	0.95	0.32	67,67,67,67	0
58	MG	AA	3005	1/1	0.95	0.17	61,61,61,61	0
58	MG	CA	3435	1/1	0.95	0.14	28,28,28,28	0
58	MG	CA	3632	1/1	0.95	0.15	54,54,54,54	0
58	MG	AA	3834	1/1	0.95	0.26	64,64,64,64	0
58	MG	AA	3501	1/1	0.95	0.12	48,48,48,48	0
58	MG	AA	3514	1/1	0.95	0.15	35,35,35,35	0
58	MG	AA	3785	1/1	0.95	0.15	70,70,70,70	0
58	MG	DA	1707	1/1	0.95	0.17	69,69,69,69	0
58	MG	AA	3295	1/1	0.95	0.28	46,46,46,46	0
58	MG	AA	3450	1/1	0.95	0.21	48,48,48,48	0
58	MG	AA	3513	1/1	0.95	0.28	58,58,58,58	0
58	MG	AA	3177	1/1	0.95	0.36	51,51,51,51	0
58	MG	AA	3768	1/1	0.95	0.35	96,96,96,96	0
58	MG	AA	3612	1/1	0.95	0.30	49,49,49,49	0
58	MG	CA	3525	1/1	0.95	0.30	40,40,40,40	0
58	MG	AA	3448	1/1	0.95	0.14	17,17,17,17	0
58	MG	BA	3040	1/1	0.95	0.27	48,48,48,48	0
58	MG	AA	3127	1/1	0.95	0.30	52,52,52,52	0
58	MG	CA	3268	1/1	0.95	0.18	69,69,69,69	0
58	MG	AA	3746	1/1	0.95	0.12	28,28,28,28	0
58	MG	AA	3329	1/1	0.96	0.17	17,17,17,17	0
58	MG	DA	1748	1/1	0.96	0.21	66,66,66,66	0
58	MG	CA	3120	1/1	0.96	0.15	127,127,127,127	0
58	MG	AA	3604	1/1	0.96	0.15	65,65,65,65	0
58	MG	DA	1756	1/1	0.96	0.20	68,68,68,68	0
58	MG	AQ	201	1/1	0.96	0.14	29,29,29,29	0
58	MG	AB	3015	1/1	0.96	0.17	38,38,38,38	0
58	MG	AB	3019	1/1	0.96	0.13	64,64,64,64	0
58	MG	CA	3640	1/1	0.96	0.25	57,57,57,57	0
58	MG	DF	3001	1/1	0.96	0.17	49,49,49,49	0
58	MG	CA	3658	1/1	0.96	0.41	50,50,50,50	0
58	MG	CA	3326	1/1	0.96	0.13	39,39,39,39	0
58	MG	CA	3021	1/1	0.96	0.15	27,27,27,27	0
58	MG	AA	3771	1/1	0.96	0.24	38,38,38,38	1
58	MG	DA	1649	1/1	0.96	0.21	60,60,60,60	0
58	MG	AA	3486	1/1	0.96	0.14	28,28,28,28	0
58	MG	CA	3253	1/1	0.96	0.13	56,56,56,56	0
58	MG	BA	3193	1/1	0.96	0.09	70,70,70,70	0
58	MG	AA	3322	1/1	0.96	0.09	33,33,33,33	0
58	MG	CA	3547	1/1	0.96	0.13	66,66,66,66	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
58	MG	AA	3363	1/1	0.96	0.31	28,28,28,28	0
58	MG	CA	3301	1/1	0.96	0.15	58,58,58,58	0
58	MG	AA	3128	1/1	0.96	0.34	71,71,71,71	0
58	MG	CA	3220	1/1	0.96	0.14	30,30,30,30	0
58	MG	CA	3492	1/1	0.96	0.22	52,52,52,52	0
58	MG	CA	3567	1/1	0.96	0.32	49,49,49,49	0
58	MG	CA	3578	1/1	0.96	0.15	38,38,38,38	0
58	MG	AA	3585	1/1	0.96	0.12	63,63,63,63	0
58	MG	AA	3358	1/1	0.96	0.12	61,61,61,61	0
58	MG	CA	3219	1/1	0.96	0.36	52,52,52,52	0
58	MG	CA	3346	1/1	0.96	0.12	40,40,40,40	0
58	MG	CA	3639	1/1	0.96	0.34	79,79,79,79	0
58	MG	AB	3022	1/1	0.96	0.06	56,56,56,56	0
58	MG	AA	3788	1/1	0.96	0.26	60,60,60,60	0
58	MG	CA	3267	1/1	0.96	0.13	39,39,39,39	0
58	MG	CA	3441	1/1	0.96	0.35	56,56,56,56	0
58	MG	AA	3457	1/1	0.96	0.23	65,65,65,65	0
60	ZN	C9	501	1/1	0.96	0.11	93,93,93,93	0
58	MG	AA	3009	1/1	0.96	0.13	23,23,23,23	0
58	MG	AA	3386	1/1	0.96	0.15	18,18,18,18	0
58	MG	CA	3614	1/1	0.96	0.60	89,89,89,89	0
58	MG	AA	3439	1/1	0.96	0.23	33,33,33,33	0
58	MG	AA	3123	1/1	0.96	0.20	53,53,53,53	0
58	MG	AA	3331	1/1	0.96	0.28	34,34,34,34	0
58	MG	DA	1721	1/1	0.96	0.18	65,65,65,65	0
58	MG	AA	3228	1/1	0.96	0.15	55,55,55,55	0
58	MG	DA	1696	1/1	0.96	0.28	64,64,64,64	0
58	MG	CA	3456	1/1	0.96	0.17	46,46,46,46	0
58	MG	AA	3233	1/1	0.96	0.24	51,51,51,51	0
58	MG	AA	3570	1/1	0.96	0.12	18,18,18,18	0
58	MG	AA	3782	1/1	0.96	0.31	72,72,72,72	0
58	MG	AA	3419	1/1	0.96	0.20	26,26,26,26	0
58	MG	AA	3227	1/1	0.96	0.21	31,31,31,31	0
58	MG	CA	3372	1/1	0.96	0.21	53,53,53,53	0
58	MG	AA	3023	1/1	0.96	0.24	37,37,37,37	0
58	MG	BA	3026	1/1	0.96	0.26	57,57,57,57	0
58	MG	AA	3033	1/1	0.96	0.31	34,34,34,34	0
58	MG	CA	3321	1/1	0.96	0.15	30,30,30,30	0
58	MG	CA	3605	1/1	0.96	0.17	63,63,63,63	0
58	MG	A7	101	1/1	0.96	0.07	44,44,44,44	0
58	MG	AU	201	1/1	0.96	0.34	44,44,44,44	0
62	GDP	BZ	801	28/28	0.96	0.15	52,52,52,52	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
58	MG	AA	3413	1/1	0.96	0.16	36,36,36,36	0
58	MG	AA	3599	1/1	0.96	0.13	52,52,52,52	0
58	MG	AA	3725	1/1	0.96	0.29	39,39,39,39	0
58	MG	CA	3270	1/1	0.96	0.24	66,66,66,66	0
58	MG	CA	3403	1/1	0.96	0.12	70,70,70,70	0
58	MG	AA	3051	1/1	0.96	0.29	34,34,34,34	0
58	MG	AA	3288	1/1	0.96	0.23	25,25,25,25	0
58	MG	CA	3022	1/1	0.96	0.10	35,35,35,35	0
58	MG	AA	3568	1/1	0.96	0.21	51,51,51,51	0
58	MG	DA	1697	1/1	0.96	0.38	65,65,65,65	0
58	MG	BA	3184	1/1	0.96	0.07	49,49,49,49	0
58	MG	CA	3615	1/1	0.96	0.28	65,65,65,65	0
58	MG	CA	3331	1/1	0.96	0.24	43,43,43,43	0
58	MG	AA	3305	1/1	0.96	0.26	53,53,53,53	0
58	MG	CA	3113	1/1	0.96	0.23	60,60,60,60	0
58	MG	CA	3333	1/1	0.96	0.21	41,41,41,41	0
58	MG	CA	3524	1/1	0.96	0.23	54,54,54,54	0
58	MG	AA	3008	1/1	0.96	0.26	18,18,18,18	0
58	MG	CA	3334	1/1	0.96	0.40	72,72,72,72	0
58	MG	AA	3390	1/1	0.96	0.18	47,47,47,47	0
58	MG	AA	3489	1/1	0.96	0.09	63,63,63,63	0
58	MG	AA	3644	1/1	0.96	0.11	49,49,49,49	0
58	MG	CA	3418	1/1	0.96	0.21	39,39,39,39	0
58	MG	A9	502	1/1	0.96	0.34	58,58,58,58	0
58	MG	AA	3812	1/1	0.96	0.31	57,57,57,57	0
58	MG	CA	3629	1/1	0.96	0.38	73,73,73,73	0
58	MG	AA	3468	1/1	0.96	0.24	51,51,51,51	0
58	MG	CA	3655	1/1	0.96	0.17	52,52,52,52	0
58	MG	AA	3747	1/1	0.96	0.20	62,62,62,62	0
58	MG	BA	3039	1/1	0.96	0.58	78,78,78,78	0
58	MG	CA	3276	1/1	0.96	0.11	51,51,51,51	0
58	MG	AB	3016	1/1	0.96	0.21	33,33,33,33	0
58	MG	AA	3719	1/1	0.96	0.13	41,41,41,41	0
58	MG	CA	3146	1/1	0.96	0.16	80,80,80,80	0
58	MG	CA	3589	1/1	0.96	0.09	35,35,35,35	0
58	MG	AE	303	1/1	0.96	0.14	40,40,40,40	0
58	MG	AA	3829	1/1	0.96	0.19	19,19,19,19	0
58	MG	AA	3290	1/1	0.96	0.27	63,63,63,63	0
58	MG	AA	3463	1/1	0.96	0.28	46,46,46,46	0
58	MG	CA	3202	1/1	0.96	0.27	58,58,58,58	0
58	MG	CA	3338	1/1	0.96	0.14	41,41,41,41	0
58	MG	DA	1681	1/1	0.96	0.19	46,46,46,46	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
58	MG	CA	3415	1/1	0.96	0.13	52,52,52,52	0
58	MG	AA	3772	1/1	0.96	0.18	22,22,22,22	1
58	MG	AA	3525	1/1	0.96	0.17	26,26,26,26	0
58	MG	AA	3583	1/1	0.96	0.30	64,64,64,64	0
58	MG	DA	1612	1/1	0.96	0.10	38,38,38,38	0
58	MG	AA	3669	1/1	0.96	0.12	34,34,34,34	0
58	MG	AA	3416	1/1	0.96	0.14	25,25,25,25	0
58	MG	CA	3475	1/1	0.96	0.30	75,75,75,75	0
58	MG	CA	3111	1/1	0.96	0.41	62,62,62,62	0
58	MG	DA	1743	1/1	0.96	0.13	60,60,60,60	0
58	MG	DA	1680	1/1	0.96	0.23	56,56,56,56	0
58	MG	AA	3245	1/1	0.96	0.29	28,28,28,28	1
58	MG	CA	3115	1/1	0.96	0.53	37,37,37,37	0
58	MG	BZ	800	1/1	0.96	0.17	44,44,44,44	0
58	MG	DA	1741	1/1	0.96	0.44	68,68,68,68	0
58	MG	AA	3643	1/1	0.96	0.22	47,47,47,47	0
58	MG	CB	3003	1/1	0.96	0.07	76,76,76,76	0
58	MG	AB	3002	1/1	0.96	0.15	58,58,58,58	0
58	MG	AA	3293	1/1	0.96	0.19	32,32,32,32	0
58	MG	CA	3236	1/1	0.96	0.22	52,52,52,52	0
58	MG	AA	3755	1/1	0.96	0.18	29,29,29,29	0
58	MG	AA	3427	1/1	0.96	0.10	34,34,34,34	0
58	MG	AB	3013	1/1	0.96	0.19	53,53,53,53	0
58	MG	CA	3454	1/1	0.96	0.20	38,38,38,38	0
58	MG	AA	3602	1/1	0.96	0.34	47,47,47,47	0
58	MG	BA	3076	1/1	0.96	0.17	42,42,42,42	0
58	MG	CA	3092	1/1	0.96	0.41	107,107,107,107	0
58	MG	AA	3731	1/1	0.96	0.28	31,31,31,31	0
58	MG	CA	3368	1/1	0.96	0.30	64,64,64,64	0
58	MG	AA	3300	1/1	0.96	0.12	51,51,51,51	0
58	MG	AA	3157	1/1	0.96	0.18	40,40,40,40	1
58	MG	AA	3790	1/1	0.96	0.11	48,48,48,48	0
58	MG	AA	3394	1/1	0.96	0.13	18,18,18,18	0
58	MG	AA	3221	1/1	0.96	0.24	55,55,55,55	0
58	MG	BA	3145	1/1	0.96	0.08	37,37,37,37	0
58	MG	AA	3773	1/1	0.96	0.33	36,36,36,36	0
58	MG	CA	3028	1/1	0.96	0.23	42,42,42,42	0
58	MG	CA	3172	1/1	0.96	0.30	53,53,53,53	0
58	MG	CA	3384	1/1	0.96	0.26	44,44,44,44	0
58	MG	AA	3426	1/1	0.96	0.14	33,33,33,33	0
58	MG	AA	3534	1/1	0.96	0.12	22,22,22,22	0
58	MG	AA	3487	1/1	0.96	0.14	39,39,39,39	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
58	MG	BA	3085	1/1	0.96	0.14	49,49,49,49	0
58	MG	AB	3012	1/1	0.96	0.20	30,30,30,30	1
58	MG	BA	3080	1/1	0.96	0.08	52,52,52,52	0
58	MG	AA	3332	1/1	0.96	0.16	44,44,44,44	0
58	MG	CA	3319	1/1	0.96	0.23	33,33,33,33	0
58	MG	DA	1708	1/1	0.96	0.32	68,68,68,68	0
58	MG	AV	201	1/1	0.96	0.27	37,37,37,37	0
58	MG	AA	3549	1/1	0.96	0.15	58,58,58,58	0
58	MG	CA	3661	1/1	0.96	0.20	60,60,60,60	0
58	MG	AA	3722	1/1	0.96	0.14	11,11,11,11	0
58	MG	AA	3405	1/1	0.96	0.09	54,54,54,54	0
58	MG	AA	3378	1/1	0.96	0.18	18,18,18,18	0
58	MG	AA	3557	1/1	0.96	0.13	39,39,39,39	0
58	MG	AA	3316	1/1	0.96	0.22	59,59,59,59	0
58	MG	AA	3697	1/1	0.96	0.23	69,69,69,69	0
58	MG	CA	3336	1/1	0.96	0.11	60,60,60,60	0
58	MG	AA	3340	1/1	0.96	0.15	58,58,58,58	0
58	MG	CA	3586	1/1	0.96	0.19	46,46,46,46	0
58	MG	AA	3623	1/1	0.96	0.12	43,43,43,43	0
58	MG	AA	3770	1/1	0.96	0.31	39,39,39,39	0
58	MG	AA	3484	1/1	0.96	0.22	35,35,35,35	0
58	MG	CA	3474	1/1	0.96	0.14	52,52,52,52	0
58	MG	DA	1614	1/1	0.96	0.24	70,70,70,70	0
58	MG	CF	304	1/1	0.96	0.16	54,54,54,54	0
58	MG	AB	3005	1/1	0.96	0.11	67,67,67,67	0
58	MG	AA	3265	1/1	0.96	0.13	60,60,60,60	0
58	MG	DA	1679	1/1	0.96	0.35	60,60,60,60	0
58	MG	CA	3051	1/1	0.96	0.51	64,64,64,64	0
58	MG	AA	3542	1/1	0.96	0.12	45,45,45,45	0
58	MG	AA	3500	1/1	0.96	0.19	55,55,55,55	0
58	MG	CA	3507	1/1	0.96	0.08	71,71,71,71	0
58	MG	AA	3346	1/1	0.96	0.17	45,45,45,45	0
58	MG	AA	3655	1/1	0.96	0.15	59,59,59,59	0
58	MG	CA	3360	1/1	0.96	0.22	43,43,43,43	0
58	MG	CA	3594	1/1	0.96	0.57	74,74,74,74	0
58	MG	AA	3298	1/1	0.96	0.08	57,57,57,57	0
58	MG	CA	3470	1/1	0.96	0.19	69,69,69,69	0
58	MG	CA	3016	1/1	0.96	0.45	79,79,79,79	0
58	MG	AA	3664	1/1	0.96	0.17	55,55,55,55	0
58	MG	AA	3558	1/1	0.97	0.22	18,18,18,18	0
58	MG	AA	3168	1/1	0.97	0.13	64,64,64,64	0
58	MG	AA	3296	1/1	0.97	0.14	18,18,18,18	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
58	MG	AA	3494	1/1	0.97	0.19	33,33,33,33	1
58	MG	CA	3382	1/1	0.97	0.15	37,37,37,37	0
58	MG	AA	3617	1/1	0.97	0.09	30,30,30,30	0
58	MG	CA	3426	1/1	0.97	0.14	51,51,51,51	0
58	MG	AA	3366	1/1	0.97	0.14	52,52,52,52	0
58	MG	CA	3554	1/1	0.97	0.08	67,67,67,67	0
58	MG	AA	3011	1/1	0.97	0.22	39,39,39,39	0
58	MG	AA	3575	1/1	0.97	0.15	30,30,30,30	0
58	MG	CA	3358	1/1	0.97	0.11	78,78,78,78	0
58	MG	AA	3632	1/1	0.97	0.21	45,45,45,45	0
58	MG	AA	3120	1/1	0.97	0.18	43,43,43,43	0
58	MG	AD	302	1/1	0.97	0.33	18,18,18,18	0
58	MG	AA	3140	1/1	0.97	0.09	56,56,56,56	0
58	MG	AA	3528	1/1	0.97	0.13	25,25,25,25	0
58	MG	AA	3446	1/1	0.97	0.10	59,59,59,59	0
58	MG	AA	3820	1/1	0.97	0.26	44,44,44,44	0
58	MG	CA	3446	1/1	0.97	0.31	39,39,39,39	0
58	MG	CA	3568	1/1	0.97	0.08	40,40,40,40	0
58	MG	AA	3301	1/1	0.97	0.25	22,22,22,22	0
58	MG	AA	3433	1/1	0.97	0.18	18,18,18,18	0
58	MG	AA	3155	1/1	0.97	0.20	48,48,48,48	0
58	MG	AA	3312	1/1	0.97	0.19	52,52,52,52	0
58	MG	AA	3497	1/1	0.97	0.12	51,51,51,51	0
58	MG	CA	3307	1/1	0.97	0.16	39,39,39,39	0
58	MG	AA	3779	1/1	0.97	0.11	61,61,61,61	0
58	MG	AA	3328	1/1	0.97	0.16	17,17,17,17	0
58	MG	AA	3734	1/1	0.97	0.33	65,65,65,65	0
58	MG	AA	3467	1/1	0.97	0.07	44,44,44,44	0
58	MG	AA	3636	1/1	0.97	0.13	24,24,24,24	0
58	MG	AA	3684	1/1	0.97	0.10	28,28,28,28	0
58	MG	CA	3631	1/1	0.97	0.23	66,66,66,66	0
58	MG	AA	3646	1/1	0.97	0.10	57,57,57,57	0
58	MG	CA	3388	1/1	0.97	0.53	68,68,68,68	0
58	MG	CA	3416	1/1	0.97	0.22	34,34,34,34	0
58	MG	AA	3131	1/1	0.97	0.25	36,36,36,36	0
58	MG	AA	3318	1/1	0.97	0.32	53,53,53,53	0
58	MG	AA	3551	1/1	0.97	0.16	46,46,46,46	0
58	MG	DA	1636	1/1	0.97	0.46	64,64,64,64	0
58	MG	BA	3086	1/1	0.97	0.25	51,51,51,51	0
58	MG	AA	3603	1/1	0.97	0.17	35,35,35,35	0
58	MG	AA	3368	1/1	0.97	0.22	39,39,39,39	0
58	MG	AA	3678	1/1	0.97	0.19	32,32,32,32	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
58	MG	CB	3011	1/1	0.97	0.32	51,51,51,51	0
58	MG	AA	3607	1/1	0.97	0.34	59,59,59,59	0
58	MG	DA	1694	1/1	0.97	0.23	65,65,65,65	0
58	MG	AA	3496	1/1	0.97	0.12	58,58,58,58	0
58	MG	CA	3561	1/1	0.97	0.15	55,55,55,55	1
58	MG	CA	3497	1/1	0.97	0.14	63,63,63,63	0
58	MG	BA	3024	1/1	0.97	0.43	63,63,63,63	0
58	MG	AA	3800	1/1	0.97	0.13	30,30,30,30	0
58	MG	AA	3072	1/1	0.97	0.64	40,40,40,40	0
58	MG	AA	3814	1/1	0.97	0.21	43,43,43,43	0
58	MG	AA	3507	1/1	0.97	0.28	31,31,31,31	0
58	MG	CA	3288	1/1	0.97	0.22	63,63,63,63	0
58	MG	AA	3654	1/1	0.97	0.30	65,65,65,65	0
58	MG	AQ	202	1/1	0.97	0.33	40,40,40,40	0
58	MG	AA	3216	1/1	0.97	0.12	36,36,36,36	0
58	MG	AA	3065	1/1	0.97	0.24	28,28,28,28	0
58	MG	AA	3376	1/1	0.97	0.18	18,18,18,18	0
58	MG	AA	3357	1/1	0.97	0.19	27,27,27,27	0
58	MG	AA	3673	1/1	0.97	0.13	66,66,66,66	0
58	MG	CA	3303	1/1	0.97	0.28	45,45,45,45	0
58	MG	CA	3621	1/1	0.97	0.51	65,65,65,65	0
58	MG	AA	3182	1/1	0.97	0.09	23,23,23,23	1
58	MG	CA	3409	1/1	0.97	0.19	61,61,61,61	0
58	MG	AA	3180	1/1	0.97	0.33	72,72,72,72	0
58	MG	CA	3504	1/1	0.97	0.19	69,69,69,69	0
58	MG	AA	3103	1/1	0.97	0.24	48,48,48,48	0
58	MG	BA	3150	1/1	0.97	0.16	47,47,47,47	0
58	MG	AA	3429	1/1	0.97	0.18	42,42,42,42	0
58	MG	CA	3558	1/1	0.97	0.10	47,47,47,47	0
58	MG	CA	3383	1/1	0.97	0.16	40,40,40,40	0
58	MG	CA	3167	1/1	0.97	0.35	43,43,43,43	0
58	MG	AA	3398	1/1	0.97	0.07	17,17,17,17	0
58	MG	AA	3220	1/1	0.97	0.11	34,34,34,34	0
58	MG	CA	3449	1/1	0.97	0.21	42,42,42,42	0
58	MG	BA	3123	1/1	0.97	0.26	54,54,54,54	0
58	MG	AA	3699	1/1	0.97	0.22	38,38,38,38	1
58	MG	CA	3423	1/1	0.97	0.19	54,54,54,54	0
58	MG	AA	3352	1/1	0.97	0.12	51,51,51,51	0
58	MG	AA	3418	1/1	0.97	0.17	30,30,30,30	0
58	MG	CA	3653	1/1	0.97	0.20	25,25,25,25	0
58	MG	AA	3530	1/1	0.97	0.15	15,15,15,15	0
58	MG	AA	3393	1/1	0.97	0.15	26,26,26,26	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
58	MG	AA	3143	1/1	0.97	0.17	28,28,28,28	0
58	MG	CA	3564	1/1	0.97	0.14	75,75,75,75	0
58	MG	AA	3236	1/1	0.97	0.31	37,37,37,37	1
58	MG	CA	3213	1/1	0.97	0.11	68,68,68,68	0
58	MG	AA	3199	1/1	0.97	0.10	55,55,55,55	0
58	MG	CA	3519	1/1	0.97	0.21	62,62,62,62	0
58	MG	AN	3003	1/1	0.97	0.10	45,45,45,45	0
58	MG	CA	3367	1/1	0.97	0.37	59,59,59,59	0
58	MG	AA	3499	1/1	0.97	0.12	35,35,35,35	0
58	MG	CA	3040	1/1	0.97	0.19	64,64,64,64	0
58	MG	CA	3660	1/1	0.97	0.17	38,38,38,38	0
58	MG	CA	3440	1/1	0.97	0.20	39,39,39,39	0
58	MG	CA	3161	1/1	0.97	0.13	40,40,40,40	0
58	MG	AA	3047	1/1	0.97	0.27	31,31,31,31	0
58	MG	AA	3085	1/1	0.97	0.15	30,30,30,30	0
58	MG	AA	3315	1/1	0.97	0.16	34,34,34,34	0
61	SF4	DD	501	8/8	0.97	0.10	90,90,90,90	0
58	MG	CA	3662	1/1	0.97	0.18	48,48,48,48	0
58	MG	AA	3146	1/1	0.97	0.14	34,34,34,34	0
58	MG	BA	3134	1/1	0.97	0.26	62,62,62,62	0
58	MG	AA	3152	1/1	0.97	0.23	49,49,49,49	0
58	MG	AA	3432	1/1	0.97	0.28	28,28,28,28	0
58	MG	BA	3064	1/1	0.97	0.07	78,78,78,78	0
58	MG	AA	3511	1/1	0.97	0.34	56,56,56,56	0
58	MG	AA	3343	1/1	0.97	0.14	65,65,65,65	0
58	MG	AA	3430	1/1	0.97	0.08	25,25,25,25	0
58	MG	AA	3628	1/1	0.97	0.13	53,53,53,53	0
58	MG	AA	3338	1/1	0.97	0.12	29,29,29,29	0
58	MG	BA	3153	1/1	0.97	0.14	48,48,48,48	0
58	MG	CA	3373	1/1	0.97	0.18	42,42,42,42	0
58	MG	AA	3506	1/1	0.97	0.17	32,32,32,32	0
58	MG	AA	3374	1/1	0.97	0.09	17,17,17,17	0
58	MG	DA	1750	1/1	0.97	0.20	71,71,71,71	0
58	MG	CA	3398	1/1	0.97	0.10	58,58,58,58	0
58	MG	CA	3208	1/1	0.97	0.28	69,69,69,69	0
58	MG	AA	3384	1/1	0.97	0.12	28,28,28,28	0
58	MG	AA	3532	1/1	0.97	0.15	60,60,60,60	0
58	MG	AA	3053	1/1	0.97	0.16	13,13,13,13	0
58	MG	AA	3465	1/1	0.97	0.15	40,40,40,40	0
58	MG	CA	3417	1/1	0.97	0.15	48,48,48,48	0
58	MG	CA	3335	1/1	0.97	0.20	43,43,43,43	0
58	MG	BX	110	1/1	0.97	0.16	57,57,57,57	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
58	MG	AA	3395	1/1	0.97	0.18	22,22,22,22	0
58	MG	AA	3438	1/1	0.97	0.13	19,19,19,19	0
58	MG	AA	3104	1/1	0.97	0.13	13,13,13,13	0
58	MG	CA	3162	1/1	0.97	0.35	63,63,63,63	0
58	MG	BA	3212	1/1	0.97	0.11	73,73,73,73	0
58	MG	AA	3661	1/1	0.97	0.33	43,43,43,43	0
58	MG	BA	3127	1/1	0.97	0.20	50,50,50,50	0
58	MG	AA	3409	1/1	0.97	0.18	30,30,30,30	0
58	MG	AA	3135	1/1	0.97	0.45	62,62,62,62	0
58	MG	AA	3075	1/1	0.97	0.31	13,13,13,13	0
58	MG	AA	3522	1/1	0.97	0.13	30,30,30,30	0
58	MG	AA	3214	1/1	0.97	0.39	39,39,39,39	1
58	MG	CA	3277	1/1	0.97	0.20	42,42,42,42	0
58	MG	AA	3327	1/1	0.97	0.16	13,13,13,13	0
58	MG	BA	3183	1/1	0.97	0.17	60,60,60,60	0
58	MG	AA	3739	1/1	0.97	0.24	74,74,74,74	0
58	MG	CA	3434	1/1	0.97	0.11	68,68,68,68	0
58	MG	BA	3118	1/1	0.97	0.15	43,43,43,43	0
58	MG	CA	3263	1/1	0.97	0.21	29,29,29,29	0
58	MG	AA	3230	1/1	0.97	0.24	49,49,49,49	0
58	MG	AA	3286	1/1	0.97	0.12	53,53,53,53	0
58	MG	CA	3462	1/1	0.97	0.25	43,43,43,43	0
58	MG	CA	3411	1/1	0.97	0.20	31,31,31,31	0
58	MG	AA	3050	1/1	0.97	0.23	53,53,53,53	0
58	MG	AF	302	1/1	0.97	0.16	40,40,40,40	0
58	MG	BA	3207	1/1	0.97	0.22	66,66,66,66	0
58	MG	DA	1647	1/1	0.97	0.09	49,49,49,49	0
58	MG	BA	3172	1/1	0.97	0.23	55,55,55,55	0
58	MG	AA	3777	1/1	0.97	0.14	20,20,20,20	0
58	MG	AA	3136	1/1	0.97	0.34	66,66,66,66	0
58	MG	BA	3180	1/1	0.97	0.07	41,41,41,41	0
58	MG	CA	3272	1/1	0.97	0.12	34,34,34,34	0
58	MG	CA	3306	1/1	0.97	0.19	61,61,61,61	0
58	MG	AB	3007	1/1	0.97	0.19	45,45,45,45	0
58	MG	AA	3022	1/1	0.97	0.11	9,9,9,9	0
58	MG	AX	101	1/1	0.97	0.16	30,30,30,30	1
58	MG	CA	3327	1/1	0.97	0.13	33,33,33,33	0
58	MG	CA	3421	1/1	0.97	0.26	69,69,69,69	0
58	MG	CA	3460	1/1	0.97	0.18	49,49,49,49	0
58	MG	CA	3630	1/1	0.97	0.23	61,61,61,61	0
58	MG	AA	3723	1/1	0.97	0.14	19,19,19,19	0
58	MG	AA	3750	1/1	0.98	0.11	14,14,14,14	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
58	MG	CA	3065	1/1	0.98	0.12	41,41,41,41	0
58	MG	AA	3031	1/1	0.98	0.23	22,22,22,22	1
58	MG	AA	3150	1/1	0.98	0.27	62,62,62,62	0
58	MG	AA	3659	1/1	0.98	0.20	14,14,14,14	0
58	MG	CA	3310	1/1	0.98	0.20	29,29,29,29	0
58	MG	CA	3518	1/1	0.98	0.08	61,61,61,61	0
58	MG	AA	3392	1/1	0.98	0.15	21,21,21,21	0
58	MG	CA	3007	1/1	0.98	0.11	27,27,27,27	0
58	MG	AA	3038	1/1	0.98	0.16	10,10,10,10	0
58	MG	CA	3442	1/1	0.98	0.26	75,75,75,75	0
58	MG	A0	104	1/1	0.98	0.13	36,36,36,36	0
58	MG	CA	3097	1/1	0.98	0.24	65,65,65,65	0
58	MG	AA	3175	1/1	0.98	0.34	60,60,60,60	0
58	MG	AA	3552	1/1	0.98	0.28	51,51,51,51	0
58	MG	DA	1727	1/1	0.98	0.09	57,57,57,57	0
58	MG	DA	1712	1/1	0.98	0.14	51,51,51,51	0
58	MG	BA	3171	1/1	0.98	0.16	61,61,61,61	0
60	ZN	C6	501	1/1	0.98	0.07	60,60,60,60	0
58	MG	AA	3403	1/1	0.98	0.17	18,18,18,18	0
58	MG	AA	3219	1/1	0.98	0.10	4,4,4,4	0
58	MG	AA	3380	1/1	0.98	0.14	15,15,15,15	0
58	MG	CO	202	1/1	0.98	0.22	52,52,52,52	0
58	MG	BA	3178	1/1	0.98	0.26	63,63,63,63	0
58	MG	CA	3618	1/1	0.98	0.19	37,37,37,37	0
58	MG	AA	3524	1/1	0.98	0.23	29,29,29,29	0
58	MG	AA	3077	1/1	0.98	0.34	92,92,92,92	0
58	MG	CA	3369	1/1	0.98	0.16	58,58,58,58	0
58	MG	AA	3420	1/1	0.98	0.18	12,12,12,12	0
58	MG	BA	3095	1/1	0.98	0.16	99,99,99,99	0
58	MG	AA	3600	1/1	0.98	0.38	57,57,57,57	0
58	MG	CA	3265	1/1	0.98	0.13	55,55,55,55	0
58	MG	AA	3370	1/1	0.98	0.20	57,57,57,57	0
58	MG	CV	201	1/1	0.98	0.21	69,69,69,69	0
58	MG	AA	3823	1/1	0.98	0.25	43,43,43,43	0
58	MG	A5	101	1/1	0.98	0.34	40,40,40,40	0
58	MG	AB	3011	1/1	0.98	0.13	31,31,31,31	0
58	MG	AA	3255	1/1	0.98	0.21	40,40,40,40	0
58	MG	CA	3165	1/1	0.98	0.31	41,41,41,41	0
58	MG	DA	1667	1/1	0.98	0.35	61,61,61,61	0
58	MG	CA	3093	1/1	0.98	0.16	68,68,68,68	0
58	MG	AP	201	1/1	0.98	0.20	31,31,31,31	0
58	MG	AA	3692	1/1	0.98	0.17	51,51,51,51	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
58	MG	AA	3320	1/1	0.98	0.24	23,23,23,23	0
58	MG	BA	3142	1/1	0.98	0.08	47,47,47,47	0
58	MG	AA	3521	1/1	0.98	0.13	37,37,37,37	0
58	MG	AA	3594	1/1	0.98	0.11	27,27,27,27	0
58	MG	AA	3406	1/1	0.98	0.17	50,50,50,50	0
58	MG	AA	3707	1/1	0.98	0.24	31,31,31,31	1
58	MG	CE	301	1/1	0.98	0.34	64,64,64,64	0
58	MG	CA	3425	1/1	0.98	0.15	54,54,54,54	0
58	MG	CA	3170	1/1	0.98	0.24	32,32,32,32	0
58	MG	AA	3504	1/1	0.98	0.14	62,62,62,62	0
58	MG	AA	3101	1/1	0.98	0.43	51,51,51,51	0
58	MG	AA	3326	1/1	0.98	0.12	59,59,59,59	0
58	MG	AA	3565	1/1	0.98	0.24	17,17,17,17	0
58	MG	CA	3350	1/1	0.98	0.20	39,39,39,39	0
58	MG	AA	3464	1/1	0.98	0.10	59,59,59,59	0
58	MG	AD	304	1/1	0.98	0.24	41,41,41,41	0
58	MG	CA	3365	1/1	0.98	0.29	29,29,29,29	0
58	MG	AA	3516	1/1	0.98	0.17	20,20,20,20	0
58	MG	AA	3797	1/1	0.98	0.22	39,39,39,39	0
58	MG	CA	3581	1/1	0.98	0.12	51,51,51,51	0
58	MG	AA	3417	1/1	0.98	0.24	42,42,42,42	0
58	MG	AA	3337	1/1	0.98	0.22	10,10,10,10	0
58	MG	CA	3304	1/1	0.98	0.26	53,53,53,53	0
58	MG	AA	3037	1/1	0.98	0.26	44,44,44,44	0
58	MG	CA	3341	1/1	0.98	0.13	48,48,48,48	0
58	MG	AU	203	1/1	0.98	0.21	34,34,34,34	1
58	MG	AA	3485	1/1	0.98	0.19	15,15,15,15	0
58	MG	AA	3810	1/1	0.98	0.27	62,62,62,62	0
58	MG	AA	3537	1/1	0.98	0.11	35,35,35,35	0
58	MG	AA	3831	1/1	0.98	0.20	51,51,51,51	0
58	MG	AA	3256	1/1	0.98	0.19	54,54,54,54	0
58	MG	DZ	703	1/1	0.98	0.22	56,56,56,56	0
58	MG	AA	3726	1/1	0.98	0.20	37,37,37,37	0
58	MG	CA	3453	1/1	0.98	0.32	59,59,59,59	0
58	MG	AA	3459	1/1	0.98	0.20	18,18,18,18	0
58	MG	AA	3571	1/1	0.98	0.17	14,14,14,14	0
58	MG	CA	3230	1/1	0.98	0.22	50,50,50,50	0
58	MG	AA	3434	1/1	0.98	0.18	22,22,22,22	0
58	MG	AA	3054	1/1	0.98	0.10	38,38,38,38	0
61	SF4	BD	501	8/8	0.98	0.06	79,79,79,79	0
58	MG	AA	3074	1/1	0.98	0.23	59,59,59,59	0
58	MG	CA	3325	1/1	0.98	0.32	39,39,39,39	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
58	MG	AA	3151	1/1	0.98	0.23	14,14,14,14	0
58	MG	AA	3356	1/1	0.98	0.23	33,33,33,33	0
58	MG	CA	3560	1/1	0.98	0.21	56,56,56,56	0
58	MG	BA	3114	1/1	0.98	0.32	55,55,55,55	0
58	MG	AA	3545	1/1	0.98	0.15	15,15,15,15	0
58	MG	CA	3023	1/1	0.98	0.17	45,45,45,45	0
58	MG	AA	3512	1/1	0.98	0.22	11,11,11,11	0
58	MG	CA	3419	1/1	0.98	0.24	40,40,40,40	0
58	MG	AA	3388	1/1	0.98	0.20	17,17,17,17	0
58	MG	CA	3642	1/1	0.98	0.32	53,53,53,53	0
58	MG	AA	3517	1/1	0.98	0.16	18,18,18,18	0
58	MG	AA	3032	1/1	0.98	0.15	37,37,37,37	0
58	MG	AA	3260	1/1	0.98	0.19	23,23,23,23	0
58	MG	AA	3526	1/1	0.98	0.25	38,38,38,38	0
58	MG	CA	3312	1/1	0.98	0.15	49,49,49,49	0
58	MG	CA	3291	1/1	0.98	0.32	40,40,40,40	0
58	MG	AA	3114	1/1	0.98	0.23	62,62,62,62	0
58	MG	AA	3666	1/1	0.98	0.16	62,62,62,62	0
58	MG	AA	3735	1/1	0.98	0.18	21,21,21,21	0
58	MG	CA	3353	1/1	0.98	0.11	66,66,66,66	0
58	MG	AA	3541	1/1	0.98	0.19	29,29,29,29	0
58	MG	AA	3084	1/1	0.98	0.23	41,41,41,41	0
60	ZN	C5	101	1/1	0.98	0.10	66,66,66,66	0
58	MG	AA	3540	1/1	0.98	0.09	29,29,29,29	0
58	MG	C3	101	1/1	0.98	0.22	69,69,69,69	0
58	MG	AA	3642	1/1	0.98	0.18	41,41,41,41	0
58	MG	AA	3351	1/1	0.98	0.16	29,29,29,29	0
58	MG	CA	3610	1/1	0.98	0.32	98,98,98,98	0
58	MG	AA	3706	1/1	0.98	0.28	29,29,29,29	1
58	MG	AA	3561	1/1	0.98	0.23	56,56,56,56	0
58	MG	AA	3377	1/1	0.98	0.15	20,20,20,20	0
58	MG	CA	3480	1/1	0.98	0.20	44,44,44,44	0
58	MG	AA	3369	1/1	0.98	0.22	27,27,27,27	0
58	MG	CA	3104	1/1	0.98	0.39	60,60,60,60	0
58	MG	AA	3826	1/1	0.98	0.29	66,66,66,66	0
58	MG	AA	3339	1/1	0.98	0.19	41,41,41,41	0
58	MG	AA	3702	1/1	0.98	0.31	46,46,46,46	1
58	MG	AA	3533	1/1	0.98	0.15	24,24,24,24	0
58	MG	AA	3694	1/1	0.99	0.15	47,47,47,47	0
58	MG	AA	3471	1/1	0.99	0.19	34,34,34,34	0
58	MG	AA	3738	1/1	0.99	0.16	28,28,28,28	0
58	MG	CA	3447	1/1	0.99	0.17	62,62,62,62	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
58	MG	AA	3724	1/1	0.99	0.17	22,22,22,22	0
58	MG	AA	3412	1/1	0.99	0.16	20,20,20,20	0
58	MG	AA	3648	1/1	0.99	0.17	38,38,38,38	0
58	MG	CA	3256	1/1	0.99	0.24	40,40,40,40	0
58	MG	AA	3287	1/1	0.99	0.36	46,46,46,46	0
58	MG	AA	3469	1/1	0.99	0.07	42,42,42,42	0
58	MG	CA	3371	1/1	0.99	0.20	46,46,46,46	0
58	MG	CA	3298	1/1	0.99	0.42	42,42,42,42	0
58	MG	AA	3348	1/1	0.99	0.23	31,31,31,31	0
58	MG	AA	3835	1/1	0.99	0.20	39,39,39,39	0
58	MG	AA	3830	1/1	0.99	0.14	40,40,40,40	0
58	MG	CE	302	1/1	0.99	0.15	46,46,46,46	0
58	MG	CA	3176	1/1	0.99	0.15	41,41,41,41	0
58	MG	AA	3361	1/1	0.99	0.23	28,28,28,28	0
58	MG	AA	3313	1/1	0.99	0.19	33,33,33,33	0
58	MG	AA	3763	1/1	0.99	0.32	62,62,62,62	0
58	MG	AA	3003	1/1	0.99	0.08	19,19,19,19	0
58	MG	AA	3307	1/1	0.99	0.23	6,6,6,6	0
58	MG	AA	3508	1/1	0.99	0.21	13,13,13,13	0
58	MG	AA	3791	1/1	0.99	0.27	15,15,15,15	0
58	MG	AA	3299	1/1	0.99	0.12	21,21,21,21	0
58	MG	AA	3708	1/1	0.99	0.21	32,32,32,32	1
58	MG	AA	3454	1/1	0.99	0.13	49,49,49,49	0
58	MG	AE	302	1/1	0.99	0.14	17,17,17,17	0
58	MG	CA	3562	1/1	0.99	0.15	36,36,36,36	0
58	MG	CA	3323	1/1	0.99	0.24	45,45,45,45	0
60	ZN	A9	501	1/1	0.99	0.10	41,41,41,41	0
58	MG	AA	3631	1/1	0.99	0.23	68,68,68,68	0
58	MG	AA	3208	1/1	0.99	0.30	26,26,26,26	1
58	MG	AA	3732	1/1	0.99	0.25	41,41,41,41	0
58	MG	AA	3535	1/1	0.99	0.17	27,27,27,27	0
60	ZN	CY	501	1/1	0.99	0.05	92,92,92,92	0
58	MG	AA	3710	1/1	0.99	0.23	32,32,32,32	1
58	MG	DA	1610	1/1	0.99	0.22	45,45,45,45	0
58	MG	BE	3001	1/1	0.99	0.04	59,59,59,59	0
58	MG	AA	3217	1/1	0.99	0.15	46,46,46,46	0
58	MG	DA	1678	1/1	0.99	0.26	57,57,57,57	0
60	ZN	A5	102	1/1	0.99	0.10	36,36,36,36	0
60	ZN	AY	501	1/1	0.99	0.06	63,63,63,63	0
58	MG	AN	3002	1/1	1.00	0.10	26,26,26,26	0
60	ZN	A6	103	1/1	1.00	0.10	46,46,46,46	0

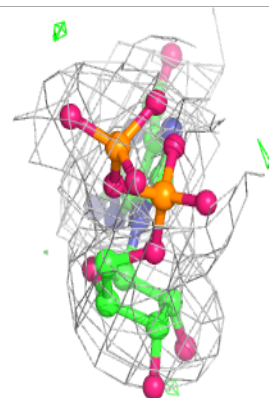
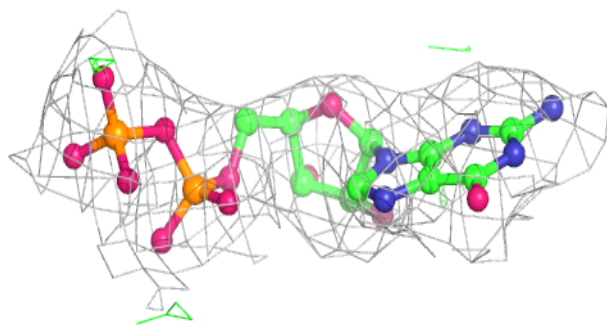
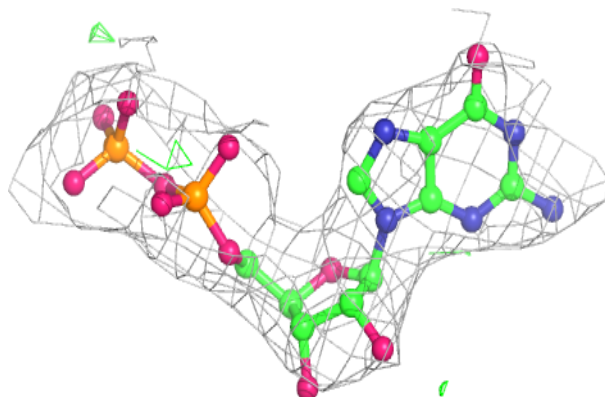
The following is a graphical depiction of the model fit to experimental electron density of all



instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

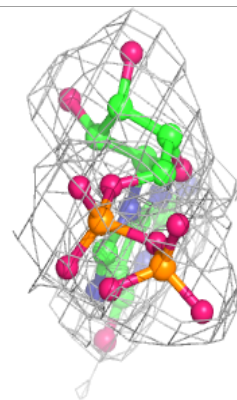
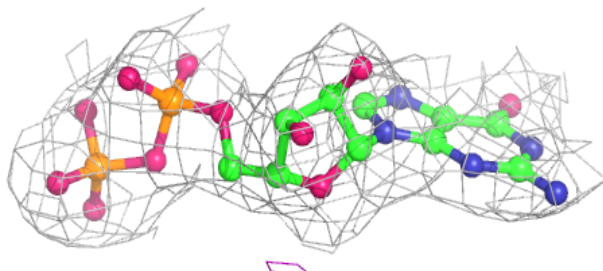
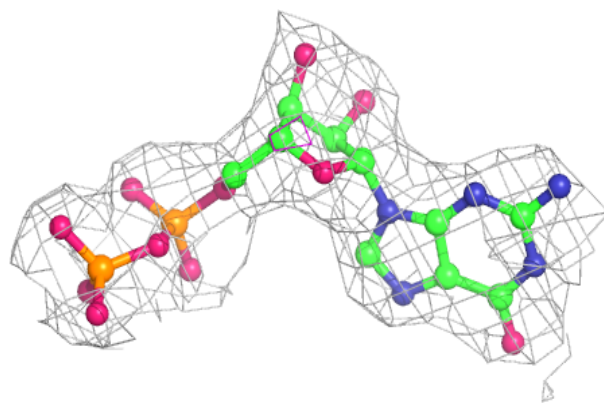
**Electron density around GDP DZ 704:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around GDP BZ 801:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



## 6.5 Other polymers [i](#)

There are no such residues in this entry.