



wwPDB X-ray Structure Validation Summary Report ⓘ

Dec 15, 2024 – 04:41 PM EST

PDB ID : 4WQF
Title : Crystal structure of the *Thermus thermophilus* 70S ribosome in complex with elongation factor G and fusidic acid in the post-translocational state
Authors : Lin, J.; Gagnon, M.G.; Steitz, T.A.
Deposited on : 2014-10-21
Resolution : 2.80 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.21
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.004 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.40

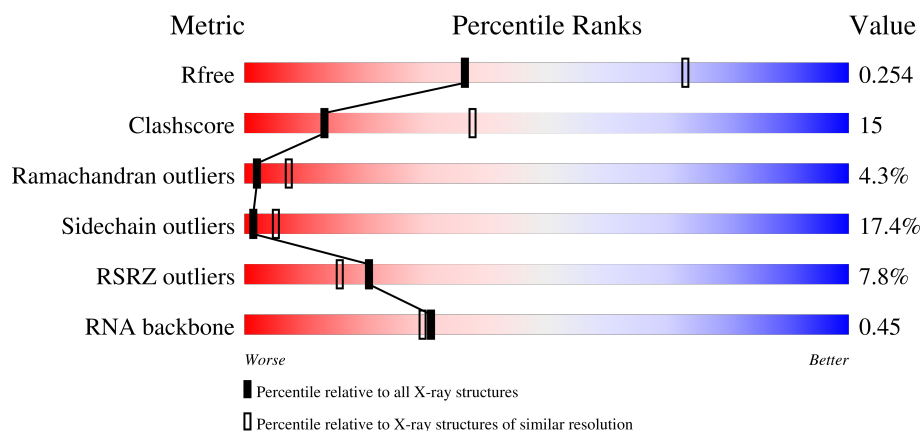
1 Overall quality at a glance

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}	164625	3657 (2.80-2.80)
Clashscore	180529	4123 (2.80-2.80)
Ramachandran outliers	177936	4071 (2.80-2.80)
Sidechain outliers	177891	4073 (2.80-2.80)
RSRZ outliers	164620	3659 (2.80-2.80)
RNA backbone	3690	1037 (3.00-2.60)

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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 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>3%</div> <div>19%</div> <div>49%</div> <div>25%</div> <div>5%</div> </div>
1	CA	2915	<div> <div>3%</div> <div>32%</div> <div>44%</div> <div>19%</div> <div>• •</div> </div>
2	AB	121	<div> <div>%</div> <div>25%</div> <div>46%</div> <div>24%</div> <div>• •</div> </div>
2	CB	121	<div> <div>2%</div> <div>44%</div> <div>41%</div> <div>13%</div> <div>• •</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	18	
55	DV	18	
56	BW	76	
56	BY	76	
56	DW	76	
56	DY	76	
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	3094	-	-	-	X
58	MG	CA	3180	-	-	-	X
60	SF4	DD	501	-	-	X	-
62	GDP	DZ	704	-	-	X	-

2 Entry composition

There are 63 unique types of molecules in this entry. The entry contains 310279 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	7	Total	C	N	O	P	0	0	0
			148	67	27	47	7			
55	DV	6	Total	C	N	O	P	0	0	0
			123	57	22	39	5			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
56	BW	76	Total	C	N	O	P	S	0	0
			1631	731	290	532	76	2		
56	BY	74	Total	C	N	O	P	S	0	0
			1581	707	285	515	73	1		
56	DW	76	Total	C	N	O	P	S	0	0
			1631	731	290	532	76	2		
56	DY	73	Total	C	N	O	P	S	0	0
			1561	698	283	507	72	1		

- 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
			5690	3616	980	1075	19			
57	DZ	730	Total	C	N	O	S	0	0	0
			5690	3616	980	1075	19			

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
58	AA	815	Total Mg 815 815	0	0
58	AB	23	Total Mg 23 23	0	0
58	AD	12	Total Mg 12 12	0	0
58	AE	5	Total Mg 5 5	0	0
58	AF	8	Total Mg 8 8	0	0
58	AG	2	Total Mg 2 2	0	0
58	AH	2	Total Mg 2 2	0	0
58	AN	3	Total Mg 3 3	0	0
58	AO	1	Total Mg 1 1	0	0
58	AP	3	Total Mg 3 3	0	0
58	AQ	3	Total Mg 3 3	0	0
58	AR	2	Total Mg 2 2	0	0
58	AU	4	Total Mg 4 4	0	0
58	AV	6	Total Mg 6 6	0	0
58	AW	4	Total Mg 4 4	0	0
58	AX	1	Total Mg 1 1	0	0
58	AY	1	Total Mg 1 1	0	0
58	AZ	2	Total Mg 2 2	0	0
58	A0	3	Total Mg 3 3	0	0
58	A2	2	Total Mg 2 2	0	0
58	A4	1	Total Mg 1 1	0	0
58	A5	4	Total Mg 4 4	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
58	A6	1	Total 1	Mg 1	0	0
58	A7	6	Total 6	Mg 6	0	0
58	A8	2	Total 2	Mg 2	0	0
58	A9	1	Total 1	Mg 1	0	0
58	BA	213	Total 213	Mg 213	0	0
58	BB	1	Total 1	Mg 1	0	0
58	BD	1	Total 1	Mg 1	0	0
58	BE	1	Total 1	Mg 1	0	0
58	BF	1	Total 1	Mg 1	0	0
58	BK	1	Total 1	Mg 1	0	0
58	BL	2	Total 2	Mg 2	0	0
58	BM	2	Total 2	Mg 2	0	0
58	BN	1	Total 1	Mg 1	0	0
58	BT	1	Total 1	Mg 1	0	0
58	BV	1	Total 1	Mg 1	0	0
58	BW	3	Total 3	Mg 3	0	0
58	BZ	2	Total 2	Mg 2	0	0
58	CA	664	Total 664	Mg 664	0	0
58	CB	13	Total 13	Mg 13	0	0
58	CD	3	Total 3	Mg 3	0	0
58	CE	6	Total 6	Mg 6	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
58	CF	5	Total 5	Mg 5	0	0
58	CG	1	Total 1	Mg 1	0	0
58	CN	1	Total 1	Mg 1	0	0
58	CO	2	Total 2	Mg 2	0	0
58	CP	3	Total 3	Mg 3	0	0
58	CQ	5	Total 5	Mg 5	0	0
58	CR	1	Total 1	Mg 1	0	0
58	CU	1	Total 1	Mg 1	0	0
58	CV	2	Total 2	Mg 2	0	0
58	CW	1	Total 1	Mg 1	0	0
58	CY	1	Total 1	Mg 1	0	0
58	C3	1	Total 1	Mg 1	0	0
58	C5	1	Total 1	Mg 1	0	0
58	C7	1	Total 1	Mg 1	0	0
58	C8	1	Total 1	Mg 1	0	0
58	DA	168	Total 168	Mg 168	0	0
58	DD	1	Total 1	Mg 1	0	0
58	DE	2	Total 2	Mg 2	0	0
58	DF	1	Total 1	Mg 1	0	0
58	DJ	1	Total 1	Mg 1	0	0
58	DK	1	Total 1	Mg 1	0	0

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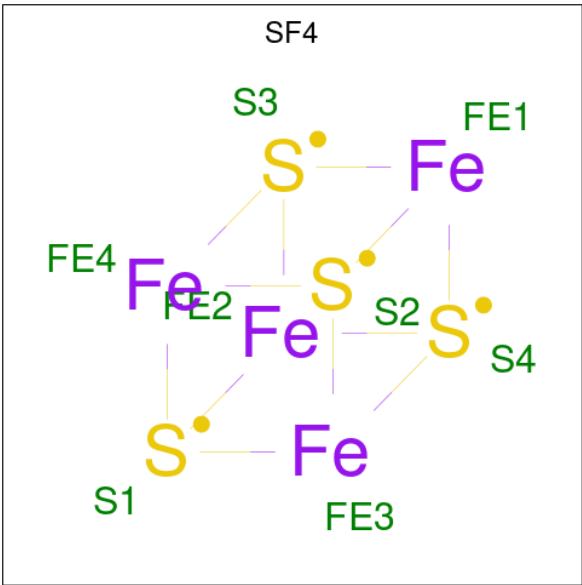
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
58	DT	1	Total 1	Mg 1	0	0
58	DW	3	Total 3	Mg 3	0	0
58	DZ	2	Total 2	Mg 2	0	0

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

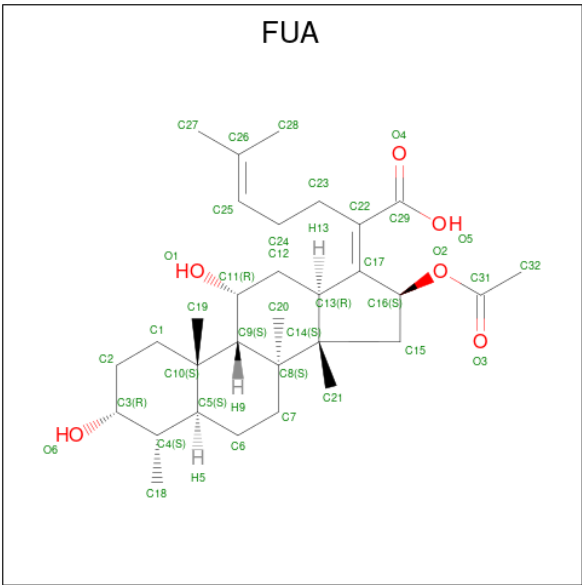
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
59	AY	1	Total 1	Zn 1	0	0
59	A4	1	Total 1	Zn 1	0	0
59	A5	1	Total 1	Zn 1	0	0
59	A6	1	Total 1	Zn 1	0	0
59	A9	1	Total 1	Zn 1	0	0
59	BN	1	Total 1	Zn 1	0	0
59	CY	1	Total 1	Zn 1	0	0
59	C4	1	Total 1	Zn 1	0	0
59	C5	1	Total 1	Zn 1	0	0
59	C6	1	Total 1	Zn 1	0	0
59	C9	1	Total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

- Molecule 60 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe₄S₄).



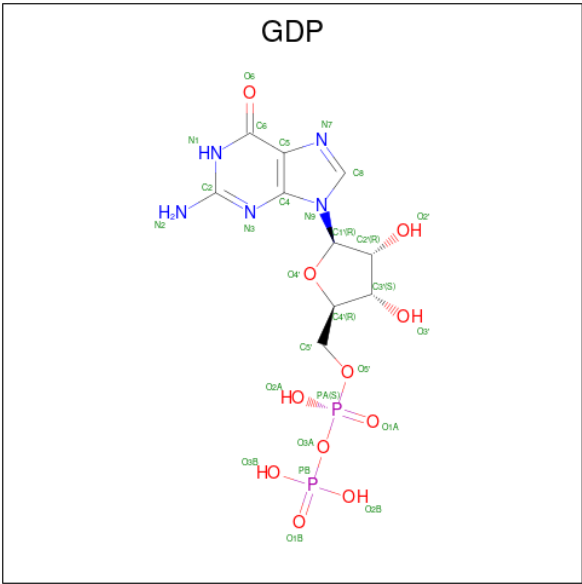
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
60	BD	1	Total	Fe	S	0	0
			8	4	4		
60	DD	1	Total	Fe	S	0	0
			8	4	4		

- Molecule 61 is FUSIDIC ACID (three-letter code: FUA) (formula: C₃₁H₄₈O₆).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
61	BZ	1	Total	C	O	0	0
			37	31	6		
61	DZ	1	Total	C	O	0	0
			37	31	6		

- Molecule 62 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula: C₁₀H₁₅N₅O₁₁P₂).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
62	BZ	1	Total	C	N	O	P	0	0
			28	10	5	11	2		
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	1408	Total	O	0	0
			1408	1408		
63	AB	36	Total	O	0	0
			36	36		
63	AD	15	Total	O	0	0
			15	15		
63	AE	19	Total	O	0	0
			19	19		
63	AF	8	Total	O	0	0
			8	8		
63	AG	3	Total	O	0	0
			3	3		
63	AH	1	Total	O	0	0
			1	1		
63	AN	2	Total	O	0	0
			2	2		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
63	AO	3	Total 3	O 3	0	0
63	AP	15	Total 15	O 15	0	0
63	AQ	3	Total 3	O 3	0	0
63	AR	3	Total 3	O 3	0	0
63	AS	1	Total 1	O 1	0	0
63	AT	2	Total 2	O 2	0	0
63	AU	6	Total 6	O 6	0	0
63	AW	1	Total 1	O 1	0	0
63	AX	2	Total 2	O 2	0	0
63	AZ	1	Total 1	O 1	0	0
63	A0	7	Total 7	O 7	0	0
63	A1	3	Total 3	O 3	0	0
63	A3	1	Total 1	O 1	0	0
63	A5	2	Total 2	O 2	0	0
63	A6	1	Total 1	O 1	0	0
63	A7	3	Total 3	O 3	0	0
63	A8	11	Total 11	O 11	0	0
63	BA	205	Total 205	O 205	0	0
63	BD	3	Total 3	O 3	0	0
63	BE	3	Total 3	O 3	0	0
63	BJ	1	Total 1	O 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
63	BL	2	Total	O	0	0
			2	2		
63	BM	1	Total	O	0	0
			1	1		
63	BO	1	Total	O	0	0
			1	1		
63	BV	2	Total	O	0	0
			2	2		
63	BW	1	Total	O	0	0
			1	1		
63	BZ	3	Total	O	0	0
			3	3		
63	CA	981	Total	O	0	0
			981	981		
63	CB	9	Total	O	0	0
			9	9		
63	CD	15	Total	O	0	0
			15	15		
63	CE	9	Total	O	0	0
			9	9		
63	CF	6	Total	O	0	0
			6	6		
63	CP	13	Total	O	0	0
			13	13		
63	CQ	1	Total	O	0	0
			1	1		
63	CT	3	Total	O	0	0
			3	3		
63	CU	4	Total	O	0	0
			4	4		
63	CV	1	Total	O	0	0
			1	1		
63	CW	1	Total	O	0	0
			1	1		
63	CX	1	Total	O	0	0
			1	1		
63	CY	1	Total	O	0	0
			1	1		
63	C0	5	Total	O	0	0
			5	5		
63	C1	3	Total	O	0	0
			3	3		

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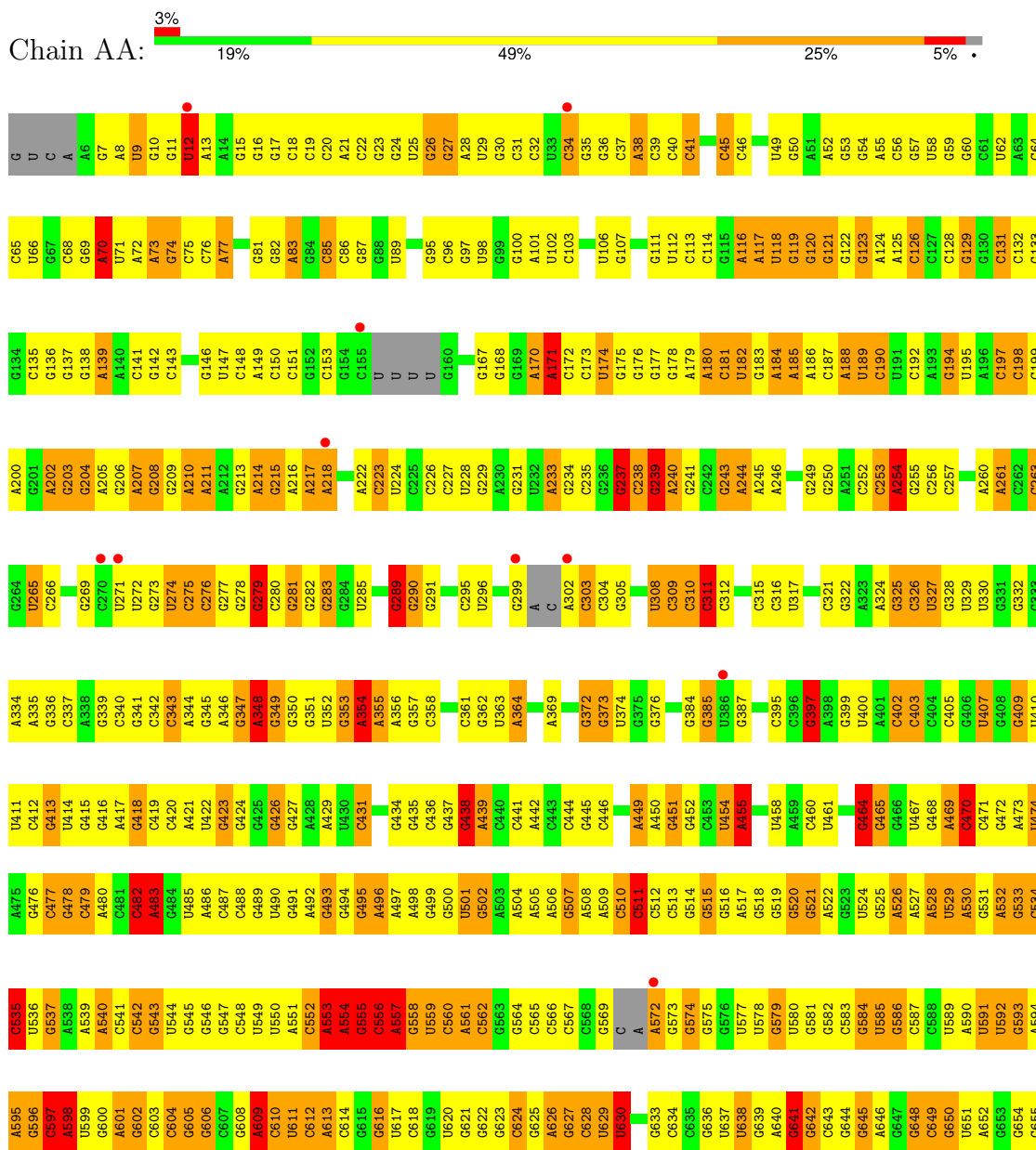
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
63	C3	1	Total 1	O 1	0	0
63	C5	1	Total 1	O 1	0	0
63	C7	3	Total 3	O 3	0	0
63	C8	3	Total 3	O 3	0	0
63	DA	153	Total 153	O 153	0	0
63	DE	2	Total 2	O 2	0	0
63	DH	1	Total 1	O 1	0	0
63	DJ	1	Total 1	O 1	0	0
63	DK	2	Total 2	O 2	0	0
63	DL	1	Total 1	O 1	0	0
63	DP	1	Total 1	O 1	0	0
63	DT	1	Total 1	O 1	0	0
63	DY	1	Total 1	O 1	0	0
63	DZ	2	Total 2	O 2	0	0

3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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.

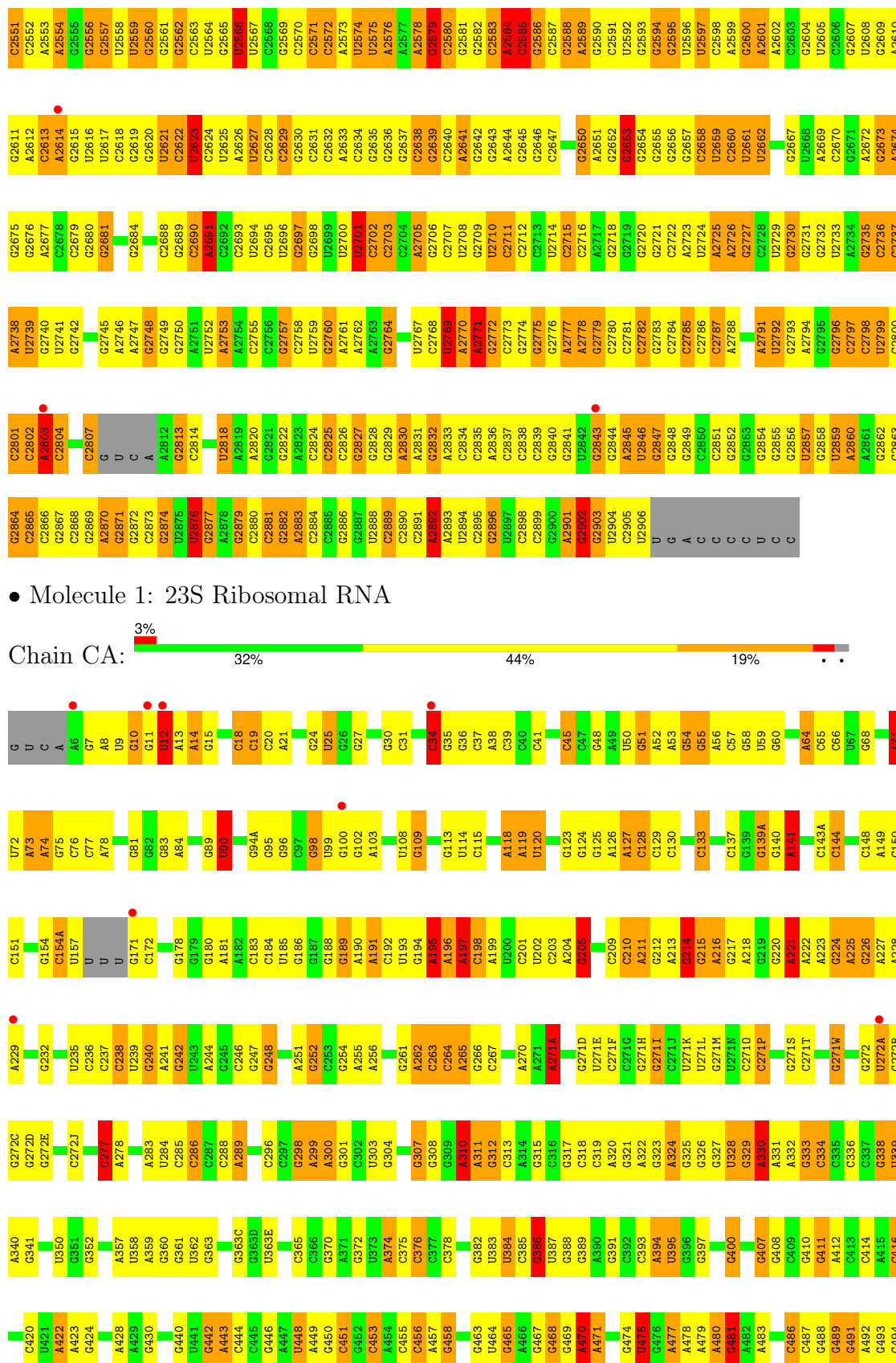
• Molecule 1: 23S Ribosomal RNA





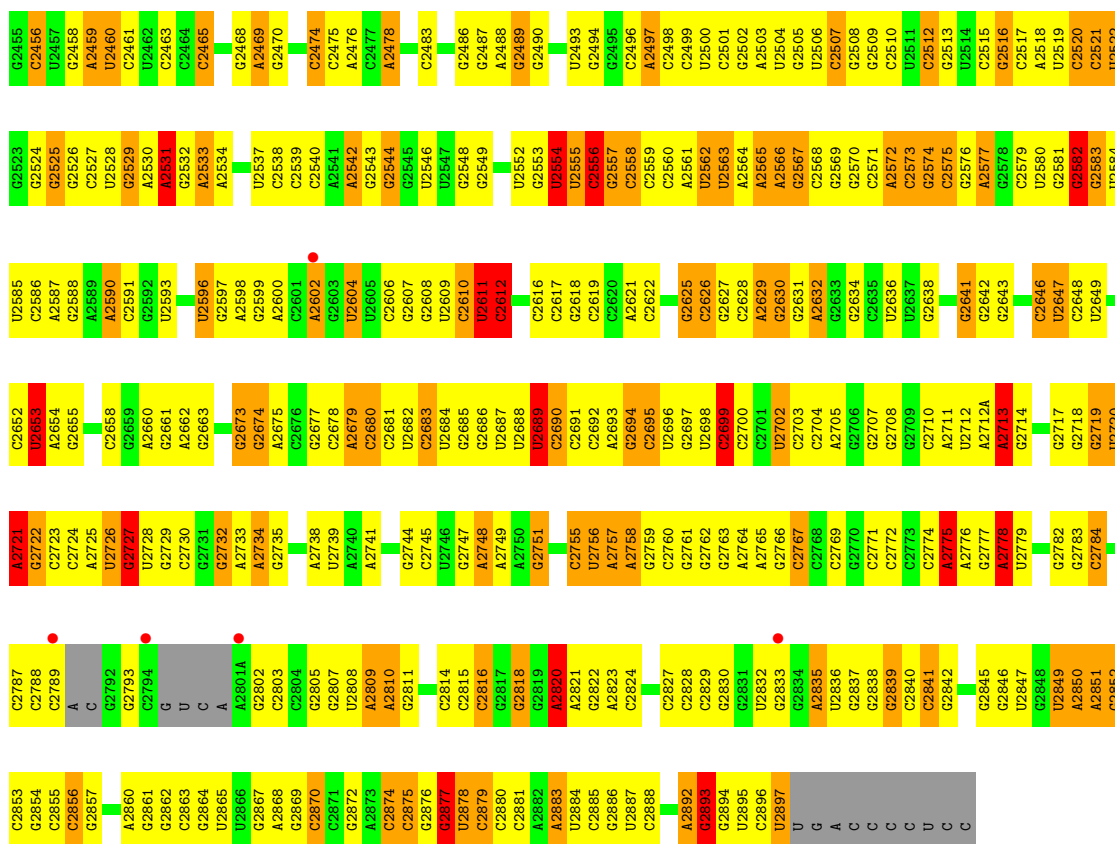
WORLDWIDE
PDB
PROTEIN DATA BANK

G2491	U2431	G2370	C2307	U2245	G2181	U2120	G2060	A1999	C1936	G1866	U1806	U1735	G1670	A1609
G2492	C2432	C2371	U2308	G2246	G2182	U2121	C2061	A2000	U1937	G1867	G1807	A1736	C1671	G1610
G2493	G2433	A2372	C2309	G2247	G2183	G2122	C2062	C2001	A1938	G1870	U1808	A1737	G1672	C1611
G2494	A2340	A2373	A2310	G2248	G2184	G2123	C2063	G2002	U1939	G1871	U1809	C1738	G1673	C1612
G2495	U2435	G2374	G2312	G2249	G2185	G2124	A2064	C2003	A1940	U1872	A1810	U1739	G1674	A1613
G2496	C2346	C2375	G2311	G2250	G2186	G2125	C2065	A2004	A1941	U1873	A1811	U1740	A1614	G1614
G2497	A2337	C2376	G2315	G2251	G2187	G2126	C2066	C2005	C1942	C1874	C1812	C1741	G1675	G1615
G2498	A2438	G2377	G2316	C2252	G2188	G2127	C2067	G2006	G1943	C1875	C1813	G1742	A1678	A1616
G2499	U2349	A2378	G2317	G2253	G2189	C2129	G2068	G2007	G1876	G1877	A1814	G1743	A1679	A1617
A2500	G2440	C2380	C2318	U2256	A2191	G2130	U2069	A2008	A1878	A1878	A1815	A1744	G1680	A1618
G2501	G2441	G2381	G2319	U2257	A2192	U2131	G2070	G2009	G1877	G1877	A1816	A1745	A1681	A1619
G2502	A2442	A2382	G2320	G2258	U2193	G2132	G2071	C2010	A1879	A1879	A1817	G1746	G1682	G1620
U2503	U2443	G2383	G2321	G2259	U2194	C2133	C2072	C2011	A1949	A1949	A1818	A1747	C1683	C1621
U2504	A2444	G2384	A2321	G2260	A2195	G2134	A2073	C2012	A1950	G1881	C1819	A1748	A1684	C1622
U2505	A2445	G2385	G2322	U2261	C2196	U2135	G2074	U2013	A1951	U1882	A1820	G1749	U1685	U1623
G2506	A2446	G2386	U2324	G2262	C2197	A2136	G2075	G2014	G1952	U1883	A1821	G1752	U1686	C1624
G2507	A2447	C2387	C2325	G2263	A2198	G2137	A2076	U2015	G1953	A1884	A1822	U1753	G1687	U1625
G2508	G2448	G2388	C2326	G2264	C2199	G2138	C2077	C2016	A1895	A1895	G1823	C1754	A1626	A1626
A2509	U2449	A2389	G2327	G2265	C2200	U2140	G2078	U2017	A1954	A1954	A1824	G1755	G1689	A1627
U2510	U2450	A2390	C2328	G2266	G2201	U2141	A2079	C2018	G1955	G1955	U1825	C1756	G1690	G1628
C2511	A2451	A2391	C2329	G2267	U2202	A2142	A2080	G2019	A1958	A1958	C1826	U1756	C1691	C1629
U2512	C2452	G2392	G2330	G2268	G2203	G2143	A2081	G2020	A1959	A1959	U1827	C1757	G1692	A1630
C2513	C2453	C2393	G2331	U2269	G2204	G2144	A2082	C2021	A1960	A1960	C1828	G1758	C1693	C1631
G2514	G2454	C2394	A2332	G2270	G2205	U2145	A2083	G2022	U1961	G1891	U1829	G1764	G1694	A1632
A2515	C2455	G2395	G2333	G2271	C2206	G2146	A2084	A2023	U1962	G1892	G1830	U1765	C1695	A1633
U2516	G2456	G2396	A2334	C2272	C2207	G2147	C2085	G2024	C1963	G1893	C1831	G1766	G1696	C1634
U2517	G2457	G2397	G2335	C2273	G2208	A2148	C2086	G2025	C1964	U1894	G1832	U1767	G1697	C1635
U2518	C2458	C2398	C2336	U2274	C2209	G2149	C2087	G2026	U1965	U1965	A1833	U1768	G1698	U1636
C2519	A2459	G2399	G2337	C2275	G2210	G2150	C2088	A2027	U1966	G1896	A1834	G1769	A1699	G1637
G2520	U2460	U2399	C2338	G2276	U2211	C2151	C2089	G2028	G1967	C1897	C1835	A1770	G1700	C1638
G2521	U2461	A2400	A2339	U2277	G2212	U2152	U2090	C2029	U1968	A1898	U1836	G1771	A1701	G1639
C2522	A2462	G2401	G2340	A2278	G2213	U2153	G2091	C2030	A1969	A1899	C1837	C1772	A1702	G1640
U2523	A2463	U2402	G2341	A2279	G2214	G2154	G2092	U2033	G1970	G1970	G1838	C1773	G1703	G1641
C2524	C2464	G2403	G2342	A2280	G2215	U2155	A2094	G2034	G1971	C1901	U1839	C1774	C1704	A1642
G2525	A2465	A2404	G2343	A2281	G2216	C2156	C2095	A2035	U1973	G1908	A1841	G1776	C1705	G1643
U2526	G2466	A2405	G2344	G2282	C2217	A2157	U2096	A2036	U1974	C1909	G1842	G1777	U1706	C1645
C2527	G2467	C2406	A2345	G2283	C2218	C2158	U2097	A2037	A1975	G1910	A1843	G1778	G1708	G1646
G2528	C2468	C2407	G2346	U2284	U2219	G2159	U2098	U2038	G1976	G1911	G1844	C1782	C1709	G1647
C2529	U2469	G2408	A2347	A2285	A2220	C2160	A2099	U2039	U1977	A1911	G1845	C1783	C1710	A1648
A2530	G2470	G2409	A2348	A2286	A2221	C2161	C2107	G2040	U1978	A1912	A1846	G1784	C1711	A1649
U2531	A2471	U2410	G2349	G2287	C2222	G2162	U2100	G2041	C1979	G1913	G1847	C1785	A1712	C1650
C2532	G2472	G2411	G2350	G2288	C2223	G2163	U2101	A2041	C1980	C1914	G1848	A1786	G1713	G1651
C2533	C2473	G2412	G2351	G2289	C2224	G2164	G2102	A2042	G1981	G1919	U1849	G1787	G1714	G1652
U2534	U2474	U2413	G2352	A2290	U2225	C2165	C2103	C2043	A1982	U1920	A1850	U1788	A1715	G1653
G2535	C2475	C2414	G2353	G2291	C2226	U2166	A2104	U2044	C1983	U1921	U1851	G1789	A1716	A1654
G2536	C2476	C2415	C2354	G2292	G2227	C2167	C2105	G2045	C1984	G1922	A1852	A1790	A1655	A1655
G2537	G2477	G2416	G2355	C2293	G2228	C2168	G2107	C2046	U1985	A1923	G1853	A1791	C1656	C1657
G2538	A2478	U2417	U2356	G2294	A2229	G2169	U2108	C2047	G1986	A1924	G1854	C1792	C1719	G1658
C2539	C2479	U2418	G2357	G2295	U2230	G2170	G2109	G2048	C1987	C1924	G1855	A1793	U1720	G1659
U2540	G2480	G2419	A2358	C2296	G2231	G2171	G2110	U2050	A1988	G1925	A1856	G1794	G1721	A1660
G2541	A2481	G2422	C2359	C2297	G2235	U2172	U2111	G2051	G1989	G1926	G1857	G1795	C1722	C1662
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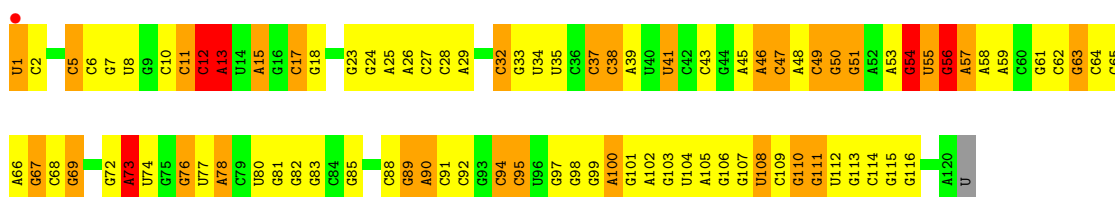




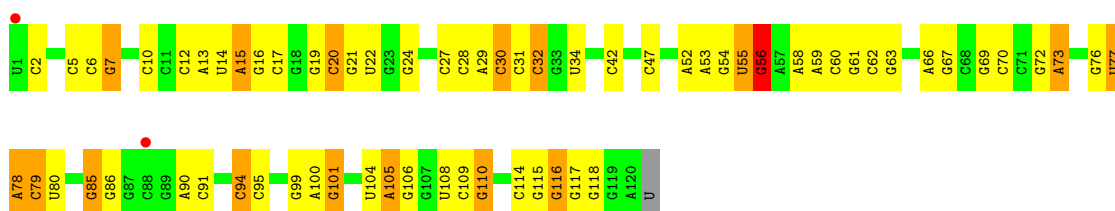
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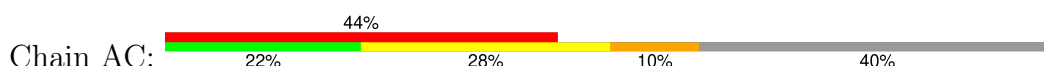
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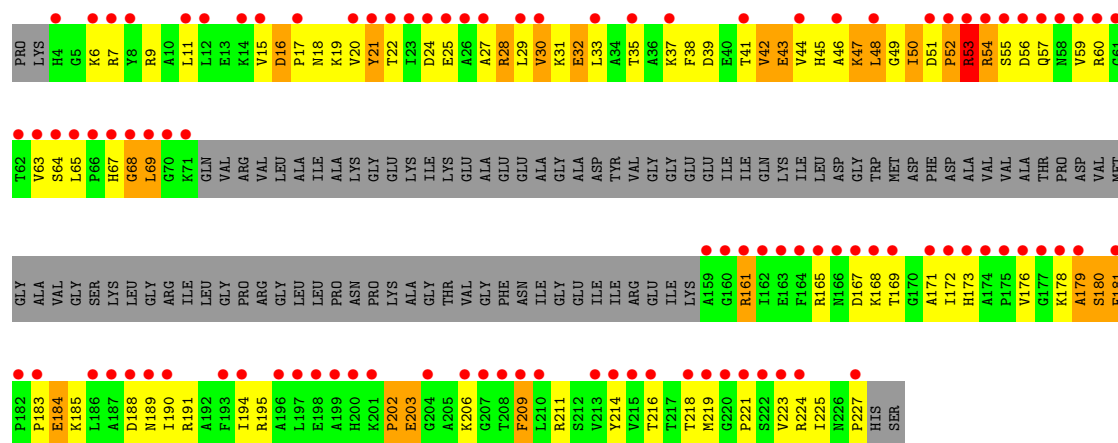


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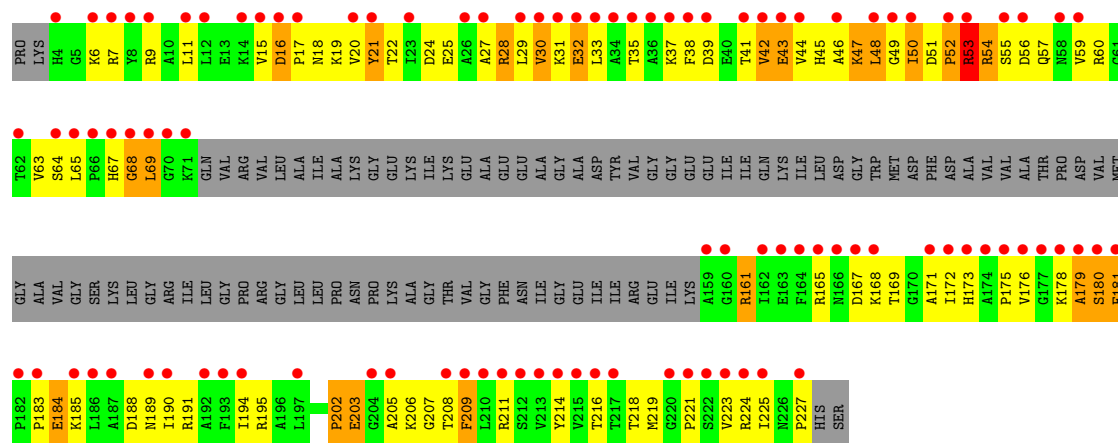
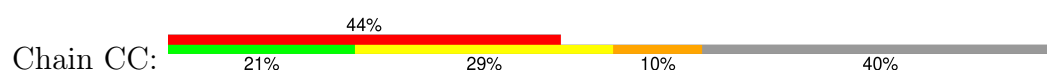


• Molecule 3: 50S ribosomal protein L1

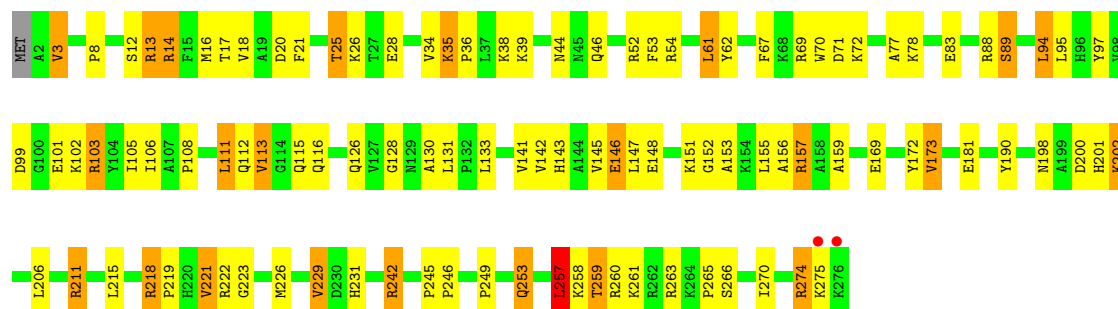




• Molecule 3: 50S ribosomal protein L1

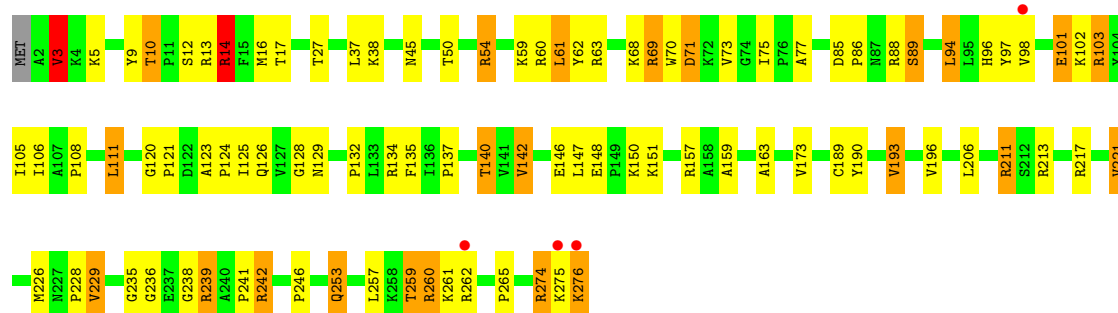


• Molecule 4: 50S ribosomal protein L2

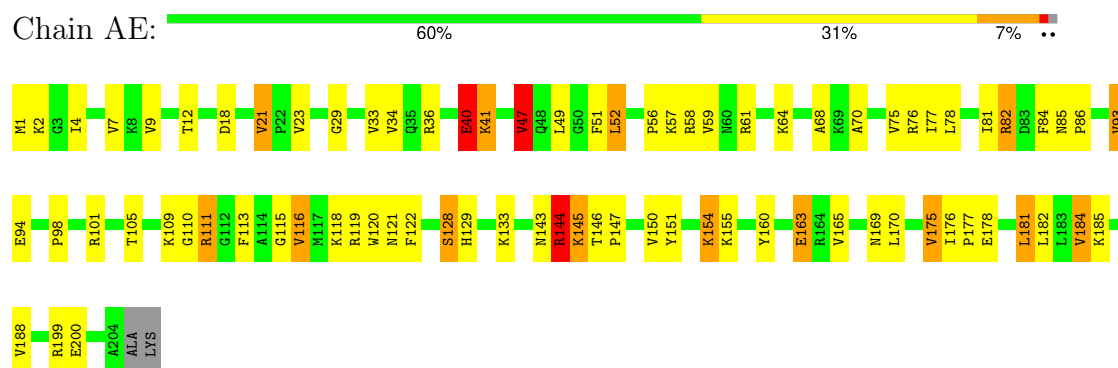


• Molecule 4: 50S ribosomal protein L2

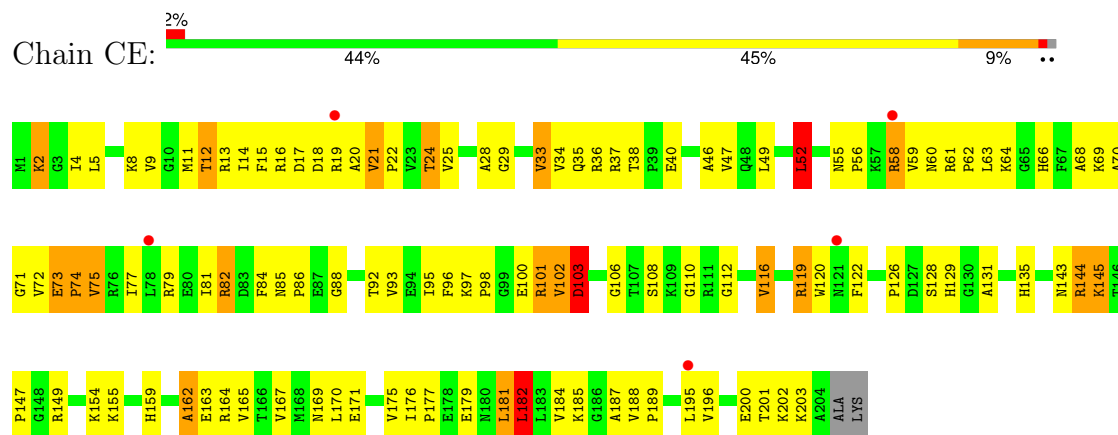




• Molecule 5: 50S ribosomal protein L3



• Molecule 5: 50S ribosomal protein L3

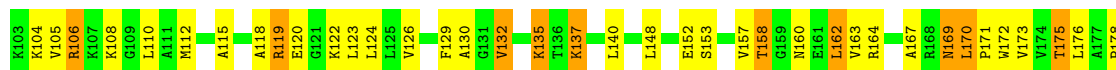
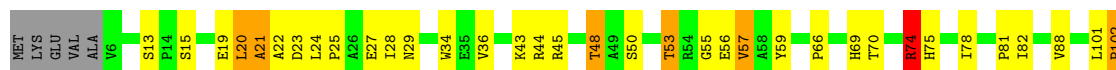


• Molecule 6: 50S ribosomal protein L4

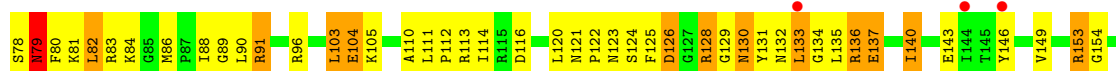
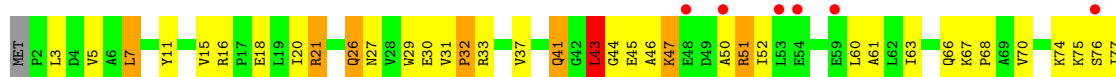




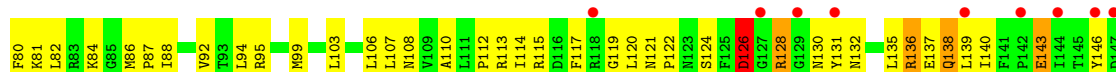
• Molecule 6: 50S ribosomal protein L4



• Molecule 7: 50S ribosomal protein L5

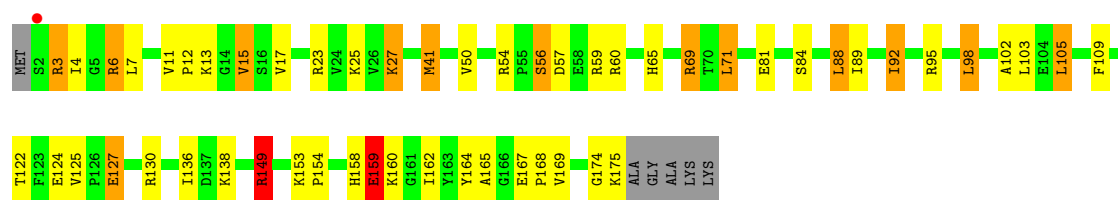


• Molecule 7: 50S ribosomal protein L5

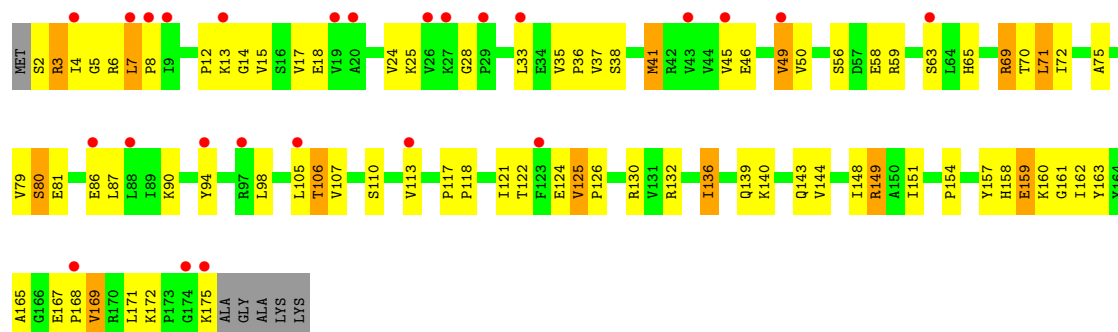


• Molecule 8: 50S ribosomal protein L6

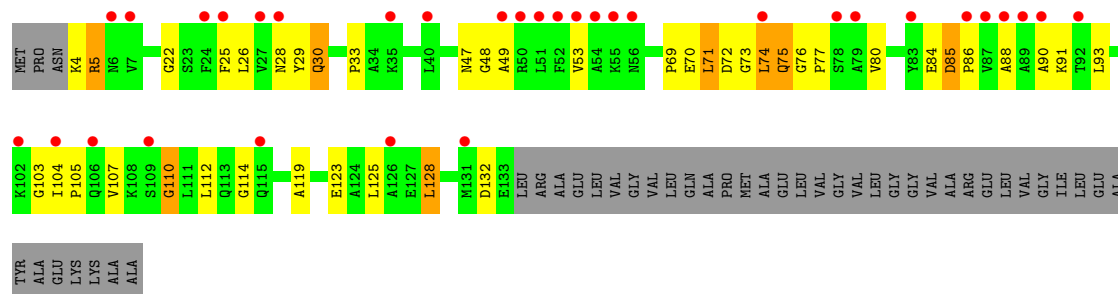




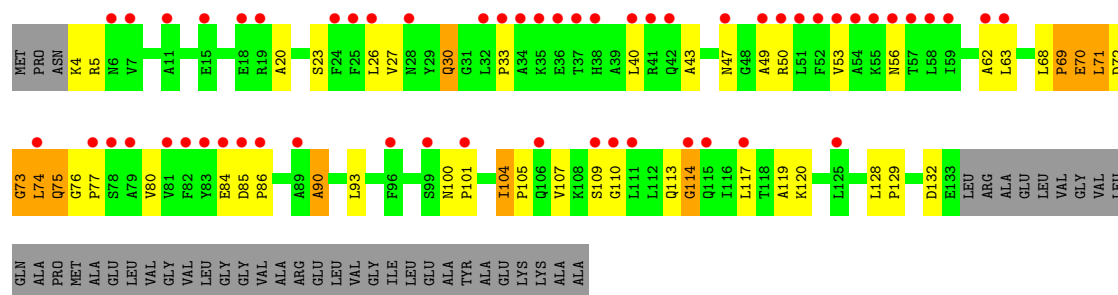
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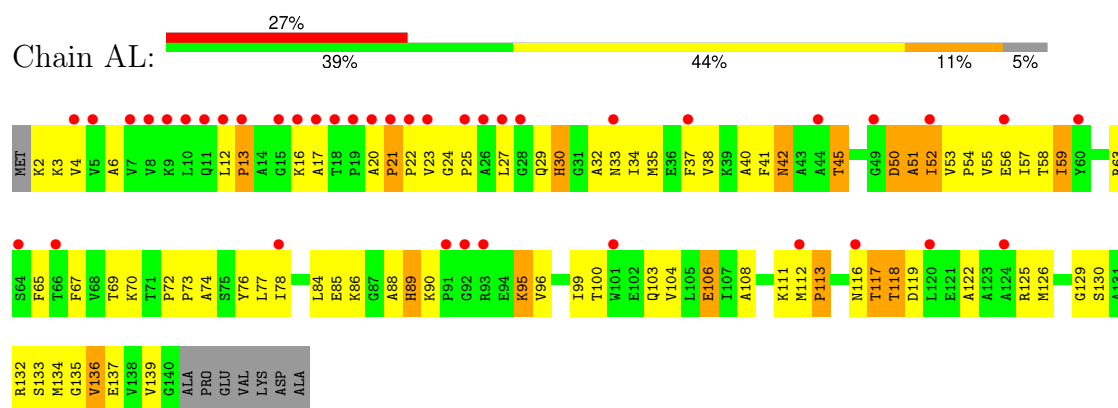
• Molecule 9: 50S ribosomal protein L10



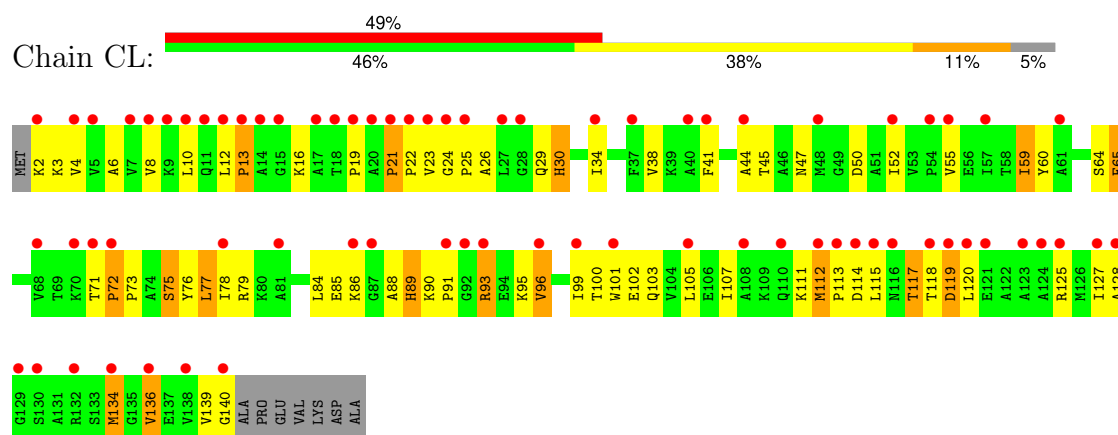
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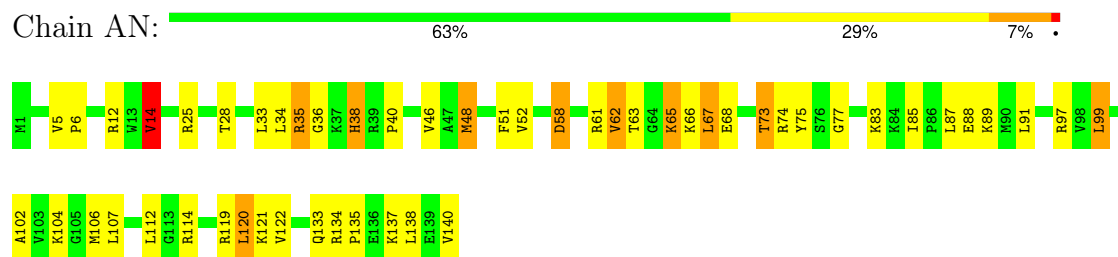
• Molecule 10: 50S ribosomal protein L11



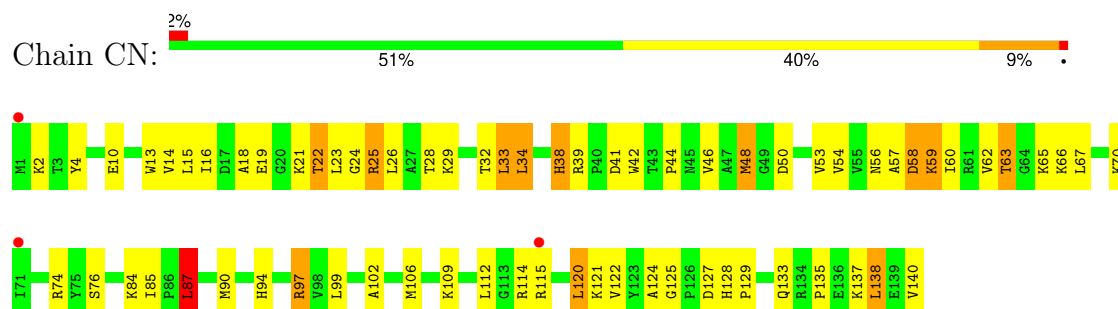
• Molecule 10: 50S ribosomal protein L11



• Molecule 11: 50S ribosomal protein L13

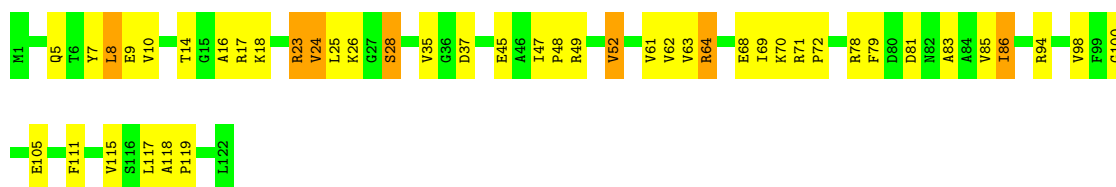


• Molecule 11: 50S ribosomal protein L13



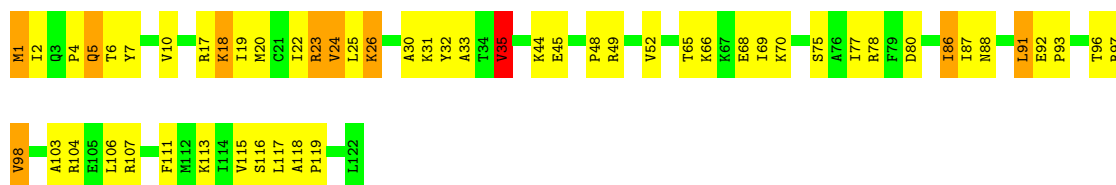
• Molecule 12: 50S ribosomal protein L14

Chain AO:  63% 31% 6%



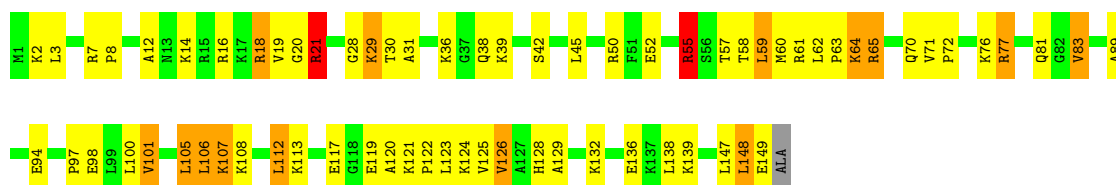
- Molecule 12: 50S ribosomal protein L14

Chain CO:  55% 37% 7%



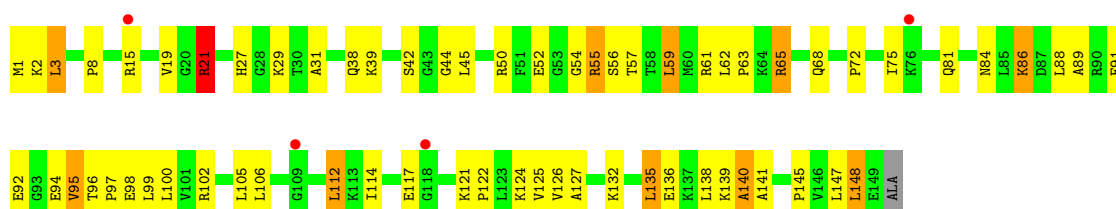
- Molecule 13: 50S ribosomal protein L15

Chain AP:  53% 35% 9%



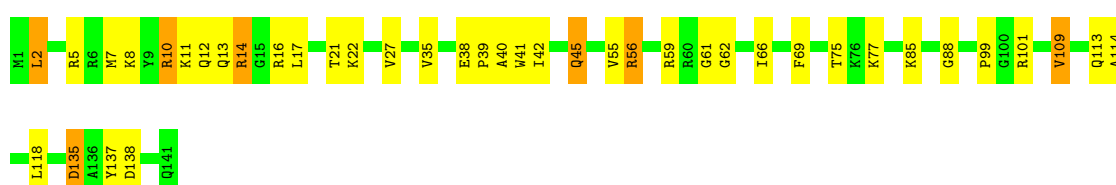
- Molecule 13: 50S ribosomal protein L15

Chain CP:  3% 56% 36% 7%

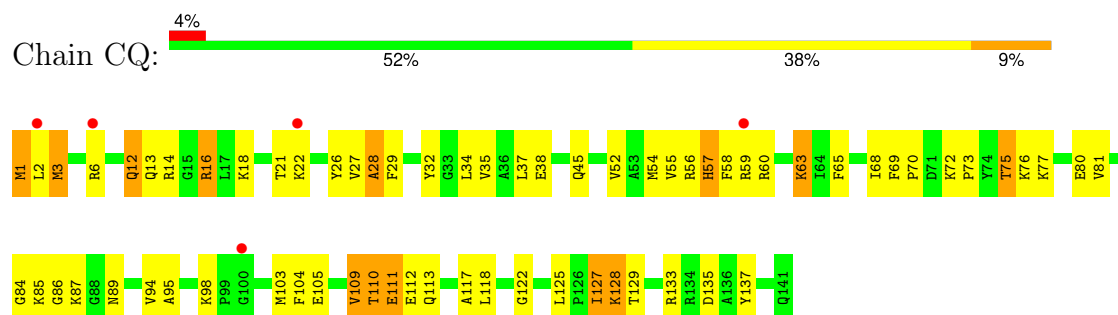


- Molecule 14: 50S ribosomal protein L16

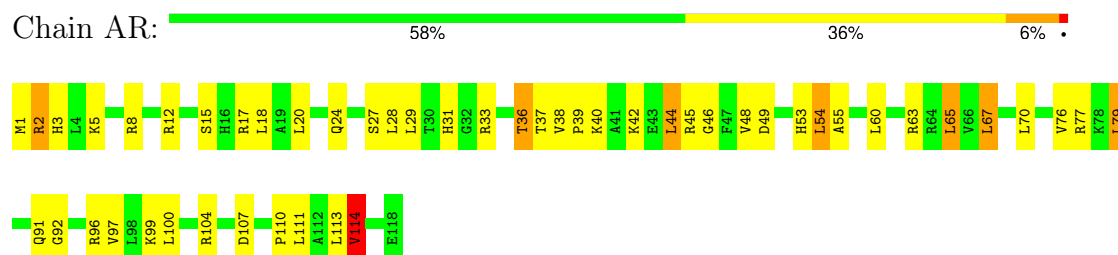
Chain AQ:  71% 24% 5%



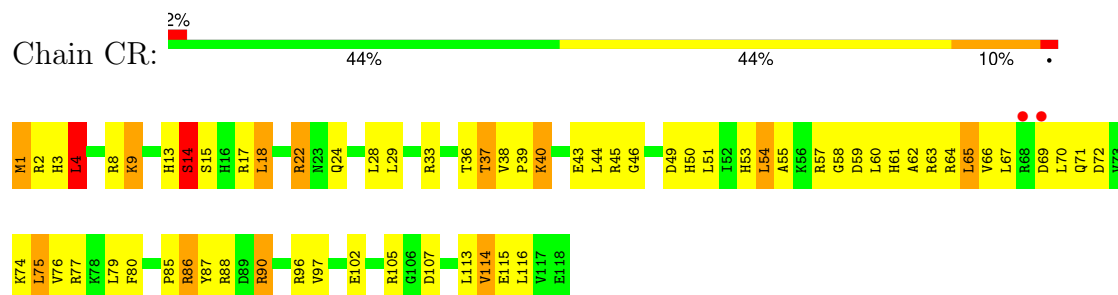
- Molecule 14: 50S ribosomal protein L16



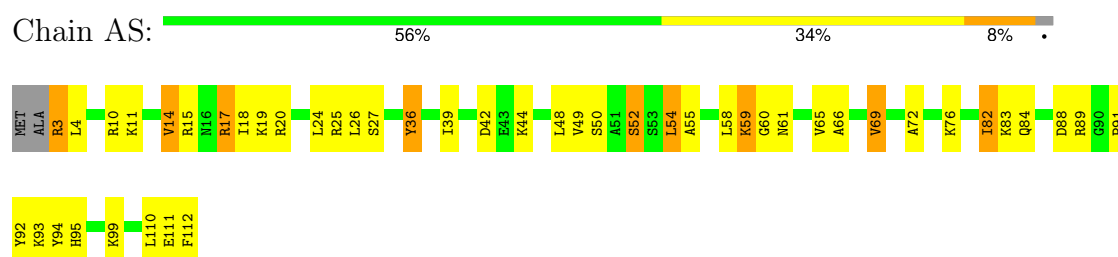
- Molecule 15: 50S ribosomal protein L17



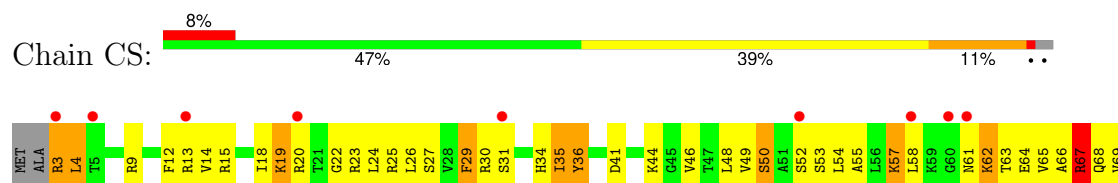
- Molecule 15: 50S ribosomal protein L17



- Molecule 16: 50S ribosomal protein L18

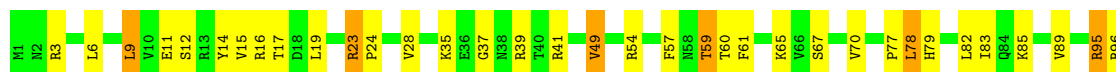


- Molecule 16: 50S ribosomal protein L18

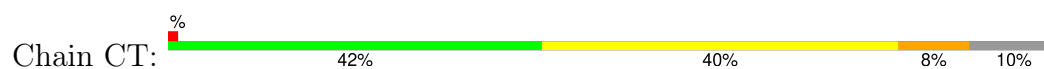




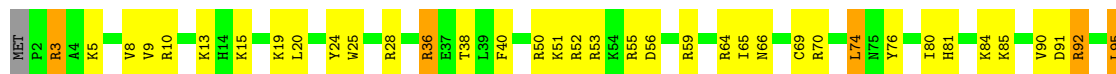
- Molecule 17: 50S ribosomal protein L19



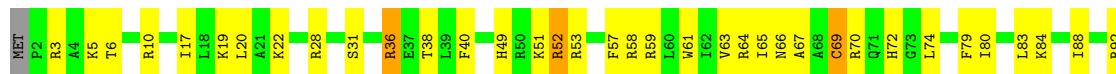
- Molecule 17: 50S ribosomal protein L19



- Molecule 18: 50S ribosomal protein L20

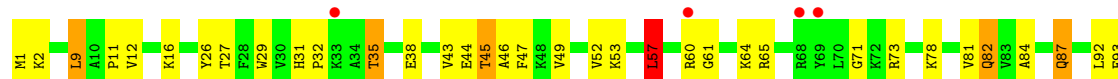


- Molecule 18: 50S ribosomal protein L20



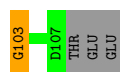
- Molecule 19: 50S ribosomal protein L21



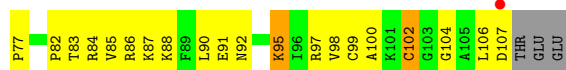
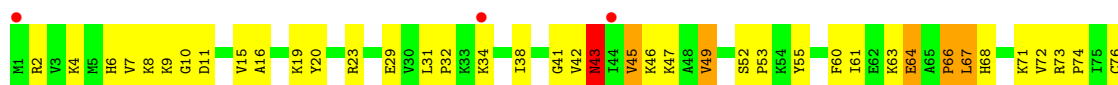
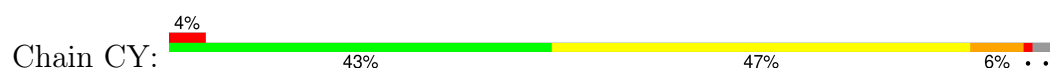




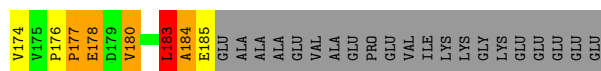
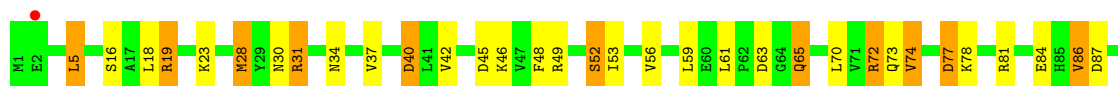
- Molecule 22: 50S ribosomal protein L24



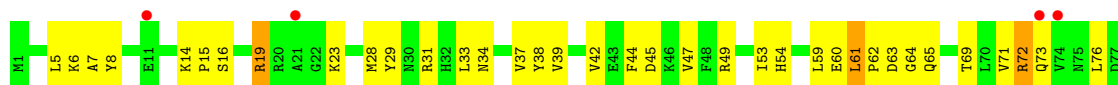
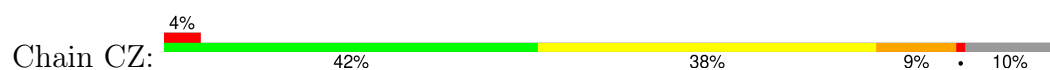
- Molecule 22: 50S ribosomal protein L24

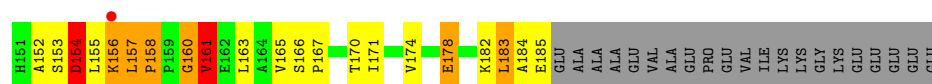


- Molecule 23: 50S ribosomal protein L25



- Molecule 23: 50S ribosomal protein L25

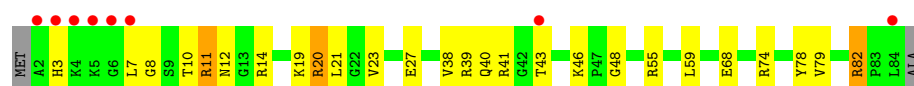




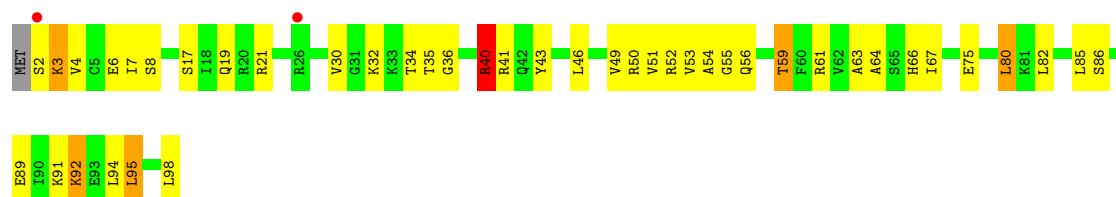
- Molecule 24: 50S ribosomal protein L27



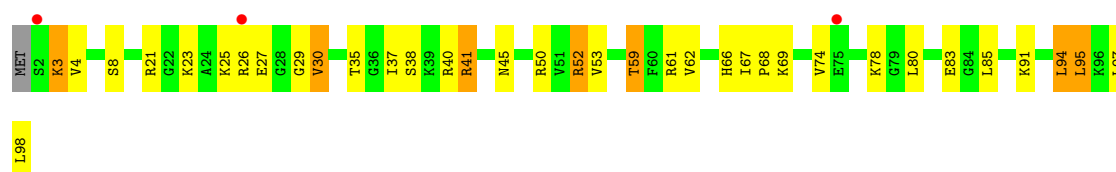
- Molecule 24: 50S ribosomal protein L27



- Molecule 25: 50S ribosomal protein L28



- Molecule 25: 50S ribosomal protein L28

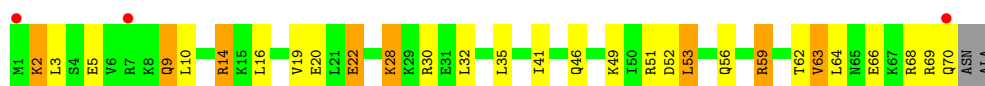


- Molecule 26: 50S ribosomal protein L29



- Molecule 26: 50S ribosomal protein L29





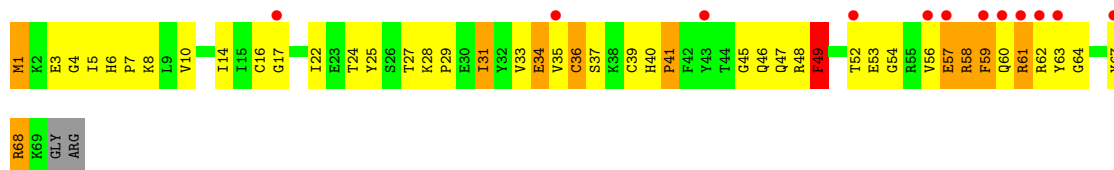
- Molecule 27: 50S ribosomal protein L30



- Molecule 27: 50S ribosomal protein L30



- Molecule 28: 50S ribosomal protein L31



- Molecule 28: 50S ribosomal protein L31



- Molecule 29: 50S ribosomal protein L32

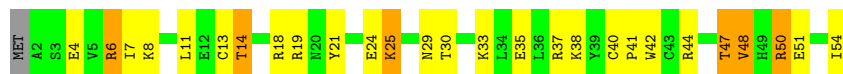


- Molecule 29: 50S ribosomal protein L32



- Molecule 30: 50S ribosomal protein L33

Chain A6: 



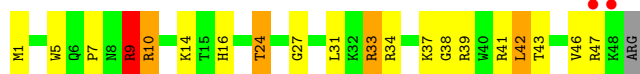
- Molecule 30: 50S ribosomal protein L33

Chain C6: 



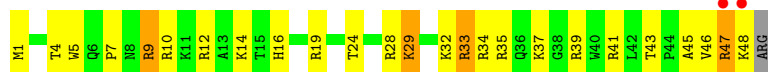
- Molecule 31: 50S ribosomal protein L34

Chain A7: 



- Molecule 31: 50S ribosomal protein L34

Chain C7: 



- Molecule 32: 50S ribosomal protein L35

Chain A8: 



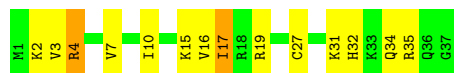
- Molecule 32: 50S ribosomal protein L35

Chain C8: 

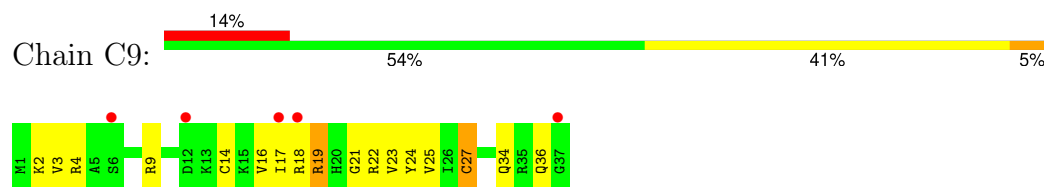


- Molecule 33: 50S ribosomal protein L36

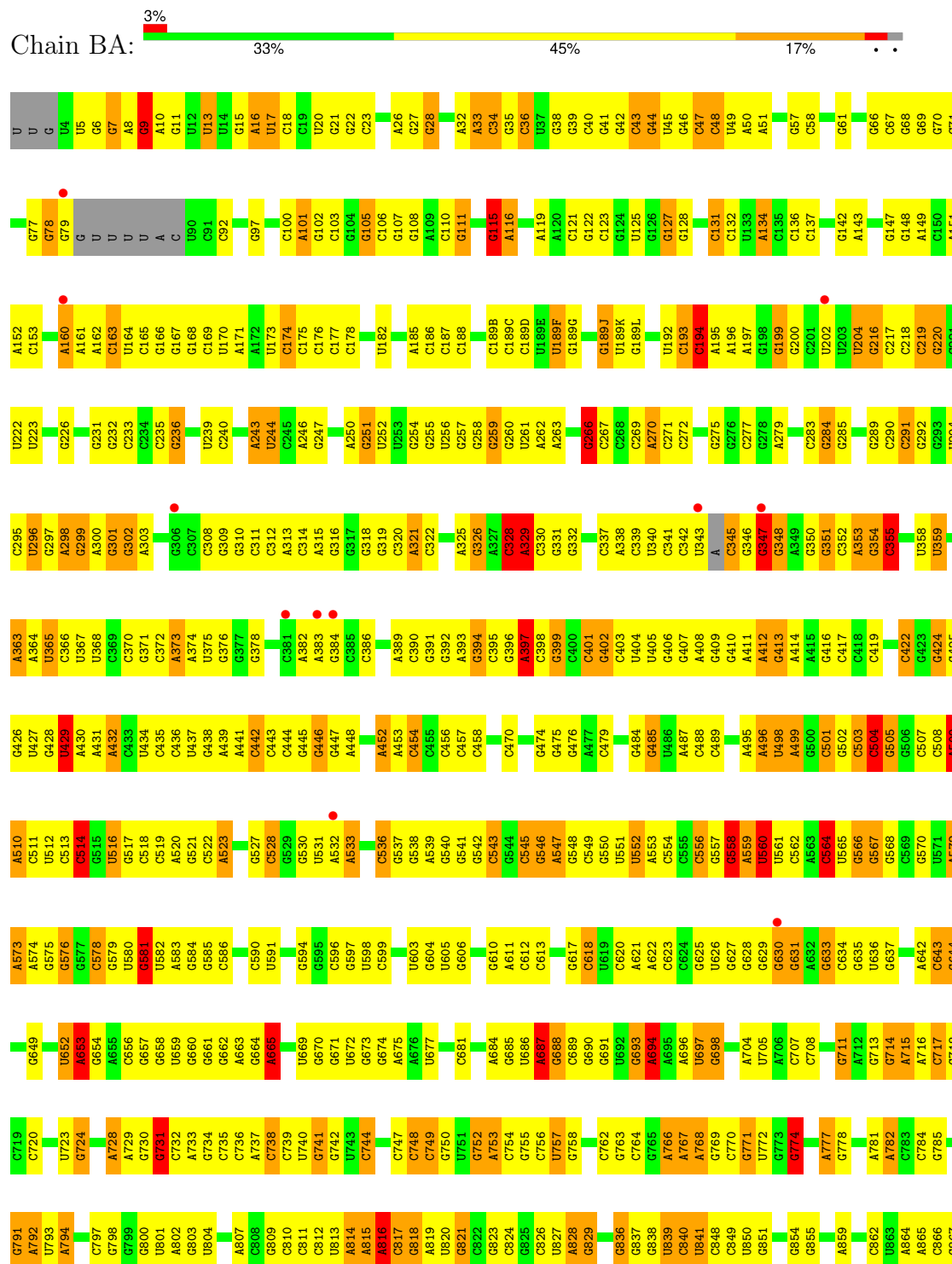
Chain A9: 



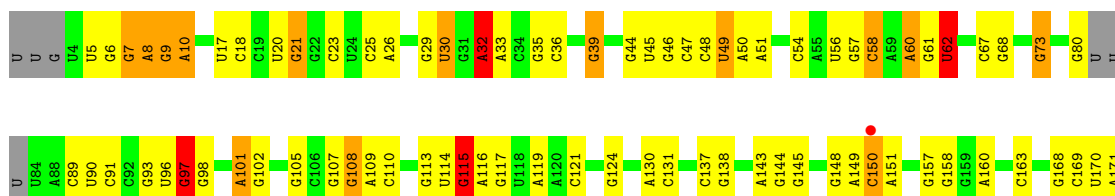
● Molecule 33: 50S ribosomal protein L36

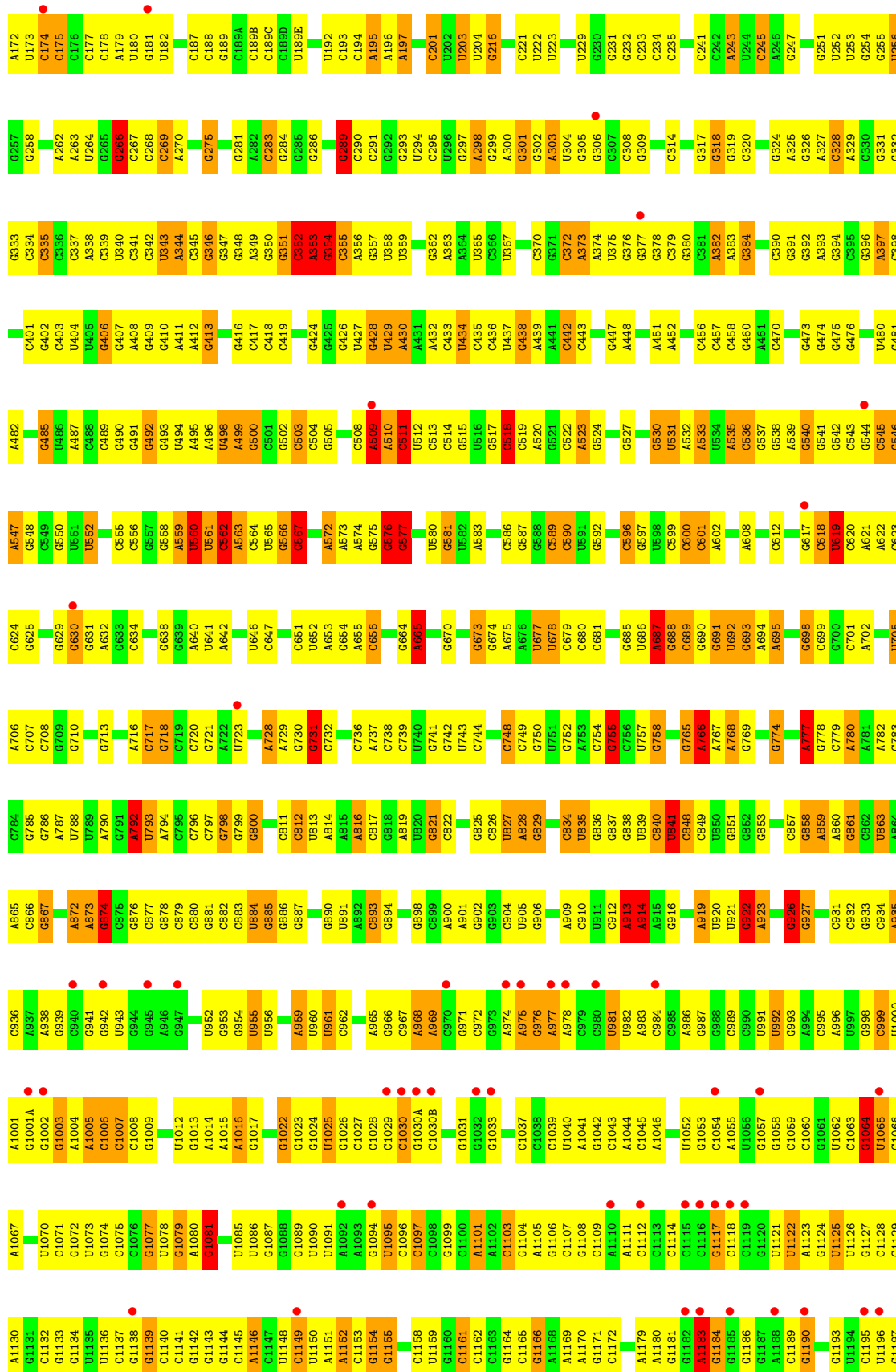


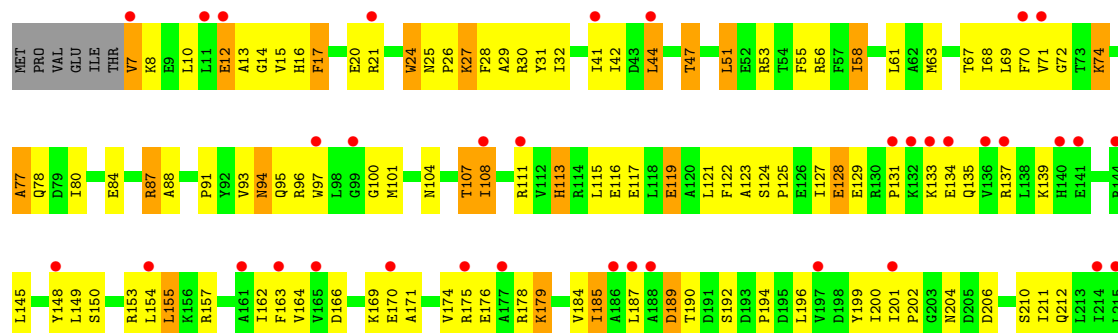
● Molecule 34: 16S Ribosomal RNA

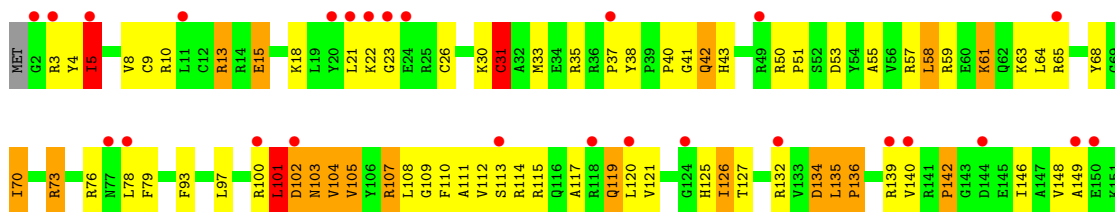


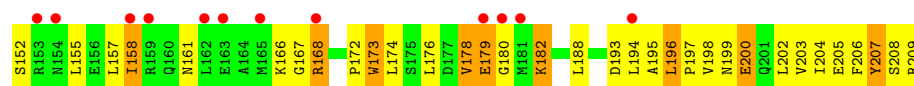
- Molecule 34: 16S Ribosomal RNA



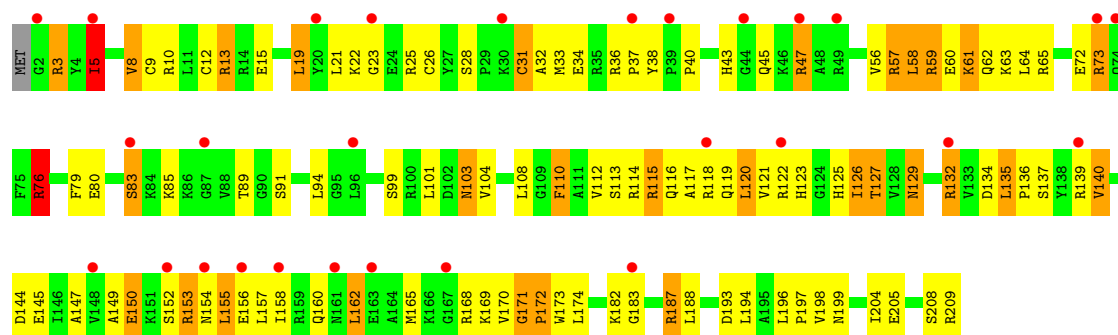




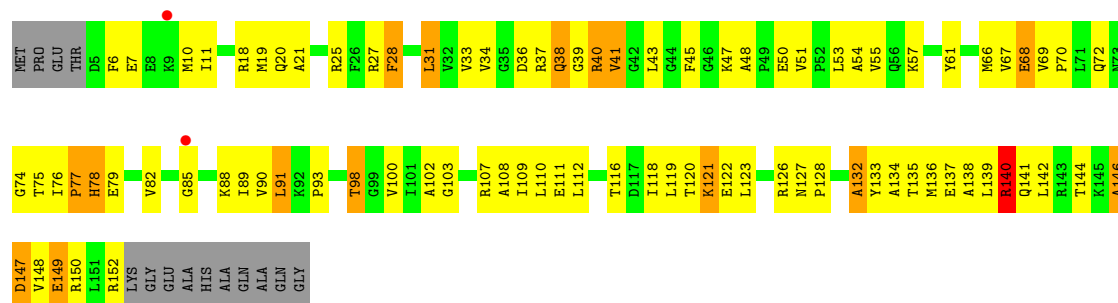




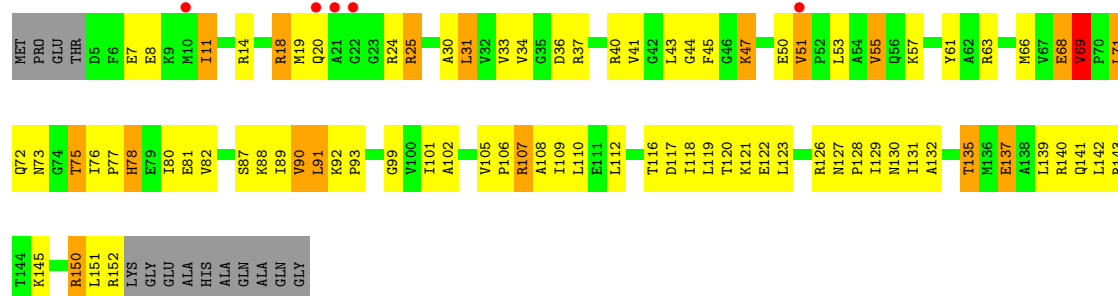
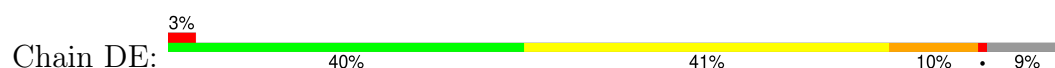
• Molecule 37: 30S ribosomal protein S4



• Molecule 38: 30S ribosomal protein S5

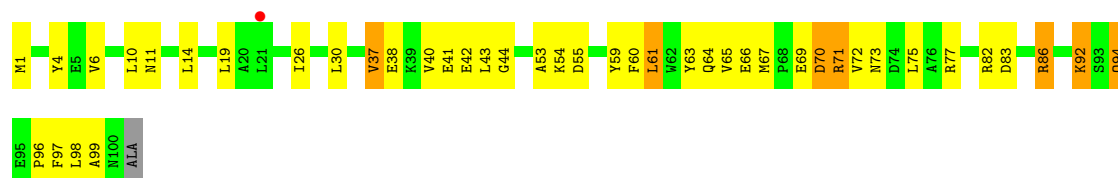


• Molecule 38: 30S ribosomal protein S5



• Molecule 39: 30S ribosomal protein S6

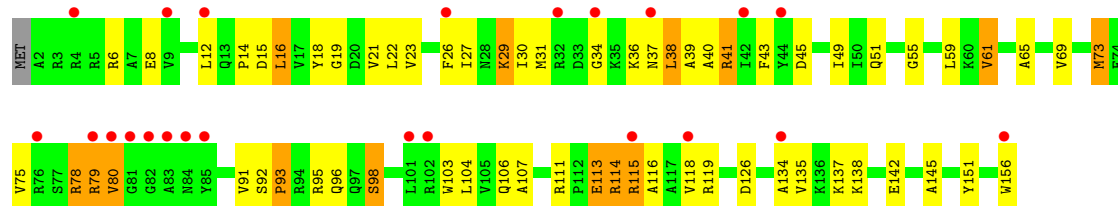




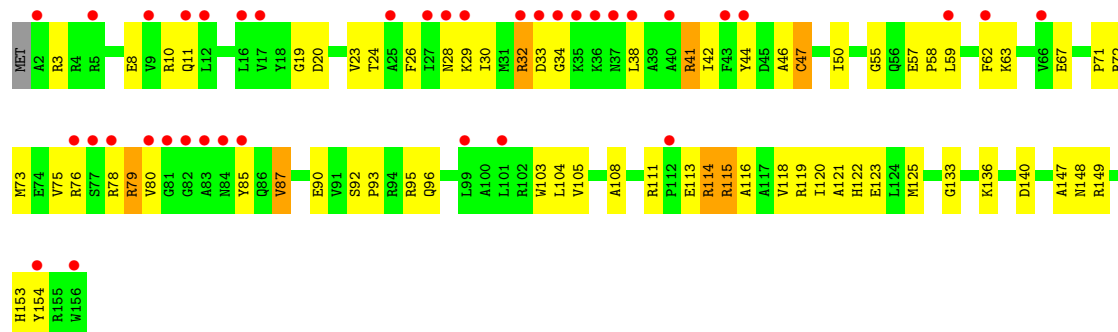
- Molecule 39: 30S ribosomal protein S6



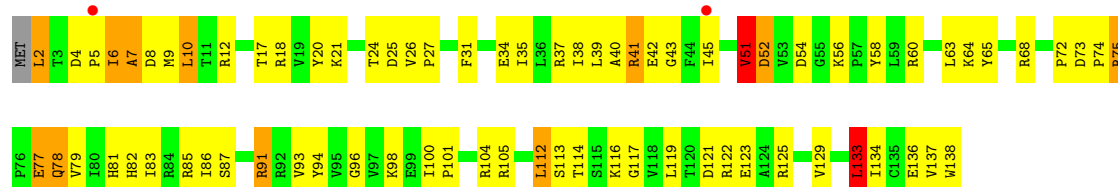
- Molecule 40: 30S ribosomal protein S7



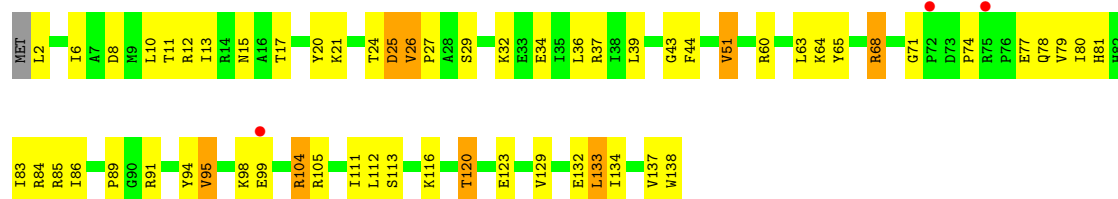
- Molecule 40: 30S ribosomal protein S7



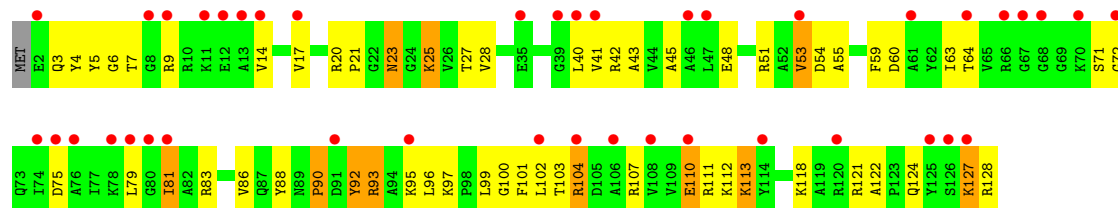
- Molecule 41: 30S ribosomal protein S8



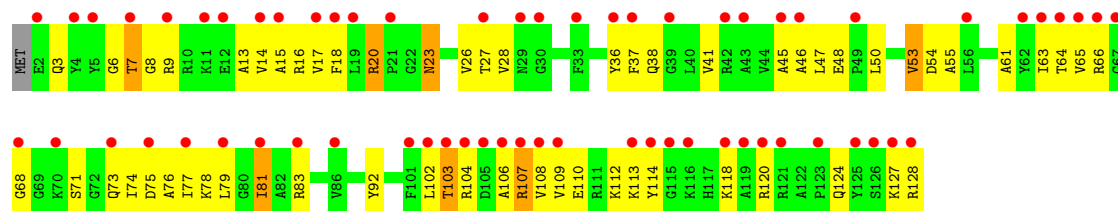
- Molecule 41: 30S ribosomal protein S8



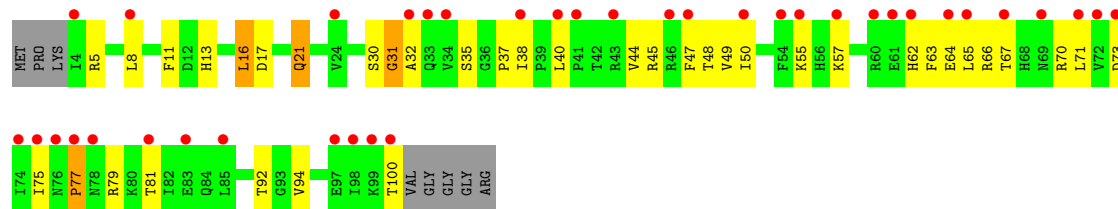
- Molecule 42: 30S ribosomal protein S9



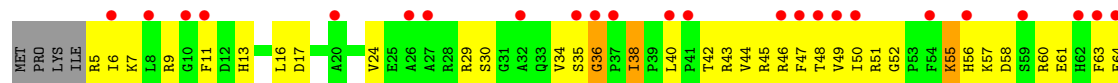
- Molecule 42: 30S ribosomal protein S9

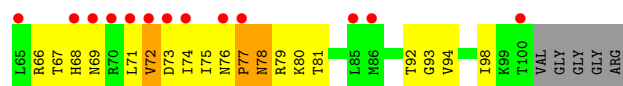


- Molecule 43: 30S ribosomal protein S10

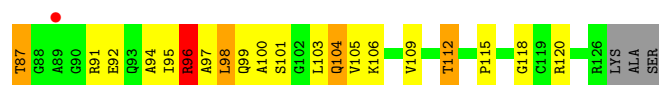
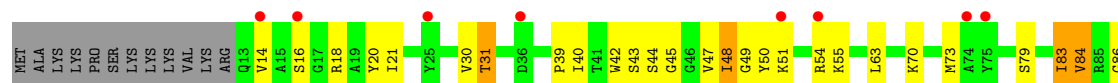


- Molecule 43: 30S ribosomal protein S10





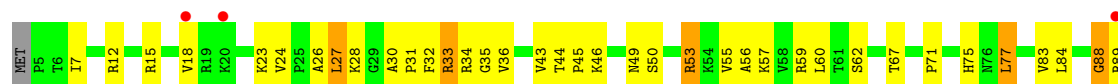
- Molecule 44: 30S ribosomal protein S11



- Molecule 44: 30S ribosomal protein S11



- Molecule 45: 30S ribosomal protein S12

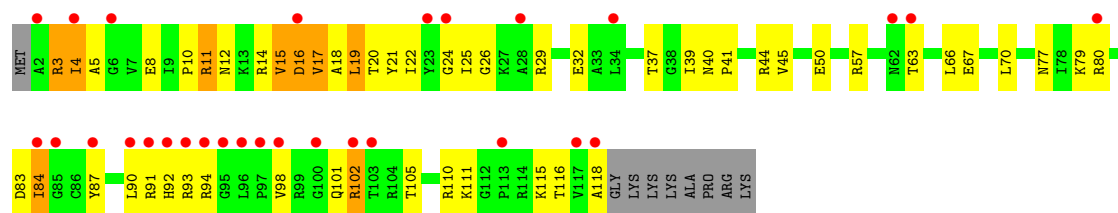


- Molecule 45: 30S ribosomal protein S12

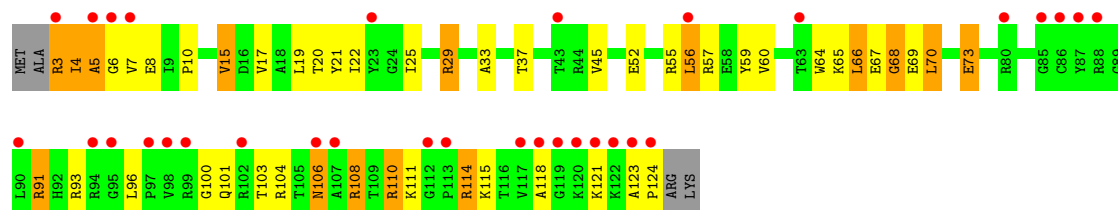


- Molecule 46: 30S ribosomal protein S13

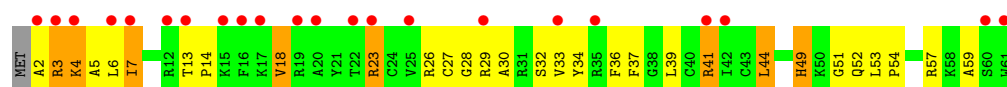




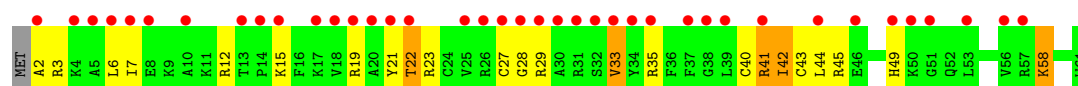
- Molecule 46: 30S ribosomal protein S13



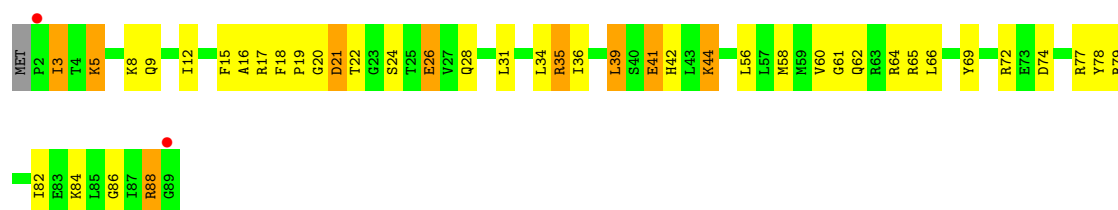
- Molecule 47: 30S ribosomal protein S14 type Z



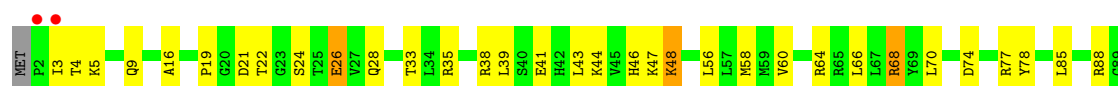
- Molecule 47: 30S ribosomal protein S14 type Z



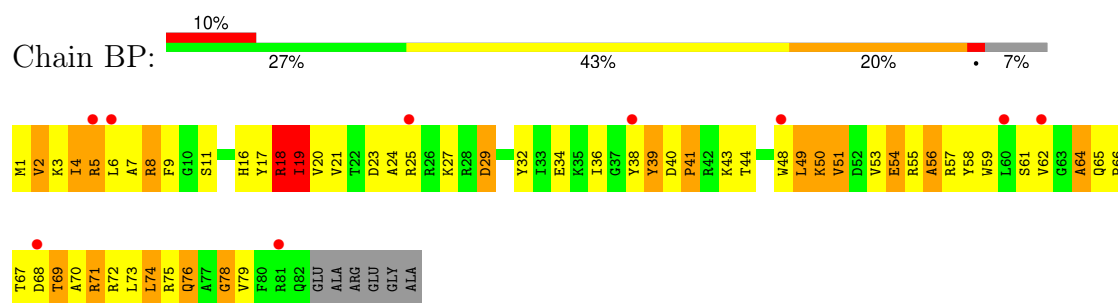
- Molecule 48: 30S ribosomal protein S15



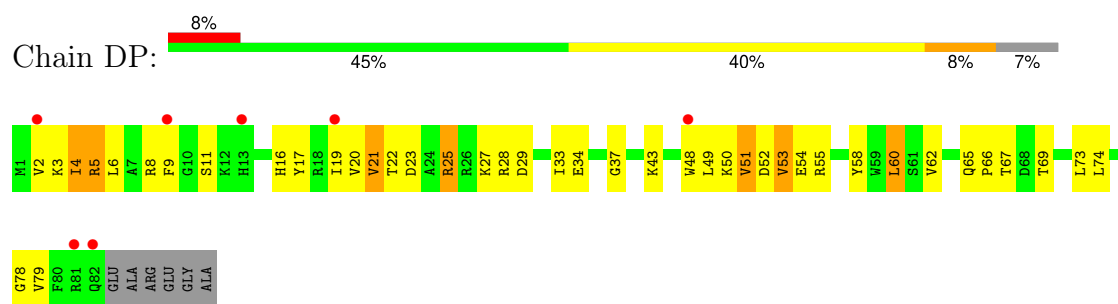
- Molecule 48: 30S ribosomal protein S15



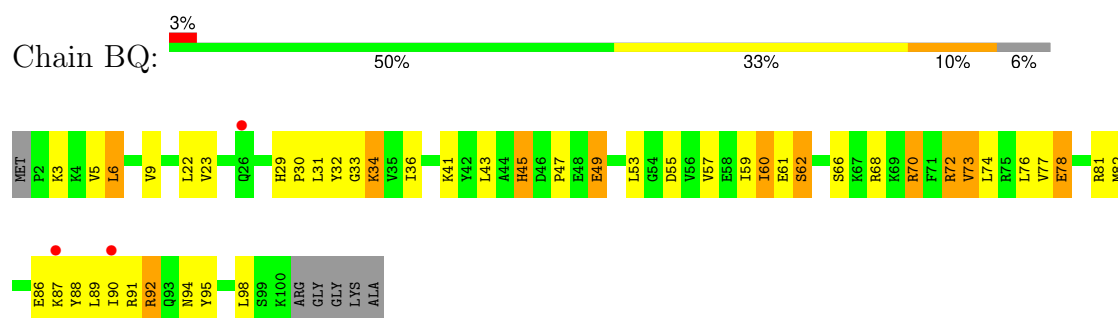
- Molecule 49: 30S ribosomal protein S16



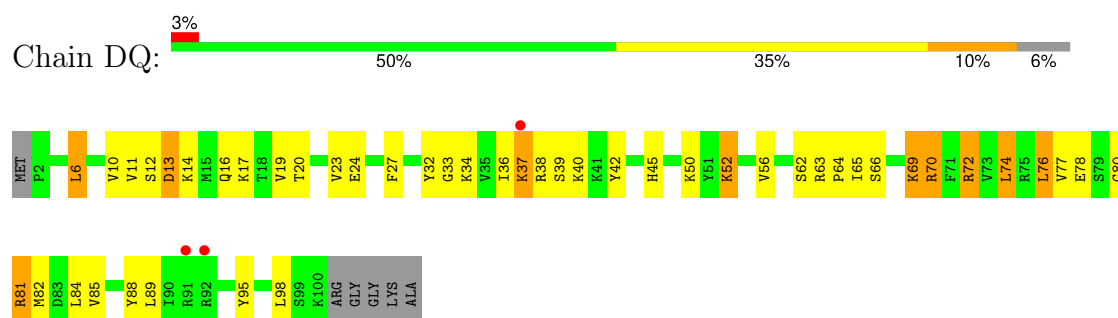
- Molecule 49: 30S ribosomal protein S16



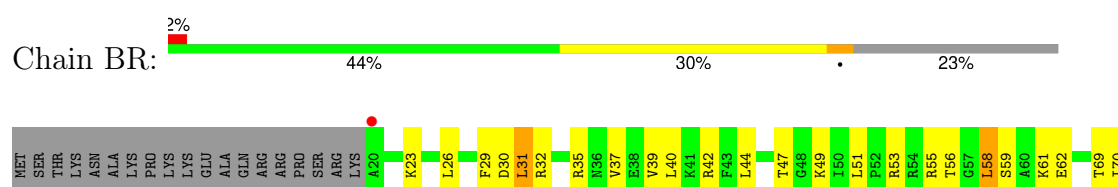
- Molecule 50: 30S ribosomal protein S17



- Molecule 50: 30S ribosomal protein S17

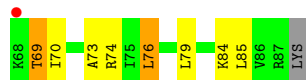
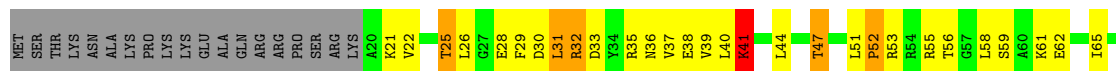


- Molecule 51: 30S ribosomal protein S18

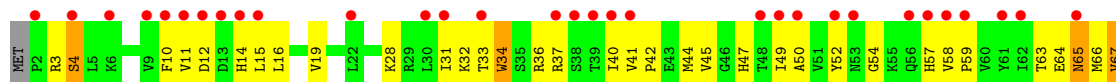
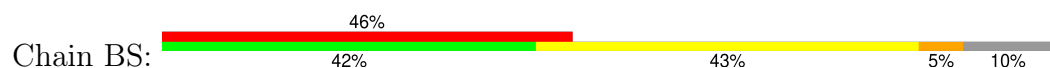




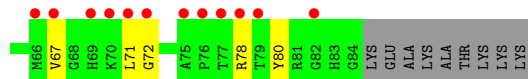
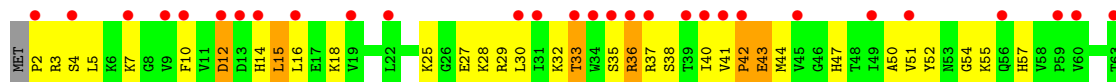
- Molecule 51: 30S ribosomal protein S18



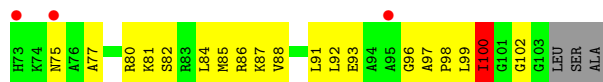
- Molecule 52: 30S ribosomal protein S19



- Molecule 52: 30S ribosomal protein S19

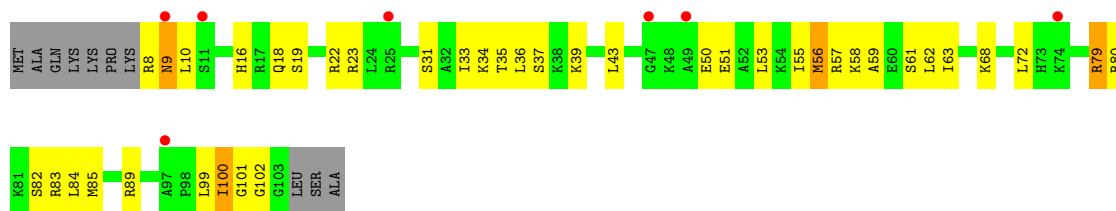


- Molecule 53: 30S ribosomal protein S20



- Molecule 53: 30S ribosomal protein S20





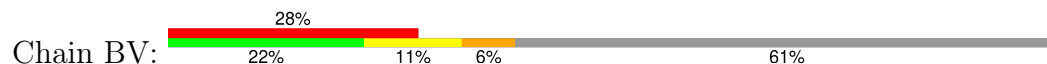
- Molecule 54: 30S ribosomal protein Thx



- Molecule 54: 30S ribosomal protein Thx



- Molecule 55: mRNA



- Molecule 55: mRNA

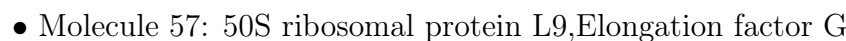


- Molecule 56: P-site tRNA

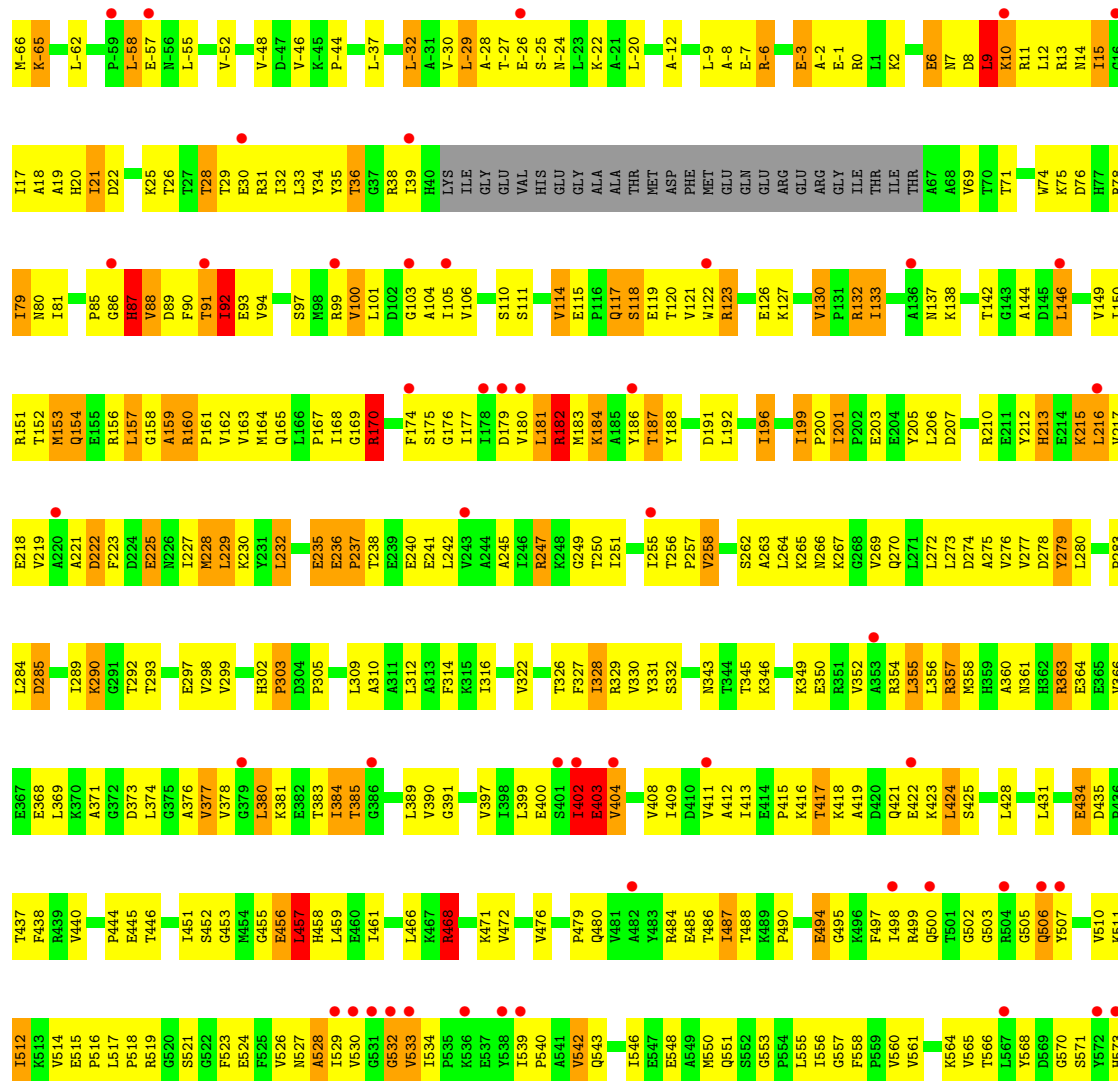


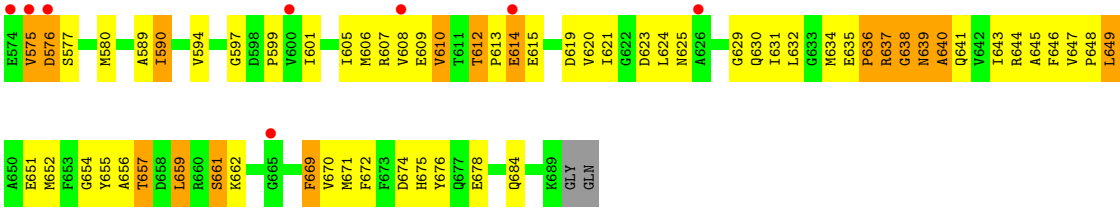
- Molecule 56: P-site tRNA





Chain DZ: 





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	210.45Å 449.00Å 625.37Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.74 – 2.80 49.74 – 2.80	Depositor EDS
% Data completeness (in resolution range)	99.8 (49.74-2.80) 99.8 (49.74-2.80)	Depositor EDS
R_{merge}	0.20	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.08 (at 2.77Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE: 1.8.2_1309)	Depositor
R, R_{free}	0.200 , 0.255 0.202 , 0.254	Depositor DCC
R_{free} test set	71854 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	54.2	Xtriage
Anisotropy	0.399	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 69.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	310279	wwPDB-VP
Average B, all atoms (Å ²)	81.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.54% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 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: MG, 4SU, ZN, FUA, 5MU, GDP, PSU, SF4, 7MG, MIA

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	1.51	654/68792 (1.0%)	2.24	4887/107377 (4.6%)
1	CA	1.01	71/68691 (0.1%)	1.68	1752/107219 (1.6%)
2	AB	1.21	5/2878 (0.2%)	2.01	141/4490 (3.1%)
2	CB	0.67	0/2878	1.30	18/4490 (0.4%)
3	AC	0.34	0/1083	0.65	0/1460
3	CC	0.34	0/1083	0.65	0/1460
4	AD	1.00	4/2186 (0.2%)	1.08	8/2944 (0.3%)
4	CD	0.76	0/2192	0.92	2/2951 (0.1%)
5	AE	1.03	5/1592 (0.3%)	1.08	4/2149 (0.2%)
5	CE	0.68	0/1592	0.85	1/2149 (0.0%)
6	AF	0.96	2/1619 (0.1%)	1.07	3/2193 (0.1%)
6	CF	0.64	0/1615	0.85	1/2188 (0.0%)
7	AG	0.55	0/1450	0.77	0/1959
7	CG	0.40	0/1449	0.63	0/1958
8	AH	0.84	0/1356	0.96	3/1834 (0.2%)
8	CH	0.42	0/1356	0.64	0/1834
9	AK	0.42	0/640	0.76	1/889 (0.1%)
9	CK	0.29	0/640	0.62	0/889
10	AL	0.34	0/1044	0.58	0/1416
10	CL	0.31	0/1044	0.53	0/1416
11	AN	1.06	2/1144 (0.2%)	1.09	3/1543 (0.2%)
11	CN	0.55	0/1144	0.76	0/1543
12	AO	1.00	0/943	1.09	2/1269 (0.2%)
12	CO	0.71	0/943	0.82	0/1269
13	AP	0.89	0/1156	1.08	9/1537 (0.6%)
13	CP	0.58	0/1152	0.86	1/1533 (0.1%)
14	AQ	0.98	0/1143	1.05	4/1527 (0.3%)
14	CQ	0.62	0/1143	0.77	0/1527
15	AR	0.98	0/982	1.15	4/1312 (0.3%)
15	CR	0.62	0/982	0.95	2/1312 (0.2%)
16	AS	0.76	0/887	0.96	0/1180
16	CS	0.56	0/880	0.83	2/1172 (0.2%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	AT	0.87	0/1105	1.04	2/1477 (0.1%)
17	CT	0.68	0/1097	0.89	0/1468
18	AU	1.18	2/977 (0.2%)	1.19	5/1301 (0.4%)
18	CU	0.67	0/977	0.78	0/1301
19	AV	1.02	1/782 (0.1%)	1.09	1/1049 (0.1%)
19	CV	0.54	0/782	0.74	0/1049
20	AW	1.21	1/897 (0.1%)	1.19	3/1205 (0.2%)
20	CW	0.77	0/897	0.91	0/1205
21	AX	0.98	1/764 (0.1%)	0.99	2/1025 (0.2%)
21	CX	0.70	0/764	0.78	1/1025 (0.1%)
22	AY	0.92	0/819	1.00	1/1095 (0.1%)
22	CY	0.62	0/819	0.77	0/1095
23	AZ	0.77	0/1483	1.00	3/2017 (0.1%)
23	CZ	0.47	0/1483	0.71	0/2017
24	A0	0.97	0/662	1.03	0/881
24	C0	0.60	0/662	0.77	0/881
25	A1	0.94	0/762	1.04	3/1014 (0.3%)
25	C1	0.70	0/762	0.86	0/1014
26	A2	0.88	0/590	0.91	0/781
26	C2	0.60	0/590	0.75	0/781
27	A3	0.99	0/474	1.09	2/635 (0.3%)
27	C3	0.51	0/469	0.78	0/630
28	A4	0.47	0/571	0.74	0/768
28	C4	0.35	0/545	0.59	0/737
29	A5	1.22	3/469 (0.6%)	1.22	4/635 (0.6%)
29	C5	0.75	0/469	0.89	2/635 (0.3%)
30	A6	0.89	0/460	1.02	1/613 (0.2%)
30	C6	0.67	0/456	0.76	0/608
31	A7	1.11	0/426	1.21	4/561 (0.7%)
31	C7	0.86	0/426	1.03	2/561 (0.4%)
32	A8	1.00	0/525	1.04	3/691 (0.4%)
32	C8	0.72	0/525	0.85	0/691
33	A9	1.09	0/310	1.04	0/407
33	C9	0.57	0/310	0.70	0/407
34	BA	0.79	7/35976 (0.0%)	1.44	496/56145 (0.9%)
34	DA	0.70	2/36119 (0.0%)	1.31	266/56370 (0.5%)
35	BB	0.47	0/1881	0.72	0/2542
35	DB	0.39	0/1860	0.64	0/2518
36	BC	0.38	0/1576	0.57	0/2130
36	DC	0.34	0/1568	0.54	0/2122
37	BD	0.52	0/1689	0.77	0/2267
37	DD	0.51	0/1708	0.77	1/2289 (0.0%)
38	BE	0.62	0/1145	0.84	0/1543

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
38	DE	0.54	0/1149	0.78	1/1548 (0.1%)
39	BF	0.54	0/825	0.75	0/1118
39	DF	0.54	0/833	0.77	2/1128 (0.2%)
40	BG	0.40	0/1250	0.60	0/1679
40	DG	0.33	0/1254	0.52	0/1683
41	BH	0.58	0/1108	0.80	1/1494 (0.1%)
41	DH	0.48	0/1108	0.70	0/1494
42	BI	0.38	0/1005	0.61	0/1350
42	DI	0.33	0/997	0.58	0/1343
43	BJ	0.38	0/722	0.59	0/982
43	DJ	0.34	0/727	0.57	0/988
44	BK	0.55	0/848	0.75	0/1149
44	DK	0.51	0/848	0.70	0/1149
45	BL	0.74	0/946	0.88	1/1274 (0.1%)
45	DL	0.58	0/946	0.81	0/1274
46	BM	0.39	0/933	0.62	0/1253
46	DM	0.34	0/961	0.55	0/1291
47	BN	0.39	0/501	0.68	1/664 (0.2%)
47	DN	0.35	0/501	0.56	0/664
48	BO	0.56	0/739	0.81	0/985
48	DO	0.53	0/739	0.72	0/985
49	BP	0.55	0/697	0.79	1/939 (0.1%)
49	DP	0.53	0/693	0.71	0/935
50	BQ	0.63	0/836	0.78	0/1117
50	DQ	0.57	0/836	0.73	0/1117
51	BR	0.55	0/560	0.80	1/746 (0.1%)
51	DR	0.51	0/560	0.71	0/746
52	BS	0.35	0/676	0.57	0/911
52	DS	0.31	0/661	0.61	0/893
53	BT	0.49	0/730	0.74	0/965
53	DT	0.49	0/733	0.71	0/969
54	BU	0.38	0/203	0.65	0/266
54	DU	0.31	0/203	0.57	0/266
55	BV	0.71	0/165	1.15	1/254 (0.4%)
55	DV	0.60	0/137	1.05	0/211
56	BW	0.89	1/1650 (0.1%)	1.64	41/2569 (1.6%)
56	BY	0.42	0/1602	0.95	1/2493 (0.0%)
56	DW	0.70	0/1650	1.36	20/2569 (0.8%)
56	DY	0.35	0/1579	0.86	0/2455
57	BZ	0.58	0/5792	0.81	4/7844 (0.1%)
57	DZ	0.49	0/5792	0.72	4/7844 (0.1%)
All	All	0.99	761/330005 (0.2%)	1.56	7729/491779 (1.6%)

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
1	CA	0	1
17	CT	0	1
19	AV	0	1
21	AX	0	1
21	CX	0	1
23	AZ	0	1
24	A0	0	1
25	A1	0	1
28	A4	0	1
53	BT	0	1
53	DT	0	1
57	BZ	0	1
57	DZ	0	3
All	All	0	15

The worst 5 of 761 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	AA	1067	A	N9-C4	-18.69	1.26	1.37
1	AA	1188	A	N9-C4	-16.21	1.28	1.37
1	AA	990	A	N9-C4	-15.62	1.28	1.37
1	AA	354	A	N9-C4	-13.34	1.29	1.37
1	AA	1988	A	N9-C4	-12.57	1.30	1.37

The worst 5 of 7729 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	1067	A	C2-N3-C4	-25.69	97.76	110.60
1	AA	1701	A	O5'-P-OP2	-25.21	80.44	110.70
1	AA	553	A	N1-C6-N6	25.19	133.71	118.60
1	AA	990	A	C5-N7-C8	-25.10	91.35	103.90
1	AA	553	A	C5-N7-C8	-23.43	92.19	103.90

There are no chirality outliers.

5 of 15 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
24	A0	11	ARG	Peptide

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Mol	Chain	Res	Type	Group
25	A1	2	SER	Peptide
19	AV	54	GLY	Peptide
21	AX	93	GLU	Peptide
23	AZ	176	PRO	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	AA	61426	0	30937	931	0
1	CA	61337	0	30928	1104	0
2	AB	2573	0	1306	39	0
2	CB	2573	0	1306	49	0
3	AC	1063	0	1089	162	0
3	CC	1063	0	1091	203	0
4	AD	2136	0	2218	72	0
4	CD	2142	0	2229	72	0
5	AE	1559	0	1618	46	0
5	CE	1559	0	1618	92	0
6	AF	1584	0	1625	58	0
6	CF	1580	0	1619	68	0
7	AG	1425	0	1443	69	0
7	CG	1424	0	1434	59	0
8	AH	1330	0	1407	40	0
8	CH	1330	0	1407	51	0
9	AK	641	0	309	13	0
9	CK	641	0	309	13	0
10	AL	1025	0	1066	54	0
10	CL	1025	0	1066	50	0
11	AN	1117	0	1184	32	0
11	CN	1117	0	1184	45	0
12	AO	933	0	996	32	0
12	CO	933	0	996	38	0
13	AP	1139	0	1223	48	0
13	CP	1135	0	1212	46	0
14	AQ	1122	0	1179	35	0
14	CQ	1122	0	1179	54	0
15	AR	968	0	1033	26	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
15	CR	968	0	1033	44	0
16	AS	877	0	938	30	0
16	CS	870	0	923	43	0
17	AT	1091	0	1151	35	0
17	CT	1083	0	1136	55	0
18	AU	959	0	1019	30	0
18	CU	959	0	1018	34	0
19	AV	771	0	829	24	0
19	CV	771	0	830	16	0
20	AW	886	0	940	26	0
20	CW	886	0	940	31	0
21	AX	750	0	814	27	0
21	CX	750	0	814	27	0
22	AY	806	0	881	23	0
22	CY	806	0	881	39	0
23	AZ	1451	0	1457	56	0
23	CZ	1451	0	1457	66	0
24	A0	653	0	674	29	0
24	C0	653	0	674	22	0
25	A1	755	0	826	24	0
25	C1	755	0	826	23	0
26	A2	588	0	643	13	0
26	C2	588	0	643	19	0
27	A3	469	0	518	13	0
27	C3	464	0	514	11	0
28	A4	558	0	547	24	0
28	C4	532	0	505	14	0
29	A5	455	0	465	18	0
29	C5	455	0	465	20	0
30	A6	453	0	473	18	0
30	C6	449	0	469	13	0
31	A7	418	0	467	17	0
31	C7	418	0	467	17	0
32	A8	517	0	582	22	0
32	C8	517	0	582	28	0
33	A9	307	0	335	10	0
33	C9	307	0	335	14	0
34	BA	32141	0	16224	674	0
34	DA	32268	0	16287	690	0
35	BB	1846	0	1867	102	0
35	DB	1825	0	1828	82	0
36	BC	1552	0	1546	59	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
36	DC	1544	0	1524	63	0
37	BD	1659	0	1678	93	0
37	DD	1678	0	1720	90	0
38	BE	1129	0	1185	65	0
38	DE	1133	0	1191	64	0
39	BF	812	0	804	27	0
39	DF	820	0	814	22	0
40	BG	1231	0	1238	42	0
40	DG	1235	0	1249	32	0
41	BH	1088	0	1126	62	0
41	DH	1088	0	1126	36	0
42	BI	986	0	995	41	0
42	DI	978	0	966	40	0
43	BJ	709	0	650	37	0
43	DJ	714	0	672	47	0
44	BK	833	0	836	31	0
44	DK	833	0	836	25	0
45	BL	930	0	980	37	0
45	DL	930	0	980	44	0
46	BM	923	0	970	29	0
46	DM	950	0	988	46	0
47	BN	492	0	529	29	0
47	DN	492	0	531	20	0
48	BO	728	0	760	29	0
48	DO	728	0	760	18	0
49	BP	681	0	697	51	0
49	DP	677	0	686	33	0
50	BQ	823	0	891	26	0
50	DQ	823	0	891	35	0
51	BR	555	0	618	22	0
51	DR	555	0	618	25	0
52	BS	661	0	675	34	0
52	DS	646	0	644	30	0
53	BT	728	0	798	35	0
53	DT	731	0	807	24	0
54	BU	199	0	208	5	0
54	DU	199	0	208	8	0
55	BV	148	0	76	5	0
55	DV	123	0	66	5	0
56	BW	1631	0	839	22	0
56	BY	1581	0	805	24	0
56	DW	1631	0	839	44	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
56	DY	1561	0	796	39	0
57	BZ	5690	0	5783	272	0
57	DZ	5690	0	5783	322	0
58	A0	3	0	0	0	0
58	A2	2	0	0	0	0
58	A4	1	0	0	0	0
58	A5	4	0	0	0	0
58	A6	1	0	0	0	0
58	A7	6	0	0	0	0
58	A8	2	0	0	0	0
58	A9	1	0	0	0	0
58	AA	815	0	0	0	0
58	AB	23	0	0	0	0
58	AD	12	0	0	0	0
58	AE	5	0	0	0	0
58	AF	8	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	3	0	0	0	0
58	AQ	3	0	0	0	0
58	AR	2	0	0	0	0
58	AU	4	0	0	0	0
58	AV	6	0	0	0	0
58	AW	4	0	0	0	0
58	AX	1	0	0	0	0
58	AY	1	0	0	0	0
58	AZ	2	0	0	0	0
58	BA	213	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	2	0	0	0	0
58	BM	2	0	0	0	0
58	BN	1	0	0	0	0
58	BT	1	0	0	0	0
58	BV	1	0	0	0	0
58	BW	3	0	0	0	0
58	BZ	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
58	C3	1	0	0	0	0
58	C5	1	0	0	0	0
58	C7	1	0	0	0	0
58	C8	1	0	0	0	0
58	CA	664	0	0	0	0
58	CB	13	0	0	0	0
58	CD	3	0	0	0	0
58	CE	6	0	0	0	0
58	CF	5	0	0	0	0
58	CG	1	0	0	0	0
58	CN	1	0	0	0	0
58	CO	2	0	0	0	0
58	CP	3	0	0	0	0
58	CQ	5	0	0	0	0
58	CR	1	0	0	0	0
58	CU	1	0	0	0	0
58	CV	2	0	0	0	0
58	CW	1	0	0	0	0
58	CY	1	0	0	0	0
58	DA	168	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	DT	1	0	0	0	0
58	DW	3	0	0	0	0
58	DZ	2	0	0	0	0
59	A4	1	0	0	0	0
59	A5	1	0	0	0	0
59	A6	1	0	0	0	0
59	A9	1	0	0	0	0
59	AY	1	0	0	0	0
59	BN	1	0	0	0	0
59	C4	1	0	0	0	0
59	C5	1	0	0	0	0
59	C6	1	0	0	0	0
59	C9	1	0	0	0	0
59	CY	1	0	0	0	0
59	DN	1	0	0	0	0
60	BD	8	0	0	1	0
60	DD	8	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
61	BZ	37	0	47	11	0
61	DZ	37	0	47	17	0
62	BZ	28	0	12	5	0
62	DZ	28	0	12	9	0
63	A0	7	0	0	1	0
63	A1	3	0	0	0	0
63	A3	1	0	0	0	0
63	A5	2	0	0	0	0
63	A6	1	0	0	0	0
63	A7	3	0	0	2	0
63	A8	11	0	0	2	0
63	AA	1408	0	0	60	0
63	AB	36	0	0	1	0
63	AD	15	0	0	1	0
63	AE	19	0	0	5	0
63	AF	8	0	0	1	0
63	AG	3	0	0	1	0
63	AH	1	0	0	0	0
63	AN	2	0	0	1	0
63	AO	3	0	0	0	0
63	AP	15	0	0	0	0
63	AQ	3	0	0	0	0
63	AR	3	0	0	0	0
63	AS	1	0	0	0	0
63	AT	2	0	0	0	0
63	AU	6	0	0	0	0
63	AW	1	0	0	0	0
63	AX	2	0	0	0	0
63	AZ	1	0	0	0	0
63	BA	205	0	0	13	0
63	BD	3	0	0	0	0
63	BE	3	0	0	0	0
63	BJ	1	0	0	0	0
63	BL	2	0	0	0	0
63	BM	1	0	0	0	0
63	BO	1	0	0	0	0
63	BV	2	0	0	0	0
63	BW	1	0	0	0	0
63	BZ	3	0	0	0	0
63	C0	5	0	0	0	0
63	C1	3	0	0	0	0
63	C3	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
63	C5	1	0	0	0	0
63	C7	3	0	0	0	0
63	C8	3	0	0	1	0
63	CA	981	0	0	65	0
63	CB	9	0	0	0	0
63	CD	15	0	0	0	0
63	CE	9	0	0	1	0
63	CF	6	0	0	0	0
63	CP	13	0	0	3	0
63	CQ	1	0	0	0	0
63	CT	3	0	0	0	0
63	CU	4	0	0	1	0
63	CV	1	0	0	0	0
63	CW	1	0	0	0	0
63	CX	1	0	0	0	0
63	CY	1	0	0	0	0
63	DA	153	0	0	11	0
63	DE	2	0	0	0	0
63	DH	1	0	0	1	0
63	DJ	1	0	0	0	0
63	DK	2	0	0	0	0
63	DL	1	0	0	0	0
63	DP	1	0	0	0	0
63	DT	1	0	0	0	0
63	DY	1	0	0	0	0
63	DZ	2	0	0	0	0
All	All	310279	0	209988	7283	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 7283 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AA:1891:G:C5'	3:AC:206:LYS:CG	1.80	1.55
1:AA:1891:G:H5''	3:AC:206:LYS:CG	1.26	1.54
1:AA:1891:G:C5'	3:AC:206:LYS:HG3	1.40	1.40
1:CA:2128:C:H5''	3:CC:219:MET:CE	1.55	1.37
1:AA:2143:G:N2	3:AC:169:THR:OG1	1.57	1.36

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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%)	249 (91%)	20 (7%)	4 (2%)	8	29
4	CD	273/276 (99%)	242 (89%)	26 (10%)	5 (2%)	7	24
5	AE	202/206 (98%)	191 (95%)	9 (4%)	2 (1%)	13	39
5	CE	202/206 (98%)	174 (86%)	19 (9%)	9 (4%)	2	7
6	AF	201/210 (96%)	187 (93%)	11 (6%)	3 (2%)	8	29
6	CF	201/210 (96%)	186 (92%)	12 (6%)	3 (2%)	8	29
7	AG	179/182 (98%)	143 (80%)	25 (14%)	11 (6%)	1	3
7	CG	179/182 (98%)	148 (83%)	20 (11%)	11 (6%)	1	3
8	AH	172/180 (96%)	150 (87%)	20 (12%)	2 (1%)	11	34
8	CH	172/180 (96%)	148 (86%)	19 (11%)	5 (3%)	3	13
9	AK	128/173 (74%)	68 (53%)	33 (26%)	27 (21%)	0	0
9	CK	128/173 (74%)	69 (54%)	24 (19%)	35 (27%)	0	0
10	AL	137/147 (93%)	105 (77%)	23 (17%)	9 (7%)	1	3
10	CL	137/147 (93%)	95 (69%)	33 (24%)	9 (7%)	1	3
11	AN	138/140 (99%)	133 (96%)	4 (3%)	1 (1%)	19	48
11	CN	138/140 (99%)	125 (91%)	11 (8%)	2 (1%)	9	30
12	AO	120/122 (98%)	114 (95%)	4 (3%)	2 (2%)	7	26
12	CO	120/122 (98%)	105 (88%)	12 (10%)	3 (2%)	4	17
13	AP	147/150 (98%)	132 (90%)	13 (9%)	2 (1%)	9	30
13	CP	147/150 (98%)	128 (87%)	16 (11%)	3 (2%)	6	21
14	AQ	139/141 (99%)	124 (89%)	13 (9%)	2 (1%)	9	30
14	CQ	139/141 (99%)	121 (87%)	15 (11%)	3 (2%)	5	20
15	AR	116/118 (98%)	100 (86%)	13 (11%)	3 (3%)	4	16

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
15	CR	116/118 (98%)	92 (79%)	16 (14%)	8 (7%)	1	2
16	AS	108/112 (96%)	92 (85%)	12 (11%)	4 (4%)	2	9
16	CS	108/112 (96%)	86 (80%)	17 (16%)	5 (5%)	2	6
17	AT	129/146 (88%)	118 (92%)	10 (8%)	1 (1%)	16	44
17	CT	129/146 (88%)	109 (84%)	15 (12%)	5 (4%)	2	9
18	AU	114/118 (97%)	111 (97%)	3 (3%)	0	100	100
18	CU	114/118 (97%)	103 (90%)	10 (9%)	1 (1%)	14	42
19	AV	99/101 (98%)	92 (93%)	5 (5%)	2 (2%)	6	21
19	CV	99/101 (98%)	87 (88%)	9 (9%)	3 (3%)	3	13
20	AW	110/113 (97%)	106 (96%)	4 (4%)	0	100	100
20	CW	110/113 (97%)	100 (91%)	10 (9%)	0	100	100
21	AX	93/96 (97%)	88 (95%)	5 (5%)	0	100	100
21	CX	93/96 (97%)	80 (86%)	11 (12%)	2 (2%)	5	20
22	AY	105/110 (96%)	91 (87%)	11 (10%)	3 (3%)	3	13
22	CY	105/110 (96%)	90 (86%)	13 (12%)	2 (2%)	6	23
23	AZ	183/206 (89%)	146 (80%)	24 (13%)	13 (7%)	1	2
23	CZ	183/206 (89%)	140 (76%)	31 (17%)	12 (7%)	1	3
24	A0	81/85 (95%)	72 (89%)	8 (10%)	1 (1%)	11	34
24	C0	81/85 (95%)	70 (86%)	11 (14%)	0	100	100
25	A1	95/98 (97%)	86 (90%)	7 (7%)	2 (2%)	5	20
25	C1	95/98 (97%)	87 (92%)	4 (4%)	4 (4%)	2	8
26	A2	68/72 (94%)	62 (91%)	5 (7%)	1 (2%)	8	29
26	C2	68/72 (94%)	63 (93%)	4 (6%)	1 (2%)	8	29
27	A3	57/60 (95%)	55 (96%)	2 (4%)	0	100	100
27	C3	57/60 (95%)	52 (91%)	5 (9%)	0	100	100
28	A4	67/71 (94%)	41 (61%)	19 (28%)	7 (10%)	0	1
28	C4	67/71 (94%)	53 (79%)	11 (16%)	3 (4%)	2	7
29	A5	57/60 (95%)	53 (93%)	4 (7%)	0	100	100
29	C5	57/60 (95%)	51 (90%)	5 (9%)	1 (2%)	7	24
30	A6	51/54 (94%)	48 (94%)	2 (4%)	1 (2%)	6	21
30	C6	51/54 (94%)	46 (90%)	4 (8%)	1 (2%)	6	21

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
31	A7	46/49 (94%)	44 (96%)	2 (4%)	0	100	100
31	C7	46/49 (94%)	43 (94%)	1 (2%)	2 (4%)	2	7
32	A8	62/65 (95%)	60 (97%)	2 (3%)	0	100	100
32	C8	62/65 (95%)	59 (95%)	2 (3%)	1 (2%)	8	27
33	A9	35/37 (95%)	35 (100%)	0	0	100	100
33	C9	35/37 (95%)	33 (94%)	2 (6%)	0	100	100
35	BB	229/256 (90%)	176 (77%)	42 (18%)	11 (5%)	2	6
35	DB	229/256 (90%)	177 (77%)	37 (16%)	15 (7%)	1	3
36	BC	204/239 (85%)	169 (83%)	28 (14%)	7 (3%)	3	11
36	DC	204/239 (85%)	175 (86%)	26 (13%)	3 (2%)	8	29
37	BD	206/209 (99%)	154 (75%)	34 (16%)	18 (9%)	0	1
37	DD	206/209 (99%)	161 (78%)	31 (15%)	14 (7%)	1	2
38	BE	146/162 (90%)	111 (76%)	26 (18%)	9 (6%)	1	3
38	DE	146/162 (90%)	122 (84%)	21 (14%)	3 (2%)	5	20
39	BF	98/101 (97%)	80 (82%)	15 (15%)	3 (3%)	3	12
39	DF	98/101 (97%)	82 (84%)	15 (15%)	1 (1%)	13	39
40	BG	153/156 (98%)	131 (86%)	17 (11%)	5 (3%)	3	11
40	DG	153/156 (98%)	133 (87%)	14 (9%)	6 (4%)	2	9
41	BH	135/138 (98%)	111 (82%)	18 (13%)	6 (4%)	2	7
41	DH	135/138 (98%)	122 (90%)	13 (10%)	0	100	100
42	BI	125/128 (98%)	104 (83%)	16 (13%)	5 (4%)	2	8
42	DI	125/128 (98%)	104 (83%)	18 (14%)	3 (2%)	5	18
43	BJ	95/105 (90%)	80 (84%)	12 (13%)	3 (3%)	3	12
43	DJ	94/105 (90%)	76 (81%)	9 (10%)	9 (10%)	0	1
44	BK	112/129 (87%)	96 (86%)	12 (11%)	4 (4%)	3	10
44	DK	112/129 (87%)	98 (88%)	11 (10%)	3 (3%)	4	15
45	BL	120/132 (91%)	111 (92%)	7 (6%)	2 (2%)	7	26
45	DL	120/132 (91%)	103 (86%)	13 (11%)	4 (3%)	3	11
46	BM	115/126 (91%)	89 (77%)	23 (20%)	3 (3%)	4	16
46	DM	120/126 (95%)	100 (83%)	12 (10%)	8 (7%)	1	3
47	BN	58/61 (95%)	47 (81%)	9 (16%)	2 (3%)	3	11

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
47	DN	58/61 (95%)	53 (91%)	5 (9%)	0	100	100
48	BO	86/89 (97%)	72 (84%)	8 (9%)	6 (7%)	1	2
48	DO	86/89 (97%)	75 (87%)	8 (9%)	3 (4%)	3	10
49	BP	80/88 (91%)	52 (65%)	19 (24%)	9 (11%)	0	1
49	DP	80/88 (91%)	65 (81%)	12 (15%)	3 (4%)	2	9
50	BQ	97/105 (92%)	82 (84%)	9 (9%)	6 (6%)	1	3
50	DQ	97/105 (92%)	87 (90%)	7 (7%)	3 (3%)	3	12
51	BR	66/88 (75%)	60 (91%)	6 (9%)	0	100	100
51	DR	66/88 (75%)	57 (86%)	7 (11%)	2 (3%)	3	13
52	BS	82/93 (88%)	66 (80%)	14 (17%)	2 (2%)	5	18
52	DS	81/93 (87%)	68 (84%)	8 (10%)	5 (6%)	1	3
53	BT	94/106 (89%)	77 (82%)	10 (11%)	7 (7%)	1	2
53	DT	94/106 (89%)	81 (86%)	10 (11%)	3 (3%)	3	12
54	BU	21/27 (78%)	20 (95%)	1 (5%)	0	100	100
54	DU	21/27 (78%)	19 (90%)	1 (5%)	1 (5%)	2	6
57	BZ	726/758 (96%)	569 (78%)	106 (15%)	51 (7%)	1	2
57	DZ	726/758 (96%)	554 (76%)	121 (17%)	51 (7%)	1	2
All	All	13389/14444 (93%)	11230 (84%)	1582 (12%)	577 (4%)	2	7

5 of 577 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%)	104 (94%)	7 (6%)	15	42
3	CC	111/180 (62%)	103 (93%)	8 (7%)	12	34
4	AD	215/218 (99%)	181 (84%)	34 (16%)	2	7
4	CD	216/218 (99%)	179 (83%)	37 (17%)	1	5
5	AE	164/166 (99%)	130 (79%)	34 (21%)	1	3
5	CE	164/166 (99%)	130 (79%)	34 (21%)	1	3
6	AF	160/166 (96%)	128 (80%)	32 (20%)	1	3
6	CF	159/166 (96%)	124 (78%)	35 (22%)	1	2
7	AG	143/156 (92%)	114 (80%)	29 (20%)	1	3
7	CG	142/156 (91%)	111 (78%)	31 (22%)	1	2
8	AH	144/148 (97%)	121 (84%)	23 (16%)	2	6
8	CH	144/148 (97%)	124 (86%)	20 (14%)	3	9
10	AL	104/111 (94%)	83 (80%)	21 (20%)	1	3
10	CL	104/111 (94%)	84 (81%)	20 (19%)	1	4
11	AN	118/119 (99%)	97 (82%)	21 (18%)	1	5
11	CN	118/119 (99%)	92 (78%)	26 (22%)	1	2
12	AO	100/100 (100%)	88 (88%)	12 (12%)	4	14
12	CO	100/100 (100%)	82 (82%)	18 (18%)	1	4
13	AP	116/116 (100%)	90 (78%)	26 (22%)	1	2
13	CP	115/116 (99%)	95 (83%)	20 (17%)	1	5
14	AQ	111/111 (100%)	99 (89%)	12 (11%)	5	17
14	CQ	111/111 (100%)	91 (82%)	20 (18%)	1	4
15	AR	101/101 (100%)	81 (80%)	20 (20%)	1	3
15	CR	101/101 (100%)	78 (77%)	23 (23%)	0	2
16	AS	87/88 (99%)	70 (80%)	17 (20%)	1	3
16	CS	85/88 (97%)	66 (78%)	19 (22%)	1	2
17	AT	115/127 (91%)	98 (85%)	17 (15%)	2	8
17	CT	113/127 (89%)	90 (80%)	23 (20%)	1	3
18	AU	93/94 (99%)	79 (85%)	14 (15%)	2	8
18	CU	93/94 (99%)	80 (86%)	13 (14%)	3	9
19	AV	80/82 (98%)	63 (79%)	17 (21%)	1	3
19	CV	80/82 (98%)	68 (85%)	12 (15%)	2	8

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
20	AW	90/92 (98%)	77 (86%)	13 (14%)	2	8
20	CW	90/92 (98%)	82 (91%)	8 (9%)	8	25
21	AX	77/78 (99%)	69 (90%)	8 (10%)	5	18
21	CX	77/78 (99%)	69 (90%)	8 (10%)	5	18
22	AY	85/91 (93%)	71 (84%)	14 (16%)	2	6
22	CY	85/91 (93%)	69 (81%)	16 (19%)	1	4
23	AZ	156/179 (87%)	121 (78%)	35 (22%)	1	2
23	CZ	156/179 (87%)	129 (83%)	27 (17%)	1	5
24	A0	65/67 (97%)	61 (94%)	4 (6%)	15	43
24	C0	65/67 (97%)	60 (92%)	5 (8%)	10	31
25	A1	80/83 (96%)	70 (88%)	10 (12%)	3	12
25	C1	80/83 (96%)	66 (82%)	14 (18%)	1	5
26	A2	65/67 (97%)	55 (85%)	10 (15%)	2	7
26	C2	65/67 (97%)	51 (78%)	14 (22%)	1	2
27	A3	51/52 (98%)	41 (80%)	10 (20%)	1	3
27	C3	50/52 (96%)	42 (84%)	8 (16%)	2	6
28	A4	60/63 (95%)	42 (70%)	18 (30%)	0	1
28	C4	53/63 (84%)	41 (77%)	12 (23%)	1	2
29	A5	50/52 (96%)	43 (86%)	7 (14%)	3	9
29	C5	50/52 (96%)	42 (84%)	8 (16%)	2	6
30	A6	51/52 (98%)	39 (76%)	12 (24%)	0	2
30	C6	50/52 (96%)	39 (78%)	11 (22%)	1	2
31	A7	41/42 (98%)	34 (83%)	7 (17%)	1	5
31	C7	41/42 (98%)	32 (78%)	9 (22%)	1	2
32	A8	54/55 (98%)	46 (85%)	8 (15%)	2	8
32	C8	54/55 (98%)	44 (82%)	10 (18%)	1	4
33	A9	34/34 (100%)	32 (94%)	2 (6%)	16	44
33	C9	34/34 (100%)	32 (94%)	2 (6%)	16	44
35	BB	192/220 (87%)	153 (80%)	39 (20%)	1	3
35	DB	187/220 (85%)	151 (81%)	36 (19%)	1	4
36	BC	143/188 (76%)	129 (90%)	14 (10%)	6	21

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
36	DC	141/188 (75%)	116 (82%)	25 (18%)	1	5
37	BD	170/181 (94%)	143 (84%)	27 (16%)	2	7
37	DD	174/181 (96%)	137 (79%)	37 (21%)	1	3
38	BE	113/123 (92%)	89 (79%)	24 (21%)	1	3
38	DE	114/123 (93%)	92 (81%)	22 (19%)	1	4
39	BF	84/90 (93%)	68 (81%)	16 (19%)	1	4
39	DF	86/90 (96%)	75 (87%)	11 (13%)	3	12
40	BG	119/127 (94%)	102 (86%)	17 (14%)	2	9
40	DG	120/127 (94%)	99 (82%)	21 (18%)	1	5
41	BH	114/119 (96%)	96 (84%)	18 (16%)	2	7
41	DH	114/119 (96%)	92 (81%)	22 (19%)	1	4
42	BI	91/99 (92%)	75 (82%)	16 (18%)	1	5
42	DI	89/99 (90%)	76 (85%)	13 (15%)	2	8
43	BJ	66/92 (72%)	61 (92%)	5 (8%)	11	32
43	DJ	69/92 (75%)	65 (94%)	4 (6%)	17	45
44	BK	83/99 (84%)	68 (82%)	15 (18%)	1	4
44	DK	83/99 (84%)	77 (93%)	6 (7%)	12	34
45	BL	97/109 (89%)	83 (86%)	14 (14%)	2	8
45	DL	97/109 (89%)	82 (84%)	15 (16%)	2	7
46	BM	91/101 (90%)	70 (77%)	21 (23%)	0	2
46	DM	92/101 (91%)	79 (86%)	13 (14%)	3	9
47	BN	49/50 (98%)	40 (82%)	9 (18%)	1	4
47	DN	49/50 (98%)	40 (82%)	9 (18%)	1	4
48	BO	78/80 (98%)	69 (88%)	9 (12%)	4	15
48	DO	78/80 (98%)	68 (87%)	10 (13%)	3	12
49	BP	69/74 (93%)	53 (77%)	16 (23%)	0	2
49	DP	68/74 (92%)	56 (82%)	12 (18%)	1	5
50	BQ	94/97 (97%)	74 (79%)	20 (21%)	1	3
50	DQ	94/97 (97%)	85 (90%)	9 (10%)	7	22
51	BR	59/77 (77%)	48 (81%)	11 (19%)	1	4
51	DR	59/77 (77%)	47 (80%)	12 (20%)	1	3

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
52	BS	70/80 (88%)	60 (86%)	10 (14%)	2	9
52	DS	67/80 (84%)	59 (88%)	8 (12%)	4	14
53	BT	70/82 (85%)	56 (80%)	14 (20%)	1	3
53	DT	71/82 (87%)	63 (89%)	8 (11%)	4	16
54	BU	18/22 (82%)	16 (89%)	2 (11%)	5	16
54	DU	18/22 (82%)	18 (100%)	0	100	100
57	BZ	609/636 (96%)	485 (80%)	124 (20%)	1	3
57	DZ	609/636 (96%)	474 (78%)	135 (22%)	1	2
All	All	10785/11672 (92%)	8911 (83%)	1874 (17%)	1	5

5 of 1874 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
57	BZ	624	LEU
57	DZ	133	ILE
12	CO	1	MET
57	DZ	22	ASP
41	DH	21	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 175 such sidechains are listed below:

Mol	Chain	Res	Type
21	CX	31	HIS
40	DG	28	ASN
23	CZ	50	GLN
36	DC	110	ASN
44	DK	117	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	AA	2845/2915 (97%)	527 (18%)	56 (1%)
1	CA	2839/2915 (97%)	579 (20%)	39 (1%)
2	AB	119/121 (98%)	23 (19%)	0
2	CB	119/121 (98%)	21 (17%)	0
34	BA	1491/1521 (98%)	310 (20%)	22 (1%)
34	DA	1498/1521 (98%)	303 (20%)	24 (1%)

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
55	BV	6/18 (33%)	1 (16%)	0
55	DV	5/18 (27%)	1 (20%)	0
56	BW	74/76 (97%)	15 (20%)	0
56	BY	71/76 (93%)	23 (32%)	2 (2%)
56	DW	74/76 (97%)	19 (25%)	2 (2%)
56	DY	69/76 (90%)	21 (30%)	1 (1%)
All	All	9210/9454 (97%)	1843 (20%)	146 (1%)

5 of 1843 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	AA	9	U
1	AA	12	U
1	AA	13	A
1	AA	34	C
1	AA	45	C

5 of 146 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	CA	2566	A
56	DW	13	C
34	DA	115	G
34	DA	748	C
1	AA	2434	A

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

28 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	PSU	BW	55	56	18,21,22	1.28	2 (11%)	21,30,33	1.94	4 (19%)
56	PSU	BW	32	56	18,21,22	1.40	3 (16%)	21,30,33	2.19	6 (28%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
56	PSU	DW	32	56	18,21,22	1.41	3 (16%)	21,30,33	1.88	4 (19%)
56	5MU	BY	54	56	19,22,23	1.53	5 (26%)	27,32,35	2.19	9 (33%)
56	PSU	DW	55	56	18,21,22	1.37	3 (16%)	21,30,33	1.87	3 (14%)
56	7MG	DY	46	56	23,26,27	1.25	3 (13%)	27,39,42	2.76	7 (25%)
56	4SU	BY	8	56	18,21,22	1.75	5 (27%)	25,30,33	2.12	6 (24%)
56	PSU	BY	39	56	18,21,22	1.38	2 (11%)	21,30,33	1.93	3 (14%)
56	5MU	BW	54	56	19,22,23	1.52	6 (31%)	27,32,35	2.29	6 (22%)
56	5MU	DY	54	56	19,22,23	1.44	6 (31%)	27,32,35	2.09	5 (18%)
56	MIA	BY	37	56	17,24,32	1.01	1 (5%)	16,35,47	1.37	2 (12%)
56	5MU	DW	54	56	19,22,23	1.48	6 (31%)	27,32,35	2.21	8 (29%)
56	PSU	DY	32	56	18,21,22	1.37	2 (11%)	21,30,33	1.96	4 (19%)
56	PSU	DY	39	56	18,21,22	1.43	2 (11%)	21,30,33	1.96	3 (14%)
56	PSU	DW	39	56	18,21,22	1.38	2 (11%)	21,30,33	2.17	5 (23%)
56	4SU	DW	8	56	18,21,22	1.73	3 (16%)	25,30,33	2.04	5 (20%)
56	MIA	BW	37	56	24,31,32	2.43	4 (16%)	22,44,47	3.24	7 (31%)
56	7MG	BY	46	56	23,26,27	1.28	3 (13%)	27,39,42	2.70	7 (25%)
56	MIA	DY	37	56	17,24,32	0.92	1 (5%)	16,35,47	1.32	2 (12%)
56	MIA	DW	37	56	24,31,32	2.46	3 (12%)	22,44,47	1.97	6 (27%)
56	PSU	BY	55	56	18,21,22	1.38	2 (11%)	21,30,33	1.99	3 (14%)
56	PSU	BY	32	56	18,21,22	1.42	2 (11%)	21,30,33	1.93	4 (19%)
56	4SU	BW	8	56	18,21,22	1.56	3 (16%)	25,30,33	2.30	5 (20%)
56	7MG	DW	46	56	23,26,27	1.32	4 (17%)	27,39,42	2.64	7 (25%)
56	4SU	DY	8	56	18,21,22	1.84	4 (22%)	25,30,33	2.34	5 (20%)
56	PSU	DY	55	56	18,21,22	1.42	3 (16%)	21,30,33	2.02	3 (14%)
56	7MG	BW	46	56	23,26,27	1.31	3 (13%)	27,39,42	2.97	7 (25%)
56	PSU	BW	39	56	18,21,22	1.37	2 (11%)	21,30,33	1.95	5 (23%)

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	PSU	BW	55	56	-	0/7/25/26	0/2/2/2
56	PSU	BW	32	56	-	4/7/25/26	0/2/2/2
56	PSU	DW	32	56	-	3/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
56	5MU	BY	54	56	-	2/7/25/26	0/2/2/2
56	PSU	DW	55	56	-	0/7/25/26	0/2/2/2
56	7MG	DY	46	56	-	3/7/37/38	0/3/3/3
56	4SU	BY	8	56	-	1/7/25/26	0/2/2/2
56	PSU	BY	39	56	-	0/7/25/26	0/2/2/2
56	5MU	BW	54	56	-	0/7/25/26	0/2/2/2
56	5MU	DY	54	56	-	2/7/25/26	0/2/2/2
56	MIA	BY	37	56	-	2/3/25/34	0/3/3/3
56	5MU	DW	54	56	-	0/7/25/26	0/2/2/2
56	PSU	DY	32	56	-	0/7/25/26	0/2/2/2
56	PSU	DY	39	56	-	2/7/25/26	0/2/2/2
56	PSU	DW	39	56	-	0/7/25/26	0/2/2/2
56	4SU	DW	8	56	-	0/7/25/26	0/2/2/2
56	MIA	BW	37	56	-	5/11/33/34	0/3/3/3
56	7MG	BY	46	56	-	4/7/37/38	0/3/3/3
56	MIA	DY	37	56	-	3/3/25/34	0/3/3/3
56	MIA	DW	37	56	-	5/11/33/34	0/3/3/3
56	PSU	BY	55	56	-	2/7/25/26	0/2/2/2
56	PSU	BY	32	56	-	0/7/25/26	0/2/2/2
56	4SU	BW	8	56	-	0/7/25/26	0/2/2/2
56	7MG	DW	46	56	-	2/7/37/38	0/3/3/3
56	4SU	DY	8	56	-	1/7/25/26	0/2/2/2
56	PSU	DY	55	56	-	3/7/25/26	0/2/2/2
56	7MG	BW	46	56	-	0/7/37/38	0/3/3/3
56	PSU	BW	39	56	-	0/7/25/26	0/2/2/2

The worst 5 of 88 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
56	DW	37	MIA	C2-S10	-8.05	1.69	1.75
56	BW	37	MIA	C13-C14	7.46	1.54	1.32
56	BW	37	MIA	C2-S10	-7.31	1.69	1.75
56	DW	37	MIA	C13-C14	7.29	1.54	1.32
56	DY	8	4SU	C4-S4	-4.87	1.60	1.68

The worst 5 of 141 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
56	BW	37	MIA	C11-S10-C2	-11.58	93.56	102.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
56	DY	46	7MG	N9-C4-N3	9.62	139.55	125.46
56	BW	46	7MG	N9-C4-N3	9.54	139.44	125.46
56	BY	46	7MG	N9-C4-N3	9.19	138.93	125.46
56	DW	46	7MG	N9-C4-N3	8.89	138.48	125.46

There are no chirality outliers.

5 of 44 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
56	BW	32	PSU	C2'-C1'-C5-C4
56	BW	32	PSU	O4'-C1'-C5-C4
56	BW	32	PSU	O4'-C1'-C5-C6
56	BW	37	MIA	N6-C12-C13-C14
56	BW	37	MIA	C12-C13-C14-C15

There are no ring outliers.

10 monomers are involved in 17 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
56	DW	55	PSU	2	0
56	DY	46	7MG	2	0
56	BY	8	4SU	1	0
56	DW	54	5MU	1	0
56	DW	39	PSU	4	0
56	BW	37	MIA	1	0
56	DY	37	MIA	1	0
56	DW	37	MIA	2	0
56	DW	46	7MG	2	0
56	DY	55	PSU	2	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 2058 ligands modelled in this entry, 2052 are monoatomic - leaving 6 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
60	SF4	DD	501	37	0,12,12	-	-	-		
62	GDP	BZ	704	58	25,30,30	1.01	1 (4%)	30,47,47	1.49	7 (23%)
61	FUA	DZ	703	-	39,40,40	1.70	7 (17%)	50,64,64	1.70	8 (16%)
61	FUA	BZ	703	-	39,40,40	1.70	7 (17%)	50,64,64	1.70	8 (16%)
60	SF4	BD	501	37	0,12,12	-	-	-		
62	GDP	DZ	704	58	25,30,30	0.92	1 (4%)	30,47,47	1.07	1 (3%)

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
60	SF4	DD	501	37	-	-	0/6/5/5
62	GDP	BZ	704	58	-	4/12/32/32	0/3/3/3
60	SF4	BD	501	37	-	-	0/6/5/5
61	FUA	DZ	703	-	-	7/16/92/92	0/4/4/4
61	FUA	BZ	703	-	-	7/16/92/92	0/4/4/4
62	GDP	DZ	704	58	-	2/12/32/32	0/3/3/3

The worst 5 of 16 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
61	BZ	703	FUA	C23-C22	-4.44	1.39	1.51
61	DZ	703	FUA	C23-C22	-4.41	1.40	1.51
61	BZ	703	FUA	C23-C24	-4.35	1.39	1.53
61	DZ	703	FUA	C23-C24	-4.34	1.39	1.53
61	BZ	703	FUA	C29-C22	4.24	1.53	1.47

The worst 5 of 24 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
61	BZ	703	FUA	C24-C23-C22	5.35	124.11	112.72
61	DZ	703	FUA	C24-C23-C22	5.34	124.09	112.72
61	BZ	703	FUA	C13-C12-C11	-4.20	105.80	111.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
61	DZ	703	FUA	C13-C12-C11	-4.16	105.85	111.90
61	DZ	703	FUA	C16-O2-C31	-3.97	111.10	117.00

There are no chirality outliers.

5 of 20 torsion outliers are listed below:

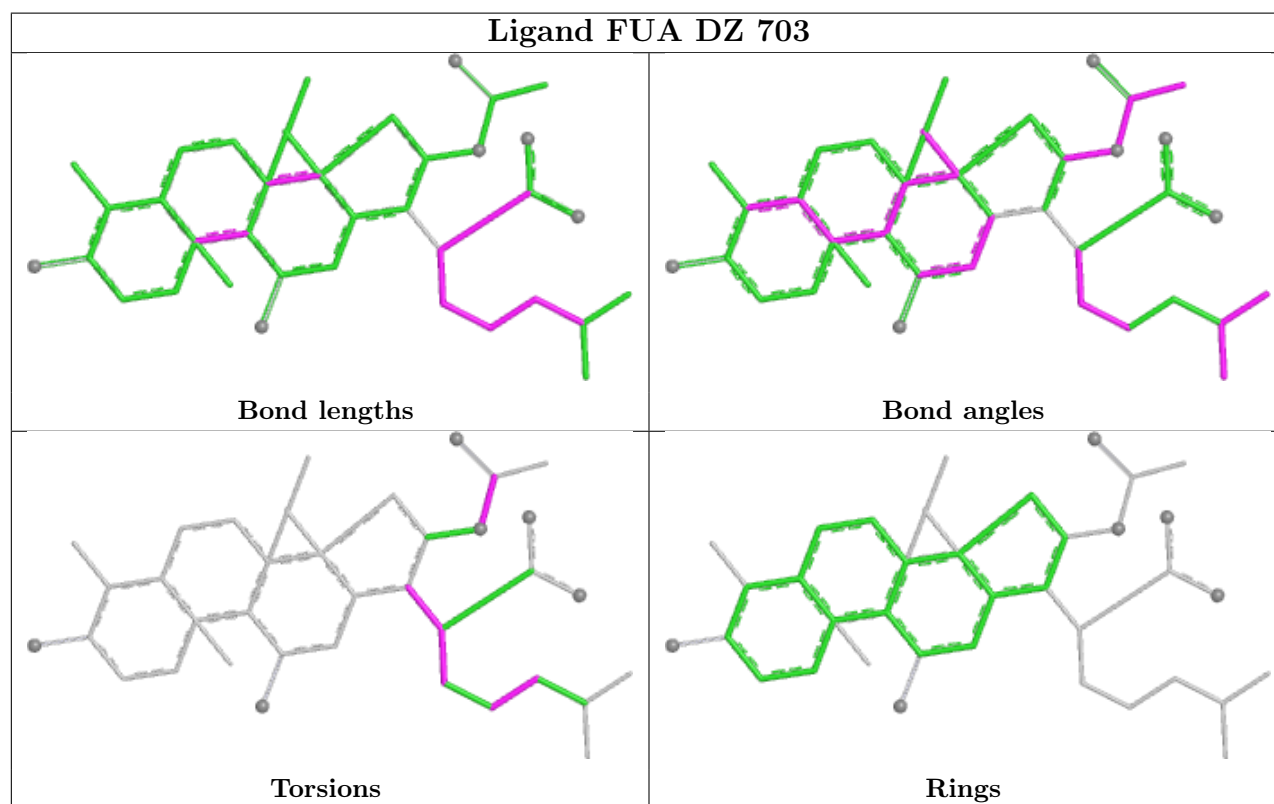
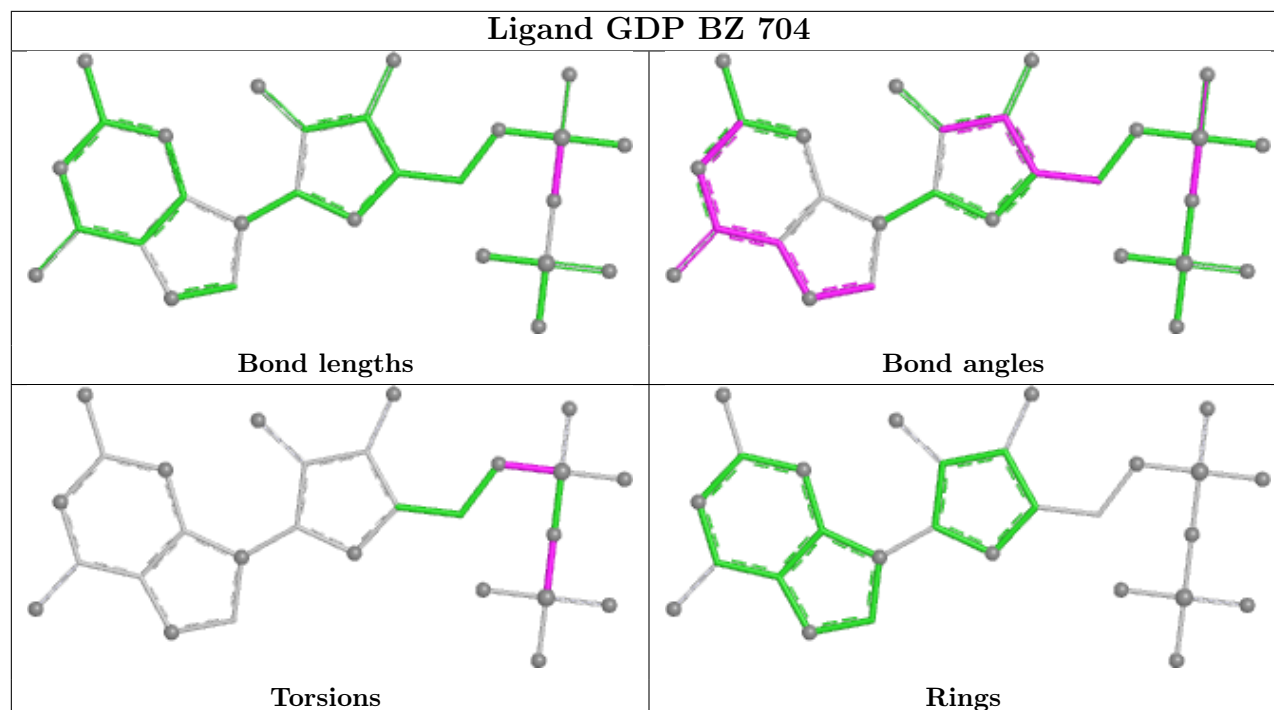
Mol	Chain	Res	Type	Atoms
61	BZ	703	FUA	C13-C17-C22-C23
61	BZ	703	FUA	C13-C17-C22-C29
61	DZ	703	FUA	C13-C17-C22-C23
61	DZ	703	FUA	C13-C17-C22-C29
62	BZ	704	GDP	PA-O3A-PB-O3B

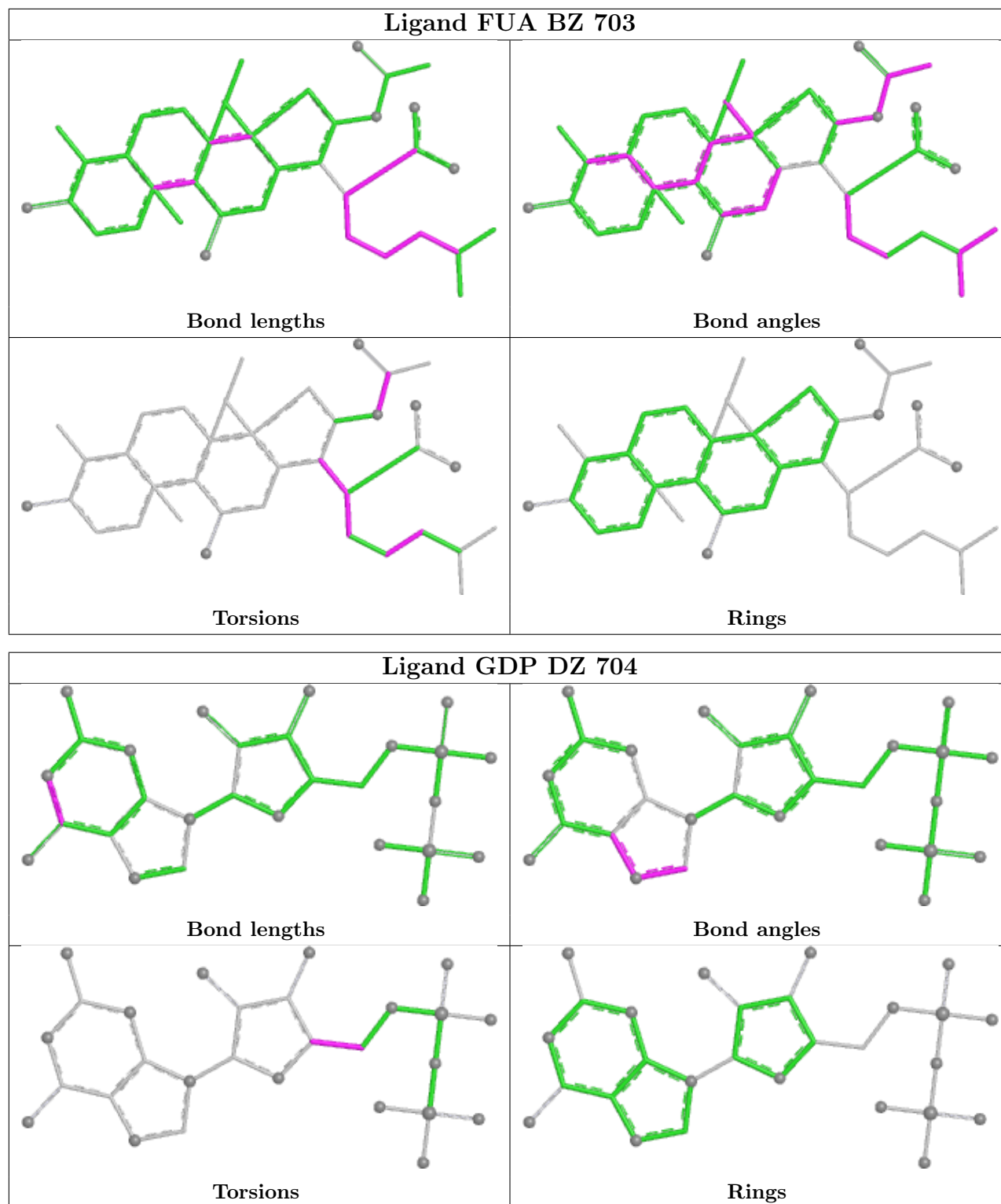
There are no ring outliers.

6 monomers are involved in 45 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
60	DD	501	SF4	2	0
62	BZ	704	GDP	5	0
61	DZ	703	FUA	17	0
61	BZ	703	FUA	11	0
60	BD	501	SF4	1	0
62	DZ	704	GDP	9	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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ > 2			OWAB(Å ²)	Q < 0.9
1	AA	2852/2915 (97%)	-0.74	77 (2%)	56	47	14, 33, 136, 352	4 (0%)
1	CA	2848/2915 (97%)	-0.21	87 (3%)	51	43	26, 56, 178, 343	0
2	AB	120/121 (99%)	-0.51	1 (0%)	82	77	22, 48, 72, 108	0
2	CB	120/121 (99%)	0.41	2 (1%)	69	61	61, 90, 117, 168	0
3	AC	137/228 (60%)	2.88	101 (73%)	0	0	258, 289, 307, 313	0
3	CC	137/228 (60%)	2.83	100 (72%)	0	0	281, 312, 331, 336	0
4	AD	275/276 (99%)	-0.64	2 (0%)	84	79	12, 34, 57, 136	0
4	CD	275/276 (99%)	-0.42	4 (1%)	71	64	16, 47, 73, 129	2 (0%)
5	AE	204/206 (99%)	-0.87	0	100	100	5, 33, 55, 75	1 (0%)
5	CE	204/206 (99%)	0.19	5 (2%)	58	49	21, 61, 106, 132	0
6	AF	203/210 (96%)	-0.73	1 (0%)	87	83	10, 35, 76, 172	0
6	CF	203/210 (96%)	-0.10	1 (0%)	87	83	21, 62, 106, 154	0
7	AG	181/182 (99%)	0.54	9 (4%)	35	28	31, 76, 134, 206	0
7	CG	181/182 (99%)	0.96	19 (10%)	13	10	72, 110, 174, 203	0
8	AH	174/180 (96%)	-0.47	1 (0%)	85	81	26, 45, 69, 111	0
8	CH	174/180 (96%)	1.10	25 (14%)	7	6	64, 111, 158, 195	0
9	AK	130/173 (75%)	1.47	33 (25%)	2	2	47, 105, 170, 221	0
9	CK	130/173 (75%)	2.03	56 (43%)	1	1	73, 159, 203, 217	0
10	AL	139/147 (94%)	1.67	40 (28%)	1	2	95, 170, 225, 245	0
10	CL	139/147 (94%)	2.19	72 (51%)	0	0	123, 192, 241, 279	1 (0%)
11	AN	140/140 (100%)	-0.87	0	100	100	13, 28, 60, 95	1 (0%)
11	CN	140/140 (100%)	0.23	3 (2%)	63	55	29, 71, 107, 150	0
12	AO	122/122 (100%)	-0.75	0	100	100	16, 37, 62, 76	0
12	CO	122/122 (100%)	-0.13	0	100	100	36, 58, 82, 104	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	AP	149/150 (99%)	-0.47	0 100 100	10, 42, 79, 102	1 (0%)
13	CP	149/150 (99%)	0.05	4 (2%) 56 47	29, 66, 115, 134	0
14	AQ	141/141 (100%)	-0.75	0 100 100	11, 33, 52, 78	0
14	CQ	141/141 (100%)	0.26	5 (3%) 47 39	35, 69, 99, 118	0
15	AR	118/118 (100%)	-0.91	0 100 100	16, 28, 43, 54	0
15	CR	118/118 (100%)	0.00	2 (1%) 69 61	32, 55, 87, 105	0
16	AS	110/112 (98%)	-0.41	0 100 100	28, 49, 79, 91	0
16	CS	110/112 (98%)	0.79	9 (8%) 19 14	43, 83, 119, 152	0
17	AT	131/146 (89%)	-0.50	3 (2%) 61 52	23, 40, 91, 164	0
17	CT	131/146 (89%)	0.13	2 (1%) 71 64	41, 64, 102, 142	0
18	AU	116/118 (98%)	-0.99	0 100 100	8, 22, 36, 89	1 (0%)
18	CU	116/118 (98%)	0.14	0 100 100	26, 64, 91, 105	0
19	AV	101/101 (100%)	-1.06	0 100 100	9, 27, 48, 73	0
19	CV	101/101 (100%)	0.11	0 100 100	34, 79, 112, 171	0
20	AW	112/113 (99%)	-0.97	0 100 100	13, 25, 43, 109	1 (0%)
20	CW	112/113 (99%)	-0.29	0 100 100	25, 48, 80, 118	0
21	AX	95/96 (98%)	-0.65	1 (1%) 77 71	16, 34, 66, 97	1 (1%)
21	CX	95/96 (98%)	0.05	4 (4%) 41 33	36, 60, 85, 106	0
22	AY	107/110 (97%)	-0.41	1 (0%) 81 75	24, 43, 86, 156	0
22	CY	107/110 (97%)	0.31	4 (3%) 45 37	45, 74, 115, 162	0
23	AZ	185/206 (89%)	-0.18	2 (1%) 77 71	28, 55, 91, 147	0
23	CZ	185/206 (89%)	0.79	8 (4%) 40 32	59, 105, 148, 213	0
24	A0	83/85 (97%)	-0.35	5 (6%) 29 22	11, 34, 77, 219	0
24	C0	83/85 (97%)	0.49	8 (9%) 15 11	39, 65, 120, 225	0
25	A1	97/98 (98%)	-0.33	2 (2%) 63 55	18, 43, 79, 99	1 (1%)
25	C1	97/98 (98%)	-0.20	3 (3%) 51 43	29, 51, 89, 125	0
26	A2	70/72 (97%)	-0.33	1 (1%) 73 66	25, 42, 67, 123	1 (1%)
26	C2	70/72 (97%)	0.28	3 (4%) 40 32	47, 70, 99, 117	0
27	A3	59/60 (98%)	-0.77	1 (1%) 69 61	13, 30, 55, 98	1 (1%)
27	C3	59/60 (98%)	0.33	2 (3%) 48 40	44, 73, 110, 150	0
28	A4	69/71 (97%)	0.97	12 (17%) 5 4	56, 116, 206, 235	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
28	C4	69/71 (97%)	1.18	11 (15%) 6 5	78, 159, 204, 220	0
29	A5	59/60 (98%)	-1.03	0 100 100	8, 25, 38, 50	0
29	C5	59/60 (98%)	-0.26	0 100 100	27, 50, 89, 102	0
30	A6	53/54 (98%)	-0.75	0 100 100	23, 40, 52, 71	0
30	C6	53/54 (98%)	-0.18	0 100 100	39, 60, 78, 103	0
31	A7	48/49 (97%)	-0.60	2 (4%) 41 33	13, 24, 69, 131	1 (2%)
31	C7	48/49 (97%)	-0.32	2 (4%) 41 33	24, 38, 95, 117	0
32	A8	64/65 (98%)	-0.80	0 100 100	16, 28, 43, 60	0
32	C8	64/65 (98%)	-0.14	1 (1%) 70 63	36, 52, 72, 80	0
33	A9	37/37 (100%)	-0.66	0 100 100	22, 34, 56, 65	1 (2%)
33	C9	37/37 (100%)	0.79	5 (13%) 8 7	44, 77, 96, 126	0
34	BA	1495/1521 (98%)	0.41	45 (3%) 52 44	30, 82, 185, 333	0
34	DA	1501/1521 (98%)	0.47	88 (5%) 29 22	37, 88, 194, 340	0
35	BB	231/256 (90%)	0.96	35 (15%) 6 5	41, 104, 170, 215	0
35	DB	231/256 (90%)	1.13	42 (18%) 4 4	68, 123, 175, 213	0
36	BC	206/239 (86%)	0.94	27 (13%) 8 7	52, 117, 172, 191	0
36	DC	206/239 (86%)	1.09	32 (15%) 6 5	67, 135, 179, 211	0
37	BD	208/209 (99%)	1.07	38 (18%) 4 4	42, 85, 137, 190	0
37	DD	208/209 (99%)	1.03	28 (13%) 8 7	58, 85, 134, 195	0
38	BE	148/162 (91%)	0.28	2 (1%) 73 66	34, 70, 104, 128	0
38	DE	148/162 (91%)	0.36	5 (3%) 48 40	45, 79, 115, 180	0
39	BF	100/101 (99%)	0.44	1 (1%) 79 73	54, 85, 116, 137	0
39	DF	100/101 (99%)	0.42	1 (1%) 79 73	45, 86, 113, 133	0
40	BG	155/156 (99%)	0.94	23 (14%) 7 6	65, 110, 182, 221	0
40	DG	155/156 (99%)	1.29	38 (24%) 2 2	68, 129, 190, 217	0
41	BH	137/138 (99%)	0.19	2 (1%) 71 64	45, 71, 97, 116	0
41	DH	137/138 (99%)	0.47	3 (2%) 62 53	53, 80, 109, 140	0
42	BI	127/128 (99%)	1.58	41 (32%) 1 1	64, 123, 164, 190	0
42	DI	127/128 (99%)	2.15	63 (49%) 0 1	89, 143, 191, 213	0
43	BJ	97/105 (92%)	1.73	38 (39%) 1 1	80, 128, 182, 213	0
43	DJ	96/105 (91%)	1.78	37 (38%) 1 1	91, 149, 196, 225	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
44	BK	114/129 (88%)	0.38	9 (7%) 20 15	34, 78, 125, 151	0
44	DK	114/129 (88%)	0.40	4 (3%) 47 39	51, 90, 115, 173	0
45	BL	122/132 (92%)	0.04	4 (3%) 49 41	35, 58, 77, 112	0
45	DL	122/132 (92%)	0.39	7 (5%) 30 24	44, 71, 95, 116	0
46	BM	117/126 (92%)	1.50	29 (24%) 2 2	76, 132, 181, 208	0
46	DM	122/126 (96%)	1.74	32 (26%) 2 2	93, 149, 195, 250	0
47	BN	60/61 (98%)	1.71	22 (36%) 1 1	66, 111, 145, 164	0
47	DN	60/61 (98%)	2.71	39 (65%) 0 0	95, 135, 176, 196	0
48	BO	88/89 (98%)	0.21	2 (2%) 61 52	34, 71, 104, 119	0
48	DO	88/89 (98%)	0.22	2 (2%) 61 52	47, 70, 104, 152	0
49	BP	82/88 (93%)	0.94	9 (10%) 12 9	46, 79, 116, 170	0
49	DP	82/88 (93%)	0.80	7 (8%) 18 14	53, 77, 111, 151	0
50	BQ	99/105 (94%)	0.30	3 (3%) 52 44	41, 70, 98, 122	0
50	DQ	99/105 (94%)	0.37	3 (3%) 52 44	42, 77, 104, 118	0
51	BR	68/88 (77%)	0.20	2 (2%) 54 45	42, 79, 122, 135	0
51	DR	68/88 (77%)	0.39	1 (1%) 71 64	52, 82, 127, 143	0
52	BS	84/93 (90%)	2.11	43 (51%) 0 0	94, 143, 191, 207	0
52	DS	83/93 (89%)	2.11	41 (49%) 0 1	86, 163, 214, 226	0
53	BT	96/106 (90%)	0.89	12 (12%) 9 8	60, 84, 121, 158	0
53	DT	96/106 (90%)	0.71	7 (7%) 22 17	56, 85, 134, 157	0
54	BU	23/27 (85%)	3.00	15 (65%) 0 0	58, 118, 156, 174	0
54	DU	23/27 (85%)	2.78	17 (73%) 0 0	92, 132, 170, 187	0
55	BV	7/18 (38%)	2.52	5 (71%) 0 0	51, 85, 207, 222	0
55	DV	6/18 (33%)	2.73	4 (66%) 0 0	82, 102, 210, 222	0
56	BW	69/76 (90%)	-0.06	3 (4%) 40 32	36, 69, 104, 210	0
56	BY	67/76 (88%)	1.68	19 (28%) 1 2	75, 278, 314, 346	0
56	DW	69/76 (90%)	0.35	4 (5%) 30 23	51, 95, 137, 251	0
56	DY	66/76 (86%)	1.79	20 (30%) 1 1	208, 287, 320, 345	0
57	BZ	730/758 (96%)	0.27	26 (3%) 46 38	35, 77, 134, 188	0
57	DZ	730/758 (96%)	0.68	57 (7%) 20 16	35, 99, 164, 218	0
All	All	22825/23898 (95%)	0.21	1779 (7%) 20 16	5, 69, 186, 352	18 (0%)

The worst 5 of 1779 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
46	DM	123	ALA	11.0
46	DM	124	PRO	8.6
47	DN	25	VAL	8.6
24	C0	2	ALA	8.5
47	DN	2	ALA	7.8

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
56	PSU	DY	32	20/21	0.14	0.21	268,268,268,268	0
56	MIA	BY	37	22/30	0.15	0.19	284,284,284,284	0
56	5MU	DY	54	21/22	0.18	0.14	305,305,305,305	1
56	PSU	BY	32	20/21	0.22	0.18	254,254,254,254	1
56	PSU	BY	55	20/21	0.22	0.15	302,302,302,302	1
56	PSU	DY	39	20/21	0.24	0.15	284,284,284,284	0
56	MIA	DY	37	22/30	0.24	0.25	319,319,319,319	1
56	PSU	DY	55	20/21	0.27	0.12	246,246,246,246	0
56	PSU	BY	39	20/21	0.29	0.14	316,316,316,316	0
56	7MG	BY	46	24/25	0.38	0.14	302,302,302,302	0
56	5MU	BY	54	21/22	0.41	0.15	315,315,315,315	0
56	4SU	BY	8	20/21	0.62	0.11	300,300,300,300	0
56	7MG	DY	46	24/25	0.69	0.13	302,302,302,302	0
56	4SU	DY	8	20/21	0.73	0.11	275,275,275,275	0
56	7MG	DW	46	24/25	0.77	0.12	114,114,114,114	2
56	PSU	DW	55	20/21	0.78	0.13	106,106,106,106	2
56	PSU	DW	32	20/21	0.85	0.12	106,106,106,106	1
56	5MU	DW	54	21/22	0.87	0.12	114,114,114,114	1
56	PSU	BW	32	20/21	0.88	0.12	81,81,81,81	1
56	7MG	BW	46	24/25	0.88	0.09	63,63,63,63	5
56	PSU	DW	39	20/21	0.89	0.17	93,93,93,93	3
56	MIA	BW	37	29/30	0.90	0.14	79,79,79,79	2
56	MIA	DW	37	29/30	0.92	0.14	94,94,94,94	0
56	4SU	DW	8	20/21	0.92	0.09	88,88,88,88	3
56	PSU	BW	55	20/21	0.93	0.08	74,74,74,74	5
56	4SU	BW	8	20/21	0.93	0.07	51,51,51,51	6
56	5MU	BW	54	21/22	0.94	0.08	74,74,74,74	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	PSU	BW	39	20/21	0.95	0.10	65,65,65,65	3

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	AA	3610	1/1	0.28	0.17	51,51,51,51	1
58	MG	CA	3107	1/1	0.28	0.24	108,108,108,108	0
58	MG	DA	1700	1/1	0.36	0.18	124,124,124,124	0
58	MG	CA	3209	1/1	0.45	0.20	93,93,93,93	0
58	MG	CA	3253	1/1	0.47	0.22	95,95,95,95	0
58	MG	CA	3624	1/1	0.48	0.21	104,104,104,104	0
58	MG	BA	1773	1/1	0.48	0.25	115,115,115,115	0
58	MG	DA	1606	1/1	0.51	0.31	84,84,84,84	0
58	MG	BA	1707	1/1	0.51	0.20	92,92,92,92	0
58	MG	DA	1660	1/1	0.52	0.32	90,90,90,90	0
58	MG	AA	3273	1/1	0.55	0.22	90,90,90,90	0
58	MG	AA	3766	1/1	0.56	0.18	72,72,72,72	0
58	MG	CA	3046	1/1	0.56	0.29	114,114,114,114	0
58	MG	BA	1711	1/1	0.56	0.20	104,104,104,104	0
58	MG	DJ	5001	1/1	0.56	0.22	105,105,105,105	0
58	MG	A4	502	1/1	0.57	0.13	123,123,123,123	0
58	MG	CB	3013	1/1	0.57	0.21	98,98,98,98	0
58	MG	CA	3126	1/1	0.57	0.35	93,93,93,93	0
58	MG	DZ	701	1/1	0.58	0.20	111,111,111,111	0
58	MG	CA	3555	1/1	0.59	0.24	83,83,83,83	0
58	MG	BZ	701	1/1	0.60	0.19	137,137,137,137	0
58	MG	CA	3590	1/1	0.61	0.15	95,95,95,95	0
58	MG	CA	3180	1/1	0.61	0.44	108,108,108,108	0
58	MG	CA	3481	1/1	0.62	0.22	91,91,91,91	0
58	MG	AA	3200	1/1	0.63	0.27	91,91,91,91	0
58	MG	DA	1755	1/1	0.64	0.20	86,86,86,86	0
58	MG	CA	3513	1/1	0.64	0.14	75,75,75,75	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	BA	1787	1/1	0.64	0.22	87,87,87,87	0
58	MG	DA	1754	1/1	0.65	0.21	81,81,81,81	0
58	MG	CA	3507	1/1	0.65	0.16	100,100,100,100	0
58	MG	CA	3205	1/1	0.66	0.18	105,105,105,105	0
58	MG	DA	1657	1/1	0.67	0.13	93,93,93,93	0
58	MG	CA	3002	1/1	0.67	0.23	114,114,114,114	0
58	MG	AA	3268	1/1	0.67	0.22	88,88,88,88	0
58	MG	BA	1618	1/1	0.67	0.21	134,134,134,134	0
58	MG	CA	3295	1/1	0.67	0.12	84,84,84,84	0
58	MG	BA	1697	1/1	0.67	0.21	98,98,98,98	0
58	MG	AA	3265	1/1	0.67	0.36	77,77,77,77	0
58	MG	BA	1617	1/1	0.68	0.14	74,74,74,74	0
58	MG	DA	1673	1/1	0.68	0.31	100,100,100,100	0
58	MG	CA	3618	1/1	0.68	0.20	65,65,65,65	0
58	MG	BA	1626	1/1	0.68	0.23	87,87,87,87	0
58	MG	BA	1691	1/1	0.68	0.19	91,91,91,91	0
58	MG	CA	3544	1/1	0.68	0.12	81,81,81,81	0
58	MG	CA	3314	1/1	0.68	0.22	77,77,77,77	0
58	MG	CA	3537	1/1	0.69	0.19	78,78,78,78	0
58	MG	CA	3080	1/1	0.69	0.37	87,87,87,87	0
58	MG	AA	3613	1/1	0.69	0.16	104,104,104,104	0
58	MG	AA	3672	1/1	0.69	0.20	25,25,25,25	1
58	MG	BA	1636	1/1	0.70	0.33	100,100,100,100	0
58	MG	DA	1706	1/1	0.70	0.28	128,128,128,128	0
58	MG	BA	1661	1/1	0.70	0.28	84,84,84,84	0
58	MG	BA	1795	1/1	0.70	0.24	86,86,86,86	0
58	MG	BA	1807	1/1	0.70	0.13	83,83,83,83	0
58	MG	AA	3758	1/1	0.70	0.26	81,81,81,81	0
58	MG	CA	3553	1/1	0.71	0.12	81,81,81,81	0
58	MG	CA	3071	1/1	0.71	0.35	97,97,97,97	0
58	MG	AB	3017	1/1	0.71	0.14	77,77,77,77	0
58	MG	AA	3751	1/1	0.71	0.22	56,56,56,56	1
58	MG	CA	3620	1/1	0.71	0.16	69,69,69,69	0
58	MG	CA	3056	1/1	0.71	0.25	85,85,85,85	0
58	MG	CA	3131	1/1	0.71	0.21	62,62,62,62	0
58	MG	CA	3300	1/1	0.71	0.20	86,86,86,86	0
58	MG	DA	1623	1/1	0.71	0.14	117,117,117,117	0
58	MG	CA	3389	1/1	0.72	0.22	75,75,75,75	0
58	MG	DA	1720	1/1	0.72	0.18	72,72,72,72	0
58	MG	AA	3784	1/1	0.72	0.19	74,74,74,74	0
58	MG	CA	3070	1/1	0.72	0.38	87,87,87,87	0
58	MG	CA	3593	1/1	0.72	0.14	73,73,73,73	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	CA	3610	1/1	0.72	0.23	98,98,98,98	0
58	MG	CA	3202	1/1	0.73	0.32	77,77,77,77	0
58	MG	AB	3018	1/1	0.73	0.15	84,84,84,84	0
58	MG	DA	1677	1/1	0.73	0.15	74,74,74,74	0
58	MG	CA	3066	1/1	0.73	0.29	84,84,84,84	0
58	MG	BA	1713	1/1	0.73	0.36	71,71,71,71	0
58	MG	CG	3001	1/1	0.73	0.22	83,83,83,83	0
58	MG	AA	3224	1/1	0.73	0.28	75,75,75,75	0
58	MG	CA	3594	1/1	0.73	0.23	80,80,80,80	0
58	MG	DA	1649	1/1	0.73	0.26	93,93,93,93	0
58	MG	CA	3076	1/1	0.73	0.16	84,84,84,84	0
58	MG	DA	1614	1/1	0.74	0.34	87,87,87,87	0
58	MG	CA	3467	1/1	0.74	0.29	80,80,80,80	0
58	MG	CA	3140	1/1	0.74	0.32	98,98,98,98	0
58	MG	AA	3108	1/1	0.74	0.39	125,125,125,125	0
58	MG	BA	1669	1/1	0.74	0.12	89,89,89,89	0
58	MG	BA	1683	1/1	0.74	0.33	84,84,84,84	0
58	MG	BA	1616	1/1	0.74	0.27	88,88,88,88	0
58	MG	CA	3460	1/1	0.75	0.30	109,109,109,109	0
58	MG	CA	3616	1/1	0.75	0.20	79,79,79,79	0
58	MG	CA	3561	1/1	0.75	0.22	95,95,95,95	0
58	MG	CA	3304	1/1	0.75	0.16	93,93,93,93	0
58	MG	AA	3690	1/1	0.75	0.17	71,71,71,71	0
58	MG	CA	3125	1/1	0.75	0.30	73,73,73,73	0
58	MG	DA	1669	1/1	0.75	0.23	84,84,84,84	0
58	MG	CA	3604	1/1	0.75	0.14	69,69,69,69	0
58	MG	AA	3744	1/1	0.76	0.17	86,86,86,86	0
58	MG	CA	3058	1/1	0.76	0.27	77,77,77,77	0
58	MG	AA	3192	1/1	0.76	0.28	76,76,76,76	0
58	MG	BA	1777	1/1	0.76	0.16	75,75,75,75	0
58	MG	CA	3290	1/1	0.76	0.30	75,75,75,75	0
58	MG	CA	3294	1/1	0.76	0.12	83,83,83,83	0
58	MG	AA	3270	1/1	0.76	0.16	54,54,54,54	0
58	MG	AA	3626	1/1	0.76	0.22	74,74,74,74	0
58	MG	AA	3112	1/1	0.76	0.36	98,98,98,98	0
58	MG	CA	3596	1/1	0.76	0.17	72,72,72,72	0
58	MG	BA	1704	1/1	0.76	0.30	89,89,89,89	0
58	MG	AA	3803	1/1	0.76	0.15	62,62,62,62	0
58	MG	CA	3008	1/1	0.76	0.38	100,100,100,100	0
58	MG	CA	3016	1/1	0.76	0.24	80,80,80,80	0
58	MG	CA	3042	1/1	0.76	0.28	95,95,95,95	0
58	MG	AA	3597	1/1	0.76	0.15	63,63,63,63	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	CA	3644	1/1	0.76	0.32	84,84,84,84	0
58	MG	CB	3001	1/1	0.76	0.20	99,99,99,99	0
58	MG	AA	3774	1/1	0.77	0.18	80,80,80,80	0
58	MG	CA	3286	1/1	0.77	0.14	64,64,64,64	0
58	MG	CA	3485	1/1	0.77	0.20	83,83,83,83	0
58	MG	AA	3105	1/1	0.77	0.17	81,81,81,81	0
58	MG	AB	3021	1/1	0.77	0.17	61,61,61,61	0
58	MG	AQ	201	1/1	0.77	0.22	62,62,62,62	0
58	MG	BA	1813	1/1	0.77	0.25	75,75,75,75	0
58	MG	BA	1721	1/1	0.77	0.18	80,80,80,80	0
58	MG	DA	1701	1/1	0.77	0.22	63,63,63,63	0
58	MG	BA	1736	1/1	0.77	0.15	81,81,81,81	0
58	MG	CB	3006	1/1	0.77	0.13	83,83,83,83	0
58	MG	CA	3363	1/1	0.77	0.13	66,66,66,66	0
58	MG	CA	3388	1/1	0.77	0.16	83,83,83,83	0
58	MG	BA	1748	1/1	0.77	0.12	83,83,83,83	0
58	MG	AA	3094	1/1	0.77	0.71	111,111,111,111	0
58	MG	BA	1768	1/1	0.78	0.16	86,86,86,86	0
58	MG	CA	3267	1/1	0.78	0.15	56,56,56,56	0
58	MG	AA	3640	1/1	0.78	0.34	77,77,77,77	0
58	MG	DA	1678	1/1	0.78	0.22	82,82,82,82	0
58	MG	DA	1687	1/1	0.78	0.14	100,100,100,100	0
58	MG	CD	302	1/1	0.78	0.26	95,95,95,95	0
58	MG	CA	3073	1/1	0.78	0.26	91,91,91,91	0
58	MG	BV	101	1/1	0.78	0.23	110,110,110,110	0
58	MG	DA	1715	1/1	0.78	0.13	76,76,76,76	0
58	MG	AD	311	1/1	0.78	0.20	57,57,57,57	0
58	MG	DA	1746	1/1	0.78	0.15	91,91,91,91	0
58	MG	AA	3621	1/1	0.78	0.15	46,46,46,46	0
58	MG	CA	3621	1/1	0.78	0.19	73,73,73,73	0
58	MG	DA	1765	1/1	0.78	0.18	95,95,95,95	0
58	MG	BA	1658	1/1	0.78	0.22	90,90,90,90	0
58	MG	CA	3500	1/1	0.78	0.20	64,64,64,64	0
58	MG	CA	3533	1/1	0.79	0.12	81,81,81,81	0
58	MG	CA	3155	1/1	0.79	0.11	86,86,86,86	0
58	MG	BA	1625	1/1	0.79	0.13	65,65,65,65	0
58	MG	AA	3248	1/1	0.79	0.20	64,64,64,64	0
58	MG	BA	1802	1/1	0.79	0.13	84,84,84,84	0
58	MG	BA	1692	1/1	0.79	0.23	89,89,89,89	0
58	MG	CA	3212	1/1	0.79	0.16	69,69,69,69	0
58	MG	CA	3220	1/1	0.79	0.23	78,78,78,78	0
58	MG	CA	3105	1/1	0.79	0.12	80,80,80,80	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	CA	3049	1/1	0.79	0.23	81,81,81,81	0
58	MG	AA	3460	1/1	0.79	0.23	72,72,72,72	0
58	MG	CA	3493	1/1	0.79	0.19	88,88,88,88	0
58	MG	AA	3476	1/1	0.79	0.16	69,69,69,69	0
58	MG	AA	3728	1/1	0.79	0.19	61,61,61,61	0
58	MG	AA	3242	1/1	0.79	0.29	72,72,72,72	0
58	MG	BD	502	1/1	0.80	0.29	82,82,82,82	0
58	MG	BA	1665	1/1	0.80	0.14	79,79,79,79	0
58	MG	AA	3028	1/1	0.80	0.26	51,51,51,51	1
58	MG	CA	3241	1/1	0.80	0.30	107,107,107,107	0
58	MG	CQ	205	1/1	0.80	0.22	81,81,81,81	0
58	MG	BA	1670	1/1	0.80	0.17	83,83,83,83	0
58	MG	CA	3543	1/1	0.80	0.14	63,63,63,63	0
58	MG	CA	3093	1/1	0.80	0.22	84,84,84,84	0
58	MG	CA	3272	1/1	0.80	0.24	75,75,75,75	0
58	MG	BA	1758	1/1	0.80	0.16	68,68,68,68	0
58	MG	AA	3464	1/1	0.80	0.13	63,63,63,63	0
58	MG	CA	3571	1/1	0.80	0.14	65,65,65,65	0
58	MG	CA	3113	1/1	0.80	0.22	92,92,92,92	0
58	MG	CA	3123	1/1	0.80	0.22	88,88,88,88	0
58	MG	CA	3032	1/1	0.80	0.32	67,67,67,67	0
58	MG	AA	3697	1/1	0.80	0.16	63,63,63,63	0
58	MG	AA	3771	1/1	0.80	0.22	31,31,31,31	1
58	MG	CA	3139	1/1	0.80	0.22	123,123,123,123	0
58	MG	AA	3630	1/1	0.80	0.26	71,71,71,71	0
58	MG	AA	3375	1/1	0.80	0.20	57,57,57,57	0
58	MG	CA	3159	1/1	0.80	0.17	69,69,69,69	0
58	MG	DA	1730	1/1	0.80	0.16	88,88,88,88	0
58	MG	BA	1652	1/1	0.80	0.22	72,72,72,72	0
58	MG	AA	3801	1/1	0.80	0.15	88,88,88,88	0
58	MG	A7	106	1/1	0.80	0.29	38,38,38,38	1
58	MG	CA	3646	1/1	0.80	0.12	95,95,95,95	0
58	MG	CA	3656	1/1	0.80	0.18	61,61,61,61	0
58	MG	CA	3208	1/1	0.80	0.22	84,84,84,84	0
61	FUA	BZ	703	37/37	0.80	0.18	69,69,69,69	0
58	MG	AZ	301	1/1	0.81	0.17	98,98,98,98	0
58	MG	CA	3024	1/1	0.81	0.38	88,88,88,88	0
58	MG	CA	3634	1/1	0.81	0.17	81,81,81,81	0
58	MG	CA	3636	1/1	0.81	0.11	80,80,80,80	0
58	MG	DA	1676	1/1	0.81	0.11	78,78,78,78	0
58	MG	CA	3641	1/1	0.81	0.21	67,67,67,67	0
58	MG	CA	3421	1/1	0.81	0.22	76,76,76,76	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	CA	3122	1/1	0.81	0.17	67,67,67,67	0
58	MG	DA	1691	1/1	0.81	0.10	85,85,85,85	0
58	MG	AA	3623	1/1	0.81	0.17	74,74,74,74	0
58	MG	CA	3661	1/1	0.81	0.20	74,74,74,74	0
58	MG	CA	3583	1/1	0.81	0.14	78,78,78,78	1
58	MG	DA	1708	1/1	0.81	0.14	87,87,87,87	0
58	MG	BA	1649	1/1	0.81	0.08	75,75,75,75	0
58	MG	DA	1716	1/1	0.81	0.20	78,78,78,78	0
58	MG	AA	3732	1/1	0.81	0.13	68,68,68,68	0
58	MG	BA	1653	1/1	0.81	0.18	102,102,102,102	0
58	MG	CA	3134	1/1	0.81	0.34	86,86,86,86	0
58	MG	BA	1624	1/1	0.81	0.33	75,75,75,75	0
58	MG	BA	1605	1/1	0.81	0.21	67,67,67,67	0
58	MG	CA	3323	1/1	0.81	0.15	67,67,67,67	0
58	MG	CA	3243	1/1	0.81	0.13	78,78,78,78	0
58	MG	DA	1639	1/1	0.81	0.30	75,75,75,75	0
58	MG	CA	3378	1/1	0.81	0.15	84,84,84,84	0
58	MG	DA	1652	1/1	0.82	0.18	71,71,71,71	0
58	MG	CA	3090	1/1	0.82	0.29	65,65,65,65	0
58	MG	AA	3575	1/1	0.82	0.10	69,69,69,69	0
58	MG	DA	1663	1/1	0.82	0.14	72,72,72,72	0
58	MG	AA	3016	1/1	0.82	0.20	59,59,59,59	0
58	MG	CA	3034	1/1	0.82	0.30	101,101,101,101	0
58	MG	AA	3193	1/1	0.82	0.25	62,62,62,62	0
58	MG	BA	1710	1/1	0.82	0.14	79,79,79,79	0
58	MG	BA	1804	1/1	0.82	0.13	68,68,68,68	1
58	MG	CA	3577	1/1	0.82	0.12	83,83,83,83	0
58	MG	AA	3067	1/1	0.82	0.18	55,55,55,55	0
58	MG	CB	3002	1/1	0.82	0.12	66,66,66,66	0
58	MG	CA	3444	1/1	0.82	0.17	91,91,91,91	0
58	MG	AA	3164	1/1	0.82	0.13	58,58,58,58	0
58	MG	AB	3004	1/1	0.82	0.29	89,89,89,89	0
58	MG	DA	1709	1/1	0.82	0.22	72,72,72,72	0
58	MG	BA	1673	1/1	0.82	0.24	75,75,75,75	0
58	MG	CO	202	1/1	0.82	0.10	53,53,53,53	0
58	MG	BA	1679	1/1	0.82	0.19	87,87,87,87	0
58	MG	DA	1603	1/1	0.82	0.16	74,74,74,74	0
58	MG	DA	1731	1/1	0.82	0.22	82,82,82,82	0
58	MG	DA	1737	1/1	0.82	0.14	72,72,72,72	0
58	MG	AB	3014	1/1	0.82	0.16	67,67,67,67	0
58	MG	DA	1607	1/1	0.82	0.19	61,61,61,61	0
58	MG	CA	3145	1/1	0.82	0.14	79,79,79,79	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	DA	1622	1/1	0.82	0.28	77,77,77,77	0
58	MG	AA	3230	1/1	0.82	0.42	80,80,80,80	0
58	MG	BA	1612	1/1	0.82	0.09	79,79,79,79	0
58	MG	CA	3178	1/1	0.82	0.18	57,57,57,57	0
58	MG	CA	3563	1/1	0.83	0.13	91,91,91,91	0
58	MG	CA	3569	1/1	0.83	0.22	79,79,79,79	0
58	MG	BA	1720	1/1	0.83	0.21	83,83,83,83	0
58	MG	AA	3713	1/1	0.83	0.27	52,52,52,52	1
58	MG	CA	3581	1/1	0.83	0.13	81,81,81,81	0
58	MG	BA	1655	1/1	0.83	0.27	78,78,78,78	0
58	MG	DA	1640	1/1	0.83	0.14	79,79,79,79	0
58	MG	DA	1641	1/1	0.83	0.09	77,77,77,77	0
58	MG	CA	3152	1/1	0.83	0.15	56,56,56,56	0
58	MG	CA	3357	1/1	0.83	0.12	80,80,80,80	0
58	MG	AB	3006	1/1	0.83	0.20	72,72,72,72	0
58	MG	BA	1750	1/1	0.83	0.14	84,84,84,84	0
58	MG	CA	3001	1/1	0.83	0.20	73,73,73,73	0
58	MG	CA	3607	1/1	0.83	0.19	97,97,97,97	0
58	MG	CA	3077	1/1	0.83	0.21	66,66,66,66	0
58	MG	CA	3189	1/1	0.83	0.11	68,68,68,68	0
58	MG	CA	3431	1/1	0.83	0.19	100,100,100,100	0
58	MG	CA	3441	1/1	0.83	0.28	77,77,77,77	0
58	MG	DA	1685	1/1	0.83	0.24	65,65,65,65	0
58	MG	CA	3199	1/1	0.83	0.25	74,74,74,74	0
58	MG	BA	1694	1/1	0.83	0.23	86,86,86,86	0
58	MG	CA	3631	1/1	0.83	0.14	77,77,77,77	0
58	MG	AA	3027	1/1	0.83	0.39	77,77,77,77	0
58	MG	BA	1701	1/1	0.83	0.20	75,75,75,75	0
58	MG	CA	3094	1/1	0.83	0.23	87,87,87,87	0
58	MG	CA	3489	1/1	0.83	0.21	80,80,80,80	0
58	MG	CA	3097	1/1	0.83	0.14	80,80,80,80	0
58	MG	CA	3018	1/1	0.83	0.29	64,64,64,64	0
58	MG	AA	3204	1/1	0.83	0.21	57,57,57,57	0
58	MG	CA	3031	1/1	0.83	0.13	76,76,76,76	0
58	MG	CA	3528	1/1	0.83	0.27	79,79,79,79	0
58	MG	CA	3115	1/1	0.83	0.22	76,76,76,76	0
58	MG	BA	1786	1/1	0.83	0.15	60,60,60,60	0
58	MG	DA	1749	1/1	0.83	0.24	80,80,80,80	0
58	MG	DA	1751	1/1	0.83	0.20	81,81,81,81	0
58	MG	DA	1753	1/1	0.83	0.16	70,70,70,70	0
58	MG	A8	5001	1/1	0.83	0.19	59,59,59,59	0
58	MG	BA	1792	1/1	0.83	0.12	72,72,72,72	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	AA	3244	1/1	0.83	0.23	100,100,100,100	0
58	MG	CQ	201	1/1	0.83	0.17	62,62,62,62	0
58	MG	DK	5001	1/1	0.83	0.07	100,100,100,100	0
58	MG	AA	3026	1/1	0.83	0.20	86,86,86,86	0
58	MG	AA	3710	1/1	0.83	0.22	75,75,75,75	0
61	FUA	DZ	703	37/37	0.83	0.18	85,85,85,85	0
58	MG	CA	3045	1/1	0.84	0.23	67,67,67,67	0
58	MG	AA	3649	1/1	0.84	0.15	92,92,92,92	0
58	MG	BA	1789	1/1	0.84	0.17	90,90,90,90	0
58	MG	DA	1625	1/1	0.84	0.32	73,73,73,73	0
58	MG	DA	1634	1/1	0.84	0.19	90,90,90,90	0
58	MG	CA	3052	1/1	0.84	0.24	69,69,69,69	0
58	MG	AA	3547	1/1	0.84	0.11	31,31,31,31	0
58	MG	AA	3755	1/1	0.84	0.11	63,63,63,63	0
58	MG	CA	3059	1/1	0.84	0.22	60,60,60,60	0
58	MG	CA	3585	1/1	0.84	0.17	78,78,78,78	0
58	MG	CA	3062	1/1	0.84	0.12	68,68,68,68	0
58	MG	AA	3041	1/1	0.84	0.23	75,75,75,75	0
58	MG	AA	3227	1/1	0.84	0.14	55,55,55,55	0
58	MG	DA	1665	1/1	0.84	0.30	61,61,61,61	0
58	MG	BA	1717	1/1	0.84	0.17	83,83,83,83	0
58	MG	DA	1672	1/1	0.84	0.31	73,73,73,73	0
58	MG	CA	3396	1/1	0.84	0.14	58,58,58,58	0
58	MG	CA	3402	1/1	0.84	0.11	70,70,70,70	0
58	MG	AA	3283	1/1	0.84	0.31	62,62,62,62	0
58	MG	CA	3190	1/1	0.84	0.24	83,83,83,83	0
58	MG	CA	3432	1/1	0.84	0.21	61,61,61,61	0
58	MG	CA	3436	1/1	0.84	0.11	75,75,75,75	0
58	MG	DA	1690	1/1	0.84	0.23	82,82,82,82	0
58	MG	AB	3023	1/1	0.84	0.34	76,76,76,76	0
58	MG	BL	201	1/1	0.84	0.10	80,80,80,80	0
58	MG	BA	1675	1/1	0.84	0.33	77,77,77,77	0
58	MG	BA	1747	1/1	0.84	0.17	66,66,66,66	0
58	MG	AD	307	1/1	0.84	0.17	53,53,53,53	1
58	MG	AA	3638	1/1	0.84	0.23	72,72,72,72	0
58	MG	AA	3639	1/1	0.84	0.14	77,77,77,77	0
58	MG	CA	3223	1/1	0.84	0.34	65,65,65,65	0
58	MG	CA	3649	1/1	0.84	0.24	85,85,85,85	0
58	MG	CA	3653	1/1	0.84	0.24	95,95,95,95	0
58	MG	CA	3499	1/1	0.84	0.22	83,83,83,83	0
58	MG	CA	3235	1/1	0.84	0.28	75,75,75,75	0
58	MG	CA	3236	1/1	0.84	0.14	87,87,87,87	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	BA	1759	1/1	0.84	0.23	65,65,65,65	0
58	MG	BA	1640	1/1	0.84	0.37	78,78,78,78	0
58	MG	CA	3245	1/1	0.84	0.22	57,57,57,57	0
58	MG	CA	3536	1/1	0.84	0.13	71,71,71,71	0
58	MG	AA	3321	1/1	0.84	0.21	70,70,70,70	0
58	MG	DA	1763	1/1	0.84	0.12	77,77,77,77	0
58	MG	CA	3538	1/1	0.84	0.10	71,71,71,71	0
58	MG	CA	3540	1/1	0.84	0.22	85,85,85,85	0
58	MG	BA	1774	1/1	0.84	0.10	70,70,70,70	0
58	MG	DW	503	1/1	0.84	0.19	84,84,84,84	0
58	MG	AA	3733	1/1	0.84	0.13	68,68,68,68	0
58	MG	BA	1785	1/1	0.84	0.26	69,69,69,69	0
58	MG	AA	3807	1/1	0.84	0.20	62,62,62,62	1
58	MG	DA	1630	1/1	0.85	0.18	61,61,61,61	0
58	MG	AA	3760	1/1	0.85	0.10	27,27,27,27	0
58	MG	BM	202	1/1	0.85	0.10	65,65,65,65	0
58	MG	AA	3269	1/1	0.85	0.19	84,84,84,84	0
58	MG	AA	3767	1/1	0.85	0.14	63,63,63,63	1
58	MG	CA	3599	1/1	0.85	0.14	80,80,80,80	0
58	MG	BA	1755	1/1	0.85	0.10	94,94,94,94	0
58	MG	CA	3081	1/1	0.85	0.12	68,68,68,68	0
58	MG	CA	3085	1/1	0.85	0.18	66,66,66,66	0
58	MG	AA	3362	1/1	0.85	0.21	69,69,69,69	0
58	MG	CA	3004	1/1	0.85	0.30	64,64,64,64	0
58	MG	CA	3619	1/1	0.85	0.23	47,47,47,47	1
58	MG	CA	3477	1/1	0.85	0.13	74,74,74,74	0
58	MG	BA	1629	1/1	0.85	0.22	87,87,87,87	0
58	MG	CA	3230	1/1	0.85	0.26	51,51,51,51	0
58	MG	CA	3625	1/1	0.85	0.16	79,79,79,79	0
58	MG	BA	1632	1/1	0.85	0.12	63,63,63,63	0
58	MG	CA	3633	1/1	0.85	0.16	68,68,68,68	0
58	MG	CA	3099	1/1	0.85	0.16	92,92,92,92	0
58	MG	AA	3221	1/1	0.85	0.17	56,56,56,56	0
58	MG	AA	3779	1/1	0.85	0.12	62,62,62,62	0
58	MG	DA	1692	1/1	0.85	0.15	76,76,76,76	0
58	MG	DA	1696	1/1	0.85	0.11	91,91,91,91	0
58	MG	BA	1646	1/1	0.85	0.19	75,75,75,75	0
58	MG	CA	3645	1/1	0.85	0.16	82,82,82,82	0
58	MG	CA	3246	1/1	0.85	0.23	59,59,59,59	0
58	MG	CA	3525	1/1	0.85	0.18	83,83,83,83	0
58	MG	BA	1647	1/1	0.85	0.08	61,61,61,61	0
58	MG	CA	3033	1/1	0.85	0.30	89,89,89,89	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	CA	3660	1/1	0.85	0.34	101,101,101,101	0
58	MG	BA	1648	1/1	0.85	0.35	75,75,75,75	0
58	MG	DA	1722	1/1	0.85	0.14	65,65,65,65	0
58	MG	CA	3273	1/1	0.85	0.20	69,69,69,69	0
58	MG	AA	3636	1/1	0.85	0.15	65,65,65,65	0
58	MG	DA	1733	1/1	0.85	0.16	83,83,83,83	0
58	MG	CA	3043	1/1	0.85	0.38	102,102,102,102	0
58	MG	DA	1739	1/1	0.85	0.20	79,79,79,79	0
58	MG	DA	1740	1/1	0.85	0.14	81,81,81,81	0
58	MG	CB	3010	1/1	0.85	0.14	55,55,55,55	0
58	MG	AA	3443	1/1	0.85	0.20	65,65,65,65	0
58	MG	CA	3133	1/1	0.85	0.17	69,69,69,69	0
58	MG	BA	1791	1/1	0.85	0.16	68,68,68,68	0
58	MG	AA	3458	1/1	0.85	0.15	72,72,72,72	0
58	MG	BA	1793	1/1	0.85	0.11	63,63,63,63	0
58	MG	AA	3611	1/1	0.85	0.17	51,51,51,51	0
58	MG	AA	3136	1/1	0.85	0.11	52,52,52,52	0
58	MG	CA	3153	1/1	0.85	0.25	78,78,78,78	0
58	MG	AA	3665	1/1	0.85	0.21	85,85,85,85	0
58	MG	CA	3579	1/1	0.85	0.11	51,51,51,51	0
58	MG	AA	3096	1/1	0.85	0.19	63,63,63,63	0
58	MG	AA	3689	1/1	0.85	0.11	55,55,55,55	1
58	MG	BA	1737	1/1	0.85	0.31	72,72,72,72	0
58	MG	AA	3739	1/1	0.86	0.28	94,94,94,94	0
58	MG	BA	1680	1/1	0.86	0.22	69,69,69,69	0
58	MG	DA	1674	1/1	0.86	0.12	62,62,62,62	0
58	MG	AA	3590	1/1	0.86	0.13	69,69,69,69	0
58	MG	CA	3116	1/1	0.86	0.21	75,75,75,75	0
58	MG	CA	3406	1/1	0.86	0.10	70,70,70,70	0
58	MG	CA	3407	1/1	0.86	0.12	55,55,55,55	0
58	MG	AA	3596	1/1	0.86	0.19	40,40,40,40	0
58	MG	A5	105	1/1	0.86	0.15	60,60,60,60	0
58	MG	AA	3814	1/1	0.86	0.12	93,93,93,93	0
58	MG	CB	3003	1/1	0.86	0.13	77,77,77,77	0
58	MG	AB	3001	1/1	0.86	0.23	87,87,87,87	0
58	MG	CA	3440	1/1	0.86	0.17	57,57,57,57	0
58	MG	CA	3067	1/1	0.86	0.21	72,72,72,72	0
58	MG	AA	3274	1/1	0.86	0.16	55,55,55,55	0
58	MG	CE	306	1/1	0.86	0.10	67,67,67,67	0
58	MG	BA	1607	1/1	0.86	0.07	67,67,67,67	0
58	MG	AA	3600	1/1	0.86	0.12	60,60,60,60	0
58	MG	CA	3595	1/1	0.86	0.11	53,53,53,53	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	AA	3059	1/1	0.86	0.13	51,51,51,51	0
58	MG	AA	3133	1/1	0.86	0.20	69,69,69,69	0
58	MG	DA	1604	1/1	0.86	0.30	76,76,76,76	0
58	MG	AA	3448	1/1	0.86	0.19	78,78,78,78	0
58	MG	BA	1663	1/1	0.86	0.19	82,82,82,82	0
58	MG	DA	1736	1/1	0.86	0.08	79,79,79,79	0
58	MG	CA	3285	1/1	0.86	0.19	57,57,57,57	0
58	MG	CA	3614	1/1	0.86	0.10	52,52,52,52	0
58	MG	CA	3082	1/1	0.86	0.15	70,70,70,70	0
58	MG	CA	3158	1/1	0.86	0.22	70,70,70,70	0
58	MG	DA	1628	1/1	0.86	0.30	74,74,74,74	0
58	MG	DA	1750	1/1	0.86	0.22	68,68,68,68	0
58	MG	BA	1620	1/1	0.86	0.20	57,57,57,57	0
58	MG	AA	3645	1/1	0.86	0.23	79,79,79,79	0
58	MG	AA	3731	1/1	0.86	0.13	42,42,42,42	0
58	MG	BA	1800	1/1	0.86	0.14	69,69,69,69	0
58	MG	CA	3532	1/1	0.86	0.09	79,79,79,79	0
58	MG	AA	3360	1/1	0.86	0.16	114,114,114,114	0
58	MG	CA	3194	1/1	0.86	0.31	72,72,72,72	0
58	MG	CA	3098	1/1	0.86	0.15	83,83,83,83	0
58	MG	BA	1739	1/1	0.86	0.19	63,63,63,63	0
58	MG	CA	3375	1/1	0.86	0.21	71,71,71,71	0
58	MG	CA	3642	1/1	0.86	0.44	80,80,80,80	0
58	MG	AA	3656	1/1	0.86	0.13	56,56,56,56	0
58	MG	AA	3599	1/1	0.87	0.17	58,58,58,58	0
58	MG	BA	1700	1/1	0.87	0.30	74,74,74,74	0
58	MG	AA	3245	1/1	0.87	0.22	69,69,69,69	0
58	MG	CA	3557	1/1	0.87	0.09	76,76,76,76	0
58	MG	AA	3445	1/1	0.87	0.19	75,75,75,75	0
58	MG	AA	3682	1/1	0.87	0.15	53,53,53,53	0
58	MG	AA	3246	1/1	0.87	0.19	72,72,72,72	0
58	MG	AA	3775	1/1	0.87	0.10	45,45,45,45	0
58	MG	CA	3574	1/1	0.87	0.08	72,72,72,72	0
58	MG	CA	3154	1/1	0.87	0.27	72,72,72,72	0
58	MG	DA	1635	1/1	0.87	0.12	65,65,65,65	0
58	MG	DA	1636	1/1	0.87	0.30	70,70,70,70	0
58	MG	CA	3360	1/1	0.87	0.09	49,49,49,49	0
58	MG	BA	1803	1/1	0.87	0.20	69,69,69,69	0
58	MG	CA	3373	1/1	0.87	0.27	58,58,58,58	0
58	MG	CA	3374	1/1	0.87	0.14	76,76,76,76	0
58	MG	CA	3586	1/1	0.87	0.09	69,69,69,69	0
58	MG	AA	3017	1/1	0.87	0.19	78,78,78,78	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	DA	1658	1/1	0.87	0.20	72,72,72,72	0
58	MG	AA	3319	1/1	0.87	0.11	69,69,69,69	0
58	MG	CA	3385	1/1	0.87	0.18	64,64,64,64	0
58	MG	CA	3172	1/1	0.87	0.26	83,83,83,83	0
58	MG	BA	1809	1/1	0.87	0.20	83,83,83,83	0
58	MG	CA	3395	1/1	0.87	0.21	65,65,65,65	0
58	MG	AA	3794	1/1	0.87	0.14	58,58,58,58	1
58	MG	BA	1601	1/1	0.87	0.11	58,58,58,58	0
58	MG	AA	3065	1/1	0.87	0.21	48,48,48,48	0
58	MG	BA	1662	1/1	0.87	0.15	70,70,70,70	0
58	MG	CA	3412	1/1	0.87	0.16	81,81,81,81	0
58	MG	DA	1684	1/1	0.87	0.34	72,72,72,72	0
58	MG	CA	3420	1/1	0.87	0.17	71,71,71,71	0
58	MG	DA	1686	1/1	0.87	0.11	53,53,53,53	0
58	MG	CA	3196	1/1	0.87	0.36	64,64,64,64	0
58	MG	AA	3201	1/1	0.87	0.24	65,65,65,65	0
58	MG	BA	1611	1/1	0.87	0.11	69,69,69,69	0
58	MG	CA	3204	1/1	0.87	0.17	74,74,74,74	0
58	MG	AA	3493	1/1	0.87	0.10	30,30,30,30	1
58	MG	CA	3088	1/1	0.87	0.42	75,75,75,75	0
58	MG	AA	3633	1/1	0.87	0.16	48,48,48,48	1
58	MG	CA	3447	1/1	0.87	0.19	80,80,80,80	0
58	MG	CA	3635	1/1	0.87	0.09	79,79,79,79	0
58	MG	CA	3454	1/1	0.87	0.12	81,81,81,81	0
58	MG	DA	1711	1/1	0.87	0.12	45,45,45,45	0
58	MG	CA	3210	1/1	0.87	0.25	75,75,75,75	0
58	MG	AA	3510	1/1	0.87	0.19	58,58,58,58	0
58	MG	DA	1718	1/1	0.87	0.11	77,77,77,77	0
58	MG	CA	3005	1/1	0.87	0.20	59,59,59,59	0
58	MG	CA	3095	1/1	0.87	0.19	64,64,64,64	0
58	MG	DA	1725	1/1	0.87	0.12	70,70,70,70	0
58	MG	CA	3484	1/1	0.87	0.16	76,76,76,76	0
58	MG	AB	3002	1/1	0.87	0.19	59,59,59,59	0
58	MG	CA	3231	1/1	0.87	0.30	57,57,57,57	0
58	MG	CA	3492	1/1	0.87	0.21	105,105,105,105	0
58	MG	CA	3010	1/1	0.87	0.08	41,41,41,41	0
58	MG	AA	3018	1/1	0.87	0.71	78,78,78,78	0
58	MG	AA	3049	1/1	0.87	0.14	52,52,52,52	0
58	MG	AA	3434	1/1	0.87	0.08	17,17,17,17	0
58	MG	DA	1748	1/1	0.87	0.14	78,78,78,78	0
58	MG	BA	1684	1/1	0.87	0.12	69,69,69,69	0
58	MG	CB	3005	1/1	0.87	0.15	62,62,62,62	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	BA	1775	1/1	0.87	0.15	78,78,78,78	0
58	MG	CB	3007	1/1	0.87	0.18	65,65,65,65	0
58	MG	CA	3527	1/1	0.87	0.08	78,78,78,78	0
58	MG	BA	1689	1/1	0.87	0.21	72,72,72,72	0
58	MG	CA	3257	1/1	0.87	0.30	57,57,57,57	0
58	MG	BA	1784	1/1	0.87	0.09	50,50,50,50	0
58	MG	DA	1768	1/1	0.87	0.19	73,73,73,73	0
58	MG	CA	3037	1/1	0.87	0.12	58,58,58,58	0
58	MG	AA	3438	1/1	0.87	0.16	57,57,57,57	0
58	MG	CA	3283	1/1	0.87	0.14	60,60,60,60	0
58	MG	AA	3442	1/1	0.87	0.13	49,49,49,49	0
58	MG	DA	1602	1/1	0.87	0.11	80,80,80,80	0
58	MG	AA	3652	1/1	0.87	0.12	77,77,77,77	0
58	MG	BA	1608	1/1	0.88	0.12	74,74,74,74	0
58	MG	CA	3221	1/1	0.88	0.16	54,54,54,54	0
58	MG	DA	1642	1/1	0.88	0.12	66,66,66,66	0
58	MG	AA	3806	1/1	0.88	0.15	61,61,61,61	0
58	MG	CA	3228	1/1	0.88	0.16	63,63,63,63	0
58	MG	CA	3100	1/1	0.88	0.26	79,79,79,79	0
58	MG	AA	3720	1/1	0.88	0.26	77,77,77,77	0
58	MG	CA	3233	1/1	0.88	0.29	71,71,71,71	0
58	MG	AA	3489	1/1	0.88	0.11	64,64,64,64	0
58	MG	AA	3029	1/1	0.88	0.13	53,53,53,53	0
58	MG	CA	3237	1/1	0.88	0.25	75,75,75,75	0
58	MG	DA	1671	1/1	0.88	0.26	83,83,83,83	0
58	MG	AA	3430	1/1	0.88	0.13	44,44,44,44	0
58	MG	AA	3538	1/1	0.88	0.19	61,61,61,61	1
58	MG	BA	1779	1/1	0.88	0.14	79,79,79,79	0
58	MG	CA	3035	1/1	0.88	0.28	60,60,60,60	0
58	MG	CA	3248	1/1	0.88	0.25	77,77,77,77	0
58	MG	AA	3252	1/1	0.88	0.16	66,66,66,66	0
58	MG	CA	3255	1/1	0.88	0.23	67,67,67,67	0
58	MG	BA	1690	1/1	0.88	0.34	70,70,70,70	0
58	MG	AA	3573	1/1	0.88	0.09	50,50,50,50	0
58	MG	AA	3750	1/1	0.88	0.09	24,24,24,24	0
58	MG	AA	3260	1/1	0.88	0.21	71,71,71,71	0
58	MG	CA	3523	1/1	0.88	0.11	40,40,40,40	0
58	MG	BA	1790	1/1	0.88	0.11	75,75,75,75	0
58	MG	AB	3019	1/1	0.88	0.11	65,65,65,65	0
58	MG	CA	3141	1/1	0.88	0.17	54,54,54,54	0
58	MG	AA	3589	1/1	0.88	0.16	21,21,21,21	1
58	MG	AA	3212	1/1	0.88	0.17	34,34,34,34	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	AA	3057	1/1	0.88	0.21	57,57,57,57	0
58	MG	AA	3347	1/1	0.88	0.08	38,38,38,38	0
58	MG	AN	3001	1/1	0.88	0.18	85,85,85,85	0
58	MG	AA	3355	1/1	0.88	0.11	58,58,58,58	0
58	MG	AA	3356	1/1	0.88	0.10	35,35,35,35	0
58	MG	CA	3350	1/1	0.88	0.10	85,85,85,85	0
58	MG	CA	3546	1/1	0.88	0.12	119,119,119,119	0
58	MG	AZ	302	1/1	0.88	0.14	68,68,68,68	0
58	MG	CE	303	1/1	0.88	0.15	54,54,54,54	0
58	MG	CE	304	1/1	0.88	0.25	68,68,68,68	0
58	MG	CA	3173	1/1	0.88	0.19	65,65,65,65	0
58	MG	DA	1732	1/1	0.88	0.17	76,76,76,76	0
58	MG	BA	1718	1/1	0.88	0.11	67,67,67,67	0
58	MG	CA	3179	1/1	0.88	0.32	75,75,75,75	0
58	MG	AA	3679	1/1	0.88	0.13	65,65,65,65	0
58	MG	CQ	203	1/1	0.88	0.17	67,67,67,67	0
58	MG	CA	3568	1/1	0.88	0.13	41,41,41,41	0
58	MG	CA	3183	1/1	0.88	0.52	86,86,86,86	0
58	MG	AA	3605	1/1	0.88	0.13	68,68,68,68	0
58	MG	BA	1732	1/1	0.88	0.10	78,78,78,78	0
58	MG	CA	3386	1/1	0.88	0.14	65,65,65,65	0
58	MG	AA	3010	1/1	0.88	0.29	68,68,68,68	0
58	MG	BT	3001	1/1	0.88	0.17	62,62,62,62	0
58	MG	DA	1619	1/1	0.88	0.15	71,71,71,71	0
58	MG	AA	3461	1/1	0.88	0.16	66,66,66,66	0
58	MG	AA	3109	1/1	0.88	0.12	50,50,50,50	0
58	MG	CA	3399	1/1	0.88	0.14	75,75,75,75	0
58	MG	DA	1766	1/1	0.88	0.09	58,58,58,58	0
58	MG	AA	3365	1/1	0.88	0.20	57,57,57,57	0
58	MG	CA	3091	1/1	0.88	0.26	111,111,111,111	0
58	MG	BA	1666	1/1	0.88	0.15	59,59,59,59	0
58	MG	DW	502	1/1	0.88	0.14	84,84,84,84	0
58	MG	BA	1668	1/1	0.88	0.32	75,75,75,75	0
58	MG	AA	3480	1/1	0.88	0.09	54,54,54,54	0
58	MG	DA	1637	1/1	0.88	0.11	76,76,76,76	0
58	MG	BA	1756	1/1	0.88	0.08	98,98,98,98	0
58	MG	BA	1716	1/1	0.89	0.15	88,88,88,88	0
58	MG	AA	3674	1/1	0.89	0.15	75,75,75,75	0
58	MG	CA	3284	1/1	0.89	0.15	92,92,92,92	0
58	MG	CA	3117	1/1	0.89	0.21	68,68,68,68	0
58	MG	AA	3765	1/1	0.89	0.14	63,63,63,63	0
58	MG	BA	1719	1/1	0.89	0.10	44,44,44,44	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	CA	3292	1/1	0.89	0.10	73,73,73,73	0
58	MG	AA	3367	1/1	0.89	0.10	52,52,52,52	0
58	MG	AA	3370	1/1	0.89	0.22	58,58,58,58	0
58	MG	AD	308	1/1	0.89	0.18	73,73,73,73	0
58	MG	CA	3132	1/1	0.89	0.07	30,30,30,30	0
58	MG	AA	3770	1/1	0.89	0.25	37,37,37,37	0
58	MG	DA	1638	1/1	0.89	0.23	83,83,83,83	0
58	MG	AA	3310	1/1	0.89	0.11	58,58,58,58	0
58	MG	AA	3070	1/1	0.89	0.23	60,60,60,60	0
58	MG	BA	1744	1/1	0.89	0.13	79,79,79,79	0
58	MG	CA	3025	1/1	0.89	0.14	77,77,77,77	0
58	MG	DA	1647	1/1	0.89	0.21	58,58,58,58	0
58	MG	AA	3696	1/1	0.89	0.15	69,69,69,69	0
58	MG	AA	3015	1/1	0.89	0.32	64,64,64,64	0
58	MG	AA	3781	1/1	0.89	0.20	44,44,44,44	1
58	MG	A5	102	1/1	0.89	0.30	88,88,88,88	0
58	MG	AA	3704	1/1	0.89	0.16	59,59,59,59	0
58	MG	BA	1667	1/1	0.89	0.12	55,55,55,55	0
58	MG	DA	1664	1/1	0.89	0.15	64,64,64,64	0
58	MG	AA	3788	1/1	0.89	0.16	58,58,58,58	1
58	MG	DA	1668	1/1	0.89	0.28	62,62,62,62	0
58	MG	CA	3387	1/1	0.89	0.13	70,70,70,70	0
58	MG	CA	3165	1/1	0.89	0.13	62,62,62,62	0
58	MG	CA	3167	1/1	0.89	0.12	60,60,60,60	0
58	MG	AA	3339	1/1	0.89	0.14	43,43,43,43	0
58	MG	BA	1770	1/1	0.89	0.09	75,75,75,75	0
58	MG	CA	3611	1/1	0.89	0.24	91,91,91,91	0
58	MG	AA	3795	1/1	0.89	0.21	68,68,68,68	1
58	MG	BA	1671	1/1	0.89	0.23	73,73,73,73	0
58	MG	BA	1672	1/1	0.89	0.22	92,92,92,92	0
58	MG	BA	1603	1/1	0.89	0.14	93,93,93,93	0
58	MG	AA	3111	1/1	0.89	0.17	48,48,48,48	0
58	MG	BA	1781	1/1	0.89	0.11	46,46,46,46	1
58	MG	CA	3060	1/1	0.89	0.22	77,77,77,77	0
58	MG	AA	3802	1/1	0.89	0.16	55,55,55,55	0
58	MG	CA	3628	1/1	0.89	0.16	66,66,66,66	0
58	MG	CA	3063	1/1	0.89	0.16	53,53,53,53	0
58	MG	DA	1698	1/1	0.89	0.25	68,68,68,68	0
58	MG	AA	3354	1/1	0.89	0.17	60,60,60,60	0
58	MG	AA	3804	1/1	0.89	0.15	68,68,68,68	0
58	MG	DA	1703	1/1	0.89	0.16	74,74,74,74	0
58	MG	AA	3271	1/1	0.89	0.27	69,69,69,69	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	DA	1707	1/1	0.89	0.12	87,87,87,87	0
58	MG	BA	1685	1/1	0.89	0.21	69,69,69,69	0
58	MG	BA	1686	1/1	0.89	0.13	81,81,81,81	0
58	MG	CA	3074	1/1	0.89	0.16	53,53,53,53	0
58	MG	CA	3075	1/1	0.89	0.19	71,71,71,71	0
58	MG	AA	3580	1/1	0.89	0.08	23,23,23,23	0
58	MG	CA	3470	1/1	0.89	0.17	72,72,72,72	0
58	MG	AA	3811	1/1	0.89	0.15	58,58,58,58	0
58	MG	CA	3480	1/1	0.89	0.17	55,55,55,55	0
58	MG	AA	3586	1/1	0.89	0.11	62,62,62,62	0
58	MG	CA	3482	1/1	0.89	0.17	70,70,70,70	0
58	MG	CA	3483	1/1	0.89	0.22	69,69,69,69	0
58	MG	CA	3662	1/1	0.89	0.21	55,55,55,55	0
58	MG	AA	3199	1/1	0.89	0.19	54,54,54,54	0
58	MG	BA	1797	1/1	0.89	0.17	69,69,69,69	0
58	MG	BA	1799	1/1	0.89	0.11	63,63,63,63	0
58	MG	AA	3455	1/1	0.89	0.17	58,58,58,58	0
58	MG	CA	3089	1/1	0.89	0.21	80,80,80,80	0
58	MG	DA	1744	1/1	0.89	0.14	79,79,79,79	0
58	MG	AA	3264	1/1	0.89	0.12	62,62,62,62	0
58	MG	BA	1699	1/1	0.89	0.17	78,78,78,78	0
58	MG	CB	3012	1/1	0.89	0.19	76,76,76,76	0
58	MG	CA	3506	1/1	0.89	0.11	58,58,58,58	0
58	MG	AB	3005	1/1	0.89	0.23	69,69,69,69	0
58	MG	BA	1628	1/1	0.89	0.19	75,75,75,75	0
58	MG	CA	3515	1/1	0.89	0.12	79,79,79,79	0
58	MG	CA	3516	1/1	0.89	0.12	62,62,62,62	0
58	MG	DA	1760	1/1	0.89	0.25	66,66,66,66	0
58	MG	CA	3244	1/1	0.89	0.28	78,78,78,78	0
58	MG	AA	3282	1/1	0.89	0.25	40,40,40,40	0
58	MG	CP	203	1/1	0.89	0.13	67,67,67,67	0
58	MG	BA	1811	1/1	0.89	0.09	68,68,68,68	0
58	MG	BA	1706	1/1	0.89	0.11	61,61,61,61	0
58	MG	AA	3364	1/1	0.89	0.25	81,81,81,81	0
58	MG	C5	101	1/1	0.89	0.29	65,65,65,65	0
58	MG	BK	201	1/1	0.89	0.12	57,57,57,57	0
58	MG	BA	1635	1/1	0.89	0.23	62,62,62,62	0
58	MG	AA	3463	1/1	0.89	0.10	46,46,46,46	0
58	MG	AA	3148	1/1	0.89	0.16	68,68,68,68	0
58	MG	CA	3252	1/1	0.90	0.18	64,64,64,64	0
58	MG	BA	1637	1/1	0.90	0.23	72,72,72,72	0
58	MG	BA	1638	1/1	0.90	0.15	64,64,64,64	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	CA	3256	1/1	0.90	0.13	40,40,40,40	0
58	MG	CA	3109	1/1	0.90	0.10	54,54,54,54	0
58	MG	CA	3534	1/1	0.90	0.11	79,79,79,79	0
58	MG	CA	3263	1/1	0.90	0.12	57,57,57,57	0
58	MG	AB	3015	1/1	0.90	0.10	40,40,40,40	0
58	MG	BA	1644	1/1	0.90	0.25	69,69,69,69	0
58	MG	AA	3294	1/1	0.90	0.14	66,66,66,66	0
58	MG	AA	3563	1/1	0.90	0.10	49,49,49,49	1
58	MG	AA	3203	1/1	0.90	0.20	46,46,46,46	1
58	MG	CA	3545	1/1	0.90	0.13	68,68,68,68	0
58	MG	AA	3437	1/1	0.90	0.12	54,54,54,54	0
58	MG	BA	1651	1/1	0.90	0.20	68,68,68,68	0
58	MG	BA	1722	1/1	0.90	0.16	62,62,62,62	0
58	MG	CA	3130	1/1	0.90	0.30	73,73,73,73	0
58	MG	BA	1725	1/1	0.90	0.16	71,71,71,71	0
58	MG	AA	3756	1/1	0.90	0.16	40,40,40,40	1
58	MG	BA	1733	1/1	0.90	0.20	63,63,63,63	0
58	MG	AD	305	1/1	0.90	0.20	63,63,63,63	0
58	MG	CA	3137	1/1	0.90	0.32	73,73,73,73	0
58	MG	AA	3647	1/1	0.90	0.20	72,72,72,72	0
58	MG	CA	3341	1/1	0.90	0.17	71,71,71,71	0
58	MG	AA	3578	1/1	0.90	0.10	55,55,55,55	0
58	MG	BA	1660	1/1	0.90	0.29	76,76,76,76	0
58	MG	AA	3762	1/1	0.90	0.14	53,53,53,53	1
58	MG	AH	3002	1/1	0.90	0.20	74,74,74,74	0
58	MG	AA	3100	1/1	0.90	0.19	53,53,53,53	0
58	MG	AA	3206	1/1	0.90	0.11	39,39,39,39	0
58	MG	CA	3591	1/1	0.90	0.11	83,83,83,83	0
58	MG	AA	3660	1/1	0.90	0.14	70,70,70,70	0
58	MG	CA	3157	1/1	0.90	0.12	55,55,55,55	0
58	MG	AA	3336	1/1	0.90	0.11	54,54,54,54	0
58	MG	AA	3208	1/1	0.90	0.16	61,61,61,61	0
58	MG	CA	3598	1/1	0.90	0.09	73,73,73,73	0
58	MG	BA	1762	1/1	0.90	0.09	89,89,89,89	0
58	MG	AA	3343	1/1	0.90	0.14	65,65,65,65	0
58	MG	CA	3168	1/1	0.90	0.28	56,56,56,56	0
58	MG	CA	3609	1/1	0.90	0.21	76,76,76,76	0
58	MG	AA	3345	1/1	0.90	0.08	68,68,68,68	0
58	MG	CA	3053	1/1	0.90	0.19	58,58,58,58	0
58	MG	CA	3174	1/1	0.90	0.32	61,61,61,61	0
58	MG	AA	3778	1/1	0.90	0.10	54,54,54,54	0
58	MG	CA	3405	1/1	0.90	0.17	91,91,91,91	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	CA	3057	1/1	0.90	0.12	49,49,49,49	0
58	MG	AA	3163	1/1	0.90	0.18	40,40,40,40	0
58	MG	CA	3409	1/1	0.90	0.12	40,40,40,40	0
58	MG	CA	3622	1/1	0.90	0.12	55,55,55,55	0
58	MG	AA	3122	1/1	0.90	0.13	54,54,54,54	0
58	MG	CA	3413	1/1	0.90	0.10	39,39,39,39	0
58	MG	AA	3223	1/1	0.90	0.12	35,35,35,35	0
58	MG	BA	1677	1/1	0.90	0.14	57,57,57,57	0
58	MG	CA	3426	1/1	0.90	0.15	55,55,55,55	0
58	MG	CA	3428	1/1	0.90	0.18	54,54,54,54	1
58	MG	AA	3694	1/1	0.90	0.09	45,45,45,45	0
58	MG	BA	1782	1/1	0.90	0.14	81,81,81,81	0
58	MG	CA	3197	1/1	0.90	0.25	64,64,64,64	0
58	MG	AA	3606	1/1	0.90	0.22	61,61,61,61	0
58	MG	AA	3462	1/1	0.90	0.28	71,71,71,71	0
58	MG	AA	3174	1/1	0.90	0.19	63,63,63,63	0
58	MG	DA	1726	1/1	0.90	0.13	77,77,77,77	0
58	MG	CA	3072	1/1	0.90	0.15	56,56,56,56	0
58	MG	AA	3708	1/1	0.90	0.23	53,53,53,53	1
58	MG	AA	3128	1/1	0.90	0.18	59,59,59,59	0
58	MG	BA	1687	1/1	0.90	0.19	50,50,50,50	0
58	MG	AA	3024	1/1	0.90	0.12	57,57,57,57	0
58	MG	CA	3472	1/1	0.90	0.34	72,72,72,72	0
58	MG	AA	3233	1/1	0.90	0.12	55,55,55,55	0
58	MG	AA	3107	1/1	0.90	0.22	76,76,76,76	0
58	MG	AA	3729	1/1	0.90	0.08	38,38,38,38	0
58	MG	CA	3226	1/1	0.90	0.21	69,69,69,69	0
58	MG	CB	3004	1/1	0.90	0.14	68,68,68,68	0
58	MG	BA	1693	1/1	0.90	0.34	74,74,74,74	0
58	MG	AA	3277	1/1	0.90	0.29	79,79,79,79	0
58	MG	BA	1695	1/1	0.90	0.15	67,67,67,67	0
58	MG	AA	3632	1/1	0.90	0.12	76,76,76,76	0
58	MG	BA	1698	1/1	0.90	0.17	68,68,68,68	0
58	MG	AA	3139	1/1	0.90	0.07	58,58,58,58	0
58	MG	DA	1757	1/1	0.90	0.14	75,75,75,75	0
58	MG	CA	3498	1/1	0.90	0.16	68,68,68,68	0
58	MG	DA	1761	1/1	0.90	0.17	66,66,66,66	0
58	MG	AA	3736	1/1	0.90	0.13	78,78,78,78	0
58	MG	CA	3239	1/1	0.90	0.25	75,75,75,75	0
58	MG	AA	3738	1/1	0.90	0.11	75,75,75,75	0
58	MG	DA	1767	1/1	0.90	0.10	74,74,74,74	0
58	MG	BA	1703	1/1	0.90	0.30	58,58,58,58	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	DE	202	1/1	0.90	0.09	94,94,94,94	0
58	MG	CA	3508	1/1	0.90	0.13	96,96,96,96	0
58	MG	CA	3512	1/1	0.90	0.28	65,65,65,65	0
58	MG	BA	1633	1/1	0.90	0.09	48,48,48,48	0
58	MG	BB	3001	1/1	0.90	0.11	75,75,75,75	0
58	MG	AA	3143	1/1	0.90	0.14	47,47,47,47	0
58	MG	CA	3518	1/1	0.90	0.21	86,86,86,86	0
58	MG	AA	3743	1/1	0.90	0.15	80,80,80,80	0
58	MG	CA	3478	1/1	0.91	0.10	58,58,58,58	0
58	MG	BA	1621	1/1	0.91	0.09	52,52,52,52	0
58	MG	CA	3224	1/1	0.91	0.39	81,81,81,81	0
58	MG	CD	301	1/1	0.91	0.28	81,81,81,81	0
58	MG	AA	3068	1/1	0.91	0.19	65,65,65,65	0
58	MG	CA	3227	1/1	0.91	0.13	53,53,53,53	0
58	MG	AA	3194	1/1	0.91	0.16	44,44,44,44	0
58	MG	AA	3741	1/1	0.91	0.14	34,34,34,34	1
58	MG	CA	3086	1/1	0.91	0.12	36,36,36,36	0
58	MG	BA	1627	1/1	0.91	0.27	57,57,57,57	0
58	MG	AA	3338	1/1	0.91	0.05	30,30,30,30	0
58	MG	AA	3151	1/1	0.91	0.14	50,50,50,50	0
58	MG	BA	1630	1/1	0.91	0.23	55,55,55,55	0
58	MG	BA	1631	1/1	0.91	0.26	64,64,64,64	0
58	MG	CA	3505	1/1	0.91	0.14	73,73,73,73	0
58	MG	CA	3240	1/1	0.91	0.12	64,64,64,64	0
58	MG	AA	3747	1/1	0.91	0.16	58,58,58,58	0
58	MG	BA	1808	1/1	0.91	0.14	81,81,81,81	0
58	MG	CA	3096	1/1	0.91	0.23	68,68,68,68	0
58	MG	BA	1702	1/1	0.91	0.18	61,61,61,61	0
58	MG	AA	3155	1/1	0.91	0.10	64,64,64,64	0
58	MG	AA	3344	1/1	0.91	0.09	84,84,84,84	0
58	MG	AA	3752	1/1	0.91	0.14	72,72,72,72	0
58	MG	CA	3521	1/1	0.91	0.14	61,61,61,61	0
58	MG	AA	3446	1/1	0.91	0.21	61,61,61,61	0
58	MG	DA	1626	1/1	0.91	0.23	49,49,49,49	0
58	MG	DA	1627	1/1	0.91	0.13	70,70,70,70	0
58	MG	BF	3001	1/1	0.91	0.16	74,74,74,74	0
58	MG	BA	1708	1/1	0.91	0.19	62,62,62,62	0
58	MG	CA	3111	1/1	0.91	0.06	71,71,71,71	0
58	MG	AA	3062	1/1	0.91	0.25	67,67,67,67	0
58	MG	CA	3114	1/1	0.91	0.17	39,39,39,39	0
58	MG	CA	3269	1/1	0.91	0.10	86,86,86,86	0
58	MG	AA	3450	1/1	0.91	0.14	53,53,53,53	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	BA	1641	1/1	0.91	0.16	49,49,49,49	0
58	MG	AA	3673	1/1	0.91	0.18	67,67,67,67	0
58	MG	CA	3118	1/1	0.91	0.14	57,57,57,57	0
58	MG	CA	3541	1/1	0.91	0.10	71,71,71,71	0
58	MG	CA	3121	1/1	0.91	0.10	45,45,45,45	0
58	MG	AA	3761	1/1	0.91	0.14	50,50,50,50	0
58	MG	AA	3452	1/1	0.91	0.14	69,69,69,69	0
58	MG	DA	1653	1/1	0.91	0.10	60,60,60,60	0
58	MG	AA	3232	1/1	0.91	0.20	79,79,79,79	0
58	MG	CA	3551	1/1	0.91	0.12	88,88,88,88	0
58	MG	DA	1659	1/1	0.91	0.12	64,64,64,64	0
58	MG	CA	3552	1/1	0.91	0.09	69,69,69,69	0
58	MG	DA	1662	1/1	0.91	0.16	64,64,64,64	0
58	MG	AA	3080	1/1	0.91	0.23	57,57,57,57	0
58	MG	CA	3127	1/1	0.91	0.12	63,63,63,63	0
58	MG	CA	3128	1/1	0.91	0.23	71,71,71,71	0
58	MG	DA	1666	1/1	0.91	0.12	66,66,66,66	0
58	MG	AA	3236	1/1	0.91	0.12	57,57,57,57	0
58	MG	CA	3562	1/1	0.91	0.15	76,76,76,76	0
58	MG	AA	3237	1/1	0.91	0.18	71,71,71,71	0
58	MG	AA	3088	1/1	0.91	0.10	34,34,34,34	0
58	MG	CA	3340	1/1	0.91	0.10	48,48,48,48	0
58	MG	CA	3013	1/1	0.91	0.08	63,63,63,63	0
58	MG	DA	1675	1/1	0.91	0.17	74,74,74,74	0
58	MG	BA	1726	1/1	0.91	0.09	64,64,64,64	0
58	MG	BA	1727	1/1	0.91	0.10	59,59,59,59	0
58	MG	CA	3578	1/1	0.91	0.14	80,80,80,80	0
58	MG	DA	1679	1/1	0.91	0.23	58,58,58,58	0
58	MG	BA	1654	1/1	0.91	0.07	69,69,69,69	0
58	MG	AW	3001	1/1	0.91	0.21	52,52,52,52	0
58	MG	CA	3030	1/1	0.91	0.19	57,57,57,57	1
58	MG	AY	502	1/1	0.91	0.16	58,58,58,58	0
58	MG	CA	3147	1/1	0.91	0.22	76,76,76,76	0
58	MG	CA	3376	1/1	0.91	0.14	66,66,66,66	0
58	MG	BA	1659	1/1	0.91	0.16	73,73,73,73	0
58	MG	CA	3379	1/1	0.91	0.10	65,65,65,65	0
58	MG	DA	1697	1/1	0.91	0.19	62,62,62,62	0
58	MG	AA	3177	1/1	0.91	0.25	61,61,61,61	0
58	MG	AA	3186	1/1	0.91	0.11	37,37,37,37	0
58	MG	A0	103	1/1	0.91	0.07	37,37,37,37	0
58	MG	DA	1702	1/1	0.91	0.07	65,65,65,65	0
58	MG	A2	101	1/1	0.91	0.09	35,35,35,35	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	DA	1705	1/1	0.91	0.12	62,62,62,62	0
58	MG	CA	3039	1/1	0.91	0.40	71,71,71,71	0
58	MG	CA	3601	1/1	0.91	0.10	75,75,75,75	0
58	MG	CA	3603	1/1	0.91	0.09	51,51,51,51	0
58	MG	CA	3393	1/1	0.91	0.09	82,82,82,82	0
58	MG	AA	3698	1/1	0.91	0.18	32,32,32,32	1
58	MG	AA	3702	1/1	0.91	0.20	35,35,35,35	1
58	MG	CA	3398	1/1	0.91	0.09	65,65,65,65	0
58	MG	AA	3209	1/1	0.91	0.11	63,63,63,63	0
58	MG	CA	3613	1/1	0.91	0.23	74,74,74,74	0
58	MG	CA	3401	1/1	0.91	0.11	69,69,69,69	0
58	MG	AA	3477	1/1	0.91	0.11	58,58,58,58	0
58	MG	AA	3785	1/1	0.91	0.10	72,72,72,72	0
58	MG	BA	1761	1/1	0.91	0.10	63,63,63,63	0
58	MG	AA	3247	1/1	0.91	0.16	63,63,63,63	0
58	MG	BA	1767	1/1	0.91	0.09	61,61,61,61	0
58	MG	AA	3309	1/1	0.91	0.19	44,44,44,44	0
58	MG	DA	1735	1/1	0.91	0.21	83,83,83,83	0
58	MG	AA	3718	1/1	0.91	0.08	43,43,43,43	0
58	MG	CA	3414	1/1	0.91	0.10	50,50,50,50	0
58	MG	DA	1738	1/1	0.91	0.15	80,80,80,80	0
58	MG	CA	3418	1/1	0.91	0.12	41,41,41,41	0
58	MG	BA	1606	1/1	0.91	0.16	65,65,65,65	0
58	MG	AA	3797	1/1	0.91	0.13	15,15,15,15	1
58	MG	BA	1676	1/1	0.91	0.11	68,68,68,68	0
58	MG	DA	1747	1/1	0.91	0.10	70,70,70,70	0
58	MG	CA	3192	1/1	0.91	0.12	58,58,58,58	0
58	MG	CA	3429	1/1	0.91	0.17	74,74,74,74	0
58	MG	CA	3430	1/1	0.91	0.20	53,53,53,53	0
58	MG	AA	3629	1/1	0.91	0.14	61,61,61,61	0
58	MG	CA	3643	1/1	0.91	0.08	76,76,76,76	0
58	MG	BA	1610	1/1	0.91	0.15	60,60,60,60	0
58	MG	CA	3433	1/1	0.91	0.16	71,71,71,71	0
58	MG	AA	3491	1/1	0.91	0.14	35,35,35,35	0
58	MG	CA	3069	1/1	0.91	0.19	81,81,81,81	0
58	MG	AA	3092	1/1	0.91	0.10	53,53,53,53	0
58	MG	BA	1614	1/1	0.91	0.08	75,75,75,75	0
58	MG	AA	3415	1/1	0.91	0.07	56,56,56,56	0
58	MG	AA	3526	1/1	0.91	0.09	20,20,20,20	0
58	MG	AA	3537	1/1	0.91	0.09	95,95,95,95	0
58	MG	CA	3663	1/1	0.91	0.23	91,91,91,91	0
58	MG	CA	3465	1/1	0.91	0.21	66,66,66,66	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	DF	3001	1/1	0.91	0.12	49,49,49,49	0
58	MG	BA	1688	1/1	0.91	0.21	52,52,52,52	0
58	MG	CA	3469	1/1	0.91	0.12	69,69,69,69	0
58	MG	BA	1619	1/1	0.91	0.08	73,73,73,73	0
58	MG	AA	3249	1/1	0.91	0.09	24,24,24,24	1
58	MG	CA	3474	1/1	0.91	0.17	76,76,76,76	0
58	MG	CA	3079	1/1	0.91	0.16	57,57,57,57	0
58	MG	CB	3009	1/1	0.91	0.12	67,67,67,67	0
58	MG	CN	5001	1/1	0.92	0.07	77,77,77,77	0
58	MG	CO	201	1/1	0.92	0.12	64,64,64,64	0
58	MG	AA	3715	1/1	0.92	0.12	66,66,66,66	0
58	MG	CA	3514	1/1	0.92	0.23	105,105,105,105	0
58	MG	BZ	702	1/1	0.92	0.18	46,46,46,46	0
58	MG	BA	1715	1/1	0.92	0.15	55,55,55,55	0
58	MG	CA	3517	1/1	0.92	0.24	64,64,64,64	0
58	MG	AA	3052	1/1	0.92	0.35	65,65,65,65	0
58	MG	AA	3457	1/1	0.92	0.12	67,67,67,67	0
58	MG	BA	1643	1/1	0.92	0.24	71,71,71,71	0
58	MG	CA	3287	1/1	0.92	0.08	52,52,52,52	0
58	MG	AA	3172	1/1	0.92	0.33	71,71,71,71	0
58	MG	AA	3358	1/1	0.92	0.18	63,63,63,63	0
58	MG	DA	1609	1/1	0.92	0.19	46,46,46,46	0
58	MG	DA	1613	1/1	0.92	0.19	72,72,72,72	0
58	MG	CA	3531	1/1	0.92	0.11	51,51,51,51	0
58	MG	DA	1618	1/1	0.92	0.26	65,65,65,65	0
58	MG	AA	3019	1/1	0.92	0.10	58,58,58,58	0
58	MG	AA	3137	1/1	0.92	0.12	56,56,56,56	0
58	MG	AA	3616	1/1	0.92	0.10	28,28,28,28	0
58	MG	CA	3302	1/1	0.92	0.19	68,68,68,68	0
58	MG	BA	1650	1/1	0.92	0.12	37,37,37,37	0
58	MG	CA	3310	1/1	0.92	0.09	48,48,48,48	0
58	MG	CA	3539	1/1	0.92	0.22	73,73,73,73	0
58	MG	AA	3618	1/1	0.92	0.10	38,38,38,38	0
58	MG	DA	1631	1/1	0.92	0.18	70,70,70,70	0
58	MG	DA	1632	1/1	0.92	0.21	61,61,61,61	0
58	MG	AA	3620	1/1	0.92	0.13	40,40,40,40	0
58	MG	CA	3542	1/1	0.92	0.22	68,68,68,68	0
58	MG	AA	3184	1/1	0.92	0.18	68,68,68,68	0
58	MG	AA	3138	1/1	0.92	0.20	50,50,50,50	0
58	MG	CA	3343	1/1	0.92	0.07	36,36,36,36	0
58	MG	AE	302	1/1	0.92	0.17	69,69,69,69	0
58	MG	AA	3625	1/1	0.92	0.11	60,60,60,60	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	CA	3148	1/1	0.92	0.18	65,65,65,65	0
58	MG	CA	3150	1/1	0.92	0.09	54,54,54,54	0
58	MG	DA	1643	1/1	0.92	0.09	55,55,55,55	0
58	MG	CA	3365	1/1	0.92	0.11	48,48,48,48	0
58	MG	DA	1648	1/1	0.92	0.14	50,50,50,50	0
58	MG	CA	3556	1/1	0.92	0.09	48,48,48,48	0
58	MG	BA	1741	1/1	0.92	0.08	93,93,93,93	0
58	MG	AA	3190	1/1	0.92	0.18	45,45,45,45	0
58	MG	AA	3042	1/1	0.92	0.19	38,38,38,38	0
58	MG	AA	3479	1/1	0.92	0.10	54,54,54,54	0
58	MG	CA	3565	1/1	0.92	0.14	51,51,51,51	0
58	MG	CA	3567	1/1	0.92	0.12	56,56,56,56	0
58	MG	AW	3004	1/1	0.92	0.18	65,65,65,65	0
58	MG	AA	3312	1/1	0.92	0.09	55,55,55,55	0
58	MG	BA	1664	1/1	0.92	0.12	53,53,53,53	0
58	MG	AA	3382	1/1	0.92	0.08	36,36,36,36	1
58	MG	CA	3051	1/1	0.92	0.24	63,63,63,63	0
58	MG	AA	3411	1/1	0.92	0.09	47,47,47,47	0
58	MG	CA	3171	1/1	0.92	0.14	55,55,55,55	0
58	MG	AA	3316	1/1	0.92	0.19	60,60,60,60	0
58	MG	AA	3424	1/1	0.92	0.09	65,65,65,65	0
58	MG	A2	102	1/1	0.92	0.10	54,54,54,54	0
58	MG	AA	3518	1/1	0.92	0.08	33,33,33,33	0
58	MG	CA	3589	1/1	0.92	0.13	79,79,79,79	0
58	MG	AA	3642	1/1	0.92	0.08	49,49,49,49	0
58	MG	CA	3400	1/1	0.92	0.09	62,62,62,62	0
58	MG	AA	3644	1/1	0.92	0.10	56,56,56,56	0
58	MG	AA	3426	1/1	0.92	0.10	50,50,50,50	0
58	MG	CA	3185	1/1	0.92	0.25	59,59,59,59	0
58	MG	BA	1674	1/1	0.92	0.15	61,61,61,61	0
58	MG	AA	3531	1/1	0.92	0.15	62,62,62,62	0
58	MG	CA	3191	1/1	0.92	0.29	65,65,65,65	0
58	MG	DA	1689	1/1	0.92	0.13	58,58,58,58	0
58	MG	AA	3317	1/1	0.92	0.11	58,58,58,58	0
58	MG	CA	3602	1/1	0.92	0.10	66,66,66,66	0
58	MG	AA	3095	1/1	0.92	0.21	82,82,82,82	0
58	MG	BA	1678	1/1	0.92	0.18	44,44,44,44	0
58	MG	CA	3606	1/1	0.92	0.18	65,65,65,65	0
58	MG	BA	1604	1/1	0.92	0.08	53,53,53,53	0
58	MG	AA	3543	1/1	0.92	0.10	52,52,52,52	1
58	MG	CA	3201	1/1	0.92	0.26	59,59,59,59	0
58	MG	CA	3424	1/1	0.92	0.10	55,55,55,55	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	AA	3772	1/1	0.92	0.24	17,17,17,17	1
58	MG	AA	3773	1/1	0.92	0.19	30,30,30,30	1
58	MG	AA	3657	1/1	0.92	0.13	43,43,43,43	1
58	MG	AA	3436	1/1	0.92	0.11	38,38,38,38	0
58	MG	AA	3661	1/1	0.92	0.18	43,43,43,43	0
58	MG	AA	3548	1/1	0.92	0.08	57,57,57,57	1
58	MG	DA	1710	1/1	0.92	0.13	70,70,70,70	0
58	MG	AA	3671	1/1	0.92	0.16	58,58,58,58	0
58	MG	DA	1713	1/1	0.92	0.20	72,72,72,72	0
58	MG	CA	3434	1/1	0.92	0.09	28,28,28,28	0
58	MG	CA	3216	1/1	0.92	0.10	66,66,66,66	0
58	MG	CA	3217	1/1	0.92	0.17	52,52,52,52	0
58	MG	BA	1794	1/1	0.92	0.20	75,75,75,75	0
58	MG	AA	3558	1/1	0.92	0.10	51,51,51,51	0
58	MG	CA	3084	1/1	0.92	0.19	59,59,59,59	1
58	MG	AA	3261	1/1	0.92	0.16	51,51,51,51	0
58	MG	AA	3571	1/1	0.92	0.10	48,48,48,48	0
58	MG	CA	3087	1/1	0.92	0.13	67,67,67,67	0
58	MG	CA	3638	1/1	0.92	0.15	55,55,55,55	0
58	MG	AA	3678	1/1	0.92	0.12	31,31,31,31	0
58	MG	CA	3468	1/1	0.92	0.11	61,61,61,61	0
58	MG	AA	3263	1/1	0.92	0.18	80,80,80,80	0
58	MG	AA	3060	1/1	0.92	0.34	65,65,65,65	0
58	MG	BA	1696	1/1	0.92	0.09	80,80,80,80	0
58	MG	CA	3473	1/1	0.92	0.08	54,54,54,54	0
58	MG	BA	1805	1/1	0.92	0.10	64,64,64,64	0
58	MG	CA	3651	1/1	0.92	0.09	31,31,31,31	0
58	MG	AA	3799	1/1	0.92	0.13	47,47,47,47	0
58	MG	AA	3118	1/1	0.92	0.19	64,64,64,64	0
58	MG	CA	3657	1/1	0.92	0.15	67,67,67,67	0
58	MG	AA	3073	1/1	0.92	0.14	58,58,58,58	0
58	MG	AA	3585	1/1	0.92	0.09	65,65,65,65	0
58	MG	BA	1812	1/1	0.92	0.12	66,66,66,66	0
58	MG	AA	3235	1/1	0.92	0.15	64,64,64,64	0
58	MG	AA	3447	1/1	0.92	0.10	61,61,61,61	0
58	MG	AA	3158	1/1	0.92	0.19	97,97,97,97	0
58	MG	CA	3488	1/1	0.92	0.10	51,51,51,51	0
58	MG	DA	1759	1/1	0.92	0.13	76,76,76,76	0
58	MG	AA	3701	1/1	0.92	0.24	43,43,43,43	1
58	MG	AA	3591	1/1	0.92	0.14	65,65,65,65	0
58	MG	AA	3592	1/1	0.92	0.17	52,52,52,52	0
58	MG	CA	3494	1/1	0.92	0.13	63,63,63,63	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	CA	3495	1/1	0.92	0.12	65,65,65,65	0
58	MG	BL	202	1/1	0.92	0.15	67,67,67,67	0
58	MG	CA	3254	1/1	0.92	0.09	42,42,42,42	0
58	MG	DD	502	1/1	0.92	0.30	62,62,62,62	0
58	MG	DE	201	1/1	0.92	0.18	84,84,84,84	0
58	MG	AA	3002	1/1	0.92	0.19	55,55,55,55	0
58	MG	BN	502	1/1	0.92	0.09	66,66,66,66	0
58	MG	AA	3451	1/1	0.92	0.14	48,48,48,48	0
58	MG	AA	3272	1/1	0.92	0.23	52,52,52,52	0
58	MG	DW	501	1/1	0.92	0.27	74,74,74,74	0
58	MG	BW	501	1/1	0.92	0.22	48,48,48,48	0
58	MG	CA	3509	1/1	0.92	0.11	76,76,76,76	0
58	MG	CF	301	1/1	0.92	0.15	63,63,63,63	0
58	MG	CF	303	1/1	0.92	0.17	62,62,62,62	0
58	MG	CA	3120	1/1	0.92	0.27	62,62,62,62	0
62	GDP	DZ	704	28/28	0.92	0.10	80,80,80,80	3
58	MG	CA	3306	1/1	0.93	0.06	41,41,41,41	0
58	MG	CR	201	1/1	0.93	0.13	51,51,51,51	0
58	MG	CV	201	1/1	0.93	0.26	100,100,100,100	0
58	MG	CA	3530	1/1	0.93	0.14	59,59,59,59	0
58	MG	C8	5001	1/1	0.93	0.12	51,51,51,51	0
58	MG	CA	3142	1/1	0.93	0.10	69,69,69,69	0
58	MG	CA	3313	1/1	0.93	0.12	50,50,50,50	0
58	MG	CA	3143	1/1	0.93	0.29	57,57,57,57	0
58	MG	DA	1605	1/1	0.93	0.14	73,73,73,73	0
58	MG	CA	3319	1/1	0.93	0.09	67,67,67,67	0
58	MG	CA	3535	1/1	0.93	0.17	69,69,69,69	0
58	MG	AU	201	1/1	0.93	0.18	45,45,45,45	0
58	MG	CA	3327	1/1	0.93	0.15	53,53,53,53	0
58	MG	CA	3332	1/1	0.93	0.08	42,42,42,42	0
58	MG	DA	1615	1/1	0.93	0.21	53,53,53,53	0
58	MG	CA	3334	1/1	0.93	0.13	44,44,44,44	0
58	MG	AV	201	1/1	0.93	0.06	17,17,17,17	1
58	MG	DA	1620	1/1	0.93	0.05	58,58,58,58	0
58	MG	BA	1751	1/1	0.93	0.08	48,48,48,48	0
58	MG	BA	1752	1/1	0.93	0.11	65,65,65,65	0
58	MG	CA	3347	1/1	0.93	0.13	59,59,59,59	0
58	MG	CA	3348	1/1	0.93	0.13	54,54,54,54	0
58	MG	AA	3658	1/1	0.93	0.17	62,62,62,62	0
58	MG	AA	3152	1/1	0.93	0.20	71,71,71,71	0
58	MG	CA	3549	1/1	0.93	0.07	57,57,57,57	0
58	MG	CA	3358	1/1	0.93	0.14	45,45,45,45	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	AX	101	1/1	0.93	0.17	75,75,75,75	0
58	MG	CA	3361	1/1	0.93	0.19	58,58,58,58	0
58	MG	AA	3368	1/1	0.93	0.07	37,37,37,37	0
58	MG	AA	3664	1/1	0.93	0.12	57,57,57,57	0
58	MG	CA	3368	1/1	0.93	0.11	59,59,59,59	0
58	MG	CA	3558	1/1	0.93	0.09	51,51,51,51	1
58	MG	AA	3262	1/1	0.93	0.32	70,70,70,70	0
58	MG	CA	3048	1/1	0.93	0.18	86,86,86,86	0
58	MG	CA	3161	1/1	0.93	0.13	66,66,66,66	0
58	MG	CA	3564	1/1	0.93	0.12	40,40,40,40	1
58	MG	BA	1765	1/1	0.93	0.11	62,62,62,62	0
58	MG	BA	1766	1/1	0.93	0.22	63,63,63,63	0
58	MG	AA	3667	1/1	0.93	0.09	28,28,28,28	0
58	MG	AA	3372	1/1	0.93	0.19	63,63,63,63	0
58	MG	DA	1650	1/1	0.93	0.23	61,61,61,61	0
58	MG	CA	3570	1/1	0.93	0.20	77,77,77,77	0
58	MG	CA	3054	1/1	0.93	0.16	71,71,71,71	0
58	MG	CA	3573	1/1	0.93	0.08	80,80,80,80	0
58	MG	AA	3373	1/1	0.93	0.17	59,59,59,59	0
58	MG	AA	3598	1/1	0.93	0.17	54,54,54,54	0
58	MG	CA	3177	1/1	0.93	0.07	36,36,36,36	0
58	MG	DA	1661	1/1	0.93	0.19	70,70,70,70	0
58	MG	AA	3468	1/1	0.93	0.18	52,52,52,52	0
58	MG	CA	3580	1/1	0.93	0.08	100,100,100,100	0
58	MG	AA	3313	1/1	0.93	0.06	35,35,35,35	0
58	MG	AA	3604	1/1	0.93	0.11	38,38,38,38	1
58	MG	CA	3181	1/1	0.93	0.20	47,47,47,47	0
58	MG	DA	1667	1/1	0.93	0.13	49,49,49,49	0
58	MG	BA	1778	1/1	0.93	0.11	64,64,64,64	0
58	MG	CA	3588	1/1	0.93	0.17	63,63,63,63	0
58	MG	AA	3153	1/1	0.93	0.14	59,59,59,59	0
58	MG	CA	3186	1/1	0.93	0.12	69,69,69,69	0
58	MG	AA	3683	1/1	0.93	0.23	67,67,67,67	0
58	MG	CA	3592	1/1	0.93	0.21	76,76,76,76	0
58	MG	AA	3686	1/1	0.93	0.11	73,73,73,73	0
58	MG	AA	3178	1/1	0.93	0.14	78,78,78,78	0
58	MG	AA	3783	1/1	0.93	0.09	54,54,54,54	0
58	MG	AA	3414	1/1	0.93	0.09	36,36,36,36	0
58	MG	CA	3597	1/1	0.93	0.13	39,39,39,39	0
58	MG	AA	3691	1/1	0.93	0.18	89,89,89,89	0
58	MG	AA	3181	1/1	0.93	0.10	56,56,56,56	0
58	MG	AA	3695	1/1	0.93	0.17	78,78,78,78	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	CA	3200	1/1	0.93	0.16	54,54,54,54	0
58	MG	AA	3612	1/1	0.93	0.14	56,56,56,56	0
58	MG	AA	3266	1/1	0.93	0.20	50,50,50,50	0
58	MG	CA	3423	1/1	0.93	0.09	50,50,50,50	0
58	MG	AA	3492	1/1	0.93	0.16	45,45,45,45	0
58	MG	DA	1693	1/1	0.93	0.12	54,54,54,54	0
58	MG	DA	1694	1/1	0.93	0.10	60,60,60,60	0
58	MG	CA	3078	1/1	0.93	0.09	47,47,47,47	0
58	MG	CA	3206	1/1	0.93	0.31	56,56,56,56	0
58	MG	BA	1615	1/1	0.93	0.06	101,101,101,101	0
58	MG	AA	3182	1/1	0.93	0.17	76,76,76,76	0
58	MG	AA	3078	1/1	0.93	0.26	66,66,66,66	0
58	MG	AA	3123	1/1	0.93	0.13	37,37,37,37	1
58	MG	CA	3215	1/1	0.93	0.16	73,73,73,73	0
58	MG	DA	1704	1/1	0.93	0.10	69,69,69,69	0
58	MG	AA	3706	1/1	0.93	0.14	27,27,27,27	1
58	MG	BA	1801	1/1	0.93	0.11	65,65,65,65	0
58	MG	AA	3622	1/1	0.93	0.07	45,45,45,45	0
58	MG	AA	3147	1/1	0.93	0.21	69,69,69,69	0
58	MG	CA	3442	1/1	0.93	0.25	67,67,67,67	0
58	MG	CA	3222	1/1	0.93	0.14	75,75,75,75	0
58	MG	CA	3446	1/1	0.93	0.09	63,63,63,63	0
58	MG	AA	3809	1/1	0.93	0.20	62,62,62,62	0
58	MG	AA	3624	1/1	0.93	0.09	65,65,65,65	0
58	MG	AA	3812	1/1	0.93	0.12	42,42,42,42	0
58	MG	AA	3214	1/1	0.93	0.06	34,34,34,34	0
58	MG	AA	3099	1/1	0.93	0.07	62,62,62,62	0
58	MG	AA	3441	1/1	0.93	0.11	51,51,51,51	1
58	MG	DA	1724	1/1	0.93	0.14	61,61,61,61	0
58	MG	CA	3640	1/1	0.93	0.12	59,59,59,59	0
58	MG	AA	3165	1/1	0.93	0.18	57,57,57,57	0
58	MG	DA	1727	1/1	0.93	0.14	66,66,66,66	0
58	MG	DA	1728	1/1	0.93	0.12	63,63,63,63	0
58	MG	AA	3348	1/1	0.93	0.07	32,32,32,32	0
58	MG	AA	3352	1/1	0.93	0.10	51,51,51,51	0
58	MG	AB	3009	1/1	0.93	0.07	56,56,56,56	0
58	MG	BA	1634	1/1	0.93	0.24	54,54,54,54	0
58	MG	DA	1734	1/1	0.93	0.15	83,83,83,83	0
58	MG	AA	3171	1/1	0.93	0.17	25,25,25,25	1
58	MG	CA	3101	1/1	0.93	0.11	78,78,78,78	0
58	MG	AA	3561	1/1	0.93	0.13	58,58,58,58	0
58	MG	AB	3016	1/1	0.93	0.10	34,34,34,34	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	BM	201	1/1	0.93	0.07	57,57,57,57	0
58	MG	AA	3735	1/1	0.93	0.08	35,35,35,35	0
58	MG	DA	1742	1/1	0.93	0.16	79,79,79,79	0
58	MG	DA	1743	1/1	0.93	0.17	72,72,72,72	0
58	MG	BA	1639	1/1	0.93	0.08	66,66,66,66	0
58	MG	AA	3250	1/1	0.93	0.13	46,46,46,46	0
58	MG	AA	3198	1/1	0.93	0.11	58,58,58,58	0
58	MG	AA	3286	1/1	0.93	0.09	52,52,52,52	0
58	MG	AA	3292	1/1	0.93	0.13	74,74,74,74	0
58	MG	AD	303	1/1	0.93	0.18	70,70,70,70	0
58	MG	AA	3256	1/1	0.93	0.09	21,21,21,21	1
58	MG	AA	3579	1/1	0.93	0.07	38,38,38,38	0
58	MG	AA	3648	1/1	0.93	0.10	40,40,40,40	0
58	MG	AD	309	1/1	0.93	0.10	37,37,37,37	0
58	MG	CA	3006	1/1	0.93	0.22	67,67,67,67	0
58	MG	CB	3008	1/1	0.93	0.10	59,59,59,59	0
58	MG	CA	3501	1/1	0.93	0.12	45,45,45,45	1
58	MG	AA	3363	1/1	0.93	0.07	28,28,28,28	0
58	MG	CB	3011	1/1	0.93	0.16	53,53,53,53	0
58	MG	AA	3456	1/1	0.93	0.08	30,30,30,30	0
58	MG	AF	304	1/1	0.93	0.17	43,43,43,43	0
58	MG	CA	3014	1/1	0.93	0.15	62,62,62,62	0
58	MG	AF	307	1/1	0.93	0.11	62,62,62,62	0
58	MG	AA	3653	1/1	0.93	0.10	68,68,68,68	0
58	MG	CA	3020	1/1	0.93	0.08	63,63,63,63	0
58	MG	BA	1740	1/1	0.93	0.19	56,56,56,56	0
58	MG	CA	3135	1/1	0.93	0.18	66,66,66,66	0
58	MG	AA	3297	1/1	0.93	0.06	20,20,20,20	1
58	MG	CF	304	1/1	0.93	0.14	65,65,65,65	0
58	MG	CA	3138	1/1	0.93	0.07	63,63,63,63	0
58	MG	CA	3298	1/1	0.93	0.10	68,68,68,68	0
58	MG	CA	3027	1/1	0.93	0.14	44,44,44,44	0
58	MG	CA	3301	1/1	0.93	0.08	47,47,47,47	0
58	MG	CA	3524	1/1	0.93	0.06	77,77,77,77	0
58	MG	AP	203	1/1	0.93	0.06	40,40,40,40	0
58	MG	AA	3129	1/1	0.93	0.18	66,66,66,66	1
58	MG	CF	302	1/1	0.94	0.08	56,56,56,56	0
58	MG	AA	3185	1/1	0.94	0.19	41,41,41,41	0
58	MG	CA	3103	1/1	0.94	0.21	62,62,62,62	0
58	MG	CF	305	1/1	0.94	0.12	51,51,51,51	0
58	MG	AA	3098	1/1	0.94	0.23	58,58,58,58	0
58	MG	CA	3106	1/1	0.94	0.22	55,55,55,55	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	AW	3003	1/1	0.94	0.15	52,52,52,52	0
58	MG	AA	3748	1/1	0.94	0.16	56,56,56,56	0
58	MG	CP	201	1/1	0.94	0.38	65,65,65,65	0
58	MG	CA	3261	1/1	0.94	0.11	29,29,29,29	0
58	MG	AA	3481	1/1	0.94	0.05	51,51,51,51	0
58	MG	CA	3112	1/1	0.94	0.10	61,61,61,61	0
58	MG	AA	3487	1/1	0.94	0.09	39,39,39,39	0
58	MG	AA	3189	1/1	0.94	0.09	40,40,40,40	0
58	MG	AA	3753	1/1	0.94	0.10	41,41,41,41	0
58	MG	CV	202	1/1	0.94	0.21	85,85,85,85	0
58	MG	CY	502	1/1	0.94	0.15	56,56,56,56	0
58	MG	CA	3278	1/1	0.94	0.09	37,37,37,37	0
58	MG	CA	3280	1/1	0.94	0.06	30,30,30,30	0
58	MG	A0	102	1/1	0.94	0.09	40,40,40,40	0
58	MG	AA	3278	1/1	0.94	0.18	36,36,36,36	0
58	MG	CA	3522	1/1	0.94	0.15	56,56,56,56	0
58	MG	AA	3279	1/1	0.94	0.24	53,53,53,53	0
58	MG	AA	3280	1/1	0.94	0.14	47,47,47,47	0
58	MG	AA	3496	1/1	0.94	0.13	52,52,52,52	0
58	MG	CA	3526	1/1	0.94	0.06	40,40,40,40	0
58	MG	DA	1610	1/1	0.94	0.07	75,75,75,75	0
58	MG	DA	1612	1/1	0.94	0.33	72,72,72,72	0
58	MG	A5	101	1/1	0.94	0.13	37,37,37,37	1
58	MG	AA	3503	1/1	0.94	0.09	64,64,64,64	0
58	MG	AA	3120	1/1	0.94	0.16	46,46,46,46	0
58	MG	A6	101	1/1	0.94	0.19	65,65,65,65	0
58	MG	AA	3763	1/1	0.94	0.17	65,65,65,65	0
58	MG	AA	3511	1/1	0.94	0.07	12,12,12,12	0
58	MG	AA	3512	1/1	0.94	0.15	60,60,60,60	0
58	MG	BA	1602	1/1	0.94	0.16	111,111,111,111	0
58	MG	DA	1624	1/1	0.94	0.06	44,44,44,44	0
58	MG	AA	3516	1/1	0.94	0.08	18,18,18,18	0
58	MG	BW	502	1/1	0.94	0.13	53,53,53,53	0
58	MG	CA	3309	1/1	0.94	0.08	29,29,29,29	0
58	MG	BW	503	1/1	0.94	0.10	45,45,45,45	0
58	MG	AA	3191	1/1	0.94	0.16	42,42,42,42	0
58	MG	AA	3651	1/1	0.94	0.09	52,52,52,52	0
58	MG	CA	3316	1/1	0.94	0.11	50,50,50,50	0
58	MG	DA	1633	1/1	0.94	0.28	73,73,73,73	0
58	MG	AA	3519	1/1	0.94	0.09	21,21,21,21	0
58	MG	AA	3284	1/1	0.94	0.22	44,44,44,44	0
58	MG	CA	3324	1/1	0.94	0.14	40,40,40,40	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	BA	1705	1/1	0.94	0.17	78,78,78,78	0
58	MG	CA	3547	1/1	0.94	0.10	61,61,61,61	0
58	MG	CA	3330	1/1	0.94	0.13	43,43,43,43	0
58	MG	CA	3331	1/1	0.94	0.12	52,52,52,52	0
58	MG	AA	3378	1/1	0.94	0.07	19,19,19,19	0
58	MG	BA	1609	1/1	0.94	0.10	62,62,62,62	0
58	MG	CA	3336	1/1	0.94	0.10	69,69,69,69	0
58	MG	DA	1644	1/1	0.94	0.17	57,57,57,57	0
58	MG	DA	1646	1/1	0.94	0.22	62,62,62,62	0
58	MG	AA	3381	1/1	0.94	0.10	27,27,27,27	0
58	MG	AA	3239	1/1	0.94	0.17	64,64,64,64	0
58	MG	CA	3012	1/1	0.94	0.12	59,59,59,59	0
58	MG	CA	3344	1/1	0.94	0.15	87,87,87,87	0
58	MG	DA	1651	1/1	0.94	0.29	59,59,59,59	0
58	MG	CA	3346	1/1	0.94	0.07	31,31,31,31	0
58	MG	AA	3390	1/1	0.94	0.11	35,35,35,35	0
58	MG	DA	1655	1/1	0.94	0.30	58,58,58,58	0
58	MG	DA	1656	1/1	0.94	0.16	75,75,75,75	0
58	MG	CA	3149	1/1	0.94	0.05	66,66,66,66	0
58	MG	AA	3546	1/1	0.94	0.08	32,32,32,32	0
58	MG	CA	3352	1/1	0.94	0.11	68,68,68,68	0
58	MG	CA	3151	1/1	0.94	0.07	50,50,50,50	0
58	MG	AA	3406	1/1	0.94	0.11	57,57,57,57	0
58	MG	CA	3017	1/1	0.94	0.21	46,46,46,46	0
58	MG	AA	3290	1/1	0.94	0.13	63,63,63,63	0
58	MG	AA	3551	1/1	0.94	0.10	52,52,52,52	0
58	MG	CA	3156	1/1	0.94	0.16	68,68,68,68	0
58	MG	CA	3366	1/1	0.94	0.17	61,61,61,61	0
58	MG	AA	3668	1/1	0.94	0.07	40,40,40,40	0
58	MG	AA	3241	1/1	0.94	0.13	69,69,69,69	0
58	MG	AA	3087	1/1	0.94	0.19	72,72,72,72	0
58	MG	AA	3422	1/1	0.94	0.07	71,71,71,71	0
58	MG	CA	3163	1/1	0.94	0.20	40,40,40,40	0
58	MG	CA	3584	1/1	0.94	0.08	46,46,46,46	0
58	MG	AA	3061	1/1	0.94	0.12	27,27,27,27	0
58	MG	CA	3166	1/1	0.94	0.20	44,44,44,44	0
58	MG	CA	3380	1/1	0.94	0.17	71,71,71,71	0
58	MG	BA	1724	1/1	0.94	0.16	55,55,55,55	0
58	MG	AA	3127	1/1	0.94	0.16	71,71,71,71	0
58	MG	CA	3169	1/1	0.94	0.12	34,34,34,34	0
58	MG	AA	3428	1/1	0.94	0.10	35,35,35,35	0
58	MG	AA	3197	1/1	0.94	0.13	37,37,37,37	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	AA	3431	1/1	0.94	0.12	25,25,25,25	0
58	MG	AA	3432	1/1	0.94	0.13	57,57,57,57	0
58	MG	CA	3040	1/1	0.94	0.17	66,66,66,66	0
58	MG	AA	3581	1/1	0.94	0.10	40,40,40,40	0
58	MG	AA	3582	1/1	0.94	0.14	66,66,66,66	0
58	MG	CA	3044	1/1	0.94	0.16	52,52,52,52	0
58	MG	BA	1738	1/1	0.94	0.07	73,73,73,73	0
58	MG	AA	3102	1/1	0.94	0.18	49,49,49,49	0
58	MG	CA	3404	1/1	0.94	0.08	54,54,54,54	0
58	MG	AA	3159	1/1	0.94	0.24	46,46,46,46	1
58	MG	CA	3605	1/1	0.94	0.17	73,73,73,73	0
58	MG	AA	3161	1/1	0.94	0.18	60,60,60,60	0
58	MG	BA	1743	1/1	0.94	0.06	46,46,46,46	0
58	MG	CA	3608	1/1	0.94	0.09	56,56,56,56	0
58	MG	AA	3091	1/1	0.94	0.12	38,38,38,38	1
58	MG	AA	3132	1/1	0.94	0.14	27,27,27,27	1
58	MG	AB	3003	1/1	0.94	0.13	51,51,51,51	0
58	MG	BA	1749	1/1	0.94	0.14	68,68,68,68	0
58	MG	CA	3195	1/1	0.94	0.16	60,60,60,60	0
58	MG	CA	3615	1/1	0.94	0.10	38,38,38,38	0
58	MG	CA	3419	1/1	0.94	0.07	60,60,60,60	0
58	MG	AA	3254	1/1	0.94	0.14	42,42,42,42	0
58	MG	AA	3699	1/1	0.94	0.14	46,46,46,46	1
58	MG	CA	3198	1/1	0.94	0.06	37,37,37,37	0
58	MG	AA	3330	1/1	0.94	0.10	69,69,69,69	0
58	MG	AB	3008	1/1	0.94	0.24	51,51,51,51	0
58	MG	BA	1642	1/1	0.94	0.12	55,55,55,55	0
58	MG	AA	3335	1/1	0.94	0.09	41,41,41,41	0
58	MG	DA	1721	1/1	0.94	0.12	67,67,67,67	0
58	MG	CA	3626	1/1	0.94	0.16	75,75,75,75	0
58	MG	DA	1723	1/1	0.94	0.18	66,66,66,66	0
58	MG	CA	3203	1/1	0.94	0.07	60,60,60,60	0
58	MG	AB	3010	1/1	0.94	0.06	47,47,47,47	1
58	MG	AA	3703	1/1	0.94	0.06	76,76,76,76	0
58	MG	AA	3106	1/1	0.94	0.20	52,52,52,52	0
58	MG	CA	3207	1/1	0.94	0.14	71,71,71,71	0
58	MG	DA	1729	1/1	0.94	0.07	57,57,57,57	0
58	MG	CA	3435	1/1	0.94	0.08	52,52,52,52	0
58	MG	CA	3637	1/1	0.94	0.26	59,59,59,59	0
58	MG	AA	3258	1/1	0.94	0.05	22,22,22,22	0
58	MG	AA	3259	1/1	0.94	0.19	20,20,20,20	1
58	MG	AA	3341	1/1	0.94	0.08	15,15,15,15	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	AA	3712	1/1	0.94	0.14	46,46,46,46	0
58	MG	CA	3213	1/1	0.94	0.18	44,44,44,44	0
58	MG	AA	3166	1/1	0.94	0.18	31,31,31,31	0
58	MG	AA	3714	1/1	0.94	0.17	56,56,56,56	0
58	MG	AD	301	1/1	0.94	0.16	43,43,43,43	0
58	MG	CA	3647	1/1	0.94	0.06	66,66,66,66	0
58	MG	CA	3456	1/1	0.94	0.13	60,60,60,60	0
58	MG	AD	302	1/1	0.94	0.15	61,61,61,61	0
58	MG	CA	3463	1/1	0.94	0.10	49,49,49,49	0
58	MG	CA	3654	1/1	0.94	0.17	51,51,51,51	0
58	MG	CA	3655	1/1	0.94	0.11	70,70,70,70	0
58	MG	BA	1656	1/1	0.94	0.10	54,54,54,54	0
58	MG	CA	3466	1/1	0.94	0.20	57,57,57,57	0
58	MG	CA	3659	1/1	0.94	0.10	77,77,77,77	0
58	MG	AA	3135	1/1	0.94	0.31	62,62,62,62	1
58	MG	DA	1752	1/1	0.94	0.12	74,74,74,74	0
58	MG	AA	3607	1/1	0.94	0.08	30,30,30,30	0
58	MG	AD	306	1/1	0.94	0.19	38,38,38,38	1
58	MG	CA	3225	1/1	0.94	0.15	65,65,65,65	0
58	MG	DA	1756	1/1	0.94	0.09	68,68,68,68	0
58	MG	CA	3664	1/1	0.94	0.11	54,54,54,54	0
58	MG	AA	3058	1/1	0.94	0.13	35,35,35,35	0
58	MG	AA	3173	1/1	0.94	0.13	60,60,60,60	0
58	MG	AA	3093	1/1	0.94	0.07	27,27,27,27	1
58	MG	DA	1762	1/1	0.94	0.06	73,73,73,73	0
58	MG	AD	310	1/1	0.94	0.14	42,42,42,42	0
58	MG	AA	3349	1/1	0.94	0.10	40,40,40,40	0
58	MG	CA	3232	1/1	0.94	0.07	60,60,60,60	0
58	MG	AA	3215	1/1	0.94	0.20	42,42,42,42	1
58	MG	AF	301	1/1	0.94	0.11	25,25,25,25	1
58	MG	AA	3353	1/1	0.94	0.09	76,76,76,76	0
58	MG	AA	3216	1/1	0.94	0.14	51,51,51,51	0
58	MG	AG	201	1/1	0.94	0.10	52,52,52,52	0
58	MG	AH	3001	1/1	0.94	0.19	52,52,52,52	0
58	MG	AA	3063	1/1	0.94	0.23	67,67,67,67	0
58	MG	CA	3490	1/1	0.94	0.10	67,67,67,67	0
58	MG	DT	3001	1/1	0.94	0.22	67,67,67,67	0
58	MG	BA	1796	1/1	0.94	0.13	77,77,77,77	0
58	MG	CE	301	1/1	0.94	0.13	66,66,66,66	0
58	MG	AA	3110	1/1	0.94	0.18	79,79,79,79	0
58	MG	AA	3055	1/1	0.94	0.11	35,35,35,35	0
58	MG	CE	305	1/1	0.94	0.14	43,43,43,43	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	AA	3146	1/1	0.94	0.14	33,33,33,33	1
58	MG	AA	3036	1/1	0.94	0.11	51,51,51,51	0
58	MG	AA	3167	1/1	0.95	0.09	65,65,65,65	0
58	MG	AA	3726	1/1	0.95	0.06	67,67,67,67	0
58	MG	AA	3196	1/1	0.95	0.18	52,52,52,52	0
58	MG	CA	3325	1/1	0.95	0.07	38,38,38,38	0
58	MG	AA	3517	1/1	0.95	0.09	19,19,19,19	0
58	MG	CA	3328	1/1	0.95	0.07	55,55,55,55	0
58	MG	AA	3168	1/1	0.95	0.16	63,63,63,63	0
58	MG	AA	3628	1/1	0.95	0.14	80,80,80,80	0
58	MG	AA	3008	1/1	0.95	0.08	19,19,19,19	0
58	MG	CA	3333	1/1	0.95	0.15	75,75,75,75	0
58	MG	AD	304	1/1	0.95	0.13	19,19,19,19	0
58	MG	DA	1616	1/1	0.95	0.18	64,64,64,64	0
58	MG	CA	3335	1/1	0.95	0.13	62,62,62,62	0
58	MG	CA	3038	1/1	0.95	0.20	48,48,48,48	0
58	MG	CA	3162	1/1	0.95	0.20	46,46,46,46	0
58	MG	AA	3525	1/1	0.95	0.18	40,40,40,40	0
58	MG	AA	3076	1/1	0.95	0.17	92,92,92,92	0
58	MG	AA	3737	1/1	0.95	0.07	29,29,29,29	0
58	MG	AA	3124	1/1	0.95	0.15	63,63,63,63	0
58	MG	AA	3634	1/1	0.95	0.08	62,62,62,62	0
58	MG	AA	3021	1/1	0.95	0.07	40,40,40,40	0
58	MG	AA	3202	1/1	0.95	0.09	47,47,47,47	0
58	MG	DA	1629	1/1	0.95	0.19	58,58,58,58	0
58	MG	AE	301	1/1	0.95	0.07	19,19,19,19	0
58	MG	CA	3353	1/1	0.95	0.09	48,48,48,48	0
58	MG	CA	3355	1/1	0.95	0.07	41,41,41,41	0
58	MG	AA	3175	1/1	0.95	0.09	51,51,51,51	0
58	MG	AE	304	1/1	0.95	0.05	41,41,41,41	0
58	MG	CA	3175	1/1	0.95	0.16	42,42,42,42	0
58	MG	AA	3281	1/1	0.95	0.28	61,61,61,61	0
58	MG	CA	3362	1/1	0.95	0.09	44,44,44,44	0
58	MG	AA	3176	1/1	0.95	0.08	50,50,50,50	0
58	MG	BA	1763	1/1	0.95	0.09	55,55,55,55	0
58	MG	CA	3055	1/1	0.95	0.16	39,39,39,39	0
58	MG	CA	3367	1/1	0.95	0.16	65,65,65,65	0
58	MG	AA	3205	1/1	0.95	0.27	64,64,64,64	0
58	MG	CA	3182	1/1	0.95	0.15	27,27,27,27	0
58	MG	BA	1657	1/1	0.95	0.16	69,69,69,69	0
58	MG	DA	1645	1/1	0.95	0.12	64,64,64,64	0
58	MG	AA	3549	1/1	0.95	0.06	54,54,54,54	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	AG	202	1/1	0.95	0.06	73,73,73,73	0
58	MG	CA	3187	1/1	0.95	0.10	37,37,37,37	0
58	MG	AA	3646	1/1	0.95	0.08	58,58,58,58	0
58	MG	CA	3061	1/1	0.95	0.27	67,67,67,67	0
58	MG	CA	3384	1/1	0.95	0.13	71,71,71,71	0
58	MG	BA	1772	1/1	0.95	0.12	56,56,56,56	0
58	MG	AA	3006	1/1	0.95	0.17	52,52,52,52	0
58	MG	CA	3065	1/1	0.95	0.09	52,52,52,52	0
58	MG	AA	3553	1/1	0.95	0.07	40,40,40,40	0
58	MG	AA	3081	1/1	0.95	0.06	40,40,40,40	0
58	MG	CA	3392	1/1	0.95	0.07	35,35,35,35	0
58	MG	BA	1776	1/1	0.95	0.08	61,61,61,61	0
58	MG	AA	3560	1/1	0.95	0.09	58,58,58,58	0
58	MG	AQ	203	1/1	0.95	0.18	41,41,41,41	0
58	MG	AA	3759	1/1	0.95	0.13	65,65,65,65	0
58	MG	BA	1780	1/1	0.95	0.06	42,42,42,42	0
58	MG	AU	203	1/1	0.95	0.14	29,29,29,29	1
58	MG	AA	3180	1/1	0.95	0.16	94,94,94,94	0
58	MG	BA	1783	1/1	0.95	0.10	62,62,62,62	0
58	MG	AV	202	1/1	0.95	0.10	20,20,20,20	0
58	MG	AV	205	1/1	0.95	0.15	55,55,55,55	1
58	MG	CA	3600	1/1	0.95	0.07	50,50,50,50	0
58	MG	AA	3291	1/1	0.95	0.07	44,44,44,44	0
58	MG	AW	3002	1/1	0.95	0.14	55,55,55,55	0
58	MG	AA	3654	1/1	0.95	0.15	66,66,66,66	0
58	MG	CA	3411	1/1	0.95	0.19	61,61,61,61	0
58	MG	AA	3655	1/1	0.95	0.11	61,61,61,61	0
58	MG	AA	3570	1/1	0.95	0.06	15,15,15,15	0
58	MG	AA	3449	1/1	0.95	0.06	15,15,15,15	0
58	MG	CA	3416	1/1	0.95	0.10	48,48,48,48	0
58	MG	AA	3361	1/1	0.95	0.07	29,29,29,29	0
58	MG	DA	1681	1/1	0.95	0.10	55,55,55,55	0
58	MG	DA	1683	1/1	0.95	0.19	54,54,54,54	0
58	MG	AA	3211	1/1	0.95	0.26	42,42,42,42	1
58	MG	AA	3576	1/1	0.95	0.10	38,38,38,38	0
58	MG	CA	3612	1/1	0.95	0.11	68,68,68,68	0
58	MG	CA	3218	1/1	0.95	0.34	54,54,54,54	0
58	MG	AA	3663	1/1	0.95	0.17	62,62,62,62	0
58	MG	AA	3025	1/1	0.95	0.08	35,35,35,35	1
58	MG	CA	3425	1/1	0.95	0.07	53,53,53,53	0
58	MG	AA	3295	1/1	0.95	0.16	47,47,47,47	0
58	MG	AA	3157	1/1	0.95	0.08	34,34,34,34	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	AA	3366	1/1	0.95	0.08	53,53,53,53	0
58	MG	DA	1695	1/1	0.95	0.13	66,66,66,66	0
58	MG	AA	3669	1/1	0.95	0.06	33,33,33,33	0
58	MG	AA	3299	1/1	0.95	0.08	20,20,20,20	0
58	MG	AA	3782	1/1	0.95	0.17	74,74,74,74	0
58	MG	A7	101	1/1	0.95	0.11	65,65,65,65	0
58	MG	CA	3229	1/1	0.95	0.15	51,51,51,51	0
58	MG	BA	1806	1/1	0.95	0.14	67,67,67,67	0
58	MG	AA	3305	1/1	0.95	0.14	55,55,55,55	0
58	MG	CA	3438	1/1	0.95	0.08	46,46,46,46	0
58	MG	AA	3307	1/1	0.95	0.06	6,6,6,6	0
58	MG	A9	502	1/1	0.95	0.17	60,60,60,60	0
58	MG	BA	1810	1/1	0.95	0.12	50,50,50,50	0
58	MG	AA	3371	1/1	0.95	0.12	62,62,62,62	0
58	MG	AA	3030	1/1	0.95	0.15	26,26,26,26	1
58	MG	AA	3789	1/1	0.95	0.15	54,54,54,54	0
58	MG	CA	3449	1/1	0.95	0.07	66,66,66,66	0
58	MG	DA	1712	1/1	0.95	0.12	81,81,81,81	0
58	MG	CA	3110	1/1	0.95	0.09	63,63,63,63	0
58	MG	AA	3113	1/1	0.95	0.14	64,64,64,64	0
58	MG	AA	3681	1/1	0.95	0.12	65,65,65,65	0
58	MG	BE	3001	1/1	0.95	0.08	60,60,60,60	0
58	MG	CA	3464	1/1	0.95	0.07	46,46,46,46	0
58	MG	AA	3466	1/1	0.95	0.07	63,63,63,63	0
58	MG	AA	3798	1/1	0.95	0.09	35,35,35,35	0
58	MG	CA	3247	1/1	0.95	0.15	66,66,66,66	0
58	MG	AA	3219	1/1	0.95	0.18	58,58,58,58	0
58	MG	CA	3251	1/1	0.95	0.12	56,56,56,56	0
58	MG	AA	3220	1/1	0.95	0.22	62,62,62,62	0
58	MG	AA	3115	1/1	0.95	0.23	67,67,67,67	1
58	MG	CA	3119	1/1	0.95	0.19	128,128,128,128	0
58	MG	AA	3162	1/1	0.95	0.10	47,47,47,47	0
58	MG	CA	3476	1/1	0.95	0.07	55,55,55,55	0
58	MG	AA	3383	1/1	0.95	0.10	54,54,54,54	0
58	MG	AA	3601	1/1	0.95	0.19	47,47,47,47	0
58	MG	CA	3479	1/1	0.95	0.12	46,46,46,46	0
58	MG	CA	3258	1/1	0.95	0.12	70,70,70,70	0
58	MG	CA	3259	1/1	0.95	0.10	47,47,47,47	0
58	MG	AA	3603	1/1	0.95	0.12	63,63,63,63	0
58	MG	CA	3124	1/1	0.95	0.18	48,48,48,48	0
58	MG	AA	3386	1/1	0.95	0.09	29,29,29,29	0
58	MG	CA	3268	1/1	0.95	0.17	69,69,69,69	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	BA	1709	1/1	0.95	0.14	50,50,50,50	0
58	MG	CA	3271	1/1	0.95	0.12	57,57,57,57	0
58	MG	AA	3484	1/1	0.95	0.09	35,35,35,35	0
58	MG	CA	3491	1/1	0.95	0.07	51,51,51,51	0
58	MG	AA	3486	1/1	0.95	0.10	27,27,27,27	0
58	MG	CA	3275	1/1	0.95	0.09	42,42,42,42	0
58	MG	CA	3277	1/1	0.95	0.09	90,90,90,90	0
58	MG	CA	3129	1/1	0.95	0.26	69,69,69,69	0
58	MG	CA	3497	1/1	0.95	0.12	73,73,73,73	0
58	MG	BA	1712	1/1	0.95	0.40	73,73,73,73	0
58	MG	AA	3117	1/1	0.95	0.16	30,30,30,30	1
58	MG	CE	302	1/1	0.95	0.09	47,47,47,47	0
58	MG	AA	3609	1/1	0.95	0.10	53,53,53,53	0
58	MG	AA	3391	1/1	0.95	0.08	45,45,45,45	0
58	MG	CA	3503	1/1	0.95	0.09	62,62,62,62	0
58	MG	BA	1623	1/1	0.95	0.11	49,49,49,49	0
58	MG	AA	3054	1/1	0.95	0.10	38,38,38,38	0
58	MG	CA	3136	1/1	0.95	0.19	53,53,53,53	0
58	MG	AA	3324	1/1	0.95	0.07	33,33,33,33	0
58	MG	CA	3293	1/1	0.95	0.10	71,71,71,71	0
58	MG	CA	3009	1/1	0.95	0.17	67,67,67,67	0
58	MG	AA	3412	1/1	0.95	0.10	43,43,43,43	0
58	MG	AA	3495	1/1	0.95	0.10	59,59,59,59	0
58	MG	CA	3299	1/1	0.95	0.08	61,61,61,61	0
58	MG	AA	3709	1/1	0.95	0.14	29,29,29,29	1
58	MG	AA	3617	1/1	0.95	0.13	49,49,49,49	0
58	MG	AA	3119	1/1	0.95	0.09	40,40,40,40	1
58	MG	CA	3520	1/1	0.95	0.12	59,59,59,59	0
58	MG	CQ	202	1/1	0.95	0.23	64,64,64,64	0
58	MG	CA	3303	1/1	0.95	0.14	54,54,54,54	0
58	MG	CA	3144	1/1	0.95	0.23	67,67,67,67	0
58	MG	AA	3619	1/1	0.95	0.07	42,42,42,42	0
58	MG	AA	3334	1/1	0.95	0.09	57,57,57,57	0
58	MG	AA	3231	1/1	0.95	0.20	53,53,53,53	0
58	MG	CW	201	1/1	0.95	0.08	39,39,39,39	0
58	MG	AA	3071	1/1	0.95	0.20	41,41,41,41	0
59	ZN	C4	501	1/1	0.95	0.06	189,189,189,189	0
58	MG	BA	1735	1/1	0.95	0.10	62,62,62,62	0
58	MG	CA	3315	1/1	0.95	0.13	60,60,60,60	0
58	MG	CA	3026	1/1	0.95	0.15	81,81,81,81	0
58	MG	CA	3184	1/1	0.96	0.13	66,66,66,66	0
58	MG	AA	3014	1/1	0.96	0.19	45,45,45,45	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	CA	3351	1/1	0.96	0.07	46,46,46,46	0
58	MG	BA	1764	1/1	0.96	0.05	52,52,52,52	1
58	MG	AA	3114	1/1	0.96	0.06	17,17,17,17	0
58	MG	DA	1608	1/1	0.96	0.08	47,47,47,47	0
58	MG	CA	3354	1/1	0.96	0.09	61,61,61,61	0
58	MG	CA	3188	1/1	0.96	0.14	58,58,58,58	0
58	MG	AA	3226	1/1	0.96	0.12	56,56,56,56	0
58	MG	AA	3195	1/1	0.96	0.14	50,50,50,50	0
58	MG	AA	3311	1/1	0.96	0.11	33,33,33,33	0
58	MG	BA	1769	1/1	0.96	0.06	58,58,58,58	0
58	MG	AA	3229	1/1	0.96	0.16	43,43,43,43	0
58	MG	AD	312	1/1	0.96	0.15	58,58,58,58	0
58	MG	CA	3068	1/1	0.96	0.12	57,57,57,57	0
58	MG	AA	3004	1/1	0.96	0.07	25,25,25,25	0
58	MG	AA	3554	1/1	0.96	0.06	49,49,49,49	0
58	MG	CA	3548	1/1	0.96	0.04	48,48,48,48	1
58	MG	AA	3740	1/1	0.96	0.08	45,45,45,45	0
58	MG	CA	3369	1/1	0.96	0.07	59,59,59,59	0
58	MG	CA	3371	1/1	0.96	0.12	55,55,55,55	0
58	MG	AA	3556	1/1	0.96	0.08	39,39,39,39	0
58	MG	AF	302	1/1	0.96	0.14	40,40,40,40	0
58	MG	AA	3267	1/1	0.96	0.21	63,63,63,63	0
58	MG	AA	3559	1/1	0.96	0.12	39,39,39,39	0
58	MG	AF	308	1/1	0.96	0.09	55,55,55,55	0
58	MG	AA	3746	1/1	0.96	0.09	64,64,64,64	0
58	MG	AA	3454	1/1	0.96	0.11	51,51,51,51	0
58	MG	AA	3142	1/1	0.96	0.15	26,26,26,26	1
58	MG	AA	3048	1/1	0.96	0.06	34,34,34,34	0
58	MG	AA	3564	1/1	0.96	0.08	19,19,19,19	0
58	MG	AO	5001	1/1	0.96	0.08	55,55,55,55	0
58	MG	CA	3083	1/1	0.96	0.16	90,90,90,90	0
58	MG	AA	3566	1/1	0.96	0.08	27,27,27,27	0
58	MG	CA	3391	1/1	0.96	0.09	63,63,63,63	0
58	MG	CA	3214	1/1	0.96	0.14	40,40,40,40	0
58	MG	AA	3144	1/1	0.96	0.09	40,40,40,40	0
58	MG	CA	3394	1/1	0.96	0.11	55,55,55,55	0
58	MG	CA	3575	1/1	0.96	0.06	43,43,43,43	1
58	MG	AA	3377	1/1	0.96	0.05	20,20,20,20	0
58	MG	AR	201	1/1	0.96	0.13	37,37,37,37	1
58	MG	CA	3397	1/1	0.96	0.08	59,59,59,59	0
58	MG	AA	3145	1/1	0.96	0.12	33,33,33,33	0
58	MG	AU	202	1/1	0.96	0.10	44,44,44,44	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	CA	3582	1/1	0.96	0.08	44,44,44,44	0
58	MG	AA	3007	1/1	0.96	0.04	21,21,21,21	0
58	MG	AA	3332	1/1	0.96	0.08	46,46,46,46	0
58	MG	AA	3577	1/1	0.96	0.05	32,32,32,32	0
58	MG	AA	3333	1/1	0.96	0.08	66,66,66,66	0
58	MG	BA	1798	1/1	0.96	0.07	70,70,70,70	0
58	MG	AV	206	1/1	0.96	0.14	38,38,38,38	0
58	MG	AA	3050	1/1	0.96	0.09	53,53,53,53	0
58	MG	CA	3408	1/1	0.96	0.08	64,64,64,64	0
58	MG	AA	3079	1/1	0.96	0.05	34,34,34,34	0
58	MG	CA	3410	1/1	0.96	0.06	31,31,31,31	0
58	MG	AA	3467	1/1	0.96	0.06	44,44,44,44	0
58	MG	AA	3662	1/1	0.96	0.15	59,59,59,59	0
58	MG	AA	3149	1/1	0.96	0.13	62,62,62,62	0
58	MG	CA	3102	1/1	0.96	0.07	56,56,56,56	0
58	MG	AA	3769	1/1	0.96	0.14	57,57,57,57	0
58	MG	CA	3104	1/1	0.96	0.07	48,48,48,48	0
58	MG	AA	3584	1/1	0.96	0.07	65,65,65,65	0
58	MG	AA	3404	1/1	0.96	0.06	19,19,19,19	0
58	MG	CA	3238	1/1	0.96	0.09	59,59,59,59	0
58	MG	CA	3422	1/1	0.96	0.12	55,55,55,55	0
58	MG	AA	3405	1/1	0.96	0.16	46,46,46,46	0
58	MG	AA	3051	1/1	0.96	0.15	36,36,36,36	0
58	MG	AA	3103	1/1	0.96	0.07	15,15,15,15	0
58	MG	CA	3242	1/1	0.96	0.04	41,41,41,41	0
58	MG	CA	3427	1/1	0.96	0.09	55,55,55,55	0
58	MG	AA	3670	1/1	0.96	0.08	33,33,33,33	0
58	MG	AA	3777	1/1	0.96	0.05	19,19,19,19	0
58	MG	AA	3011	1/1	0.96	0.05	40,40,40,40	0
58	MG	AA	3125	1/1	0.96	0.10	23,23,23,23	1
58	MG	AA	3780	1/1	0.96	0.12	42,42,42,42	0
58	MG	AA	3594	1/1	0.96	0.09	43,43,43,43	0
58	MG	CA	3250	1/1	0.96	0.07	52,52,52,52	0
58	MG	AA	3595	1/1	0.96	0.10	55,55,55,55	0
58	MG	A7	104	1/1	0.96	0.09	49,49,49,49	1
58	MG	AA	3676	1/1	0.96	0.09	66,66,66,66	0
58	MG	AA	3677	1/1	0.96	0.05	41,41,41,41	0
58	MG	AA	3183	1/1	0.96	0.10	35,35,35,35	1
58	MG	AA	3419	1/1	0.96	0.08	31,31,31,31	0
58	MG	CA	3623	1/1	0.96	0.07	64,64,64,64	0
58	MG	AA	3680	1/1	0.96	0.09	59,59,59,59	0
58	MG	CA	3445	1/1	0.96	0.13	40,40,40,40	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	AA	3790	1/1	0.96	0.05	49,49,49,49	0
58	MG	AA	3793	1/1	0.96	0.08	28,28,28,28	0
58	MG	CA	3448	1/1	0.96	0.08	43,43,43,43	0
58	MG	AA	3420	1/1	0.96	0.13	26,26,26,26	0
58	MG	CA	3451	1/1	0.96	0.10	63,63,63,63	0
58	MG	CA	3452	1/1	0.96	0.16	61,61,61,61	0
58	MG	CA	3262	1/1	0.96	0.06	61,61,61,61	0
58	MG	CA	3455	1/1	0.96	0.14	47,47,47,47	0
58	MG	AA	3490	1/1	0.96	0.06	50,50,50,50	0
58	MG	CA	3264	1/1	0.96	0.10	59,59,59,59	0
58	MG	CA	3462	1/1	0.96	0.08	49,49,49,49	0
58	MG	AA	3796	1/1	0.96	0.11	50,50,50,50	0
58	MG	AA	3086	1/1	0.96	0.10	47,47,47,47	0
58	MG	AA	3685	1/1	0.96	0.10	47,47,47,47	0
58	MG	AA	3423	1/1	0.96	0.06	22,22,22,22	0
58	MG	BA	1714	1/1	0.96	0.11	61,61,61,61	0
58	MG	DA	1714	1/1	0.96	0.06	51,51,51,51	0
58	MG	CA	3003	1/1	0.96	0.13	45,45,45,45	0
58	MG	CA	3648	1/1	0.96	0.14	53,53,53,53	0
58	MG	DA	1717	1/1	0.96	0.10	52,52,52,52	0
58	MG	AA	3688	1/1	0.96	0.07	25,25,25,25	1
58	MG	CA	3276	1/1	0.96	0.16	50,50,50,50	0
58	MG	AA	3602	1/1	0.96	0.11	37,37,37,37	0
58	MG	AA	3213	1/1	0.96	0.06	58,58,58,58	0
58	MG	AA	3032	1/1	0.96	0.10	36,36,36,36	0
58	MG	CA	3475	1/1	0.96	0.23	55,55,55,55	0
58	MG	AA	3805	1/1	0.96	0.10	35,35,35,35	1
58	MG	AA	3427	1/1	0.96	0.06	33,33,33,33	0
58	MG	CA	3011	1/1	0.96	0.09	47,47,47,47	0
58	MG	AA	3499	1/1	0.96	0.07	51,51,51,51	1
58	MG	AA	3066	1/1	0.96	0.19	50,50,50,50	0
58	MG	CA	3288	1/1	0.96	0.07	54,54,54,54	0
58	MG	BA	1723	1/1	0.96	0.08	60,60,60,60	0
58	MG	CA	3015	1/1	0.96	0.17	85,85,85,85	0
58	MG	AA	3504	1/1	0.96	0.09	58,58,58,58	0
58	MG	AA	3505	1/1	0.96	0.05	31,31,31,31	0
58	MG	AA	3813	1/1	0.96	0.26	54,54,54,54	0
58	MG	CA	3297	1/1	0.96	0.18	56,56,56,56	0
58	MG	AA	3508	1/1	0.96	0.17	49,49,49,49	0
58	MG	BA	1728	1/1	0.96	0.20	52,52,52,52	0
58	MG	BA	1730	1/1	0.96	0.07	52,52,52,52	0
58	MG	BA	1731	1/1	0.96	0.09	49,49,49,49	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	DA	1741	1/1	0.96	0.10	78,78,78,78	0
58	MG	AA	3429	1/1	0.96	0.11	41,41,41,41	0
58	MG	AA	3351	1/1	0.96	0.05	30,30,30,30	0
58	MG	CA	3496	1/1	0.96	0.10	63,63,63,63	0
58	MG	AA	3614	1/1	0.96	0.07	56,56,56,56	0
58	MG	AA	3615	1/1	0.96	0.06	35,35,35,35	1
58	MG	AA	3705	1/1	0.96	0.16	24,24,24,24	1
58	MG	AA	3090	1/1	0.96	0.16	30,30,30,30	1
58	MG	AA	3513	1/1	0.96	0.07	35,35,35,35	0
58	MG	CA	3502	1/1	0.96	0.12	70,70,70,70	0
58	MG	CA	3036	1/1	0.96	0.08	44,44,44,44	0
58	MG	CA	3504	1/1	0.96	0.09	62,62,62,62	0
58	MG	AA	3255	1/1	0.96	0.11	53,53,53,53	0
58	MG	AA	3013	1/1	0.96	0.07	35,35,35,35	0
58	MG	CA	3164	1/1	0.96	0.12	41,41,41,41	0
58	MG	CA	3322	1/1	0.96	0.13	45,45,45,45	0
58	MG	BA	1742	1/1	0.96	0.09	50,50,50,50	0
58	MG	CA	3511	1/1	0.96	0.06	68,68,68,68	0
58	MG	AA	3711	1/1	0.96	0.13	34,34,34,34	1
58	MG	AA	3056	1/1	0.96	0.09	63,63,63,63	0
58	MG	CA	3326	1/1	0.96	0.08	34,34,34,34	0
58	MG	AA	3069	1/1	0.96	0.06	34,34,34,34	0
58	MG	AA	3298	1/1	0.96	0.07	59,59,59,59	0
58	MG	CP	202	1/1	0.96	0.15	71,71,71,71	0
58	MG	AA	3222	1/1	0.96	0.13	28,28,28,28	0
58	MG	AA	3301	1/1	0.96	0.07	23,23,23,23	0
58	MG	CA	3047	1/1	0.96	0.15	61,61,61,61	0
58	MG	AA	3719	1/1	0.96	0.07	58,58,58,58	0
58	MG	CQ	204	1/1	0.96	0.10	61,61,61,61	0
58	MG	AA	3535	1/1	0.96	0.04	15,15,15,15	0
58	MG	CA	3176	1/1	0.96	0.21	50,50,50,50	0
58	MG	BA	1754	1/1	0.96	0.13	48,48,48,48	0
58	MG	AA	3724	1/1	0.96	0.11	40,40,40,40	0
58	MG	AA	3725	1/1	0.96	0.08	39,39,39,39	0
58	MG	AA	3302	1/1	0.96	0.07	56,56,56,56	0
58	MG	C3	3001	1/1	0.96	0.10	69,69,69,69	0
58	MG	BA	1645	1/1	0.96	0.06	58,58,58,58	0
58	MG	C7	101	1/1	0.96	0.21	42,42,42,42	1
58	MG	AA	3627	1/1	0.96	0.11	54,54,54,54	0
58	MG	AA	3444	1/1	0.96	0.09	63,63,63,63	0
58	MG	AA	3482	1/1	0.97	0.10	65,65,65,65	0
58	MG	AA	3156	1/1	0.97	0.15	33,33,33,33	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	AA	3325	1/1	0.97	0.07	66,66,66,66	0
58	MG	AA	3326	1/1	0.97	0.09	58,58,58,58	0
58	MG	AA	3786	1/1	0.97	0.19	59,59,59,59	0
58	MG	AA	3787	1/1	0.97	0.09	53,53,53,53	0
58	MG	A7	103	1/1	0.97	0.08	49,49,49,49	0
58	MG	AA	3593	1/1	0.97	0.06	25,25,25,25	1
58	MG	AA	3101	1/1	0.97	0.20	52,52,52,52	0
58	MG	AA	3020	1/1	0.97	0.04	25,25,25,25	0
58	MG	AA	3792	1/1	0.97	0.13	45,45,45,45	0
58	MG	AA	3684	1/1	0.97	0.06	29,29,29,29	0
58	MG	AA	3077	1/1	0.97	0.17	50,50,50,50	0
58	MG	AA	3104	1/1	0.97	0.06	28,28,28,28	0
58	MG	AA	3687	1/1	0.97	0.06	45,45,45,45	0
58	MG	AA	3417	1/1	0.97	0.06	25,25,25,25	0
58	MG	AA	3418	1/1	0.97	0.07	43,43,43,43	0
58	MG	CA	3417	1/1	0.97	0.10	37,37,37,37	0
58	MG	AA	3131	1/1	0.97	0.14	55,55,55,55	0
58	MG	AA	3497	1/1	0.97	0.04	46,46,46,46	0
58	MG	AA	3692	1/1	0.97	0.10	53,53,53,53	0
58	MG	AA	3039	1/1	0.97	0.08	39,39,39,39	1
58	MG	AA	3502	1/1	0.97	0.06	51,51,51,51	1
58	MG	CA	3260	1/1	0.97	0.11	65,65,65,65	0
58	MG	AA	3421	1/1	0.97	0.10	12,12,12,12	0
58	MG	BA	1613	1/1	0.97	0.09	31,31,31,31	0
58	MG	AA	3234	1/1	0.97	0.08	30,30,30,30	1
58	MG	AA	3005	1/1	0.97	0.07	62,62,62,62	0
58	MG	CA	3266	1/1	0.97	0.12	69,69,69,69	0
58	MG	AA	3506	1/1	0.97	0.08	32,32,32,32	0
58	MG	AA	3810	1/1	0.97	0.08	54,54,54,54	0
58	MG	AA	3608	1/1	0.97	0.07	73,73,73,73	0
58	MG	BA	1729	1/1	0.97	0.05	45,45,45,45	0
58	MG	AA	3022	1/1	0.97	0.03	9,9,9,9	0
58	MG	AA	3043	1/1	0.97	0.12	31,31,31,31	0
58	MG	CA	3274	1/1	0.97	0.05	50,50,50,50	1
58	MG	CA	3022	1/1	0.97	0.12	38,38,38,38	0
58	MG	CA	3437	1/1	0.97	0.05	48,48,48,48	0
58	MG	CA	3023	1/1	0.97	0.12	46,46,46,46	0
58	MG	CA	3439	1/1	0.97	0.06	38,38,38,38	0
58	MG	AA	3238	1/1	0.97	0.12	61,61,61,61	0
58	MG	BA	1622	1/1	0.97	0.06	37,37,37,37	0
58	MG	AA	3084	1/1	0.97	0.09	32,32,32,32	0
58	MG	CA	3281	1/1	0.97	0.08	51,51,51,51	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	CA	3282	1/1	0.97	0.05	50,50,50,50	0
58	MG	AA	3240	1/1	0.97	0.18	30,30,30,30	0
58	MG	AA	3044	1/1	0.97	0.11	34,34,34,34	0
58	MG	AA	3169	1/1	0.97	0.09	39,39,39,39	0
58	MG	AA	3285	1/1	0.97	0.06	45,45,45,45	0
58	MG	AA	3433	1/1	0.97	0.06	28,28,28,28	0
58	MG	AB	3007	1/1	0.97	0.05	45,45,45,45	0
58	MG	CA	3289	1/1	0.97	0.11	42,42,42,42	0
58	MG	AA	3522	1/1	0.97	0.11	28,28,28,28	0
58	MG	DA	1670	1/1	0.97	0.07	75,75,75,75	0
58	MG	AA	3046	1/1	0.97	0.08	34,34,34,34	0
58	MG	CA	3457	1/1	0.97	0.09	47,47,47,47	0
58	MG	CA	3458	1/1	0.97	0.07	49,49,49,49	0
58	MG	AA	3287	1/1	0.97	0.13	47,47,47,47	0
58	MG	CA	3461	1/1	0.97	0.07	43,43,43,43	0
58	MG	AA	3530	1/1	0.97	0.05	53,53,53,53	0
58	MG	CA	3160	1/1	0.97	0.08	42,42,42,42	0
58	MG	CA	3296	1/1	0.97	0.08	42,42,42,42	0
58	MG	AA	3717	1/1	0.97	0.13	47,47,47,47	0
58	MG	DA	1680	1/1	0.97	0.10	62,62,62,62	0
58	MG	AA	3288	1/1	0.97	0.06	24,24,24,24	0
58	MG	DA	1682	1/1	0.97	0.14	47,47,47,47	0
58	MG	CA	3627	1/1	0.97	0.09	63,63,63,63	0
58	MG	AA	3532	1/1	0.97	0.11	25,25,25,25	0
58	MG	CA	3630	1/1	0.97	0.09	63,63,63,63	0
58	MG	AA	3533	1/1	0.97	0.07	22,22,22,22	0
58	MG	CA	3632	1/1	0.97	0.06	79,79,79,79	0
58	MG	AA	3721	1/1	0.97	0.05	10,10,10,10	0
58	MG	BA	1753	1/1	0.97	0.07	58,58,58,58	0
58	MG	AA	3141	1/1	0.97	0.09	40,40,40,40	0
58	MG	AA	3047	1/1	0.97	0.12	34,34,34,34	0
58	MG	CA	3305	1/1	0.97	0.07	62,62,62,62	0
58	MG	AA	3064	1/1	0.97	0.05	29,29,29,29	0
58	MG	CA	3639	1/1	0.97	0.13	55,55,55,55	0
58	MG	CA	3307	1/1	0.97	0.13	52,52,52,52	0
58	MG	CA	3170	1/1	0.97	0.18	47,47,47,47	0
58	MG	BA	1757	1/1	0.97	0.12	38,38,38,38	0
58	MG	CA	3050	1/1	0.97	0.05	44,44,44,44	0
58	MG	AA	3541	1/1	0.97	0.08	43,43,43,43	0
58	MG	AA	3359	1/1	0.97	0.06	51,51,51,51	0
58	MG	AA	3023	1/1	0.97	0.17	33,33,33,33	1
58	MG	CA	3317	1/1	0.97	0.05	44,44,44,44	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	AA	3631	1/1	0.97	0.08	46,46,46,46	0
58	MG	CA	3321	1/1	0.97	0.05	31,31,31,31	0
58	MG	CA	3486	1/1	0.97	0.16	69,69,69,69	0
58	MG	CA	3652	1/1	0.97	0.07	53,53,53,53	0
58	MG	CA	3487	1/1	0.97	0.12	70,70,70,70	0
58	MG	AA	3001	1/1	0.97	0.06	37,37,37,37	0
58	MG	AA	3210	1/1	0.97	0.13	24,24,24,24	1
58	MG	AA	3031	1/1	0.97	0.15	10,10,10,10	1
58	MG	AA	3550	1/1	0.97	0.09	47,47,47,47	0
58	MG	AA	3637	1/1	0.97	0.06	45,45,45,45	0
58	MG	AA	3253	1/1	0.97	0.16	29,29,29,29	1
58	MG	AA	3552	1/1	0.97	0.07	63,63,63,63	0
58	MG	CA	3329	1/1	0.97	0.07	29,29,29,29	0
58	MG	AA	3300	1/1	0.97	0.08	50,50,50,50	0
58	MG	DA	1719	1/1	0.97	0.06	74,74,74,74	0
58	MG	BA	1771	1/1	0.97	0.11	63,63,63,63	0
58	MG	CA	3064	1/1	0.97	0.06	43,43,43,43	0
58	MG	AA	3641	1/1	0.97	0.09	41,41,41,41	0
58	MG	AA	3009	1/1	0.97	0.04	24,24,24,24	0
58	MG	AA	3745	1/1	0.97	0.06	29,29,29,29	0
58	MG	AA	3179	1/1	0.97	0.11	71,71,71,71	0
58	MG	CA	3337	1/1	0.97	0.06	41,41,41,41	0
58	MG	CA	3338	1/1	0.97	0.10	63,63,63,63	0
58	MG	AF	303	1/1	0.97	0.09	41,41,41,41	1
58	MG	AA	3557	1/1	0.97	0.05	19,19,19,19	0
58	MG	CA	3193	1/1	0.97	0.07	64,64,64,64	0
58	MG	AF	306	1/1	0.97	0.12	50,50,50,50	0
58	MG	AA	3303	1/1	0.97	0.11	56,56,56,56	0
58	MG	CA	3510	1/1	0.97	0.06	65,65,65,65	0
58	MG	AA	3453	1/1	0.97	0.15	56,56,56,56	0
58	MG	AA	3033	1/1	0.97	0.18	29,29,29,29	1
58	MG	CA	3349	1/1	0.97	0.16	41,41,41,41	0
58	MG	AA	3257	1/1	0.97	0.03	14,14,14,14	0
58	MG	AA	3562	1/1	0.97	0.05	48,48,48,48	1
58	MG	AA	3053	1/1	0.97	0.08	14,14,14,14	0
58	MG	AA	3150	1/1	0.97	0.10	15,15,15,15	0
58	MG	AN	3002	1/1	0.97	0.09	27,27,27,27	0
58	MG	CA	3519	1/1	0.97	0.10	79,79,79,79	0
58	MG	AN	3003	1/1	0.97	0.07	47,47,47,47	0
58	MG	BA	1788	1/1	0.97	0.10	66,66,66,66	0
58	MG	DA	1745	1/1	0.97	0.12	61,61,61,61	0
58	MG	AA	3757	1/1	0.97	0.05	55,55,55,55	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	AP	201	1/1	0.97	0.24	65,65,65,65	0
58	MG	AP	202	1/1	0.97	0.13	28,28,28,28	1
58	MG	AA	3374	1/1	0.97	0.07	18,18,18,18	0
58	MG	AA	3567	1/1	0.97	0.07	51,51,51,51	0
58	MG	AQ	202	1/1	0.97	0.11	31,31,31,31	0
58	MG	CA	3211	1/1	0.97	0.11	40,40,40,40	0
58	MG	CA	3529	1/1	0.97	0.06	57,57,57,57	0
58	MG	AA	3569	1/1	0.97	0.08	19,19,19,19	0
58	MG	AA	3218	1/1	0.97	0.11	38,38,38,38	0
58	MG	AR	202	1/1	0.97	0.07	32,32,32,32	0
58	MG	AA	3121	1/1	0.97	0.14	70,70,70,70	0
58	MG	CA	3092	1/1	0.97	0.09	70,70,70,70	0
58	MG	AA	3572	1/1	0.97	0.04	32,32,32,32	0
58	MG	AA	3764	1/1	0.97	0.09	55,55,55,55	0
58	MG	CU	201	1/1	0.97	0.18	64,64,64,64	0
58	MG	AA	3034	1/1	0.97	0.11	57,57,57,57	0
58	MG	CA	3377	1/1	0.97	0.05	80,80,80,80	0
58	MG	AA	3574	1/1	0.97	0.06	30,30,30,30	1
58	MG	AA	3315	1/1	0.97	0.10	34,34,34,34	0
58	MG	AA	3768	1/1	0.97	0.15	99,99,99,99	0
58	MG	AA	3072	1/1	0.97	0.05	26,26,26,26	0
58	MG	AA	3154	1/1	0.97	0.14	46,46,46,46	0
58	MG	AA	3666	1/1	0.97	0.06	64,64,64,64	0
58	MG	DA	1601	1/1	0.97	0.09	61,61,61,61	0
58	MG	AA	3384	1/1	0.97	0.06	34,34,34,34	0
58	MG	AA	3318	1/1	0.97	0.10	51,51,51,51	1
58	MG	AA	3470	1/1	0.97	0.05	29,29,29,29	0
58	MG	AA	3188	1/1	0.97	0.07	13,13,13,13	0
58	MG	AA	3035	1/1	0.97	0.08	57,57,57,57	0
58	MG	AA	3395	1/1	0.97	0.09	18,18,18,18	0
58	MG	AA	3397	1/1	0.97	0.05	15,15,15,15	0
58	MG	DZ	702	1/1	0.97	0.11	57,57,57,57	0
58	MG	CA	3234	1/1	0.97	0.15	54,54,54,54	0
60	SF4	BD	501	8/8	0.97	0.04	80,80,80,80	0
60	SF4	DD	501	8/8	0.97	0.05	90,90,90,90	1
58	MG	CA	3554	1/1	0.97	0.12	67,67,67,67	0
58	MG	AA	3401	1/1	0.97	0.06	33,33,33,33	0
62	GDP	BZ	704	28/28	0.97	0.06	53,53,53,53	1
58	MG	AA	3587	1/1	0.97	0.09	53,53,53,53	0
58	MG	BA	1682	1/1	0.98	0.03	53,53,53,53	0
58	MG	A5	103	1/1	0.98	0.07	45,45,45,45	0
58	MG	AA	3089	1/1	0.98	0.12	47,47,47,47	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	AA	3350	1/1	0.98	0.10	31,31,31,31	0
58	MG	AA	3396	1/1	0.98	0.03	22,22,22,22	0
58	MG	A7	102	1/1	0.98	0.07	38,38,38,38	0
58	MG	CA	3390	1/1	0.98	0.03	64,64,64,64	0
58	MG	AA	3588	1/1	0.98	0.08	38,38,38,38	0
58	MG	AA	3659	1/1	0.98	0.06	14,14,14,14	0
58	MG	A7	105	1/1	0.98	0.06	43,43,43,43	0
58	MG	AA	3097	1/1	0.98	0.09	26,26,26,26	0
58	MG	AA	3400	1/1	0.98	0.11	39,39,39,39	0
58	MG	A8	5002	1/1	0.98	0.06	31,31,31,31	0
58	MG	AA	3742	1/1	0.98	0.08	82,82,82,82	0
58	MG	AA	3251	1/1	0.98	0.07	42,42,42,42	0
58	MG	AA	3402	1/1	0.98	0.10	33,33,33,33	0
58	MG	AB	3011	1/1	0.98	0.06	30,30,30,30	0
58	MG	AB	3012	1/1	0.98	0.10	29,29,29,29	1
58	MG	AB	3013	1/1	0.98	0.08	54,54,54,54	0
58	MG	CA	3403	1/1	0.98	0.05	91,91,91,91	0
58	MG	CA	3279	1/1	0.98	0.03	34,34,34,34	0
58	MG	CA	3658	1/1	0.98	0.08	50,50,50,50	0
58	MG	AA	3217	1/1	0.98	0.04	6,6,6,6	0
58	MG	AA	3523	1/1	0.98	0.08	30,30,30,30	0
58	MG	AA	3134	1/1	0.98	0.20	59,59,59,59	1
58	MG	AA	3293	1/1	0.98	0.11	32,32,32,32	0
58	MG	AA	3527	1/1	0.98	0.08	26,26,26,26	0
58	MG	AA	3528	1/1	0.98	0.05	28,28,28,28	0
58	MG	AB	3020	1/1	0.98	0.10	55,55,55,55	0
58	MG	AA	3529	1/1	0.98	0.07	16,16,16,16	0
58	MG	AB	3022	1/1	0.98	0.04	58,58,58,58	0
58	MG	AA	3408	1/1	0.98	0.04	20,20,20,20	0
58	MG	AA	3754	1/1	0.98	0.03	29,29,29,29	0
58	MG	DA	1688	1/1	0.98	0.09	66,66,66,66	0
58	MG	CA	3291	1/1	0.98	0.05	27,27,27,27	0
58	MG	AA	3410	1/1	0.98	0.07	30,30,30,30	0
58	MG	AA	3160	1/1	0.98	0.07	57,57,57,57	0
58	MG	AA	3357	1/1	0.98	0.06	27,27,27,27	0
58	MG	AA	3534	1/1	0.98	0.06	27,27,27,27	0
58	MG	AA	3322	1/1	0.98	0.04	32,32,32,32	1
58	MG	AA	3536	1/1	0.98	0.03	35,35,35,35	0
58	MG	AA	3323	1/1	0.98	0.03	22,22,22,22	0
58	MG	AA	3083	1/1	0.98	0.11	38,38,38,38	1
58	MG	AA	3540	1/1	0.98	0.04	29,29,29,29	0
58	MG	CD	303	1/1	0.98	0.18	37,37,37,37	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	AA	3296	1/1	0.98	0.05	17,17,17,17	0
58	MG	CA	3550	1/1	0.98	0.08	33,33,33,33	0
58	MG	AA	3542	1/1	0.98	0.08	63,63,63,63	0
58	MG	AA	3040	1/1	0.98	0.15	40,40,40,40	1
58	MG	AA	3544	1/1	0.98	0.05	16,16,16,16	0
58	MG	AA	3545	1/1	0.98	0.05	51,51,51,51	1
58	MG	AE	305	1/1	0.98	0.07	30,30,30,30	0
58	MG	AA	3469	1/1	0.98	0.07	43,43,43,43	0
58	MG	CA	3308	1/1	0.98	0.04	41,41,41,41	0
58	MG	AA	3327	1/1	0.98	0.03	13,13,13,13	0
58	MG	CA	3559	1/1	0.98	0.08	52,52,52,52	1
58	MG	AA	3471	1/1	0.98	0.09	34,34,34,34	0
58	MG	CA	3311	1/1	0.98	0.07	48,48,48,48	0
58	MG	AA	3474	1/1	0.98	0.09	53,53,53,53	0
58	MG	AF	305	1/1	0.98	0.15	41,41,41,41	0
58	MG	AA	3328	1/1	0.98	0.04	18,18,18,18	0
58	MG	CA	3566	1/1	0.98	0.05	41,41,41,41	0
58	MG	AA	3275	1/1	0.98	0.12	47,47,47,47	1
58	MG	AA	3693	1/1	0.98	0.08	48,48,48,48	0
58	MG	CA	3318	1/1	0.98	0.05	33,33,33,33	0
58	MG	BA	1734	1/1	0.98	0.04	71,71,71,71	0
58	MG	AA	3478	1/1	0.98	0.05	40,40,40,40	0
58	MG	AA	3331	1/1	0.98	0.12	34,34,34,34	0
58	MG	AA	3276	1/1	0.98	0.15	47,47,47,47	1
58	MG	AA	3425	1/1	0.98	0.07	18,18,18,18	0
58	MG	CA	3576	1/1	0.98	0.04	36,36,36,36	0
58	MG	CA	3450	1/1	0.98	0.05	48,48,48,48	0
58	MG	CA	3108	1/1	0.98	0.14	60,60,60,60	0
58	MG	AA	3116	1/1	0.98	0.11	51,51,51,51	0
58	MG	CA	3007	1/1	0.98	0.04	28,28,28,28	0
58	MG	AA	3483	1/1	0.98	0.04	43,43,43,43	1
58	MG	AA	3369	1/1	0.98	0.08	27,27,27,27	0
58	MG	AA	3126	1/1	0.98	0.14	50,50,50,50	0
58	MG	AA	3085	1/1	0.98	0.09	53,53,53,53	0
58	MG	CA	3459	1/1	0.98	0.07	48,48,48,48	0
58	MG	AA	3488	1/1	0.98	0.06	20,20,20,20	0
58	MG	CA	3219	1/1	0.98	0.09	31,31,31,31	0
58	MG	BA	1745	1/1	0.98	0.05	52,52,52,52	0
58	MG	BA	1746	1/1	0.98	0.04	37,37,37,37	0
58	MG	AA	3225	1/1	0.98	0.06	27,27,27,27	1
58	MG	AA	3337	1/1	0.98	0.03	10,10,10,10	0
58	MG	AA	3707	1/1	0.98	0.17	29,29,29,29	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	AA	3565	1/1	0.98	0.07	29,29,29,29	0
58	MG	CA	3019	1/1	0.98	0.05	28,28,28,28	0
58	MG	AA	3304	1/1	0.98	0.10	30,30,30,30	0
58	MG	CA	3021	1/1	0.98	0.04	29,29,29,29	0
58	MG	CA	3471	1/1	0.98	0.08	45,45,45,45	0
58	MG	CA	3345	1/1	0.98	0.07	38,38,38,38	0
58	MG	DA	1617	1/1	0.98	0.10	48,48,48,48	0
58	MG	AA	3243	1/1	0.98	0.11	24,24,24,24	1
58	MG	AA	3568	1/1	0.98	0.07	16,16,16,16	0
58	MG	AA	3306	1/1	0.98	0.09	47,47,47,47	0
58	MG	AA	3494	1/1	0.98	0.09	50,50,50,50	0
58	MG	AU	204	1/1	0.98	0.18	62,62,62,62	0
58	MG	AA	3435	1/1	0.98	0.05	20,20,20,20	0
58	MG	CA	3029	1/1	0.98	0.06	33,33,33,33	0
58	MG	AA	3342	1/1	0.98	0.05	5,5,5,5	0
58	MG	DA	1758	1/1	0.98	0.12	71,71,71,71	0
58	MG	AV	203	1/1	0.98	0.09	40,40,40,40	0
58	MG	AV	204	1/1	0.98	0.07	38,38,38,38	0
58	MG	AA	3716	1/1	0.98	0.05	57,57,57,57	0
58	MG	AA	3800	1/1	0.98	0.04	30,30,30,30	0
58	MG	CA	3359	1/1	0.98	0.10	42,42,42,42	0
58	MG	DA	1764	1/1	0.98	0.04	55,55,55,55	0
58	MG	AA	3379	1/1	0.98	0.05	30,30,30,30	0
58	MG	AA	3643	1/1	0.98	0.08	49,49,49,49	0
58	MG	AA	3380	1/1	0.98	0.04	15,15,15,15	0
58	MG	AA	3500	1/1	0.98	0.05	47,47,47,47	0
58	MG	CA	3364	1/1	0.98	0.09	29,29,29,29	0
58	MG	AA	3012	1/1	0.98	0.07	34,34,34,34	0
58	MG	AA	3003	1/1	0.98	0.03	20,20,20,20	0
58	MG	CA	3041	1/1	0.98	0.17	31,31,31,31	0
58	MG	AA	3130	1/1	0.98	0.06	37,37,37,37	0
58	MG	CA	3249	1/1	0.98	0.06	46,46,46,46	0
58	MG	CA	3370	1/1	0.98	0.06	47,47,47,47	0
58	MG	AA	3808	1/1	0.98	0.09	28,28,28,28	1
58	MG	CA	3146	1/1	0.98	0.07	60,60,60,60	0
58	MG	AA	3346	1/1	0.98	0.07	46,46,46,46	0
58	MG	AA	3650	1/1	0.98	0.04	60,60,60,60	0
58	MG	CA	3629	1/1	0.98	0.07	55,55,55,55	0
59	ZN	A4	501	1/1	0.98	0.04	137,137,137,137	0
59	ZN	BN	501	1/1	0.98	0.05	123,123,123,123	0
58	MG	AA	3082	1/1	0.98	0.15	23,23,23,23	1
59	ZN	DN	501	1/1	0.98	0.05	129,129,129,129	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	AA	3507	1/1	0.98	0.06	14,14,14,14	0
58	MG	AA	3387	1/1	0.98	0.03	17,17,17,17	0
58	MG	AA	3170	1/1	0.98	0.10	53,53,53,53	0
58	MG	AA	3815	1/1	0.98	0.05	29,29,29,29	1
58	MG	CA	3381	1/1	0.98	0.06	38,38,38,38	0
58	MG	DA	1654	1/1	0.98	0.04	30,30,30,30	0
58	MG	CA	3339	1/1	0.99	0.04	34,34,34,34	0
58	MG	AA	3730	1/1	0.99	0.10	30,30,30,30	0
58	MG	AA	3413	1/1	0.99	0.03	20,20,20,20	0
58	MG	CA	3342	1/1	0.99	0.07	45,45,45,45	0
58	MG	AA	3340	1/1	0.99	0.08	59,59,59,59	0
58	MG	AA	3555	1/1	0.99	0.06	38,38,38,38	0
58	MG	AA	3734	1/1	0.99	0.05	22,22,22,22	0
58	MG	AA	3515	1/1	0.99	0.04	20,20,20,20	0
58	MG	AA	3388	1/1	0.99	0.05	25,25,25,25	0
58	MG	CA	3617	1/1	0.99	0.04	31,31,31,31	0
58	MG	AA	3416	1/1	0.99	0.04	30,30,30,30	0
58	MG	AA	3389	1/1	0.99	0.06	17,17,17,17	0
58	MG	CA	3415	1/1	0.99	0.03	31,31,31,31	1
58	MG	BA	1681	1/1	0.99	0.08	36,36,36,36	0
58	MG	AA	3228	1/1	0.99	0.07	51,51,51,51	0
58	MG	AA	3520	1/1	0.99	0.03	38,38,38,38	0
58	MG	AA	3521	1/1	0.99	0.05	29,29,29,29	0
58	MG	AA	3314	1/1	0.99	0.11	28,28,28,28	0
58	MG	A0	101	1/1	0.99	0.04	43,43,43,43	0
58	MG	CA	3356	1/1	0.99	0.04	57,57,57,57	0
58	MG	AA	3392	1/1	0.99	0.04	42,42,42,42	0
58	MG	AA	3524	1/1	0.99	0.05	28,28,28,28	0
58	MG	AA	3393	1/1	0.99	0.07	21,21,21,21	0
58	MG	CA	3560	1/1	0.99	0.02	36,36,36,36	0
58	MG	AA	3485	1/1	0.99	0.04	14,14,14,14	0
58	MG	AA	3394	1/1	0.99	0.07	27,27,27,27	0
58	MG	AA	3075	1/1	0.99	0.03	9,9,9,9	0
58	MG	AA	3749	1/1	0.99	0.03	14,14,14,14	0
58	MG	AA	3329	1/1	0.99	0.05	17,17,17,17	0
58	MG	AA	3700	1/1	0.99	0.08	35,35,35,35	0
58	MG	AA	3038	1/1	0.99	0.05	11,11,11,11	0
58	MG	CA	3028	1/1	0.99	0.18	35,35,35,35	1
58	MG	AA	3399	1/1	0.99	0.03	18,18,18,18	0
58	MG	AA	3376	1/1	0.99	0.05	19,19,19,19	0
58	MG	AA	3045	1/1	0.99	0.10	43,43,43,43	0
58	MG	CA	3572	1/1	0.99	0.05	54,54,54,54	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	AA	3207	1/1	0.99	0.07	22,22,22,22	1
58	MG	CA	3372	1/1	0.99	0.03	42,42,42,42	0
58	MG	AA	3459	1/1	0.99	0.04	18,18,18,18	0
58	MG	AA	3403	1/1	0.99	0.04	28,28,28,28	0
58	MG	CA	3312	1/1	0.99	0.04	51,51,51,51	0
58	MG	AA	3037	1/1	0.99	0.06	45,45,45,45	0
58	MG	CA	3650	1/1	0.99	0.14	27,27,27,27	0
58	MG	CA	3443	1/1	0.99	0.03	36,36,36,36	0
58	MG	DA	1611	1/1	0.99	0.03	38,38,38,38	0
58	MG	AA	3320	1/1	0.99	0.06	24,24,24,24	0
58	MG	AA	3539	1/1	0.99	0.03	28,28,28,28	0
58	MG	AA	3498	1/1	0.99	0.04	37,37,37,37	0
58	MG	BA	1760	1/1	0.99	0.02	57,57,57,57	0
58	MG	AA	3308	1/1	0.99	0.03	30,30,30,30	0
58	MG	CA	3382	1/1	0.99	0.04	40,40,40,40	0
58	MG	AA	3583	1/1	0.99	0.02	13,13,13,13	0
58	MG	CA	3587	1/1	0.99	0.03	34,34,34,34	0
58	MG	CA	3320	1/1	0.99	0.05	30,30,30,30	0
58	MG	DA	1621	1/1	0.99	0.08	44,44,44,44	0
58	MG	AA	3407	1/1	0.99	0.04	49,49,49,49	0
58	MG	CA	3453	1/1	0.99	0.04	39,39,39,39	0
58	MG	AA	3465	1/1	0.99	0.04	39,39,39,39	0
58	MG	DA	1699	1/1	0.99	0.06	75,75,75,75	0
58	MG	AA	3187	1/1	0.99	0.13	32,32,32,32	0
58	MG	CA	3265	1/1	0.99	0.04	40,40,40,40	0
58	MG	AA	3409	1/1	0.99	0.08	45,45,45,45	0
58	MG	AA	3289	1/1	0.99	0.03	27,27,27,27	0
58	MG	AA	3074	1/1	0.99	0.09	15,15,15,15	0
58	MG	AA	3675	1/1	0.99	0.05	38,38,38,38	0
58	MG	CA	3270	1/1	0.99	0.08	35,35,35,35	0
58	MG	AA	3439	1/1	0.99	0.12	17,17,17,17	0
58	MG	AA	3723	1/1	0.99	0.05	21,21,21,21	0
58	MG	AA	3440	1/1	0.99	0.10	31,31,31,31	0
58	MG	AA	3509	1/1	0.99	0.06	49,49,49,49	0
58	MG	AA	3776	1/1	0.99	0.02	40,40,40,40	0
58	MG	AA	3635	1/1	0.99	0.03	23,23,23,23	0
58	MG	AA	3727	1/1	0.99	0.04	49,49,49,49	0
58	MG	AA	3140	1/1	0.99	0.06	50,50,50,50	0
58	MG	AA	3475	1/1	0.99	0.04	62,62,62,62	0
59	ZN	AY	501	1/1	1.00	0.01	65,65,65,65	0
58	MG	AA	3472	1/1	1.00	0.03	24,24,24,24	0
59	ZN	A5	104	1/1	1.00	0.01	36,36,36,36	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
59	ZN	A6	102	1/1	1.00	0.02	46,46,46,46	0
59	ZN	A9	501	1/1	1.00	0.02	42,42,42,42	0
58	MG	AA	3791	1/1	1.00	0.08	16,16,16,16	0
59	ZN	CY	501	1/1	1.00	0.02	93,93,93,93	0
58	MG	AA	3501	1/1	1.00	0.02	24,24,24,24	0
59	ZN	C5	102	1/1	1.00	0.03	68,68,68,68	0
59	ZN	C6	501	1/1	1.00	0.02	61,61,61,61	0
59	ZN	C9	501	1/1	1.00	0.03	94,94,94,94	0
58	MG	AA	3722	1/1	1.00	0.03	18,18,18,18	0
58	MG	AA	3473	1/1	1.00	0.03	15,15,15,15	0
58	MG	AA	3398	1/1	1.00	0.01	15,15,15,15	0
58	MG	AA	3514	1/1	1.00	0.03	18,18,18,18	0
58	MG	AE	303	1/1	1.00	0.07	18,18,18,18	0
58	MG	AA	3385	1/1	1.00	0.05	28,28,28,28	0
58	MG	CA	3383	1/1	1.00	0.07	44,44,44,44	0

6.5 Other polymers [i](#)

There are no such residues in this entry.