



wwPDB X-ray Structure Validation Summary Report ⓘ

May 14, 2020 – 05:52 am BST

PDB ID : 4WQU
Title : Crystal structure of the *Thermus thermophilus* 70S ribosome in complex with elongation factor G trapped by the antibiotic dityromycin
Authors : Lin, J.; Gagnon, M.G.; Steitz, T.A.
Deposited on : 2014-10-22
Resolution : 2.80 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

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

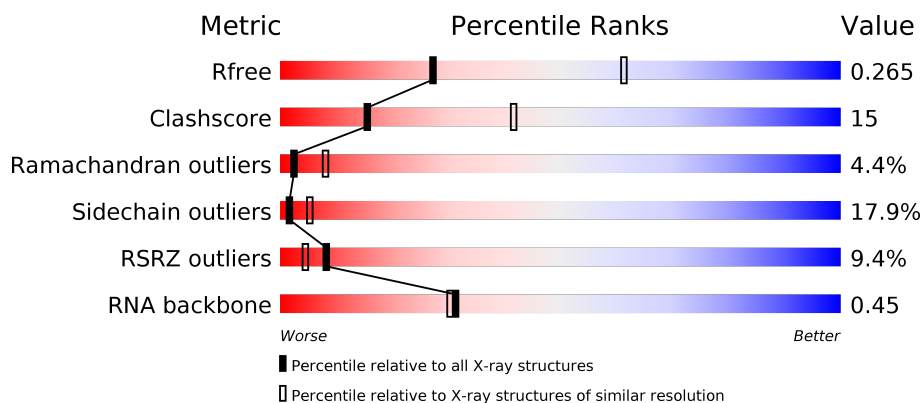
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

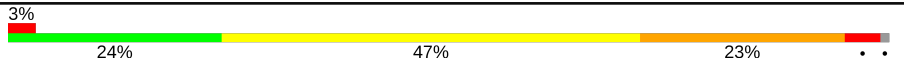
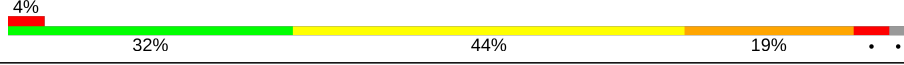

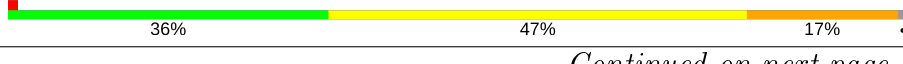
The reported resolution of this entry is 2.80 Å.

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



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

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 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	
1	CA	2915	
2	AB	121	
2	CB	121	




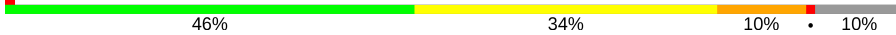





















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Mol	Chain	Length	Quality of chain
3	AC	228	
3	CC	228	
4	AD	276	
4	CD	276	
5	AE	206	
5	CE	206	
6	AF	210	
6	CF	210	
7	AG	182	
7	CG	182	
8	AH	180	
8	CH	180	
9	AK	173	
9	CK	173	
10	AL	147	
10	CL	147	
11	AN	140	
11	CN	140	
12	AO	122	
12	CO	122	
13	AP	150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

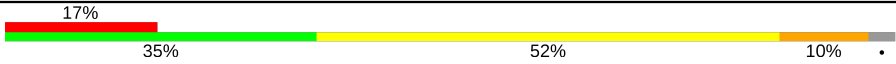



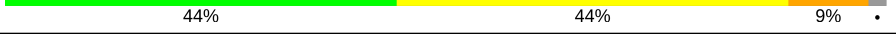

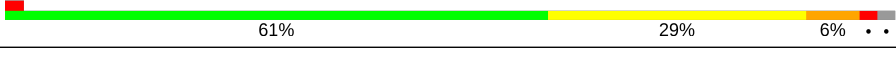




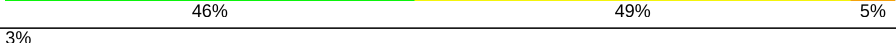
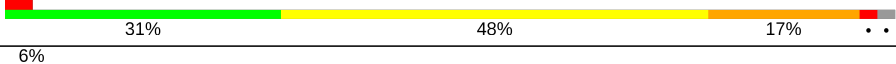

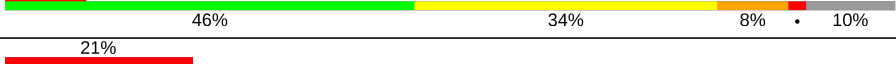




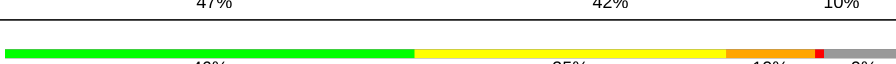
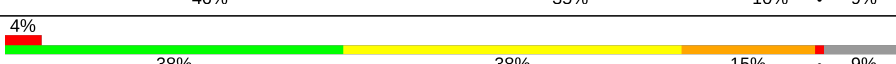



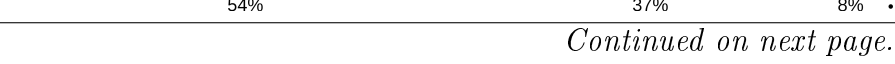
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Mol	Chain	Length	Quality of chain
15	CR	118	
16	AS	112	
16	CS	112	
17	AT	146	
17	CT	146	
18	AU	118	
18	CU	118	
19	AV	101	
19	CV	101	
20	AW	113	
20	CW	113	
21	AX	96	
21	CX	96	
22	AY	110	
22	CY	110	
23	AZ	206	
23	CZ	206	
24	A0	85	
24	C0	85	
25	A1	98	
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	
58	BX	10	
58	DX	10	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
56	PSU	BY	32	-	-	-	X
56	MIA	BY	37	-	-	-	X
56	PSU	BY	39	-	-	-	X
56	5MU	BY	54	-	-	-	X
56	PSU	BY	55	-	-	-	X
56	PSU	DY	32	-	-	-	X
56	MIA	DY	37	-	-	-	X
56	PSU	DY	39	-	-	-	X
56	7MG	DY	46	-	-	-	X
56	5MU	DY	54	-	-	-	X
56	PSU	DY	55	-	-	-	X
56	4SU	DY	8	-	-	-	X
58	2QY	DX	10	-	-	X	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
59	MG	AA	3016	-	-	-	X
59	MG	AA	3067	-	-	-	X
59	MG	AA	3108	-	-	-	X
59	MG	AA	3122	-	-	-	X
59	MG	AA	3140	-	-	-	X
59	MG	AA	3212	-	-	-	X
59	MG	AA	3238	-	-	-	X
59	MG	AA	3266	-	-	-	X
59	MG	AA	3273	-	-	-	X
59	MG	AA	3277	-	-	-	X
59	MG	AA	3582	-	-	-	X
59	MG	AA	3712	-	-	-	X
59	MG	AA	3717	-	-	-	X
59	MG	AA	3773	-	-	-	X
59	MG	AA	3814	-	-	-	X
59	MG	AA	3816	-	-	-	X
59	MG	AA	3820	-	-	-	X
59	MG	AD	305	-	-	-	X
59	MG	AE	301	-	-	-	X
59	MG	AF	305	-	-	-	X
59	MG	BA	1665	-	-	-	X
59	MG	BA	1691	-	-	-	X
59	MG	BA	1697	-	-	-	X
59	MG	BA	1698	-	-	-	X
59	MG	BA	1767	-	-	-	X
59	MG	CA	3030	-	-	-	X
59	MG	CA	3037	-	-	-	X
59	MG	CA	3040	-	-	-	X
59	MG	CA	3041	-	-	-	X
59	MG	CA	3075	-	-	-	X
59	MG	CA	3082	-	-	-	X
59	MG	CA	3084	-	-	-	X
59	MG	CA	3089	-	-	-	X
59	MG	CA	3092	-	-	-	X
59	MG	CA	3093	-	-	-	X
59	MG	CA	3101	-	-	-	X
59	MG	CA	3127	-	-	-	X
59	MG	CA	3139	-	-	-	X
59	MG	CA	3146	-	-	-	X
59	MG	CA	3186	-	-	-	X
59	MG	CA	3205	-	-	-	X
59	MG	CA	3208	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
59	MG	CA	3216	-	-	-	X
59	MG	CA	3236	-	-	-	X
59	MG	CA	3237	-	-	-	X
59	MG	CA	3240	-	-	-	X
59	MG	CA	3460	-	-	-	X
59	MG	CA	3499	-	-	-	X
59	MG	CA	3501	-	-	-	X
59	MG	CA	3502	-	-	-	X
59	MG	CA	3514	-	-	-	X
59	MG	CA	3542	-	-	-	X
59	MG	CA	3600	-	-	-	X
59	MG	CA	3620	-	-	-	X
59	MG	CV	201	-	-	-	X
59	MG	DA	1639	-	-	-	X
59	MG	DA	1724	-	-	-	X
59	MG	DA	1738	-	-	-	X
59	MG	DA	1754	-	-	-	X
59	MG	DA	1756	-	-	-	X
59	MG	DA	1757	-	-	-	X
59	MG	DA	1769	-	-	-	X
59	MG	DT	3001	-	-	-	X
61	SF4	DD	501	-	-	X	-

2 Entry composition [i](#)

There are 63 unique types of molecules in this entry. The entry contains 310038 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	2872	Total	C	N	O	P	0	0	0
			61861	27532	11574	19884	2871			
1	CA	2868	Total	C	N	O	P	0	0	0
			61771	27492	11554	19858	2867			

- 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	66	Total	C	N	O	S	0	0	0
			498	310	93	92	3			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	CL	66	Total	C	N	O	S	0	0	0
			498	310	93	92	3			

- 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	77	Total	C	N	O	S	0	0	0
			608	375	129	103	1			
24	C0	77	Total	C	N	O	S	0	0	0
			608	375	129	103	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	116	Total	C	N	O	S	0	0	0
			907	558	188	159	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	728	Total	C	N	O	S	0	0	0
			5663	3599	973	1072	19			
57	DZ	730	Total	C	N	O	S	0	0	0
			5682	3611	978	1074	19			

- Molecule 58 is a protein called Dityromycin.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
58	BX	10	Total	C	N	O	0	0	0
			93	67	10	16			
58	DX	10	Total	C	N	O	0	0	0
			93	67	10	16			

- Molecule 59 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
59	AP	3	Total	Mg	0	0
			3	3		
59	CR	1	Total	Mg	0	0
			1	1		
59	BA	215	Total	Mg	0	0
			215	215		
59	CA	664	Total	Mg	0	0
			664	664		
59	C5	1	Total	Mg	0	0
			1	1		
59	AB	23	Total	Mg	0	0
			23	23		
59	BL	2	Total	Mg	0	0
			2	2		
59	CV	2	Total	Mg	0	0
			2	2		
59	A6	2	Total	Mg	0	0
			2	2		
59	BE	1	Total	Mg	0	0
			1	1		
59	AW	3	Total	Mg	0	0
			3	3		
59	C1	1	Total	Mg	0	0
			1	1		
59	AN	3	Total	Mg	0	0
			3	3		
59	DZ	2	Total	Mg	0	0
			2	2		
59	AX	1	Total	Mg	0	0
			1	1		
59	CN	1	Total	Mg	0	0
			1	1		
59	A2	1	Total	Mg	0	0
			1	1		
59	C8	1	Total	Mg	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
59	DD	1	Total 1	Mg 1	0	0
59	BB	1	Total 1	Mg 1	0	0
59	BT	1	Total 1	Mg 1	0	0
59	AE	5	Total 5	Mg 5	0	0
59	BM	1	Total 1	Mg 1	0	0
59	CU	1	Total 1	Mg 1	0	0
59	BF	1	Total 1	Mg 1	0	0
59	AV	2	Total 2	Mg 2	0	0
59	DA	171	Total 171	Mg 171	0	0
59	CB	13	Total 13	Mg 13	0	0
59	C0	1	Total 1	Mg 1	0	0
59	AA	832	Total 832	Mg 832	0	0
59	CQ	4	Total 4	Mg 4	0	0
59	A5	1	Total 1	Mg 1	0	0
59	AR	1	Total 1	Mg 1	0	0
59	CG	1	Total 1	Mg 1	0	0
59	DK	1	Total 1	Mg 1	0	0
59	DF	1	Total 1	Mg 1	0	0
59	AD	10	Total 10	Mg 10	0	0
59	BN	2	Total 2	Mg 2	0	0
59	DJ	1	Total 1	Mg 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
59	C7	1	Total 1	Mg 1	0	0
59	C3	1	Total 1	Mg 1	0	0
59	AZ	1	Total 1	Mg 1	0	0
59	BK	1	Total 1	Mg 1	0	0
59	AU	5	Total 5	Mg 5	0	0
59	DW	3	Total 3	Mg 3	0	0
59	A9	1	Total 1	Mg 1	0	0
59	CF	4	Total 4	Mg 4	0	0
59	CX	1	Total 1	Mg 1	0	0
59	A0	5	Total 5	Mg 5	0	0
59	AG	2	Total 2	Mg 2	0	0
59	DE	2	Total 2	Mg 2	0	0
59	AQ	4	Total 4	Mg 4	0	0
59	CE	5	Total 5	Mg 5	0	0
59	AH	1	Total 1	Mg 1	0	0
59	BZ	1	Total 1	Mg 1	0	0
59	CO	1	Total 1	Mg 1	0	0
59	CP	1	Total 1	Mg 1	0	0
59	BS	1	Total 1	Mg 1	0	0
59	CW	1	Total 1	Mg 1	0	0
59	A7	1	Total 1	Mg 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
59	CD	4	Total 4	Mg 4	0	0
59	BD	1	Total 1	Mg 1	0	0
59	DT	1	Total 1	Mg 1	0	0
59	A8	1	Total 1	Mg 1	0	0
59	AO	1	Total 1	Mg 1	0	0
59	BW	3	Total 3	Mg 3	0	0
59	AY	1	Total 1	Mg 1	0	0
59	AF	6	Total 6	Mg 6	0	0

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

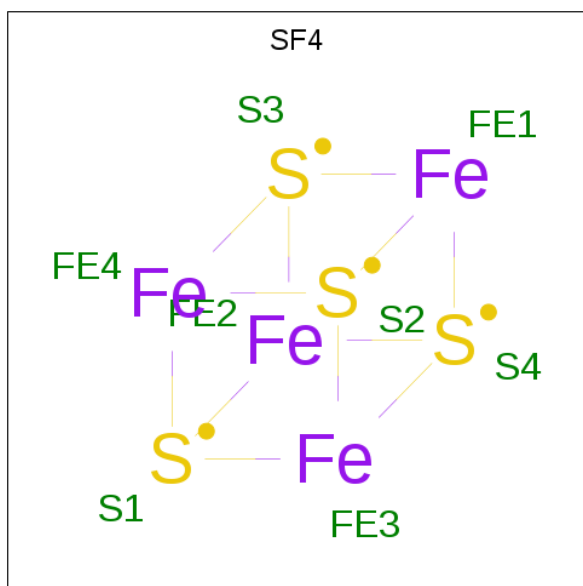
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
60	AY	1	Total 1	Zn 1	0	0
60	BN	1	Total 1	Zn 1	0	0
60	C4	1	Total 1	Zn 1	0	0
60	C5	1	Total 1	Zn 1	0	0
60	C6	1	Total 1	Zn 1	0	0
60	A6	1	Total 1	Zn 1	0	0
60	C9	1	Total 1	Zn 1	0	0
60	DN	1	Total 1	Zn 1	0	0
60	A4	1	Total 1	Zn 1	0	0
60	A5	1	Total 1	Zn 1	0	0
60	A9	1	Total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

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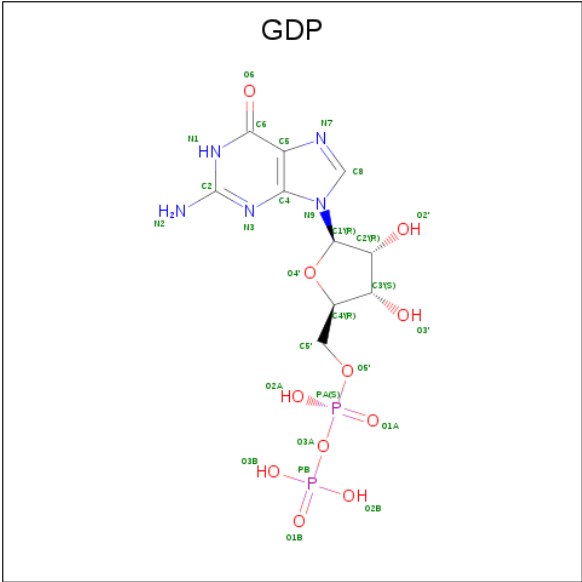
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
60	CY	1	Total	Zn	0	0
			1	1		

- Molecule 61 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe₄S₄).



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

- Molecule 62 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula: 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	1413	Total	O	0	0
			1413	1413		
63	AB	38	Total	O	0	0
			38	38		
63	AD	10	Total	O	0	0
			10	10		
63	AE	17	Total	O	0	0
			17	17		
63	AF	11	Total	O	0	0
			11	11		
63	AG	3	Total	O	0	0
			3	3		
63	AH	1	Total	O	0	0
			1	1		
63	AN	1	Total	O	0	0
			1	1		
63	AO	3	Total	O	0	0
			3	3		
63	AP	16	Total	O	0	0
			16	16		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
63	AQ	4	Total	O	0	0
			4	4		
63	AR	2	Total	O	0	0
			2	2		
63	AS	1	Total	O	0	0
			1	1		
63	AT	1	Total	O	0	0
			1	1		
63	AU	4	Total	O	0	0
			4	4		
63	AV	1	Total	O	0	0
			1	1		
63	AW	1	Total	O	0	0
			1	1		
63	AX	3	Total	O	0	0
			3	3		
63	AZ	1	Total	O	0	0
			1	1		
63	A0	6	Total	O	0	0
			6	6		
63	A1	2	Total	O	0	0
			2	2		
63	A3	2	Total	O	0	0
			2	2		
63	A5	3	Total	O	0	0
			3	3		
63	A6	1	Total	O	0	0
			1	1		
63	A7	2	Total	O	0	0
			2	2		
63	A8	10	Total	O	0	0
			10	10		
63	A9	1	Total	O	0	0
			1	1		
63	BA	213	Total	O	0	0
			213	213		
63	BD	1	Total	O	0	0
			1	1		
63	BM	1	Total	O	0	0
			1	1		
63	BO	1	Total	O	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
63	BP	1	Total	O	0	0
			1	1		
63	BV	1	Total	O	0	0
			1	1		
63	BW	1	Total	O	0	0
			1	1		
63	BZ	2	Total	O	0	0
			2	2		
63	CA	983	Total	O	0	0
			983	983		
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	CN	1	Total	O	0	0
			1	1		
63	CO	1	Total	O	0	0
			1	1		
63	CP	11	Total	O	0	0
			11	11		
63	CQ	2	Total	O	0	0
			2	2		
63	CT	3	Total	O	0	0
			3	3		
63	CU	2	Total	O	0	0
			2	2		
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	2	Total	O	0	0
			2	2		
63	C0	4	Total	O	0	0
			4	4		
63	C3	2	Total	O	0	0
			2	2		

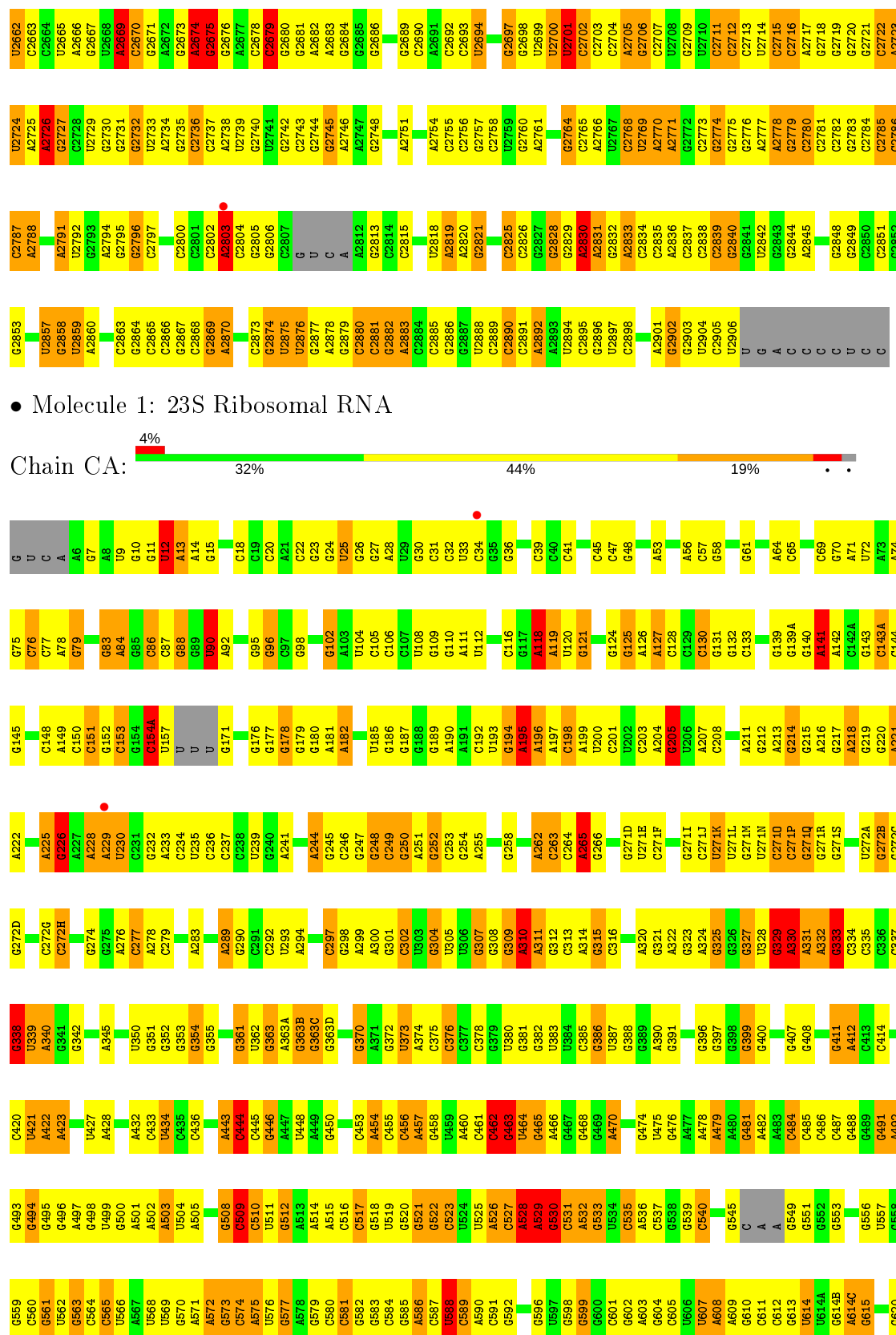
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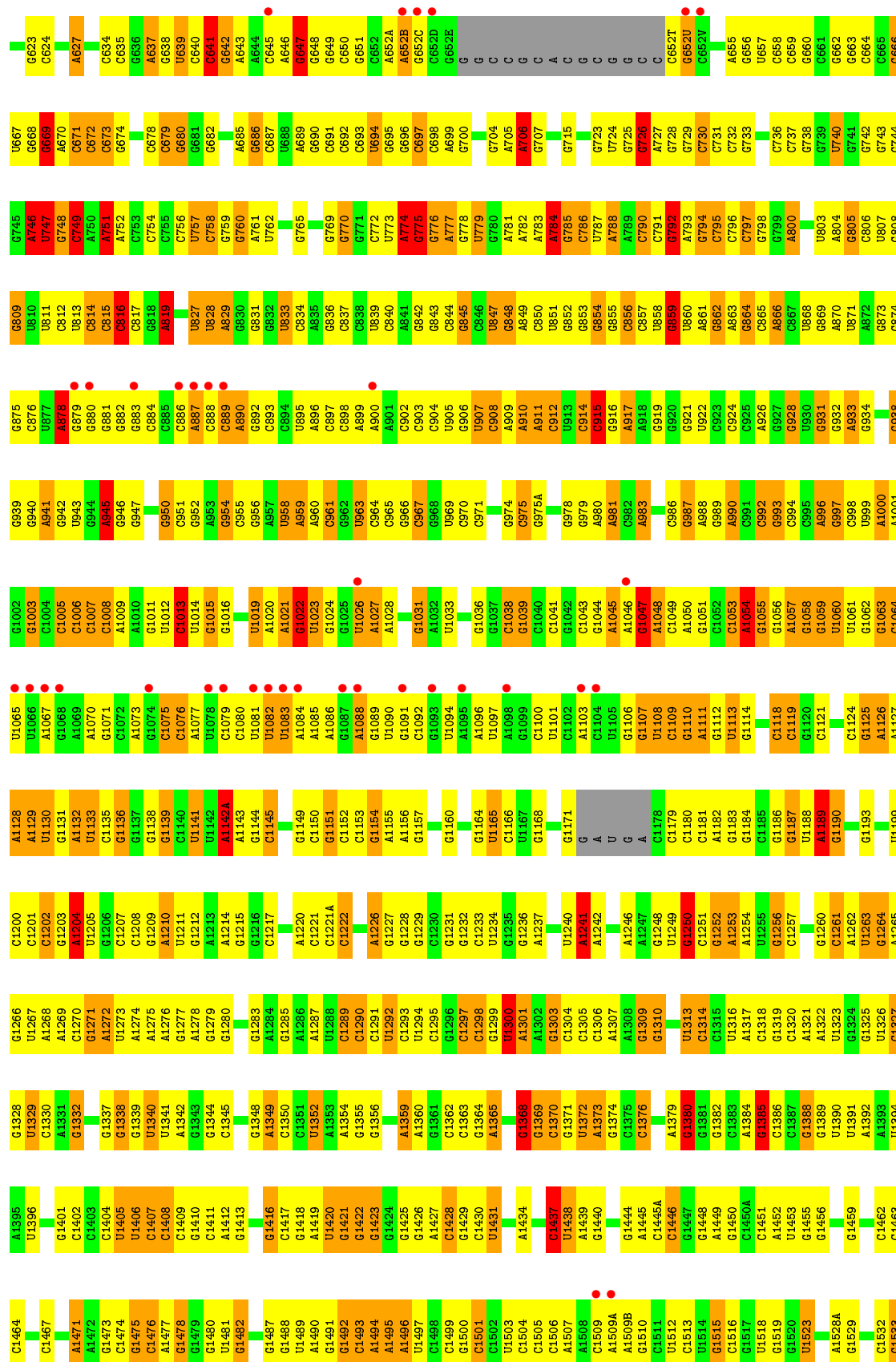
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
63	C5	1	Total	O	0	0
			1	1		
63	C7	2	Total	O	0	0
			2	2		
63	C8	4	Total	O	0	0
			4	4		
63	DA	157	Total	O	0	0
			157	157		
63	DD	1	Total	O	0	0
			1	1		
63	DE	2	Total	O	0	0
			2	2		
63	DH	1	Total	O	0	0
			1	1		
63	DJ	1	Total	O	0	0
			1	1		
63	DK	2	Total	O	0	0
			2	2		
63	DL	1	Total	O	0	0
			1	1		
63	DT	1	Total	O	0	0
			1	1		

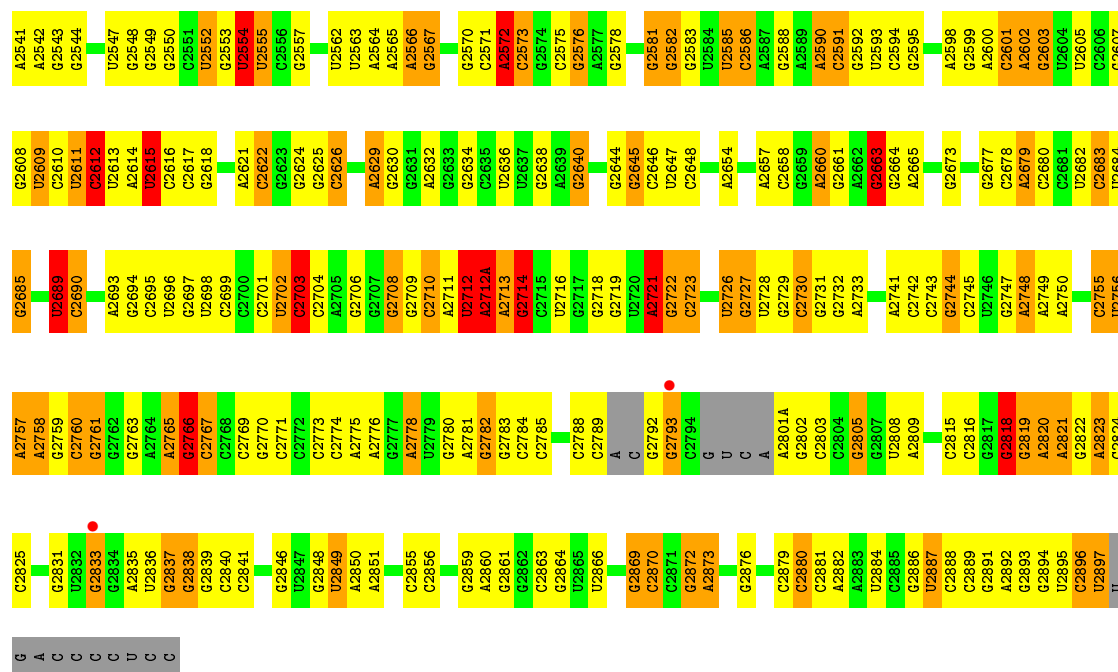
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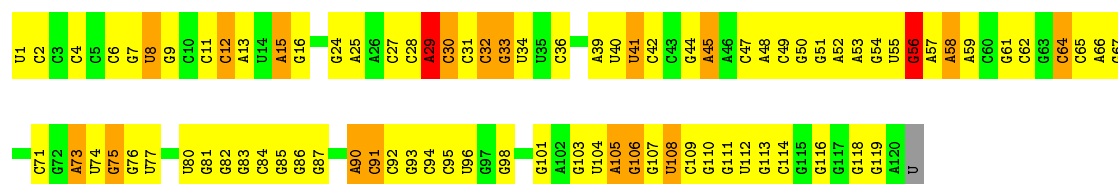


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C2474	U2401	A2336	G2192	U2132	G2056	G1992	C1920	C1832	G1772	C1611	A
A2475	C2404	G2340	G2193	A2133	U1833	U1993	G1921	U1833	A1773	G1612	C1536
A2476	G2405	G2340	A2134	A2134	A2057	U1993	G1922	U1834	U1680	G1613	
A2477	U2406	G2343	C2195	C2135	A2060	G1994	U1923	G1835	U1775	G1614	G1539
A2478	G2407	G2344	C2196	C2136	G2061	U1995		G1836	G1776	C1615	U1540
G2479	U2408	U2344	U2197	C2137	A2062	G1996	U1926	C1837	U1777	A1616	G1541
	U2409	A2345	A2198	C2138	C2063	G1997	A1927	G1838	U1778	C1617	A1542
G2485	G2410	G2346	C2199	C2139	C2064	G1998	A1928	G1839	U1779	A1618	C1543
G2486	G2411	G2347	G2200	C2140	C2065	G1999	A1929	G1840	G1780	G1619	
G2487	C2281	U2348	C2201	G2141	G1930	U1841	G1930	U1841	C1781	A1690	C1547
A2488	G2412	G2349	C2202	C2142	U1931	G1931	U1931	G1842	C1782	C1691	C1548
G2489	G2413	G2350	U2203	C2143	G2069	A2001	A1932	C1843	A1783	U1692	C1549
G2490	C2414	G2351	G2204	U2144	G2070	G2003	G1933	C1844	A1784	G1623	C1550
U2491	A2417	G2352	G2205	C2145	A2071	G2004	C1934			G1624	
U2492	A2418	C2355	G2206	C2146	G2072	A2005	G1935	A1847	A1785		A1553
U2493	A2419	A2356	A2207	G2147	C2073	C2006	A1936	A1848	G1696		C1556
G2494	U2420	U2357	U2218	G2148	U2074	G2007	A1937	G1849	G1697	A1632	C1557
G2495	G2421	G2358	G2222	C2149	U2075		A1938	G1850	A1789	A1633	A1558
	A2422	G2359		U2150		G2010	U1939		C1790	G1634	G1559
C2496	A2423	G2360	A2225	G2151	C2078	A2013	G1940	G1857	A1791	A1637	
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U2500	G2425	G2362	C2227	C2153	G2080	A2015	G1945	A1859	C1793	G1703	G1561
C2501	G2426	G2363	A2228	G2154	C2081	U2016	U1946	G1860	U1794	U1638	
G2502	A2430	C2364	C2229	G2155	A2082			G1861	G1795	U1639	C1564
U2503	U2431	G2365		G2156					U1796	C1640	G1565
U2504		A2366	U2233	G2157	U2086	A2020	G1949	U1864	C1797	A1641	
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G2509	U2437	G2370	C2237	C2161		G2024	G1953	A1877	A1701	G1638	
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C2512	C2440	G2373	G2240	C2164	G2104	C2027	U1956	G1883	G1704	C1640	G1565
G2513	G2441	C2374	U2243	G2165	C2105	U2028	G1957	C1886	C1646	A1652	
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G2536	C2465	G2395	C2264	G2186	A2126	C2050	G1984	A1913	C1826	C1672	C1605
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C2538	G2467	G2396	C2266	U2188	C2128	G2052		U1917	G1768	G1674	C1607
C2539	G2468		A2268	U2189	C2129	G2053		A1918	G1769	C1675	A1608
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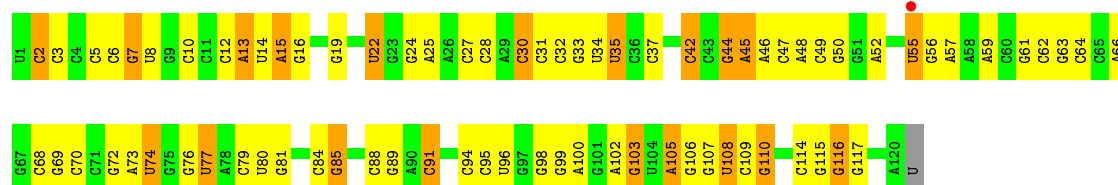
• Molecule 2: 5S Ribosomal RNA

Chain AB: 28% 55% 14%



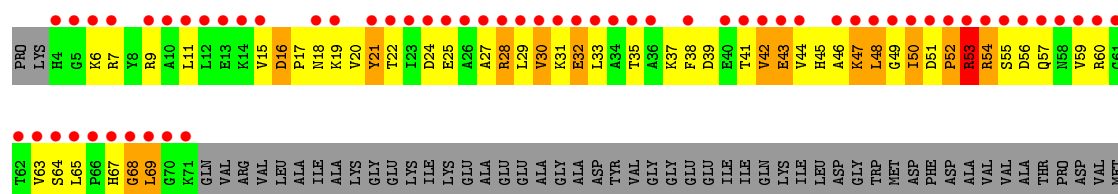
• Molecule 2: 5S Ribosomal RNA

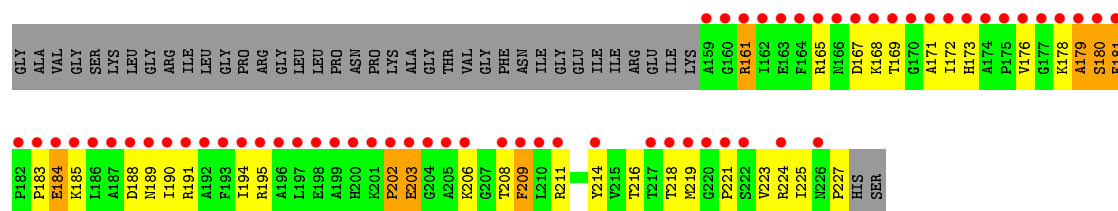
Chain CB: 36% 47% 17%



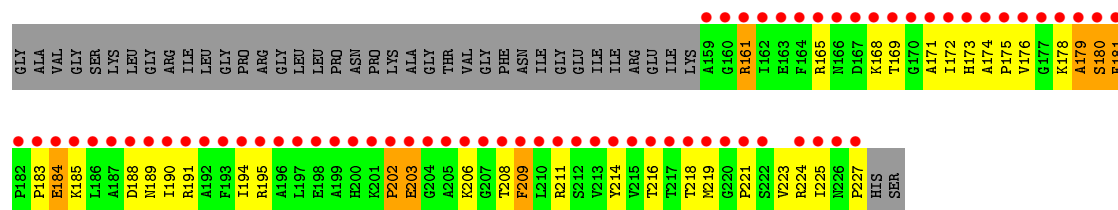
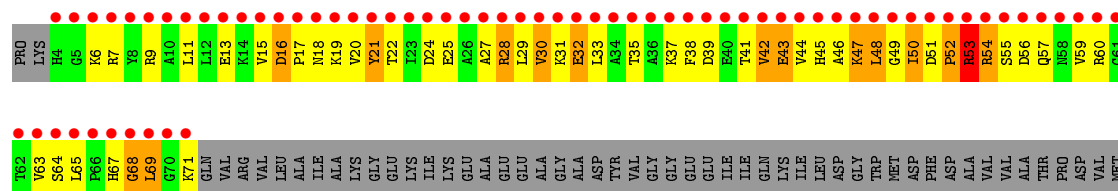
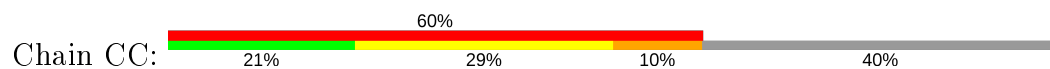
• Molecule 3: 50S ribosomal protein L1

Chain AC: 22% 54% 10% 40%

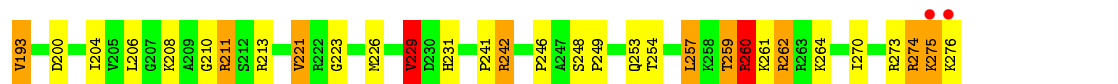
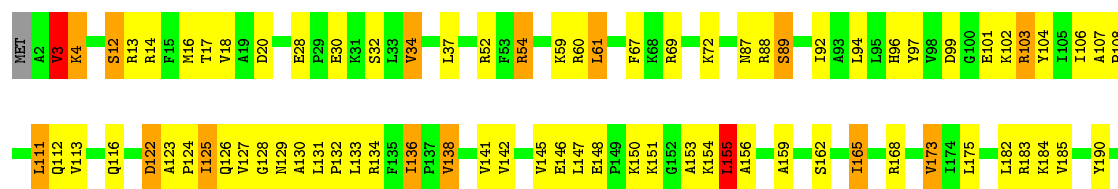




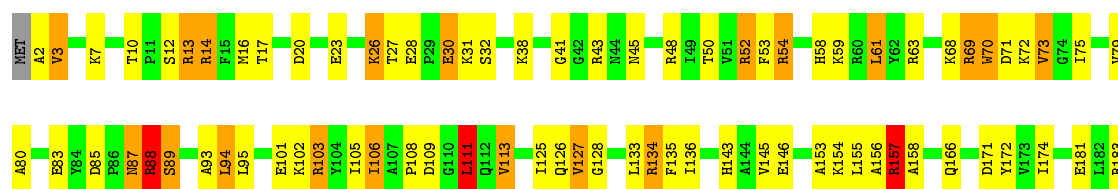
• Molecule 3: 50S ribosomal protein L1

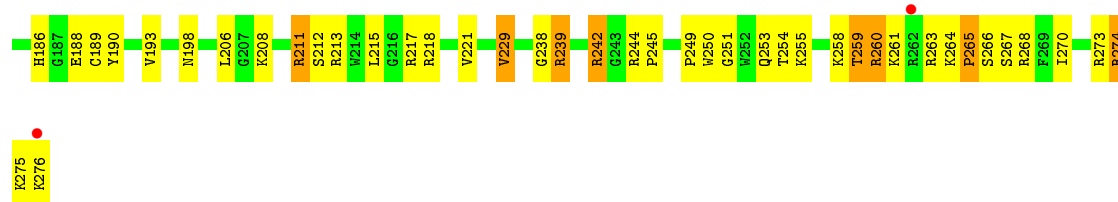


• Molecule 4: 50S ribosomal protein L2



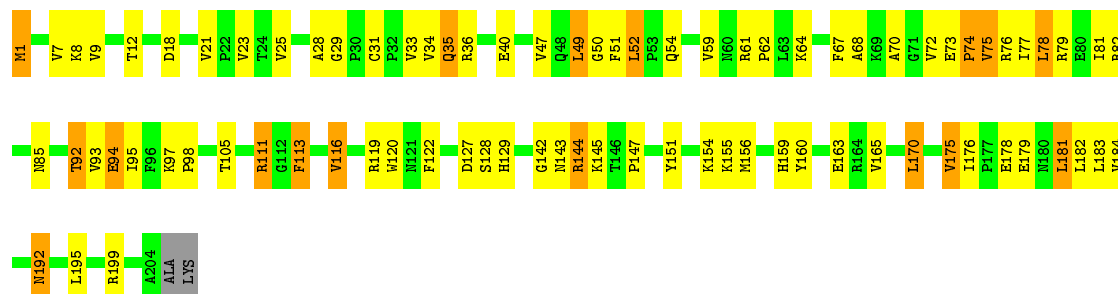
• Molecule 4: 50S ribosomal protein L2





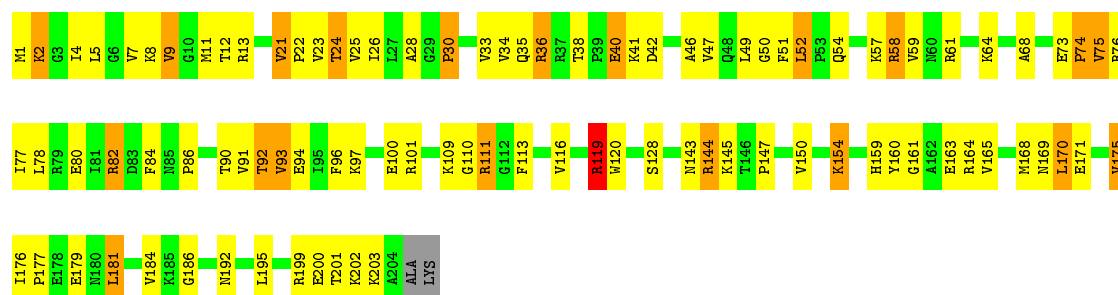
• Molecule 5: 50S ribosomal protein L3

Chain AE: 59% 32% 8%



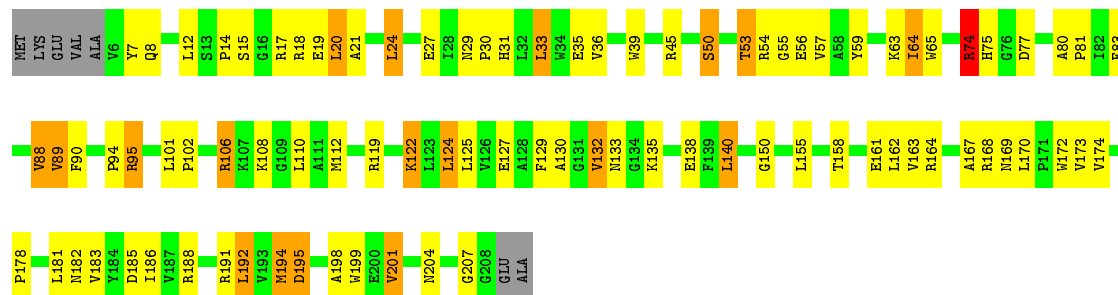
• Molecule 5: 50S ribosomal protein L3

Chain CE: 52% 36% 10%



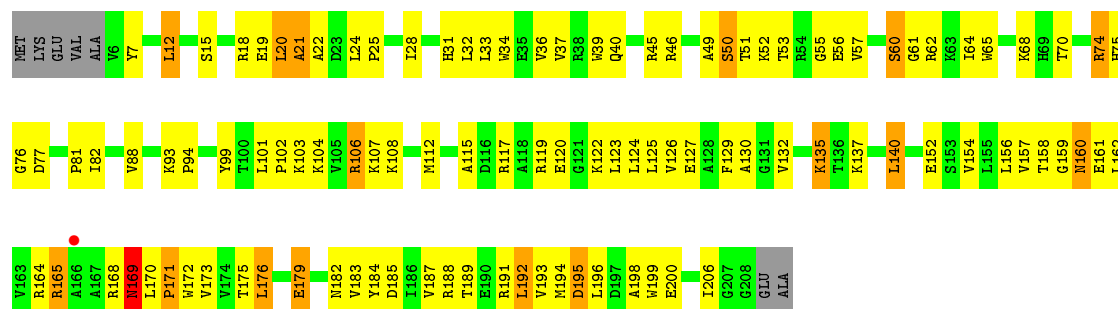
• Molecule 6: 50S ribosomal protein L4

Chain AF: 54% 33% 9%

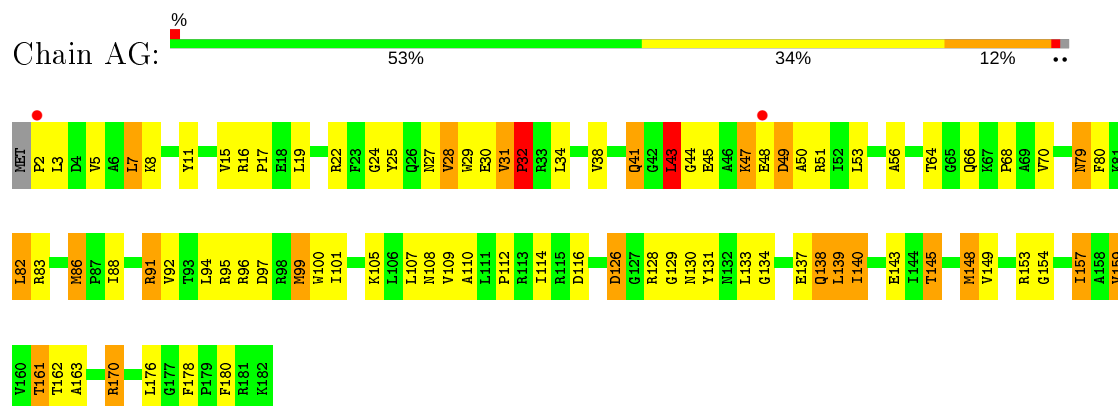


• Molecule 6: 50S ribosomal protein L4

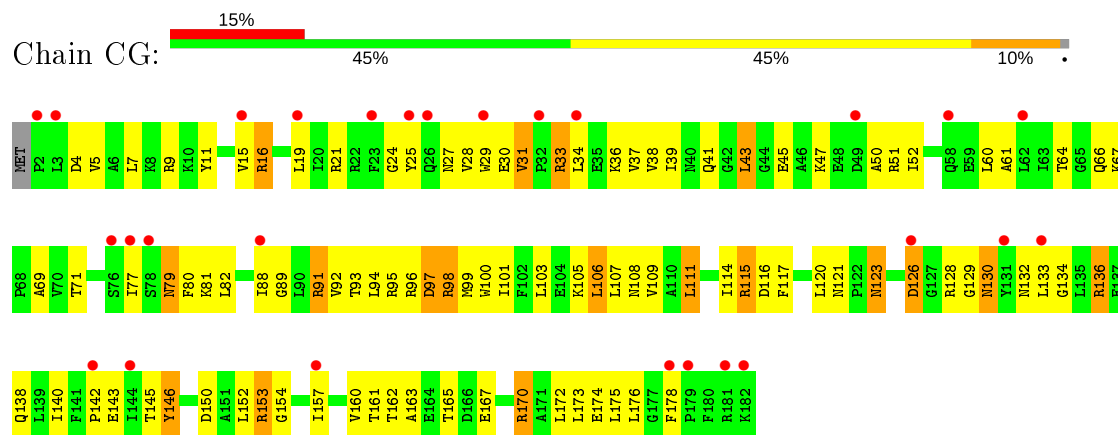
Chain CF: 46% 43% 8%



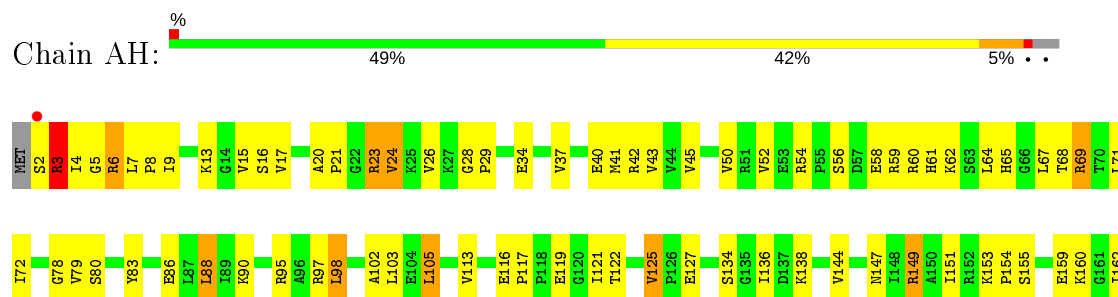
• Molecule 7: 50S ribosomal protein L5



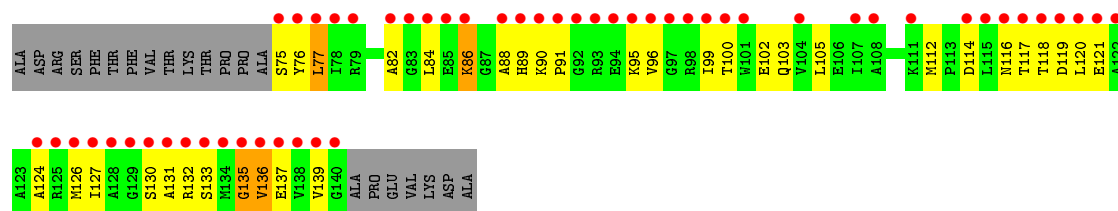
• Molecule 7: 50S ribosomal protein L5



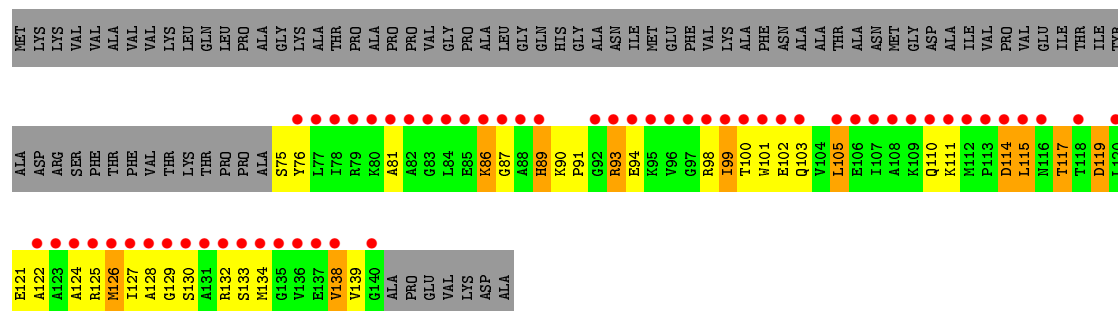
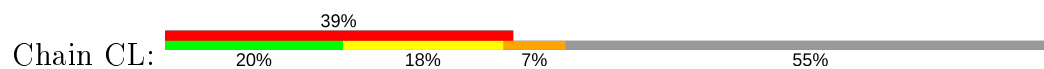
• Molecule 8: 50S ribosomal protein L6



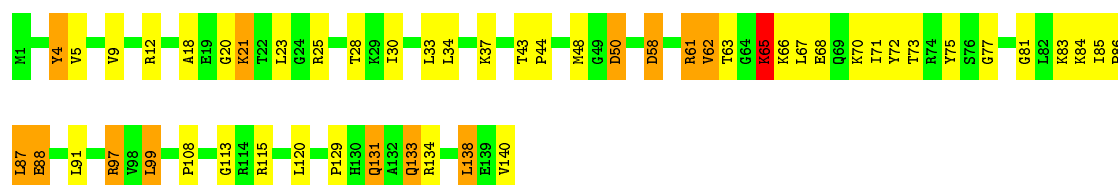




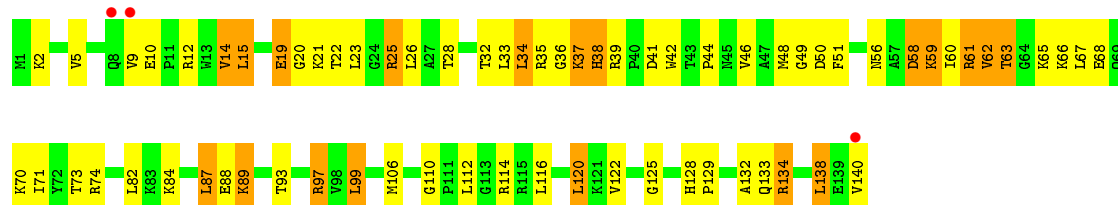
• Molecule 10: 50S ribosomal protein L11



• Molecule 11: 50S ribosomal protein L13



• Molecule 11: 50S ribosomal protein L13



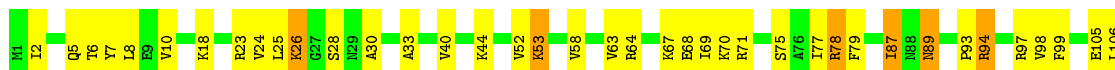
• Molecule 12: 50S ribosomal protein L14





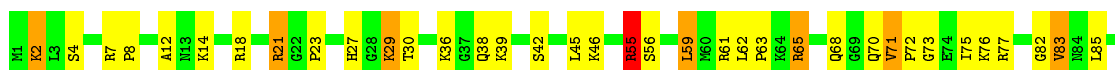
- Molecule 12: 50S ribosomal protein L14

Chain CO: 64% 31% 5%



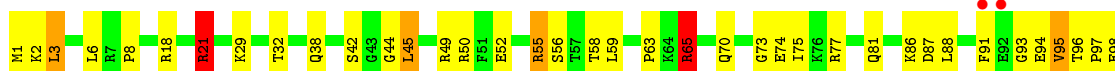
- Molecule 13: 50S ribosomal protein L15

Chain AP: 58% 33% 7% ..



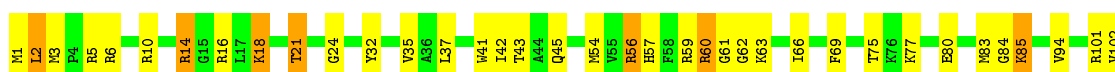
- Molecule 13: 50S ribosomal protein L15

Chain CP: 5% 58% 33% 7% ..



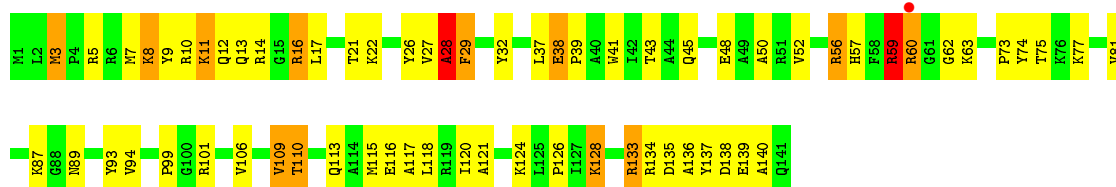
- Molecule 14: 50S ribosomal protein L16

Chain AQ: 65% 28% 8%

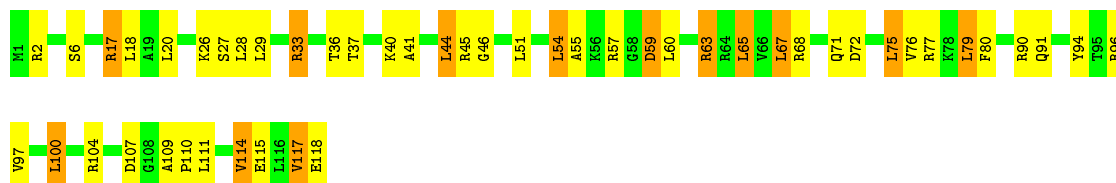


- Molecule 14: 50S ribosomal protein L16

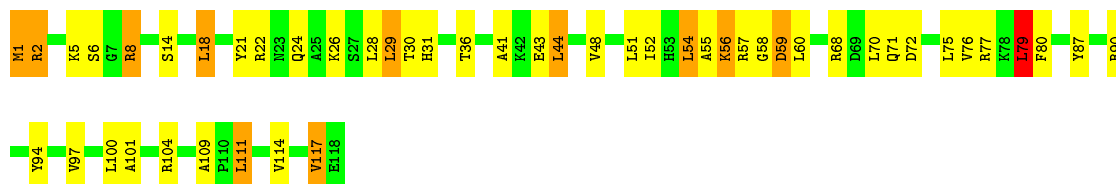
Chain CQ: 53% 37% 9% .



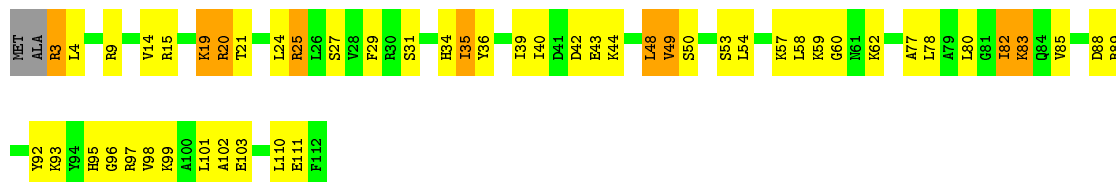
• Molecule 15: 50S ribosomal protein L17



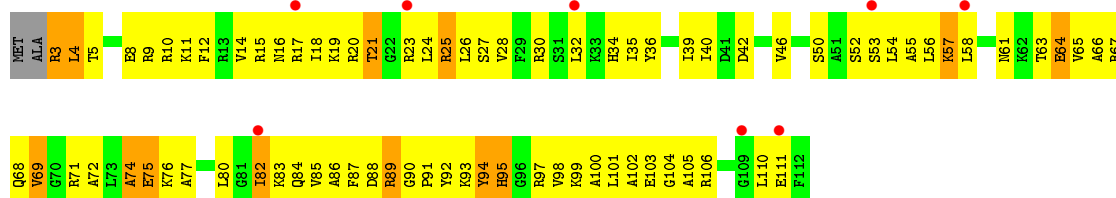
• Molecule 15: 50S ribosomal protein L17



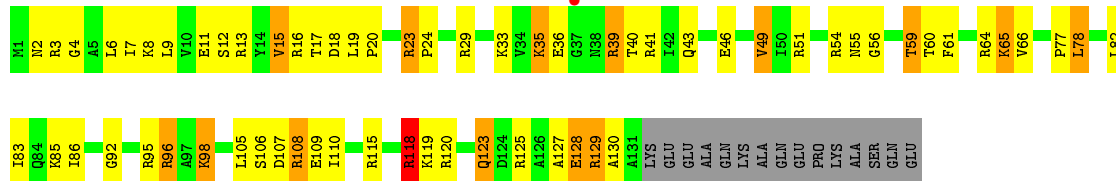
• Molecule 16: 50S ribosomal protein L18



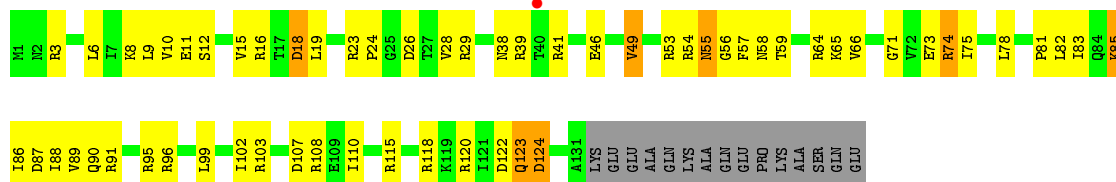
• Molecule 16: 50S ribosomal protein L18



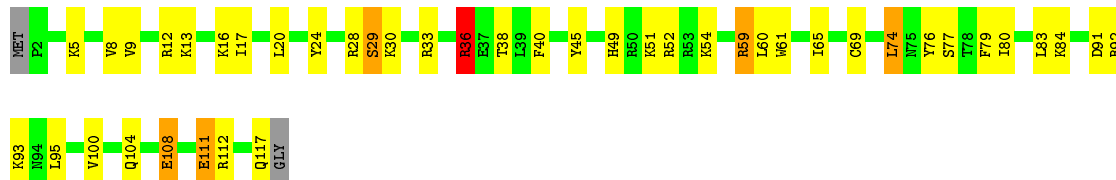
• Molecule 17: 50S ribosomal protein L19



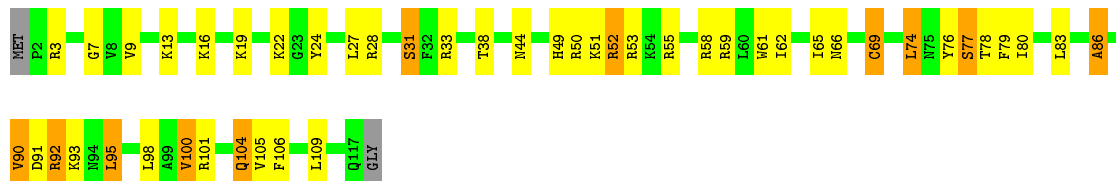
- Molecule 17: 50S ribosomal protein L19



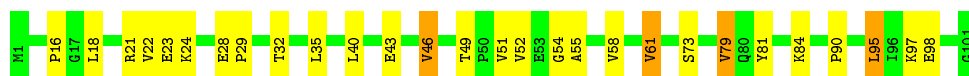
- Molecule 18: 50S ribosomal protein L20



- Molecule 18: 50S ribosomal protein L20

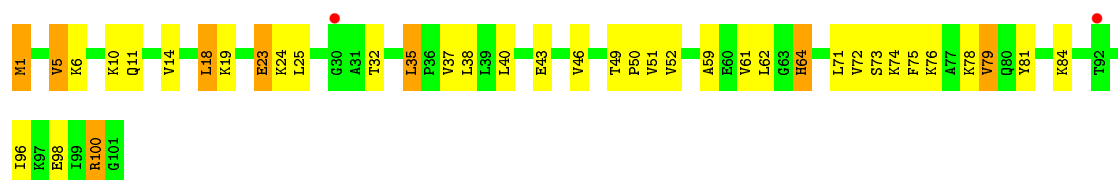


- Molecule 19: 50S ribosomal protein L21



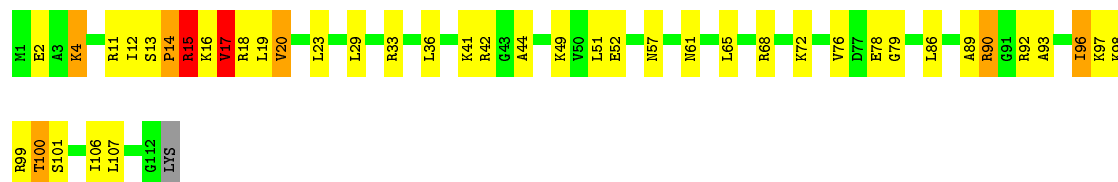
- Molecule 19: 50S ribosomal protein L21





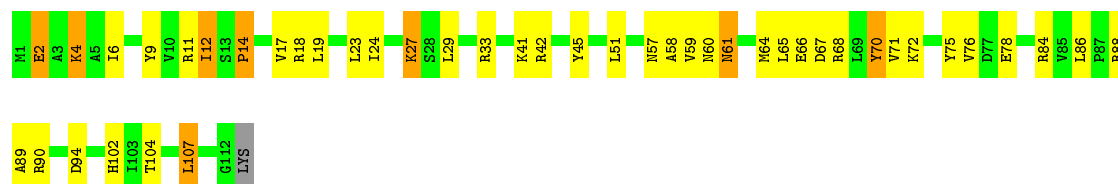
- Molecule 20: 50S ribosomal protein L22

Chain AW: 61% 31% 5% ..



- Molecule 20: 50S ribosomal protein L22

Chain CW: 60% 32% 7% ..



- Molecule 21: 50S ribosomal protein L23

Chain AX: 68% 27% ..



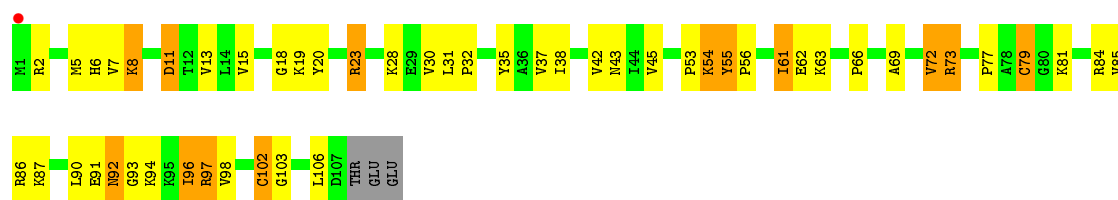
- Molecule 21: 50S ribosomal protein L23

Chain CX: 4% 51% 43% ..

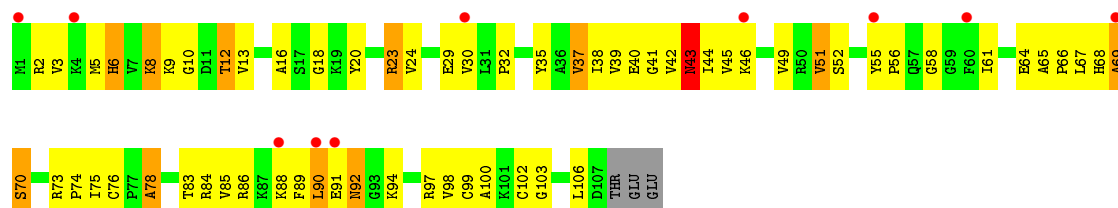
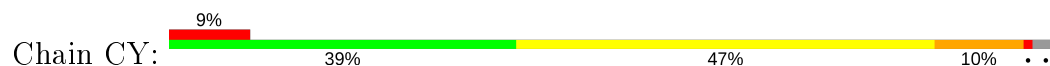


- Molecule 22: 50S ribosomal protein L24

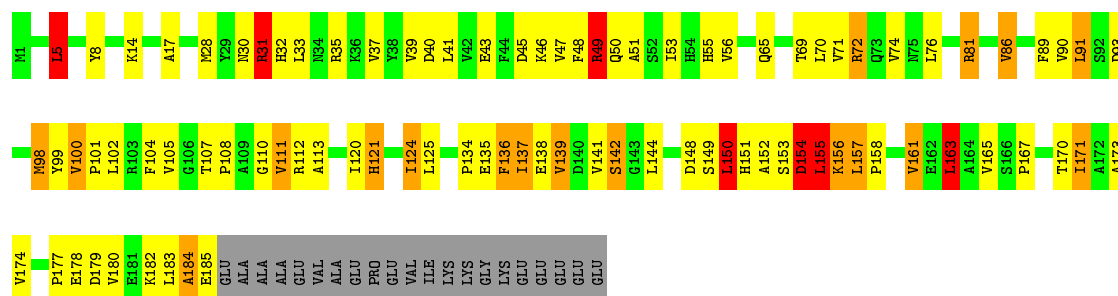
Chain AY: 51% 35% 12% ..



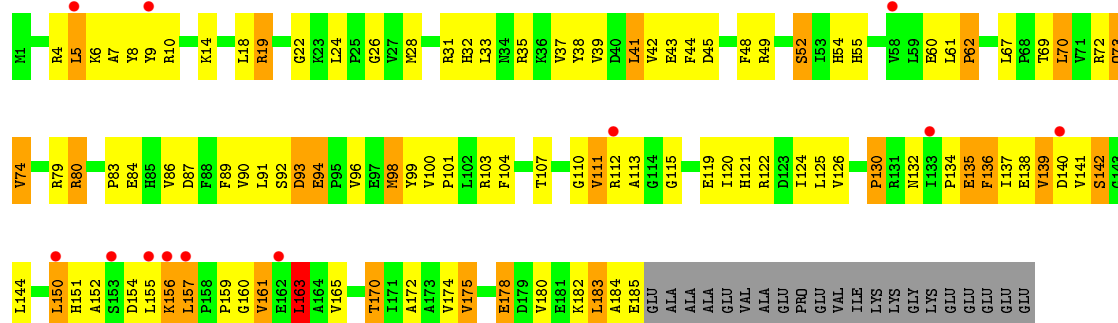
- Molecule 22: 50S ribosomal protein L24



- Molecule 23: 50S ribosomal protein L25

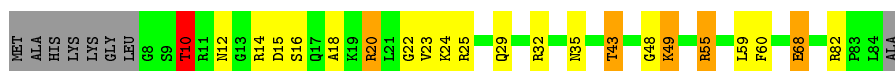


- Molecule 23: 50S ribosomal protein L25

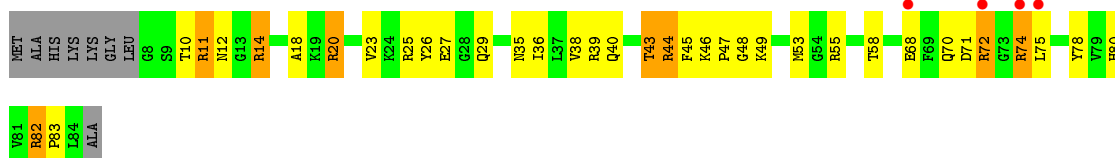


- Molecule 24: 50S ribosomal protein L27

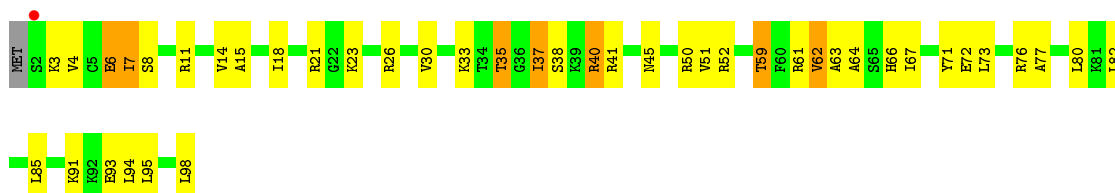




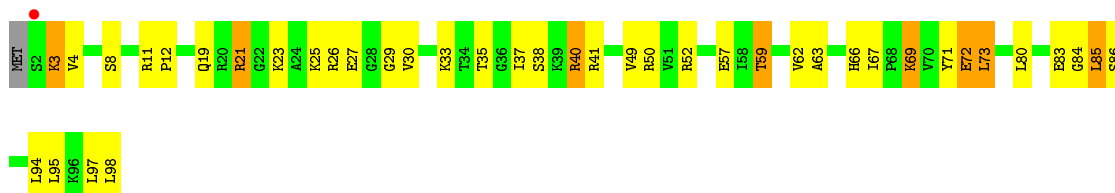
- Molecule 24: 50S ribosomal protein L27



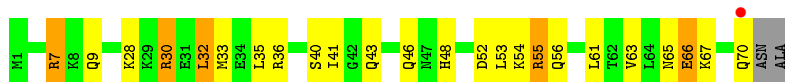
- Molecule 25: 50S ribosomal protein L28



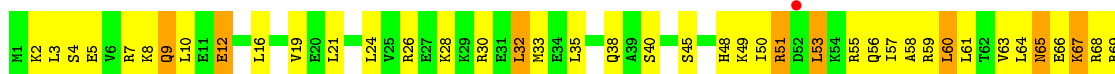
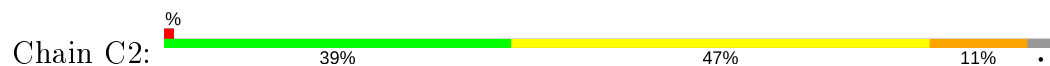
- Molecule 25: 50S ribosomal protein L28



- Molecule 26: 50S ribosomal protein L29



- Molecule 26: 50S ribosomal protein L29





- Molecule 27: 50S ribosomal protein L30



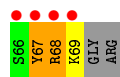
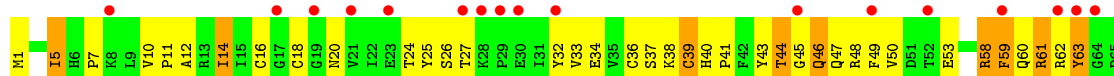
- Molecule 27: 50S ribosomal protein L30



- Molecule 28: 50S ribosomal protein L31



- Molecule 28: 50S ribosomal protein L31



- Molecule 29: 50S ribosomal protein L32



- Molecule 29: 50S ribosomal protein L32





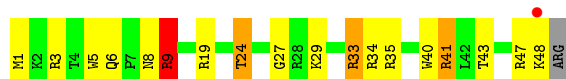
- Molecule 30: 50S ribosomal protein L33



- Molecule 30: 50S ribosomal protein L33



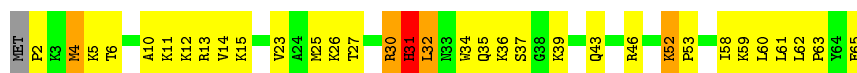
- Molecule 31: 50S ribosomal protein L34



- Molecule 31: 50S ribosomal protein L34



- Molecule 32: 50S ribosomal protein L35

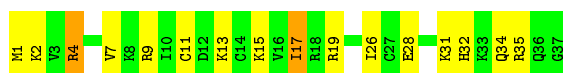


- Molecule 32: 50S ribosomal protein L35



- Molecule 33: 50S ribosomal protein L36





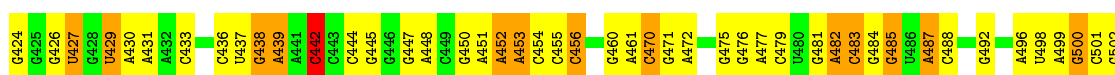
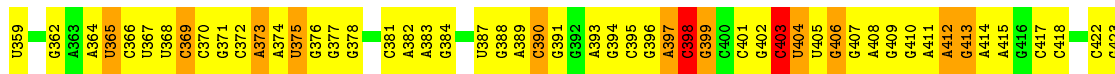
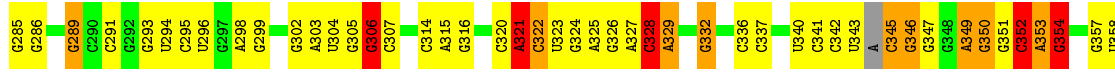
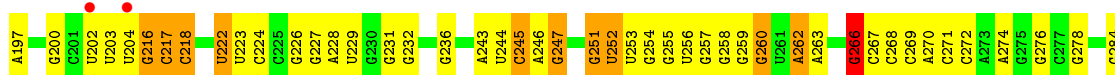
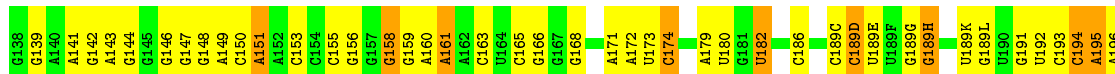
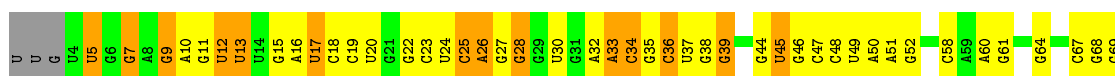
- Molecule 33: 50S ribosomal protein L36

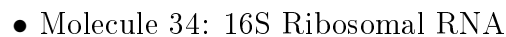
Chain C9: 46% 49% 5%



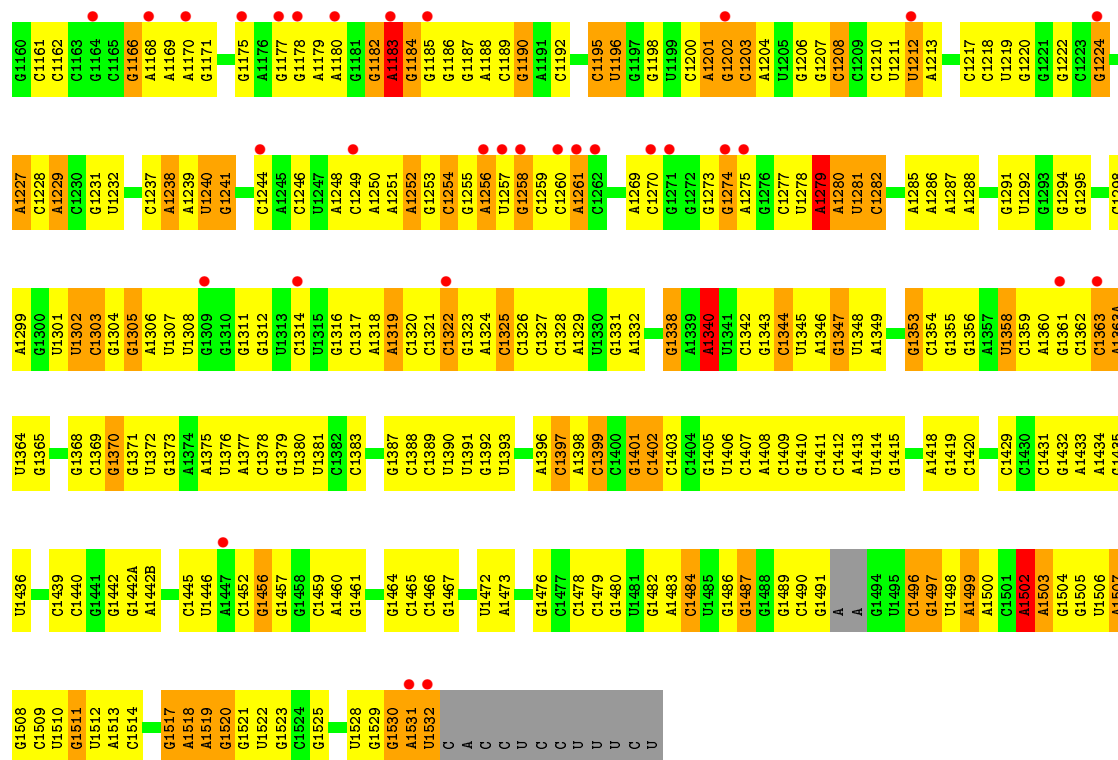
- Molecule 34: 16S Ribosomal RNA

Chain BA: 3% 31% 48% 17%

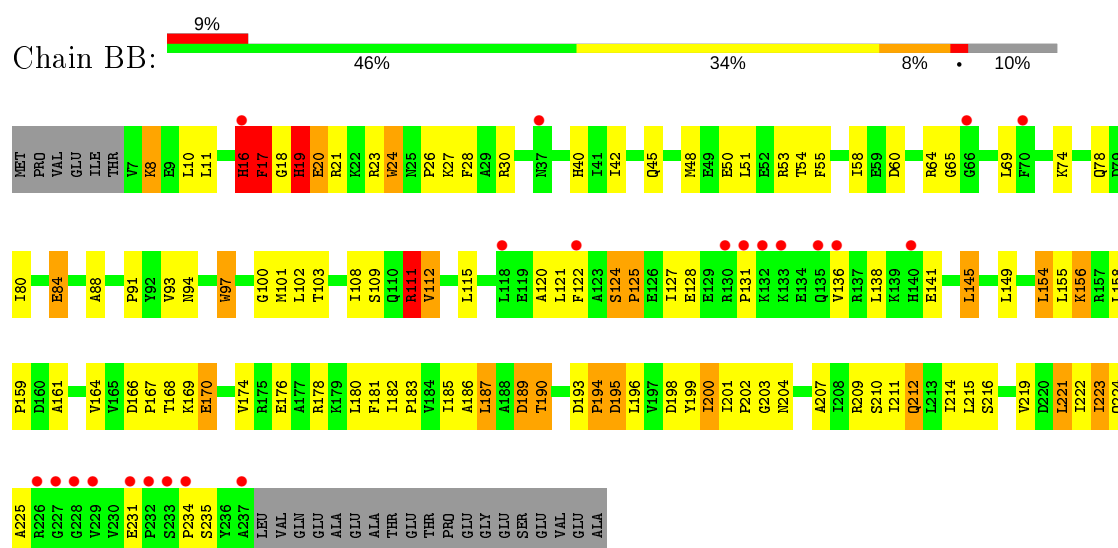




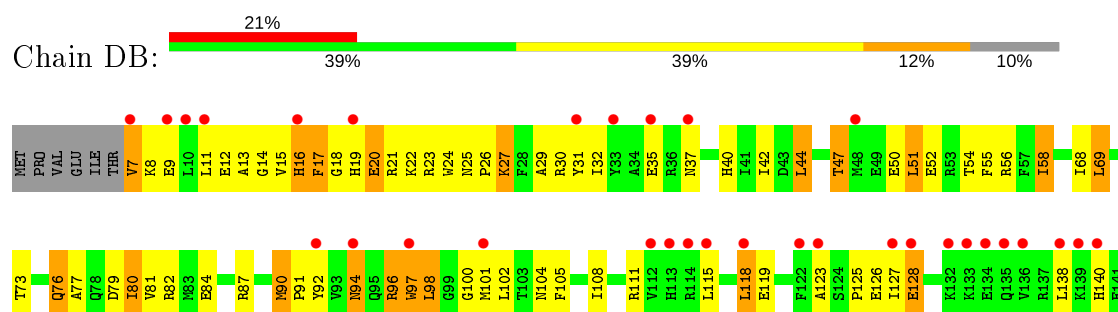
G1098	G1036	A978	C904	G825	U757	G683	C596	G527	A448	G379	C308	C236	A161	C67
G1099	C1037	C979	U905	C826	G758	A684	G697	U531	A449	G380	G309	G236	A162	G70
A1100	C1038	C980	G906	U827	A759	A687	U598	A532	C449	C381	C237	C237	C163	C71
A1101	C1039	U981	A907	A828	G760	G688	C599	A533	A450	A382	C314	C240	U164	C72
A1102	A1040	U982	A908	G829	G761	C689	C600	A534	A451	A383	C315	C241	C165	G73
A1103	A1041	C983	A909	G830	G762	G690	A602	C536	A452	G384	C316	C242	C166	
A1104	C1042	C984	C912	U831	G763	G691		C537	A453	G388	C320	C243	A171	G79
A1105	A1043	C985	A913	C832	G764	U892	A607	C538	A454	A389	A321	A244	U	
A1106	A1044	A986	G914	U833	G765	G692	A608	C539	C455	C390	A322	C245	U	
A1107	C1045	C987	A915	C834	A766	A694	A609	A540		G391	C323	C246		
A1108	A1046	G988	A916	U835	A767	A695	G610	C541	A461	C392	C324	A247	U84	
A1109	G1047	C989	G916	G836	G769	A696	G611	C542	C470	A393	A325	C247	C174	
A1110	G1048	C990	G917	G837	C770	U697	A612	C543	A471	G394	A326	C248	C175	
A1111	U1049	U991	A918	G838	C771	G698	C613	C544	A472	C395	G327	C249	A88	
A1112	C1050	G992	A919	U839	G773				A473	C396	C328	C250	C176	
A1113	C1051	G993	U920	C840	G774				A474	C397	A329	C251	C177	
A1114	U1052	A994	U921	U841	G775	C701	U619	A547	C475	A398	C330	C252	A179	
A1115	C1053	C995	G922	C848	G776	A702	U618	C548	C476	C399	C331	C253	U180	
A1116	C1054	A996	A823	C849	A777	G703	C620	C549	C477	C400	G332	C254	U181	
A1117	A1055	C997		U850	G778		A621	G550	C478	C401	G333	C255	U182	
A1118	U1056	G998	G926	G851	C779	C707	A622	C551	C479	U403	G334	C256	C186	
A1119	G1057	C999	G927	G852	A780	C708	C623	U552	U480	U404	G335	C257	C187	
A1120	C1058	U1000		G853	A781	G709	C624	A553	U481	U405	G336	C258	C188	
U1121	C1059	A1001	G932	G854	A782	G713	U625	C554	C483	C407	G337	C259	C189	
U1122	C1060	G1001A	G933	G855	C783	G714	U626	C555	C484	U408	A338	C260	G104	
A1123	G1061	G1002	C934	C856	C784	A715	G627	C556	C485	U409	C339	C261	G105	
U1124	U1062	G1003	A935	C857	G785	A716		C557	C486	C410		C262	G106	
U1125	C1063	A1004	C936	G858	G786			C558	A487	G411	A344	C263	G107	
U1126	G1064	A1005	A937	A859	A787	C719	U630	U559	U487	A412	C345	C264	U189E	
U1127	U1065	C1006	A938	A860	G790	C720	U638	U560	C488	U413	C346	C265	U189F	
C1128	C1066	C1007	G939	G861	A791	G721	U639	U561	C489	U414	C347	C266	U189G	
C1129		C1008	C940	C862	G792	A722		C562	C491	U415	A349	C267	G189H	
A1130	C1069	G1009	G941	U863	A793	U723	A642	A563	C492	U416	G350	C268	G189I	
G1131	U1070	G1010	G942	C864	C794	G725	U643	C564	A496	C417	G351	C269	U189J	
G1132	G944	G1011		A865	A795	G726	U644	U565	U498	U418	C352	C270	U190	
G1133	G945	U1012	C945	C866	C796	G727		U566	U499	C419	C353	C271	U191	
U1134	A946	G1013	G946	G867	G798	A728	U649	C567	A499	U421	G354	C272	U192	
U1135	C1075	A1014		C868		A729	U650			C422	C355	C273	C193	
C1076	C1077	A1015		G869	A802	G730	C851	G570	C503	U425	A356	C274	C194	
C1077		A1016			G803	C731	U652	U571	C504	U426	G357	C275	C195	
U1078	U1078	G1021	G954	G874	U804	C732	A653	A572	C505	G428	U358	C276	U125	
A1080	A1080	G1022	U955	G875	C805	A733	U656	A573	G505	U427	U359	C277	U126	
G1081	G1081	G1023	U956	G876	C806			A574		G429	A360	C278	G127	
G1082	U1082	G1024	A957	G877	A807	C736	C656	G575	A509	U429	G361	C279	G128	
U1083	U1083	U1025	A958	G878	C807	A737	U662	G576	A510	U430	G362	C280	U129	
G1084	G1084	G1026	U959	C879	C810	C738	A663	G577	C511	A431	A363	C281	U130	
U1085	U1085	C1027	U960	C880	C811	C739	U664	C578	U512	A432	A364	C282	G129A	
U1086	U1086	G1028	U961	G881	C812	U740	A665	C579	C513	C433	U365	C283	A130	
G1087	G1087	C1029	C867	G882	C813	G741	U669	U580	C514	C434	C366	C284	C131	
U1088	U1088	C1030	A968	C883	U813	G742	U670	G581	U515	U434	U367	C285	A134	
U1089	A969	G1030A	A968	U884	A814	U743	G670		U516	C435	U368	C286	A143	
U1090	C1030B	C970	A969	G885	A815	C747	G671	C586	C517	U436	G371	C287	G144	
U1091	G1030C	G971	A970	U891	A816	C748	U672	G587	C518	U437	U222	C288	G145	
A1092	A1030D	C972	G973	U892	C817	C749	G673	G588	C519	U438	C372	C289	G146	
G1093	G973		C809	C809	G818	C749	U674	G589	A520	A439	A373	C290	G147	
G1094	A974		A900	A900	G819	A753	U675	C590	A521	A441	U375	C291	A148	
U1095	A975		A901	A901	C822	C754	U676	U591	C522	C442	G376	C292	A149	
G1096	G1034		A902	A902	G823	C755	U677	G592	A523	C443	G377	C293	C150	
C1097	A1035		G903	G903	C824	C756	U678	G595	A524	C444	G378	C294	G158	

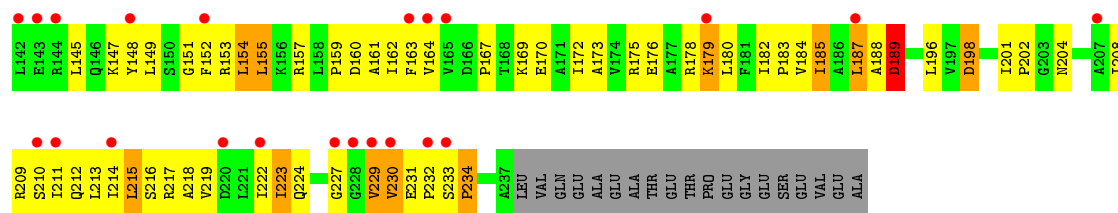


• Molecule 35: 30S ribosomal protein S2

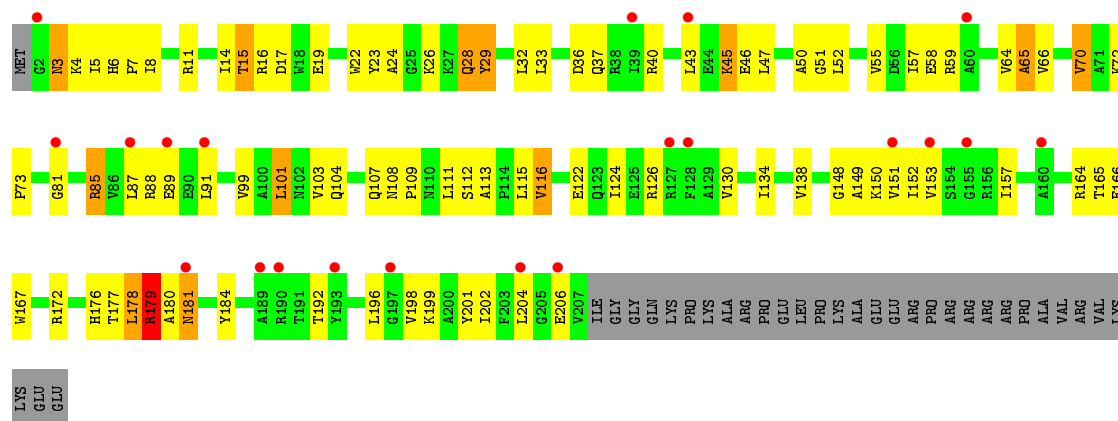


• Molecule 35: 30S ribosomal protein S2

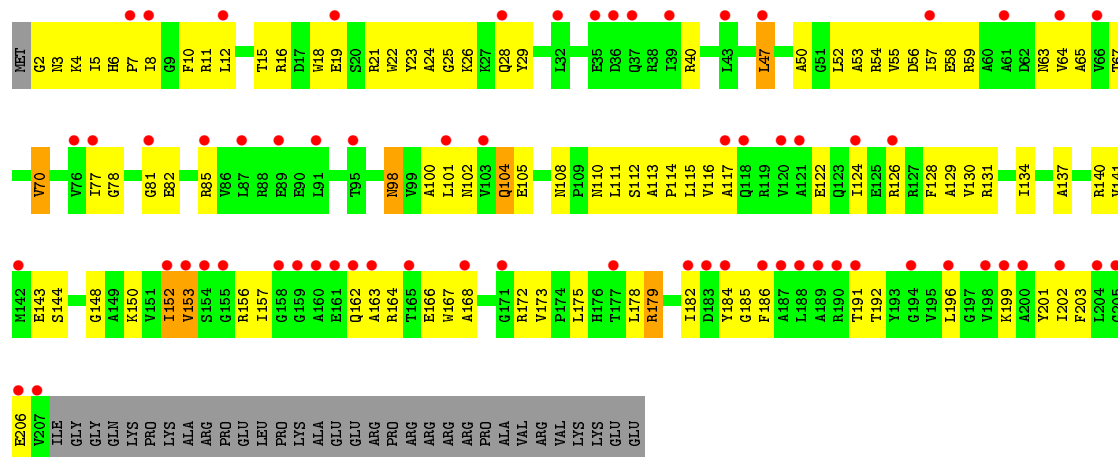




• Molecule 36: 30S ribosomal protein S3

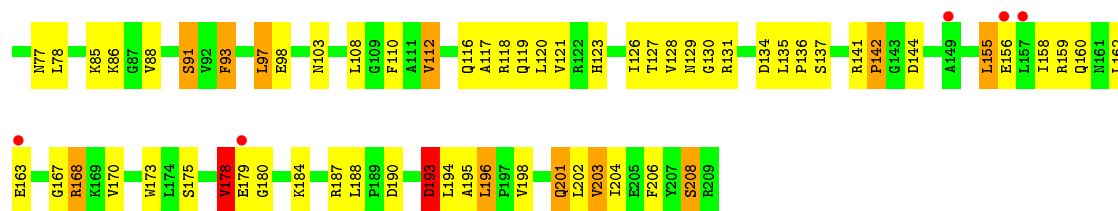


• Molecule 36: 30S ribosomal protein S3

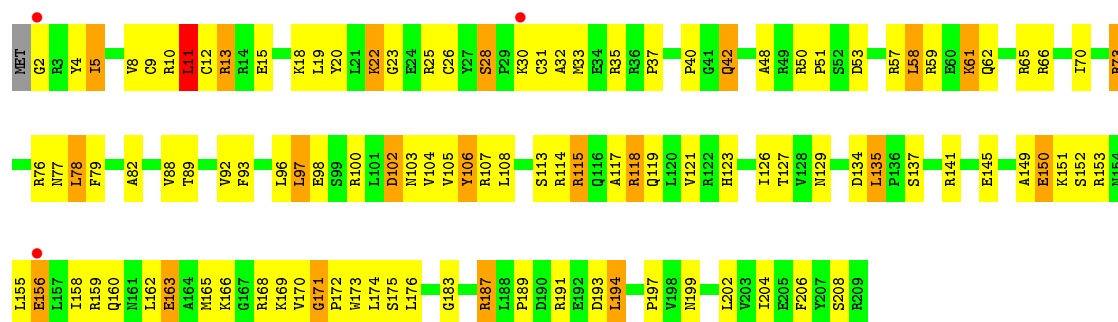


• Molecule 37: 30S ribosomal protein S4

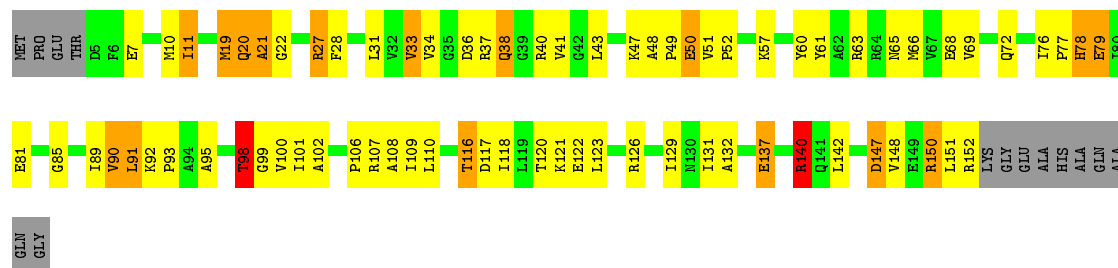




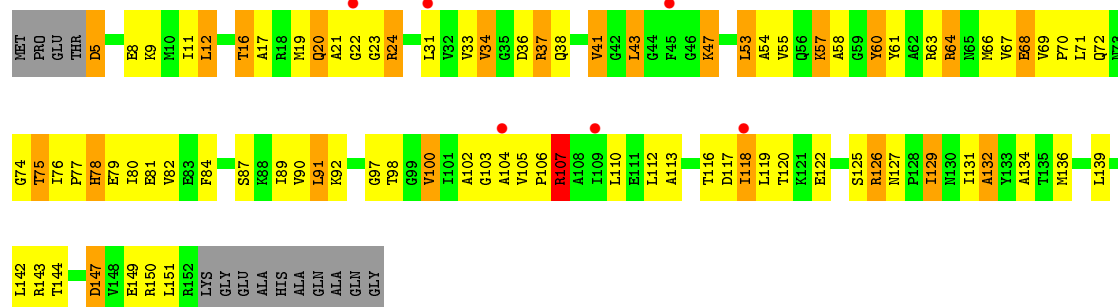
• Molecule 37: 30S ribosomal protein S4



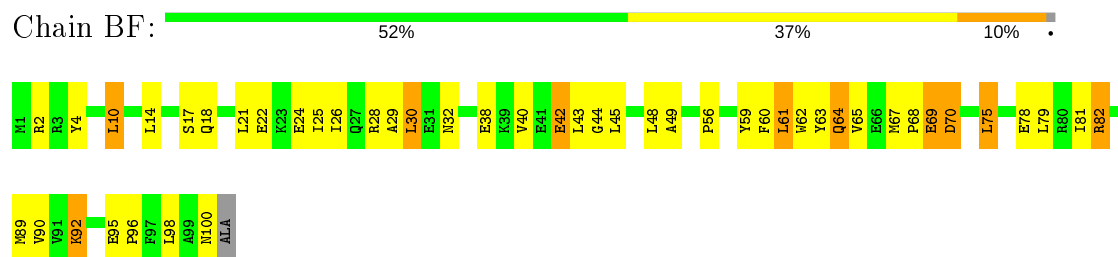
• Molecule 38: 30S ribosomal protein S5



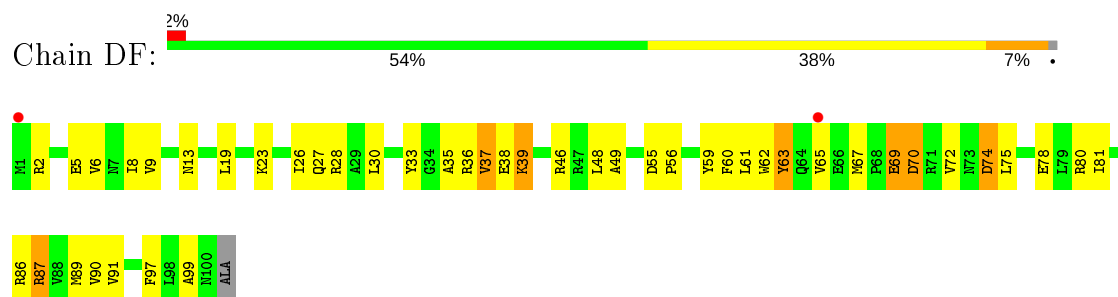
• Molecule 38: 30S ribosomal protein S5



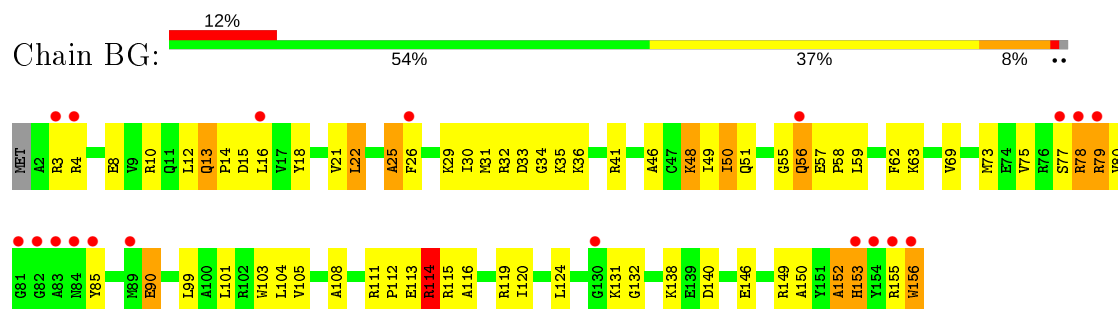
• Molecule 39: 30S ribosomal protein S6



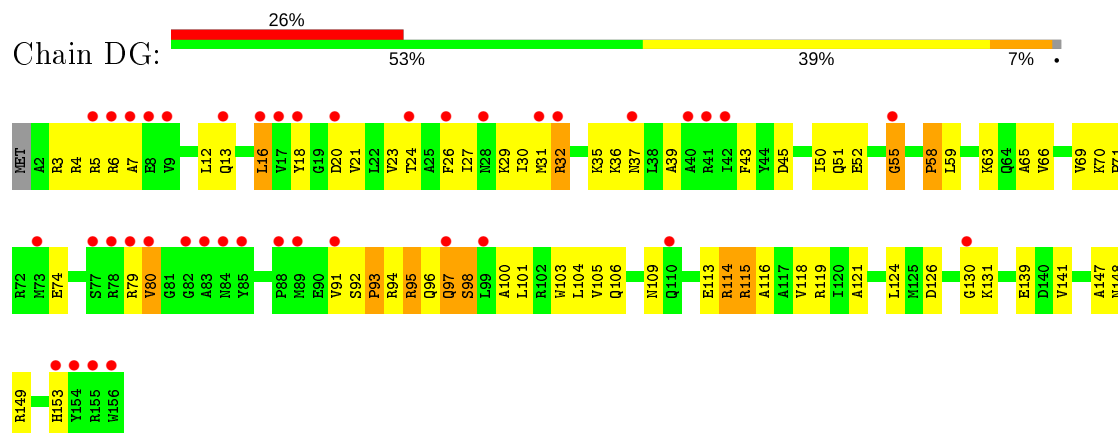
- Molecule 39: 30S ribosomal protein S6



- Molecule 40: 30S ribosomal protein S7

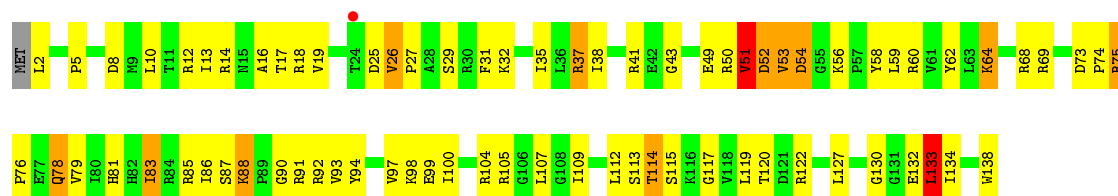


- Molecule 40: 30S ribosomal protein S7

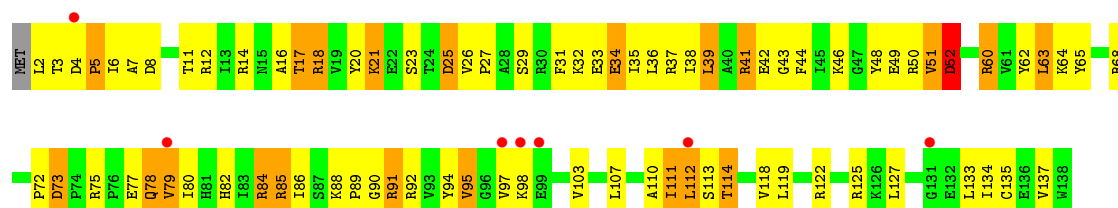
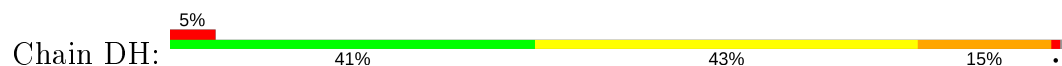


- Molecule 41: 30S ribosomal protein S8

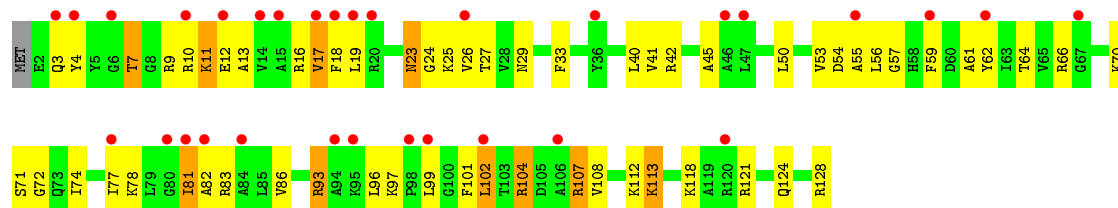




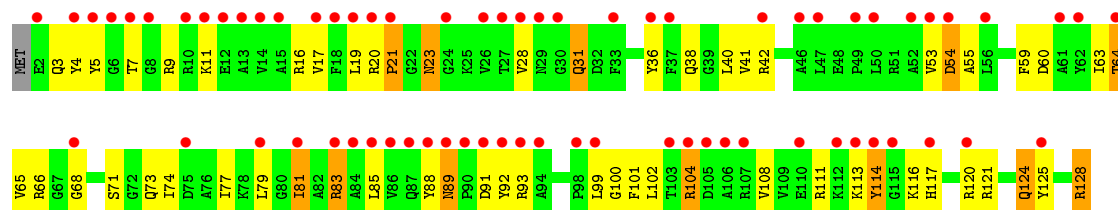
• Molecule 41: 30S ribosomal protein S8



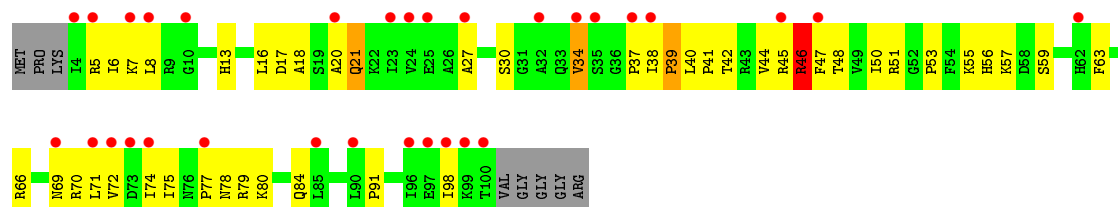
• Molecule 42: 30S ribosomal protein S9



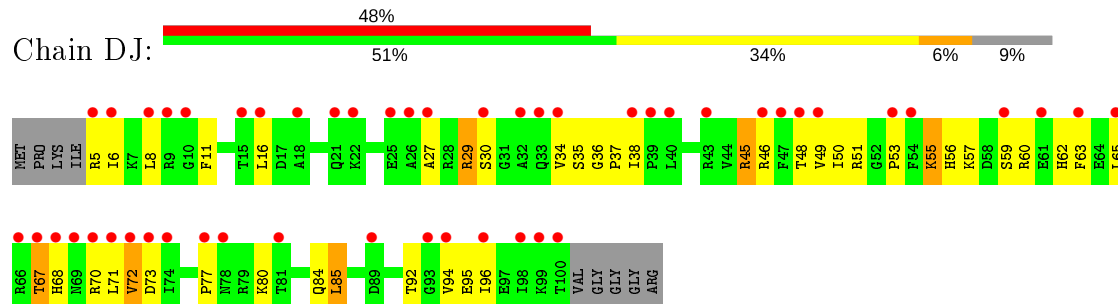
• Molecule 42: 30S ribosomal protein S9



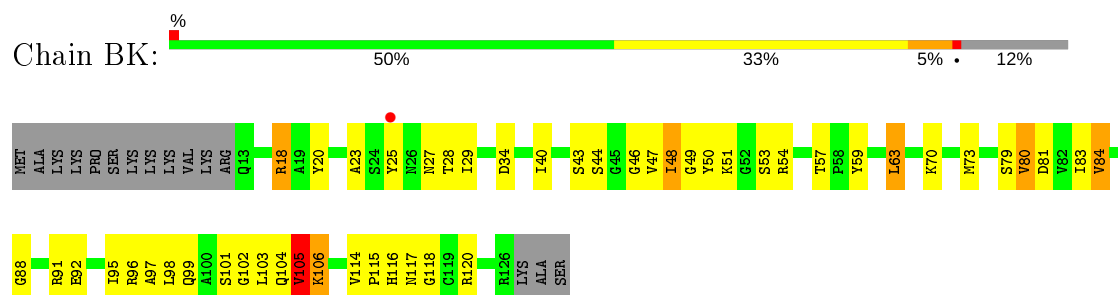
• Molecule 43: 30S ribosomal protein S10



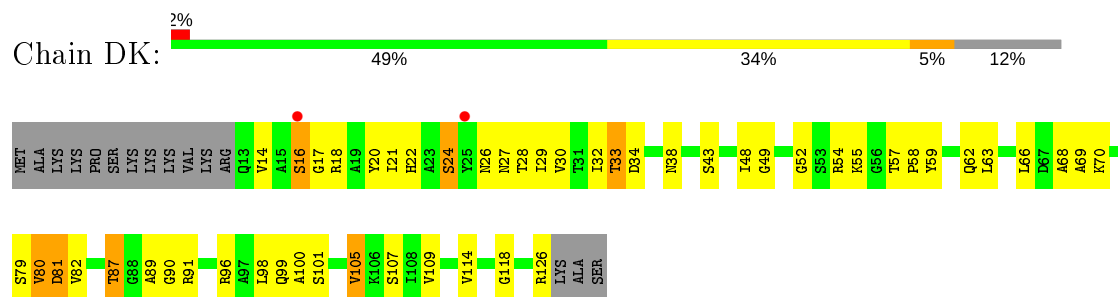
- Molecule 43: 30S ribosomal protein S10



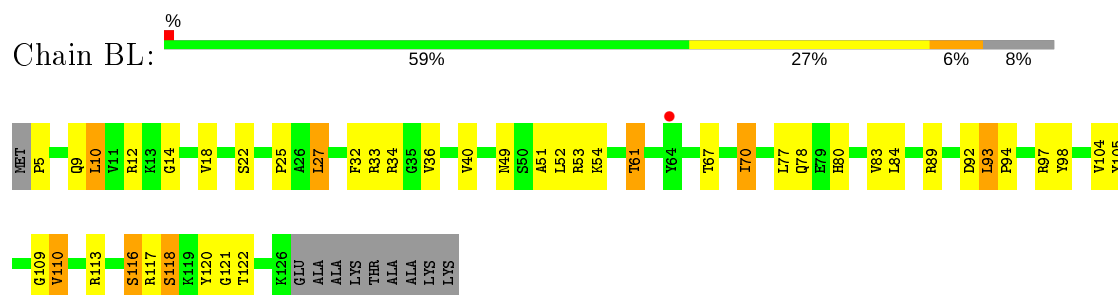
- Molecule 44: 30S ribosomal protein S11



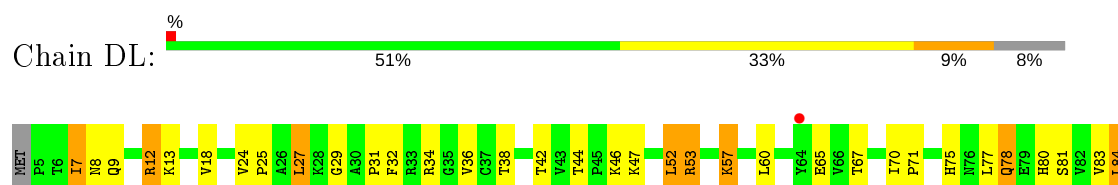
- Molecule 44: 30S ribosomal protein S11



- Molecule 45: 30S ribosomal protein S12



- Molecule 45: 30S ribosomal protein S12

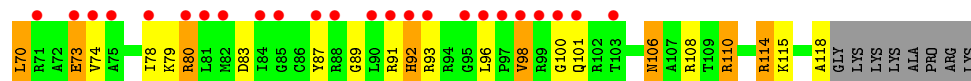
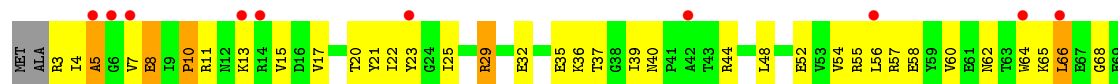




- Molecule 46: 30S ribosomal protein S13



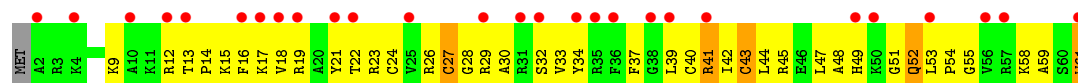
- Molecule 46: 30S ribosomal protein S13



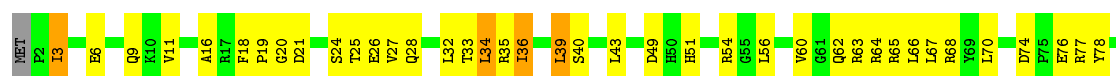
- Molecule 47: 30S ribosomal protein S14 type Z



- Molecule 47: 30S ribosomal protein S14 type Z



- Molecule 48: 30S ribosomal protein S15



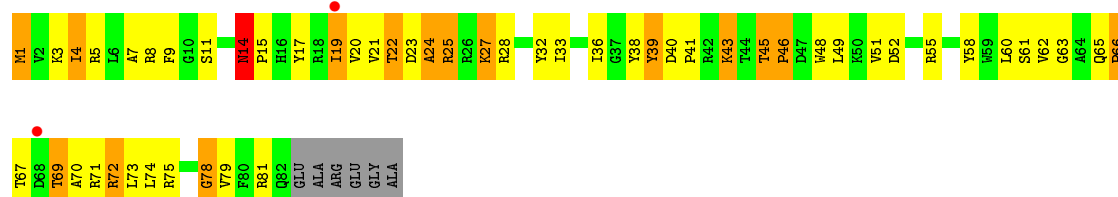
- Molecule 48: 30S ribosomal protein S15

Chain DO: 




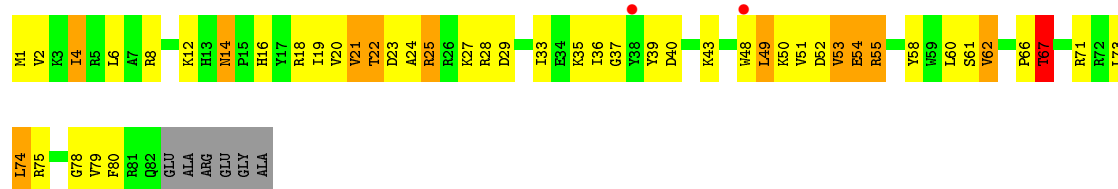
- Molecule 49: 30S ribosomal protein S16

Chain BP: 



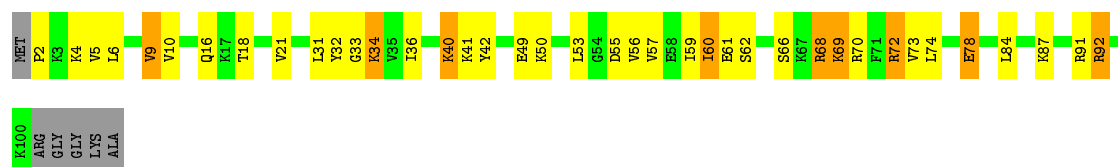
- Molecule 49: 30S ribosomal protein S16

Chain DP: 



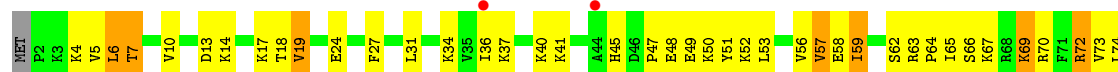
- Molecule 50: 30S ribosomal protein S17

Chain BQ: 

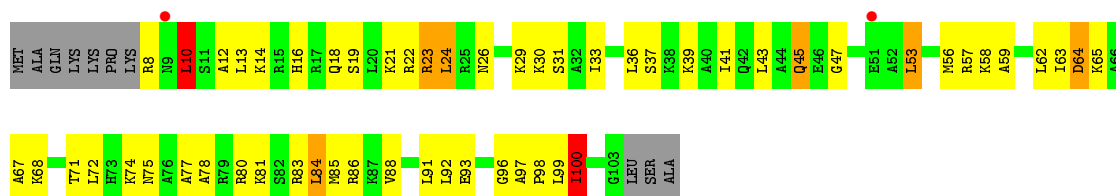


- Molecule 50: 30S ribosomal protein S17

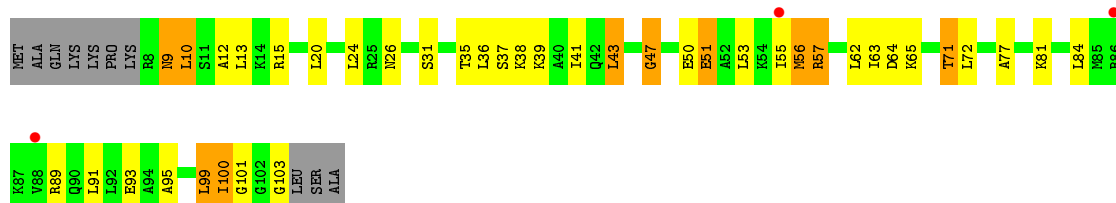
Chain DQ: 







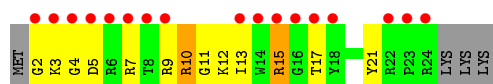
- Molecule 53: 30S ribosomal protein S20



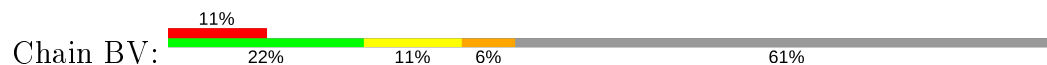
- Molecule 54: 30S ribosomal protein Thx



- Molecule 54: 30S ribosomal protein Thx



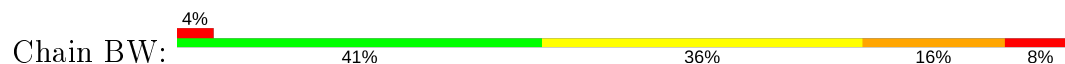
- Molecule 55: mRNA

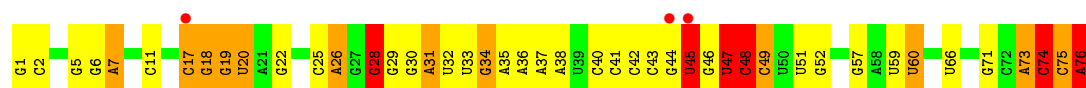


- Molecule 55: mRNA

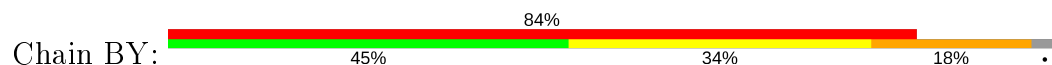


- Molecule 56: P-site tRNA

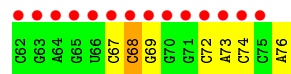
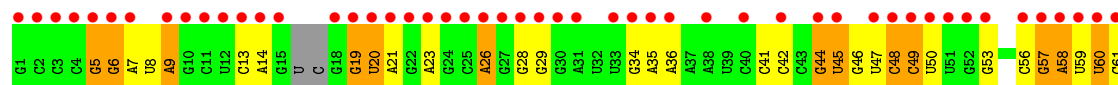




● Molecule 56: P-site tRNA



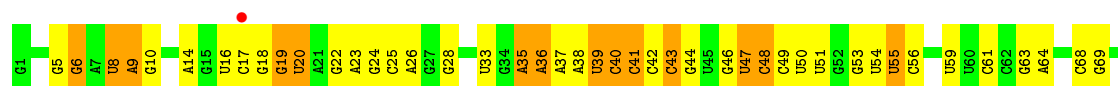
Chain BY:



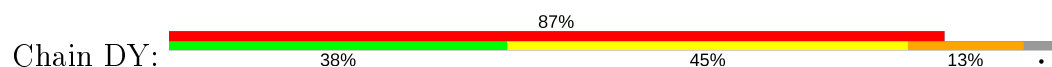
● Molecule 56: P-site tRNA



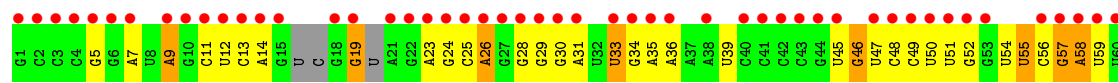
Chain DW:



● Molecule 56: P-site tRNA



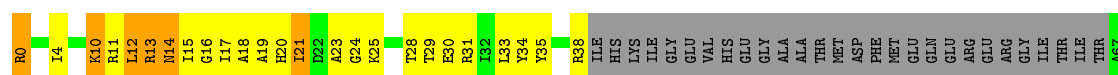
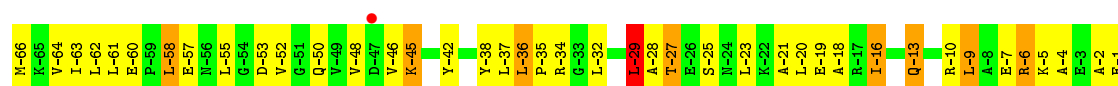
Chain DY:

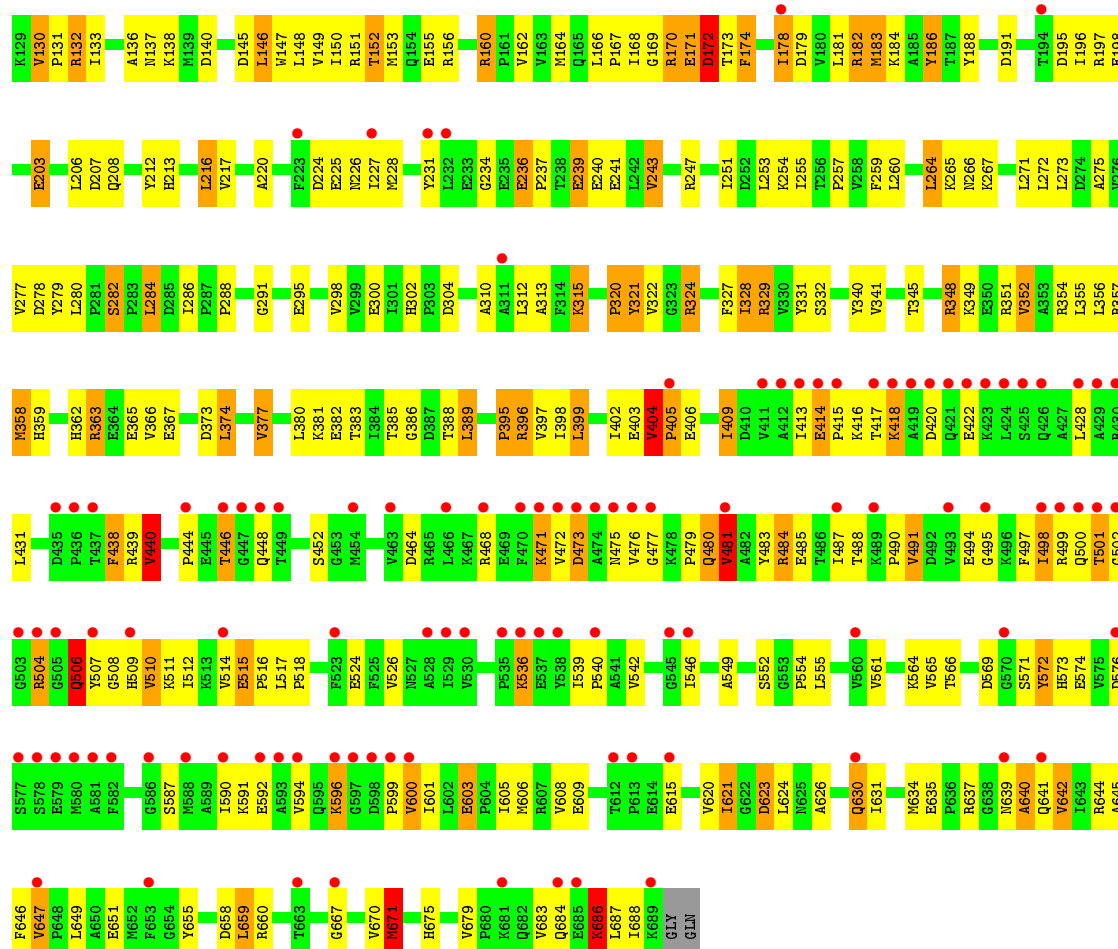


● Molecule 57: 50S ribosomal protein L9,Elongation factor G

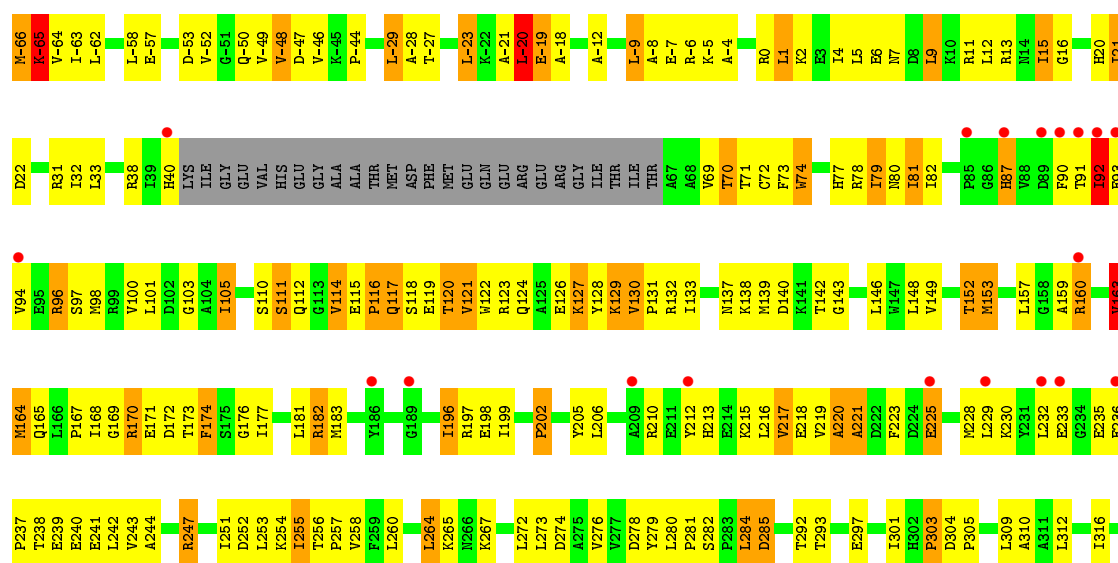


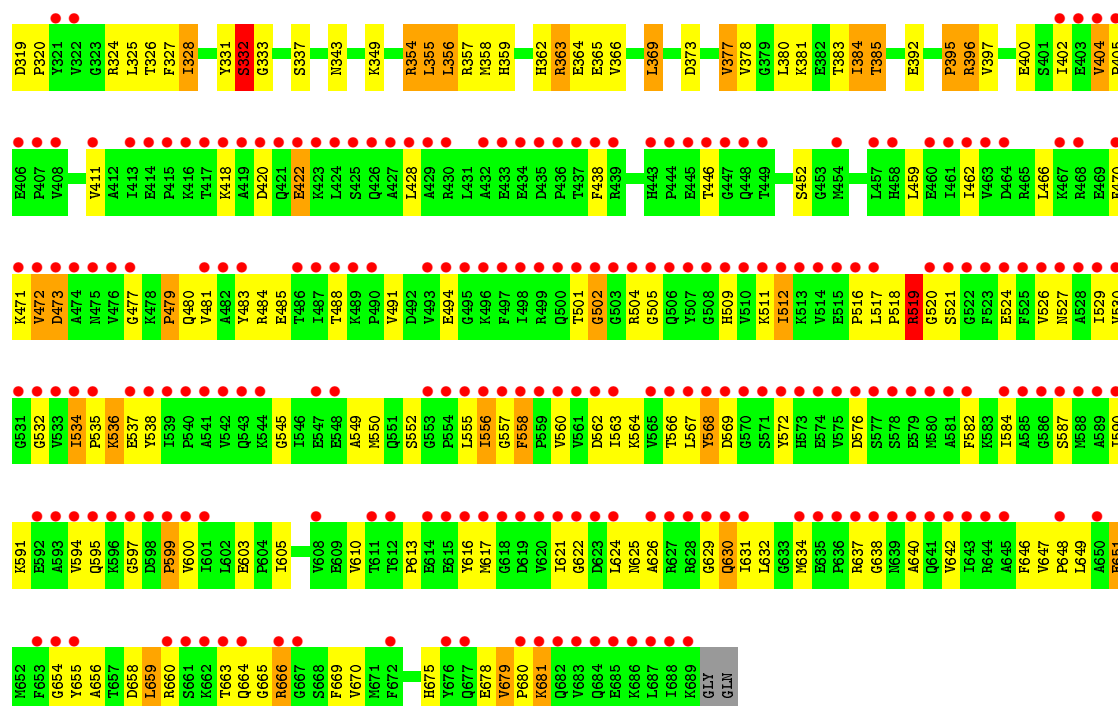
Chain BZ:





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





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	209.84Å 450.58Å 623.43Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.81 – 2.80 49.80 – 2.80	Depositor EDS
% Data completeness (in resolution range)	94.5 (49.81-2.80) 94.5 (49.80-2.80)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.61 (at 2.81Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE: 1.8.2_1309)	Depositor
R, R_{free}	0.209 , 0.264 0.210 , 0.265	Depositor DCC
R_{free} test set	67916 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	56.0	Xtriage
Anisotropy	0.111	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 73.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	310038	wwPDB-VP
Average B, all atoms (Å ²)	79.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.56% 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: 5MU, GDP, ZN, MIA, 7MG, SF4, 2QZ, MG, 2QY, MVA, 004, 4SU, 2R3, 2R1, PSU

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	AA	1.41	444/69281 (0.6%)	2.07	3848/108144 (3.6%)
1	CA	1.00	75/69179 (0.1%)	1.66	1653/107984 (1.5%)
2	AB	1.17	7/2878 (0.2%)	1.92	120/4490 (2.7%)
2	CB	0.66	0/2878	1.33	24/4490 (0.5%)
3	AC	0.34	0/1083	0.65	0/1460
3	CC	0.34	0/1083	0.65	0/1460
4	AD	0.94	2/2186 (0.1%)	1.04	5/2944 (0.2%)
4	CD	0.74	0/2192	0.95	6/2951 (0.2%)
5	AE	0.93	0/1592	1.08	2/2149 (0.1%)
5	CE	0.72	0/1592	0.91	1/2149 (0.0%)
6	AF	0.91	2/1619 (0.1%)	1.01	4/2193 (0.2%)
6	CF	0.63	0/1615	0.83	1/2188 (0.0%)
7	AG	0.60	0/1450	0.83	2/1959 (0.1%)
7	CG	0.36	0/1449	0.62	0/1958
8	AH	0.84	0/1356	0.96	1/1834 (0.1%)
8	CH	0.49	0/1356	0.67	0/1834
9	AK	0.34	0/640	0.67	0/889
9	CK	0.28	0/640	0.61	0/889
10	AL	0.31	0/503	0.54	0/673
10	CL	0.34	0/503	0.60	0/673
11	AN	0.95	0/1144	1.01	3/1543 (0.2%)
11	CN	0.61	0/1144	0.81	0/1543
12	AO	0.91	1/943 (0.1%)	1.02	3/1269 (0.2%)
12	CO	0.77	0/943	0.87	0/1269
13	AP	0.85	0/1156	1.03	4/1537 (0.3%)
13	CP	0.57	0/1152	0.87	2/1533 (0.1%)
14	AQ	0.91	0/1143	0.97	2/1527 (0.1%)
14	CQ	0.64	0/1143	0.82	1/1527 (0.1%)
15	AR	0.90	0/982	1.07	4/1312 (0.3%)
15	CR	0.65	0/982	0.88	1/1312 (0.1%)
16	AS	0.76	0/887	0.95	1/1180 (0.1%)
16	CS	0.49	0/880	0.74	0/1172

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	AT	0.89	0/1105	1.02	3/1477 (0.2%)
17	CT	0.65	0/1097	0.89	1/1468 (0.1%)
18	AU	1.11	3/977 (0.3%)	1.05	1/1301 (0.1%)
18	CU	0.69	1/977 (0.1%)	0.79	0/1301
19	AV	0.98	0/782	1.08	2/1049 (0.2%)
19	CV	0.58	0/782	0.79	0/1049
20	AW	1.10	2/897 (0.2%)	1.09	7/1205 (0.6%)
20	CW	0.80	0/897	0.92	0/1205
21	AX	0.96	0/764	0.99	0/1025
21	CX	0.67	0/764	0.83	1/1025 (0.1%)
22	AY	0.88	0/819	0.97	0/1095
22	CY	0.56	0/819	0.72	0/1095
23	AZ	0.72	1/1483 (0.1%)	0.93	4/2017 (0.2%)
23	CZ	0.45	0/1483	0.73	0/2017
24	A0	0.87	0/616	1.05	1/821 (0.1%)
24	C0	0.60	0/616	0.76	0/821
25	A1	0.87	0/762	0.92	0/1014
25	C1	0.67	0/762	0.89	1/1014 (0.1%)
26	A2	0.79	0/590	0.93	1/781 (0.1%)
26	C2	0.59	0/590	0.73	0/781
27	A3	1.01	0/474	1.06	0/635
27	C3	0.57	0/469	0.81	0/630
28	A4	0.50	0/571	0.72	0/768
28	C4	0.35	0/545	0.59	0/737
29	A5	0.99	0/469	1.05	0/635
29	C5	0.76	1/469 (0.2%)	0.86	0/635
30	A6	0.95	0/460	1.03	1/613 (0.2%)
30	C6	0.71	0/456	0.81	1/608 (0.2%)
31	A7	0.99	0/426	1.11	3/561 (0.5%)
31	C7	0.77	0/426	0.99	1/561 (0.2%)
32	A8	0.95	0/525	0.94	0/691
32	C8	0.63	0/525	0.82	0/691
33	A9	0.98	0/310	1.05	0/407
33	C9	0.64	0/310	0.80	0/407
34	BA	0.77	3/35976 (0.0%)	1.42	439/56145 (0.8%)
34	DA	0.68	1/36119 (0.0%)	1.30	238/56370 (0.4%)
35	BB	0.45	0/1881	0.69	1/2542 (0.0%)
35	DB	0.38	0/1860	0.66	0/2518
36	BC	0.40	0/1576	0.61	0/2130
36	DC	0.35	0/1568	0.55	0/2122
37	BD	0.49	0/1689	0.71	0/2267
37	DD	0.51	0/1708	0.73	1/2289 (0.0%)
38	BE	0.60	0/1145	0.79	0/1543

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
38	DE	0.51	0/1149	0.77	0/1548
39	BF	0.50	0/825	0.77	0/1118
39	DF	0.51	0/833	0.72	0/1128
40	BG	0.43	0/1250	0.60	0/1679
40	DG	0.35	0/1254	0.58	0/1683
41	BH	0.55	0/1108	0.76	0/1494
41	DH	0.45	0/1108	0.75	1/1494 (0.1%)
42	BI	0.44	0/1005	0.64	0/1350
42	DI	0.34	0/997	0.56	0/1343
43	BJ	0.39	0/722	0.71	2/982 (0.2%)
43	DJ	0.34	0/727	0.59	0/988
44	BK	0.56	0/848	0.72	0/1149
44	DK	0.48	0/848	0.63	0/1149
45	BL	0.65	0/946	0.79	0/1274
45	DL	0.64	0/946	0.84	1/1274 (0.1%)
46	BM	0.42	0/933	0.67	0/1253
46	DM	0.30	0/917	0.52	0/1234
47	BN	0.45	0/501	0.67	0/664
47	DN	0.33	0/501	0.60	0/664
48	BO	0.57	0/739	0.74	0/985
48	DO	0.50	0/739	0.70	0/985
49	BP	0.55	0/697	0.81	1/939 (0.1%)
49	DP	0.49	0/693	0.72	0/935
50	BQ	0.58	0/836	0.78	0/1117
50	DQ	0.51	0/836	0.72	0/1117
51	BR	0.55	0/560	0.83	0/746
51	DR	0.48	0/560	0.70	0/746
52	BS	0.34	0/676	0.59	0/911
52	DS	0.31	0/661	0.66	0/893
53	BT	0.50	0/730	0.81	0/965
53	DT	0.46	0/733	0.72	0/969
54	BU	0.42	0/203	0.69	0/266
54	DU	0.38	0/203	0.59	0/266
55	BV	0.64	0/165	1.06	0/254
55	DV	0.54	0/137	1.11	0/211
56	BW	0.86	0/1650	1.64	45/2569 (1.8%)
56	BY	0.42	0/1602	0.95	1/2493 (0.0%)
56	DW	0.65	0/1650	1.29	7/2569 (0.3%)
56	DY	0.35	0/1579	0.86	0/2455
57	BZ	0.49	0/5763	0.72	1/7804 (0.0%)
57	DZ	0.45	0/5784	0.69	1/7835 (0.0%)
58	BX	0.67	0/20	0.66	0/23
58	DX	0.70	0/20	1.43	0/23

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
All	All	0.95	543/329767 (0.2%)	1.50	6455/491645 (1.3%)

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
5	AE	0	1
6	AF	0	1
19	AV	0	1
35	BB	0	1
57	DZ	0	1
58	BX	0	1
All	All	0	6

The worst 5 of 543 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	AA	1067	A	N9-C4	-15.28	1.28	1.37
1	AA	354	A	N9-C4	-13.92	1.29	1.37
1	AA	2299	A	N9-C4	-13.50	1.29	1.37
1	AA	1188	A	N9-C4	-13.32	1.29	1.37
1	AA	990	A	N9-C4	-11.81	1.30	1.37

The worst 5 of 6455 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	553	A	N1-C6-N6	26.84	134.71	118.60
1	AA	990	A	N1-C2-N3	21.55	140.07	129.30
1	AA	990	A	C6-C5-N7	-21.18	117.48	132.30
1	AA	354	A	C2-N3-C4	-21.03	100.09	110.60
1	AA	553	A	C6-C5-N7	-20.90	117.67	132.30

There are no chirality outliers.

5 of 6 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
5	AE	74	PRO	Peptide
6	AF	194	MET	Peptide
19	AV	54	GLY	Peptide

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Mol	Chain	Res	Type	Group
35	BB	93	VAL	Peptide
58	BX	3	004	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	61861	0	31172	850	0
1	CA	61771	0	31146	1166	0
2	AB	2573	0	1306	27	0
2	CB	2573	0	1306	57	0
3	AC	1063	0	1091	153	4
3	CC	1063	0	1090	186	17
4	AD	2136	0	2218	84	0
4	CD	2142	0	2229	85	0
5	AE	1559	0	1618	58	0
5	CE	1559	0	1618	76	0
6	AF	1584	0	1625	62	0
6	CF	1580	0	1619	75	0
7	AG	1425	0	1443	64	0
7	CG	1424	0	1434	82	0
8	AH	1330	0	1407	53	0
8	CH	1330	0	1407	54	0
9	AK	641	0	309	15	0
9	CK	641	0	309	9	0
10	AL	498	0	521	20	0
10	CL	498	0	521	29	0
11	AN	1117	0	1184	31	0
11	CN	1117	0	1184	38	0
12	AO	933	0	996	30	0
12	CO	933	0	996	26	0
13	AP	1139	0	1223	44	0
13	CP	1135	0	1212	57	0
14	AQ	1122	0	1179	37	0
14	CQ	1122	0	1179	54	0
15	AR	968	0	1033	32	0
15	CR	968	0	1033	37	0
16	AS	877	0	938	42	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
16	CS	870	0	923	67	0
17	AT	1091	0	1151	48	0
17	CT	1083	0	1136	42	0
18	AU	959	0	1019	29	0
18	CU	959	0	1018	40	0
19	AV	771	0	830	11	0
19	CV	771	0	830	24	0
20	AW	886	0	940	23	0
20	CW	886	0	940	40	0
21	AX	750	0	814	24	0
21	CX	750	0	814	28	0
22	AY	806	0	881	37	0
22	CY	806	0	882	45	0
23	AZ	1451	0	1457	61	0
23	CZ	1451	0	1457	72	0
24	A0	608	0	622	20	0
24	C0	608	0	622	27	0
25	A1	755	0	826	29	0
25	C1	755	0	826	23	0
26	A2	588	0	643	16	0
26	C2	588	0	643	28	0
27	A3	469	0	518	12	0
27	C3	464	0	514	25	0
28	A4	558	0	545	31	0
28	C4	532	0	507	28	0
29	A5	455	0	465	15	0
29	C5	455	0	465	16	0
30	A6	453	0	473	17	0
30	C6	449	0	469	20	0
31	A7	418	0	467	16	0
31	C7	418	0	467	12	0
32	A8	517	0	582	25	0
32	C8	517	0	582	24	0
33	A9	307	0	335	11	0
33	C9	307	0	335	13	0
34	BA	32141	0	16224	681	0
34	DA	32268	0	16287	742	0
35	BB	1846	0	1867	78	0
35	DB	1825	0	1828	101	0
36	BC	1552	0	1546	65	0
36	DC	1544	0	1524	63	0
37	BD	1659	0	1679	68	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
37	DD	1678	0	1719	86	0
38	BE	1129	0	1185	51	0
38	DE	1133	0	1191	69	0
39	BF	812	0	804	29	0
39	DF	820	0	814	37	0
40	BG	1231	0	1238	45	0
40	DG	1235	0	1249	52	0
41	BH	1088	0	1126	53	0
41	DH	1088	0	1126	74	0
42	BI	986	0	995	52	0
42	DI	978	0	966	56	0
43	BJ	709	0	650	32	0
43	DJ	714	0	672	32	0
44	BK	833	0	836	34	0
44	DK	833	0	836	26	0
45	BL	930	0	980	39	0
45	DL	930	0	980	45	0
46	BM	923	0	970	37	0
46	DM	907	0	934	39	0
47	BN	492	0	529	30	0
47	DN	492	0	531	46	0
48	BO	728	0	760	29	0
48	DO	728	0	760	29	0
49	BP	681	0	697	50	0
49	DP	677	0	686	36	0
50	BQ	823	0	891	32	0
50	DQ	823	0	891	35	0
51	BR	555	0	618	24	0
51	DR	555	0	618	30	0
52	BS	661	0	675	36	0
52	DS	646	0	644	34	0
53	BT	728	0	798	36	0
53	DT	731	0	807	27	0
54	BU	199	0	208	7	0
54	DU	199	0	208	9	0
55	BV	148	0	76	3	0
55	DV	123	0	66	1	0
56	BW	1631	0	839	25	0
56	BY	1581	0	805	24	0
56	DW	1631	0	839	33	0
56	DY	1561	0	796	34	0
57	BZ	5663	0	5747	265	17

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
57	DZ	5682	0	5766	236	4
58	BX	93	0	85	14	0
58	DX	93	0	85	15	0
59	A0	5	0	0	0	0
59	A2	1	0	0	0	0
59	A5	1	0	0	0	0
59	A6	2	0	0	0	0
59	A7	1	0	0	0	0
59	A8	1	0	0	0	0
59	A9	1	0	0	0	0
59	AA	832	0	0	0	0
59	AB	23	0	0	0	0
59	AD	10	0	0	0	0
59	AE	5	0	0	0	0
59	AF	6	0	0	0	0
59	AG	2	0	0	0	0
59	AH	1	0	0	0	0
59	AN	3	0	0	0	0
59	AO	1	0	0	0	0
59	AP	3	0	0	0	0
59	AQ	4	0	0	0	0
59	AR	1	0	0	0	0
59	AU	5	0	0	0	0
59	AV	2	0	0	0	0
59	AW	3	0	0	0	0
59	AX	1	0	0	0	0
59	AY	1	0	0	0	0
59	AZ	1	0	0	0	0
59	BA	215	0	0	0	0
59	BB	1	0	0	0	0
59	BD	1	0	0	0	0
59	BE	1	0	0	0	0
59	BF	1	0	0	0	0
59	BK	1	0	0	0	0
59	BL	2	0	0	0	0
59	BM	1	0	0	0	0
59	BN	2	0	0	0	0
59	BS	1	0	0	0	0
59	BT	1	0	0	0	0
59	BW	3	0	0	0	0
59	BZ	1	0	0	0	0
59	C0	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
59	C1	1	0	0	0	0
59	C3	1	0	0	0	0
59	C5	1	0	0	0	0
59	C7	1	0	0	0	0
59	C8	1	0	0	0	0
59	CA	664	0	0	0	0
59	CB	13	0	0	0	0
59	CD	4	0	0	0	0
59	CE	5	0	0	0	0
59	CF	4	0	0	0	0
59	CG	1	0	0	0	0
59	CN	1	0	0	0	0
59	CO	1	0	0	0	0
59	CP	1	0	0	0	0
59	CQ	4	0	0	0	0
59	CR	1	0	0	0	0
59	CU	1	0	0	0	0
59	CV	2	0	0	0	0
59	CW	1	0	0	0	0
59	CX	1	0	0	0	0
59	DA	171	0	0	0	0
59	DD	1	0	0	0	0
59	DE	2	0	0	0	0
59	DF	1	0	0	0	0
59	DJ	1	0	0	0	0
59	DK	1	0	0	0	0
59	DT	1	0	0	0	0
59	DW	3	0	0	0	0
59	DZ	2	0	0	0	0
60	A4	1	0	0	0	0
60	A5	1	0	0	0	0
60	A6	1	0	0	0	0
60	A9	1	0	0	0	0
60	AY	1	0	0	0	0
60	BN	1	0	0	0	0
60	C4	1	0	0	0	0
60	C5	1	0	0	0	0
60	C6	1	0	0	0	0
60	C9	1	0	0	0	0
60	CY	1	0	0	0	0
60	DN	1	0	0	0	0
61	BD	8	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
61	DD	8	0	0	2	0
62	BZ	28	0	12	5	0
62	DZ	28	0	12	7	0
63	A0	6	0	0	0	0
63	A1	2	0	0	0	0
63	A3	2	0	0	0	0
63	A5	3	0	0	0	0
63	A6	1	0	0	0	0
63	A7	2	0	0	1	0
63	A8	10	0	0	1	0
63	A9	1	0	0	0	0
63	AA	1413	0	0	66	0
63	AB	38	0	0	3	0
63	AD	10	0	0	2	0
63	AE	17	0	0	4	0
63	AF	11	0	0	1	0
63	AG	3	0	0	1	0
63	AH	1	0	0	0	0
63	AN	1	0	0	0	0
63	AO	3	0	0	0	0
63	AP	16	0	0	1	0
63	AQ	4	0	0	1	0
63	AR	2	0	0	0	0
63	AS	1	0	0	1	0
63	AT	1	0	0	0	0
63	AU	4	0	0	0	0
63	AV	1	0	0	0	0
63	AW	1	0	0	0	0
63	AX	3	0	0	0	0
63	AZ	1	0	0	0	0
63	BA	213	0	0	19	0
63	BD	1	0	0	0	0
63	BM	1	0	0	0	0
63	BO	1	0	0	0	0
63	BP	1	0	0	0	0
63	BV	1	0	0	0	0
63	BW	1	0	0	0	0
63	BZ	2	0	0	0	0
63	C0	4	0	0	0	0
63	C3	2	0	0	0	0
63	C5	1	0	0	0	0
63	C7	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
63	C8	4	0	0	0	0
63	CA	983	0	0	79	0
63	CB	9	0	0	1	0
63	CD	15	0	0	1	0
63	CE	9	0	0	1	0
63	CF	6	0	0	0	0
63	CN	1	0	0	0	0
63	CO	1	0	0	0	0
63	CP	11	0	0	2	0
63	CQ	2	0	0	1	0
63	CT	3	0	0	0	0
63	CU	2	0	0	0	0
63	CV	1	0	0	1	0
63	CW	1	0	0	0	0
63	CX	1	0	0	0	0
63	CY	2	0	0	1	0
63	DA	157	0	0	13	0
63	DD	1	0	0	0	0
63	DE	2	0	0	2	0
63	DH	1	0	0	0	0
63	DJ	1	0	0	0	0
63	DK	2	0	0	0	0
63	DL	1	0	0	0	0
63	DT	1	0	0	0	0
All	All	310038	0	209219	7358	21

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 7358 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:H5''	3:AC:206:LYS:CG	1.32	1.59
1:AA:1891:G:C5'	3:AC:206:LYS:HD2	1.36	1.52
1:CA:2128:C:H5''	3:CC:219:MET:CE	1.36	1.51
1:CA:2132:U:C4	3:CC:6:LYS:HE3	1.51	1.41
1:AA:1891:G:C5'	3:AC:206:LYS:CD	2.01	1.37

The worst 5 of 21 symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
57:BZ:502:GLY:CA	3:CC:9:ARG:CD[2_655]	1.16	1.04
3:AC:9:ARG:NH2	57:DZ:504:ARG:NH1[3_654]	1.36	0.84
57:BZ:502:GLY:N	3:CC:9:ARG:CB[2_655]	1.54	0.66
57:BZ:502:GLY:N	3:CC:9:ARG:CD[2_655]	1.69	0.51
57:BZ:573:HIS:CE1	3:CC:13:GLU:OE1[2_655]	1.71	0.49

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	AC	133/228 (58%)	90 (68%)	25 (19%)	18 (14%)	0	0
3	CC	133/228 (58%)	90 (68%)	25 (19%)	18 (14%)	0	0
4	AD	273/276 (99%)	249 (91%)	19 (7%)	5 (2%)	8	28
4	CD	273/276 (99%)	234 (86%)	26 (10%)	13 (5%)	2	7
5	AE	202/206 (98%)	186 (92%)	14 (7%)	2 (1%)	15	44
5	CE	202/206 (98%)	179 (89%)	20 (10%)	3 (2%)	10	33
6	AF	201/210 (96%)	182 (90%)	18 (9%)	1 (0%)	29	61
6	CF	201/210 (96%)	177 (88%)	17 (8%)	7 (4%)	3	12
7	AG	179/182 (98%)	154 (86%)	19 (11%)	6 (3%)	3	13
7	CG	179/182 (98%)	141 (79%)	31 (17%)	7 (4%)	3	10
8	AH	172/180 (96%)	154 (90%)	15 (9%)	3 (2%)	9	29
8	CH	172/180 (96%)	144 (84%)	17 (10%)	11 (6%)	1	3
9	AK	128/173 (74%)	66 (52%)	36 (28%)	26 (20%)	0	0
9	CK	128/173 (74%)	76 (59%)	27 (21%)	25 (20%)	0	0
10	AL	64/147 (44%)	43 (67%)	17 (27%)	4 (6%)	1	3
10	CL	64/147 (44%)	42 (66%)	19 (30%)	3 (5%)	2	7
11	AN	138/140 (99%)	129 (94%)	8 (6%)	1 (1%)	22	53
11	CN	138/140 (99%)	120 (87%)	15 (11%)	3 (2%)	6	22

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
12	AO	120/122 (98%)	113 (94%)	7 (6%)	0	100	100
12	CO	120/122 (98%)	107 (89%)	10 (8%)	3 (2%)	5	19
13	AP	147/150 (98%)	130 (88%)	15 (10%)	2 (1%)	11	34
13	CP	147/150 (98%)	119 (81%)	25 (17%)	3 (2%)	7	24
14	AQ	139/141 (99%)	126 (91%)	12 (9%)	1 (1%)	22	53
14	CQ	139/141 (99%)	123 (88%)	14 (10%)	2 (1%)	11	34
15	AR	116/118 (98%)	106 (91%)	10 (9%)	0	100	100
15	CR	116/118 (98%)	102 (88%)	11 (10%)	3 (3%)	5	18
16	AS	108/112 (96%)	88 (82%)	16 (15%)	4 (4%)	3	11
16	CS	108/112 (96%)	83 (77%)	20 (18%)	5 (5%)	2	7
17	AT	129/146 (88%)	114 (88%)	13 (10%)	2 (2%)	9	31
17	CT	129/146 (88%)	116 (90%)	11 (8%)	2 (2%)	9	31
18	AU	114/118 (97%)	111 (97%)	3 (3%)	0	100	100
18	CU	114/118 (97%)	100 (88%)	11 (10%)	3 (3%)	5	18
19	AV	99/101 (98%)	95 (96%)	3 (3%)	1 (1%)	15	44
19	CV	99/101 (98%)	86 (87%)	10 (10%)	3 (3%)	4	15
20	AW	110/113 (97%)	104 (94%)	6 (6%)	0	100	100
20	CW	110/113 (97%)	105 (96%)	5 (4%)	0	100	100
21	AX	93/96 (97%)	85 (91%)	6 (6%)	2 (2%)	6	22
21	CX	93/96 (97%)	77 (83%)	11 (12%)	5 (5%)	2	5
22	AY	105/110 (96%)	93 (89%)	9 (9%)	3 (3%)	4	15
22	CY	105/110 (96%)	86 (82%)	14 (13%)	5 (5%)	2	7
23	AZ	183/206 (89%)	147 (80%)	24 (13%)	12 (7%)	1	3
23	CZ	183/206 (89%)	134 (73%)	33 (18%)	16 (9%)	1	1
24	A0	75/85 (88%)	70 (93%)	5 (7%)	0	100	100
24	C0	75/85 (88%)	67 (89%)	7 (9%)	1 (1%)	12	36
25	A1	95/98 (97%)	90 (95%)	5 (5%)	0	100	100
25	C1	95/98 (97%)	85 (90%)	7 (7%)	3 (3%)	4	13
26	A2	68/72 (94%)	62 (91%)	6 (9%)	0	100	100
26	C2	68/72 (94%)	60 (88%)	7 (10%)	1 (2%)	10	33
27	A3	57/60 (95%)	51 (90%)	6 (10%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
27	C3	57/60 (95%)	50 (88%)	5 (9%)	2 (4%)	3	12
28	A4	67/71 (94%)	46 (69%)	12 (18%)	9 (13%)	0	0
28	C4	67/71 (94%)	43 (64%)	15 (22%)	9 (13%)	0	0
29	A5	57/60 (95%)	51 (90%)	6 (10%)	0	100	100
29	C5	57/60 (95%)	53 (93%)	3 (5%)	1 (2%)	8	28
30	A6	51/54 (94%)	49 (96%)	2 (4%)	0	100	100
30	C6	51/54 (94%)	42 (82%)	8 (16%)	1 (2%)	7	24
31	A7	46/49 (94%)	45 (98%)	1 (2%)	0	100	100
31	C7	46/49 (94%)	41 (89%)	4 (9%)	1 (2%)	6	22
32	A8	62/65 (95%)	60 (97%)	1 (2%)	1 (2%)	9	31
32	C8	62/65 (95%)	54 (87%)	7 (11%)	1 (2%)	9	31
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%)	182 (80%)	33 (14%)	14 (6%)	1	4
35	DB	229/256 (90%)	170 (74%)	41 (18%)	18 (8%)	1	2
36	BC	204/239 (85%)	155 (76%)	38 (19%)	11 (5%)	2	5
36	DC	204/239 (85%)	169 (83%)	29 (14%)	6 (3%)	4	15
37	BD	206/209 (99%)	166 (81%)	28 (14%)	12 (6%)	1	4
37	DD	206/209 (99%)	171 (83%)	27 (13%)	8 (4%)	3	10
38	BE	146/162 (90%)	114 (78%)	24 (16%)	8 (6%)	2	5
38	DE	146/162 (90%)	117 (80%)	22 (15%)	7 (5%)	2	7
39	BF	98/101 (97%)	84 (86%)	11 (11%)	3 (3%)	4	14
39	DF	98/101 (97%)	90 (92%)	5 (5%)	3 (3%)	4	14
40	BG	153/156 (98%)	128 (84%)	13 (8%)	12 (8%)	1	2
40	DG	153/156 (98%)	126 (82%)	22 (14%)	5 (3%)	4	13
41	BH	135/138 (98%)	110 (82%)	22 (16%)	3 (2%)	6	22
41	DH	135/138 (98%)	114 (84%)	14 (10%)	7 (5%)	2	6
42	BI	125/128 (98%)	103 (82%)	15 (12%)	7 (6%)	2	5
42	DI	125/128 (98%)	100 (80%)	21 (17%)	4 (3%)	4	13
43	BJ	95/105 (90%)	76 (80%)	12 (13%)	7 (7%)	1	2
43	DJ	94/105 (90%)	75 (80%)	16 (17%)	3 (3%)	4	13

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
44	BK	112/129 (87%)	96 (86%)	14 (12%)	2 (2%)	8	28
44	DK	112/129 (87%)	92 (82%)	16 (14%)	4 (4%)	3	11
45	BL	120/132 (91%)	108 (90%)	11 (9%)	1 (1%)	19	49
45	DL	120/132 (91%)	100 (83%)	16 (13%)	4 (3%)	4	13
46	BM	115/126 (91%)	93 (81%)	18 (16%)	4 (4%)	3	12
46	DM	114/126 (90%)	88 (77%)	17 (15%)	9 (8%)	1	2
47	BN	58/61 (95%)	46 (79%)	9 (16%)	3 (5%)	2	6
47	DN	58/61 (95%)	49 (84%)	7 (12%)	2 (3%)	3	13
48	BO	86/89 (97%)	67 (78%)	16 (19%)	3 (4%)	3	12
48	DO	86/89 (97%)	72 (84%)	10 (12%)	4 (5%)	2	7
49	BP	80/88 (91%)	54 (68%)	17 (21%)	9 (11%)	0	1
49	DP	80/88 (91%)	58 (72%)	18 (22%)	4 (5%)	2	6
50	BQ	97/105 (92%)	87 (90%)	7 (7%)	3 (3%)	4	14
50	DQ	97/105 (92%)	87 (90%)	10 (10%)	0	100	100
51	BR	66/88 (75%)	57 (86%)	7 (11%)	2 (3%)	4	15
51	DR	66/88 (75%)	60 (91%)	6 (9%)	0	100	100
52	BS	82/93 (88%)	64 (78%)	14 (17%)	4 (5%)	2	7
52	DS	81/93 (87%)	63 (78%)	15 (18%)	3 (4%)	3	11
53	BT	94/106 (89%)	78 (83%)	12 (13%)	4 (4%)	2	8
53	DT	94/106 (89%)	75 (80%)	13 (14%)	6 (6%)	1	3
54	BU	21/27 (78%)	20 (95%)	1 (5%)	0	100	100
54	DU	21/27 (78%)	17 (81%)	2 (10%)	2 (10%)	0	1
57	BZ	722/758 (95%)	563 (78%)	107 (15%)	52 (7%)	1	2
57	DZ	726/758 (96%)	537 (74%)	132 (18%)	57 (8%)	1	2
58	BX	3/10 (30%)	1 (33%)	0	2 (67%)	0	0
58	DX	3/10 (30%)	0	2 (67%)	1 (33%)	0	0
All	All	13227/14464 (91%)	10975 (83%)	1666 (13%)	586 (4%)	2	8

5 of 586 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	AC	42	VAL
3	AC	47	LYS

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Mol	Chain	Res	Type
3	AC	68	GLY
3	AC	180	SER
3	AC	181	PHE

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	AC	111/180 (62%)	103 (93%)	8 (7%)	14	38
3	CC	111/180 (62%)	103 (93%)	8 (7%)	14	38
4	AD	215/218 (99%)	173 (80%)	42 (20%)	1	4
4	CD	216/218 (99%)	178 (82%)	38 (18%)	2	5
5	AE	164/166 (99%)	138 (84%)	26 (16%)	2	7
5	CE	164/166 (99%)	137 (84%)	27 (16%)	2	7
6	AF	160/166 (96%)	132 (82%)	28 (18%)	2	6
6	CF	159/166 (96%)	126 (79%)	33 (21%)	1	3
7	AG	143/156 (92%)	115 (80%)	28 (20%)	1	4
7	CG	142/156 (91%)	114 (80%)	28 (20%)	1	4
8	AH	144/148 (97%)	120 (83%)	24 (17%)	2	6
8	CH	144/148 (97%)	118 (82%)	26 (18%)	1	5
10	AL	50/111 (45%)	39 (78%)	11 (22%)	1	2
10	CL	50/111 (45%)	35 (70%)	15 (30%)	0	1
11	AN	118/119 (99%)	93 (79%)	25 (21%)	1	3
11	CN	118/119 (99%)	85 (72%)	33 (28%)	0	1
12	AO	100/100 (100%)	87 (87%)	13 (13%)	4	13
12	CO	100/100 (100%)	86 (86%)	14 (14%)	3	11
13	AP	116/116 (100%)	97 (84%)	19 (16%)	2	7
13	CP	115/116 (99%)	95 (83%)	20 (17%)	2	6
14	AQ	111/111 (100%)	94 (85%)	17 (15%)	2	8

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
14	CQ	111/111 (100%)	83 (75%)	28 (25%)	0	1
15	AR	101/101 (100%)	80 (79%)	21 (21%)	1	3
15	CR	101/101 (100%)	87 (86%)	14 (14%)	3	11
16	AS	87/88 (99%)	71 (82%)	16 (18%)	1	5
16	CS	85/88 (97%)	68 (80%)	17 (20%)	1	4
17	AT	115/127 (91%)	96 (84%)	19 (16%)	2	7
17	CT	113/127 (89%)	98 (87%)	15 (13%)	4	12
18	AU	93/94 (99%)	77 (83%)	16 (17%)	2	6
18	CU	93/94 (99%)	81 (87%)	12 (13%)	4	13
19	AV	80/82 (98%)	67 (84%)	13 (16%)	2	7
19	CV	80/82 (98%)	65 (81%)	15 (19%)	1	5
20	AW	90/92 (98%)	76 (84%)	14 (16%)	2	8
20	CW	90/92 (98%)	75 (83%)	15 (17%)	2	6
21	AX	77/78 (99%)	67 (87%)	10 (13%)	4	13
21	CX	77/78 (99%)	66 (86%)	11 (14%)	3	10
22	AY	85/91 (93%)	66 (78%)	19 (22%)	1	2
22	CY	85/91 (93%)	66 (78%)	19 (22%)	1	2
23	AZ	156/179 (87%)	120 (77%)	36 (23%)	1	2
23	CZ	156/179 (87%)	125 (80%)	31 (20%)	1	4
24	A0	61/67 (91%)	55 (90%)	6 (10%)	8	24
24	C0	61/67 (91%)	50 (82%)	11 (18%)	1	5
25	A1	80/83 (96%)	66 (82%)	14 (18%)	2	6
25	C1	80/83 (96%)	66 (82%)	14 (18%)	2	6
26	A2	65/67 (97%)	56 (86%)	9 (14%)	3	11
26	C2	65/67 (97%)	51 (78%)	14 (22%)	1	3
27	A3	51/52 (98%)	41 (80%)	10 (20%)	1	4
27	C3	50/52 (96%)	38 (76%)	12 (24%)	0	2
28	A4	60/63 (95%)	52 (87%)	8 (13%)	4	12
28	C4	53/63 (84%)	39 (74%)	14 (26%)	0	1
29	A5	50/52 (96%)	43 (86%)	7 (14%)	3	11
29	C5	50/52 (96%)	42 (84%)	8 (16%)	2	7

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
30	A6	51/52 (98%)	37 (72%)	14 (28%)	0	1
30	C6	50/52 (96%)	43 (86%)	7 (14%)	3	11
31	A7	41/42 (98%)	35 (85%)	6 (15%)	3	9
31	C7	41/42 (98%)	35 (85%)	6 (15%)	3	9
32	A8	54/55 (98%)	43 (80%)	11 (20%)	1	4
32	C8	54/55 (98%)	48 (89%)	6 (11%)	6	19
33	A9	34/34 (100%)	30 (88%)	4 (12%)	5	16
33	C9	34/34 (100%)	30 (88%)	4 (12%)	5	16
35	BB	192/220 (87%)	157 (82%)	35 (18%)	1	5
35	DB	187/220 (85%)	148 (79%)	39 (21%)	1	3
36	BC	143/188 (76%)	127 (89%)	16 (11%)	6	18
36	DC	141/188 (75%)	113 (80%)	28 (20%)	1	4
37	BD	170/181 (94%)	136 (80%)	34 (20%)	1	4
37	DD	174/181 (96%)	143 (82%)	31 (18%)	2	5
38	BE	113/123 (92%)	86 (76%)	27 (24%)	0	2
38	DE	114/123 (93%)	82 (72%)	32 (28%)	0	1
39	BF	84/90 (93%)	70 (83%)	14 (17%)	2	6
39	DF	86/90 (96%)	74 (86%)	12 (14%)	3	11
40	BG	119/127 (94%)	99 (83%)	20 (17%)	2	6
40	DG	120/127 (94%)	104 (87%)	16 (13%)	4	12
41	BH	114/119 (96%)	90 (79%)	24 (21%)	1	3
41	DH	114/119 (96%)	86 (75%)	28 (25%)	0	2
42	BI	91/99 (92%)	78 (86%)	13 (14%)	3	10
42	DI	89/99 (90%)	73 (82%)	16 (18%)	1	5
43	BJ	66/92 (72%)	58 (88%)	8 (12%)	5	15
43	DJ	69/92 (75%)	58 (84%)	11 (16%)	2	7
44	BK	83/99 (84%)	65 (78%)	18 (22%)	1	3
44	DK	83/99 (84%)	64 (77%)	19 (23%)	1	2
45	BL	97/109 (89%)	83 (86%)	14 (14%)	3	10
45	DL	97/109 (89%)	74 (76%)	23 (24%)	1	2
46	BM	91/101 (90%)	80 (88%)	11 (12%)	5	15

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
46	DM	88/101 (87%)	75 (85%)	13 (15%)	3	9
47	BN	49/50 (98%)	38 (78%)	11 (22%)	1	2
47	DN	49/50 (98%)	42 (86%)	7 (14%)	3	10
48	BO	78/80 (98%)	70 (90%)	8 (10%)	7	21
48	DO	78/80 (98%)	66 (85%)	12 (15%)	2	8
49	BP	69/74 (93%)	54 (78%)	15 (22%)	1	3
49	DP	68/74 (92%)	51 (75%)	17 (25%)	0	2
50	BQ	94/97 (97%)	82 (87%)	12 (13%)	4	13
50	DQ	94/97 (97%)	80 (85%)	14 (15%)	3	9
51	BR	59/77 (77%)	49 (83%)	10 (17%)	2	6
51	DR	59/77 (77%)	52 (88%)	7 (12%)	5	16
52	BS	70/80 (88%)	59 (84%)	11 (16%)	2	8
52	DS	67/80 (84%)	55 (82%)	12 (18%)	2	5
53	BT	70/82 (85%)	53 (76%)	17 (24%)	0	2
53	DT	71/82 (87%)	59 (83%)	12 (17%)	2	6
54	BU	18/22 (82%)	17 (94%)	1 (6%)	21	51
54	DU	18/22 (82%)	16 (89%)	2 (11%)	6	19
57	BZ	604/636 (95%)	477 (79%)	127 (21%)	1	3
57	DZ	607/636 (95%)	509 (84%)	98 (16%)	2	7
58	BX	3/3 (100%)	3 (100%)	0	100	100
58	DX	3/3 (100%)	3 (100%)	0	100	100
All	All	10664/11678 (91%)	8760 (82%)	1904 (18%)	2	5

5 of 1904 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
57	BZ	186	TYR
7	CG	136	ARG
50	DQ	6	LEU
57	BZ	354	ARG
4	CD	113	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 172 such sidechains are listed below:

Mol	Chain	Res	Type
57	BZ	573	HIS
13	CP	38	GLN
48	DO	28	GLN
3	CC	67	HIS
6	CF	203	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	AA	2865/2915 (98%)	526 (18%)	51 (1%)
1	CA	2860/2915 (98%)	611 (21%)	39 (1%)
2	AB	119/121 (98%)	15 (12%)	0
2	CB	119/121 (98%)	27 (22%)	0
34	BA	1491/1521 (98%)	331 (22%)	20 (1%)
34	DA	1498/1521 (98%)	350 (23%)	22 (1%)
55	BV	6/18 (33%)	2 (33%)	0
55	DV	5/18 (27%)	1 (20%)	0
56	BW	74/76 (97%)	16 (21%)	1 (1%)
56	BY	71/76 (93%)	23 (32%)	2 (2%)
56	DW	74/76 (97%)	23 (31%)	2 (2%)
56	DY	69/76 (90%)	21 (30%)	1 (1%)
All	All	9251/9454 (97%)	1946 (21%)	138 (1%)

5 of 1946 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	AA	12	U
1	AA	13	A
1	AA	15	G
1	AA	34	C
1	AA	45	C

5 of 138 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
34	BA	991	U
1	CA	249	C
34	DA	991	U
34	BA	1067	A
34	BA	1530	G

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

42 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$
58	2QZ	BX	1	58	7,8,9	0.76	0	8,10,12	4.49	5 (62%)
56	7MG	DY	46	56	22,26,27	1.75	4 (18%)	28,39,42	2.94	11 (39%)
58	MVA	DX	9	58	6,7,8	1.13	1 (16%)	7,8,10	1.45	1 (14%)
56	MIA	DY	37	56	18,24,32	1.10	2 (11%)	18,35,47	1.31	2 (11%)
56	PSU	BY	39	56	17,21,22	1.44	2 (11%)	20,30,33	3.23	6 (30%)
58	004	BX	3	58	9,10,11	1.28	1 (11%)	9,12,14	2.45	2 (22%)
56	MIA	BW	37	56	24,31,32	2.37	5 (20%)	26,44,47	2.38	9 (34%)
56	5MU	BY	54	56	15,22,23	1.06	1 (6%)	16,32,35	1.86	1 (6%)
56	7MG	BW	46	56	22,26,27	1.65	4 (18%)	28,39,42	2.96	8 (28%)
58	004	DX	3	58	9,10,11	1.30	1 (11%)	9,12,14	1.10	0
58	2QZ	DX	1	58	7,8,9	0.51	0	8,10,12	4.28	3 (37%)
58	2R1	DX	6	58	10,10,11	1.62	2 (20%)	6,13,15	2.53	3 (50%)
56	PSU	BW	39	56	17,21,22	1.60	3 (17%)	20,30,33	3.04	6 (30%)
56	PSU	DY	39	56	17,21,22	1.54	3 (17%)	20,30,33	3.28	6 (30%)
56	PSU	DW	39	56	17,21,22	1.44	2 (11%)	20,30,33	3.76	8 (40%)
56	5MU	DY	54	56	15,22,23	1.08	1 (6%)	16,32,35	1.89	2 (12%)
56	PSU	DY	32	56	17,21,22	1.40	2 (11%)	20,30,33	3.16	6 (30%)
56	PSU	BW	55	56	17,21,22	1.48	2 (11%)	20,30,33	3.26	6 (30%)
58	2R3	DX	8	58	12,14,15	0.58	0	16,18,20	1.76	5 (31%)
56	7MG	DW	46	56	22,26,27	1.67	4 (18%)	28,39,42	2.81	10 (35%)
58	2QY	DX	10	58	12,13,14	1.86	1 (8%)	13,16,18	3.06	5 (38%)
56	5MU	DW	54	56	15,22,23	1.17	1 (6%)	16,32,35	1.85	2 (12%)
56	4SU	DW	8	56	14,21,22	1.39	1 (7%)	15,30,33	1.39	2 (13%)
56	4SU	BW	8	56	14,21,22	1.20	1 (7%)	15,30,33	1.49	2 (13%)
56	MIA	DW	37	56	24,31,32	2.19	4 (16%)	26,44,47	2.29	9 (34%)
56	PSU	BY	32	56	17,21,22	1.38	2 (11%)	20,30,33	3.12	5 (25%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
56	PSU	BW	32	56	17,21,22	1.60	3 (17%)	20,30,33	3.54	7 (35%)
56	PSU	DW	55	56	17,21,22	1.51	2 (11%)	20,30,33	3.28	8 (40%)
56	7MG	BY	46	56	22,26,27	1.77	4 (18%)	28,39,42	2.80	9 (32%)
58	MVA	BX	5	58	6,7,8	0.51	0	7,8,10	1.35	1 (14%)
56	PSU	BY	55	56	17,21,22	1.46	3 (17%)	20,30,33	3.13	6 (30%)
58	2R3	BX	8	58	12,14,15	0.67	0	16,18,20	2.12	7 (43%)
56	5MU	BW	54	56	15,22,23	1.20	1 (6%)	16,32,35	2.18	1 (6%)
56	4SU	BY	8	56	14,21,22	1.20	1 (7%)	15,30,33	1.66	3 (20%)
56	PSU	DY	55	56	17,21,22	1.55	4 (23%)	20,30,33	3.12	6 (30%)
58	MVA	DX	5	58	6,7,8	1.04	0	7,8,10	1.44	1 (14%)
56	4SU	DY	8	56	14,21,22	1.30	1 (7%)	15,30,33	1.52	2 (13%)
58	2QY	BX	10	58	12,13,14	1.87	1 (8%)	13,16,18	3.61	5 (38%)
58	2R1	BX	6	58	10,10,11	1.99	3 (30%)	6,13,15	4.42	2 (33%)
58	MVA	BX	9	58	6,7,8	0.76	0	7,8,10	1.41	0
56	PSU	DW	32	56	17,21,22	1.31	1 (5%)	20,30,33	3.21	7 (35%)
56	MIA	BY	37	56	18,24,32	1.19	2 (11%)	18,35,47	1.37	3 (16%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
58	2QZ	BX	1	58	-	2/6/10/12	-
56	7MG	DY	46	56	-	2/7/37/38	0/3/3/3
58	MVA	DX	9	58	-	4/6/8/10	-
56	MIA	DY	37	56	-	3/3/25/34	0/3/3/3
56	PSU	BY	39	56	-	0/7/25/26	0/2/2/2
58	004	BX	3	58	-	0/4/6/8	0/1/1/1
56	MIA	BW	37	56	-	5/11/33/34	0/3/3/3
56	5MU	BY	54	56	-	3/5/25/26	0/2/2/2
56	7MG	BW	46	56	-	1/7/37/38	0/3/3/3
58	004	DX	3	58	-	0/4/6/8	0/1/1/1
58	2QZ	DX	1	58	-	2/6/10/12	-
58	2R1	DX	6	58	-	2/2/14/16	0/1/1/1
56	PSU	BW	39	56	-	0/7/25/26	0/2/2/2
56	PSU	DY	39	56	-	2/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
56	PSU	DW	39	56	-	1/7/25/26	0/2/2/2
56	5MU	DY	54	56	-	2/5/25/26	0/2/2/2
56	PSU	DY	32	56	-	0/7/25/26	0/2/2/2
56	PSU	BW	55	56	-	0/7/25/26	0/2/2/2
58	2R3	DX	8	58	-	6/11/12/14	0/1/1/1
56	7MG	DW	46	56	-	5/7/37/38	0/3/3/3
58	2QY	DX	10	58	-	3/4/8/10	0/1/1/1
56	5MU	DW	54	56	-	0/5/25/26	0/2/2/2
56	4SU	DW	8	56	-	0/5/25/26	0/2/2/2
56	4SU	BW	8	56	-	0/5/25/26	0/2/2/2
56	MIA	DW	37	56	-	7/11/33/34	0/3/3/3
56	PSU	BY	32	56	-	0/7/25/26	0/2/2/2
56	PSU	BW	32	56	-	2/7/25/26	0/2/2/2
56	PSU	DW	55	56	-	0/7/25/26	0/2/2/2
56	7MG	BY	46	56	-	5/7/37/38	0/3/3/3
58	MVA	BX	5	58	-	4/6/8/10	-
56	PSU	BY	55	56	-	0/7/25/26	0/2/2/2
58	2R3	BX	8	58	-	6/11/12/14	0/1/1/1
56	5MU	BW	54	56	-	0/5/25/26	0/2/2/2
56	4SU	BY	8	56	-	1/5/25/26	0/2/2/2
56	PSU	DY	55	56	-	5/7/25/26	0/2/2/2
58	MVA	DX	5	58	-	4/6/8/10	-
56	4SU	DY	8	56	-	1/5/25/26	0/2/2/2
58	2QY	BX	10	58	-	3/4/8/10	0/1/1/1
58	2R1	BX	6	58	-	1/2/14/16	0/1/1/1
58	MVA	BX	9	58	-	2/6/8/10	-
56	PSU	DW	32	56	-	2/7/25/26	0/2/2/2
56	MIA	BY	37	56	-	2/3/25/34	0/3/3/3

The worst 5 of 76 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
56	BW	37	MIA	C13-C14	7.83	1.54	1.32
56	DW	37	MIA	C13-C14	7.42	1.53	1.32
56	BW	37	MIA	C2-S10	-6.89	1.69	1.75
58	DX	10	2QY	C-CA	6.02	1.52	1.43
58	BX	10	2QY	C-CA	5.64	1.51	1.43

The worst 5 of 193 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
58	BX	1	2QZ	OG1-CB-CG2	11.55	143.95	109.74
58	DX	1	2QZ	OG1-CB-CG2	11.24	143.03	109.74
58	BX	10	2QY	CN-N-CA	-10.66	107.25	123.45
56	BW	32	PSU	N1-C2-N3	-10.54	120.05	128.43
56	BW	46	7MG	N3-C4-N9	9.90	139.62	126.91

There are no chirality outliers.

5 of 88 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
58	BX	1	2QZ	N-CA-CB-OG1
56	DY	46	7MG	O4'-C4'-C5'-O5'
58	DX	9	MVA	N-CA-CB-CG1
58	DX	9	MVA	N-CA-CB-CG2
58	DX	9	MVA	C-CA-CB-CG2

There are no ring outliers.

23 monomers are involved in 48 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
56	DY	46	7MG	2	0
58	DX	9	MVA	4	0
58	BX	3	004	4	0
56	BW	37	MIA	2	0
58	DX	3	004	1	0
58	DX	1	2QZ	2	0
58	DX	6	2R1	2	0
56	DW	39	PSU	6	0
58	DX	8	2R3	2	0
58	DX	10	2QY	9	0
56	DW	54	5MU	1	0
56	DW	8	4SU	1	0
56	DW	37	MIA	2	0
56	BW	32	PSU	1	0
56	DW	55	PSU	1	0
58	BX	5	MVA	2	0
58	BX	8	2R3	2	0
56	BY	8	4SU	1	0
56	DY	55	PSU	3	0
58	DX	5	MVA	2	0
58	BX	10	2QY	1	0
58	BX	6	2R1	5	0
58	BX	9	MVA	2	0

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 2056 ligands modelled in this entry, 2052 are monoatomic - leaving 4 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
62	GDP	BZ	702	59	24,30,30	1.24	2 (8%)	31,47,47	2.14	9 (29%)
61	SF4	BD	501	-	0,12,12	0.00	-	-		
61	SF4	DD	501	37	0,12,12	0.00	-	-		
62	GDP	DZ	703	59	24,30,30	1.22	2 (8%)	31,47,47	2.08	7 (22%)

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
62	GDP	BZ	702	59	-	3/12/32/32	0/3/3/3
61	SF4	BD	501	-	-	-	0/6/5/5
61	SF4	DD	501	37	-	-	0/6/5/5
62	GDP	DZ	703	59	-	1/12/32/32	0/3/3/3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
62	BZ	702	GDP	C6-C5	4.01	1.48	1.41
62	DZ	703	GDP	C6-C5	3.83	1.48	1.41
62	BZ	702	GDP	C5-C4	2.72	1.48	1.40
62	DZ	703	GDP	C5-C4	2.60	1.47	1.40

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
62	BZ	702	GDP	C5-C6-N1	-5.60	115.77	123.43
62	BZ	702	GDP	C6-N1-C2	5.07	123.99	115.93
62	DZ	703	GDP	C5-C6-N1	-4.91	116.72	123.43
62	DZ	703	GDP	C6-N1-C2	4.88	123.68	115.93
62	BZ	702	GDP	PA-O3A-PB	-4.62	116.96	132.83

There are no chirality outliers.

All (4) torsion outliers are listed below:

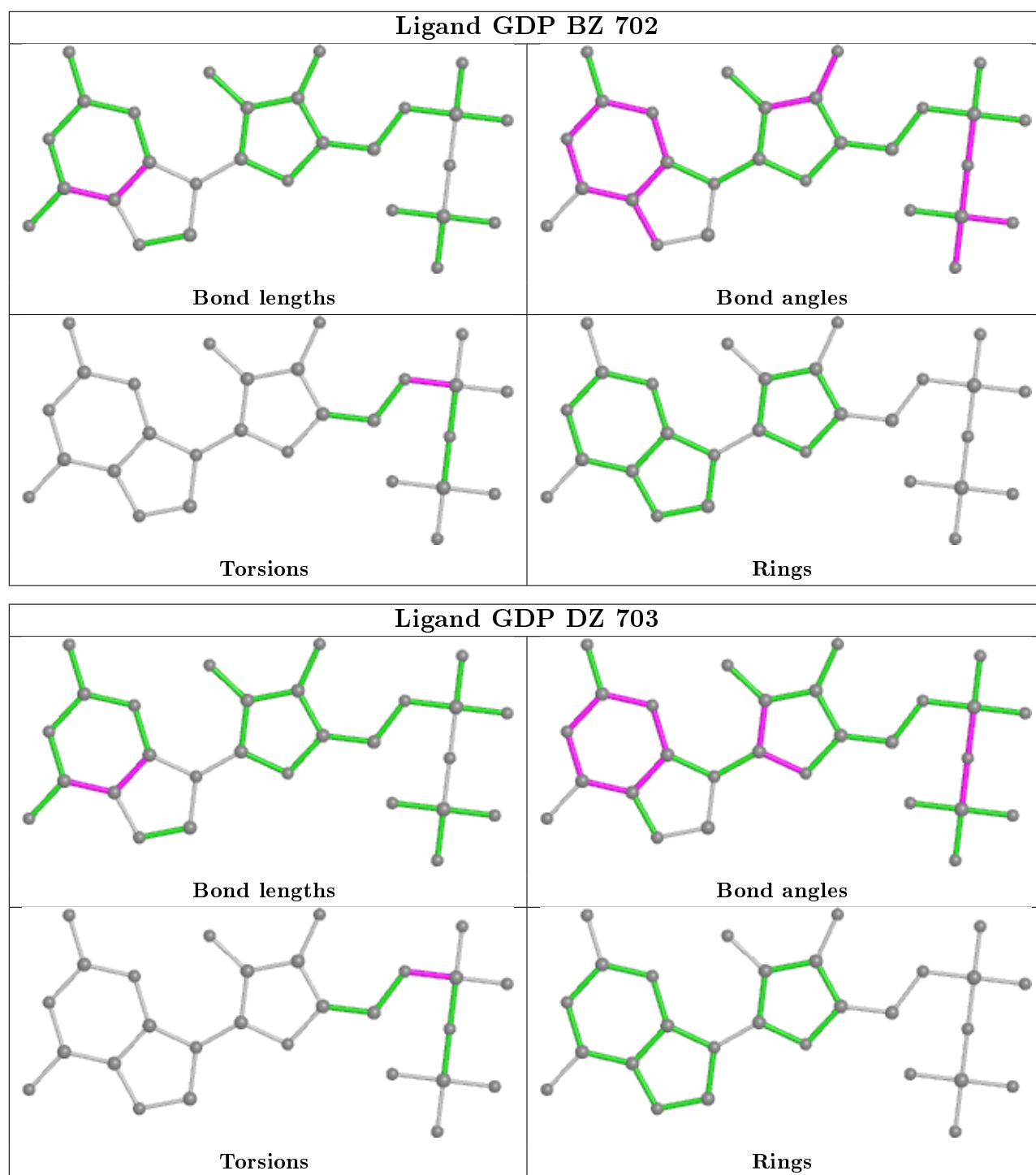
Mol	Chain	Res	Type	Atoms
62	BZ	702	GDP	C5'-O5'-PA-O3A
62	BZ	702	GDP	C5'-O5'-PA-O1A
62	BZ	702	GDP	C5'-O5'-PA-O2A
62	DZ	703	GDP	C5'-O5'-PA-O1A

There are no ring outliers.

4 monomers are involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
62	BZ	702	GDP	5	0
61	BD	501	SF4	1	0
61	DD	501	SF4	2	0
62	DZ	703	GDP	7	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 [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	AA	2872/2915 (98%)	-0.06	94 (3%) 46 36	13, 31, 166, 313	0
1	CA	2868/2915 (98%)	0.06	122 (4%) 35 25	24, 55, 177, 331	0
2	AB	120/121 (99%)	-0.41	0 100 100	24, 47, 66, 112	0
2	CB	120/121 (99%)	0.01	1 (0%) 86 81	56, 104, 146, 178	0
3	AC	137/228 (60%)	5.85	122 (89%) 0 0	89, 187, 231, 259	0
3	CC	137/228 (60%)	8.38	136 (99%) 0 0	142, 205, 249, 270	0
4	AD	275/276 (99%)	-0.46	2 (0%) 87 84	8, 30, 56, 122	0
4	CD	275/276 (99%)	-0.37	2 (0%) 87 84	13, 44, 77, 134	0
5	AE	204/206 (99%)	-0.47	0 100 100	7, 31, 60, 100	0
5	CE	204/206 (99%)	-0.31	0 100 100	16, 51, 87, 143	0
6	AF	203/210 (96%)	-0.41	0 100 100	6, 32, 76, 141	0
6	CF	203/210 (96%)	-0.19	1 (0%) 91 88	20, 66, 123, 158	0
7	AG	181/182 (99%)	-0.28	2 (1%) 80 75	34, 67, 114, 180	0
7	CG	181/182 (99%)	0.82	27 (14%) 2 1	75, 125, 183, 211	0
8	AH	174/180 (96%)	-0.46	2 (1%) 80 75	21, 46, 74, 199	0
8	CH	174/180 (96%)	0.66	11 (6%) 20 12	52, 92, 139, 174	0
9	AK	130/173 (75%)	1.27	30 (23%) 0 0	65, 131, 198, 223	0
9	CK	130/173 (75%)	2.85	78 (60%) 0 0	85, 163, 212, 233	0
10	AL	66/147 (44%)	4.23	54 (81%) 0 0	112, 182, 229, 247	0
10	CL	66/147 (44%)	5.46	58 (87%) 0 0	105, 183, 232, 263	0
11	AN	140/140 (100%)	-0.58	0 100 100	11, 28, 57, 97	0
11	CN	140/140 (100%)	-0.12	3 (2%) 63 54	35, 59, 92, 143	0
12	AO	122/122 (100%)	-0.43	0 100 100	16, 35, 66, 93	0
12	CO	122/122 (100%)	-0.32	0 100 100	30, 49, 80, 94	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	AP	149/150 (99%)	-0.35	0 100 100	8, 38, 78, 128	0
13	CP	149/150 (99%)	0.27	7 (4%) 31 22	26, 75, 123, 155	0
14	AQ	141/141 (100%)	-0.48	0 100 100	9, 32, 54, 99	0
14	CQ	141/141 (100%)	-0.27	1 (0%) 87 84	19, 63, 95, 146	0
15	AR	118/118 (100%)	-0.48	0 100 100	14, 27, 52, 76	0
15	CR	118/118 (100%)	-0.32	0 100 100	26, 49, 75, 106	0
16	AS	110/112 (98%)	-0.28	0 100 100	24, 47, 76, 86	0
16	CS	110/112 (98%)	0.66	8 (7%) 15 8	61, 96, 140, 166	0
17	AT	131/146 (89%)	-0.30	1 (0%) 86 81	20, 40, 95, 219	0
17	CT	131/146 (89%)	-0.22	1 (0%) 86 81	36, 56, 104, 152	0
18	AU	116/118 (98%)	-0.51	0 100 100	7, 22, 39, 87	0
18	CU	116/118 (98%)	-0.18	0 100 100	31, 55, 88, 107	0
19	AV	101/101 (100%)	-0.60	0 100 100	11, 27, 58, 77	0
19	CV	101/101 (100%)	-0.07	2 (1%) 65 56	29, 69, 102, 162	0
20	AW	112/113 (99%)	-0.47	0 100 100	10, 24, 49, 145	0
20	CW	112/113 (99%)	-0.21	0 100 100	26, 45, 76, 159	0
21	AX	95/96 (98%)	-0.48	0 100 100	12, 33, 64, 108	0
21	CX	95/96 (98%)	0.15	4 (4%) 36 26	37, 63, 100, 173	0
22	AY	107/110 (97%)	-0.40	1 (0%) 84 80	18, 43, 88, 120	0
22	CY	107/110 (97%)	0.57	10 (9%) 8 4	48, 81, 124, 171	0
23	AZ	185/206 (89%)	-0.44	0 100 100	28, 56, 94, 136	0
23	CZ	185/206 (89%)	0.39	12 (6%) 18 11	52, 98, 145, 175	0
24	A0	77/85 (90%)	-0.42	0 100 100	10, 31, 54, 82	0
24	C0	77/85 (90%)	0.28	4 (5%) 27 18	27, 69, 104, 127	0
25	A1	97/98 (98%)	-0.31	1 (1%) 82 77	15, 39, 80, 98	0
25	C1	97/98 (98%)	-0.16	1 (1%) 82 77	31, 56, 95, 144	0
26	A2	70/72 (97%)	-0.39	1 (1%) 75 70	15, 43, 65, 135	0
26	C2	70/72 (97%)	-0.03	1 (1%) 75 70	47, 79, 110, 151	0
27	A3	59/60 (98%)	-0.40	1 (1%) 70 63	11, 26, 53, 112	0
27	C3	59/60 (98%)	0.39	2 (3%) 45 35	31, 63, 103, 162	0
28	A4	69/71 (97%)	0.73	12 (17%) 1 1	47, 102, 188, 221	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
28	C4	69/71 (97%)	1.31	21 (30%) 0 0	88, 158, 196, 229	0
29	A5	59/60 (98%)	-0.51	0 100 100	11, 23, 50, 68	0
29	C5	59/60 (98%)	-0.26	1 (1%) 70 63	16, 47, 82, 121	0
30	A6	53/54 (98%)	-0.44	0 100 100	17, 36, 62, 77	0
30	C6	53/54 (98%)	-0.11	0 100 100	41, 63, 86, 104	0
31	A7	48/49 (97%)	-0.34	1 (2%) 63 54	11, 21, 54, 100	0
31	C7	48/49 (97%)	-0.22	0 100 100	23, 36, 96, 120	0
32	A8	64/65 (98%)	-0.43	0 100 100	14, 26, 39, 63	0
32	C8	64/65 (98%)	-0.20	0 100 100	27, 53, 71, 94	0
33	A9	37/37 (100%)	-0.29	0 100 100	20, 33, 64, 67	0
33	C9	37/37 (100%)	0.05	0 100 100	44, 62, 90, 101	0
34	BA	1495/1521 (98%)	0.14	50 (3%) 46 36	24, 82, 180, 330	0
34	DA	1501/1521 (98%)	0.33	93 (6%) 20 13	40, 94, 207, 307	0
35	BB	231/256 (90%)	0.50	22 (9%) 8 4	53, 104, 167, 195	0
35	DB	231/256 (90%)	1.21	54 (23%) 0 0	67, 135, 197, 228	0
36	BC	206/239 (86%)	0.73	21 (10%) 6 3	74, 114, 169, 187	0
36	DC	206/239 (86%)	1.71	66 (32%) 0 0	88, 151, 198, 221	0
37	BD	208/209 (99%)	0.27	11 (5%) 26 17	54, 91, 141, 182	0
37	DD	208/209 (99%)	0.13	3 (1%) 75 70	53, 88, 134, 199	0
38	BE	148/162 (91%)	-0.09	0 100 100	37, 72, 110, 150	0
38	DE	148/162 (91%)	0.35	6 (4%) 37 27	43, 90, 131, 177	0
39	BF	100/101 (99%)	-0.12	0 100 100	43, 81, 124, 145	0
39	DF	100/101 (99%)	0.02	2 (2%) 65 56	49, 90, 133, 146	0
40	BG	155/156 (99%)	0.62	19 (12%) 4 2	66, 100, 155, 194	0
40	DG	155/156 (99%)	1.52	40 (25%) 0 0	81, 131, 178, 214	0
41	BH	137/138 (99%)	0.11	1 (0%) 87 84	45, 73, 105, 121	0
41	DH	137/138 (99%)	0.35	7 (5%) 28 19	52, 92, 126, 160	0
42	BI	127/128 (99%)	1.37	31 (24%) 0 0	59, 115, 169, 192	0
42	DI	127/128 (99%)	2.47	69 (54%) 0 0	79, 154, 192, 248	0
43	BJ	97/105 (92%)	1.59	31 (31%) 0 0	75, 123, 173, 194	0
43	DJ	96/105 (91%)	2.40	50 (52%) 0 0	77, 160, 201, 221	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
44	BK	114/129 (88%)	-0.28	1 (0%) 84 80	30, 73, 117, 125	0
44	DK	114/129 (88%)	0.23	2 (1%) 68 61	61, 93, 139, 170	0
45	BL	122/132 (92%)	-0.21	1 (0%) 86 81	27, 61, 88, 110	0
45	DL	122/132 (92%)	0.04	1 (0%) 86 81	41, 70, 101, 142	0
46	BM	117/126 (92%)	0.53	9 (7%) 13 7	62, 108, 154, 187	0
46	DM	116/126 (92%)	1.46	34 (29%) 0 0	64, 156, 202, 235	0
47	BN	60/61 (98%)	0.80	5 (8%) 11 6	60, 110, 153, 173	0
47	DN	60/61 (98%)	1.97	27 (45%) 0 0	95, 142, 192, 210	0
48	BO	88/89 (98%)	-0.17	0 100 100	36, 69, 107, 139	0
48	DO	88/89 (98%)	0.09	0 100 100	50, 83, 115, 140	0
49	BP	82/88 (93%)	0.20	2 (2%) 59 49	46, 81, 126, 151	0
49	DP	82/88 (93%)	0.30	2 (2%) 59 49	50, 76, 108, 121	0
50	BQ	99/105 (94%)	-0.09	0 100 100	46, 72, 103, 119	0
50	DQ	99/105 (94%)	0.22	2 (2%) 65 56	47, 80, 116, 148	0
51	BR	68/88 (77%)	0.25	3 (4%) 34 24	45, 71, 115, 136	0
51	DR	68/88 (77%)	0.52	6 (8%) 10 5	58, 90, 129, 147	0
52	BS	84/93 (90%)	2.00	36 (42%) 0 0	68, 127, 168, 222	0
52	DS	83/93 (89%)	3.09	60 (72%) 0 0	98, 164, 213, 222	0
53	BT	96/106 (90%)	0.31	2 (2%) 63 54	49, 84, 117, 160	0
53	DT	96/106 (90%)	0.16	3 (3%) 49 39	48, 81, 126, 145	0
54	BU	23/27 (85%)	1.34	6 (26%) 0 0	60, 100, 114, 154	0
54	DU	23/27 (85%)	2.81	17 (73%) 0 0	78, 134, 159, 181	0
55	BV	7/18 (38%)	1.22	2 (28%) 0 0	61, 69, 175, 190	0
55	DV	6/18 (33%)	1.85	3 (50%) 0 0	89, 95, 181, 204	0
56	BW	69/76 (90%)	0.28	3 (4%) 35 25	38, 69, 118, 210	0
56	BY	67/76 (88%)	4.14	64 (95%) 0 0	76, 232, 280, 304	0
56	DW	69/76 (90%)	0.56	1 (1%) 75 70	48, 108, 151, 254	0
56	DY	66/76 (86%)	6.43	66 (100%) 0 0	145, 283, 315, 338	0
57	BZ	728/758 (96%)	0.71	113 (15%) 2 1	38, 97, 190, 248	0
57	DZ	730/758 (96%)	1.48	242 (33%) 0 0	27, 113, 212, 264	0
58	BX	3/10 (30%)	-0.18	0 100 100	83, 83, 83, 83	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
58	DX	3/10 (30%)	0.19	0 100 100	81, 81, 81, 81	0
All	All	22705/23918 (94%)	0.37	2127 (9%) 8 4	6, 70, 189, 338	0

The worst 5 of 2127 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	CC	166	ASN	26.6
3	CC	167	ASP	25.1
3	CC	179	ALA	24.3
3	AC	171	ALA	21.6
3	CC	175	PRO	19.2

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	1.13	275,275,275,275	0
56	PSU	DY	39	20/21	0.18	1.02	291,291,291,291	0
56	PSU	BY	55	20/21	0.27	0.51	243,243,243,243	0
56	PSU	DY	55	20/21	0.29	0.66	252,252,252,252	0
56	5MU	DY	54	21/22	0.38	0.84	303,303,303,303	0
56	4SU	DY	8	20/21	0.40	0.42	277,277,277,277	0
56	MIA	DY	37	22/30	0.46	0.85	271,271,271,271	0
56	PSU	BY	32	20/21	0.47	0.55	226,226,226,226	0
56	5MU	BY	54	21/22	0.47	0.58	246,246,246,246	0
56	7MG	BY	46	24/25	0.49	0.34	276,276,276,276	0
56	7MG	DY	46	24/25	0.52	0.40	266,266,266,266	0
56	4SU	BY	8	20/21	0.52	0.34	239,239,239,239	0
56	PSU	BY	39	20/21	0.68	0.54	197,197,197,197	0
56	MIA	BY	37	22/30	0.72	0.42	186,186,186,186	0
56	PSU	DW	32	20/21	0.82	0.31	126,126,126,126	0
58	2R1	DX	6	10/11	0.83	0.15	81,81,81,81	0
58	004	DX	3	10/11	0.83	0.19	81,81,81,81	0
56	PSU	DW	39	20/21	0.86	0.28	112,112,112,112	1
56	7MG	DW	46	24/25	0.87	0.23	124,124,124,124	0
58	MVA	BX	5	8/9	0.87	0.15	82,82,82,82	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	PSU	DW	55	20/21	0.88	0.19	92,92,92,92	0
58	2R1	BX	6	10/11	0.89	0.16	82,82,82,82	1
56	7MG	BW	46	24/25	0.89	0.19	76,76,76,76	3
56	5MU	DW	54	21/22	0.89	0.20	95,95,95,95	1
58	MVA	BX	9	8/9	0.90	0.31	82,82,82,82	0
58	2QY	BX	10	13/14	0.90	0.19	82,82,82,82	0
58	004	BX	3	10/11	0.90	0.12	82,82,82,82	0
56	4SU	DW	8	20/21	0.91	0.14	103,103,103,103	0
56	MIA	DW	37	29/30	0.91	0.24	109,109,109,109	0
56	PSU	BW	55	20/21	0.91	0.17	79,79,79,79	0
56	5MU	BW	54	21/22	0.92	0.18	80,80,80,80	0
58	2QY	DX	10	13/14	0.92	0.17	81,81,81,81	0
58	2R3	BX	8	14/15	0.92	0.14	82,82,82,82	0
58	2QZ	BX	1	9/10	0.93	0.25	82,82,82,82	0
58	2QZ	DX	1	9/10	0.94	0.24	81,81,81,81	0
56	PSU	BW	32	20/21	0.94	0.20	73,73,73,73	1
56	MIA	BW	37	29/30	0.94	0.22	79,79,79,79	0
58	MVA	DX	9	8/9	0.94	0.24	81,81,81,81	0
58	MVA	DX	5	8/9	0.95	0.36	81,81,81,81	0
56	PSU	BW	39	20/21	0.96	0.14	65,65,65,65	0
58	2R3	DX	8	14/15	0.96	0.13	81,81,81,81	0
56	4SU	BW	8	20/21	0.96	0.14	60,60,60,60	1

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. 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
59	MG	BA	1660	1/1	0.10	0.39	82,82,82,82	0
59	MG	CA	3460	1/1	0.11	0.95	104,104,104,104	0
59	MG	DA	1757	1/1	0.26	1.14	111,111,111,111	0
59	MG	DA	1738	1/1	0.29	0.48	95,95,95,95	0
59	MG	CA	3155	1/1	0.31	0.23	112,112,112,112	0
59	MG	CA	3096	1/1	0.32	0.24	125,125,125,125	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
59	MG	CA	3139	1/1	0.32	0.70	126,126,126,126	0
59	MG	CA	3646	1/1	0.36	0.16	91,91,91,91	0
59	MG	BA	1755	1/1	0.38	0.14	86,86,86,86	0
59	MG	AA	3108	1/1	0.40	0.64	101,101,101,101	0
59	MG	AA	3040	1/1	0.42	0.17	113,113,113,113	0
59	MG	BA	1767	1/1	0.44	0.42	96,96,96,96	0
59	MG	AA	3212	1/1	0.45	0.82	81,81,81,81	0
59	MG	CA	3565	1/1	0.47	0.19	95,95,95,95	0
59	MG	DA	1626	1/1	0.47	0.30	71,71,71,71	0
59	MG	BA	1657	1/1	0.47	0.25	78,78,78,78	0
59	MG	DA	1754	1/1	0.48	0.40	120,120,120,120	0
59	MG	BA	1812	1/1	0.48	0.20	79,79,79,79	0
59	MG	AA	3747	1/1	0.48	0.33	85,85,85,85	0
59	MG	CA	3620	1/1	0.48	0.64	96,96,96,96	0
59	MG	CA	3100	1/1	0.49	0.25	81,81,81,81	0
59	MG	AA	3266	1/1	0.49	0.78	90,90,90,90	0
59	MG	AA	3807	1/1	0.50	0.31	77,77,77,77	0
59	MG	AA	3617	1/1	0.53	0.15	77,77,77,77	0
59	MG	AA	3122	1/1	0.53	0.70	99,99,99,99	0
59	MG	CA	3244	1/1	0.54	0.30	89,89,89,89	0
59	MG	BA	1616	1/1	0.54	0.27	122,122,122,122	0
59	MG	DA	1639	1/1	0.55	0.55	69,69,69,69	0
59	MG	AA	3269	1/1	0.55	0.33	63,63,63,63	0
59	MG	CA	3546	1/1	0.56	0.15	88,88,88,88	0
59	MG	CA	3127	1/1	0.56	0.41	94,94,94,94	0
59	MG	CA	3485	1/1	0.56	0.30	85,85,85,85	0
59	MG	DA	1733	1/1	0.56	0.34	92,92,92,92	0
59	MG	AF	305	1/1	0.57	0.53	76,76,76,76	0
59	MG	BA	1775	1/1	0.57	0.34	90,90,90,90	0
59	MG	CA	3101	1/1	0.58	1.12	84,84,84,84	0
59	MG	BA	1786	1/1	0.58	0.22	82,82,82,82	0
59	MG	AA	3754	1/1	0.58	0.25	64,64,64,64	0
59	MG	CA	3080	1/1	0.58	0.24	75,75,75,75	0
59	MG	AB	3017	1/1	0.59	0.17	59,59,59,59	0
59	MG	CA	3149	1/1	0.59	0.17	100,100,100,100	0
59	MG	DA	1717	1/1	0.59	0.28	95,95,95,95	0
59	MG	CA	3186	1/1	0.59	0.61	77,77,77,77	0
59	MG	BA	1691	1/1	0.59	0.45	86,86,86,86	0
59	MG	BA	1673	1/1	0.60	0.20	80,80,80,80	0
59	MG	BA	1764	1/1	0.60	0.09	71,71,71,71	0
59	MG	CA	3040	1/1	0.61	0.47	79,79,79,79	0
59	MG	BA	1790	1/1	0.61	0.15	96,96,96,96	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
59	MG	CA	3075	1/1	0.62	0.65	90,90,90,90	0
59	MG	CB	3013	1/1	0.62	0.17	100,100,100,100	0
59	MG	CA	3146	1/1	0.63	0.95	82,82,82,82	0
59	MG	BA	1741	1/1	0.63	0.19	88,88,88,88	0
59	MG	DT	3001	1/1	0.64	0.42	60,60,60,60	0
59	MG	BA	1776	1/1	0.64	0.21	97,97,97,97	0
59	MG	CQ	202	1/1	0.64	0.29	74,74,74,74	0
59	MG	DA	1655	1/1	0.64	0.24	83,83,83,83	0
59	MG	AA	3242	1/1	0.64	0.29	85,85,85,85	0
59	MG	AA	3240	1/1	0.65	0.16	69,69,69,69	0
59	MG	CP	201	1/1	0.65	0.16	62,62,62,62	1
59	MG	DK	5001	1/1	0.65	0.16	76,76,76,76	0
59	MG	CA	3108	1/1	0.65	0.27	78,78,78,78	0
59	MG	AA	3016	1/1	0.65	0.45	64,64,64,64	0
59	MG	AA	3241	1/1	0.65	0.21	65,65,65,65	0
59	MG	DA	1623	1/1	0.65	0.24	72,72,72,72	0
59	MG	AA	3195	1/1	0.65	0.37	69,69,69,69	0
59	MG	CA	3624	1/1	0.65	0.16	118,118,118,118	0
59	MG	BA	1638	1/1	0.66	0.21	66,66,66,66	0
59	MG	AA	3541	1/1	0.66	0.12	74,74,74,74	0
59	MG	DA	1746	1/1	0.66	0.10	81,81,81,81	0
59	MG	CA	3654	1/1	0.66	0.40	90,90,90,90	0
59	MG	DA	1718	1/1	0.67	0.32	101,101,101,101	0
59	MG	CA	3587	1/1	0.67	0.34	70,70,70,70	0
59	MG	DA	1642	1/1	0.67	0.20	62,62,62,62	0
59	MG	BL	201	1/1	0.67	0.37	84,84,84,84	0
59	MG	BA	1654	1/1	0.67	0.23	76,76,76,76	0
59	MG	DA	1634	1/1	0.68	0.29	66,66,66,66	0
59	MG	AA	3680	1/1	0.69	0.33	79,79,79,79	0
59	MG	DA	1659	1/1	0.69	0.29	78,78,78,78	0
59	MG	CA	3061	1/1	0.69	0.35	68,68,68,68	0
59	MG	AA	3582	1/1	0.69	0.58	76,76,76,76	0
59	MG	BA	1643	1/1	0.69	0.34	66,66,66,66	0
59	MG	CA	3237	1/1	0.69	0.49	94,94,94,94	0
59	MG	CA	3501	1/1	0.70	0.45	74,74,74,74	0
59	MG	AE	302	1/1	0.70	0.24	57,57,57,57	0
59	MG	AA	3238	1/1	0.70	0.44	76,76,76,76	0
59	MG	CA	3117	1/1	0.70	0.28	67,67,67,67	0
59	MG	AD	305	1/1	0.70	0.63	86,86,86,86	0
59	MG	CA	3154	1/1	0.70	0.20	64,64,64,64	0
59	MG	AA	3717	1/1	0.70	0.56	68,68,68,68	0
59	MG	CA	3548	1/1	0.70	0.10	90,90,90,90	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
59	MG	BA	1802	1/1	0.70	0.24	76,76,76,76	0
59	MG	CA	3579	1/1	0.70	0.22	65,65,65,65	0
59	MG	CA	3242	1/1	0.70	0.39	82,82,82,82	0
59	MG	CA	3304	1/1	0.70	0.12	67,67,67,67	0
59	MG	CA	3538	1/1	0.70	0.15	72,72,72,72	0
59	MG	DA	1654	1/1	0.71	0.35	63,63,63,63	0
59	MG	DA	1756	1/1	0.71	0.57	86,86,86,86	0
59	MG	BA	1602	1/1	0.72	0.18	79,79,79,79	0
59	MG	AA	3296	1/1	0.72	0.25	67,67,67,67	0
59	MG	CA	3294	1/1	0.72	0.09	72,72,72,72	0
59	MG	DA	1611	1/1	0.72	0.39	89,89,89,89	0
59	MG	AA	3739	1/1	0.72	0.17	38,38,38,38	0
59	MG	AA	3140	1/1	0.72	0.58	62,62,62,62	0
59	MG	CA	3499	1/1	0.72	0.49	62,62,62,62	0
59	MG	CA	3325	1/1	0.72	0.13	38,38,38,38	0
59	MG	BA	1758	1/1	0.72	0.36	76,76,76,76	0
59	MG	CA	3135	1/1	0.72	0.31	59,59,59,59	0
59	MG	BA	1697	1/1	0.72	1.08	99,99,99,99	0
59	MG	CA	3378	1/1	0.72	0.24	97,97,97,97	0
59	MG	AA	3277	1/1	0.72	0.69	99,99,99,99	0
59	MG	BA	1631	1/1	0.72	0.17	71,71,71,71	0
59	MG	CA	3112	1/1	0.72	0.38	69,69,69,69	0
59	MG	AB	3004	1/1	0.72	0.32	69,69,69,69	0
59	MG	CA	3152	1/1	0.72	0.35	64,64,64,64	0
59	MG	CA	3536	1/1	0.73	0.26	84,84,84,84	0
59	MG	CA	3486	1/1	0.73	0.24	81,81,81,81	0
59	MG	AA	3769	1/1	0.73	0.17	63,63,63,63	0
59	MG	CA	3205	1/1	0.73	0.53	81,81,81,81	0
59	MG	CB	3008	1/1	0.73	0.20	66,66,66,66	0
59	MG	BA	1601	1/1	0.73	0.34	95,95,95,95	0
59	MG	AA	3571	1/1	0.73	0.34	94,94,94,94	0
59	MG	AA	3536	1/1	0.74	0.24	66,66,66,66	0
59	MG	DA	1724	1/1	0.74	0.41	70,70,70,70	0
59	MG	CA	3350	1/1	0.74	0.09	82,82,82,82	0
59	MG	CA	3420	1/1	0.74	0.33	69,69,69,69	0
59	MG	CA	3093	1/1	0.74	0.71	75,75,75,75	0
59	MG	CA	3505	1/1	0.74	0.09	67,67,67,67	0
59	MG	BA	1716	1/1	0.74	0.24	86,86,86,86	0
59	MG	AA	3363	1/1	0.74	0.20	82,82,82,82	0
59	MG	CA	3553	1/1	0.74	0.19	90,90,90,90	0
59	MG	BA	1612	1/1	0.74	0.25	92,92,92,92	0
59	MG	CA	3502	1/1	0.75	0.66	90,90,90,90	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
59	MG	AA	3773	1/1	0.75	0.45	35,35,35,35	1
59	MG	AA	3067	1/1	0.75	0.42	61,61,61,61	0
59	MG	CQ	204	1/1	0.75	0.33	74,74,74,74	0
59	MG	DA	1742	1/1	0.75	0.21	72,72,72,72	0
59	MG	CA	3089	1/1	0.75	0.47	87,87,87,87	0
59	MG	BA	1604	1/1	0.75	0.19	63,63,63,63	0
59	MG	CA	3602	1/1	0.75	0.10	84,84,84,84	0
59	MG	CA	3082	1/1	0.75	0.75	76,76,76,76	0
59	MG	AA	3814	1/1	0.75	0.59	72,72,72,72	0
59	MG	CA	3216	1/1	0.75	0.47	79,79,79,79	0
59	MG	AA	3625	1/1	0.75	0.21	51,51,51,51	0
59	MG	BA	1714	1/1	0.75	0.28	74,74,74,74	0
59	MG	BA	1707	1/1	0.75	0.11	72,72,72,72	0
59	MG	BA	1721	1/1	0.75	0.20	66,66,66,66	0
59	MG	AA	3767	1/1	0.75	0.35	67,67,67,67	0
59	MG	CA	3041	1/1	0.75	0.41	61,61,61,61	0
59	MG	BA	1670	1/1	0.75	0.23	69,69,69,69	0
59	MG	CA	3542	1/1	0.75	0.41	87,87,87,87	0
59	MG	AA	3712	1/1	0.76	0.69	70,70,70,70	0
59	MG	CA	3390	1/1	0.76	0.23	80,80,80,80	0
59	MG	DA	1769	1/1	0.76	0.44	74,74,74,74	0
59	MG	CA	3517	1/1	0.76	0.16	62,62,62,62	0
59	MG	AE	301	1/1	0.76	0.57	69,69,69,69	0
59	MG	DA	1631	1/1	0.76	0.09	74,74,74,74	0
59	MG	CA	3084	1/1	0.77	0.41	56,56,56,56	0
59	MG	CA	3279	1/1	0.77	0.17	26,26,26,26	0
59	MG	CA	3236	1/1	0.77	0.68	81,81,81,81	0
59	MG	CA	3348	1/1	0.77	0.28	44,44,44,44	0
59	MG	CV	201	1/1	0.77	0.81	117,117,117,117	0
59	MG	DA	1674	1/1	0.77	0.28	77,77,77,77	0
59	MG	BA	1788	1/1	0.77	0.19	79,79,79,79	0
59	MG	BA	1665	1/1	0.77	0.45	73,73,73,73	0
59	MG	CA	3194	1/1	0.77	0.23	52,52,52,52	0
59	MG	CA	3097	1/1	0.77	0.29	66,66,66,66	0
59	MG	DA	1622	1/1	0.77	0.35	60,60,60,60	0
59	MG	AA	3323	1/1	0.77	0.21	64,64,64,64	0
59	MG	BA	1614	1/1	0.78	0.14	72,72,72,72	0
59	MG	AA	3225	1/1	0.78	0.15	73,73,73,73	0
59	MG	CA	3550	1/1	0.78	0.09	62,62,62,62	1
59	MG	AA	3002	1/1	0.78	0.21	57,57,57,57	0
59	MG	CA	3092	1/1	0.78	0.78	79,79,79,79	0
59	MG	AA	3066	1/1	0.78	0.14	51,51,51,51	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
59	MG	DA	1715	1/1	0.78	0.28	79,79,79,79	0
59	MG	AA	3732	1/1	0.78	0.28	70,70,70,70	0
59	MG	CA	3572	1/1	0.78	0.16	70,70,70,70	0
59	MG	CA	3055	1/1	0.78	0.12	77,77,77,77	0
59	MG	CA	3494	1/1	0.78	0.24	97,97,97,97	0
59	MG	CA	3630	1/1	0.78	0.10	65,65,65,65	0
59	MG	CA	3388	1/1	0.78	0.14	90,90,90,90	0
59	MG	AA	3644	1/1	0.78	0.33	56,56,56,56	0
59	MG	CA	3007	1/1	0.78	0.40	92,92,92,92	0
59	MG	CA	3158	1/1	0.78	0.37	54,54,54,54	0
59	MG	CA	3541	1/1	0.78	0.28	63,63,63,63	0
59	MG	CA	3240	1/1	0.78	0.48	71,71,71,71	0
59	MG	BA	1698	1/1	0.78	0.42	63,63,63,63	0
59	MG	AA	3181	1/1	0.78	0.33	79,79,79,79	0
59	MG	BB	3001	1/1	0.78	0.16	91,91,91,91	0
59	MG	DA	1722	1/1	0.79	0.13	77,77,77,77	0
59	MG	AA	3281	1/1	0.79	0.29	75,75,75,75	0
59	MG	CA	3180	1/1	0.79	0.36	62,62,62,62	0
59	MG	AX	3001	1/1	0.79	0.31	52,52,52,52	0
59	MG	BA	1634	1/1	0.79	0.39	64,64,64,64	0
59	MG	CA	3514	1/1	0.79	0.42	64,64,64,64	0
59	MG	CA	3044	1/1	0.79	0.21	89,89,89,89	0
59	MG	AA	3167	1/1	0.79	0.19	45,45,45,45	0
59	MG	AA	3827	1/1	0.79	0.37	38,38,38,38	0
59	MG	BA	1644	1/1	0.79	0.19	74,74,74,74	0
59	MG	CA	3150	1/1	0.79	0.19	57,57,57,57	0
59	MG	CA	3591	1/1	0.79	0.11	60,60,60,60	0
59	MG	CA	3490	1/1	0.79	0.13	50,50,50,50	0
59	MG	CA	3600	1/1	0.79	0.52	86,86,86,86	0
59	MG	BA	1811	1/1	0.79	0.20	77,77,77,77	0
59	MG	CA	3389	1/1	0.79	0.34	59,59,59,59	0
59	MG	CA	3037	1/1	0.79	0.72	57,57,57,57	0
59	MG	AA	3780	1/1	0.79	0.40	72,72,72,72	0
59	MG	AA	3708	1/1	0.80	0.30	61,61,61,61	0
59	MG	BA	1619	1/1	0.80	0.21	59,59,59,59	0
59	MG	AA	3012	1/1	0.80	0.35	49,49,49,49	0
59	MG	AA	3273	1/1	0.80	0.77	90,90,90,90	0
59	MG	AA	3352	1/1	0.80	0.36	47,47,47,47	0
59	MG	CA	3555	1/1	0.80	0.14	71,71,71,71	0
59	MG	AA	3816	1/1	0.80	0.70	66,66,66,66	0
59	MG	AA	3820	1/1	0.80	0.43	85,85,85,85	0
59	MG	BA	1778	1/1	0.80	0.16	54,54,54,54	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
59	MG	AA	3219	1/1	0.80	0.21	61,61,61,61	0
59	MG	BA	1704	1/1	0.80	0.31	71,71,71,71	0
59	MG	CA	3077	1/1	0.80	0.24	42,42,42,42	0
59	MG	CA	3605	1/1	0.80	0.21	70,70,70,70	0
59	MG	BA	1628	1/1	0.80	0.30	87,87,87,87	0
59	MG	CA	3030	1/1	0.80	0.51	59,59,59,59	0
59	MG	CA	3038	1/1	0.80	0.51	97,97,97,97	0
59	MG	DA	1633	1/1	0.80	0.27	55,55,55,55	0
59	MG	AA	3768	1/1	0.80	0.19	58,58,58,58	0
59	MG	AA	3586	1/1	0.80	0.35	74,74,74,74	0
59	MG	AA	3761	1/1	0.80	0.38	92,92,92,92	0
59	MG	CA	3208	1/1	0.80	0.63	74,74,74,74	0
59	MG	CA	3307	1/1	0.80	0.31	60,60,60,60	0
59	MG	BA	1655	1/1	0.80	0.15	59,59,59,59	0
59	MG	CA	3034	1/1	0.80	0.29	77,77,77,77	0
59	MG	BA	1668	1/1	0.80	0.16	69,69,69,69	0
59	MG	CA	3583	1/1	0.80	0.16	80,80,80,80	0
59	MG	CA	3005	1/1	0.80	0.19	48,48,48,48	0
59	MG	BS	101	1/1	0.80	0.16	79,79,79,79	0
59	MG	CA	3557	1/1	0.80	0.22	76,76,76,76	0
59	MG	CA	3072	1/1	0.80	0.38	66,66,66,66	0
59	MG	CA	3563	1/1	0.80	0.09	75,75,75,75	0
59	MG	AB	3003	1/1	0.80	0.23	60,60,60,60	0
59	MG	CA	3289	1/1	0.80	0.28	65,65,65,65	0
59	MG	AA	3629	1/1	0.81	0.17	77,77,77,77	0
59	MG	CA	3145	1/1	0.81	0.44	76,76,76,76	0
59	MG	CA	3122	1/1	0.81	0.70	58,58,58,58	0
59	MG	CA	3013	1/1	0.81	0.23	42,42,42,42	0
59	MG	AW	3002	1/1	0.81	0.25	47,47,47,47	0
59	MG	CA	3068	1/1	0.81	0.43	66,66,66,66	0
59	MG	AA	3109	1/1	0.81	0.34	56,56,56,56	0
59	MG	AA	3627	1/1	0.81	0.15	76,76,76,76	0
59	MG	BA	1810	1/1	0.81	0.13	82,82,82,82	0
59	MG	AA	3206	1/1	0.81	0.54	106,106,106,106	0
59	MG	BA	1713	1/1	0.81	0.58	68,68,68,68	0
59	MG	DA	1704	1/1	0.81	0.18	49,49,49,49	0
59	MG	AA	3227	1/1	0.81	0.18	22,22,22,22	0
59	MG	DA	1727	1/1	0.81	0.13	61,61,61,61	0
59	MG	AA	3817	1/1	0.81	0.18	75,75,75,75	0
59	MG	AA	3556	1/1	0.81	0.32	66,66,66,66	0
59	MG	AA	3128	1/1	0.81	0.47	89,89,89,89	0
59	MG	AA	3675	1/1	0.81	0.14	64,64,64,64	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
59	MG	CA	3631	1/1	0.81	0.11	65,65,65,65	0
59	MG	CA	3202	1/1	0.81	0.71	73,73,73,73	0
59	MG	AA	3643	1/1	0.81	0.24	84,84,84,84	0
59	MG	AA	3051	1/1	0.81	0.47	48,48,48,48	0
59	MG	BA	1693	1/1	0.81	0.47	76,76,76,76	0
59	MG	AA	3653	1/1	0.81	0.22	60,60,60,60	0
59	MG	CA	3513	1/1	0.81	0.16	70,70,70,70	0
59	MG	CA	3078	1/1	0.81	0.48	57,57,57,57	0
59	MG	AB	3008	1/1	0.82	0.38	52,52,52,52	0
59	MG	CA	3125	1/1	0.82	0.32	78,78,78,78	0
59	MG	BA	1690	1/1	0.82	0.40	71,71,71,71	0
59	MG	A0	101	1/1	0.82	0.20	69,69,69,69	0
59	MG	AA	3693	1/1	0.82	0.14	69,69,69,69	0
59	MG	AA	3315	1/1	0.82	0.22	65,65,65,65	0
59	MG	DA	1610	1/1	0.82	0.71	71,71,71,71	0
59	MG	CA	3333	1/1	0.82	0.36	68,68,68,68	0
59	MG	CA	3457	1/1	0.82	0.26	43,43,43,43	0
59	MG	CA	3575	1/1	0.82	0.21	71,71,71,71	0
59	MG	BA	1689	1/1	0.82	0.51	71,71,71,71	0
59	MG	CA	3060	1/1	0.82	0.39	72,72,72,72	0
59	MG	AA	3258	1/1	0.82	0.44	68,68,68,68	0
59	MG	CA	3413	1/1	0.82	0.22	39,39,39,39	0
59	MG	BA	1648	1/1	0.82	0.11	74,74,74,74	0
59	MG	DA	1614	1/1	0.82	0.18	65,65,65,65	0
59	MG	AA	3558	1/1	0.82	0.08	48,48,48,48	0
59	MG	AA	3660	1/1	0.82	0.22	61,61,61,61	0
59	MG	AA	3601	1/1	0.82	0.11	61,61,61,61	0
59	MG	A7	101	1/1	0.82	0.16	55,55,55,55	0
59	MG	CA	3528	1/1	0.82	0.10	38,38,38,38	0
59	MG	AA	3018	1/1	0.82	1.43	67,67,67,67	0
59	MG	BA	1635	1/1	0.82	0.51	65,65,65,65	0
59	MG	AA	3087	1/1	0.82	0.48	55,55,55,55	0
59	MG	CA	3050	1/1	0.82	0.45	75,75,75,75	0
59	MG	DA	1669	1/1	0.82	0.20	65,65,65,65	0
59	MG	AA	3149	1/1	0.82	0.33	51,51,51,51	0
59	MG	CA	3406	1/1	0.82	0.13	77,77,77,77	0
59	MG	DA	1632	1/1	0.82	0.29	57,57,57,57	0
59	MG	AA	3640	1/1	0.82	0.21	68,68,68,68	0
59	MG	BA	1723	1/1	0.82	0.24	70,70,70,70	0
59	MG	CA	3172	1/1	0.83	0.35	81,81,81,81	0
59	MG	CA	3367	1/1	0.83	0.21	63,63,63,63	0
59	MG	AA	3300	1/1	0.83	0.16	22,22,22,22	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
59	MG	AA	3019	1/1	0.83	0.29	70,70,70,70	0
59	MG	CA	3518	1/1	0.83	0.11	65,65,65,65	0
59	MG	CA	3566	1/1	0.83	0.35	30,30,30,30	1
59	MG	DA	1770	1/1	0.83	0.15	63,63,63,63	0
59	MG	DA	1656	1/1	0.83	0.13	63,63,63,63	0
59	MG	CA	3323	1/1	0.83	0.40	87,87,87,87	0
59	MG	AA	3583	1/1	0.83	0.14	63,63,63,63	0
59	MG	CA	3377	1/1	0.83	0.10	52,52,52,52	0
59	MG	CA	3598	1/1	0.83	0.15	65,65,65,65	0
59	MG	AA	3776	1/1	0.83	0.12	69,69,69,69	0
59	MG	CA	3608	1/1	0.83	0.32	50,50,50,50	1
59	MG	AA	3450	1/1	0.83	0.10	58,58,58,58	0
59	MG	CA	3176	1/1	0.83	0.42	60,60,60,60	0
59	MG	CA	3225	1/1	0.83	0.34	64,64,64,64	0
59	MG	AA	3714	1/1	0.83	0.24	70,70,70,70	0
59	MG	BA	1633	1/1	0.83	0.25	63,63,63,63	0
59	MG	AA	3656	1/1	0.83	0.23	80,80,80,80	0
59	MG	DA	1605	1/1	0.83	0.33	105,105,105,105	0
59	MG	AA	3596	1/1	0.83	0.31	65,65,65,65	0
59	MG	CA	3159	1/1	0.83	0.59	69,69,69,69	0
59	MG	AA	3809	1/1	0.83	0.29	57,57,57,57	0
59	MG	AA	3622	1/1	0.83	0.22	60,60,60,60	0
59	MG	C7	101	1/1	0.83	0.43	56,56,56,56	0
59	MG	AA	3070	1/1	0.83	0.40	81,81,81,81	0
59	MG	CA	3559	1/1	0.83	0.12	75,75,75,75	0
59	MG	A0	102	1/1	0.83	0.09	56,56,56,56	0
59	MG	CA	3023	1/1	0.83	0.42	68,68,68,68	0
59	MG	CA	3193	1/1	0.83	0.44	89,89,89,89	0
59	MG	CA	3058	1/1	0.83	0.33	67,67,67,67	0
59	MG	CA	3644	1/1	0.83	0.20	66,66,66,66	0
59	MG	AA	3056	1/1	0.83	1.05	96,96,96,96	0
59	MG	CD	302	1/1	0.83	0.53	56,56,56,56	0
59	MG	DA	1771	1/1	0.83	0.12	60,60,60,60	0
59	MG	CA	3001	1/1	0.83	0.25	64,64,64,64	0
59	MG	BA	1603	1/1	0.83	0.11	61,61,61,61	0
59	MG	BA	1750	1/1	0.84	0.20	55,55,55,55	0
59	MG	CA	3200	1/1	0.84	0.30	51,51,51,51	0
59	MG	AA	3786	1/1	0.84	0.17	53,53,53,53	0
59	MG	CA	3432	1/1	0.84	0.27	32,32,32,32	0
59	MG	BA	1624	1/1	0.84	0.18	58,58,58,58	0
59	MG	DA	1644	1/1	0.84	0.35	94,94,94,94	0
59	MG	CA	3521	1/1	0.84	0.22	74,74,74,74	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
59	MG	AA	3409	1/1	0.84	0.08	60,60,60,60	0
59	MG	DA	1618	1/1	0.84	0.64	91,91,91,91	0
59	MG	AP	203	1/1	0.84	0.18	59,59,59,59	0
59	MG	CA	3124	1/1	0.84	0.26	65,65,65,65	0
59	MG	DA	1665	1/1	0.84	0.20	63,63,63,63	0
59	MG	CA	3120	1/1	0.84	0.21	42,42,42,42	0
59	MG	AD	307	1/1	0.84	0.24	56,56,56,56	0
59	MG	AA	3479	1/1	0.84	0.23	55,55,55,55	0
59	MG	BA	1696	1/1	0.84	0.16	98,98,98,98	0
59	MG	CA	3633	1/1	0.84	0.26	68,68,68,68	0
59	MG	AA	3626	1/1	0.84	0.18	35,35,35,35	0
59	MG	CA	3363	1/1	0.84	0.17	88,88,88,88	0
59	MG	AA	3026	1/1	0.84	0.23	47,47,47,47	0
59	MG	AA	3792	1/1	0.84	0.13	48,48,48,48	0
59	MG	AA	3169	1/1	0.84	0.34	35,35,35,35	0
59	MG	BA	1772	1/1	0.84	0.12	66,66,66,66	0
59	MG	AA	3614	1/1	0.84	0.28	50,50,50,50	1
59	MG	CA	3530	1/1	0.84	0.51	71,71,71,71	0
59	MG	BA	1756	1/1	0.84	0.07	85,85,85,85	0
59	MG	CA	3273	1/1	0.84	0.35	58,58,58,58	0
59	MG	CA	3296	1/1	0.84	0.15	79,79,79,79	0
59	MG	AA	3544	1/1	0.84	0.22	26,26,26,26	0
59	MG	AA	3461	1/1	0.84	0.19	62,62,62,62	0
59	MG	CA	3629	1/1	0.84	0.08	55,55,55,55	0
59	MG	DA	1732	1/1	0.84	0.15	85,85,85,85	0
59	MG	BA	1719	1/1	0.84	0.15	62,62,62,62	0
59	MG	CA	3153	1/1	0.84	0.23	73,73,73,73	0
59	MG	BA	1792	1/1	0.84	0.19	80,80,80,80	0
59	MG	AA	3061	1/1	0.84	0.57	59,59,59,59	0
59	MG	CA	3603	1/1	0.84	0.35	49,49,49,49	0
59	MG	AB	3006	1/1	0.84	0.19	57,57,57,57	0
59	MG	BA	1646	1/1	0.84	0.95	66,66,66,66	0
59	MG	DA	1603	1/1	0.84	0.10	72,72,72,72	0
59	MG	AA	3808	1/1	0.84	0.40	72,72,72,72	0
59	MG	CA	3070	1/1	0.84	0.16	60,60,60,60	0
59	MG	CA	3392	1/1	0.84	0.19	43,43,43,43	0
59	MG	AA	3467	1/1	0.84	0.31	49,49,49,49	0
59	MG	CA	3599	1/1	0.84	0.08	70,70,70,70	0
59	MG	BA	1682	1/1	0.84	0.82	70,70,70,70	0
59	MG	DA	1624	1/1	0.84	0.12	82,82,82,82	0
59	MG	CA	3203	1/1	0.84	0.19	73,73,73,73	0
59	MG	CA	3081	1/1	0.84	0.31	63,63,63,63	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
59	MG	BA	1729	1/1	0.84	0.16	53,53,53,53	0
59	MG	CA	3634	1/1	0.84	0.23	82,82,82,82	0
59	MG	CA	3284	1/1	0.84	0.17	75,75,75,75	0
59	MG	AA	3093	1/1	0.84	1.05	92,92,92,92	0
59	MG	AA	3818	1/1	0.84	0.31	61,61,61,61	0
59	MG	AA	3010	1/1	0.84	0.45	46,46,46,46	0
59	MG	AA	3208	1/1	0.84	0.42	54,54,54,54	0
59	MG	AB	3001	1/1	0.84	0.37	74,74,74,74	0
59	MG	CA	3456	1/1	0.84	0.09	54,54,54,54	0
59	MG	CA	3581	1/1	0.84	0.12	38,38,38,38	0
59	MG	AA	3480	1/1	0.84	0.31	88,88,88,88	0
59	MG	BA	1727	1/1	0.85	0.09	77,77,77,77	0
59	MG	CA	3111	1/1	0.85	0.24	79,79,79,79	0
59	MG	AA	3041	1/1	0.85	0.26	37,37,37,37	0
59	MG	CA	3373	1/1	0.85	0.29	58,58,58,58	0
59	MG	BA	1814	1/1	0.85	0.21	69,69,69,69	0
59	MG	DE	202	1/1	0.85	0.08	100,100,100,100	0
59	MG	AA	3180	1/1	0.85	0.26	69,69,69,69	0
59	MG	CA	3408	1/1	0.85	0.11	58,58,58,58	0
59	MG	DA	1749	1/1	0.85	0.33	77,77,77,77	0
59	MG	CA	3647	1/1	0.85	0.15	85,85,85,85	0
59	MG	CF	301	1/1	0.85	0.47	61,61,61,61	0
59	MG	BA	1685	1/1	0.85	0.14	50,50,50,50	0
59	MG	CA	3352	1/1	0.85	0.18	79,79,79,79	0
59	MG	DA	1761	1/1	0.85	0.29	72,72,72,72	0
59	MG	CA	3251	1/1	0.85	0.18	82,82,82,82	0
59	MG	AA	3344	1/1	0.85	0.23	22,22,22,22	0
59	MG	DA	1643	1/1	0.85	0.24	79,79,79,79	0
59	MG	CA	3088	1/1	0.85	0.31	67,67,67,67	0
59	MG	CA	3091	1/1	0.85	0.28	69,69,69,69	0
59	MG	AA	3575	1/1	0.85	0.14	35,35,35,35	0
59	MG	BA	1815	1/1	0.85	0.22	53,53,53,53	0
59	MG	BA	1679	1/1	0.85	0.31	59,59,59,59	0
59	MG	CA	3069	1/1	0.85	0.72	81,81,81,81	0
59	MG	AA	3057	1/1	0.85	0.18	46,46,46,46	0
59	MG	CA	3276	1/1	0.85	0.18	44,44,44,44	0
59	MG	AA	3095	1/1	0.85	0.32	75,75,75,75	0
59	MG	CA	3014	1/1	0.85	0.24	50,50,50,50	0
59	MG	CA	3184	1/1	0.85	0.33	77,77,77,77	0
59	MG	AA	3083	1/1	0.85	0.38	61,61,61,61	0
59	MG	CA	3507	1/1	0.85	0.27	83,83,83,83	0
59	MG	AA	3215	1/1	0.85	0.33	59,59,59,59	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
59	MG	AA	3649	1/1	0.85	0.33	62,62,62,62	0
59	MG	CA	3560	1/1	0.85	0.23	79,79,79,79	0
59	MG	CA	3510	1/1	0.85	0.11	95,95,95,95	0
59	MG	CA	3288	1/1	0.85	0.17	49,49,49,49	0
59	MG	CA	3454	1/1	0.85	0.16	81,81,81,81	0
59	MG	DA	1729	1/1	0.85	0.17	49,49,49,49	0
59	MG	AA	3551	1/1	0.85	0.12	39,39,39,39	0
59	MG	BA	1610	1/1	0.85	0.08	78,78,78,78	0
59	MG	AA	3611	1/1	0.85	0.18	47,47,47,47	0
59	MG	AA	3249	1/1	0.85	0.17	59,59,59,59	0
59	MG	CA	3488	1/1	0.85	0.15	88,88,88,88	0
59	MG	CA	3226	1/1	0.85	0.33	52,52,52,52	0
59	MG	AA	3740	1/1	0.85	0.29	61,61,61,61	0
59	MG	BA	1791	1/1	0.85	0.18	72,72,72,72	0
59	MG	CA	3210	1/1	0.85	0.34	62,62,62,62	0
59	MG	CA	3379	1/1	0.85	0.23	83,83,83,83	0
59	MG	A0	103	1/1	0.85	0.10	70,70,70,70	0
59	MG	CA	3577	1/1	0.85	0.16	51,51,51,51	1
59	MG	BA	1694	1/1	0.85	0.24	83,83,83,83	0
59	MG	AA	3634	1/1	0.85	0.19	76,76,76,76	0
59	MG	BA	1625	1/1	0.85	0.15	86,86,86,86	0
59	MG	AA	3542	1/1	0.85	0.23	58,58,58,58	0
59	MG	CA	3229	1/1	0.85	0.19	53,53,53,53	0
59	MG	CA	3130	1/1	0.85	0.16	55,55,55,55	0
59	MG	CA	3016	1/1	0.86	0.25	52,52,52,52	0
59	MG	AA	3253	1/1	0.86	0.35	64,64,64,64	0
59	MG	BA	1613	1/1	0.86	0.12	76,76,76,76	0
59	MG	AD	303	1/1	0.86	0.16	50,50,50,50	0
59	MG	CA	3087	1/1	0.86	0.81	68,68,68,68	0
59	MG	AA	3035	1/1	0.86	0.15	48,48,48,48	0
59	MG	CA	3319	1/1	0.86	0.14	65,65,65,65	0
59	MG	AA	3657	1/1	0.86	0.17	63,63,63,63	0
59	MG	AA	3158	1/1	0.86	0.88	68,68,68,68	0
59	MG	CA	3140	1/1	0.86	0.38	63,63,63,63	0
59	MG	BA	1652	1/1	0.86	0.12	59,59,59,59	0
59	MG	CA	3115	1/1	0.86	0.41	67,67,67,67	0
59	MG	BA	1669	1/1	0.86	0.37	66,66,66,66	0
59	MG	BA	1659	1/1	0.86	0.33	67,67,67,67	0
59	MG	CA	3516	1/1	0.86	0.35	79,79,79,79	0
59	MG	AA	3481	1/1	0.86	0.13	78,78,78,78	0
59	MG	CA	3376	1/1	0.86	0.09	78,78,78,78	0
59	MG	CA	3340	1/1	0.86	0.17	66,66,66,66	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
59	MG	AA	3705	1/1	0.86	0.57	53,53,53,53	1
59	MG	CA	3095	1/1	0.86	0.32	58,58,58,58	0
59	MG	DA	1662	1/1	0.86	0.23	75,75,75,75	0
59	MG	AA	3751	1/1	0.86	0.34	61,61,61,61	0
59	MG	BA	1695	1/1	0.86	0.08	83,83,83,83	0
59	MG	CA	3612	1/1	0.86	0.36	83,83,83,83	0
59	MG	AA	3274	1/1	0.86	0.38	75,75,75,75	0
59	MG	CA	3656	1/1	0.86	0.57	63,63,63,63	0
59	MG	CA	3165	1/1	0.86	0.25	57,57,57,57	0
59	MG	BA	1700	1/1	0.86	0.14	52,52,52,52	0
59	MG	AE	304	1/1	0.86	0.19	52,52,52,52	0
59	MG	AB	3020	1/1	0.86	0.18	62,62,62,62	0
59	MG	AA	3327	1/1	0.86	0.17	31,31,31,31	0
59	MG	AA	3237	1/1	0.86	0.38	76,76,76,76	0
59	MG	CA	3235	1/1	0.86	0.28	78,78,78,78	0
59	MG	AA	3150	1/1	0.86	0.28	45,45,45,45	0
59	MG	CA	3481	1/1	0.86	0.21	64,64,64,64	0
59	MG	BD	502	1/1	0.86	0.53	64,64,64,64	0
59	MG	BA	1803	1/1	0.86	0.12	64,64,64,64	0
59	MG	DA	1609	1/1	0.86	0.30	89,89,89,89	0
59	MG	BA	1662	1/1	0.86	0.72	70,70,70,70	0
59	MG	AA	3603	1/1	0.86	0.62	76,76,76,76	0
59	MG	CA	3256	1/1	0.86	0.29	65,65,65,65	0
59	MG	BA	1784	1/1	0.86	0.27	68,68,68,68	0
59	MG	CA	3341	1/1	0.86	0.34	73,73,73,73	0
59	MG	AA	3695	1/1	0.86	0.08	67,67,67,67	0
59	MG	AA	3177	1/1	0.86	0.28	59,59,59,59	0
59	MG	DA	1636	1/1	0.86	0.50	62,62,62,62	0
59	MG	AA	3213	1/1	0.86	0.65	76,76,76,76	0
59	MG	AA	3202	1/1	0.86	0.11	61,61,61,61	0
59	MG	CA	3291	1/1	0.86	0.41	48,48,48,48	0
59	MG	AA	3736	1/1	0.86	0.30	59,59,59,59	0
59	MG	CA	3540	1/1	0.86	0.07	54,54,54,54	0
59	MG	AA	3331	1/1	0.86	0.16	15,15,15,15	0
59	MG	CA	3395	1/1	0.86	0.42	50,50,50,50	0
59	MG	AA	3275	1/1	0.86	0.34	89,89,89,89	0
59	MG	AA	3604	1/1	0.86	0.43	81,81,81,81	0
59	MG	CA	3544	1/1	0.86	0.32	60,60,60,60	0
59	MG	BA	1709	1/1	0.87	0.29	50,50,50,50	0
59	MG	DA	1683	1/1	0.87	0.32	58,58,58,58	0
59	MG	AA	3444	1/1	0.87	0.24	66,66,66,66	0
59	MG	DA	1681	1/1	0.87	0.37	70,70,70,70	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
59	MG	BA	1663	1/1	0.87	0.23	43,43,43,43	0
59	MG	BA	1683	1/1	0.87	0.21	71,71,71,71	0
59	MG	AA	3157	1/1	0.87	0.48	91,91,91,91	0
59	MG	AA	3445	1/1	0.87	0.13	23,23,23,23	0
59	MG	CA	3260	1/1	0.87	0.15	35,35,35,35	0
59	MG	AA	3197	1/1	0.87	0.19	45,45,45,45	0
59	MG	CA	3065	1/1	0.87	0.55	56,56,56,56	0
59	MG	CA	3059	1/1	0.87	0.43	58,58,58,58	0
59	MG	AA	3592	1/1	0.87	0.15	26,26,26,26	0
59	MG	A6	101	1/1	0.87	0.23	60,60,60,60	0
59	MG	CB	3012	1/1	0.87	0.26	62,62,62,62	0
59	MG	DZ	701	1/1	0.87	0.25	72,72,72,72	0
59	MG	DA	1641	1/1	0.87	0.25	74,74,74,74	0
59	MG	AA	3694	1/1	0.87	0.15	53,53,53,53	0
59	MG	BA	1605	1/1	0.87	0.13	73,73,73,73	0
59	MG	AA	3677	1/1	0.87	0.10	69,69,69,69	0
59	MG	BA	1630	1/1	0.87	0.29	61,61,61,61	0
59	MG	CA	3098	1/1	0.87	0.14	70,70,70,70	0
59	MG	BA	1737	1/1	0.87	0.20	79,79,79,79	0
59	MG	CA	3116	1/1	0.87	0.32	52,52,52,52	0
59	MG	AA	3126	1/1	0.87	0.36	79,79,79,79	0
59	MG	DA	1686	1/1	0.87	0.19	56,56,56,56	0
59	MG	CQ	203	1/1	0.87	0.34	54,54,54,54	0
59	MG	AA	3153	1/1	0.87	0.32	59,59,59,59	0
59	MG	DA	1737	1/1	0.87	0.20	69,69,69,69	0
59	MG	BA	1712	1/1	0.87	0.40	57,57,57,57	0
59	MG	AA	3065	1/1	0.87	0.58	62,62,62,62	0
59	MG	A2	3001	1/1	0.87	0.25	53,53,53,53	0
59	MG	BA	1622	1/1	0.87	0.51	65,65,65,65	0
59	MG	AA	3229	1/1	0.87	0.36	67,67,67,67	0
59	MG	CA	3478	1/1	0.87	0.31	65,65,65,65	0
59	MG	DA	1708	1/1	0.87	0.25	77,77,77,77	0
59	MG	BA	1687	1/1	0.87	0.22	52,52,52,52	0
59	MG	AB	3021	1/1	0.87	0.26	65,65,65,65	0
59	MG	CA	3511	1/1	0.87	0.20	81,81,81,81	0
59	MG	CA	3204	1/1	0.87	0.19	54,54,54,54	0
59	MG	CA	3246	1/1	0.87	0.50	57,57,57,57	0
59	MG	CA	3317	1/1	0.87	0.14	49,49,49,49	0
59	MG	CA	3118	1/1	0.87	0.64	65,65,65,65	0
59	MG	CA	3545	1/1	0.87	0.46	86,86,86,86	0
59	MG	AA	3164	1/1	0.87	0.63	71,71,71,71	0
59	MG	BA	1658	1/1	0.87	0.61	66,66,66,66	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
59	MG	AA	3025	1/1	0.87	0.43	68,68,68,68	0
59	MG	DA	1692	1/1	0.87	0.16	53,53,53,53	0
59	MG	CA	3411	1/1	0.87	0.24	57,57,57,57	0
59	MG	DA	1660	1/1	0.87	0.15	80,80,80,80	0
59	MG	AA	3068	1/1	0.87	0.56	73,73,73,73	0
59	MG	AA	3264	1/1	0.87	0.41	51,51,51,51	0
59	MG	AA	3079	1/1	0.87	0.12	27,27,27,27	0
59	MG	CA	3551	1/1	0.87	0.07	63,63,63,63	0
59	MG	AP	202	1/1	0.88	0.18	44,44,44,44	0
59	MG	CB	3011	1/1	0.88	0.23	56,56,56,56	0
59	MG	BA	1609	1/1	0.88	0.12	62,62,62,62	0
59	MG	AA	3664	1/1	0.88	0.20	62,62,62,62	0
59	MG	AA	3142	1/1	0.88	0.25	64,64,64,64	0
59	MG	AA	3293	1/1	0.88	0.15	27,27,27,27	0
59	MG	DA	1663	1/1	0.88	0.42	91,91,91,91	0
59	MG	BW	503	1/1	0.88	0.20	60,60,60,60	0
59	MG	CA	3224	1/1	0.88	0.53	59,59,59,59	0
59	MG	AA	3047	1/1	0.88	0.18	29,29,29,29	0
59	MG	AN	3003	1/1	0.88	0.08	55,55,55,55	0
59	MG	AA	3015	1/1	0.88	0.35	57,57,57,57	0
59	MG	CA	3264	1/1	0.88	0.19	60,60,60,60	0
59	MG	AA	3285	1/1	0.88	0.30	51,51,51,51	0
59	MG	DA	1739	1/1	0.88	0.12	73,73,73,73	0
59	MG	AA	3235	1/1	0.88	0.45	93,93,93,93	0
59	MG	CA	3496	1/1	0.88	0.13	56,56,56,56	0
59	MG	CA	3035	1/1	0.88	0.28	69,69,69,69	0
59	MG	AA	3031	1/1	0.88	0.48	63,63,63,63	0
59	MG	AA	3723	1/1	0.88	0.09	49,49,49,49	0
59	MG	AA	3414	1/1	0.88	0.17	37,37,37,37	0
59	MG	CA	3569	1/1	0.88	0.19	41,41,41,41	0
59	MG	AA	3194	1/1	0.88	0.26	82,82,82,82	0
59	MG	AA	3005	1/1	0.88	0.16	64,64,64,64	0
59	MG	AA	3464	1/1	0.88	0.40	66,66,66,66	0
59	MG	BA	1703	1/1	0.88	0.30	51,51,51,51	0
59	MG	DA	1638	1/1	0.88	0.29	80,80,80,80	0
59	MG	AA	3171	1/1	0.88	0.27	54,54,54,54	0
59	MG	AA	3156	1/1	0.88	0.43	49,49,49,49	0
59	MG	BA	1744	1/1	0.88	0.17	57,57,57,57	0
59	MG	CA	3173	1/1	0.88	0.36	61,61,61,61	0
59	MG	AA	3659	1/1	0.88	0.18	73,73,73,73	0
59	MG	AA	3619	1/1	0.88	0.12	47,47,47,47	0
59	MG	CA	3474	1/1	0.88	0.22	59,59,59,59	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
59	MG	CA	3328	1/1	0.88	0.20	35,35,35,35	0
59	MG	CA	3189	1/1	0.88	0.14	50,50,50,50	0
59	MG	DA	1679	1/1	0.88	0.12	70,70,70,70	0
59	MG	AA	3440	1/1	0.88	0.24	63,63,63,63	0
59	MG	AA	3642	1/1	0.88	0.34	71,71,71,71	0
59	MG	CA	3114	1/1	0.88	0.19	66,66,66,66	0
59	MG	CA	3090	1/1	0.88	0.28	77,77,77,77	0
59	MG	DA	1652	1/1	0.88	0.84	80,80,80,80	0
59	MG	AA	3699	1/1	0.88	0.27	71,71,71,71	0
59	MG	CA	3535	1/1	0.88	0.22	77,77,77,77	0
59	MG	CA	3336	1/1	0.88	0.09	64,64,64,64	0
59	MG	AA	3796	1/1	0.88	0.50	78,78,78,78	0
59	MG	CA	3057	1/1	0.88	0.29	60,60,60,60	0
59	MG	CA	3534	1/1	0.88	0.11	73,73,73,73	0
59	MG	AA	3724	1/1	0.88	0.23	47,47,47,47	0
59	MG	CA	3492	1/1	0.88	0.24	59,59,59,59	0
59	MG	AE	305	1/1	0.88	0.35	48,48,48,48	0
59	MG	AA	3175	1/1	0.88	0.56	63,63,63,63	0
59	MG	AA	3196	1/1	0.88	0.19	55,55,55,55	0
59	MG	CA	3191	1/1	0.88	0.22	46,46,46,46	0
59	MG	AR	201	1/1	0.88	0.16	28,28,28,28	0
59	MG	AA	3636	1/1	0.88	0.34	86,86,86,86	0
59	MG	AA	3788	1/1	0.88	0.28	61,61,61,61	0
59	MG	CA	3503	1/1	0.88	0.35	52,52,52,52	0
59	MG	DA	1646	1/1	0.88	0.12	57,57,57,57	0
59	MG	CQ	201	1/1	0.88	0.23	72,72,72,72	0
59	MG	CE	301	1/1	0.88	0.32	53,53,53,53	0
59	MG	AF	302	1/1	0.88	0.11	41,41,41,41	0
59	MG	CA	3495	1/1	0.88	0.21	70,70,70,70	0
59	MG	DA	1735	1/1	0.88	0.12	73,73,73,73	0
59	MG	AA	3034	1/1	0.89	0.31	49,49,49,49	0
59	MG	CA	3426	1/1	0.89	0.20	38,38,38,38	0
59	MG	AA	3027	1/1	0.89	0.51	75,75,75,75	0
59	MG	CB	3007	1/1	0.89	0.22	52,52,52,52	0
59	MG	CA	3371	1/1	0.89	0.18	52,52,52,52	0
59	MG	AA	3485	1/1	0.89	0.11	48,48,48,48	0
59	MG	CA	3417	1/1	0.89	0.21	56,56,56,56	0
59	MG	DA	1684	1/1	0.89	0.18	69,69,69,69	0
59	MG	AA	3295	1/1	0.89	0.14	57,57,57,57	0
59	MG	CB	3001	1/1	0.89	0.28	72,72,72,72	0
59	MG	AA	3418	1/1	0.89	0.13	74,74,74,74	0
59	MG	CA	3509	1/1	0.89	0.11	83,83,83,83	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
59	MG	AA	3744	1/1	0.89	0.15	34,34,34,34	0
59	MG	AA	3616	1/1	0.89	0.17	57,57,57,57	0
59	MG	CA	3626	1/1	0.89	0.18	61,61,61,61	0
59	MG	DA	1617	1/1	0.89	0.17	64,64,64,64	0
59	MG	AA	3655	1/1	0.89	0.33	55,55,55,55	0
59	MG	CA	3310	1/1	0.89	0.17	47,47,47,47	0
59	MG	CA	3593	1/1	0.89	0.60	61,61,61,61	0
59	MG	AA	3825	1/1	0.89	0.40	63,63,63,63	0
59	MG	CA	3223	1/1	0.89	0.15	59,59,59,59	0
59	MG	DA	1689	1/1	0.89	0.17	56,56,56,56	0
59	MG	BA	1661	1/1	0.89	0.32	63,63,63,63	0
59	MG	DA	1702	1/1	0.89	0.13	63,63,63,63	0
59	MG	CA	3649	1/1	0.89	0.26	51,51,51,51	0
59	MG	AA	3357	1/1	0.89	0.15	55,55,55,55	0
59	MG	CA	3615	1/1	0.89	0.20	28,28,28,28	0
59	MG	AA	3499	1/1	0.89	0.13	48,48,48,48	0
59	MG	AW	3001	1/1	0.89	0.29	54,54,54,54	0
59	MG	CA	3625	1/1	0.89	0.26	64,64,64,64	0
59	MG	CA	3113	1/1	0.89	0.39	38,38,38,38	0
59	MG	CA	3270	1/1	0.89	0.28	76,76,76,76	0
59	MG	AA	3088	1/1	0.89	0.42	39,39,39,39	0
59	MG	BA	1607	1/1	0.89	0.27	64,64,64,64	0
59	MG	CA	3241	1/1	0.89	0.18	72,72,72,72	0
59	MG	DA	1666	1/1	0.89	0.19	53,53,53,53	0
59	MG	BA	1796	1/1	0.89	0.26	57,57,57,57	0
59	MG	AA	3557	1/1	0.89	0.19	37,37,37,37	0
59	MG	AA	3584	1/1	0.89	0.13	17,17,17,17	0
59	MG	A0	104	1/1	0.89	0.35	51,51,51,51	0
59	MG	CA	3582	1/1	0.89	0.08	99,99,99,99	0
59	MG	BA	1671	1/1	0.89	0.21	101,101,101,101	0
59	MG	CA	3257	1/1	0.89	0.16	35,35,35,35	0
59	MG	AA	3803	1/1	0.89	0.33	45,45,45,45	0
59	MG	CE	304	1/1	0.89	0.36	75,75,75,75	0
59	MG	AA	3209	1/1	0.89	0.30	62,62,62,62	0
59	MG	BA	1730	1/1	0.89	0.18	53,53,53,53	0
59	MG	CA	3500	1/1	0.89	0.23	75,75,75,75	0
59	MG	AA	3385	1/1	0.89	0.21	49,49,49,49	0
59	MG	CA	3215	1/1	0.89	0.07	54,54,54,54	0
59	MG	CA	3398	1/1	0.89	0.15	67,67,67,67	0
59	MG	AA	3371	1/1	0.89	0.23	53,53,53,53	0
59	MG	BA	1779	1/1	0.89	0.19	85,85,85,85	0
59	MG	CA	3573	1/1	0.89	0.12	65,65,65,65	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
59	MG	DA	1767	1/1	0.89	0.13	74,74,74,74	0
59	MG	CA	3467	1/1	0.89	0.62	77,77,77,77	0
59	MG	AA	3143	1/1	0.89	0.23	48,48,48,48	0
59	MG	BA	1645	1/1	0.89	0.18	74,74,74,74	0
59	MG	BA	1711	1/1	0.89	0.14	61,61,61,61	0
59	MG	AA	3233	1/1	0.89	0.18	46,46,46,46	0
59	MG	CA	3129	1/1	0.89	0.59	64,64,64,64	0
59	MG	CA	3628	1/1	0.89	0.18	54,54,54,54	0
59	MG	BA	1641	1/1	0.89	0.20	54,54,54,54	0
59	MG	CA	3046	1/1	0.89	0.29	68,68,68,68	0
59	MG	AA	3168	1/1	0.89	0.31	47,47,47,47	0
59	MG	CA	3385	1/1	0.89	0.37	61,61,61,61	0
59	MG	AA	3795	1/1	0.89	0.25	22,22,22,22	0
59	MG	AA	3492	1/1	0.89	0.18	26,26,26,26	0
59	MG	AA	3635	1/1	0.89	0.31	49,49,49,49	0
59	MG	CA	3419	1/1	0.89	0.15	59,59,59,59	0
59	MG	DA	1604	1/1	0.89	0.12	80,80,80,80	0
59	MG	CA	3632	1/1	0.89	0.18	74,74,74,74	0
59	MG	DA	1627	1/1	0.89	0.08	77,77,77,77	0
59	MG	CA	3428	1/1	0.89	0.26	58,58,58,58	0
59	MG	AA	3782	1/1	0.89	0.20	44,44,44,44	0
59	MG	DA	1621	1/1	0.89	0.09	42,42,42,42	0
59	MG	AA	3230	1/1	0.89	0.28	69,69,69,69	0
59	MG	CA	3663	1/1	0.89	0.11	64,64,64,64	0
59	MG	DA	1736	1/1	0.89	0.12	78,78,78,78	0
59	MG	BA	1768	1/1	0.89	0.10	64,64,64,64	0
59	MG	CA	3141	1/1	0.89	0.45	68,68,68,68	0
59	MG	AA	3162	1/1	0.89	0.26	67,67,67,67	0
59	MG	AA	3055	1/1	0.89	0.28	65,65,65,65	0
59	MG	CA	3450	1/1	0.90	0.11	54,54,54,54	0
59	MG	AA	3683	1/1	0.90	0.27	62,62,62,62	0
59	MG	AA	3308	1/1	0.90	0.22	18,18,18,18	0
59	MG	AA	3810	1/1	0.90	0.27	67,67,67,67	0
59	MG	DA	1753	1/1	0.90	0.29	79,79,79,79	0
59	MG	CA	3465	1/1	0.90	0.30	70,70,70,70	0
59	MG	AA	3280	1/1	0.90	0.29	53,53,53,53	0
59	MG	AA	3252	1/1	0.90	0.20	44,44,44,44	0
59	MG	BA	1656	1/1	0.90	0.32	75,75,75,75	0
59	MG	AA	3715	1/1	0.90	0.54	33,33,33,33	1
59	MG	AD	302	1/1	0.90	0.15	17,17,17,17	0
59	MG	BA	1642	1/1	0.90	0.15	60,60,60,60	0
59	MG	CF	302	1/1	0.90	0.53	69,69,69,69	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
59	MG	AA	3017	1/1	0.90	0.10	61,61,61,61	0
59	MG	CA	3066	1/1	0.90	0.16	69,69,69,69	0
59	MG	AA	3138	1/1	0.90	0.13	38,38,38,38	0
59	MG	AA	3313	1/1	0.90	0.16	39,39,39,39	0
59	MG	BA	1797	1/1	0.90	0.17	59,59,59,59	0
59	MG	BA	1806	1/1	0.90	0.33	55,55,55,55	0
59	MG	AA	3787	1/1	0.90	0.20	82,82,82,82	0
59	MG	AA	3618	1/1	0.90	0.15	72,72,72,72	0
59	MG	CA	3021	1/1	0.90	0.44	69,69,69,69	0
59	MG	AA	3756	1/1	0.90	0.14	49,49,49,49	0
59	MG	AA	3191	1/1	0.90	0.11	16,16,16,16	0
59	MG	DA	1703	1/1	0.90	0.21	89,89,89,89	0
59	MG	CA	3086	1/1	0.90	0.26	85,85,85,85	0
59	MG	BA	1739	1/1	0.90	0.19	62,62,62,62	0
59	MG	AA	3822	1/1	0.90	0.31	47,47,47,47	0
59	MG	AA	3155	1/1	0.90	0.21	93,93,93,93	0
59	MG	AA	3139	1/1	0.90	0.33	60,60,60,60	0
59	MG	AA	3607	1/1	0.90	0.14	60,60,60,60	1
59	MG	CA	3031	1/1	0.90	0.48	68,68,68,68	0
59	MG	AA	3123	1/1	0.90	0.34	54,54,54,54	0
59	MG	CA	3192	1/1	0.90	0.11	45,45,45,45	0
59	MG	CA	3595	1/1	0.90	0.10	70,70,70,70	0
59	MG	BA	1608	1/1	0.90	0.52	57,57,57,57	0
59	MG	CA	3512	1/1	0.90	0.15	53,53,53,53	0
59	MG	BA	1705	1/1	0.90	0.23	53,53,53,53	0
59	MG	CA	3280	1/1	0.90	0.15	48,48,48,48	0
59	MG	CA	3171	1/1	0.90	0.37	56,56,56,56	0
59	MG	AA	3256	1/1	0.90	0.34	49,49,49,49	0
59	MG	AA	3783	1/1	0.90	0.49	53,53,53,53	1
59	MG	AA	3028	1/1	0.90	0.28	39,39,39,39	0
59	MG	CA	3506	1/1	0.90	0.12	63,63,63,63	0
59	MG	CA	3033	1/1	0.90	0.40	55,55,55,55	0
59	MG	DA	1658	1/1	0.90	0.33	51,51,51,51	0
59	MG	AA	3466	1/1	0.90	0.20	76,76,76,76	0
59	MG	A0	105	1/1	0.90	0.08	30,30,30,30	0
59	MG	AA	3576	1/1	0.90	0.18	52,52,52,52	0
59	MG	CA	3298	1/1	0.90	0.36	57,57,57,57	0
59	MG	BW	502	1/1	0.90	0.10	59,59,59,59	0
59	MG	CA	3249	1/1	0.90	0.15	61,61,61,61	0
59	MG	DA	1616	1/1	0.90	0.23	51,51,51,51	0
59	MG	AD	301	1/1	0.90	0.71	58,58,58,58	0
59	MG	CA	3586	1/1	0.90	0.17	93,93,93,93	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
59	MG	CA	3458	1/1	0.90	0.22	54,54,54,54	0
59	MG	CA	3134	1/1	0.90	0.66	71,71,71,71	0
59	MG	AA	3282	1/1	0.90	0.12	33,33,33,33	0
59	MG	DA	1608	1/1	0.90	0.17	57,57,57,57	0
59	MG	CA	3472	1/1	0.90	0.47	62,62,62,62	0
59	MG	CX	5001	1/1	0.90	0.14	65,65,65,65	0
59	MG	AA	3763	1/1	0.90	0.26	47,47,47,47	0
59	MG	BA	1813	1/1	0.90	0.07	55,55,55,55	0
59	MG	AA	3591	1/1	0.90	0.26	52,52,52,52	0
59	MG	AA	3608	1/1	0.90	0.36	60,60,60,60	0
59	MG	CA	3453	1/1	0.90	0.16	35,35,35,35	0
59	MG	BA	1701	1/1	0.90	0.09	54,54,54,54	0
59	MG	AD	306	1/1	0.90	0.14	65,65,65,65	0
59	MG	AA	3267	1/1	0.90	0.35	53,53,53,53	0
59	MG	AA	3120	1/1	0.90	0.24	33,33,33,33	0
59	MG	CR	201	1/1	0.90	0.26	34,34,34,34	0
59	MG	AA	3226	1/1	0.90	0.22	46,46,46,46	0
59	MG	AA	3199	1/1	0.90	0.34	41,41,41,41	0
59	MG	DA	1664	1/1	0.90	0.12	66,66,66,66	0
59	MG	DF	3001	1/1	0.90	0.20	54,54,54,54	0
59	MG	CB	3003	1/1	0.90	0.09	65,65,65,65	0
59	MG	AA	3633	1/1	0.90	0.16	48,48,48,48	0
59	MG	CA	3020	1/1	0.90	0.18	47,47,47,47	0
59	MG	CB	3002	1/1	0.90	0.10	63,63,63,63	0
59	MG	BA	1774	1/1	0.90	0.27	50,50,50,50	0
59	MG	BA	1728	1/1	0.90	0.19	47,47,47,47	0
59	MG	CA	3250	1/1	0.90	0.14	38,38,38,38	0
59	MG	DA	1635	1/1	0.90	0.28	75,75,75,75	0
59	MG	AA	3183	1/1	0.90	0.35	58,58,58,58	0
59	MG	AA	3676	1/1	0.90	0.15	26,26,26,26	0
59	MG	AA	3105	1/1	0.90	0.15	52,52,52,52	0
59	MG	DA	1730	1/1	0.90	0.25	71,71,71,71	0
59	MG	AA	3472	1/1	0.90	0.23	42,42,42,42	0
59	MG	AA	3347	1/1	0.90	0.13	88,88,88,88	0
59	MG	AA	3700	1/1	0.90	0.21	70,70,70,70	0
59	MG	AA	3679	1/1	0.90	0.08	36,36,36,36	0
59	MG	CA	3539	1/1	0.90	0.18	90,90,90,90	0
59	MG	DA	1667	1/1	0.90	0.06	66,66,66,66	0
59	MG	BA	1620	1/1	0.91	0.17	52,52,52,52	0
59	MG	CA	3042	1/1	0.91	0.31	65,65,65,65	0
59	MG	BA	1746	1/1	0.91	0.12	33,33,33,33	0
59	MG	AA	3654	1/1	0.91	0.06	67,67,67,67	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
59	MG	BA	1706	1/1	0.91	0.20	63,63,63,63	0
59	MG	CA	3616	1/1	0.91	0.64	74,74,74,74	0
59	MG	AA	3205	1/1	0.91	0.15	42,42,42,42	0
59	MG	BA	1647	1/1	0.91	0.51	57,57,57,57	0
59	MG	AA	3486	1/1	0.91	0.21	67,67,67,67	0
59	MG	AA	3211	1/1	0.91	0.27	56,56,56,56	0
59	MG	CA	3524	1/1	0.91	0.24	52,52,52,52	0
59	MG	AA	3624	1/1	0.91	0.12	42,42,42,42	0
59	MG	AA	3358	1/1	0.91	0.12	45,45,45,45	0
59	MG	AA	3014	1/1	0.91	0.12	31,31,31,31	0
59	MG	CA	3610	1/1	0.91	0.13	69,69,69,69	0
59	MG	AA	3090	1/1	0.91	0.38	53,53,53,53	0
59	MG	AA	3284	1/1	0.91	0.58	60,60,60,60	0
59	MG	AA	3106	1/1	0.91	0.17	33,33,33,33	0
59	MG	AA	3078	1/1	0.91	0.32	70,70,70,70	0
59	MG	CA	3442	1/1	0.91	0.59	74,74,74,74	0
59	MG	AA	3630	1/1	0.91	0.34	72,72,72,72	0
59	MG	CA	3409	1/1	0.91	0.28	42,42,42,42	0
59	MG	AA	3446	1/1	0.91	0.09	59,59,59,59	0
59	MG	CA	3126	1/1	0.91	0.31	62,62,62,62	0
59	MG	AF	301	1/1	0.91	0.21	35,35,35,35	1
59	MG	AA	3288	1/1	0.91	0.27	39,39,39,39	0
59	MG	CA	3174	1/1	0.91	0.52	50,50,50,50	0
59	MG	CA	3137	1/1	0.91	0.23	69,69,69,69	0
59	MG	CA	3274	1/1	0.91	0.15	52,52,52,52	0
59	MG	AA	3826	1/1	0.91	0.28	46,46,46,46	0
59	MG	AA	3179	1/1	0.91	0.50	45,45,45,45	1
59	MG	AQ	203	1/1	0.91	0.29	32,32,32,32	0
59	MG	CA	3199	1/1	0.91	0.22	55,55,55,55	0
59	MG	BA	1738	1/1	0.91	0.08	66,66,66,66	0
59	MG	CA	3623	1/1	0.91	0.15	64,64,64,64	0
59	MG	AA	3772	1/1	0.91	0.62	61,61,61,61	1
59	MG	AA	3043	1/1	0.91	0.30	45,45,45,45	0
59	MG	DA	1620	1/1	0.91	0.21	57,57,57,57	0
59	MG	AA	3246	1/1	0.91	0.13	52,52,52,52	0
59	MG	CA	3271	1/1	0.91	0.18	48,48,48,48	0
59	MG	AA	3449	1/1	0.91	0.23	50,50,50,50	0
59	MG	AY	502	1/1	0.91	0.28	60,60,60,60	0
59	MG	CA	3604	1/1	0.91	0.09	62,62,62,62	0
59	MG	CA	3239	1/1	0.91	0.17	69,69,69,69	0
59	MG	BN	503	1/1	0.91	0.14	62,62,62,62	0
59	MG	AA	3270	1/1	0.91	0.55	55,55,55,55	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
59	MG	AA	3701	1/1	0.91	0.15	81,81,81,81	0
59	MG	AA	3069	1/1	0.91	0.09	28,28,28,28	0
59	MG	BA	1753	1/1	0.91	0.11	48,48,48,48	0
59	MG	AB	3009	1/1	0.91	0.09	50,50,50,50	0
59	MG	AA	3224	1/1	0.91	0.24	56,56,56,56	0
59	MG	AA	3232	1/1	0.91	0.25	58,58,58,58	0
59	MG	AA	3602	1/1	0.91	0.15	51,51,51,51	0
59	MG	CA	3278	1/1	0.91	0.12	58,58,58,58	0
59	MG	CA	3636	1/1	0.91	0.19	64,64,64,64	0
59	MG	DA	1601	1/1	0.91	0.42	74,74,74,74	0
59	MG	AA	3373	1/1	0.91	0.16	48,48,48,48	0
59	MG	CA	3448	1/1	0.91	0.21	37,37,37,37	0
59	MG	CA	3234	1/1	0.91	0.35	50,50,50,50	0
59	MG	AA	3579	1/1	0.91	0.18	54,54,54,54	0
59	MG	CA	3343	1/1	0.91	0.12	32,32,32,32	0
59	MG	AA	3391	1/1	0.91	0.20	19,19,19,19	0
59	MG	CA	3036	1/1	0.91	0.28	32,32,32,32	0
59	MG	DA	1677	1/1	0.91	0.42	78,78,78,78	0
59	MG	BA	1724	1/1	0.91	0.19	67,67,67,67	0
59	MG	AA	3612	1/1	0.91	0.14	68,68,68,68	0
59	MG	AA	3118	1/1	0.91	0.40	76,76,76,76	0
59	MG	DA	1699	1/1	0.91	0.19	74,74,74,74	0
59	MG	CA	3597	1/1	0.91	0.21	58,58,58,58	0
59	MG	CA	3444	1/1	0.91	0.10	67,67,67,67	0
59	MG	AA	3166	1/1	0.91	0.41	40,40,40,40	0
59	MG	AA	3722	1/1	0.91	0.12	37,37,37,37	0
59	MG	AA	3310	1/1	0.91	0.15	56,56,56,56	0
59	MG	DA	1606	1/1	0.91	0.30	85,85,85,85	0
59	MG	BA	1733	1/1	0.91	0.20	78,78,78,78	0
59	MG	CA	3071	1/1	0.91	0.27	45,45,45,45	0
59	MG	CA	3594	1/1	0.91	0.11	73,73,73,73	0
59	MG	BA	1699	1/1	0.91	0.18	72,72,72,72	0
59	MG	BA	1649	1/1	0.91	0.16	35,35,35,35	0
59	MG	BA	1794	1/1	0.91	0.07	38,38,38,38	0
59	MG	CA	3374	1/1	0.91	0.30	60,60,60,60	0
59	MG	CA	3148	1/1	0.91	0.34	62,62,62,62	0
59	MG	BN	502	1/1	0.91	0.17	87,87,87,87	0
59	MG	DA	1705	1/1	0.91	0.10	68,68,68,68	0
59	MG	CA	3079	1/1	0.91	0.10	41,41,41,41	0
59	MG	CA	3110	1/1	0.91	0.26	56,56,56,56	0
59	MG	BA	1807	1/1	0.91	0.12	61,61,61,61	0
59	MG	DA	1701	1/1	0.91	0.24	68,68,68,68	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
59	MG	DA	1694	1/1	0.91	0.35	106,106,106,106	0
59	MG	CA	3473	1/1	0.91	0.16	51,51,51,51	0
59	MG	DW	503	1/1	0.91	0.22	85,85,85,85	0
59	MG	AA	3339	1/1	0.91	0.17	49,49,49,49	0
59	MG	DA	1672	1/1	0.91	0.23	77,77,77,77	0
59	MG	CA	3314	1/1	0.91	0.29	57,57,57,57	0
59	MG	CA	3187	1/1	0.91	0.22	37,37,37,37	0
59	MG	BA	1708	1/1	0.91	0.22	64,64,64,64	0
59	MG	AA	3781	1/1	0.91	0.20	72,72,72,72	0
59	MG	CA	3638	1/1	0.91	0.34	76,76,76,76	0
59	MG	CA	3221	1/1	0.91	0.58	65,65,65,65	0
59	MG	AA	3638	1/1	0.91	0.35	71,71,71,71	0
59	MG	CA	3580	1/1	0.91	0.23	76,76,76,76	0
59	MG	CA	3477	1/1	0.91	0.14	69,69,69,69	0
59	MG	BA	1736	1/1	0.91	0.17	67,67,67,67	0
59	MG	CA	3032	1/1	0.91	0.55	100,100,100,100	0
59	MG	AA	3009	1/1	0.91	0.09	22,22,22,22	0
59	MG	BA	1637	1/1	0.91	0.46	72,72,72,72	0
59	MG	AA	3135	1/1	0.91	0.55	55,55,55,55	0
59	MG	AA	3516	1/1	0.91	0.23	65,65,65,65	0
59	MG	CA	3067	1/1	0.91	0.19	63,63,63,63	0
59	MG	AA	3080	1/1	0.92	0.50	61,61,61,61	0
59	MG	BA	1718	1/1	0.92	0.09	63,63,63,63	0
59	MG	BA	1611	1/1	0.92	0.13	31,31,31,31	0
59	MG	AN	3001	1/1	0.92	0.32	58,58,58,58	0
59	MG	CA	3026	1/1	0.92	0.22	32,32,32,32	1
59	MG	AB	3010	1/1	0.92	0.11	62,62,62,62	0
59	MG	AA	3110	1/1	0.92	0.48	52,52,52,52	0
59	MG	CA	3243	1/1	0.92	0.28	58,58,58,58	0
59	MG	CA	3431	1/1	0.92	0.20	75,75,75,75	0
59	MG	CA	3043	1/1	0.92	0.41	61,61,61,61	0
59	MG	CE	303	1/1	0.92	0.40	51,51,51,51	0
59	MG	AA	3085	1/1	0.92	0.20	46,46,46,46	0
59	MG	BA	1623	1/1	0.92	0.62	67,67,67,67	0
59	MG	DA	1728	1/1	0.92	0.08	71,71,71,71	0
59	MG	AA	3696	1/1	0.92	0.17	66,66,66,66	0
59	MG	AA	3707	1/1	0.92	0.09	59,59,59,59	0
59	MG	AA	3161	1/1	0.92	0.23	43,43,43,43	0
59	MG	BA	1805	1/1	0.92	0.25	71,71,71,71	0
59	MG	AA	3716	1/1	0.92	0.24	66,66,66,66	0
59	MG	AA	3033	1/1	0.92	0.27	55,55,55,55	0
59	MG	CA	3168	1/1	0.92	0.42	58,58,58,58	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
59	MG	CA	3529	1/1	0.92	0.07	68,68,68,68	0
59	MG	CA	3259	1/1	0.92	0.26	80,80,80,80	0
59	MG	AA	3189	1/1	0.92	0.20	62,62,62,62	0
59	MG	CA	3549	1/1	0.92	0.16	70,70,70,70	0
59	MG	BA	1800	1/1	0.92	0.46	77,77,77,77	0
59	MG	CA	3396	1/1	0.92	0.23	39,39,39,39	0
59	MG	AA	3487	1/1	0.92	0.03	49,49,49,49	0
59	MG	AA	3771	1/1	0.92	0.24	60,60,60,60	0
59	MG	CA	3345	1/1	0.92	0.17	46,46,46,46	0
59	MG	DE	201	1/1	0.92	0.17	84,84,84,84	0
59	MG	DA	1751	1/1	0.92	0.16	64,64,64,64	0
59	MG	AA	3077	1/1	0.92	0.27	43,43,43,43	0
59	MG	CA	3576	1/1	0.92	0.11	71,71,71,71	0
59	MG	AA	3483	1/1	0.92	0.20	46,46,46,46	0
59	MG	BA	1618	1/1	0.92	0.31	52,52,52,52	0
59	MG	BA	1650	1/1	0.92	0.15	55,55,55,55	0
59	MG	DA	1661	1/1	0.92	0.18	66,66,66,66	0
59	MG	AA	3244	1/1	0.92	0.25	52,52,52,52	0
59	MG	CA	3212	1/1	0.92	0.24	84,84,84,84	0
59	MG	BA	1760	1/1	0.92	0.17	53,53,53,53	0
59	MG	AA	3133	1/1	0.92	0.33	50,50,50,50	0
59	MG	AA	3134	1/1	0.92	0.23	62,62,62,62	0
59	MG	AA	3427	1/1	0.92	0.12	61,61,61,61	0
59	MG	DA	1675	1/1	0.92	0.41	70,70,70,70	0
59	MG	CA	3589	1/1	0.92	0.23	71,71,71,71	0
59	MG	BA	1748	1/1	0.92	0.14	63,63,63,63	0
59	MG	CA	3368	1/1	0.92	0.16	44,44,44,44	0
59	MG	CA	3312	1/1	0.92	0.18	38,38,38,38	0
59	MG	BA	1754	1/1	0.92	0.13	49,49,49,49	0
59	MG	AA	3186	1/1	0.92	0.29	48,48,48,48	0
59	MG	CA	3207	1/1	0.92	0.28	75,75,75,75	0
59	MG	DA	1726	1/1	0.92	0.29	60,60,60,60	0
59	MG	AA	3287	1/1	0.92	0.39	43,43,43,43	0
59	MG	DA	1678	1/1	0.92	0.28	66,66,66,66	0
59	MG	A6	103	1/1	0.92	0.36	72,72,72,72	0
59	MG	AA	3698	1/1	0.92	0.16	41,41,41,41	0
59	MG	CA	3462	1/1	0.92	0.11	63,63,63,63	0
59	MG	CA	3527	1/1	0.92	0.14	76,76,76,76	0
59	MG	DA	1713	1/1	0.92	0.17	49,49,49,49	0
59	MG	AA	3641	1/1	0.92	0.28	51,51,51,51	0
59	MG	AA	3678	1/1	0.92	0.15	77,77,77,77	0
59	MG	AA	3749	1/1	0.92	0.17	73,73,73,73	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
59	MG	AA	3184	1/1	0.92	0.24	75,75,75,75	0
59	MG	AA	3718	1/1	0.92	0.21	42,42,42,42	0
60	ZN	C4	501	1/1	0.92	0.11	194,194,194,194	0
59	MG	DA	1670	1/1	0.92	0.12	49,49,49,49	0
59	MG	CA	3508	1/1	0.92	0.18	52,52,52,52	0
59	MG	CA	3403	1/1	0.92	0.07	70,70,70,70	0
59	MG	DA	1637	1/1	0.92	0.39	68,68,68,68	0
59	MG	BA	1675	1/1	0.92	0.07	100,100,100,100	0
59	MG	DW	502	1/1	0.92	0.08	58,58,58,58	0
59	MG	CA	3619	1/1	0.92	0.38	40,40,40,40	0
59	MG	CA	3131	1/1	0.92	0.23	26,26,26,26	0
59	MG	CA	3247	1/1	0.92	0.28	39,39,39,39	0
59	MG	BA	1666	1/1	0.92	0.37	61,61,61,61	0
59	MG	C3	3001	1/1	0.92	0.39	72,72,72,72	0
59	MG	AA	3394	1/1	0.92	0.16	39,39,39,39	0
59	MG	AA	3797	1/1	0.92	0.17	52,52,52,52	0
59	MG	AA	3800	1/1	0.92	0.16	35,35,35,35	0
59	MG	CA	3083	1/1	0.92	0.41	61,61,61,61	0
59	MG	CA	3532	1/1	0.92	0.23	49,49,49,49	0
59	MG	BA	1629	1/1	0.92	0.28	61,61,61,61	0
59	MG	CA	3387	1/1	0.92	0.33	50,50,50,50	0
59	MG	CA	3609	1/1	0.92	0.16	52,52,52,52	0
59	MG	AA	3746	1/1	0.92	0.17	73,73,73,73	0
59	MG	CA	3520	1/1	0.92	0.16	73,73,73,73	0
59	MG	CA	3596	1/1	0.92	0.12	51,51,51,51	0
59	MG	CA	3143	1/1	0.92	0.56	41,41,41,41	0
59	MG	AA	3476	1/1	0.92	0.17	28,28,28,28	0
59	MG	CA	3301	1/1	0.92	0.19	60,60,60,60	0
59	MG	AA	3447	1/1	0.92	0.34	56,56,56,56	0
59	MG	CD	303	1/1	0.92	0.08	70,70,70,70	0
59	MG	CA	3391	1/1	0.92	0.07	51,51,51,51	0
59	MG	CA	3515	1/1	0.92	0.20	54,54,54,54	0
59	MG	CA	3585	1/1	0.92	0.16	36,36,36,36	1
59	MG	DA	1741	1/1	0.92	0.35	67,67,67,67	0
59	MG	DA	1748	1/1	0.92	0.18	70,70,70,70	0
59	MG	DA	1691	1/1	0.92	0.18	63,63,63,63	0
59	MG	AA	3102	1/1	0.92	0.23	47,47,47,47	0
59	MG	AA	3203	1/1	0.92	0.07	59,59,59,59	0
59	MG	BA	1667	1/1	0.92	0.25	74,74,74,74	0
59	MG	AA	3319	1/1	0.92	0.19	58,58,58,58	0
59	MG	AA	3645	1/1	0.92	0.21	58,58,58,58	0
59	MG	AA	3045	1/1	0.92	0.32	55,55,55,55	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
59	MG	BA	1731	1/1	0.92	0.17	45,45,45,45	0
59	MG	CA	3558	1/1	0.92	0.09	64,64,64,64	0
59	MG	AA	3268	1/1	0.92	0.07	66,66,66,66	0
59	MG	CA	3128	1/1	0.92	0.39	50,50,50,50	0
59	MG	AA	3141	1/1	0.92	0.09	68,68,68,68	0
59	MG	BA	1676	1/1	0.92	0.20	61,61,61,61	0
59	MG	AA	3115	1/1	0.92	0.34	44,44,44,44	0
59	MG	DA	1625	1/1	0.92	0.15	50,50,50,50	0
59	MG	CA	3238	1/1	0.92	0.24	69,69,69,69	0
59	MG	DA	1613	1/1	0.92	0.24	48,48,48,48	0
59	MG	CA	3222	1/1	0.92	0.34	57,57,57,57	0
59	MG	CA	3201	1/1	0.93	0.23	45,45,45,45	0
59	MG	BA	1793	1/1	0.93	0.09	65,65,65,65	0
59	MG	BA	1787	1/1	0.93	0.27	55,55,55,55	0
59	MG	AA	3101	1/1	0.93	0.64	68,68,68,68	0
59	MG	CA	3164	1/1	0.93	0.56	64,64,64,64	0
59	MG	AA	3651	1/1	0.93	0.22	77,77,77,77	0
59	MG	AA	3823	1/1	0.93	0.48	39,39,39,39	0
59	MG	CA	3614	1/1	0.93	0.24	62,62,62,62	0
59	MG	DA	1759	1/1	0.93	0.17	53,53,53,53	0
59	MG	CN	5001	1/1	0.93	0.16	65,65,65,65	0
59	MG	CA	3022	1/1	0.93	0.52	69,69,69,69	0
59	MG	CB	3005	1/1	0.93	0.38	63,63,63,63	0
59	MG	AA	3589	1/1	0.93	0.08	55,55,55,55	0
59	MG	CA	3056	1/1	0.93	0.09	63,63,63,63	0
59	MG	AA	3577	1/1	0.93	0.08	42,42,42,42	0
59	MG	DA	1755	1/1	0.93	0.51	88,88,88,88	0
59	MG	CA	3651	1/1	0.93	0.53	76,76,76,76	0
59	MG	AA	3304	1/1	0.93	0.15	47,47,47,47	0
59	MG	CA	3156	1/1	0.93	0.38	52,52,52,52	0
59	MG	DA	1744	1/1	0.93	0.22	66,66,66,66	0
59	MG	AA	3062	1/1	0.93	0.17	47,47,47,47	0
59	MG	DA	1650	1/1	0.93	0.28	50,50,50,50	0
59	MG	AA	3832	1/1	0.93	0.42	55,55,55,55	0
59	MG	DA	1758	1/1	0.93	0.17	75,75,75,75	0
59	MG	CA	3313	1/1	0.93	0.26	38,38,38,38	0
59	MG	AZ	301	1/1	0.93	0.14	55,55,55,55	0
59	MG	AA	3124	1/1	0.93	0.73	62,62,62,62	0
59	MG	CA	3412	1/1	0.93	0.18	59,59,59,59	0
59	MG	AA	3286	1/1	0.93	0.45	40,40,40,40	0
59	MG	DA	1629	1/1	0.93	0.42	59,59,59,59	0
59	MG	CA	3052	1/1	0.93	0.18	44,44,44,44	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
59	MG	AA	3661	1/1	0.93	0.24	41,41,41,41	1
59	MG	BA	1672	1/1	0.93	0.30	65,65,65,65	0
59	MG	AD	308	1/1	0.93	0.42	46,46,46,46	0
59	MG	CA	3275	1/1	0.93	0.10	61,61,61,61	0
59	MG	CA	3233	1/1	0.93	0.12	59,59,59,59	0
59	MG	CA	3655	1/1	0.93	0.41	52,52,52,52	0
59	MG	CA	3293	1/1	0.93	0.16	60,60,60,60	0
59	MG	AA	3163	1/1	0.93	0.25	72,72,72,72	0
59	MG	BA	1617	1/1	0.93	0.12	118,118,118,118	0
59	MG	AA	3024	1/1	0.93	0.13	48,48,48,48	0
59	MG	AQ	202	1/1	0.93	0.25	35,35,35,35	0
59	MG	DA	1690	1/1	0.93	0.19	73,73,73,73	0
59	MG	AA	3231	1/1	0.93	0.21	64,64,64,64	0
59	MG	BA	1710	1/1	0.93	0.25	81,81,81,81	0
60	ZN	BN	501	1/1	0.93	0.10	132,132,132,132	0
59	MG	CA	3076	1/1	0.93	0.34	64,64,64,64	0
59	MG	AA	3609	1/1	0.93	0.11	58,58,58,58	0
59	MG	DA	1700	1/1	0.93	0.16	61,61,61,61	0
59	MG	AA	3063	1/1	0.93	0.26	54,54,54,54	0
59	MG	AA	3058	1/1	0.93	0.14	22,22,22,22	0
59	MG	AA	3314	1/1	0.93	0.26	57,57,57,57	0
59	MG	BA	1734	1/1	0.93	0.13	61,61,61,61	0
59	MG	AA	3198	1/1	0.93	0.15	63,63,63,63	0
59	MG	AA	3086	1/1	0.93	0.40	55,55,55,55	0
59	MG	AA	3046	1/1	0.93	0.33	35,35,35,35	0
59	MG	BA	1757	1/1	0.93	0.22	43,43,43,43	0
59	MG	BA	1720	1/1	0.93	0.21	61,61,61,61	0
59	MG	AA	3731	1/1	0.93	0.14	51,51,51,51	0
59	MG	AA	3775	1/1	0.93	0.59	25,25,25,25	1
59	MG	BA	1780	1/1	0.93	0.36	60,60,60,60	0
59	MG	BK	201	1/1	0.93	0.10	44,44,44,44	0
59	MG	CA	3245	1/1	0.93	0.41	62,62,62,62	0
59	MG	AA	3234	1/1	0.93	0.29	36,36,36,36	0
59	MG	AA	3673	1/1	0.93	0.11	38,38,38,38	0
59	MG	CB	3004	1/1	0.93	0.13	55,55,55,55	0
59	MG	DJ	5001	1/1	0.93	0.32	82,82,82,82	0
59	MG	AA	3376	1/1	0.93	0.21	35,35,35,35	0
59	MG	CA	3526	1/1	0.93	0.21	58,58,58,58	0
59	MG	AA	3204	1/1	0.93	0.33	54,54,54,54	0
59	MG	AA	3429	1/1	0.93	0.19	31,31,31,31	0
59	MG	BA	1621	1/1	0.93	0.11	51,51,51,51	0
59	MG	BA	1759	1/1	0.93	0.32	63,63,63,63	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
59	MG	AA	3748	1/1	0.93	0.20	45,45,45,45	0
59	MG	CA	3547	1/1	0.93	0.13	69,69,69,69	0
59	MG	AA	3172	1/1	0.93	0.22	47,47,47,47	0
59	MG	DA	1668	1/1	0.93	0.38	65,65,65,65	0
59	MG	CA	3178	1/1	0.93	0.13	54,54,54,54	0
59	MG	AA	3648	1/1	0.93	0.17	41,41,41,41	0
59	MG	CA	3642	1/1	0.93	0.52	52,52,52,52	0
59	MG	CA	3157	1/1	0.93	0.55	81,81,81,81	0
59	MG	AA	3733	1/1	0.93	0.15	49,49,49,49	0
59	MG	AA	3667	1/1	0.93	0.29	41,41,41,41	0
59	MG	CA	3167	1/1	0.93	0.08	50,50,50,50	0
59	MG	AA	3356	1/1	0.93	0.15	80,80,80,80	0
59	MG	CA	3254	1/1	0.93	0.16	85,85,85,85	0
59	MG	CA	3434	1/1	0.93	0.16	32,32,32,32	0
59	MG	CA	3414	1/1	0.93	0.19	34,34,34,34	1
59	MG	CA	3588	1/1	0.93	0.12	32,32,32,32	0
59	MG	AA	3261	1/1	0.93	0.31	25,25,25,25	0
59	MG	AA	3514	1/1	0.93	0.18	42,42,42,42	0
59	MG	AA	3456	1/1	0.93	0.14	56,56,56,56	0
59	MG	CA	3463	1/1	0.93	0.23	56,56,56,56	0
59	MG	AB	3002	1/1	0.93	0.17	52,52,52,52	0
59	MG	DA	1682	1/1	0.93	0.33	52,52,52,52	0
59	MG	AA	3669	1/1	0.93	0.18	81,81,81,81	0
59	MG	BE	3001	1/1	0.93	0.11	78,78,78,78	0
59	MG	DA	1607	1/1	0.93	0.10	86,86,86,86	0
59	MG	CA	3430	1/1	0.93	0.36	41,41,41,41	0
59	MG	CA	3660	1/1	0.93	0.19	60,60,60,60	0
59	MG	CA	3436	1/1	0.93	0.11	64,64,64,64	0
59	MG	AA	3646	1/1	0.93	0.22	53,53,53,53	0
59	MG	AA	3454	1/1	0.93	0.24	61,61,61,61	0
59	MG	CA	3073	1/1	0.93	0.26	49,49,49,49	0
59	MG	BA	1732	1/1	0.93	0.25	70,70,70,70	0
59	MG	CA	3161	1/1	0.93	0.25	57,57,57,57	0
59	MG	DA	1680	1/1	0.93	0.17	56,56,56,56	0
59	MG	AA	3764	1/1	0.93	0.16	73,73,73,73	0
59	MG	DA	1688	1/1	0.93	0.25	51,51,51,51	0
59	MG	AA	3096	1/1	0.93	0.20	59,59,59,59	0
59	MG	CA	3029	1/1	0.93	0.09	56,56,56,56	0
59	MG	CF	303	1/1	0.93	0.14	51,51,51,51	0
59	MG	AA	3738	1/1	0.93	0.19	24,24,24,24	0
59	MG	CA	3094	1/1	0.93	0.21	59,59,59,59	0
59	MG	BA	1639	1/1	0.93	0.46	61,61,61,61	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
59	MG	CA	3402	1/1	0.93	0.09	66,66,66,66	0
59	MG	BA	1763	1/1	0.93	0.17	76,76,76,76	0
59	MG	CA	3484	1/1	0.93	0.26	78,78,78,78	0
59	MG	CA	3476	1/1	0.93	0.17	38,38,38,38	0
59	MG	CA	3051	1/1	0.93	0.74	57,57,57,57	0
59	MG	BA	1782	1/1	0.93	0.19	47,47,47,47	0
59	MG	AA	3178	1/1	0.93	0.36	48,48,48,48	0
59	MG	CA	3658	1/1	0.93	0.39	64,64,64,64	0
59	MG	AA	3038	1/1	0.93	0.45	29,29,29,29	1
59	MG	CA	3177	1/1	0.93	0.15	29,29,29,29	0
59	MG	BA	1664	1/1	0.94	0.14	56,56,56,56	0
59	MG	AA	3148	1/1	0.94	0.45	29,29,29,29	1
59	MG	AA	3276	1/1	0.94	0.24	67,67,67,67	0
59	MG	AA	3828	1/1	0.94	0.38	38,38,38,38	0
59	MG	AA	3759	1/1	0.94	0.10	57,57,57,57	0
59	MG	CA	3170	1/1	0.94	0.15	32,32,32,32	0
59	MG	CA	3421	1/1	0.94	0.20	57,57,57,57	0
59	MG	DA	1768	1/1	0.94	0.07	59,59,59,59	0
59	MG	CA	3166	1/1	0.94	0.31	27,27,27,27	0
59	MG	AD	310	1/1	0.94	0.39	78,78,78,78	0
59	MG	AA	3001	1/1	0.94	0.14	25,25,25,25	0
59	MG	A5	502	1/1	0.94	0.16	51,51,51,51	0
59	MG	CA	3661	1/1	0.94	0.23	27,27,27,27	0
59	MG	CA	3664	1/1	0.94	0.13	48,48,48,48	0
59	MG	AA	3370	1/1	0.94	0.15	47,47,47,47	0
59	MG	CA	3357	1/1	0.94	0.12	66,66,66,66	0
59	MG	BA	1726	1/1	0.94	0.20	46,46,46,46	0
59	MG	CA	3606	1/1	0.94	0.48	73,73,73,73	0
59	MG	CA	3370	1/1	0.94	0.14	41,41,41,41	0
59	MG	CA	3196	1/1	0.94	0.66	68,68,68,68	0
59	MG	DA	1602	1/1	0.94	0.10	45,45,45,45	0
59	MG	C1	101	1/1	0.94	0.18	57,57,57,57	0
59	MG	AA	3594	1/1	0.94	0.24	56,56,56,56	0
59	MG	AA	3628	1/1	0.94	0.23	70,70,70,70	0
59	MG	AA	3766	1/1	0.94	0.17	54,54,54,54	0
59	MG	AA	3615	1/1	0.94	0.25	43,43,43,43	0
59	MG	AA	3255	1/1	0.94	0.22	38,38,38,38	0
59	MG	AA	3081	1/1	0.94	0.21	56,56,56,56	0
59	MG	CA	3142	1/1	0.94	0.43	61,61,61,61	0
59	MG	AA	3289	1/1	0.94	0.43	53,53,53,53	0
59	MG	CA	3008	1/1	0.94	0.38	46,46,46,46	0
59	MG	AA	3451	1/1	0.94	0.07	57,57,57,57	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
59	MG	AA	3408	1/1	0.94	0.34	41,41,41,41	0
59	MG	DA	1647	1/1	0.94	0.15	51,51,51,51	0
59	MG	CA	3621	1/1	0.94	0.21	61,61,61,61	0
59	MG	CA	3316	1/1	0.94	0.17	43,43,43,43	0
59	MG	AA	3190	1/1	0.94	0.13	24,24,24,24	0
59	MG	AA	3672	1/1	0.94	0.15	48,48,48,48	0
59	MG	AA	3819	1/1	0.94	0.51	57,57,57,57	0
59	MG	AD	309	1/1	0.94	0.25	37,37,37,37	0
59	MG	CA	3283	1/1	0.94	0.12	31,31,31,31	0
59	MG	CA	3285	1/1	0.94	0.19	63,63,63,63	0
59	MG	CA	3607	1/1	0.94	0.09	64,64,64,64	0
59	MG	BA	1781	1/1	0.94	0.14	63,63,63,63	0
59	MG	AA	3573	1/1	0.94	0.16	12,12,12,12	0
59	MG	AA	3365	1/1	0.94	0.39	77,77,77,77	0
59	MG	CA	3533	1/1	0.94	0.18	45,45,45,45	0
59	MG	AA	3173	1/1	0.94	0.29	46,46,46,46	0
59	MG	AA	3743	1/1	0.94	0.16	67,67,67,67	0
59	MG	CA	3151	1/1	0.94	0.16	38,38,38,38	0
59	MG	AA	3279	1/1	0.94	0.23	34,34,34,34	0
59	MG	CA	3183	1/1	0.94	0.21	49,49,49,49	0
59	MG	CA	3359	1/1	0.94	0.08	33,33,33,33	0
59	MG	CA	3104	1/1	0.94	0.15	80,80,80,80	0
59	MG	AA	3245	1/1	0.94	0.17	11,11,11,11	0
59	MG	BA	1795	1/1	0.94	0.10	59,59,59,59	0
59	MG	DA	1723	1/1	0.94	0.13	53,53,53,53	0
59	MG	AA	3555	1/1	0.94	0.15	45,45,45,45	0
59	MG	AA	3387	1/1	0.94	0.08	29,29,29,29	0
59	MG	AA	3378	1/1	0.94	0.17	56,56,56,56	0
59	MG	CA	3269	1/1	0.94	0.14	81,81,81,81	0
59	MG	BA	1789	1/1	0.94	0.15	72,72,72,72	0
59	MG	AA	3455	1/1	0.94	0.20	32,32,32,32	1
59	MG	AA	3367	1/1	0.94	0.17	60,60,60,60	0
59	MG	AA	3337	1/1	0.94	0.16	75,75,75,75	0
59	MG	CA	3568	1/1	0.94	0.10	39,39,39,39	0
59	MG	CA	3248	1/1	0.94	0.42	53,53,53,53	0
59	MG	AA	3174	1/1	0.94	0.44	59,59,59,59	0
59	MG	DA	1640	1/1	0.94	0.31	77,77,77,77	0
59	MG	AA	3089	1/1	0.94	0.28	49,49,49,49	0
59	MG	AQ	204	1/1	0.94	0.23	86,86,86,86	0
59	MG	CA	3522	1/1	0.94	0.13	54,54,54,54	0
59	MG	DA	1706	1/1	0.94	0.33	66,66,66,66	0
59	MG	BA	1742	1/1	0.94	0.18	48,48,48,48	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
59	MG	BA	1651	1/1	0.94	0.33	55,55,55,55	0
59	MG	AA	3580	1/1	0.94	0.22	54,54,54,54	0
59	MG	AA	3071	1/1	0.94	0.60	40,40,40,40	0
59	MG	AA	3359	1/1	0.94	0.18	31,31,31,31	0
59	MG	CA	3003	1/1	0.94	0.30	62,62,62,62	0
59	MG	CA	3188	1/1	0.94	0.80	94,94,94,94	0
59	MG	CA	3643	1/1	0.94	0.17	79,79,79,79	0
59	MG	AA	3251	1/1	0.94	0.35	56,56,56,56	0
59	MG	AA	3606	1/1	0.94	0.24	34,34,34,34	0
59	MG	CA	3452	1/1	0.94	0.20	36,36,36,36	0
59	MG	CA	3048	1/1	0.94	0.10	47,47,47,47	0
59	MG	CA	3561	1/1	0.94	0.14	41,41,41,41	1
59	MG	AA	3448	1/1	0.94	0.12	62,62,62,62	0
59	MG	A8	5001	1/1	0.94	0.27	30,30,30,30	0
59	MG	AA	3620	1/1	0.94	0.11	22,22,22,22	0
59	MG	CA	3489	1/1	0.94	0.10	39,39,39,39	0
59	MG	AA	3254	1/1	0.94	0.25	52,52,52,52	0
59	MG	AB	3018	1/1	0.94	0.22	69,69,69,69	0
59	MG	AA	3704	1/1	0.94	0.19	49,49,49,49	0
59	MG	AA	3518	1/1	0.94	0.17	14,14,14,14	0
59	MG	CA	3410	1/1	0.94	0.22	25,25,25,25	0
59	MG	AA	3361	1/1	0.94	0.16	53,53,53,53	0
59	MG	BA	1745	1/1	0.94	0.20	46,46,46,46	0
59	MG	AA	3050	1/1	0.94	0.27	28,28,28,28	0
59	MG	AA	3413	1/1	0.94	0.19	25,25,25,25	0
59	MG	CA	3393	1/1	0.94	0.07	68,68,68,68	0
59	MG	AA	3207	1/1	0.94	0.20	60,60,60,60	0
59	MG	AA	3711	1/1	0.94	0.35	43,43,43,43	1
59	MG	CA	3253	1/1	0.94	0.17	70,70,70,70	0
59	MG	AA	3265	1/1	0.94	0.17	43,43,43,43	0
59	MG	AA	3217	1/1	0.94	0.44	29,29,29,29	1
59	MG	BW	501	1/1	0.94	0.22	47,47,47,47	0
59	MG	AA	3236	1/1	0.94	0.14	57,57,57,57	0
59	MG	CA	3504	1/1	0.94	0.13	79,79,79,79	0
59	MG	AA	3474	1/1	0.94	0.15	18,18,18,18	1
59	MG	DA	1710	1/1	0.94	0.25	104,104,104,104	0
59	MG	CA	3063	1/1	0.94	0.10	34,34,34,34	0
59	MG	AA	3443	1/1	0.94	0.19	33,33,33,33	0
59	MG	CA	3590	1/1	0.94	0.10	59,59,59,59	0
59	MG	CD	304	1/1	0.94	0.29	28,28,28,28	0
59	MG	CA	3441	1/1	0.94	0.23	56,56,56,56	0
59	MG	AA	3324	1/1	0.94	0.14	15,15,15,15	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
59	MG	CA	3190	1/1	0.94	0.23	66,66,66,66	0
59	MG	CA	3635	1/1	0.94	0.23	48,48,48,48	0
59	MG	AA	3572	1/1	0.94	0.20	17,17,17,17	0
59	MG	AA	3662	1/1	0.94	0.07	60,60,60,60	0
59	MG	AA	3549	1/1	0.94	0.05	66,66,66,66	0
59	MG	CA	3018	1/1	0.94	0.08	41,41,41,41	0
59	MG	AA	3004	1/1	0.94	0.15	21,21,21,21	0
59	MG	AA	3610	1/1	0.94	0.22	59,59,59,59	0
59	MG	AA	3257	1/1	0.94	0.32	54,54,54,54	0
59	MG	CA	3399	1/1	0.94	0.07	57,57,57,57	0
59	MG	AA	3351	1/1	0.94	0.21	29,29,29,29	0
59	MG	DA	1698	1/1	0.94	0.33	97,97,97,97	0
59	MG	CA	3493	1/1	0.94	0.52	65,65,65,65	0
59	MG	CA	3132	1/1	0.94	0.16	48,48,48,48	0
59	MG	DA	1743	1/1	0.94	0.13	59,59,59,59	0
60	ZN	A4	501	1/1	0.94	0.07	117,117,117,117	0
59	MG	BA	1801	1/1	0.94	0.09	65,65,65,65	0
59	MG	AA	3719	1/1	0.94	0.10	59,59,59,59	0
59	MG	AA	3039	1/1	0.94	0.52	34,34,34,34	1
59	MG	DA	1762	1/1	0.94	0.20	61,61,61,61	0
59	MG	CA	3429	1/1	0.94	0.26	59,59,59,59	0
59	MG	DA	1709	1/1	0.94	0.16	70,70,70,70	0
59	MG	CA	3578	1/1	0.94	0.09	38,38,38,38	0
59	MG	DA	1695	1/1	0.94	0.17	63,63,63,63	0
59	MG	AA	3495	1/1	0.94	0.15	35,35,35,35	0
59	MG	AA	3030	1/1	0.94	0.29	24,24,24,24	1
59	MG	AA	3374	1/1	0.94	0.31	49,49,49,49	0
59	MG	AA	3170	1/1	0.94	0.19	54,54,54,54	0
59	MG	CA	3483	1/1	0.94	0.32	64,64,64,64	0
59	MG	AA	3278	1/1	0.94	0.21	60,60,60,60	0
59	MG	AA	3784	1/1	0.94	0.21	59,59,59,59	0
59	MG	CA	3470	1/1	0.94	0.19	74,74,74,74	0
59	MG	AA	3218	1/1	0.94	0.09	67,67,67,67	0
59	MG	BA	1636	1/1	0.94	0.17	57,57,57,57	0
59	MG	CA	3531	1/1	0.94	0.09	47,47,47,47	0
59	MG	DA	1612	1/1	0.94	0.13	57,57,57,57	0
59	MG	CA	3182	1/1	0.94	0.31	38,38,38,38	0
59	MG	CA	3622	1/1	0.94	0.17	50,50,50,50	0
59	MG	AA	3490	1/1	0.94	0.16	27,27,27,27	0
59	MG	AA	3048	1/1	0.95	0.16	28,28,28,28	0
59	MG	AB	3022	1/1	0.95	0.12	61,61,61,61	0
59	MG	AA	3509	1/1	0.95	0.16	40,40,40,40	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
59	MG	AA	3187	1/1	0.95	0.29	56,56,56,56	0
59	MG	AA	3333	1/1	0.95	0.20	11,11,11,11	0
59	MG	DA	1685	1/1	0.95	0.10	46,46,46,46	0
59	MG	BA	1809	1/1	0.95	0.23	61,61,61,61	0
59	MG	DA	1747	1/1	0.95	0.14	48,48,48,48	0
59	MG	AA	3588	1/1	0.95	0.15	47,47,47,47	0
59	MG	AA	3590	1/1	0.95	0.17	60,60,60,60	0
59	MG	AA	3658	1/1	0.95	0.21	42,42,42,42	0
59	MG	AA	3271	1/1	0.95	0.33	34,34,34,34	0
59	MG	DA	1707	1/1	0.95	0.07	61,61,61,61	0
59	MG	AA	3112	1/1	0.95	0.14	61,61,61,61	0
59	MG	BA	1692	1/1	0.95	0.28	55,55,55,55	0
59	MG	CA	3281	1/1	0.95	0.23	21,21,21,21	0
59	MG	AA	3689	1/1	0.95	0.09	35,35,35,35	0
59	MG	AA	3420	1/1	0.95	0.15	25,25,25,25	1
59	MG	AW	3003	1/1	0.95	0.25	28,28,28,28	0
59	MG	AB	3013	1/1	0.95	0.15	53,53,53,53	0
59	MG	AA	3757	1/1	0.95	0.07	14,14,14,14	0
59	MG	AA	3176	1/1	0.95	0.32	70,70,70,70	0
59	MG	CA	3185	1/1	0.95	0.29	48,48,48,48	0
59	MG	C5	101	1/1	0.95	0.49	66,66,66,66	0
59	MG	AA	3013	1/1	0.95	0.18	28,28,28,28	0
59	MG	AA	3685	1/1	0.95	0.19	72,72,72,72	0
59	MG	CA	3107	1/1	0.95	0.26	77,77,77,77	0
59	MG	AA	3384	1/1	0.95	0.21	22,22,22,22	0
59	MG	AF	306	1/1	0.95	0.24	57,57,57,57	0
59	MG	CA	3268	1/1	0.95	0.17	52,52,52,52	0
59	MG	AA	3221	1/1	0.95	0.15	30,30,30,30	0
59	MG	AA	3006	1/1	0.95	0.34	52,52,52,52	0
59	MG	CA	3346	1/1	0.95	0.19	30,30,30,30	0
59	MG	CA	3318	1/1	0.95	0.21	24,24,24,24	0
59	MG	CA	3147	1/1	0.95	0.29	55,55,55,55	0
59	MG	CA	3375	1/1	0.95	0.34	68,68,68,68	0
59	MG	AA	3478	1/1	0.95	0.24	33,33,33,33	0
59	MG	AA	3697	1/1	0.95	0.23	40,40,40,40	0
59	MG	CA	3213	1/1	0.95	0.27	51,51,51,51	0
59	MG	AA	3132	1/1	0.95	0.21	41,41,41,41	0
59	MG	AA	3762	1/1	0.95	0.14	23,23,23,23	0
59	MG	BA	1749	1/1	0.95	0.32	61,61,61,61	0
59	MG	AA	3330	1/1	0.95	0.06	66,66,66,66	0
59	MG	CA	3009	1/1	0.95	0.10	27,27,27,27	0
59	MG	DA	1750	1/1	0.95	0.08	67,67,67,67	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
59	MG	AA	3652	1/1	0.95	0.14	53,53,53,53	0
59	MG	A9	502	1/1	0.95	0.24	41,41,41,41	0
59	MG	DA	1760	1/1	0.95	0.14	61,61,61,61	0
59	MG	AA	3637	1/1	0.95	0.33	17,17,17,17	1
59	MG	AH	201	1/1	0.95	0.85	64,64,64,64	0
59	MG	BA	1717	1/1	0.95	0.18	78,78,78,78	0
59	MG	AD	304	1/1	0.95	0.35	41,41,41,41	0
59	MG	CA	3440	1/1	0.95	0.31	49,49,49,49	0
59	MG	CA	3198	1/1	0.95	0.23	34,34,34,34	0
59	MG	CA	3144	1/1	0.95	0.23	40,40,40,40	0
59	MG	DA	1615	1/1	0.95	0.25	58,58,58,58	0
59	MG	AA	3510	1/1	0.95	0.24	17,17,17,17	0
59	MG	CW	201	1/1	0.95	0.36	46,46,46,46	0
59	MG	AA	3064	1/1	0.95	0.13	32,32,32,32	0
59	MG	CA	3469	1/1	0.95	0.22	61,61,61,61	0
59	MG	AA	3104	1/1	0.95	0.32	54,54,54,54	0
59	MG	BA	1680	1/1	0.95	0.19	40,40,40,40	0
59	MG	CA	3552	1/1	0.95	0.18	30,30,30,30	0
59	MG	BA	1674	1/1	0.95	0.57	48,48,48,48	0
59	MG	AA	3521	1/1	0.95	0.18	19,19,19,19	0
59	MG	AA	3574	1/1	0.95	0.17	12,12,12,12	0
59	MG	CE	305	1/1	0.95	0.04	58,58,58,58	0
59	MG	AA	3200	1/1	0.95	0.22	30,30,30,30	0
59	MG	AA	3806	1/1	0.95	0.18	42,42,42,42	0
59	MG	AA	3632	1/1	0.95	0.20	54,54,54,54	0
59	MG	AA	3530	1/1	0.95	0.19	20,20,20,20	1
59	MG	AA	3513	1/1	0.95	0.10	41,41,41,41	0
59	MG	AA	3494	1/1	0.95	0.09	34,34,34,34	0
59	MG	AO	5001	1/1	0.95	0.09	34,34,34,34	0
59	MG	AA	3706	1/1	0.95	0.54	41,41,41,41	1
59	MG	CA	3303	1/1	0.95	0.35	43,43,43,43	0
59	MG	AA	3441	1/1	0.95	0.29	58,58,58,58	0
59	MG	AA	3684	1/1	0.95	0.25	51,51,51,51	0
59	MG	BA	1626	1/1	0.95	0.12	41,41,41,41	0
59	MG	CA	3543	1/1	0.95	0.19	71,71,71,71	0
59	MG	AA	3425	1/1	0.95	0.05	77,77,77,77	0
59	MG	AA	3290	1/1	0.95	0.13	64,64,64,64	0
59	MG	AA	3501	1/1	0.95	0.06	49,49,49,49	0
59	MG	CA	3562	1/1	0.95	0.14	29,29,29,29	0
59	MG	AA	3493	1/1	0.95	0.10	77,77,77,77	0
59	MG	CA	3265	1/1	0.95	0.29	61,61,61,61	0
59	MG	AA	3117	1/1	0.95	0.24	25,25,25,25	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
59	MG	DA	1687	1/1	0.95	0.42	56,56,56,56	0
59	MG	CA	3337	1/1	0.95	0.14	20,20,20,20	0
59	MG	DA	1763	1/1	0.95	0.30	76,76,76,76	0
59	MG	AA	3392	1/1	0.95	0.24	17,17,17,17	0
59	MG	CA	3601	1/1	0.95	0.13	57,57,57,57	0
59	MG	AA	3299	1/1	0.95	0.26	47,47,47,47	0
59	MG	CA	3480	1/1	0.95	0.21	50,50,50,50	0
59	MG	CA	3455	1/1	0.95	0.28	49,49,49,49	0
59	MG	CA	3416	1/1	0.95	0.14	44,44,44,44	0
59	MG	DA	1719	1/1	0.95	0.38	61,61,61,61	0
59	MG	AA	3417	1/1	0.95	0.18	25,25,25,25	0
59	MG	AA	3829	1/1	0.95	0.24	47,47,47,47	0
59	MG	CA	3354	1/1	0.95	0.25	49,49,49,49	0
59	MG	AA	3325	1/1	0.95	0.16	70,70,70,70	0
59	MG	AA	3508	1/1	0.95	0.18	43,43,43,43	0
59	MG	AA	3520	1/1	0.95	0.14	17,17,17,17	0
59	MG	CA	3397	1/1	0.95	0.15	57,57,57,57	0
59	MG	AA	3790	1/1	0.95	0.46	57,57,57,57	0
59	MG	CA	3445	1/1	0.95	0.20	22,22,22,22	0
59	MG	AA	3160	1/1	0.95	0.15	30,30,30,30	0
59	MG	AA	3137	1/1	0.95	0.63	53,53,53,53	0
59	MG	CA	3349	1/1	0.95	0.20	23,23,23,23	0
59	MG	BA	1771	1/1	0.95	0.21	65,65,65,65	0
59	MG	AA	3671	1/1	0.95	0.23	19,19,19,19	0
59	MG	BA	1783	1/1	0.95	0.18	57,57,57,57	0
59	MG	DA	1752	1/1	0.95	0.16	52,52,52,52	0
59	MG	AA	3560	1/1	0.95	0.13	29,29,29,29	0
59	MG	DA	1734	1/1	0.95	0.14	65,65,65,65	0
59	MG	AA	3737	1/1	0.95	0.16	54,54,54,54	0
59	MG	CA	3121	1/1	0.95	0.13	49,49,49,49	0
59	MG	AA	3348	1/1	0.95	0.06	53,53,53,53	0
59	MG	AA	3686	1/1	0.95	0.20	61,61,61,61	0
59	MG	AA	3794	1/1	0.95	0.42	60,60,60,60	0
59	MG	CA	3263	1/1	0.95	0.14	64,64,64,64	0
59	MG	CA	3024	1/1	0.95	0.29	100,100,100,100	0
59	MG	AA	3052	1/1	0.95	0.16	11,11,11,11	0
59	MG	AA	3502	1/1	0.95	0.13	29,29,29,29	1
59	MG	CA	3321	1/1	0.95	0.13	28,28,28,28	0
59	MG	CA	3639	1/1	0.95	0.59	61,61,61,61	0
59	MG	CA	3252	1/1	0.95	0.19	62,62,62,62	0
59	MG	AA	3393	1/1	0.95	0.20	23,23,23,23	0
59	MG	AA	3522	1/1	0.95	0.16	30,30,30,30	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
59	MG	CA	3645	1/1	0.95	0.11	69,69,69,69	0
59	MG	AA	3400	1/1	0.95	0.17	13,13,13,13	0
59	MG	CU	201	1/1	0.95	0.48	74,74,74,74	0
59	MG	AA	3044	1/1	0.95	0.37	52,52,52,52	0
59	MG	DA	1725	1/1	0.95	0.17	58,58,58,58	0
59	MG	DA	1619	1/1	0.95	0.59	59,59,59,59	0
59	MG	AA	3193	1/1	0.95	0.20	40,40,40,40	0
59	MG	DA	1766	1/1	0.95	0.12	74,74,74,74	0
59	MG	AA	3812	1/1	0.95	0.17	41,41,41,41	0
59	MG	AA	3431	1/1	0.95	0.15	25,25,25,25	0
59	MG	AA	3533	1/1	0.95	0.17	22,22,22,22	0
59	MG	AA	3804	1/1	0.95	0.18	50,50,50,50	0
59	MG	AA	3188	1/1	0.95	0.18	31,31,31,31	0
59	MG	BA	1799	1/1	0.95	0.13	64,64,64,64	0
59	MG	AA	3548	1/1	0.95	0.11	7,7,7,7	0
59	MG	AA	3824	1/1	0.95	0.58	72,72,72,72	0
59	MG	BA	1627	1/1	0.95	0.23	51,51,51,51	0
59	MG	AG	202	1/1	0.95	0.06	54,54,54,54	0
59	MG	AA	3785	1/1	0.95	0.15	61,61,61,61	0
59	MG	AA	3036	1/1	0.95	0.24	25,25,25,25	0
59	MG	AA	3022	1/1	0.95	0.12	5,5,5,5	0
59	MG	CA	3451	1/1	0.95	0.21	62,62,62,62	0
59	MG	AA	3260	1/1	0.95	0.17	21,21,21,21	0
59	MG	AA	3503	1/1	0.95	0.06	54,54,54,54	0
59	MG	AU	205	1/1	0.95	0.26	45,45,45,45	0
59	MG	AA	3099	1/1	0.95	0.10	53,53,53,53	0
59	MG	AA	3674	1/1	0.95	0.14	30,30,30,30	0
59	MG	AA	3504	1/1	0.95	0.09	29,29,29,29	0
59	MG	CA	3305	1/1	0.95	0.27	48,48,48,48	0
59	MG	AA	3021	1/1	0.95	0.13	33,33,33,33	0
59	MG	CA	3356	1/1	0.95	0.19	44,44,44,44	0
59	MG	AA	3687	1/1	0.95	0.29	52,52,52,52	0
59	MG	CA	3012	1/1	0.95	0.15	65,65,65,65	0
59	MG	AN	3002	1/1	0.96	0.45	69,69,69,69	0
62	GDP	DZ	703	28/28	0.96	0.14	66,66,66,66	1
59	MG	CA	3286	1/1	0.96	0.20	58,58,58,58	0
59	MG	AA	3507	1/1	0.96	0.15	50,50,50,50	0
59	MG	AA	3538	1/1	0.96	0.15	15,15,15,15	0
59	MG	CA	3574	1/1	0.96	0.15	37,37,37,37	0
59	MG	C0	101	1/1	0.96	0.17	59,59,59,59	0
59	MG	AA	3581	1/1	0.96	0.17	52,52,52,52	0
59	MG	AA	3239	1/1	0.96	0.27	25,25,25,25	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
59	MG	CA	3102	1/1	0.96	0.50	62,62,62,62	0
59	MG	AA	3728	1/1	0.96	0.26	29,29,29,29	0
59	MG	BA	1681	1/1	0.96	0.09	53,53,53,53	0
59	MG	AA	3116	1/1	0.96	0.63	35,35,35,35	0
59	MG	AA	3605	1/1	0.96	0.32	45,45,45,45	0
59	MG	AA	3263	1/1	0.96	0.42	24,24,24,24	1
59	MG	CA	3347	1/1	0.96	0.15	45,45,45,45	0
59	MG	AA	3725	1/1	0.96	0.15	13,13,13,13	0
59	MG	AA	3029	1/1	0.96	0.24	28,28,28,28	0
59	MG	BA	1808	1/1	0.96	0.16	54,54,54,54	0
59	MG	CA	3299	1/1	0.96	0.14	64,64,64,64	0
59	MG	CA	3662	1/1	0.96	0.32	33,33,33,33	0
59	MG	CA	3162	1/1	0.96	0.39	31,31,31,31	0
59	MG	AA	3389	1/1	0.96	0.15	25,25,25,25	0
59	MG	AA	3529	1/1	0.96	0.20	30,30,30,30	0
59	MG	CA	3028	1/1	0.96	0.63	51,51,51,51	0
59	MG	AA	3350	1/1	0.96	0.08	36,36,36,36	0
59	MG	BL	202	1/1	0.96	0.17	54,54,54,54	0
59	MG	CA	3464	1/1	0.96	0.18	36,36,36,36	0
59	MG	CA	3366	1/1	0.96	0.16	49,49,49,49	0
59	MG	BA	1678	1/1	0.96	0.21	54,54,54,54	0
59	MG	CA	3295	1/1	0.96	0.26	66,66,66,66	0
59	MG	BT	3001	1/1	0.96	0.12	46,46,46,46	0
59	MG	AU	202	1/1	0.96	0.45	82,82,82,82	0
59	MG	AA	3403	1/1	0.96	0.34	42,42,42,42	0
59	MG	CA	3461	1/1	0.96	0.15	34,34,34,34	0
59	MG	BM	201	1/1	0.96	0.04	62,62,62,62	0
59	MG	AA	3349	1/1	0.96	0.17	47,47,47,47	0
59	MG	AF	304	1/1	0.96	0.29	36,36,36,36	0
59	MG	DA	1740	1/1	0.96	0.57	68,68,68,68	0
59	MG	CA	3335	1/1	0.96	0.20	66,66,66,66	0
59	MG	AA	3435	1/1	0.96	0.17	52,52,52,52	0
59	MG	BA	1798	1/1	0.96	0.41	73,73,73,73	0
59	MG	CA	3277	1/1	0.96	0.18	55,55,55,55	0
59	MG	AA	3119	1/1	0.96	0.31	47,47,47,47	0
59	MG	CA	3160	1/1	0.96	0.39	57,57,57,57	0
59	MG	DA	1765	1/1	0.96	0.13	64,64,64,64	0
59	MG	CA	3611	1/1	0.96	0.15	59,59,59,59	0
59	MG	AA	3471	1/1	0.96	0.08	56,56,56,56	0
59	MG	CA	3360	1/1	0.96	0.17	38,38,38,38	0
59	MG	AA	3798	1/1	0.96	0.22	25,25,25,25	0
59	MG	DD	502	1/1	0.96	0.48	50,50,50,50	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
60	ZN	DN	501	1/1	0.96	0.08	117,117,117,117	0
59	MG	AA	3312	1/1	0.96	0.10	23,23,23,23	0
59	MG	AA	3670	1/1	0.96	0.08	54,54,54,54	0
59	MG	AA	3343	1/1	0.96	0.10	46,46,46,46	0
59	MG	CA	3218	1/1	0.96	0.36	40,40,40,40	0
59	MG	BA	1632	1/1	0.96	0.08	48,48,48,48	0
59	MG	CA	3327	1/1	0.96	0.16	38,38,38,38	0
59	MG	AA	3506	1/1	0.96	0.10	48,48,48,48	0
59	MG	AA	3322	1/1	0.96	0.20	61,61,61,61	0
59	MG	AA	3007	1/1	0.96	0.14	12,12,12,12	0
59	MG	AA	3426	1/1	0.96	0.17	20,20,20,20	0
59	MG	CB	3006	1/1	0.96	0.06	71,71,71,71	0
59	MG	CA	3637	1/1	0.96	0.47	61,61,61,61	0
59	MG	BA	1606	1/1	0.96	0.28	126,126,126,126	0
59	MG	AA	3462	1/1	0.96	0.09	54,54,54,54	0
59	MG	AA	3404	1/1	0.96	0.20	27,27,27,27	0
59	MG	CA	3262	1/1	0.96	0.12	11,11,11,11	0
59	MG	AA	3621	1/1	0.96	0.07	17,17,17,17	0
59	MG	CA	3418	1/1	0.96	0.29	34,34,34,34	0
59	MG	CA	3344	1/1	0.96	0.07	68,68,68,68	0
59	MG	CA	3330	1/1	0.96	0.21	36,36,36,36	0
59	MG	AA	3092	1/1	0.96	0.17	39,39,39,39	0
59	MG	AA	3272	1/1	0.96	0.16	55,55,55,55	0
59	MG	AA	3386	1/1	0.96	0.12	45,45,45,45	0
59	MG	DA	1714	1/1	0.96	0.15	68,68,68,68	0
59	MG	DA	1671	1/1	0.96	0.36	56,56,56,56	0
59	MG	CA	3491	1/1	0.96	0.06	44,44,44,44	0
59	MG	AA	3690	1/1	0.96	0.20	50,50,50,50	0
59	MG	AA	3668	1/1	0.96	0.17	54,54,54,54	0
59	MG	BA	1715	1/1	0.96	0.11	60,60,60,60	0
59	MG	CA	3362	1/1	0.96	0.12	43,43,43,43	0
59	MG	DA	1720	1/1	0.96	0.10	60,60,60,60	0
59	MG	CA	3584	1/1	0.96	0.15	32,32,32,32	0
59	MG	DZ	702	1/1	0.96	0.22	57,57,57,57	0
59	MG	CA	3004	1/1	0.96	0.14	49,49,49,49	0
59	MG	AA	3259	1/1	0.96	0.34	41,41,41,41	1
59	MG	AA	3532	1/1	0.96	0.20	20,20,20,20	0
59	MG	AA	3353	1/1	0.96	0.22	39,39,39,39	0
59	MG	CB	3010	1/1	0.96	0.13	51,51,51,51	0
59	MG	AA	3340	1/1	0.96	0.22	3,3,3,3	0
59	MG	AA	3710	1/1	0.96	0.51	29,29,29,29	1
59	MG	AA	3805	1/1	0.96	0.21	58,58,58,58	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
59	MG	CA	3300	1/1	0.96	0.12	47,47,47,47	0
59	MG	AA	3593	1/1	0.96	0.22	15,15,15,15	1
59	MG	CD	301	1/1	0.96	0.44	43,43,43,43	0
59	MG	AA	3305	1/1	0.96	0.16	25,25,25,25	0
59	MG	DA	1628	1/1	0.96	0.09	39,39,39,39	0
59	MG	CA	3324	1/1	0.96	0.17	26,26,26,26	0
59	MG	CA	3617	1/1	0.96	0.13	41,41,41,41	0
59	MG	CA	3290	1/1	0.96	0.33	34,34,34,34	0
59	MG	CA	3355	1/1	0.96	0.14	35,35,35,35	0
59	MG	AA	3692	1/1	0.96	0.15	36,36,36,36	1
59	MG	AA	3136	1/1	0.96	0.64	63,63,63,63	0
59	MG	AA	3703	1/1	0.96	0.23	56,56,56,56	0
59	MG	AA	3301	1/1	0.96	0.30	39,39,39,39	0
59	MG	AA	3382	1/1	0.96	0.12	37,37,37,37	0
59	MG	AA	3247	1/1	0.96	0.16	55,55,55,55	0
59	MG	AA	3599	1/1	0.96	0.16	59,59,59,59	0
59	MG	CA	3232	1/1	0.96	0.17	54,54,54,54	0
59	MG	DA	1693	1/1	0.96	0.14	67,67,67,67	0
59	MG	CA	3099	1/1	0.96	0.25	58,58,58,58	0
59	MG	AA	3550	1/1	0.96	0.20	38,38,38,38	0
59	MG	AA	3396	1/1	0.96	0.17	16,16,16,16	0
59	MG	AA	3566	1/1	0.96	0.05	56,56,56,56	0
59	MG	AA	3201	1/1	0.96	0.09	53,53,53,53	0
59	MG	AA	3129	1/1	0.96	0.18	34,34,34,34	1
59	MG	AA	3341	1/1	0.96	0.19	25,25,25,25	0
59	MG	AA	3032	1/1	0.96	0.33	59,59,59,59	0
59	MG	AA	3720	1/1	0.96	0.16	55,55,55,55	0
59	MG	AA	3500	1/1	0.96	0.12	59,59,59,59	0
59	MG	AA	3570	1/1	0.96	0.15	14,14,14,14	0
59	MG	AA	3131	1/1	0.96	0.26	63,63,63,63	0
59	MG	AA	3094	1/1	0.96	0.24	80,80,80,80	0
59	MG	AA	3228	1/1	0.96	0.30	32,32,32,32	0
59	MG	DA	1764	1/1	0.96	0.08	71,71,71,71	0
59	MG	AV	202	1/1	0.96	0.23	33,33,33,33	0
59	MG	CA	3062	1/1	0.96	0.29	38,38,38,38	0
59	MG	BA	1766	1/1	0.96	0.14	62,62,62,62	0
59	MG	AA	3802	1/1	0.96	0.15	86,86,86,86	0
59	MG	AA	3791	1/1	0.96	0.17	51,51,51,51	0
59	MG	AA	3813	1/1	0.96	0.19	29,29,29,29	1
59	MG	DA	1731	1/1	0.96	0.09	49,49,49,49	0
59	MG	AA	3647	1/1	0.96	0.11	43,43,43,43	0
59	MG	DA	1630	1/1	0.96	0.71	62,62,62,62	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
59	MG	AA	3758	1/1	0.96	0.28	43,43,43,43	1
59	MG	BA	1653	1/1	0.96	0.10	56,56,56,56	0
59	MG	BZ	701	1/1	0.96	0.19	49,49,49,49	0
59	MG	CA	3338	1/1	0.96	0.14	64,64,64,64	0
59	MG	AA	3375	1/1	0.96	0.29	48,48,48,48	0
59	MG	CA	3439	1/1	0.96	0.23	32,32,32,32	0
59	MG	AA	3688	1/1	0.96	0.15	25,25,25,25	0
59	MG	DA	1721	1/1	0.96	0.09	80,80,80,80	0
59	MG	CA	3394	1/1	0.96	0.12	69,69,69,69	0
59	MG	CA	3074	1/1	0.96	0.33	49,49,49,49	0
59	MG	BA	1615	1/1	0.96	0.28	62,62,62,62	0
59	MG	AB	3007	1/1	0.96	0.07	39,39,39,39	0
59	MG	AA	3546	1/1	0.96	0.14	60,60,60,60	0
59	MG	AA	3336	1/1	0.96	0.14	51,51,51,51	0
59	MG	AA	3121	1/1	0.96	0.16	53,53,53,53	0
59	MG	AA	3423	1/1	0.96	0.20	16,16,16,16	0
59	MG	AA	3185	1/1	0.96	0.16	76,76,76,76	0
59	MG	AA	3084	1/1	0.96	0.10	23,23,23,23	0
59	MG	CA	3320	1/1	0.96	0.16	36,36,36,36	0
59	MG	AA	3491	1/1	0.96	0.09	46,46,46,46	0
59	MG	BF	3001	1/1	0.96	0.17	49,49,49,49	0
59	MG	CA	3123	1/1	0.96	0.09	29,29,29,29	0
59	MG	AA	3059	1/1	0.96	0.36	40,40,40,40	0
59	MG	AA	3399	1/1	0.96	0.15	16,16,16,16	0
59	MG	AA	3468	1/1	0.96	0.06	55,55,55,55	0
59	MG	CO	5001	1/1	0.96	0.17	50,50,50,50	0
59	MG	AA	3547	1/1	0.96	0.26	60,60,60,60	0
59	MG	CA	3054	1/1	0.96	0.25	36,36,36,36	0
59	MG	AA	3742	1/1	0.96	0.12	68,68,68,68	0
59	MG	CA	3471	1/1	0.96	0.19	33,33,33,33	0
59	MG	CA	3326	1/1	0.96	0.24	28,28,28,28	0
59	MG	AA	3114	1/1	0.96	0.21	26,26,26,26	0
59	MG	CA	3659	1/1	0.96	0.10	55,55,55,55	0
59	MG	AA	3318	1/1	0.96	0.16	23,23,23,23	0
59	MG	AA	3113	1/1	0.96	0.32	45,45,45,45	0
59	MG	AA	3537	1/1	0.96	0.17	20,20,20,20	0
59	MG	AA	3042	1/1	0.96	0.24	32,32,32,32	0
59	MG	AA	3307	1/1	0.96	0.34	61,61,61,61	0
59	MG	AA	3107	1/1	0.96	0.12	49,49,49,49	0
59	MG	AA	3511	1/1	0.96	0.20	14,14,14,14	0
59	MG	CA	3106	1/1	0.96	0.13	66,66,66,66	0
59	MG	DA	1711	1/1	0.96	0.12	60,60,60,60	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
59	MG	AA	3531	1/1	0.96	0.13	24,24,24,24	0
59	MG	CA	3381	1/1	0.96	0.14	50,50,50,50	0
59	MG	CA	3519	1/1	0.96	0.22	48,48,48,48	0
59	MG	AA	3008	1/1	0.96	0.21	26,26,26,26	0
59	MG	CA	3010	1/1	0.96	0.19	43,43,43,43	0
59	MG	AA	3383	1/1	0.96	0.16	20,20,20,20	0
59	MG	CA	3047	1/1	0.96	0.16	84,84,84,84	0
59	MG	AB	3023	1/1	0.96	0.35	54,54,54,54	0
59	MG	AP	201	1/1	0.96	0.32	21,21,21,21	1
59	MG	DA	1696	1/1	0.96	0.17	53,53,53,53	0
59	MG	AA	3469	1/1	0.96	0.12	32,32,32,32	0
59	MG	BA	1684	1/1	0.96	0.27	61,61,61,61	0
59	MG	AA	3291	1/1	0.96	0.28	45,45,45,45	0
59	MG	AA	3388	1/1	0.96	0.08	28,28,28,28	0
59	MG	DA	1716	1/1	0.96	0.10	57,57,57,57	0
59	MG	AA	3306	1/1	0.96	0.25	52,52,52,52	0
59	MG	CG	3001	1/1	0.96	0.10	65,65,65,65	0
59	MG	AA	3262	1/1	0.96	0.14	15,15,15,15	0
59	MG	AA	3568	1/1	0.96	0.18	15,15,15,15	0
59	MG	AA	3210	1/1	0.96	0.31	59,59,59,59	1
59	MG	DA	1649	1/1	0.96	0.33	69,69,69,69	0
59	MG	DA	1645	1/1	0.96	0.10	58,58,58,58	0
59	MG	CA	3255	1/1	0.96	0.24	28,28,28,28	0
59	MG	BA	1770	1/1	0.96	0.12	54,54,54,54	0
59	MG	AA	3567	1/1	0.96	0.11	26,26,26,26	0
59	MG	AA	3564	1/1	0.96	0.20	44,44,44,44	0
59	MG	AA	3750	1/1	0.96	0.33	51,51,51,51	0
59	MG	AA	3329	1/1	0.96	0.08	40,40,40,40	1
59	MG	CA	3133	1/1	0.97	0.20	85,85,85,85	0
59	MG	BA	1752	1/1	0.97	0.27	59,59,59,59	0
59	MG	AA	3098	1/1	0.97	0.27	51,51,51,51	0
59	MG	AA	3334	1/1	0.97	0.14	63,63,63,63	0
59	MG	AA	3517	1/1	0.97	0.07	23,23,23,23	0
59	MG	AA	3713	1/1	0.97	0.22	27,27,27,27	0
59	MG	AA	3691	1/1	0.97	0.23	62,62,62,62	0
59	MG	AA	3100	1/1	0.97	0.24	29,29,29,29	0
60	ZN	CY	501	1/1	0.97	0.06	101,101,101,101	0
59	MG	AA	3665	1/1	0.97	0.30	40,40,40,40	0
59	MG	AA	3223	1/1	0.97	0.11	15,15,15,15	0
59	MG	AA	3543	1/1	0.97	0.22	32,32,32,32	0
59	MG	AA	3554	1/1	0.97	0.19	40,40,40,40	0
59	MG	CA	3497	1/1	0.97	0.09	45,45,45,45	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
59	MG	AA	3379	1/1	0.97	0.26	23,23,23,23	0
59	MG	AU	201	1/1	0.97	0.19	25,25,25,25	0
59	MG	AA	3497	1/1	0.97	0.13	44,44,44,44	0
59	MG	CA	3556	1/1	0.97	0.18	62,62,62,62	0
59	MG	BA	1785	1/1	0.97	0.17	62,62,62,62	0
59	MG	CA	3554	1/1	0.97	0.09	66,66,66,66	0
60	ZN	C6	501	1/1	0.97	0.10	66,66,66,66	0
59	MG	AA	3821	1/1	0.97	0.19	38,38,38,38	0
59	MG	CA	3220	1/1	0.97	0.07	59,59,59,59	0
59	MG	AA	3111	1/1	0.97	0.23	24,24,24,24	0
59	MG	AA	3125	1/1	0.97	0.16	22,22,22,22	1
59	MG	AA	3430	1/1	0.97	0.16	39,39,39,39	0
59	MG	BA	1761	1/1	0.97	0.16	62,62,62,62	0
59	MG	AA	3473	1/1	0.97	0.07	53,53,53,53	0
59	MG	CA	3571	1/1	0.97	0.26	45,45,45,45	0
59	MG	CA	3652	1/1	0.97	0.13	23,23,23,23	0
59	MG	AA	3539	1/1	0.97	0.14	34,34,34,34	0
59	MG	BA	1725	1/1	0.97	0.24	54,54,54,54	0
59	MG	CA	3231	1/1	0.97	0.72	60,60,60,60	0
59	MG	CA	3422	1/1	0.97	0.24	43,43,43,43	0
59	MG	AA	3283	1/1	0.97	0.33	43,43,43,43	0
59	MG	CA	3109	1/1	0.97	0.22	35,35,35,35	0
59	MG	AA	3406	1/1	0.97	0.09	20,20,20,20	0
59	MG	CA	3217	1/1	0.97	0.26	62,62,62,62	0
59	MG	CA	3364	1/1	0.97	0.10	22,22,22,22	0
59	MG	BA	1777	1/1	0.97	0.29	71,71,71,71	0
59	MG	CA	3351	1/1	0.97	0.14	46,46,46,46	0
59	MG	AA	3075	1/1	0.97	0.28	49,49,49,49	0
59	MG	AA	3811	1/1	0.97	0.15	56,56,56,56	0
59	MG	AA	3598	1/1	0.97	0.24	51,51,51,51	0
59	MG	BA	1735	1/1	0.97	0.20	41,41,41,41	0
59	MG	CA	3332	1/1	0.97	0.24	29,29,29,29	0
59	MG	CA	3653	1/1	0.97	0.20	32,32,32,32	0
59	MG	AA	3222	1/1	0.97	0.17	4,4,4,4	0
59	MG	CE	302	1/1	0.97	0.13	64,64,64,64	0
59	MG	AA	3326	1/1	0.97	0.09	36,36,36,36	1
59	MG	AA	3552	1/1	0.97	0.18	63,63,63,63	0
59	MG	AA	3650	1/1	0.97	0.11	49,49,49,49	0
59	MG	AA	3460	1/1	0.97	0.14	27,27,27,27	0
59	MG	CA	3006	1/1	0.97	0.08	22,22,22,22	0
59	MG	AA	3770	1/1	0.97	0.12	43,43,43,43	0
59	MG	CA	3407	1/1	0.97	0.19	36,36,36,36	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
59	MG	AA	3074	1/1	0.97	0.29	14,14,14,14	0
59	MG	CA	3027	1/1	0.97	0.06	31,31,31,31	0
59	MG	CA	3404	1/1	0.97	0.16	65,65,65,65	0
59	MG	AA	3559	1/1	0.97	0.23	46,46,46,46	0
59	MG	AA	3366	1/1	0.97	0.23	35,35,35,35	1
59	MG	DA	1657	1/1	0.97	0.10	23,23,23,23	0
59	MG	AA	3534	1/1	0.97	0.19	14,14,14,14	0
59	MG	AA	3159	1/1	0.97	0.27	55,55,55,55	0
59	MG	CA	3019	1/1	0.97	0.11	22,22,22,22	0
59	MG	CA	3365	1/1	0.97	0.19	55,55,55,55	0
59	MG	CA	3175	1/1	0.97	0.19	31,31,31,31	0
59	MG	CA	3315	1/1	0.97	0.13	47,47,47,47	0
59	MG	AA	3463	1/1	0.97	0.16	15,15,15,15	0
59	MG	CF	304	1/1	0.97	0.13	65,65,65,65	0
59	MG	AA	3298	1/1	0.97	0.15	58,58,58,58	0
59	MG	CA	3641	1/1	0.97	0.21	46,46,46,46	0
59	MG	AA	3442	1/1	0.97	0.14	23,23,23,23	0
59	MG	CA	3537	1/1	0.97	0.30	59,59,59,59	0
59	MG	AA	3563	1/1	0.97	0.21	34,34,34,34	0
59	MG	AA	3397	1/1	0.97	0.13	13,13,13,13	0
59	MG	AA	3360	1/1	0.97	0.23	22,22,22,22	0
59	MG	CA	3163	1/1	0.97	0.30	30,30,30,30	0
59	MG	AA	3127	1/1	0.97	0.34	57,57,57,57	0
59	MG	AA	3145	1/1	0.97	0.29	44,44,44,44	0
59	MG	CA	3487	1/1	0.97	0.20	60,60,60,60	0
59	MG	AA	3779	1/1	0.97	0.12	22,22,22,22	0
59	MG	AA	3054	1/1	0.97	0.17	21,21,21,21	0
59	MG	BA	1773	1/1	0.97	0.13	40,40,40,40	0
59	MG	AB	3011	1/1	0.97	0.16	29,29,29,29	0
59	MG	CA	3386	1/1	0.97	0.20	50,50,50,50	0
59	MG	CA	3627	1/1	0.97	0.19	60,60,60,60	0
60	ZN	C5	102	1/1	0.97	0.10	66,66,66,66	0
59	MG	AA	3395	1/1	0.97	0.17	54,54,54,54	0
59	MG	AA	3398	1/1	0.97	0.22	31,31,31,31	0
59	MG	CA	3138	1/1	0.97	0.04	86,86,86,86	0
59	MG	CA	3197	1/1	0.97	0.40	45,45,45,45	0
59	MG	CA	3103	1/1	0.97	0.19	53,53,53,53	0
59	MG	AA	3525	1/1	0.97	0.18	35,35,35,35	0
59	MG	BA	1702	1/1	0.97	0.19	46,46,46,46	0
59	MG	AA	3496	1/1	0.97	0.36	31,31,31,31	0
59	MG	AA	3527	1/1	0.97	0.16	27,27,27,27	0
59	MG	CB	3009	1/1	0.97	0.18	67,67,67,67	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
59	MG	C8	5001	1/1	0.97	0.34	37,37,37,37	0
59	MG	CA	3053	1/1	0.97	0.45	32,32,32,32	0
59	MG	CA	3017	1/1	0.97	0.14	30,30,30,30	0
59	MG	CA	3064	1/1	0.97	0.09	48,48,48,48	0
59	MG	AA	3419	1/1	0.97	0.17	20,20,20,20	0
59	MG	AA	3565	1/1	0.97	0.21	44,44,44,44	0
59	MG	AA	3355	1/1	0.97	0.16	57,57,57,57	0
59	MG	CA	3468	1/1	0.97	0.06	53,53,53,53	0
59	MG	CA	3105	1/1	0.97	0.25	39,39,39,39	0
59	MG	AA	3535	1/1	0.97	0.13	48,48,48,48	0
59	MG	CA	3119	1/1	0.97	0.54	55,55,55,55	0
59	MG	AA	3562	1/1	0.97	0.09	56,56,56,56	0
59	MG	AA	3342	1/1	0.97	0.23	51,51,51,51	0
62	GDP	BZ	702	28/28	0.97	0.12	57,57,57,57	0
59	MG	CA	3211	1/1	0.97	0.09	29,29,29,29	0
59	MG	DA	1676	1/1	0.97	0.15	74,74,74,74	0
59	MG	AQ	201	1/1	0.97	0.44	48,48,48,48	0
59	MG	AA	3623	1/1	0.97	0.17	28,28,28,28	0
59	MG	AB	3005	1/1	0.97	0.20	44,44,44,44	0
59	MG	AA	3214	1/1	0.97	0.81	58,58,58,58	1
59	MG	CA	3657	1/1	0.97	0.39	41,41,41,41	0
59	MG	CA	3334	1/1	0.97	0.21	47,47,47,47	0
59	MG	BA	1769	1/1	0.97	0.10	58,58,58,58	0
59	MG	AA	3613	1/1	0.97	0.17	48,48,48,48	0
59	MG	CA	3475	1/1	0.97	0.25	50,50,50,50	0
59	MG	CA	3002	1/1	0.97	0.23	28,28,28,28	0
59	MG	AA	3049	1/1	0.97	0.18	35,35,35,35	0
59	MG	AA	3721	1/1	0.97	0.20	40,40,40,40	0
59	MG	AA	3216	1/1	0.97	0.60	38,38,38,38	0
59	MG	AA	3309	1/1	0.97	0.25	46,46,46,46	0
59	MG	AA	3639	1/1	0.97	0.13	18,18,18,18	0
59	MG	CA	3339	1/1	0.97	0.14	24,24,24,24	0
59	MG	AA	3390	1/1	0.97	0.16	23,23,23,23	0
59	MG	AA	3428	1/1	0.97	0.19	18,18,18,18	0
59	MG	AU	203	1/1	0.97	0.21	31,31,31,31	0
59	MG	AA	3073	1/1	0.97	0.14	31,31,31,31	0
59	MG	CA	3425	1/1	0.97	0.12	50,50,50,50	0
59	MG	CA	3482	1/1	0.97	0.17	61,61,61,61	0
59	MG	CA	3437	1/1	0.97	0.18	64,64,64,64	0
59	MG	BA	1751	1/1	0.97	0.12	48,48,48,48	0
59	MG	AA	3317	1/1	0.97	0.16	24,24,24,24	0
59	MG	AA	3830	1/1	0.97	0.27	47,47,47,47	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
59	MG	AA	3422	1/1	0.97	0.18	23,23,23,23	0
59	MG	CA	3498	1/1	0.97	0.12	49,49,49,49	0
59	MG	CA	3230	1/1	0.97	0.33	49,49,49,49	0
59	MG	AA	3755	1/1	0.97	0.64	78,78,78,78	0
59	MG	CA	3136	1/1	0.97	0.10	63,63,63,63	0
59	MG	CA	3272	1/1	0.97	0.32	49,49,49,49	0
59	MG	AB	3015	1/1	0.97	0.14	28,28,28,28	0
59	MG	AA	3060	1/1	0.97	0.32	20,20,20,20	0
59	MG	CA	3447	1/1	0.97	0.25	73,73,73,73	0
59	MG	BA	1743	1/1	0.97	0.06	41,41,41,41	0
59	MG	AA	3144	1/1	0.97	0.35	50,50,50,50	0
59	MG	AU	204	1/1	0.97	0.38	25,25,25,25	0
59	MG	AA	3515	1/1	0.97	0.22	12,12,12,12	0
59	MG	AA	3682	1/1	0.97	0.17	31,31,31,31	0
59	MG	CA	3449	1/1	0.97	0.07	55,55,55,55	0
59	MG	CA	3424	1/1	0.97	0.19	66,66,66,66	0
59	MG	AA	3730	1/1	0.97	0.17	75,75,75,75	0
59	MG	AA	3578	1/1	0.97	0.13	28,28,28,28	0
59	MG	AA	3815	1/1	0.97	0.17	30,30,30,30	0
59	MG	CA	3297	1/1	0.97	0.34	36,36,36,36	0
59	MG	AA	3147	1/1	0.97	0.52	40,40,40,40	1
59	MG	BA	1762	1/1	0.97	0.06	74,74,74,74	0
59	MG	AB	3016	1/1	0.97	0.14	34,34,34,34	0
59	MG	AA	3681	1/1	0.97	0.13	42,42,42,42	0
59	MG	AA	3459	1/1	0.97	0.20	53,53,53,53	0
59	MG	CA	3011	1/1	0.97	0.38	63,63,63,63	0
59	MG	AA	3453	1/1	0.97	0.23	39,39,39,39	0
59	MG	AA	3524	1/1	0.97	0.19	41,41,41,41	0
59	MG	CA	3309	1/1	0.97	0.24	22,22,22,22	0
59	MG	CA	3219	1/1	0.97	0.25	42,42,42,42	0
59	MG	AB	3019	1/1	0.97	0.12	70,70,70,70	0
59	MG	BA	1747	1/1	0.97	0.19	65,65,65,65	0
59	MG	AG	201	1/1	0.97	0.07	38,38,38,38	0
59	MG	BA	1804	1/1	0.97	0.10	45,45,45,45	0
59	MG	AA	3424	1/1	0.97	0.18	14,14,14,14	0
59	MG	AA	3666	1/1	0.97	0.14	41,41,41,41	0
59	MG	AA	3489	1/1	0.97	0.18	15,15,15,15	0
59	MG	CA	3564	1/1	0.97	0.13	80,80,80,80	0
59	MG	AA	3369	1/1	0.97	0.12	47,47,47,47	0
59	MG	AA	3519	1/1	0.97	0.23	27,27,27,27	0
59	MG	CA	3329	1/1	0.98	0.14	21,21,21,21	0
59	MG	AA	3595	1/1	0.98	0.15	42,42,42,42	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
59	MG	CA	3353	1/1	0.98	0.22	45,45,45,45	0
59	MG	AA	3663	1/1	0.98	0.19	11,11,11,11	0
59	MG	AA	3437	1/1	0.98	0.18	17,17,17,17	0
59	MG	CA	3438	1/1	0.98	0.14	24,24,24,24	0
59	MG	AA	3765	1/1	0.98	0.38	60,60,60,60	0
59	MG	AA	3243	1/1	0.98	0.23	43,43,43,43	0
59	MG	AA	3152	1/1	0.98	0.24	10,10,10,10	0
59	MG	AA	3302	1/1	0.98	0.06	51,51,51,51	0
59	MG	AA	3439	1/1	0.98	0.28	37,37,37,37	0
59	MG	CA	3049	1/1	0.98	0.36	46,46,46,46	0
59	MG	CA	3331	1/1	0.98	0.26	52,52,52,52	0
59	MG	CA	3369	1/1	0.98	0.14	48,48,48,48	0
59	MG	AA	3407	1/1	0.98	0.20	10,10,10,10	0
59	MG	AA	3377	1/1	0.98	0.06	20,20,20,20	0
59	MG	AA	3523	1/1	0.98	0.16	13,13,13,13	0
59	MG	AA	3597	1/1	0.98	0.11	33,33,33,33	0
59	MG	CA	3435	1/1	0.98	0.11	55,55,55,55	0
59	MG	BA	1765	1/1	0.98	0.23	54,54,54,54	0
59	MG	DA	1673	1/1	0.98	0.13	82,82,82,82	0
59	MG	AA	3505	1/1	0.98	0.15	30,30,30,30	0
59	MG	CA	3446	1/1	0.98	0.18	33,33,33,33	0
59	MG	AA	3457	1/1	0.98	0.13	30,30,30,30	0
59	MG	AA	3320	1/1	0.98	0.13	37,37,37,37	0
59	MG	CA	3427	1/1	0.98	0.19	37,37,37,37	0
61	SF4	BD	501	8/8	0.98	0.10	78,78,78,78	0
59	MG	AA	3569	1/1	0.98	0.22	17,17,17,17	0
59	MG	AA	3545	1/1	0.98	0.19	43,43,43,43	0
59	MG	AA	3091	1/1	0.98	0.75	47,47,47,47	1
59	MG	AA	3362	1/1	0.98	0.16	46,46,46,46	0
59	MG	AA	3182	1/1	0.98	0.22	46,46,46,46	0
59	MG	AA	3250	1/1	0.98	0.18	123,123,123,123	0
59	MG	AA	3037	1/1	0.98	0.11	4,4,4,4	0
59	MG	CA	3342	1/1	0.98	0.11	33,33,33,33	0
60	ZN	C9	501	1/1	0.98	0.09	75,75,75,75	0
59	MG	CA	3384	1/1	0.98	0.11	55,55,55,55	0
59	MG	CA	3525	1/1	0.98	0.28	23,23,23,23	0
59	MG	CA	3287	1/1	0.98	0.22	45,45,45,45	0
59	MG	AA	3165	1/1	0.98	0.16	52,52,52,52	0
59	MG	AA	3498	1/1	0.98	0.24	47,47,47,47	0
59	MG	CA	3640	1/1	0.98	0.28	43,43,43,43	0
59	MG	AA	3436	1/1	0.98	0.17	12,12,12,12	0
59	MG	CA	3214	1/1	0.98	0.11	22,22,22,22	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
59	MG	BA	1686	1/1	0.98	0.15	36,36,36,36	0
59	MG	CA	3567	1/1	0.98	0.22	26,26,26,26	0
59	MG	AA	3434	1/1	0.98	0.06	17,17,17,17	0
59	MG	CA	3613	1/1	0.98	0.22	57,57,57,57	0
59	MG	AA	3587	1/1	0.98	0.14	28,28,28,28	0
59	MG	AE	303	1/1	0.98	0.21	19,19,19,19	0
59	MG	AA	3372	1/1	0.98	0.23	37,37,37,37	0
59	MG	AA	3082	1/1	0.98	0.27	60,60,60,60	0
59	MG	AA	3416	1/1	0.98	0.14	14,14,14,14	0
59	MG	CA	3401	1/1	0.98	0.22	28,28,28,28	0
59	MG	AA	3488	1/1	0.98	0.18	36,36,36,36	0
59	MG	AA	3411	1/1	0.98	0.14	12,12,12,12	0
59	MG	BA	1722	1/1	0.98	0.29	51,51,51,51	0
59	MG	AA	3311	1/1	0.98	0.14	2,2,2,2	0
59	MG	AB	3014	1/1	0.98	0.11	56,56,56,56	0
59	MG	AA	3220	1/1	0.98	0.15	62,62,62,62	0
59	MG	CA	3206	1/1	0.98	0.40	44,44,44,44	0
59	MG	AA	3335	1/1	0.98	0.24	15,15,15,15	0
59	MG	AA	3432	1/1	0.98	0.23	42,42,42,42	0
59	MG	CA	3258	1/1	0.98	0.36	51,51,51,51	0
59	MG	CA	3302	1/1	0.98	0.28	37,37,37,37	0
59	MG	AA	3292	1/1	0.98	0.20	24,24,24,24	0
59	MG	AA	3778	1/1	0.98	0.14	43,43,43,43	0
59	MG	AA	3553	1/1	0.98	0.05	43,43,43,43	0
59	MG	BA	1677	1/1	0.98	0.17	28,28,28,28	0
59	MG	AA	3452	1/1	0.98	0.14	14,14,14,14	0
59	MG	AB	3012	1/1	0.98	0.15	23,23,23,23	1
59	MG	BA	1740	1/1	0.98	0.30	50,50,50,50	0
59	MG	AA	3777	1/1	0.98	0.12	41,41,41,41	0
59	MG	AA	3831	1/1	0.98	0.20	37,37,37,37	0
59	MG	CA	3306	1/1	0.98	0.08	24,24,24,24	0
59	MG	AA	3332	1/1	0.98	0.18	17,17,17,17	0
59	MG	DW	501	1/1	0.98	0.17	44,44,44,44	0
59	MG	CA	3466	1/1	0.98	0.40	56,56,56,56	0
59	MG	AA	3072	1/1	0.98	0.08	19,19,19,19	0
59	MG	CA	3266	1/1	0.98	0.15	36,36,36,36	0
59	MG	CA	3382	1/1	0.98	0.22	38,38,38,38	0
59	MG	CA	3459	1/1	0.98	0.09	28,28,28,28	0
59	MG	CA	3025	1/1	0.98	0.39	59,59,59,59	0
59	MG	AA	3484	1/1	0.98	0.11	53,53,53,53	0
59	MG	CA	3443	1/1	0.98	0.18	28,28,28,28	0
59	MG	AA	3600	1/1	0.98	0.15	25,25,25,25	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
59	MG	AA	3528	1/1	0.98	0.16	19,19,19,19	0
59	MG	AA	3003	1/1	0.98	0.06	8,8,8,8	0
59	MG	AA	3752	1/1	0.98	0.12	42,42,42,42	0
59	MG	AA	3793	1/1	0.98	0.22	7,7,7,7	0
59	MG	AA	3154	1/1	0.98	0.18	57,57,57,57	0
59	MG	BA	1640	1/1	0.98	0.44	52,52,52,52	0
59	MG	DA	1651	1/1	0.98	0.11	63,63,63,63	0
59	MG	AA	3470	1/1	0.98	0.08	39,39,39,39	0
59	MG	CA	3358	1/1	0.98	0.29	36,36,36,36	0
59	MG	CA	3195	1/1	0.98	0.31	47,47,47,47	0
59	MG	AA	3734	1/1	0.98	0.24	26,26,26,26	0
59	MG	AA	3433	1/1	0.98	0.14	37,37,37,37	0
59	MG	CA	3267	1/1	0.98	0.13	38,38,38,38	0
59	MG	CA	3648	1/1	0.98	0.34	52,52,52,52	0
59	MG	AA	3561	1/1	0.98	0.20	21,21,21,21	0
59	MG	AA	3368	1/1	0.98	0.24	49,49,49,49	0
59	MG	AA	3760	1/1	0.98	0.37	55,55,55,55	0
59	MG	CA	3650	1/1	0.98	0.25	14,14,14,14	0
59	MG	AA	3774	1/1	0.98	0.35	25,25,25,25	1
59	MG	AA	3727	1/1	0.98	0.14	23,23,23,23	0
59	MG	AA	3753	1/1	0.98	0.15	30,30,30,30	0
59	MG	DA	1653	1/1	0.98	0.30	55,55,55,55	0
59	MG	CV	202	1/1	0.98	0.21	38,38,38,38	0
59	MG	AA	3585	1/1	0.98	0.17	35,35,35,35	0
59	MG	AA	3023	1/1	0.98	0.62	53,53,53,53	0
59	MG	CA	3179	1/1	0.98	0.32	60,60,60,60	0
59	MG	AA	3381	1/1	0.98	0.16	16,16,16,16	0
59	MG	AA	3192	1/1	0.98	0.23	30,30,30,30	0
59	MG	AA	3631	1/1	0.98	0.18	46,46,46,46	0
61	SF4	DD	501	8/8	0.98	0.11	82,82,82,82	1
59	MG	AA	3421	1/1	0.98	0.21	28,28,28,28	0
59	MG	AA	3097	1/1	0.98	0.20	22,22,22,22	0
59	MG	CA	3169	1/1	0.98	0.21	34,34,34,34	0
59	MG	CA	3405	1/1	0.98	0.10	55,55,55,55	0
59	MG	CA	3228	1/1	0.98	0.36	59,59,59,59	0
59	MG	CA	3383	1/1	0.98	0.20	30,30,30,30	0
59	MG	CA	3209	1/1	0.98	0.13	73,73,73,73	0
59	MG	CA	3415	1/1	0.98	0.26	34,34,34,34	0
59	MG	CA	3361	1/1	0.98	0.20	43,43,43,43	0
59	MG	AA	3338	1/1	0.98	0.08	28,28,28,28	0
59	MG	AA	3294	1/1	0.98	0.17	37,37,37,37	0
59	MG	DA	1697	1/1	0.98	0.17	48,48,48,48	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
59	MG	AA	3130	1/1	0.98	0.23	34,34,34,34	0
59	MG	CA	3039	1/1	0.98	0.28	37,37,37,37	0
59	MG	CA	3523	1/1	0.98	0.14	37,37,37,37	0
59	MG	AA	3729	1/1	0.98	0.20	41,41,41,41	0
59	MG	CA	3308	1/1	0.98	0.10	39,39,39,39	0
59	MG	CA	3592	1/1	0.98	0.14	64,64,64,64	0
59	MG	AA	3316	1/1	0.98	0.23	36,36,36,36	0
59	MG	AA	3412	1/1	0.98	0.20	39,39,39,39	0
59	MG	AA	3020	1/1	0.98	0.18	11,11,11,11	0
59	MG	AA	3789	1/1	0.98	0.21	44,44,44,44	0
59	MG	CA	3045	1/1	0.98	0.17	60,60,60,60	0
59	MG	CA	3400	1/1	0.98	0.13	57,57,57,57	0
59	MG	AA	3465	1/1	0.98	0.20	42,42,42,42	0
59	MG	AF	303	1/1	0.98	0.20	19,19,19,19	0
59	MG	CA	3292	1/1	0.98	0.09	12,12,12,12	0
59	MG	CA	3227	1/1	0.99	0.22	41,41,41,41	0
59	MG	CA	3479	1/1	0.99	0.17	50,50,50,50	0
59	MG	AA	3482	1/1	0.99	0.11	41,41,41,41	0
59	MG	AA	3726	1/1	0.99	0.16	12,12,12,12	0
60	ZN	A5	501	1/1	0.99	0.13	30,30,30,30	0
59	MG	CA	3380	1/1	0.99	0.21	59,59,59,59	0
59	MG	BA	1688	1/1	0.99	0.43	61,61,61,61	0
59	MG	DA	1648	1/1	0.99	0.12	40,40,40,40	0
59	MG	AA	3248	1/1	0.99	0.14	22,22,22,22	0
59	MG	AA	3354	1/1	0.99	0.12	27,27,27,27	0
59	MG	CA	3372	1/1	0.99	0.18	35,35,35,35	0
59	MG	AA	3735	1/1	0.99	0.13	25,25,25,25	0
59	MG	AA	3345	1/1	0.99	0.13	6,6,6,6	0
59	MG	CA	3015	1/1	0.99	0.28	51,51,51,51	0
59	MG	CA	3181	1/1	0.99	0.16	40,40,40,40	0
60	ZN	AY	501	1/1	0.99	0.09	61,61,61,61	0
59	MG	CA	3322	1/1	0.99	0.26	40,40,40,40	0
59	MG	AA	3380	1/1	0.99	0.12	18,18,18,18	0
59	MG	CA	3085	1/1	0.99	0.16	25,25,25,25	0
59	MG	DA	1712	1/1	0.99	0.33	53,53,53,53	0
59	MG	AA	3458	1/1	0.99	0.09	40,40,40,40	0
59	MG	CA	3282	1/1	0.99	0.18	36,36,36,36	0
59	MG	DA	1745	1/1	0.99	0.38	50,50,50,50	0
59	MG	AA	3321	1/1	0.99	0.10	61,61,61,61	0
59	MG	AA	3801	1/1	0.99	0.15	27,27,27,27	0
59	MG	AA	3540	1/1	0.99	0.09	36,36,36,36	0
59	MG	AA	3477	1/1	0.99	0.18	14,14,14,14	0

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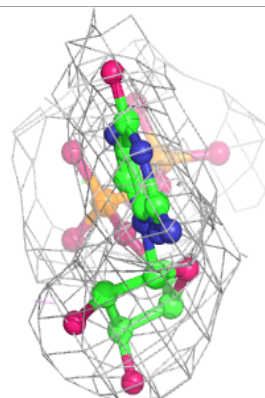
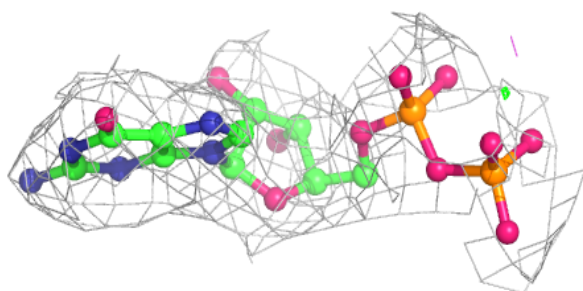
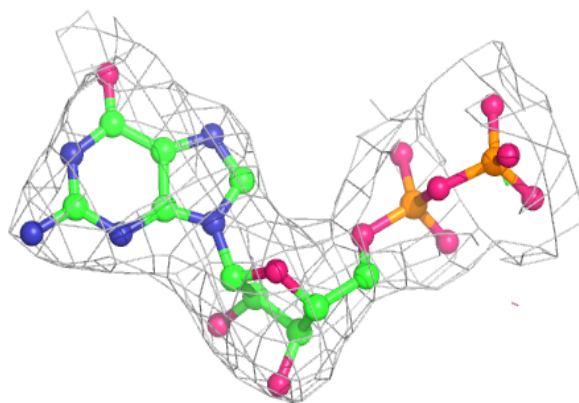
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
59	MG	AA	3076	1/1	0.99	0.13	0,0,0,0	0
59	MG	AA	3799	1/1	0.99	0.33	42,42,42,42	0
59	MG	AA	3328	1/1	0.99	0.16	42,42,42,42	0
59	MG	AA	3401	1/1	0.99	0.14	21,21,21,21	0
59	MG	AA	3053	1/1	0.99	0.18	19,19,19,19	0
59	MG	AA	3709	1/1	0.99	0.42	23,23,23,23	1
59	MG	AA	3475	1/1	0.99	0.25	45,45,45,45	0
59	MG	AA	3011	1/1	0.99	0.08	16,16,16,16	0
59	MG	AA	3702	1/1	0.99	0.20	14,14,14,14	0
59	MG	AV	201	1/1	0.99	0.25	42,42,42,42	0
59	MG	CA	3570	1/1	0.99	0.12	36,36,36,36	0
59	MG	AA	3526	1/1	0.99	0.20	19,19,19,19	0
59	MG	AA	3146	1/1	0.99	0.08	29,29,29,29	0
59	MG	AA	3410	1/1	0.99	0.14	57,57,57,57	0
59	MG	AA	3745	1/1	0.99	0.18	68,68,68,68	0
59	MG	AA	3438	1/1	0.99	0.15	17,17,17,17	0
60	ZN	A6	102	1/1	0.99	0.12	40,40,40,40	0
59	MG	AA	3415	1/1	0.99	0.23	62,62,62,62	0
59	MG	AA	3364	1/1	0.99	0.18	23,23,23,23	0
59	MG	AA	3402	1/1	0.99	0.13	27,27,27,27	0
59	MG	AA	3346	1/1	0.99	0.13	59,59,59,59	0
59	MG	CA	3433	1/1	0.99	0.12	82,82,82,82	0
59	MG	CA	3311	1/1	0.99	0.14	50,50,50,50	0
59	MG	AA	3303	1/1	0.99	0.15	24,24,24,24	0
59	MG	AA	3151	1/1	0.99	0.23	62,62,62,62	0
59	MG	AA	3103	1/1	0.99	0.03	5,5,5,5	0
59	MG	CA	3261	1/1	0.99	0.16	47,47,47,47	0
59	MG	CA	3618	1/1	0.99	0.30	40,40,40,40	0
59	MG	AA	3741	1/1	0.99	0.10	21,21,21,21	0
59	MG	AA	3405	1/1	0.99	0.27	44,44,44,44	0
59	MG	CA	3423	1/1	0.99	0.23	46,46,46,46	0
59	MG	AA	3297	1/1	0.99	0.23	27,27,27,27	0
59	MG	AA	3512	1/1	0.99	0.15	38,38,38,38	0
60	ZN	A9	501	1/1	1.00	0.12	42,42,42,42	0

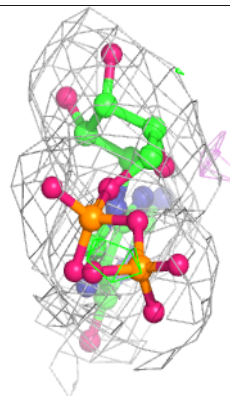
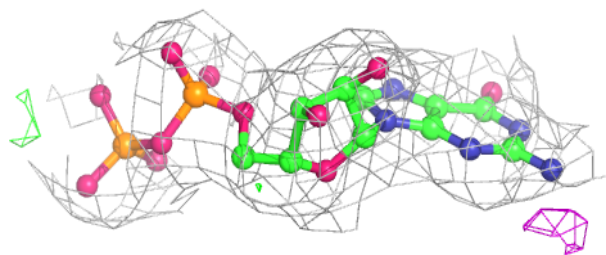
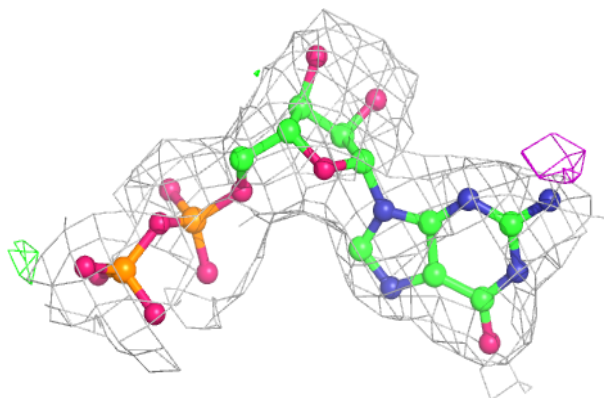
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around GDP DZ 703:

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

**Electron density around GDP BZ 702:**

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



6.5 Other polymers [i](#)

There are no such residues in this entry.