



wwPDB X-ray Structure Validation Summary Report ⓘ

May 17, 2020 – 12:21 am BST

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

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The 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

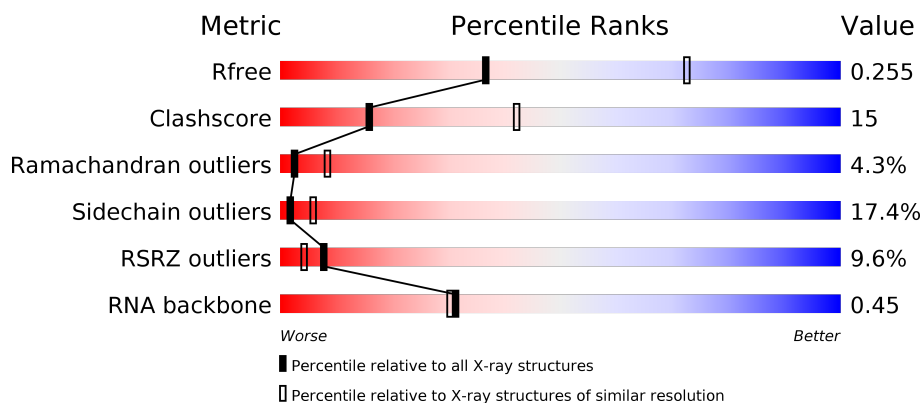
1 Overall quality at a glance

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	<div> <div>4%</div> <div>19%</div> <div>49%</div> <div>25%</div> <div>5%</div> </div>
1	CA	2915	<div> <div>4%</div> <div>32%</div> <div>44%</div> <div>19%</div> </div>
2	AB	121	<div> <div>25%</div> <div>46%</div> <div>24%</div> </div>
2	CB	121	<div> <div>%</div> <div>44%</div> <div>41%</div> <div>13%</div> </div>





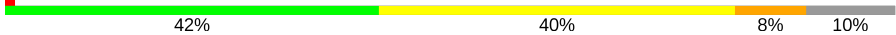




















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Mol	Chain	Length	Quality of chain
3	AC	228	
3	CC	228	
4	AD	276	
4	CD	276	
5	AE	206	
5	CE	206	
6	AF	210	
6	CF	210	
7	AG	182	
7	CG	182	
8	AH	180	
8	CH	180	
9	AK	173	
9	CK	173	
10	AL	147	
10	CL	147	
11	AN	140	
11	CN	140	
12	AO	122	
12	CO	122	
13	AP	150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

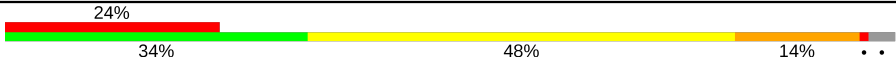

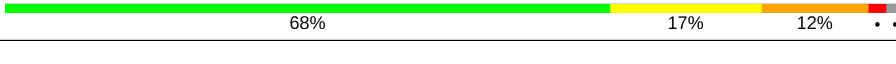


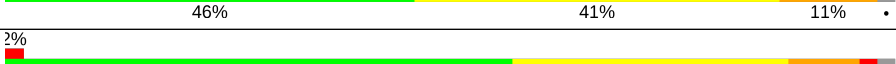

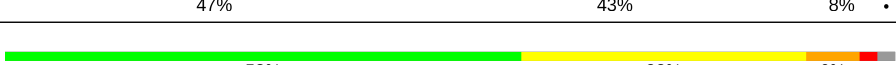

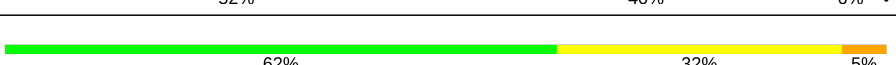
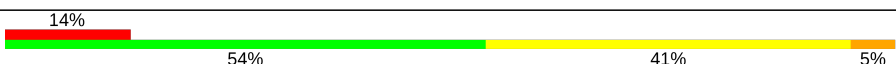
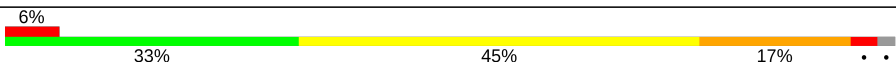
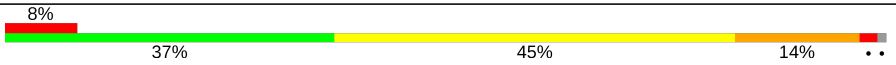


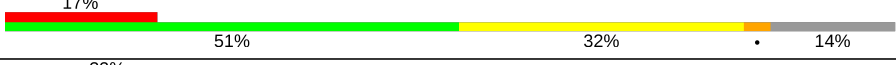

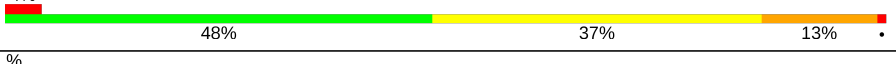
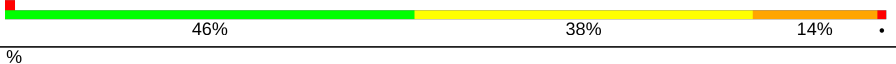

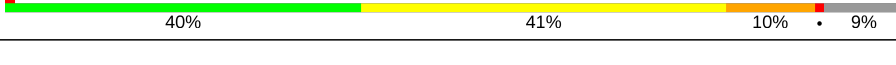


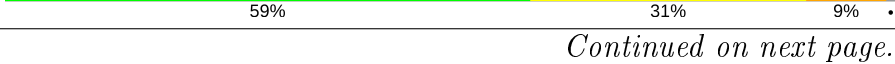

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Mol	Chain	Length	Quality of chain
15	CR	118	
16	AS	112	
16	CS	112	
17	AT	146	
17	CT	146	
18	AU	118	
18	CU	118	
19	AV	101	
19	CV	101	
20	AW	113	
20	CW	113	
21	AX	96	
21	CX	96	
22	AY	110	
22	CY	110	
23	AZ	206	
23	CZ	206	
24	A0	85	
24	C0	85	
25	A1	98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

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

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

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Mol	Chain	Length	Quality of chain
53	BT	106	
53	DT	106	
54	BU	27	
54	DU	27	
55	BV	18	
55	DV	18	
56	BW	76	
56	BY	76	
56	DW	76	
56	DY	76	
57	BZ	758	
57	DZ	758	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
56	PSU	BY	32	-	-	-	X
56	MIA	BY	37	-	-	-	X
56	PSU	BY	39	-	-	-	X
56	7MG	BY	46	-	-	-	X
56	5MU	BY	54	-	-	-	X
56	PSU	BY	55	-	-	-	X
56	4SU	BY	8	-	-	-	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	MG	A4	502	-	-	-	X
58	MG	AA	3010	-	-	-	X
58	MG	AA	3095	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
58	MG	AA	3108	-	-	-	X
58	MG	AA	3112	-	-	-	X
58	MG	AA	3115	-	-	-	X
58	MG	AA	3178	-	-	-	X
58	MG	AA	3192	-	-	-	X
58	MG	AA	3248	-	-	-	X
58	MG	AA	3252	-	-	-	X
58	MG	AA	3269	-	-	-	X
58	MG	AA	3272	-	-	-	X
58	MG	AA	3640	-	-	-	X
58	MG	AA	3713	-	-	-	X
58	MG	AA	3739	-	-	-	X
58	MG	AA	3751	-	-	-	X
58	MG	AB	3001	-	-	-	X
58	MG	AD	305	-	-	-	X
58	MG	AN	3001	-	-	-	X
58	MG	AQ	201	-	-	-	X
58	MG	AX	101	-	-	-	X
58	MG	BA	1616	-	-	-	X
58	MG	BA	1622	-	-	-	X
58	MG	BA	1634	-	-	-	X
58	MG	BA	1645	-	-	-	X
58	MG	BA	1661	-	-	-	X
58	MG	BA	1666	-	-	-	X
58	MG	BA	1673	-	-	-	X
58	MG	BA	1681	-	-	-	X
58	MG	BA	1689	-	-	-	X
58	MG	BA	1711	-	-	-	X
58	MG	BA	1771	-	-	-	X
58	MG	CA	3015	-	-	-	X
58	MG	CA	3033	-	-	-	X
58	MG	CA	3042	-	-	-	X
58	MG	CA	3043	-	-	-	X
58	MG	CA	3058	-	-	-	X
58	MG	CA	3066	-	-	-	X
58	MG	CA	3070	-	-	-	X
58	MG	CA	3071	-	-	-	X
58	MG	CA	3076	-	-	-	X
58	MG	CA	3083	-	-	-	X
58	MG	CA	3085	-	-	-	X
58	MG	CA	3088	-	-	-	X
58	MG	CA	3089	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
58	MG	CA	3093	-	-	-	X
58	MG	CA	3107	-	-	-	X
58	MG	CA	3134	-	-	-	X
58	MG	CA	3140	-	-	-	X
58	MG	CA	3173	-	-	-	X
58	MG	CA	3174	-	-	-	X
58	MG	CA	3180	-	-	-	X
58	MG	CA	3183	-	-	-	X
58	MG	CA	3202	-	-	-	X
58	MG	CA	3205	-	-	-	X
58	MG	CA	3209	-	-	-	X
58	MG	CA	3224	-	-	-	X
58	MG	CA	3236	-	-	-	X
58	MG	CA	3241	-	-	-	X
58	MG	CA	3244	-	-	-	X
58	MG	CA	3246	-	-	-	X
58	MG	CA	3290	-	-	-	X
58	MG	CA	3314	-	-	-	X
58	MG	CA	3374	-	-	-	X
58	MG	CA	3389	-	-	-	X
58	MG	CA	3460	-	-	-	X
58	MG	CA	3492	-	-	-	X
58	MG	CA	3500	-	-	-	X
58	MG	CA	3514	-	-	-	X
58	MG	CA	3611	-	-	-	X
58	MG	CA	3616	-	-	-	X
58	MG	CA	3660	-	-	-	X
58	MG	CD	301	-	-	-	X
58	MG	CQ	205	-	-	-	X
58	MG	DA	1606	-	-	-	X
58	MG	DA	1614	-	-	-	X
58	MG	DA	1649	-	-	-	X
58	MG	DA	1660	-	-	-	X
58	MG	DA	1672	-	-	-	X
58	MG	DA	1755	-	-	-	X
58	MG	DJ	5001	-	-	-	X
58	MG	DZ	701	-	-	-	X
60	SF4	DD	501	-	-	X	-
62	GDP	DZ	704	-	-	X	-

2 Entry composition

There are 63 unique types of molecules in this entry. The entry contains 310279 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a RNA chain called 23S Ribosomal RNA.

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

- Molecule 55 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
55	BV	7	Total	C	N	O	P	0	0	0
			148	67	27	47	7			
55	DV	6	Total	C	N	O	P	0	0	0
			123	57	22	39	5			

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
57	BZ	730	Total	C	N	O	S	0	0	0
			5690	3616	980	1075	19			
57	DZ	730	Total	C	N	O	S	0	0	0
			5690	3616	980	1075	19			

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
58	AP	2	Total 2 Mg 2	0	0
58	CR	1	Total 1 Mg 1	0	0
58	BA	211	Total 211 Mg 211	0	0
58	CA	664	Total 664 Mg 664	0	0
58	C8	1	Total 1 Mg 1	0	0
58	C5	1	Total 1 Mg 1	0	0
58	AB	23	Total 23 Mg 23	0	0
58	BL	2	Total 2 Mg 2	0	0
58	CV	2	Total 2 Mg 2	0	0
58	A6	1	Total 1 Mg 1	0	0
58	BE	1	Total 1 Mg 1	0	0
58	AW	4	Total 4 Mg 4	0	0
58	AN	3	Total 3 Mg 3	0	0
58	DZ	2	Total 2 Mg 2	0	0
58	AX	1	Total 1 Mg 1	0	0
58	CN	1	Total 1 Mg 1	0	0
58	A2	2	Total 2 Mg 2	0	0
58	CY	1	Total 1 Mg 1	0	0
58	DD	1	Total 1 Mg 1	0	0
58	BB	1	Total 1 Mg 1	0	0
58	BT	1	Total 1 Mg 1	0	0
58	AE	4	Total 4 Mg 4	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
58	BM	2	Total 2	Mg 2	0	0
58	CU	1	Total 1	Mg 1	0	0
58	BF	1	Total 1	Mg 1	0	0
58	AV	3	Total 3	Mg 3	0	0
58	DA	168	Total 168	Mg 168	0	0
58	CB	13	Total 13	Mg 13	0	0
58	AA	835	Total 835	Mg 835	0	0
58	CQ	5	Total 5	Mg 5	0	0
58	A5	1	Total 1	Mg 1	0	0
58	AR	1	Total 1	Mg 1	0	0
58	CG	1	Total 1	Mg 1	0	0
58	DK	1	Total 1	Mg 1	0	0
58	DF	1	Total 1	Mg 1	0	0
58	AD	10	Total 10	Mg 10	0	0
58	BN	1	Total 1	Mg 1	0	0
58	DJ	1	Total 1	Mg 1	0	0
58	C7	1	Total 1	Mg 1	0	0
58	C3	1	Total 1	Mg 1	0	0
58	AZ	2	Total 2	Mg 2	0	0
58	A4	1	Total 1	Mg 1	0	0
58	BK	1	Total 1	Mg 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
58	AU	3	Total 3	Mg 3	0	0
58	DW	3	Total 3	Mg 3	0	0
58	A9	1	Total 1	Mg 1	0	0
58	CF	5	Total 5	Mg 5	0	0
58	BV	1	Total 1	Mg 1	0	0
58	A0	3	Total 3	Mg 3	0	0
58	AG	2	Total 2	Mg 2	0	0
58	DE	2	Total 2	Mg 2	0	0
58	AQ	3	Total 3	Mg 3	0	0
58	CE	6	Total 6	Mg 6	0	0
58	AH	2	Total 2	Mg 2	0	0
58	BZ	2	Total 2	Mg 2	0	0
58	CO	2	Total 2	Mg 2	0	0
58	CP	3	Total 3	Mg 3	0	0
58	CW	1	Total 1	Mg 1	0	0
58	A7	3	Total 3	Mg 3	0	0
58	CD	3	Total 3	Mg 3	0	0
58	BD	1	Total 1	Mg 1	0	0
58	DT	1	Total 1	Mg 1	0	0
58	A8	2	Total 2	Mg 2	0	0
58	AO	1	Total 1	Mg 1	0	0

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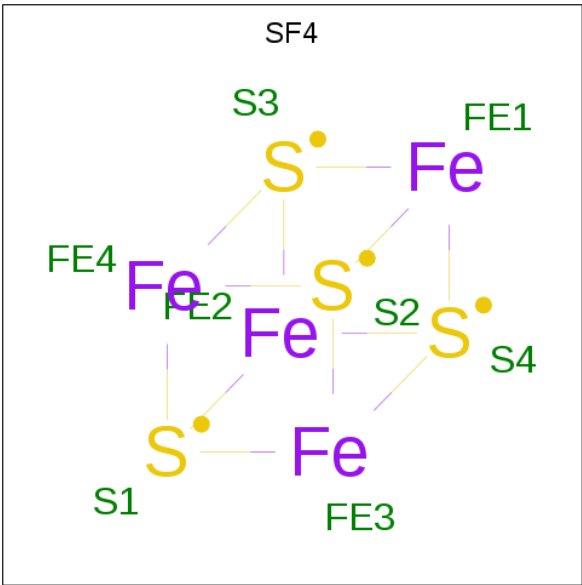
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
58	BW	3	Total 3	Mg 3	0	0
58	AY	1	Total 1	Mg 1	0	0
58	AF	5	Total 5	Mg 5	0	0

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

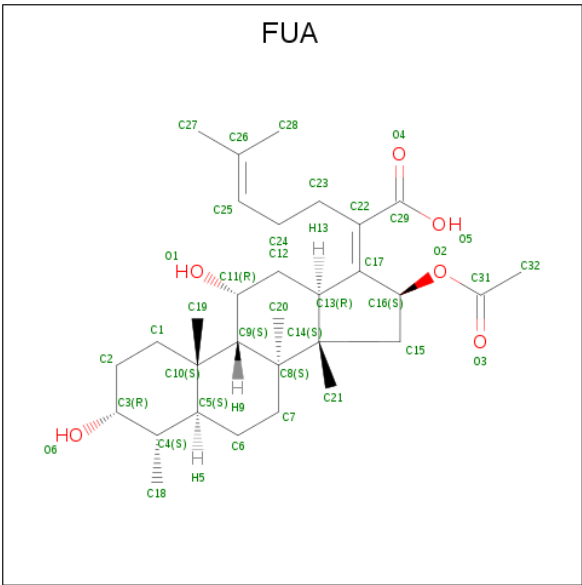
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
59	AY	1	Total 1	Zn 1	0	0
59	BN	1	Total 1	Zn 1	0	0
59	C4	1	Total 1	Zn 1	0	0
59	C5	1	Total 1	Zn 1	0	0
59	C6	1	Total 1	Zn 1	0	0
59	A6	1	Total 1	Zn 1	0	0
59	C9	1	Total 1	Zn 1	0	0
59	DN	1	Total 1	Zn 1	0	0
59	A4	1	Total 1	Zn 1	0	0
59	A5	1	Total 1	Zn 1	0	0
59	A9	1	Total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

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



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

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



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

-
- The image displays the chemical structure of Guanosine Diphosphate (GDP). It consists of a guanine base (a purine ring system with an amino group at C2 and a carbonyl group at C6) linked to a ribose sugar via a glycosidic bond at the C1 position. The ribose sugar is further linked to two phosphate groups (diphosphate) via a pyrophosphate bridge. The structure is labeled with atom names and numbers, including N1, C2, N3, C4, N5, C6, N7, C8, N9, C10, C11, C12, C13, C14, C15, C16, C17, C18, C19, C20, C21, C22, C23, C24, C25, C26, C27, C28, C29, C30, C31, C32, C33, C34, C35, C36, C37, C38, C39, C40, C41, C42, C43, C44, C45, C46, C47, C48, C49, C50, C51, C52, C53, C54, C55, C56, C57, C58, C59, C60, C61, C62, C63, C64, C65, C66, C67, C68, C69, C70, C71, C72, C73, C74, C75, C76, C77, C78, C79, C80, C81, C82, C83, C84, C85, C86, C87, C88, C89, C90, C91, C92, C93, C94, C95, C96, C97, C98, C99, C100, C101, C102, C103, C104, C105, C106, C107, C108, C109, C110, C111, C112, C113, C114, C115, C116, C117, C118, C119, C120, C121, C122, C123, C124, C125, C126, C127, C128, C129, C130, C131, C132, C133, C134, C135, C136, C137, C138, C139, C140, C141, C142, C143, C144, C145, C146, C147, C148, C149, C150, C151, C152, C153, C154, C155, C156, C157, C158, C159, C160, C161, C162, C163, C164, C165, C166, C167, C168, C169, C170, C171, C172, C173, C174, C175, C176, C177, C178, C179, C180, C181, C182, C183, C184, C185, C186, C187, C188, C189, C190, C191, C192, C193, C194, C195, C196, C197, C198, C199, C200, C201, C202, C203, C204, C205, C206, C207, C208, C209, C210, C211, C212, C213, C214, C215, C216, C217, C218, C219, C220, C221, C222, C223, C224, C225, C226, C227, C228, C229, C230, C231, C232, C233, C234, C235, C236, C237, C238, C239, C240, C241, C242, C243, C244, C245, C246, C247, C248, C249, C250, C251, C252, C253, C254, C255, C256, C257, C258, C259, C260, C261, C262, C263, C264, C265, C266, C267, C268, C269, C270, C271, C272, C273, C274, C275, C276, C277, C278, C279, C280, C281, C282, C283, C284, C285, C286, C287, C288, C289, C290, C291, C292, C293, C294, C295, C296, C297, C298, C299, C300, C301, C302, C303, C304, C305, C306, C307, C308, C309, C310, C311, C312, C313, C314, C315, C316, C317, C318, C319, C320, C321, C322, C323, C324, C325, C326, C327, C328, C329, C330, C331, C332, C333, C334, C335, C336, C337, C338, C339, C340, C341, C342, C343, C344, C345, C346, C347, C348, C349, C350, C351, C352, C353, C354, C355, C356, C357, C358, C359, C360, C361, C362, C363, C364, C365, C366, C367, C368, C369, C370, C371, C372, C373, C374, C375, C376, C377, C378, C379, C380, C381, C382, C383, C384, C385, C386, C387, C388, C389, C390, C391, C392, C393, C394, C395, C396, C397, C398, C399, C400, C401, C402, C403, C404, C405, C406, C407, C408, C409, C410, C411, C412, C413, C414, C415, C416, C417, C418, C419, C420, C421, C422, C423, C424, C425, C426, C427, C428, C429, C430, C431, C432, C433, C434, C435, C436, C437, C438, C439, C440, C441, C442, C443, C444, C445, C446, C447, C448, C449, C450, C451, C452, C453, C454, C455, C456, C457, C458, C459, C460, C461, C462, C463, C464, C465, C466, C467, C468, C469, C470, C471, C472, C473, C474, C475, C476, C477, C478, C479, C480, C481, C482, C483, C484, C485, C486, C487, C488, C489, C490, C491, C492, C493, C494, C495, C496, C497, C498, C499, C500, C501, C502, C503, C504, C505, C506, C507, C508, C509, C510, C511, C512, C513, C514, C515, C516, C517, C518, C519, C520, C521, C522, C523, C524, C525, C526, C527, C528, C529, C530, C531, C532, C533, C534, C535, C536, C537, C538, C539, C540, C541, C542, C543, C544, C545, C546, C547, C548, C549, C550, C551, C552, C553, C554, C555, C556, C557, C558, C559, C560, C561, C562, C563, C564, C565, C566, C567, C568, C569, C570, C571, C572, C573, C574, C575, C576, C577, C578, C579, C580, C581, C582, C583, C584, C585, C586, C587, C588, C589, C590, C591, C592, C593, C594, C595, C596, C597, C598, C599, C600, C601, C602, C603, C604, C605, C606, C607, C608, C609, C610, C611, C612, C613, C614, C615, C616, C617, C618, C619, C620, C621, C622, C623, C624, C625, C626, C627, C628, C629, C630, C631, C632, C633, C634, C635, C636, C637, C638, C639, C640, C641, C642, C643, C644, C645, C646, C647, C648, C649, C650, C651, C652, C653, C654, C655, C656, C657, C658, C659, C660, C661, C662, C663, C664, C665, C666, C667, C668, C669, C670, C671, C672, C673, C674, C675, C676, C677, C678, C679, C680, C681, C682, C683, C684, C685, C686, C687, C688, C689, C690, C691, C692, C693, C694, C695, C696, C697, C698, C699, C700, C701, C702, C703, C704, C705, C706, C707, C708, C709, C710, C711, C712, C713, C714, C715, C716, C717, C718, C719, C720, C721, C722, C723, C724, C725, C726, C727, C728, C729, C730, C731, C732, C733, C734, C735, C736, C737, C738, C739, C740, C741, C742, C743, C744, C745, C746, C747, C748, C749, C750, C751, C752, C753, C754, C755, C756, C757, C758, C759, C760, C761, C762, C763, C764, C765, C766, C767, C768, C769, C770, C771, C772, C773, C774, C775, C776, C777, C778, C779, C780, C781, C782, C783, C784, C785, C786, C787, C788, C789, C790, C791, C792, C793, C794, C795, C796, C797, C798, C799, C800, C801, C802, C803, C804, C805, C806, C807, C808, C809, C810, C811, C812, C813, C814

- Molecule 63 is water.

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

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

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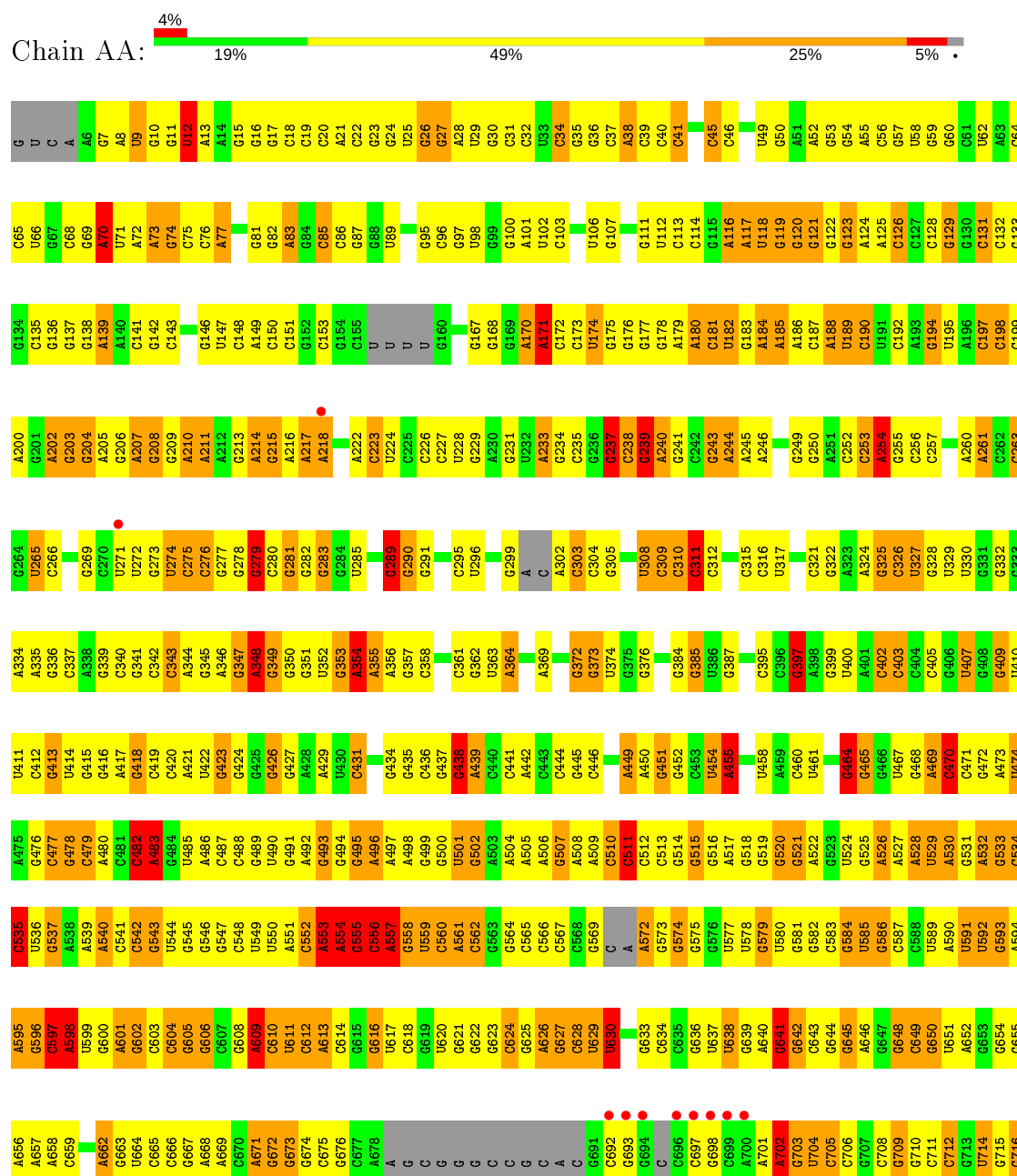
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
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63	C5	1	Total 1	O 1	0	0
63	C7	3	Total 3	O 3	0	0
63	C8	3	Total 3	O 3	0	0
63	DA	153	Total 153	O 153	0	0
63	DE	2	Total 2	O 2	0	0
63	DH	1	Total 1	O 1	0	0
63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

3 Residue-property plots

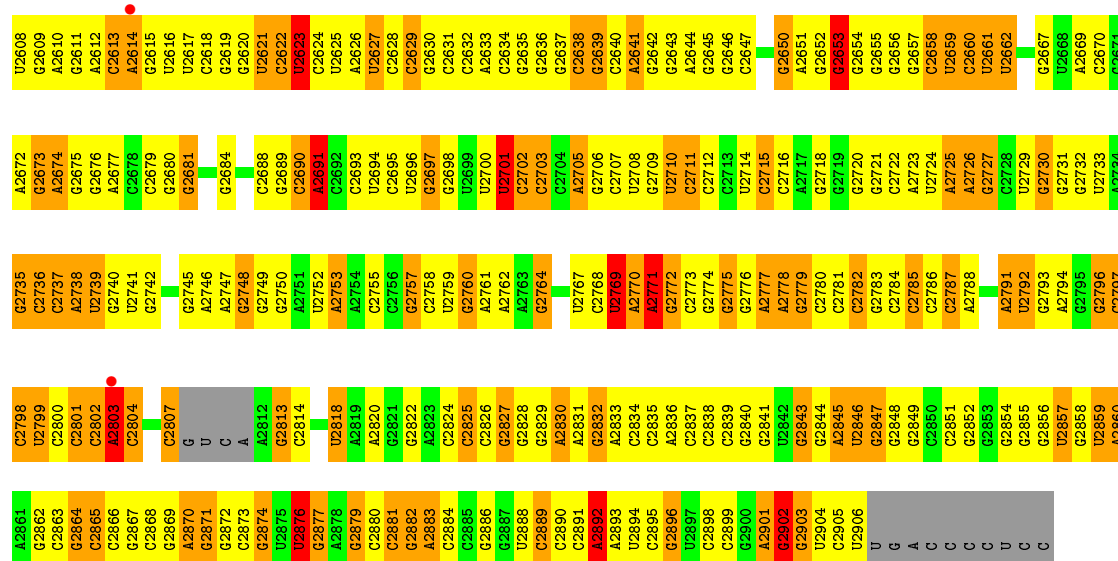
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are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

• Molecule 1: 23S Ribosomal RNA

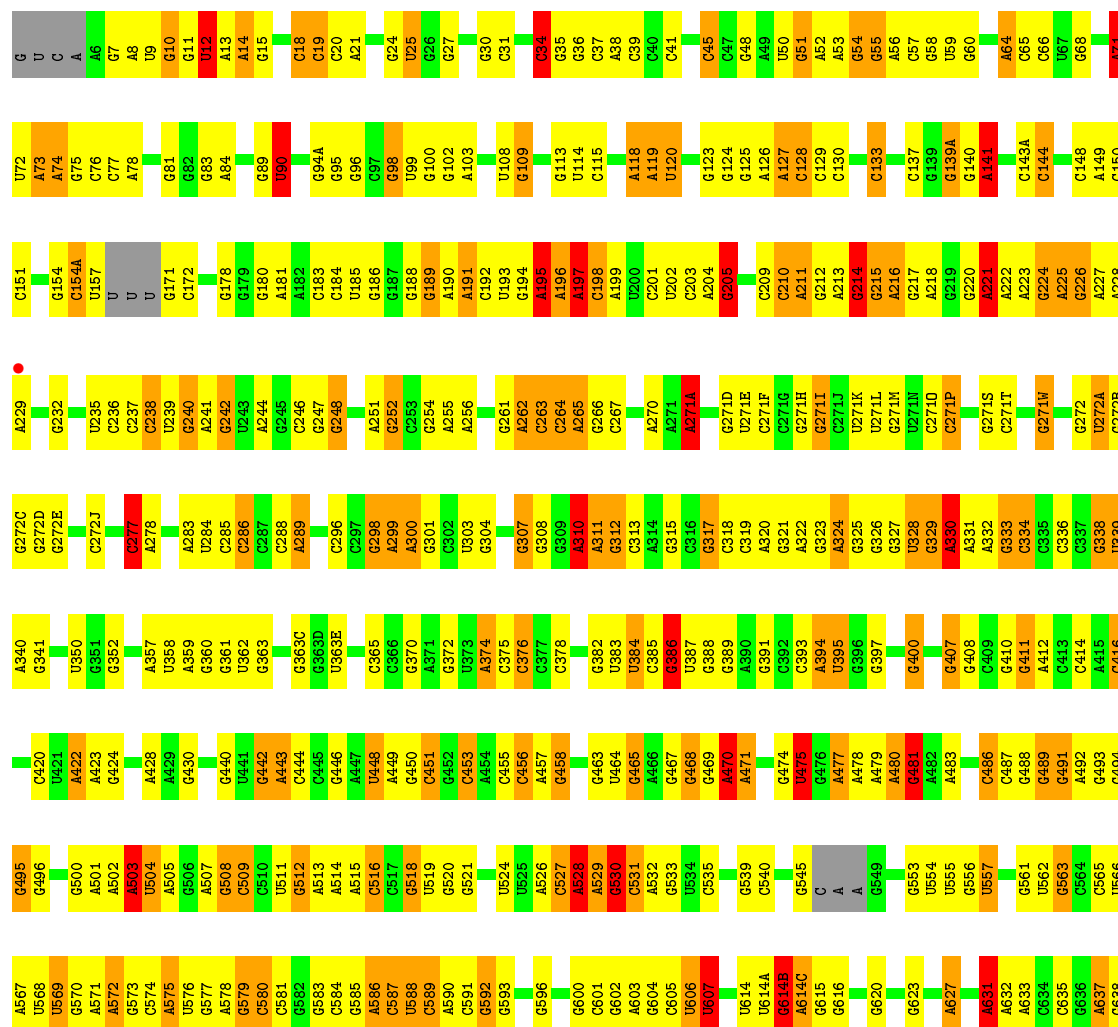




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C2550	A2490	A2430	C2369	C2306	U2244	G2181	U2121	C2061	A2000	U1937		U1807	A1736	C1671
C2551	G2491	G2431	G2370	C2307	U2245	G2182	U2122	C2062	C2001	A1938	G1870	U1808	A1737	G1672
C2552	C2492	C2432	G2371	U2308	G2246	C2183	G2123	U2063	G2002	U1939	G1871	U1809	G1738	G1673
C2553	G2493	G2433	C2372	C2309	G2247	G2184	U2124	C2064	A2003	A1940	U1872	U1810	U1739	G1674
A2554	G2494	A2434	A2373	A2310	C2248	C2185	C2125	C2065	C2004	A1941	A1871	A1811	U1740	U1675
G2555	G2495	U2435	G2374	G2311	C2249	G2186	G2126	C2066	C2005	C1942	G1873	A1812	C1741	
G2556	G2496	C2436	C2375	G2312	G2250	G2187	U2127	C2067	G2006	C1943	C1874	C1813	G1742	A1678
G2557	G2497	A2376	C2376		C2251	U2188	G2128	G2068	G2007	G1944	G1875	A1814	G1743	A1679
U2558	G2498	A2377	C2377	G2313	C2252	U2189	G2129	U2069	A2008	G1945	G1876	A1815	G1744	G1680
G2559	G2499	G2378	G2378	G2314	U2255	G2190	C2130	G2070	G2009	U1948	A1878	A1816	A1745	A1681
G2560	A2500	G2379	A2317	A2317	U2256	A2191	U2131	G2071	C2010	U1949	A1879	A1817	G1746	G1682
G2561	G2502	G2441	C2360	G2318	U2257	A2192	G2132	C2072	G2011	A1950	G1880	A1818	A1747	C1683
G2562	G2503	A2442	A2381	G2319	U2257	A2193	C2133	A2073	C2012	A1951	U1881	A1819	A1684	C1684
U2563	U2504	U2443	G2382	G2320		U2194	G2134	G2074	U2013	G1952	U1882	A1820	G1749	
U2564	A2444	A2444	G2383	A2321		A2195	U2135	G2075	G2014	U1953	C1883	C1821	U1686	U1686
G2565	U2505	A2445	G2384			A2196	A2136	A2076	U2015	U1954	A1884	A1822	G1752	C1687
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G2567	G2507	A2447	G2386	U2324	G2262	A2198	U2138	G2078	U2017	G1956	G1886	C1824	G1754	G1689
U2568	C2508	G2448	G2387	C2325	G2263	A2199	U2139	A2079	C2018		G1887	U1825	G1755	G1690
G2569	A2509	U2449	A2388	C2326	G2264	C2200	U2140	A2080	G2019	A1958	C1888	C1826	C1756	C1691
C2570	C2510	U2450	C2389	G2327	C2265	G2201	A2141	A2081	G2020	A1959	G1889	U1827	U1757	G1692
C2571	C2511	A2451	A2390	C2329	G2267	U2202	G2142	A2082	C2021	U1960	C1891	C1828		C1693
G2572	U2512	C2452	G2391	G2330	G2268	G2203	G2143	G2083	G2022	U1961	G1891	U1829	G1764	G1694
A2573	C2513	C2453	C2392	G2331	U2269	G2204	U2144	A2084	A2023	U1962	G1892	G1830	U1765	C1695
U2574	G2514	C2454	G2393	A2332	C2270	G2205	G2145	C2085	G2024	C1963	G1893	C1831	G1766	G1696
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G2582	C2522	A2462	G2402	A2340	A2278	G2213	G2153	A2093	U2033	G1971	G1900	C1901	C1774	G1704
C2583	U2523	A2463	U2403	G2341	A2279	G2214	U2154	G2094	C2034	G1972	C1902	A1840	C1775	C1705
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C2587	C2527	G2467	G2406	A2345	G2283	C2218	C2158	U2098	U2038	G1976	G1910	G1844	C1782	G1709
G2588	G2528	C2468	C2407	G2346	U2284	U2219	G2159	A2099	U2039	U1977	A1911	G1845	G1783	C1710
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G2590	A2530	G2470	A2348	A2348	A2286	A2221	C2161	U2101	G2041	C1979	G1913	A1847	G1785	A1712
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A2601	G2541	A2481		G2359	C2297	G2236	U2172	C1989	A2052	G1990	C1927	G1858	C1796	A1723
G2602	A2542	C2482	G2422	U2360	A2298	G2237	G2173	U2113	G2053	A1991	G1928	G1859	A1724	U1797
C2603	G2543	C2483	G2423	G2361	A2299	A2237	G2174	U2114	G2054	A1992		A1860	G1725	
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G2606	C2546	C2486	G2426		G2302	A2240	G2177	C2117	G2057	G1995	U1933	C1863	G1803	
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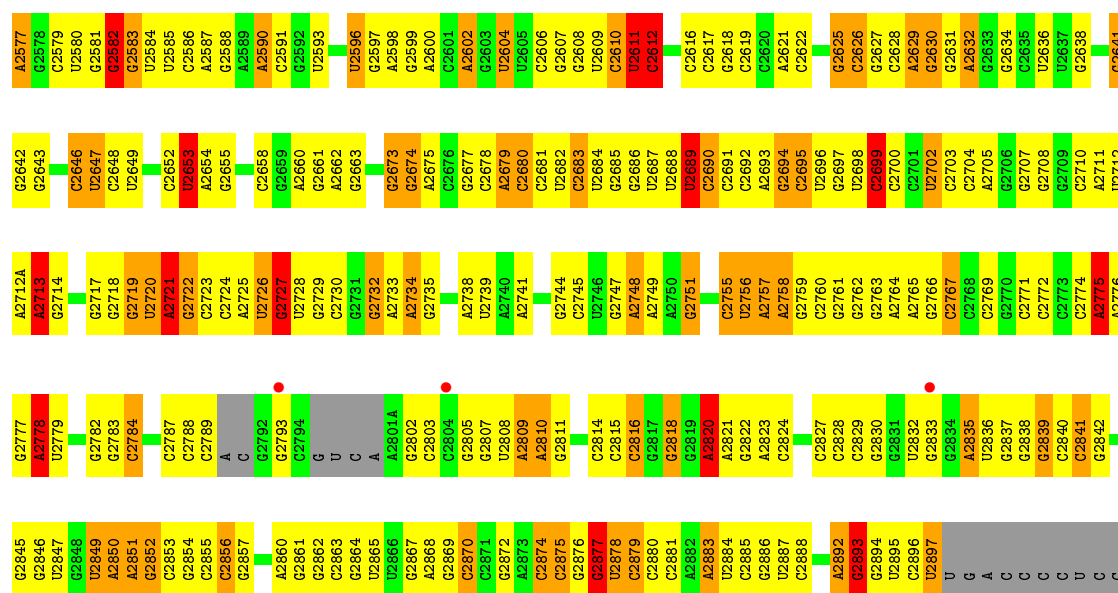


• Molecule 1: 23S Ribosomal RNA

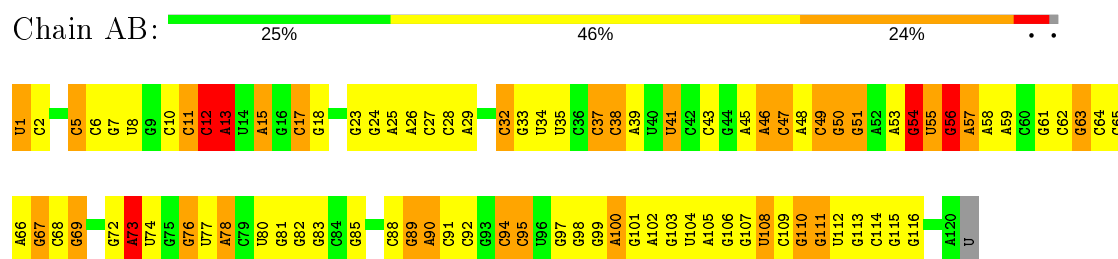




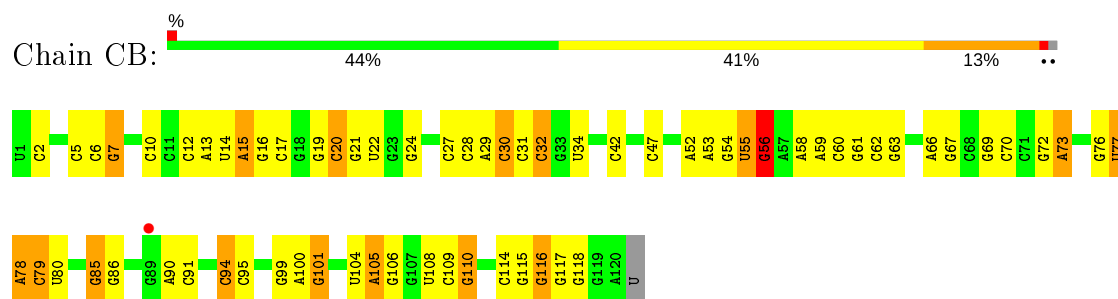
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A2518	A2450	G2383	G2306	G2240	G2185	C2105	C2044	C1979	U1915	G1831			C1675	C1607
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C2521	A2453	G2386	A2309	U2243	G2188	C2108	U2047	C1982	A1918	U1834		G1768	C1612	C1611
U2522	G2454	U2387	A2310	U2244	A2189	U2109	G2048	C1983	A1919	G1835		G1769	U1680	C1612
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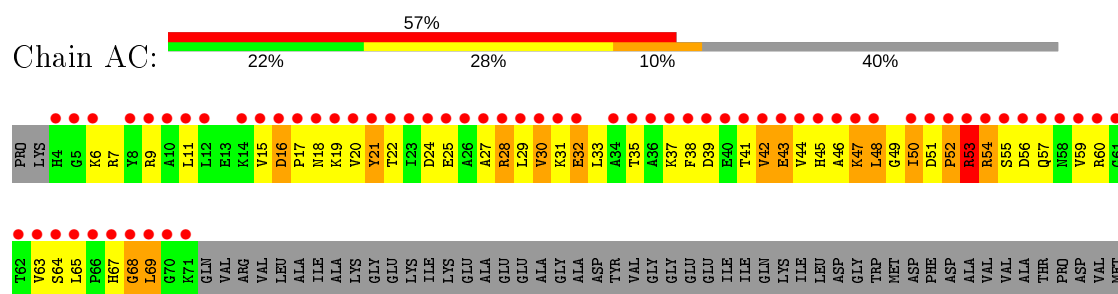
• Molecule 2: 5S Ribosomal RNA

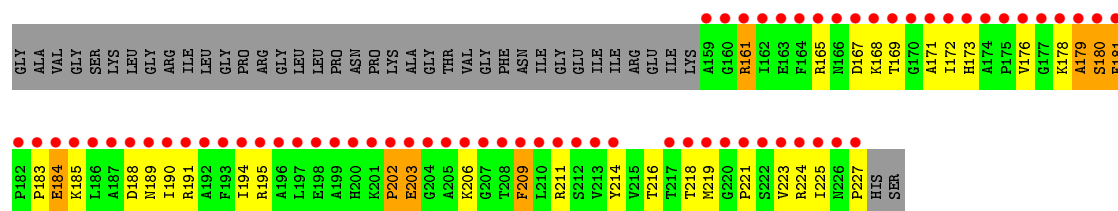


• Molecule 2: 5S Ribosomal RNA

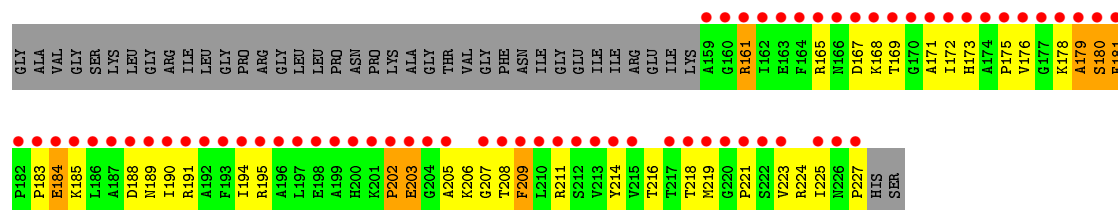
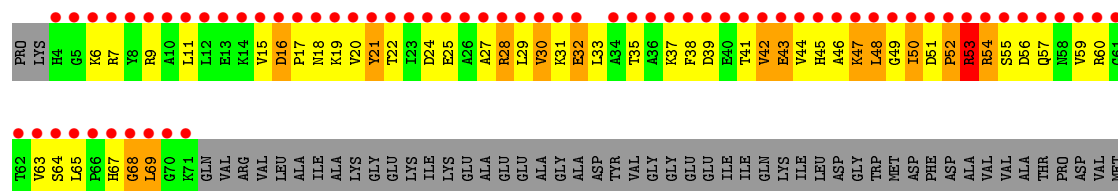
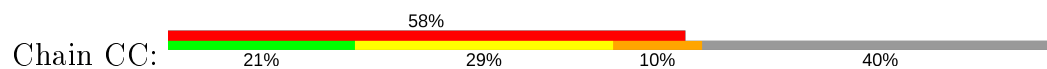


• Molecule 3: 50S ribosomal protein L1

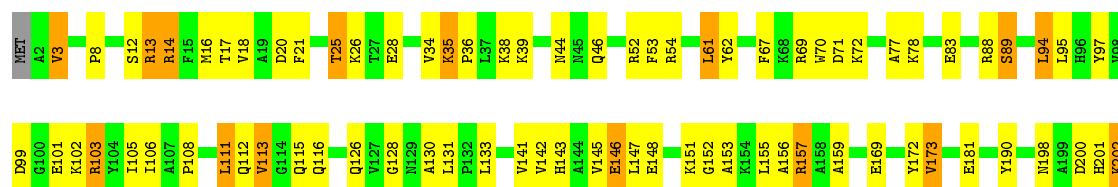




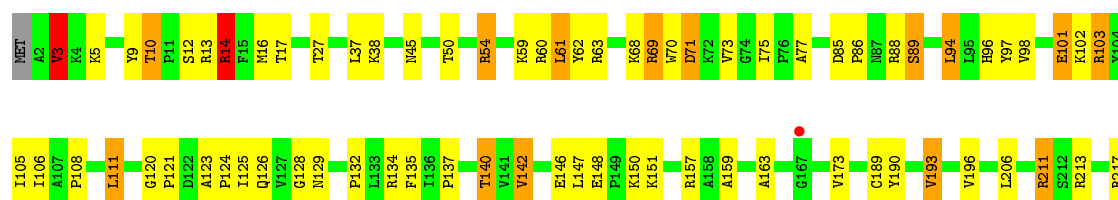
• Molecule 3: 50S ribosomal protein L1



• Molecule 4: 50S ribosomal protein L2



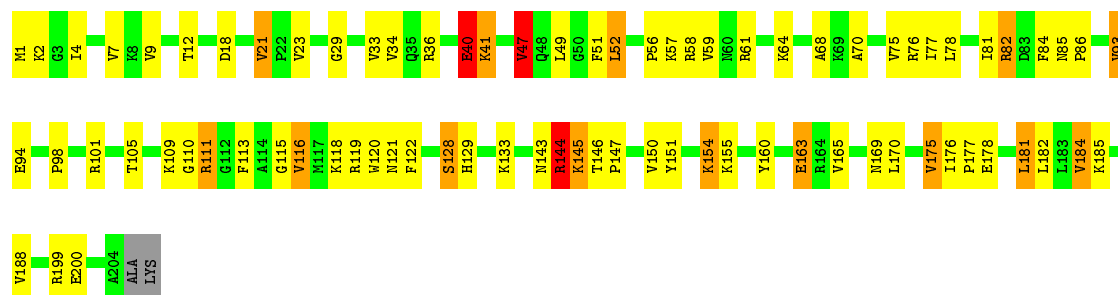
• Molecule 4: 50S ribosomal protein L2





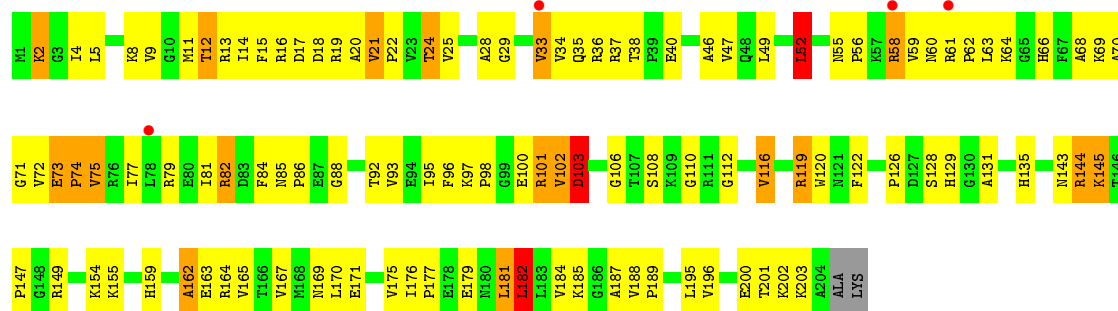
- Molecule 5: 50S ribosomal protein L3

Chain AE: 60% 31% 7% ..



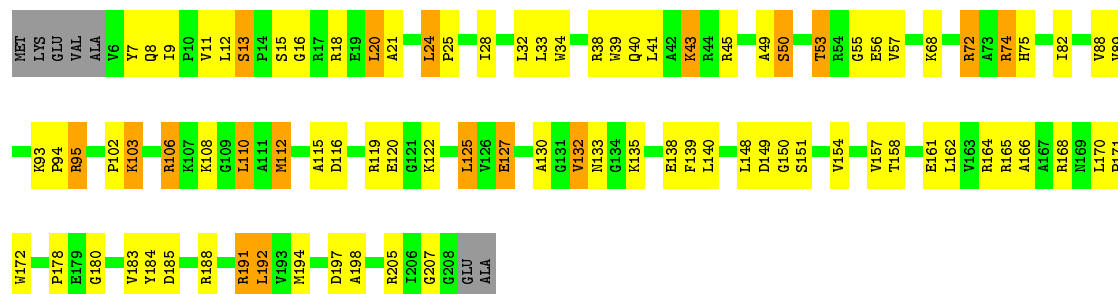
- Molecule 5: 50S ribosomal protein L3

Chain CE: 44% 45% 9% ..



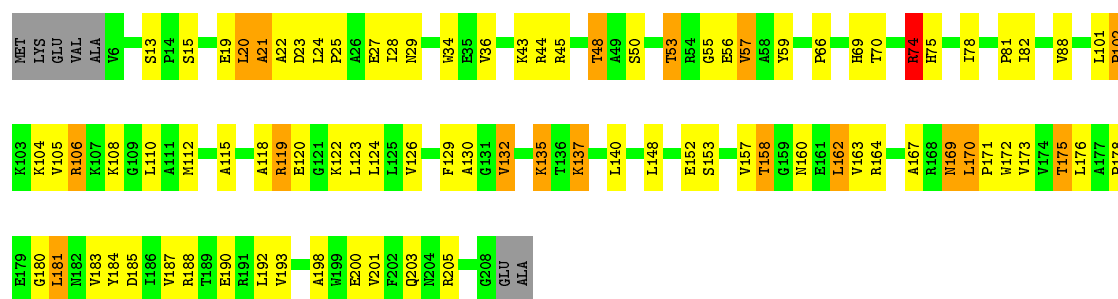
- Molecule 6: 50S ribosomal protein L4

Chain AF: 55% 33% 9% .

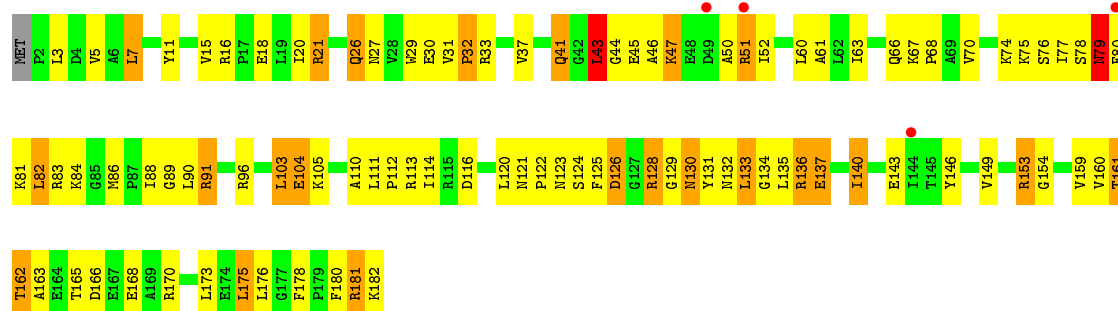


- Molecule 6: 50S ribosomal protein L4

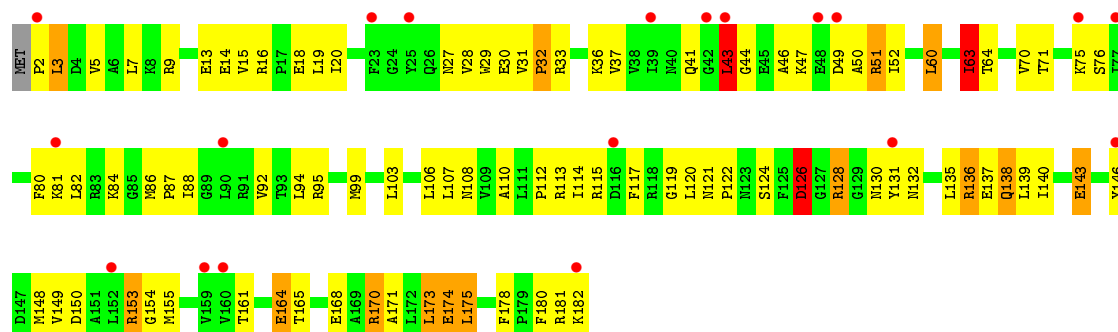
Chain CF: 55% 33% 8% .



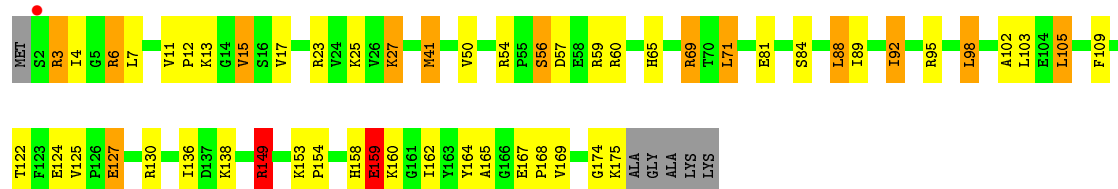
• Molecule 7: 50S ribosomal protein L5



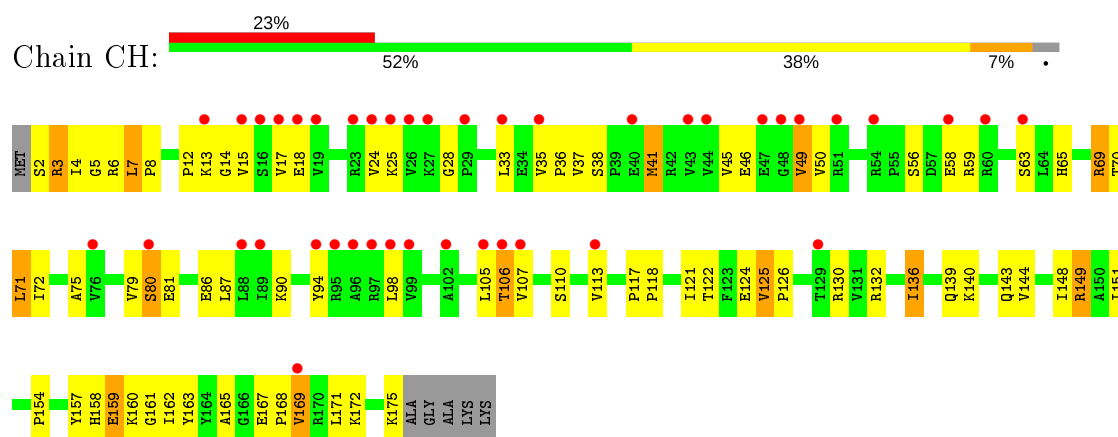
• Molecule 7: 50S ribosomal protein L5



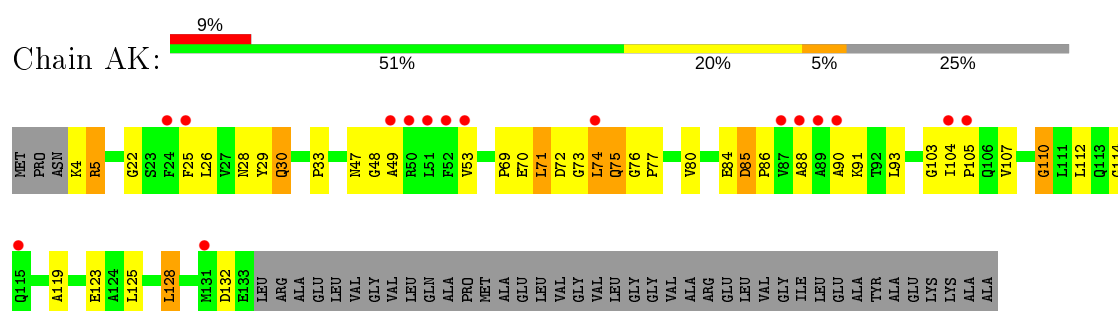
• Molecule 8: 50S ribosomal protein L6



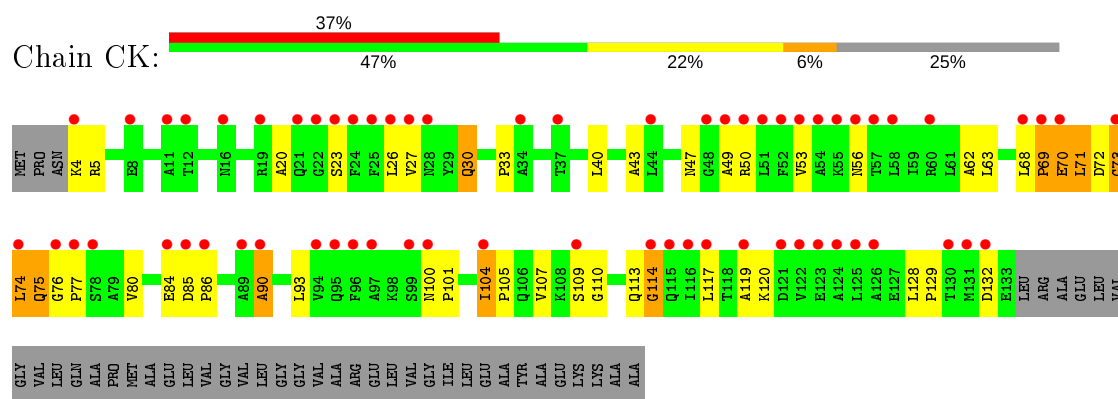
• Molecule 8: 50S ribosomal protein L6



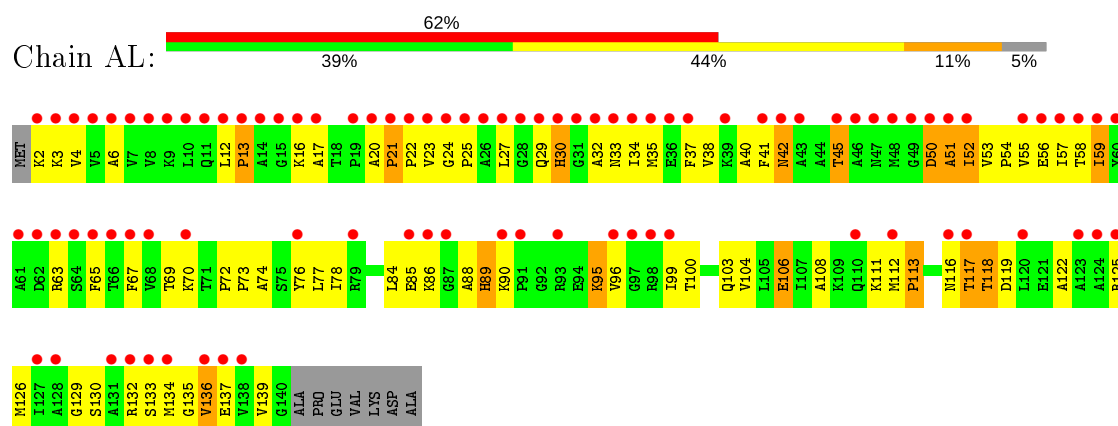
• Molecule 9: 50S ribosomal protein L10



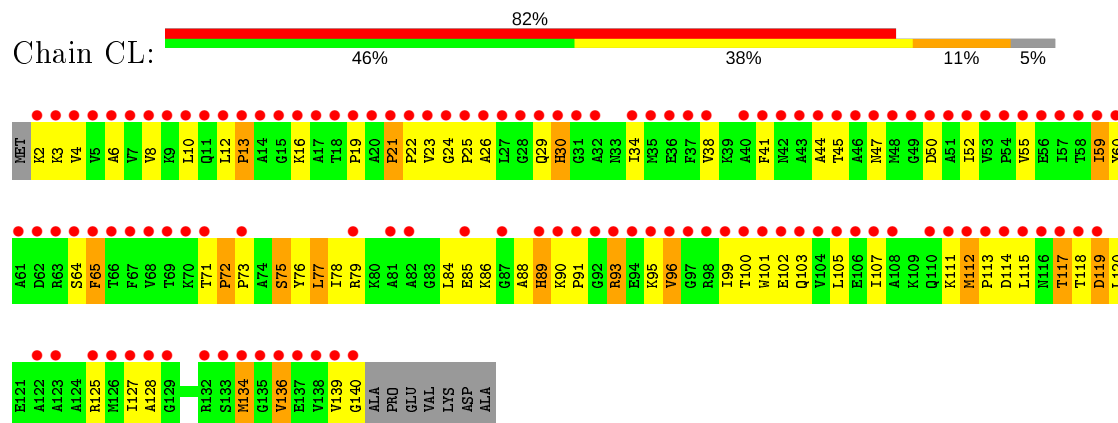
• Molecule 9: 50S ribosomal protein L10



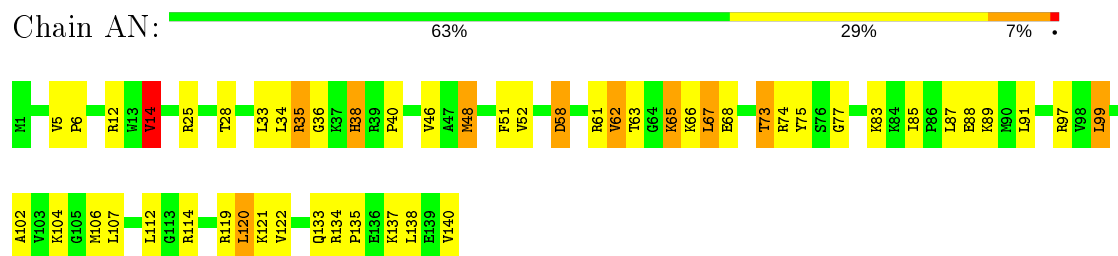
• Molecule 10: 50S ribosomal protein L11



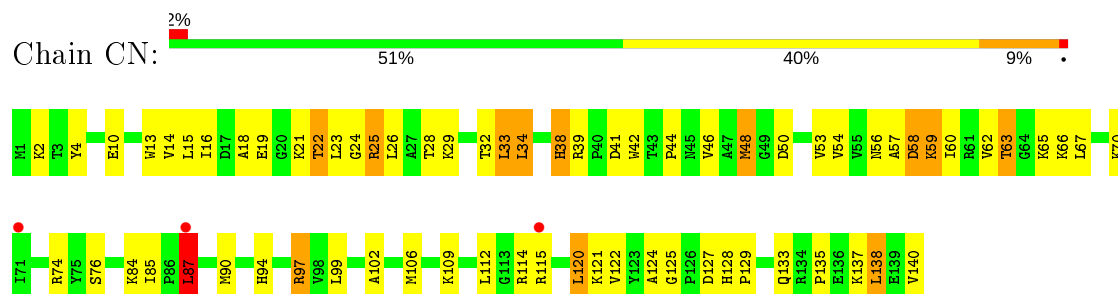
- Molecule 10: 50S ribosomal protein L11



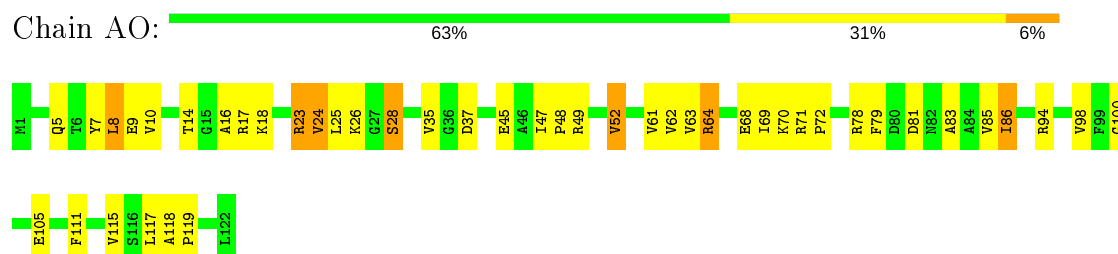
- Molecule 11: 50S ribosomal protein L13



- Molecule 11: 50S ribosomal protein L13

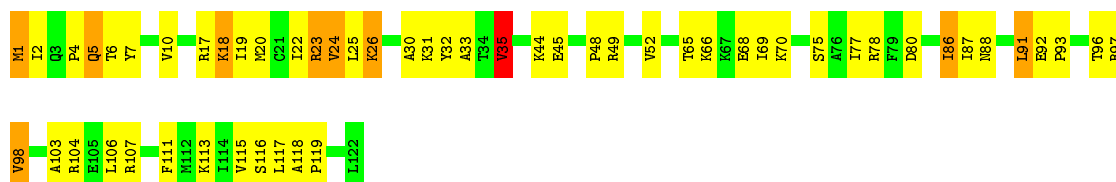


- Molecule 12: 50S ribosomal protein L14



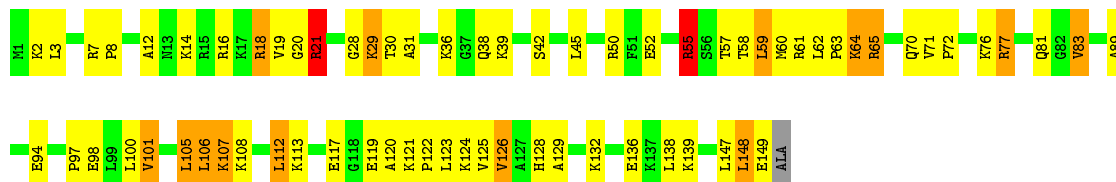
- Molecule 12: 50S ribosomal protein L14





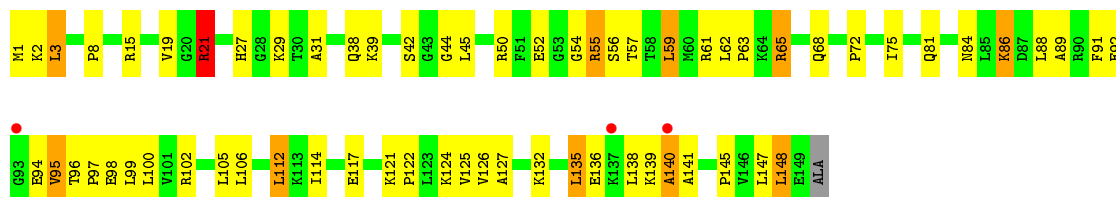
- Molecule 13: 50S ribosomal protein L15

Chain AP: 53% 35% 9% ..



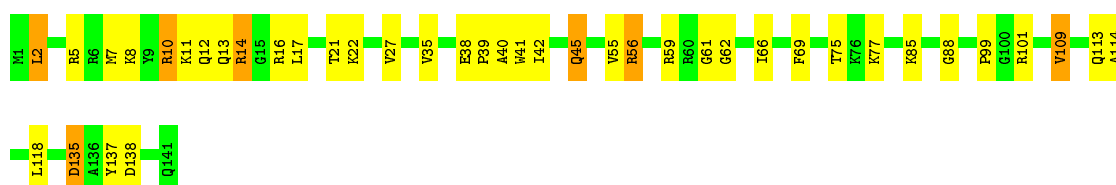
- Molecule 13: 50S ribosomal protein L15

Chain CP: 2% 56% 36% 7% ..



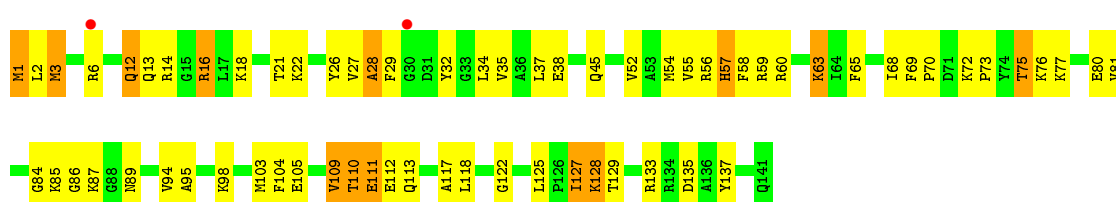
- Molecule 14: 50S ribosomal protein L16

Chain AQ: 71% 24% 5%



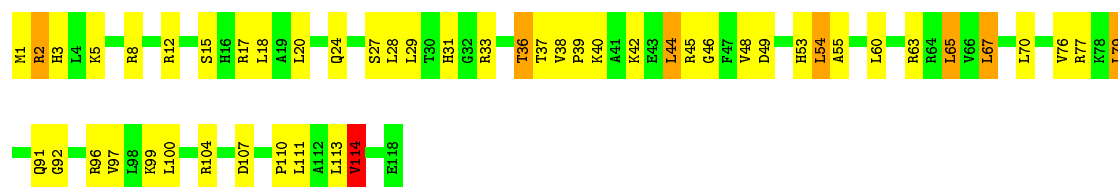
- Molecule 14: 50S ribosomal protein L16

Chain CQ: % 52% 38% 9%



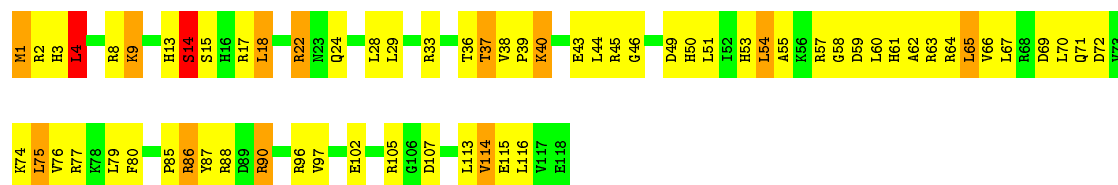
- Molecule 15: 50S ribosomal protein L17

Chain AR: 



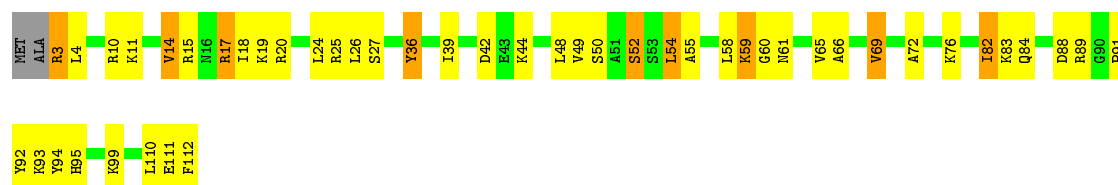
- Molecule 15: 50S ribosomal protein L17

Chain CR: 



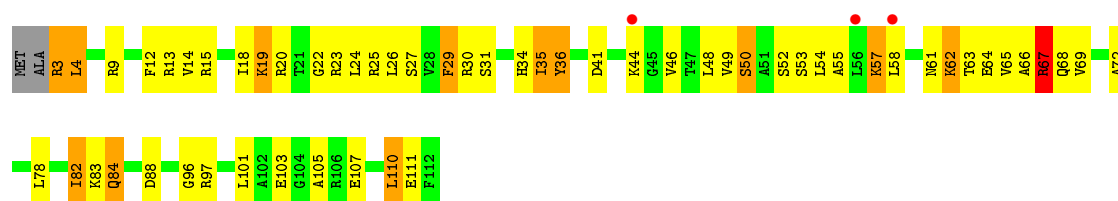
- Molecule 16: 50S ribosomal protein L18

Chain AS: 



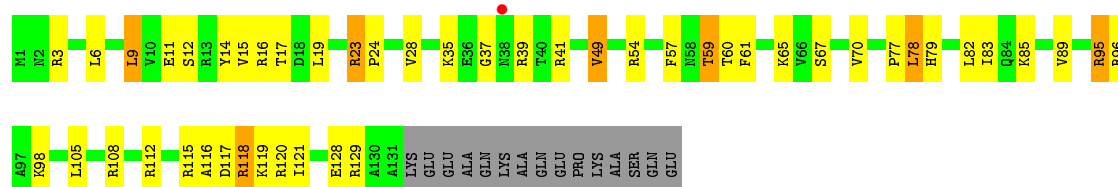
- Molecule 16: 50S ribosomal protein L18

Chain CS: 

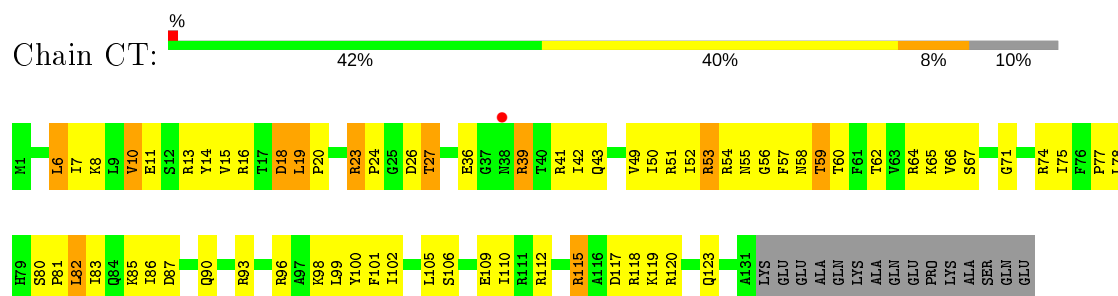


- Molecule 17: 50S ribosomal protein L19

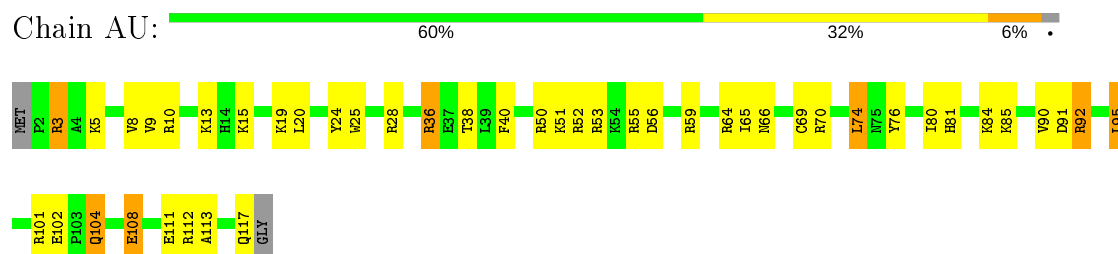
Chain AT: 



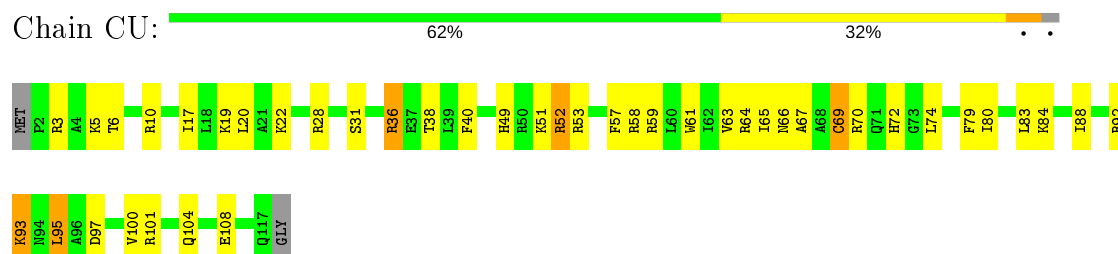
- Molecule 17: 50S ribosomal protein L19



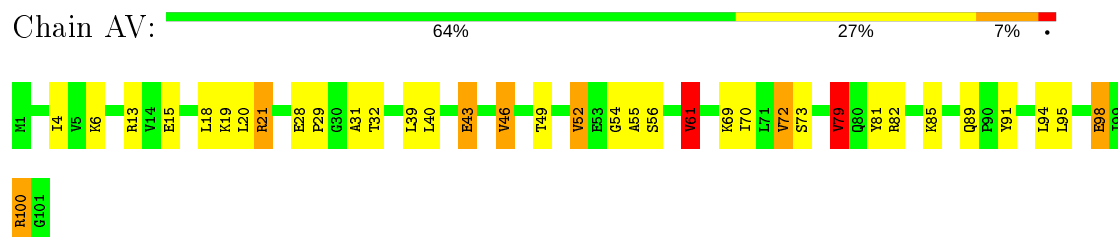
- Molecule 18: 50S ribosomal protein L20



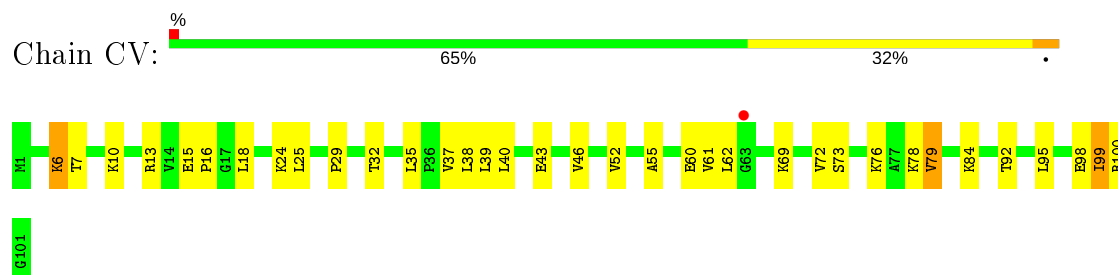
- Molecule 18: 50S ribosomal protein L20



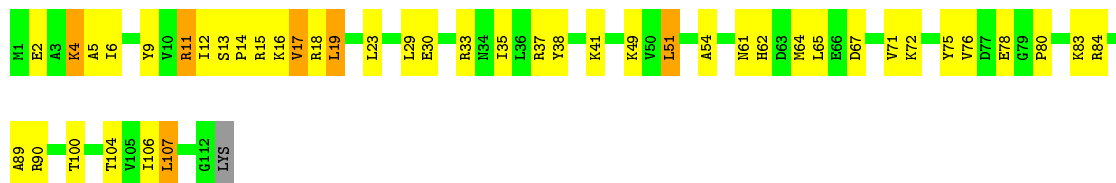
- Molecule 19: 50S ribosomal protein L21



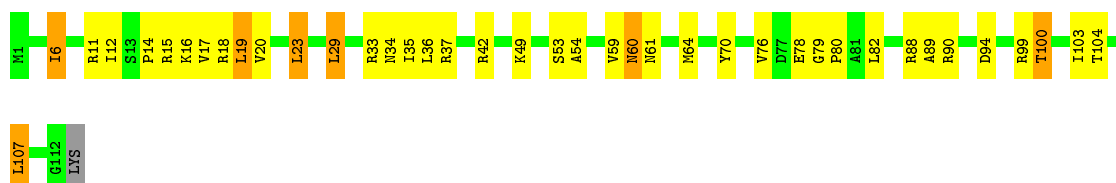
- Molecule 19: 50S ribosomal protein L21



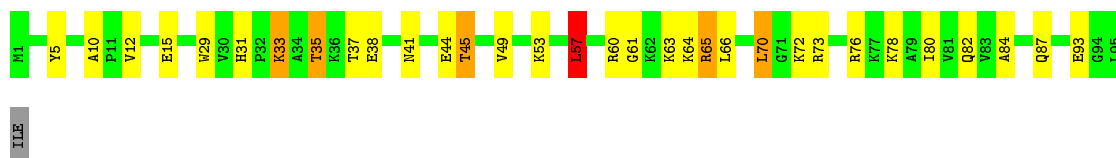
• Molecule 20: 50S ribosomal protein L22

Chain AW: 

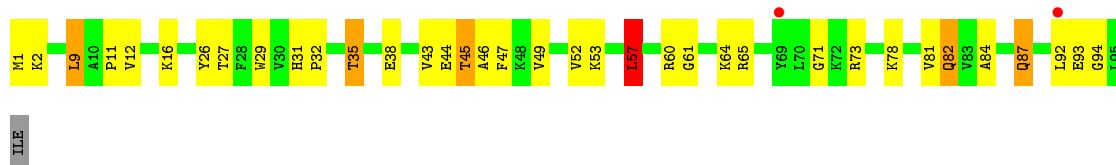
• Molecule 20: 50S ribosomal protein L22

Chain CW: 

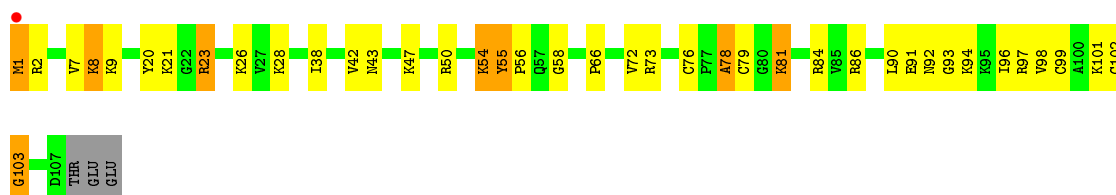
• Molecule 21: 50S ribosomal protein L23

Chain AX: 

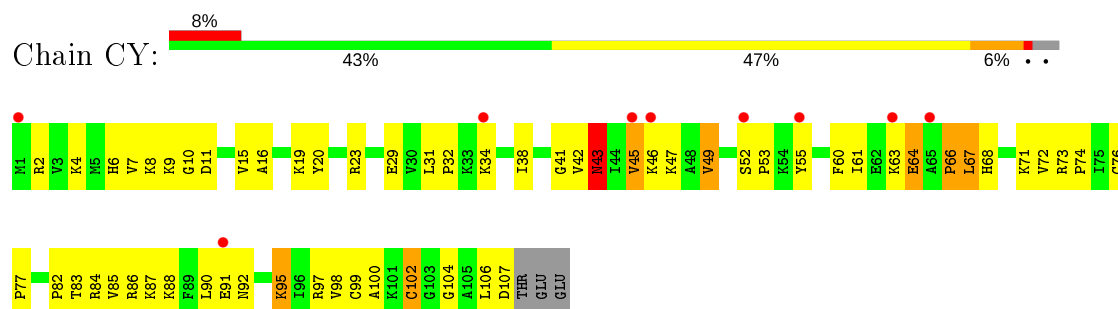
• Molecule 21: 50S ribosomal protein L23

Chain CX: 

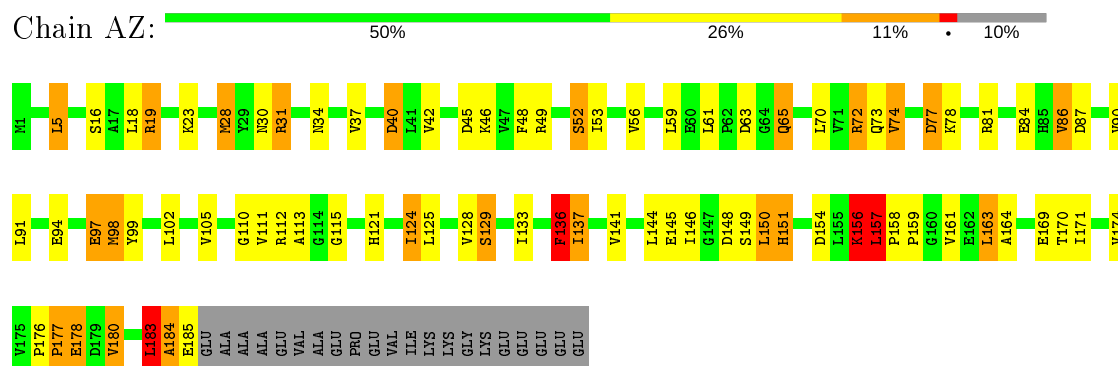
• Molecule 22: 50S ribosomal protein L24

Chain AY: 

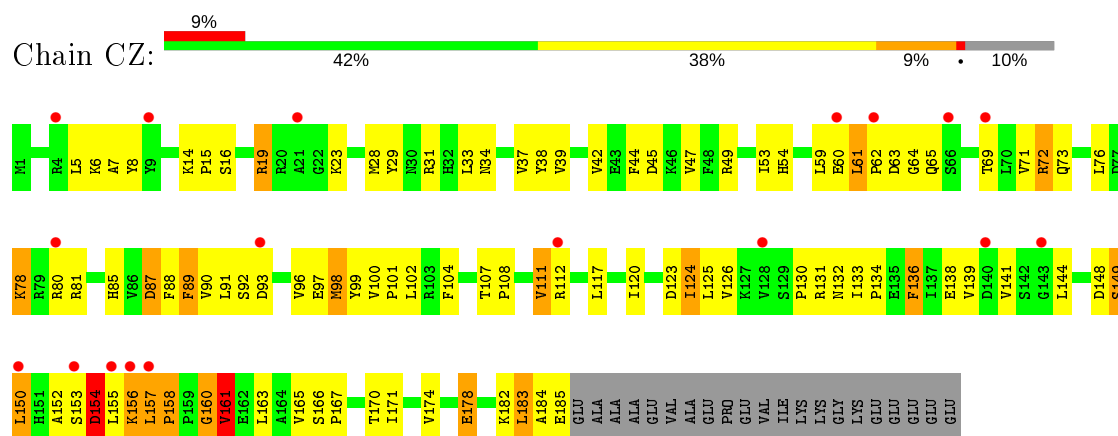
• Molecule 22: 50S ribosomal protein L24



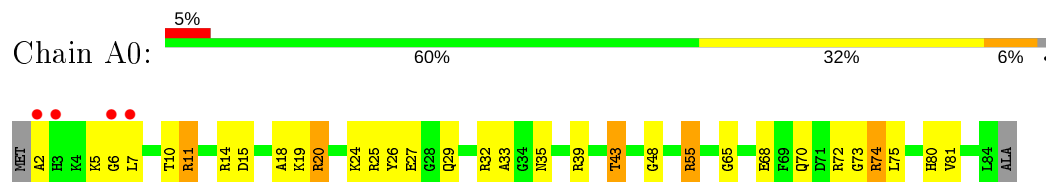
• Molecule 23: 50S ribosomal protein L25



• Molecule 23: 50S ribosomal protein L25

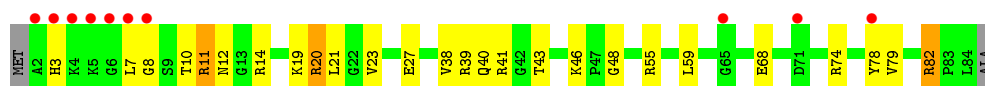


• Molecule 24: 50S ribosomal protein L27



• Molecule 24: 50S ribosomal protein L27

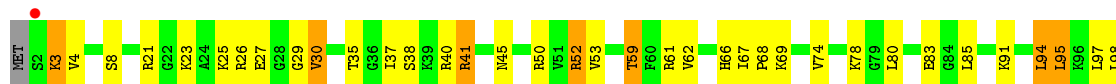




- Molecule 25: 50S ribosomal protein L28



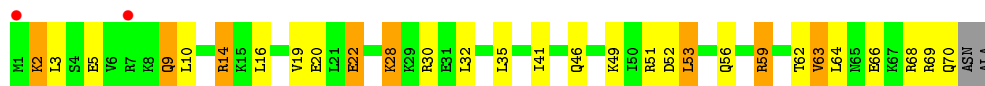
- Molecule 25: 50S ribosomal protein L28



- Molecule 26: 50S ribosomal protein L29



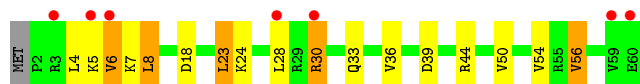
- Molecule 26: 50S ribosomal protein L29



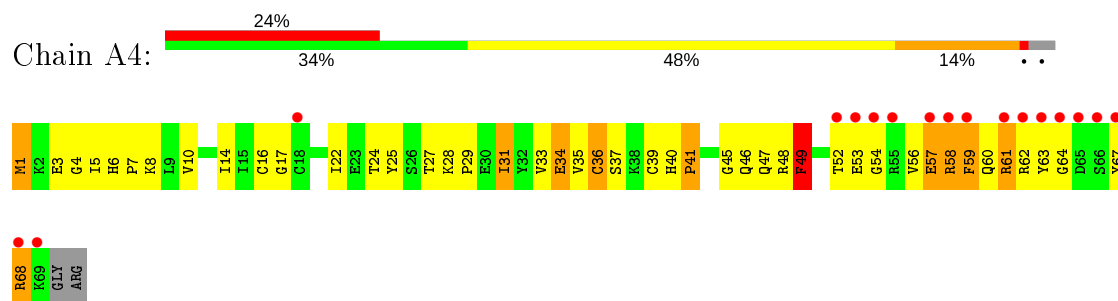
- Molecule 27: 50S ribosomal protein L30



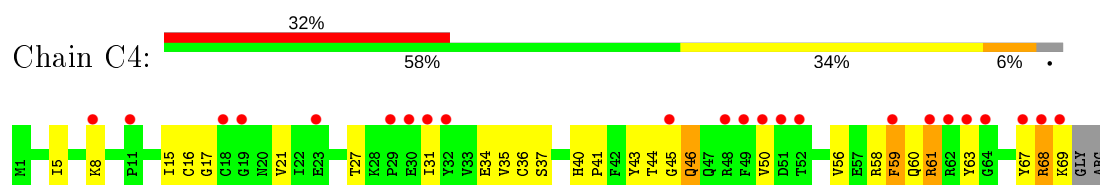
- Molecule 27: 50S ribosomal protein L30



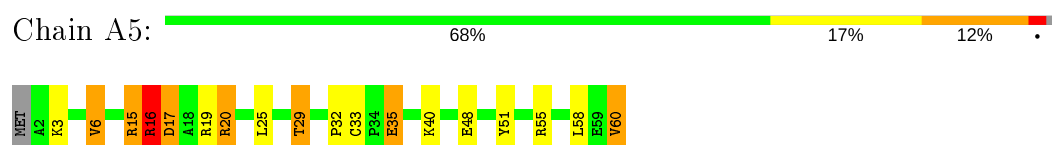
• Molecule 28: 50S ribosomal protein L31



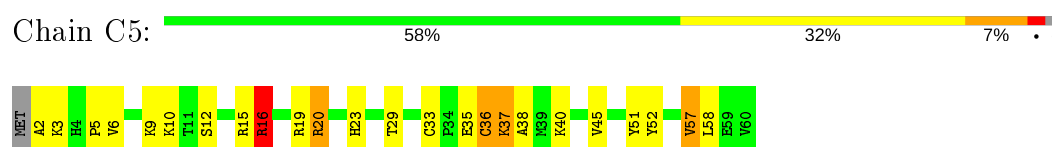
• Molecule 28: 50S ribosomal protein L31



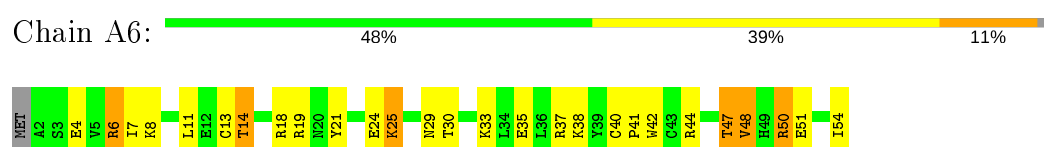
• Molecule 29: 50S ribosomal protein L32



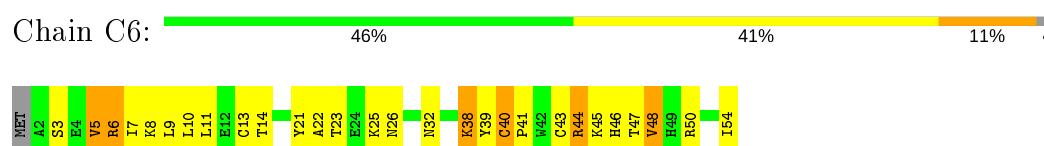
• Molecule 29: 50S ribosomal protein L32



• Molecule 30: 50S ribosomal protein L33

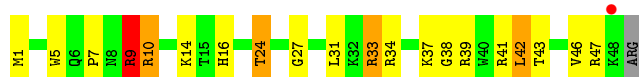


• Molecule 30: 50S ribosomal protein L33

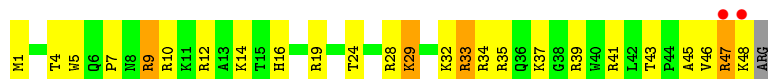


• Molecule 31: 50S ribosomal protein L34





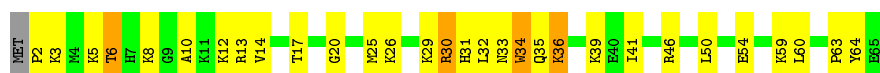
- Molecule 31: 50S ribosomal protein L34



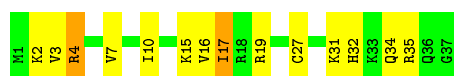
- Molecule 32: 50S ribosomal protein L35



- Molecule 32: 50S ribosomal protein L35



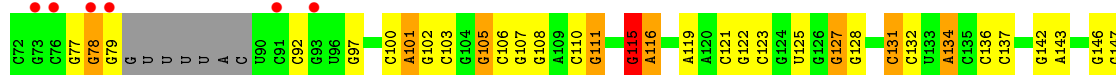
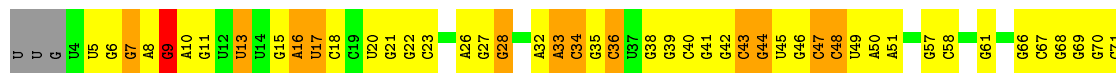
- Molecule 33: 50S ribosomal protein L36



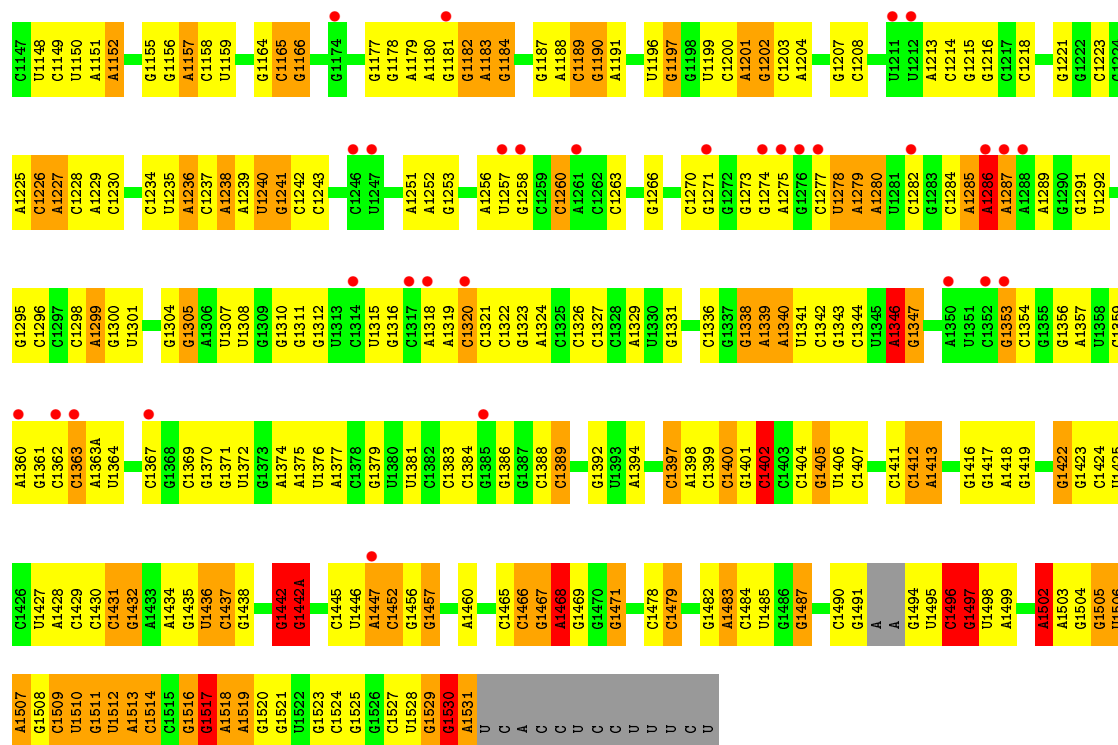
- Molecule 33: 50S ribosomal protein L36



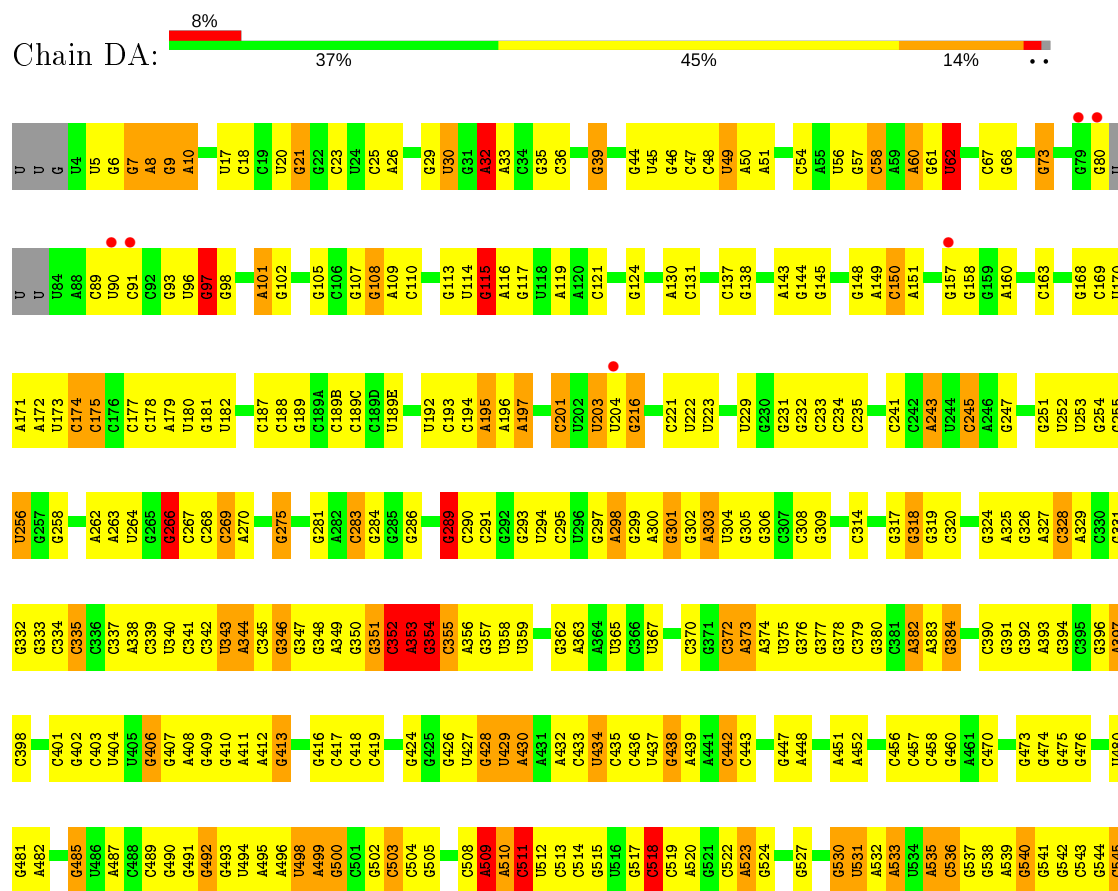
- Molecule 34: 16S Ribosomal RNA







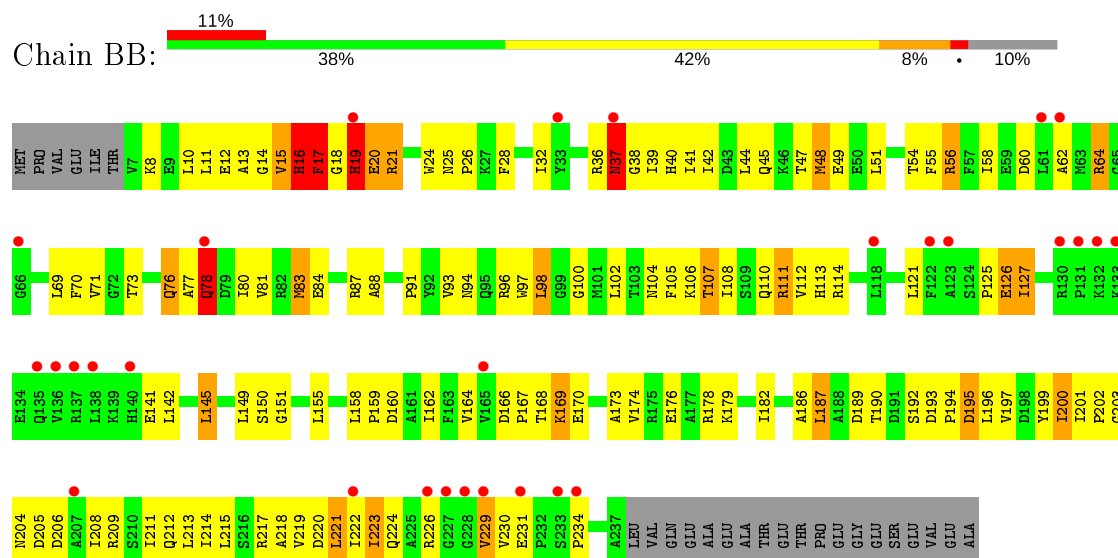
• Molecule 34: 16S Ribosomal RNA



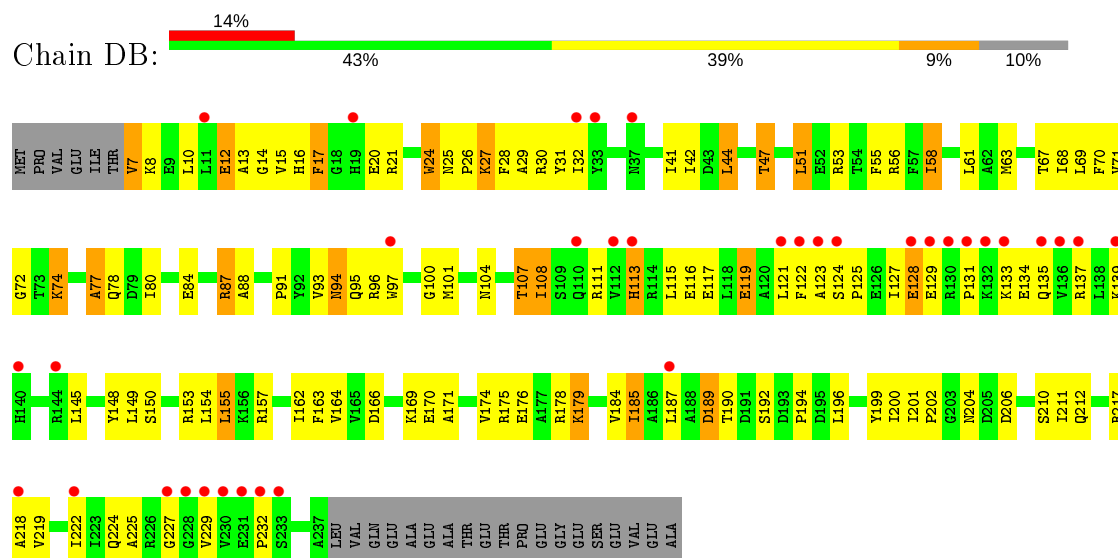
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G1469	C1384	C1320	A1257	G1195	C1129	U1065	A1005	A938	C867	G766	C708	C626	C549
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C1478	G1386	G1322	C1259	U1196	G1132	C1067	C1007	G940	A873	G768	G710	G631	U551
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U U C U

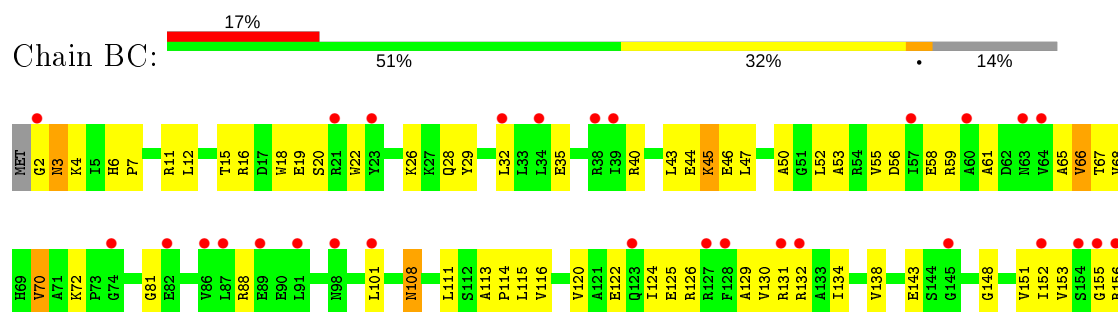
• Molecule 35: 30S ribosomal protein S2

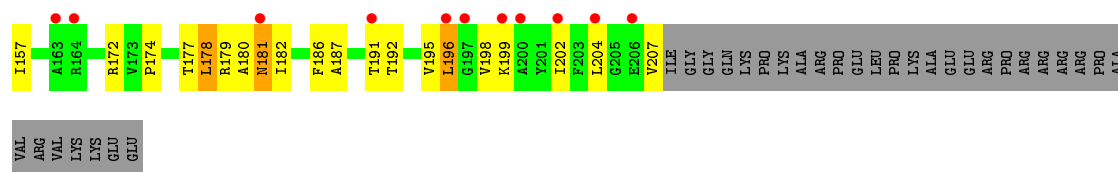


• Molecule 35: 30S ribosomal protein S2

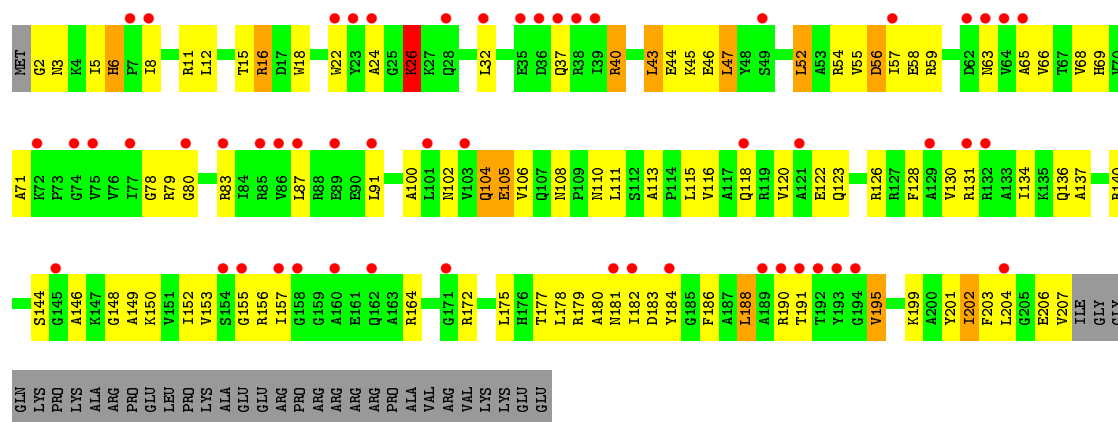


• Molecule 36: 30S ribosomal protein S3

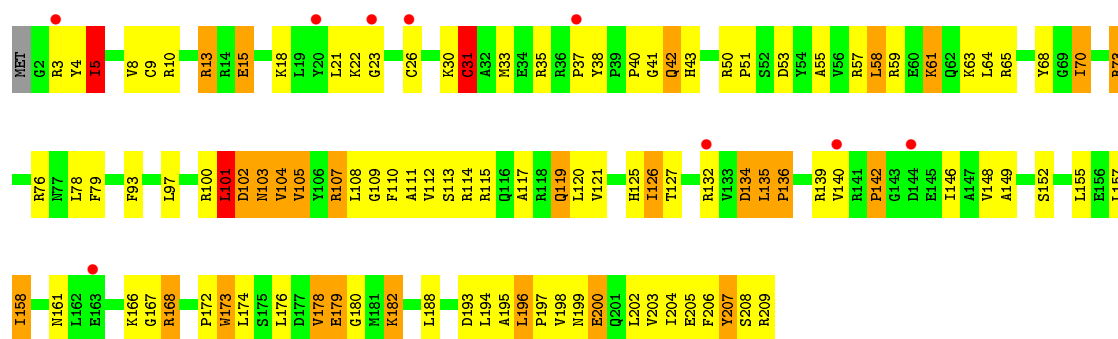




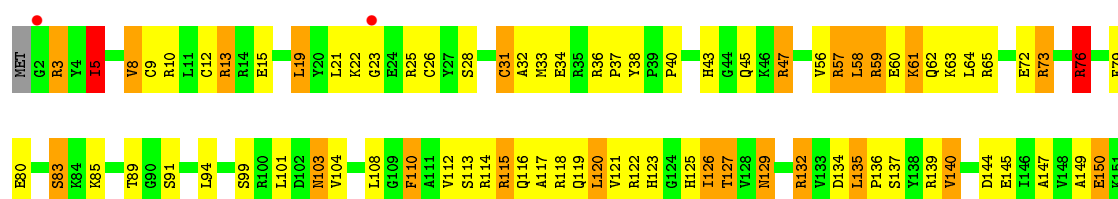
• Molecule 36: 30S ribosomal protein S3

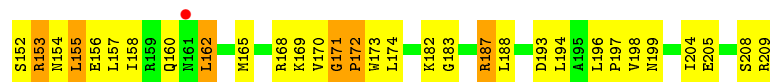


• Molecule 37: 30S ribosomal protein S4

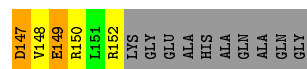
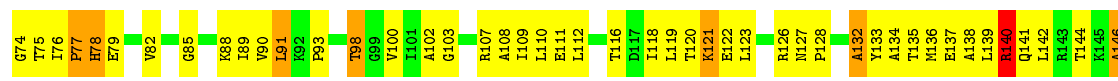
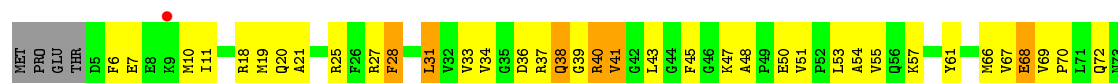


• Molecule 37: 30S ribosomal protein S4

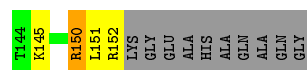
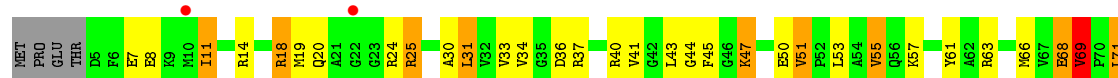




- Molecule 38: 30S ribosomal protein S5



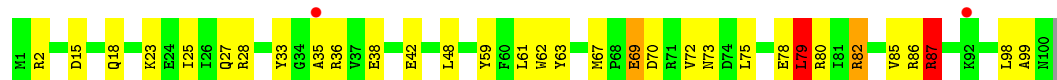
- Molecule 38: 30S ribosomal protein S5



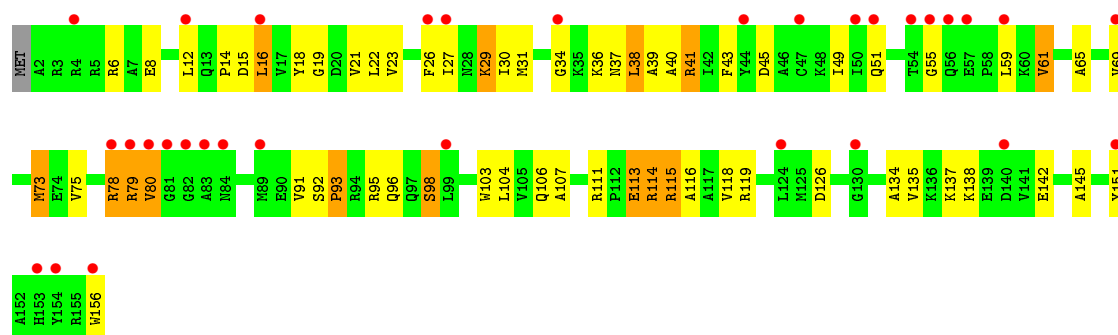
- Molecule 39: 30S ribosomal protein S6



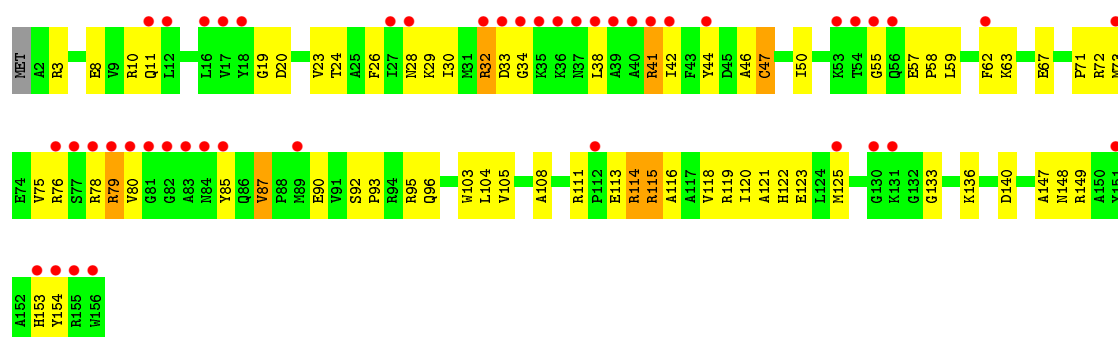
- Molecule 39: 30S ribosomal protein S6



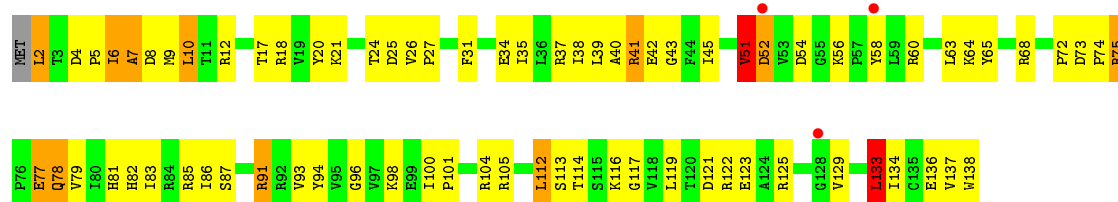
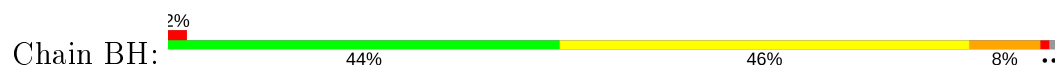
- Molecule 40: 30S ribosomal protein S7



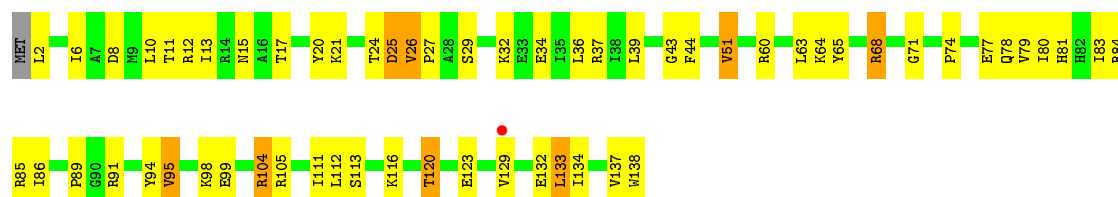
- Molecule 40: 30S ribosomal protein S7



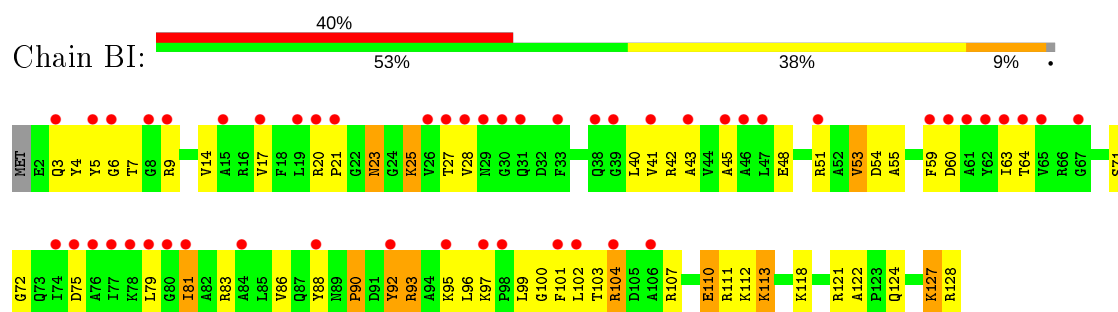
- Molecule 41: 30S ribosomal protein S8



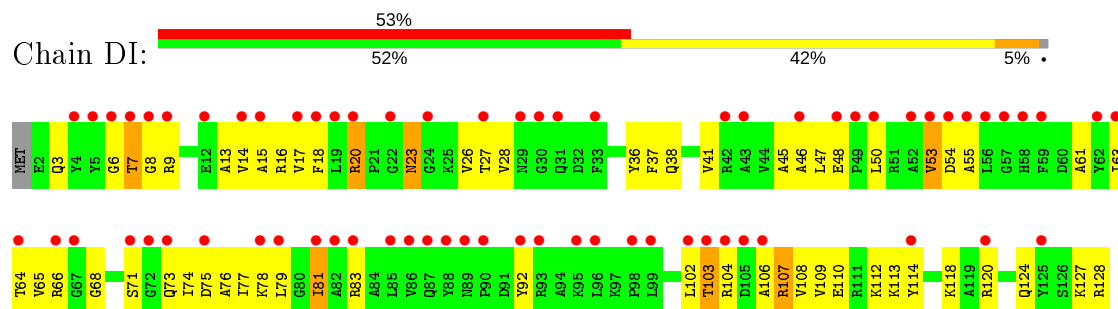
- Molecule 41: 30S ribosomal protein S8



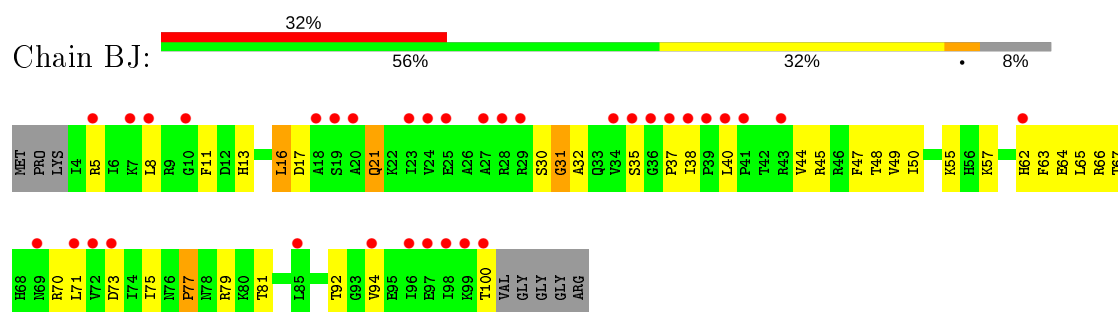
- Molecule 42: 30S ribosomal protein S9



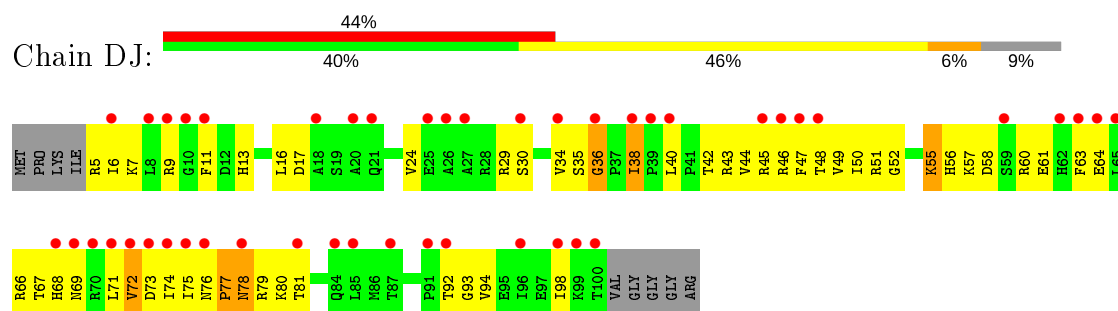
- Molecule 42: 30S ribosomal protein S9



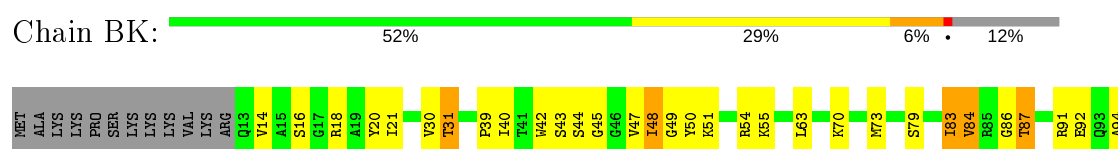
- Molecule 43: 30S ribosomal protein S10



- Molecule 43: 30S ribosomal protein S10

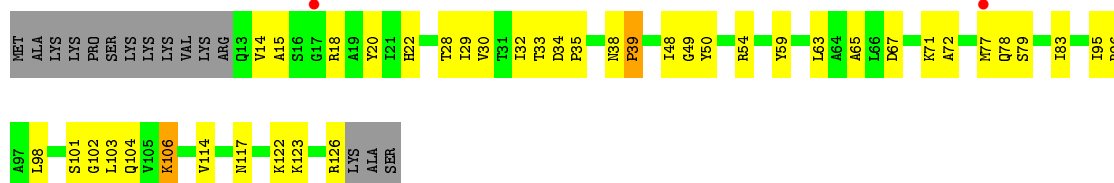


- Molecule 44: 30S ribosomal protein S11

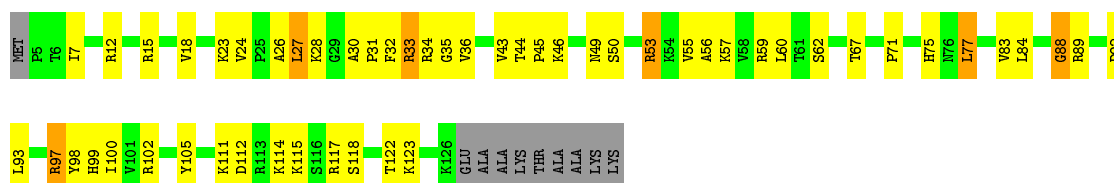




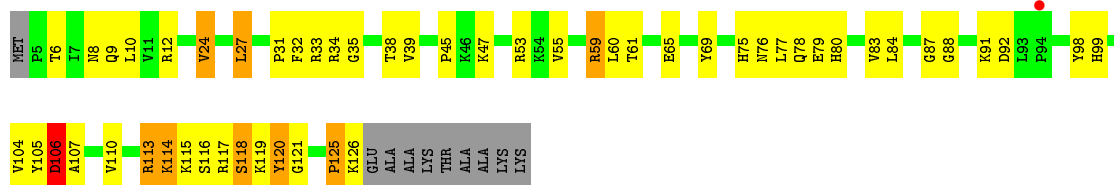
- Molecule 44: 30S ribosomal protein S11



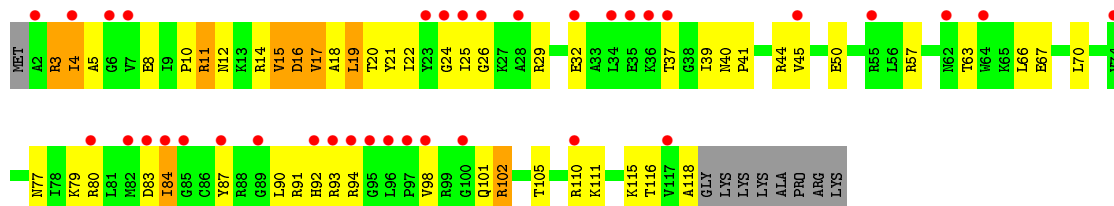
- Molecule 45: 30S ribosomal protein S12



- Molecule 45: 30S ribosomal protein S12

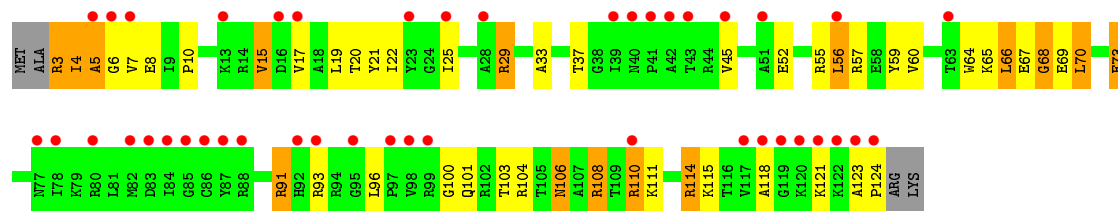


- Molecule 46: 30S ribosomal protein S13

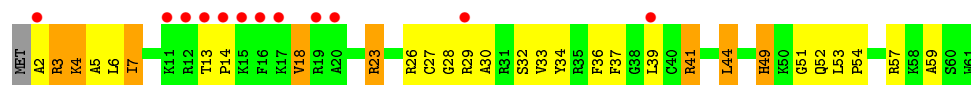


- Molecule 46: 30S ribosomal protein S13

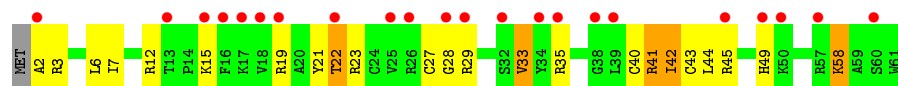




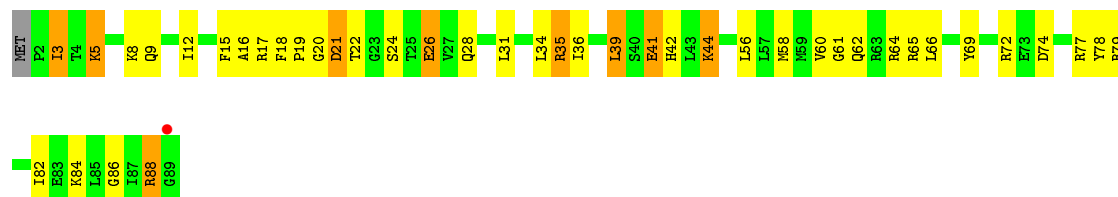
- Molecule 47: 30S ribosomal protein S14 type Z



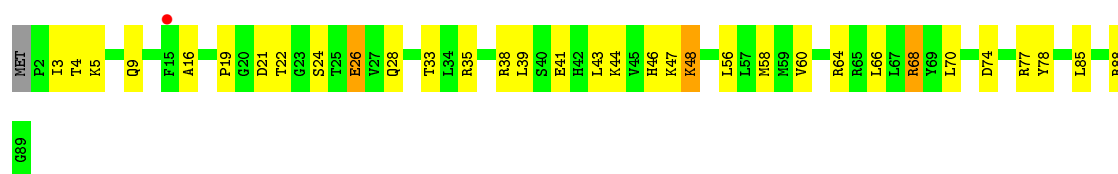
- Molecule 47: 30S ribosomal protein S14 type Z



- Molecule 48: 30S ribosomal protein S15

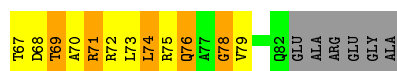


- Molecule 48: 30S ribosomal protein S15

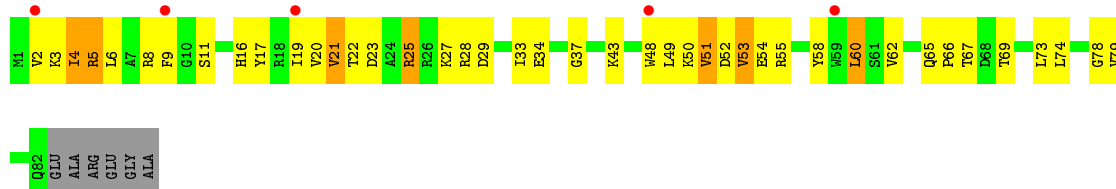


- Molecule 49: 30S ribosomal protein S16

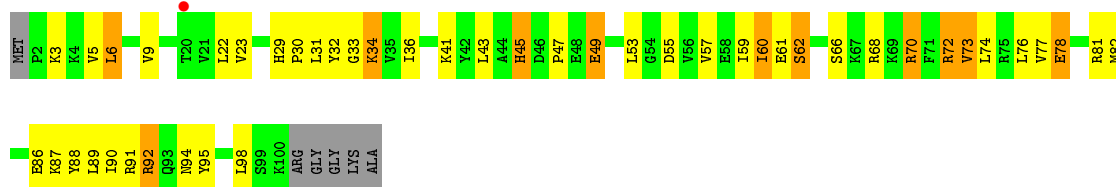




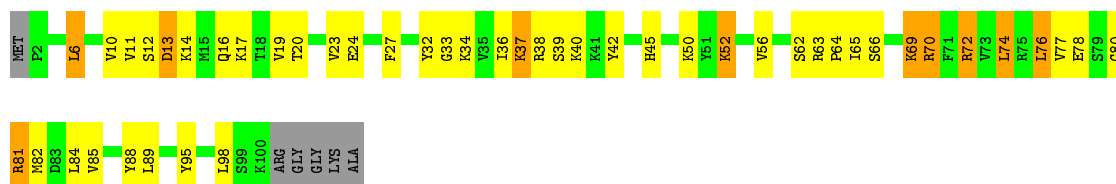
- Molecule 49: 30S ribosomal protein S16



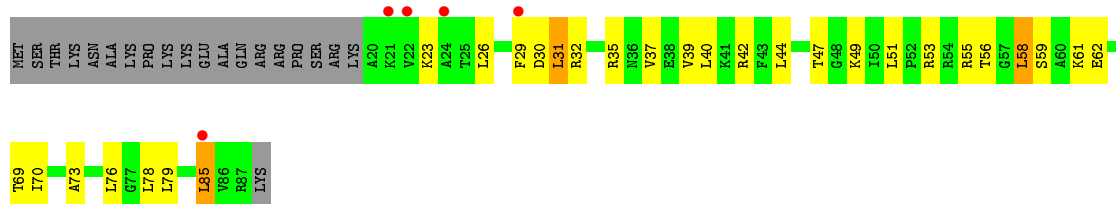
- Molecule 50: 30S ribosomal protein S17



- Molecule 50: 30S ribosomal protein S17

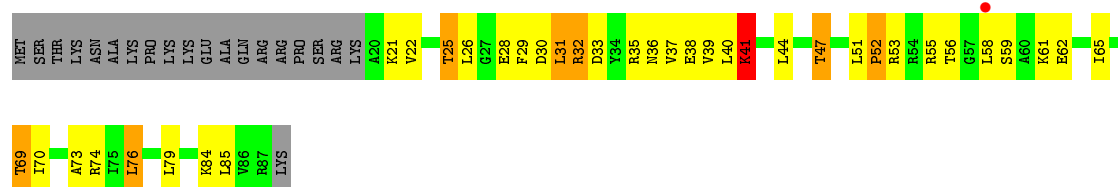


- Molecule 51: 30S ribosomal protein S18

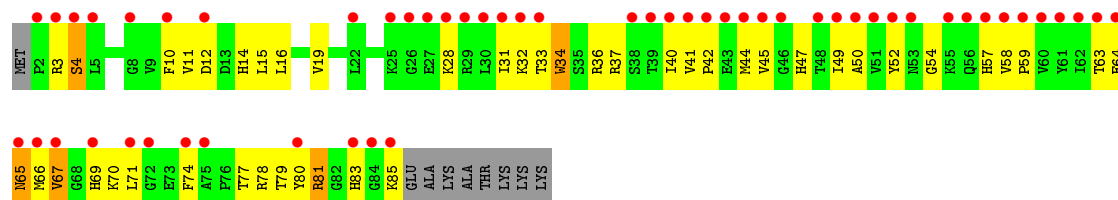


- Molecule 51: 30S ribosomal protein S18

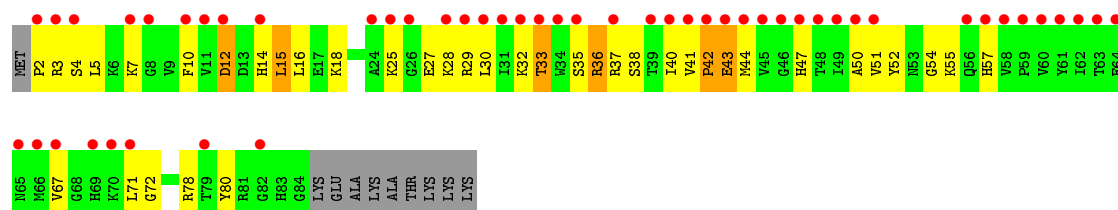




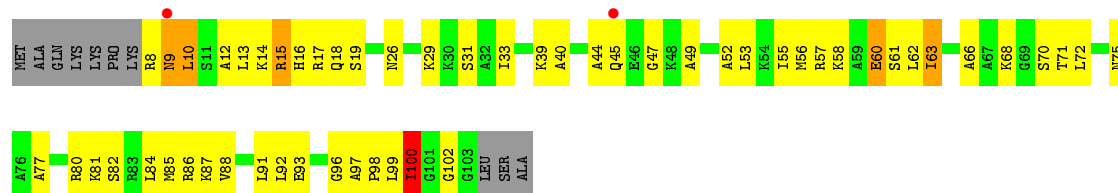
• Molecule 52: 30S ribosomal protein S19



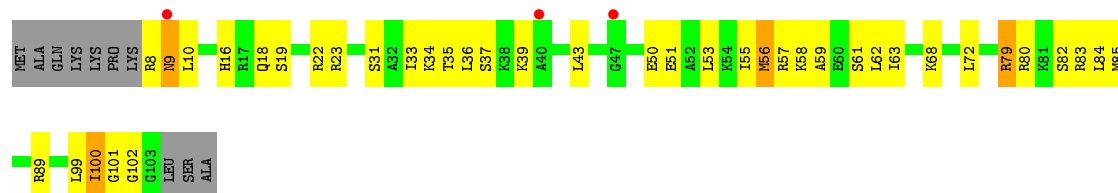
• Molecule 52: 30S ribosomal protein S19



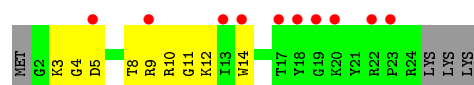
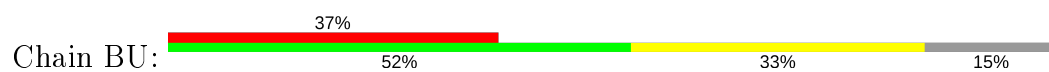
• Molecule 53: 30S ribosomal protein S20



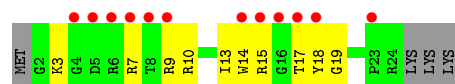
• Molecule 53: 30S ribosomal protein S20



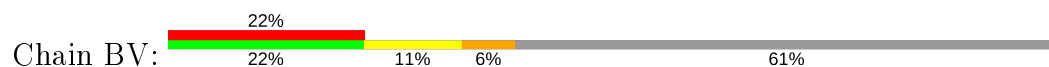
• Molecule 54: 30S ribosomal protein Thx



- Molecule 54: 30S ribosomal protein Thx



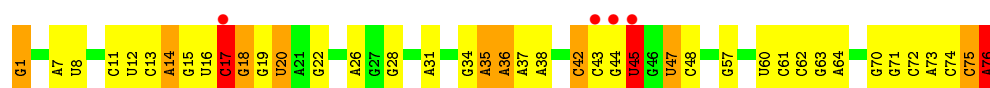
- Molecule 55: mRNA



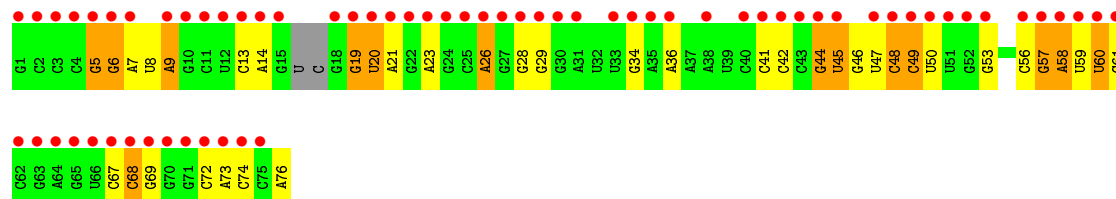
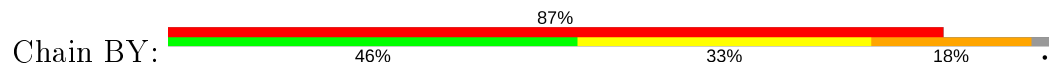
- Molecule 55: mRNA



- Molecule 56: P-site tRNA

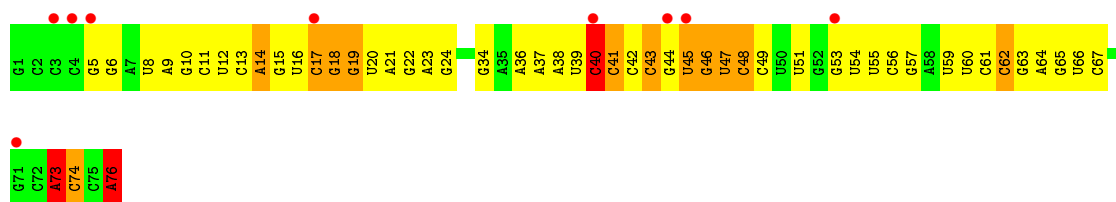


- Molecule 56: P-site tRNA

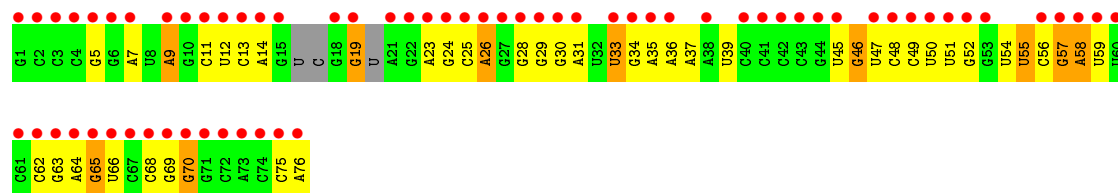
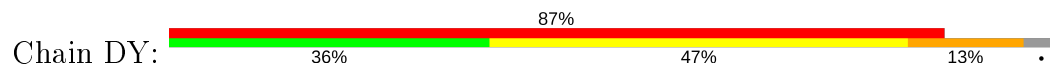


- Molecule 56: P-site tRNA

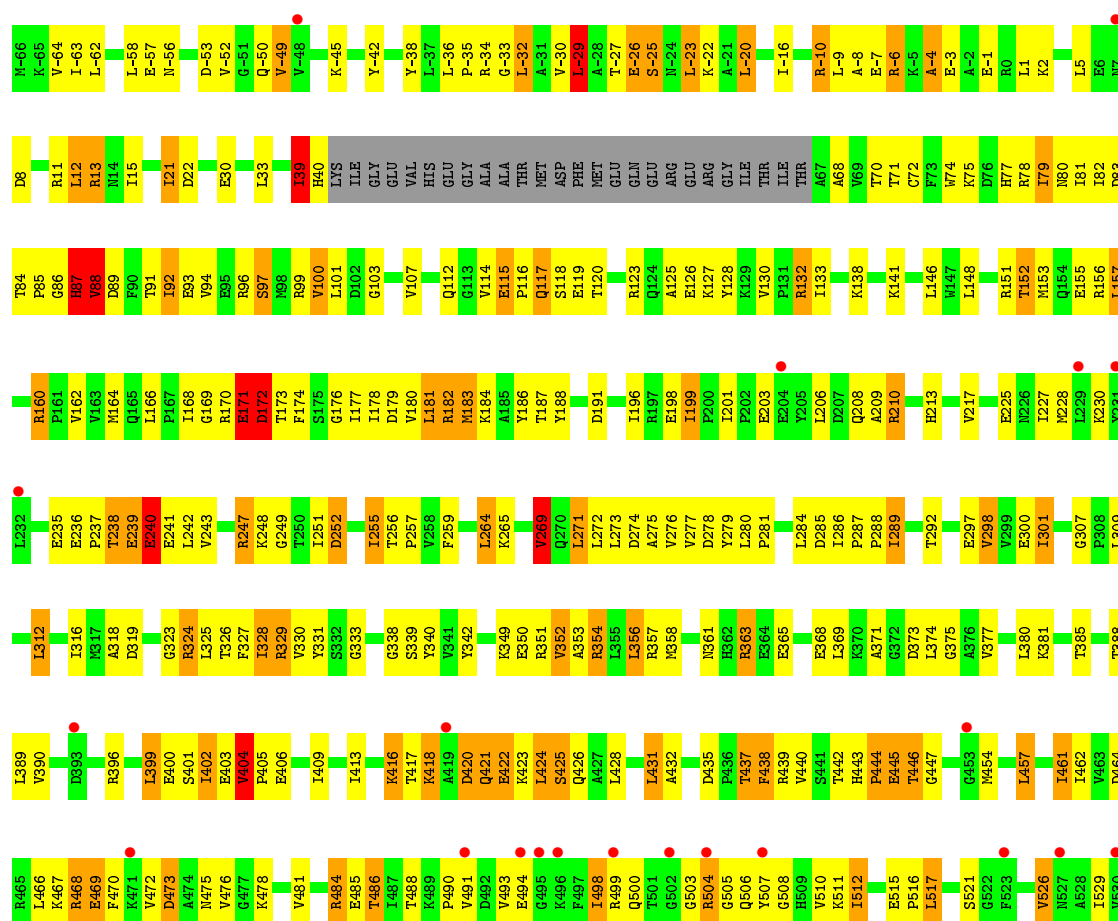


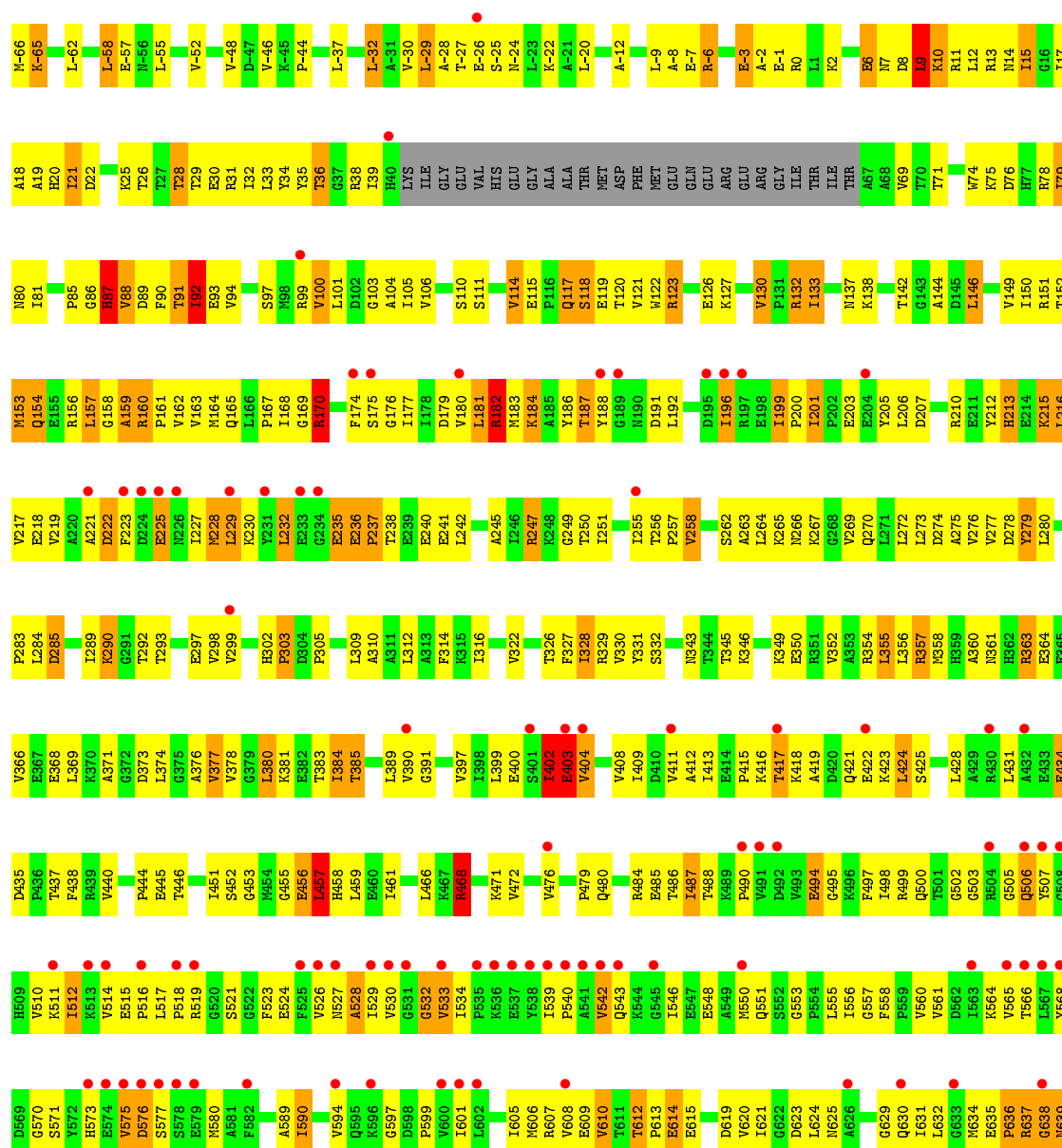


• Molecule 56: P-site tRNA



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





A640	Q641	V642	I643	R644	A645	P646	V647	P648	L649	A650	E651	M652	F653	G654	Y655	A656	T657	D658	L659	R660	S661	K662		R669	V670	M671	F672	F673	D674	H675	Y676	Q677	E678		K681	Q682	V683	Q684	E685		K689	GLY	GLN
------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	--	------	------	------	------	------	------	------	------	------	------	--	------	------	------	------	------	--	------	-----	-----

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	210.45Å 449.00Å 625.37Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.74 – 2.80 49.74 – 2.79	Depositor EDS
% Data completeness (in resolution range)	99.8 (49.74-2.80) 99.1 (49.74-2.79)	Depositor EDS
R_{merge}	0.20	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.08 (at 2.77Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE: 1.8.2_1309)	Depositor
R, R_{free}	0.200 , 0.255 0.200 , 0.255	Depositor DCC
R_{free} test set	72267 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	54.2	Xtriage
Anisotropy	0.399	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.26 , 68.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	310279	wwPDB-VP
Average B, all atoms (Å ²)	81.0	wwPDB-VP

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

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: 5MU, GDP, ZN, MIA, SF4, MG, FUA, 4SU, 7MG, 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	1.51	654/68792 (1.0%)	2.24	4887/107377 (4.6%)
1	CA	1.01	71/68691 (0.1%)	1.68	1752/107219 (1.6%)
2	AB	1.21	5/2878 (0.2%)	2.01	141/4490 (3.1%)
2	CB	0.67	0/2878	1.30	18/4490 (0.4%)
3	AC	0.34	0/1083	0.65	0/1460
3	CC	0.34	0/1083	0.65	0/1460
4	AD	1.00	4/2186 (0.2%)	1.08	8/2944 (0.3%)
4	CD	0.76	0/2192	0.92	2/2951 (0.1%)
5	AE	1.03	5/1592 (0.3%)	1.08	4/2149 (0.2%)
5	CE	0.68	0/1592	0.85	1/2149 (0.0%)
6	AF	0.96	2/1619 (0.1%)	1.07	3/2193 (0.1%)
6	CF	0.64	0/1615	0.85	1/2188 (0.0%)
7	AG	0.55	0/1450	0.77	0/1959
7	CG	0.40	0/1449	0.63	0/1958
8	AH	0.84	0/1356	0.96	3/1834 (0.2%)
8	CH	0.42	0/1356	0.64	0/1834
9	AK	0.42	0/640	0.76	1/889 (0.1%)
9	CK	0.29	0/640	0.62	0/889
10	AL	0.34	0/1044	0.58	0/1416
10	CL	0.31	0/1044	0.53	0/1416
11	AN	1.06	2/1144 (0.2%)	1.09	3/1543 (0.2%)
11	CN	0.55	0/1144	0.76	0/1543
12	AO	1.00	0/943	1.09	2/1269 (0.2%)
12	CO	0.71	0/943	0.82	0/1269
13	AP	0.89	0/1156	1.08	9/1537 (0.6%)
13	CP	0.58	0/1152	0.86	1/1533 (0.1%)
14	AQ	0.98	0/1143	1.05	4/1527 (0.3%)
14	CQ	0.62	0/1143	0.77	0/1527
15	AR	0.98	0/982	1.15	4/1312 (0.3%)
15	CR	0.62	0/982	0.95	2/1312 (0.2%)
16	AS	0.76	0/887	0.96	0/1180
16	CS	0.56	0/880	0.83	2/1172 (0.2%)

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

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

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

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

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

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

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

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

There are no chirality outliers.

5 of 15 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
24	A0	11	ARG	Peptide

Continued on next page...

Continued from previous page...

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

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	AA	61426	0	30937	933	0
1	CA	61337	0	30928	1107	0
2	AB	2573	0	1306	39	0
2	CB	2573	0	1306	49	0
3	AC	1063	0	1089	162	0
3	CC	1063	0	1091	203	0
4	AD	2136	0	2218	72	0
4	CD	2142	0	2229	72	0
5	AE	1559	0	1618	46	0
5	CE	1559	0	1618	92	0
6	AF	1584	0	1625	58	0
6	CF	1580	0	1619	68	0
7	AG	1425	0	1443	69	0
7	CG	1424	0	1434	59	0
8	AH	1330	0	1407	40	0
8	CH	1330	0	1407	51	0
9	AK	641	0	309	13	0
9	CK	641	0	309	13	0
10	AL	1025	0	1066	54	0
10	CL	1025	0	1066	50	0
11	AN	1117	0	1184	32	0
11	CN	1117	0	1184	45	0
12	AO	933	0	996	32	0
12	CO	933	0	996	38	0
13	AP	1139	0	1223	48	0
13	CP	1135	0	1212	46	0
14	AQ	1122	0	1179	35	0
14	CQ	1122	0	1179	54	0
15	AR	968	0	1033	26	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
15	CR	968	0	1033	44	0
16	AS	877	0	938	30	0
16	CS	870	0	923	43	0
17	AT	1091	0	1151	35	0
17	CT	1083	0	1136	55	0
18	AU	959	0	1019	30	0
18	CU	959	0	1018	34	0
19	AV	771	0	829	24	0
19	CV	771	0	830	16	0
20	AW	886	0	940	26	0
20	CW	886	0	940	31	0
21	AX	750	0	814	27	0
21	CX	750	0	814	27	0
22	AY	806	0	881	23	0
22	CY	806	0	881	39	0
23	AZ	1451	0	1457	56	0
23	CZ	1451	0	1457	66	0
24	A0	653	0	674	29	0
24	C0	653	0	674	22	0
25	A1	755	0	826	24	0
25	C1	755	0	826	23	0
26	A2	588	0	643	13	0
26	C2	588	0	643	19	0
27	A3	469	0	518	13	0
27	C3	464	0	514	11	0
28	A4	558	0	547	24	0
28	C4	532	0	505	14	0
29	A5	455	0	465	18	0
29	C5	455	0	465	20	0
30	A6	453	0	473	18	0
30	C6	449	0	469	13	0
31	A7	418	0	467	17	0
31	C7	418	0	467	17	0
32	A8	517	0	582	22	0
32	C8	517	0	582	28	0
33	A9	307	0	335	10	0
33	C9	307	0	335	14	0
34	BA	32141	0	16224	675	0
34	DA	32268	0	16287	690	0
35	BB	1846	0	1867	102	0
35	DB	1825	0	1828	82	0
36	BC	1552	0	1546	59	0

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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
56	DY	1561	0	796	40	0
57	BZ	5690	0	5783	272	0
57	DZ	5690	0	5783	322	0
58	A0	3	0	0	0	0
58	A2	2	0	0	0	0
58	A4	1	0	0	0	0
58	A5	1	0	0	0	0
58	A6	1	0	0	0	0
58	A7	3	0	0	0	0
58	A8	2	0	0	0	0
58	A9	1	0	0	0	0
58	AA	835	0	0	0	0
58	AB	23	0	0	0	0
58	AD	10	0	0	0	0
58	AE	4	0	0	0	0
58	AF	5	0	0	0	0
58	AG	2	0	0	0	0
58	AH	2	0	0	0	0
58	AN	3	0	0	0	0
58	AO	1	0	0	0	0
58	AP	2	0	0	0	0
58	AQ	3	0	0	0	0
58	AR	1	0	0	0	0
58	AU	3	0	0	0	0
58	AV	3	0	0	0	0
58	AW	4	0	0	0	0
58	AX	1	0	0	0	0
58	AY	1	0	0	0	0
58	AZ	2	0	0	0	0
58	BA	211	0	0	0	0
58	BB	1	0	0	0	0
58	BD	1	0	0	0	0
58	BE	1	0	0	0	0
58	BF	1	0	0	0	0
58	BK	1	0	0	0	0
58	BL	2	0	0	0	0
58	BM	2	0	0	0	0
58	BN	1	0	0	0	0
58	BT	1	0	0	0	0
58	BV	1	0	0	0	0
58	BW	3	0	0	0	0
58	BZ	2	0	0	0	0

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

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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
63	C5	1	0	0	0	0
63	C7	3	0	0	0	0
63	C8	3	0	0	1	0
63	CA	981	0	0	65	0
63	CB	9	0	0	0	0
63	CD	15	0	0	0	0
63	CE	9	0	0	1	0
63	CF	6	0	0	0	0
63	CP	13	0	0	3	0
63	CQ	1	0	0	0	0
63	CT	3	0	0	0	0
63	CU	4	0	0	1	0
63	CV	1	0	0	0	0
63	CW	1	0	0	0	0
63	CX	1	0	0	0	0
63	CY	1	0	0	0	0
63	DA	153	0	0	11	0
63	DE	2	0	0	0	0
63	DH	1	0	0	1	0
63	DJ	1	0	0	0	0
63	DK	2	0	0	0	0
63	DL	1	0	0	0	0
63	DP	1	0	0	0	0
63	DT	1	0	0	0	0
63	DY	1	0	0	0	0
63	DZ	2	0	0	0	0
All	All	310279	0	209988	7291	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 15.

The worst 5 of 7291 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

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

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	AC	133/228 (58%)	90 (68%)	25 (19%)	18 (14%)	0	0
3	CC	133/228 (58%)	90 (68%)	25 (19%)	18 (14%)	0	0
4	AD	273/276 (99%)	249 (91%)	20 (7%)	4 (2%)	10	33
4	CD	273/276 (99%)	242 (89%)	26 (10%)	5 (2%)	8	28
5	AE	202/206 (98%)	191 (95%)	9 (4%)	2 (1%)	15	44
5	CE	202/206 (98%)	174 (86%)	19 (9%)	9 (4%)	2	8
6	AF	201/210 (96%)	187 (93%)	11 (6%)	3 (2%)	10	33
6	CF	201/210 (96%)	186 (92%)	12 (6%)	3 (2%)	10	33
7	AG	179/182 (98%)	143 (80%)	25 (14%)	11 (6%)	1	4
7	CG	179/182 (98%)	148 (83%)	20 (11%)	11 (6%)	1	4
8	AH	172/180 (96%)	150 (87%)	20 (12%)	2 (1%)	13	39
8	CH	172/180 (96%)	148 (86%)	19 (11%)	5 (3%)	4	15
9	AK	128/173 (74%)	68 (53%)	33 (26%)	27 (21%)	0	0
9	CK	128/173 (74%)	69 (54%)	24 (19%)	35 (27%)	0	0
10	AL	137/147 (93%)	105 (77%)	23 (17%)	9 (7%)	1	3
10	CL	137/147 (93%)	95 (69%)	33 (24%)	9 (7%)	1	3
11	AN	138/140 (99%)	133 (96%)	4 (3%)	1 (1%)	22	53
11	CN	138/140 (99%)	125 (91%)	11 (8%)	2 (1%)	11	34
12	AO	120/122 (98%)	114 (95%)	4 (3%)	2 (2%)	9	29
12	CO	120/122 (98%)	105 (88%)	12 (10%)	3 (2%)	5	19
13	AP	147/150 (98%)	132 (90%)	13 (9%)	2 (1%)	11	34
13	CP	147/150 (98%)	128 (87%)	16 (11%)	3 (2%)	7	24
14	AQ	139/141 (99%)	124 (89%)	13 (9%)	2 (1%)	11	34
14	CQ	139/141 (99%)	121 (87%)	15 (11%)	3 (2%)	6	22
15	AR	116/118 (98%)	100 (86%)	13 (11%)	3 (3%)	5	18

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
15	CR	116/118 (98%)	92 (79%)	16 (14%)	8 (7%)	1	3
16	AS	108/112 (96%)	92 (85%)	12 (11%)	4 (4%)	3	11
16	CS	108/112 (96%)	86 (80%)	17 (16%)	5 (5%)	2	7
17	AT	129/146 (88%)	118 (92%)	10 (8%)	1 (1%)	19	49
17	CT	129/146 (88%)	109 (84%)	15 (12%)	5 (4%)	3	10
18	AU	114/118 (97%)	111 (97%)	3 (3%)	0	100	100
18	CU	114/118 (97%)	103 (90%)	10 (9%)	1 (1%)	17	46
19	AV	99/101 (98%)	92 (93%)	5 (5%)	2 (2%)	7	24
19	CV	99/101 (98%)	87 (88%)	9 (9%)	3 (3%)	4	15
20	AW	110/113 (97%)	106 (96%)	4 (4%)	0	100	100
20	CW	110/113 (97%)	100 (91%)	10 (9%)	0	100	100
21	AX	93/96 (97%)	88 (95%)	5 (5%)	0	100	100
21	CX	93/96 (97%)	80 (86%)	11 (12%)	2 (2%)	6	22
22	AY	105/110 (96%)	91 (87%)	11 (10%)	3 (3%)	4	15
22	CY	105/110 (96%)	90 (86%)	13 (12%)	2 (2%)	8	26
23	AZ	183/206 (89%)	146 (80%)	24 (13%)	13 (7%)	1	2
23	CZ	183/206 (89%)	140 (76%)	31 (17%)	12 (7%)	1	3
24	A0	81/85 (95%)	72 (89%)	8 (10%)	1 (1%)	13	39
24	C0	81/85 (95%)	70 (86%)	11 (14%)	0	100	100
25	A1	95/98 (97%)	86 (90%)	7 (7%)	2 (2%)	7	23
25	C1	95/98 (97%)	87 (92%)	4 (4%)	4 (4%)	3	9
26	A2	68/72 (94%)	62 (91%)	5 (7%)	1 (2%)	10	33
26	C2	68/72 (94%)	63 (93%)	4 (6%)	1 (2%)	10	33
27	A3	57/60 (95%)	55 (96%)	2 (4%)	0	100	100
27	C3	57/60 (95%)	52 (91%)	5 (9%)	0	100	100
28	A4	67/71 (94%)	41 (61%)	19 (28%)	7 (10%)	0	1
28	C4	67/71 (94%)	53 (79%)	11 (16%)	3 (4%)	2	8
29	A5	57/60 (95%)	53 (93%)	4 (7%)	0	100	100
29	C5	57/60 (95%)	51 (90%)	5 (9%)	1 (2%)	8	28
30	A6	51/54 (94%)	48 (94%)	2 (4%)	1 (2%)	7	24
30	C6	51/54 (94%)	46 (90%)	4 (8%)	1 (2%)	7	24

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

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

5 of 577 Ramachandran outliers are listed below:

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

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	AC	111/180 (62%)	104 (94%)	7 (6%)	18	46
3	CC	111/180 (62%)	103 (93%)	8 (7%)	14	38
4	AD	215/218 (99%)	181 (84%)	34 (16%)	2	8
4	CD	216/218 (99%)	179 (83%)	37 (17%)	2	6
5	AE	164/166 (99%)	130 (79%)	34 (21%)	1	3
5	CE	164/166 (99%)	130 (79%)	34 (21%)	1	3
6	AF	160/166 (96%)	128 (80%)	32 (20%)	1	4
6	CF	159/166 (96%)	124 (78%)	35 (22%)	1	2
7	AG	143/156 (92%)	114 (80%)	29 (20%)	1	4
7	CG	142/156 (91%)	111 (78%)	31 (22%)	1	3
8	AH	144/148 (97%)	121 (84%)	23 (16%)	2	7
8	CH	144/148 (97%)	124 (86%)	20 (14%)	3	11
10	AL	104/111 (94%)	83 (80%)	21 (20%)	1	4
10	CL	104/111 (94%)	84 (81%)	20 (19%)	1	4
11	AN	118/119 (99%)	97 (82%)	21 (18%)	2	5
11	CN	118/119 (99%)	92 (78%)	26 (22%)	1	2
12	AO	100/100 (100%)	88 (88%)	12 (12%)	5	15
12	CO	100/100 (100%)	82 (82%)	18 (18%)	1	5
13	AP	116/116 (100%)	90 (78%)	26 (22%)	1	2
13	CP	115/116 (99%)	95 (83%)	20 (17%)	2	6
14	AQ	111/111 (100%)	99 (89%)	12 (11%)	6	19
14	CQ	111/111 (100%)	91 (82%)	20 (18%)	1	5
15	AR	101/101 (100%)	81 (80%)	20 (20%)	1	4
15	CR	101/101 (100%)	78 (77%)	23 (23%)	1	2
16	AS	87/88 (99%)	70 (80%)	17 (20%)	1	4
16	CS	85/88 (97%)	66 (78%)	19 (22%)	1	2
17	AT	115/127 (91%)	98 (85%)	17 (15%)	3	9
17	CT	113/127 (89%)	90 (80%)	23 (20%)	1	4
18	AU	93/94 (99%)	79 (85%)	14 (15%)	3	9
18	CU	93/94 (99%)	80 (86%)	13 (14%)	3	11
19	AV	80/82 (98%)	63 (79%)	17 (21%)	1	3
19	CV	80/82 (98%)	68 (85%)	12 (15%)	3	9

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
20	AW	90/92 (98%)	77 (86%)	13 (14%)	3	10
20	CW	90/92 (98%)	82 (91%)	8 (9%)	9	28
21	AX	77/78 (99%)	69 (90%)	8 (10%)	7	21
21	CX	77/78 (99%)	69 (90%)	8 (10%)	7	21
22	AY	85/91 (93%)	71 (84%)	14 (16%)	2	7
22	CY	85/91 (93%)	69 (81%)	16 (19%)	1	5
23	AZ	156/179 (87%)	121 (78%)	35 (22%)	1	2
23	CZ	156/179 (87%)	129 (83%)	27 (17%)	2	6
24	A0	65/67 (97%)	61 (94%)	4 (6%)	18	47
24	C0	65/67 (97%)	60 (92%)	5 (8%)	13	35
25	A1	80/83 (96%)	70 (88%)	10 (12%)	4	14
25	C1	80/83 (96%)	66 (82%)	14 (18%)	2	6
26	A2	65/67 (97%)	55 (85%)	10 (15%)	2	8
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%)	42 (84%)	8 (16%)	2	7
28	A4	60/63 (95%)	42 (70%)	18 (30%)	0	1
28	C4	53/63 (84%)	41 (77%)	12 (23%)	1	2
29	A5	50/52 (96%)	43 (86%)	7 (14%)	3	11
29	C5	50/52 (96%)	42 (84%)	8 (16%)	2	7
30	A6	51/52 (98%)	39 (76%)	12 (24%)	1	2
30	C6	50/52 (96%)	39 (78%)	11 (22%)	1	2
31	A7	41/42 (98%)	34 (83%)	7 (17%)	2	6
31	C7	41/42 (98%)	32 (78%)	9 (22%)	1	2
32	A8	54/55 (98%)	46 (85%)	8 (15%)	3	9
32	C8	54/55 (98%)	44 (82%)	10 (18%)	1	5
33	A9	34/34 (100%)	32 (94%)	2 (6%)	19	49
33	C9	34/34 (100%)	32 (94%)	2 (6%)	19	49
35	BB	192/220 (87%)	153 (80%)	39 (20%)	1	4
35	DB	187/220 (85%)	151 (81%)	36 (19%)	1	4
36	BC	143/188 (76%)	129 (90%)	14 (10%)	8	24

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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
52	BS	70/80 (88%)	60 (86%)	10 (14%)	3	10
52	DS	67/80 (84%)	59 (88%)	8 (12%)	5	16
53	BT	70/82 (85%)	56 (80%)	14 (20%)	1	4
53	DT	71/82 (87%)	63 (89%)	8 (11%)	6	18
54	BU	18/22 (82%)	16 (89%)	2 (11%)	6	19
54	DU	18/22 (82%)	18 (100%)	0	100	100
57	BZ	609/636 (96%)	485 (80%)	124 (20%)	1	4
57	DZ	609/636 (96%)	474 (78%)	135 (22%)	1	2
All	All	10785/11672 (92%)	8911 (83%)	1874 (17%)	2	6

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

Mol	Chain	Res	Type
57	BZ	130	VAL
7	CG	3	LEU
53	DT	8	ARG
57	BZ	286	ILE
4	CD	71	ASP

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

Mol	Chain	Res	Type
57	BZ	475	ASN
6	CF	169	ASN
53	DT	16	HIS
57	BZ	573	HIS
4	CD	126	GLN

5.3.3 RNA ⓘ

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

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

5 of 1843 RNA backbone outliers are listed below:

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

5 of 146 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
34	BA	748	C
1	CA	195	A
34	DA	884	U
34	BA	793	U
34	BA	1165	C

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
56	4SU	BY	8	56	14,21,22	1.22	1 (7%)	15,30,33	1.66	3 (20%)
56	5MU	DY	54	56	15,22,23	1.07	1 (6%)	16,32,35	1.87	2 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
56	PSU	DW	39	56	17,21,22	1.50	2 (11%)	20,30,33	3.43	8 (40%)
56	7MG	DW	46	56	22,26,27	1.78	4 (18%)	28,39,42	2.80	11 (39%)
56	MIA	DW	37	56	24,31,32	2.48	4 (16%)	26,44,47	2.07	8 (30%)
56	5MU	BW	54	56	15,22,23	1.05	1 (6%)	16,32,35	1.74	2 (12%)
56	4SU	DY	8	56	14,21,22	1.32	1 (7%)	15,30,33	1.50	2 (13%)
56	PSU	BY	39	56	17,21,22	1.46	2 (11%)	20,30,33	3.23	6 (30%)
56	PSU	BW	55	56	17,21,22	1.50	2 (11%)	20,30,33	3.31	6 (30%)
56	PSU	BY	55	56	17,21,22	1.45	2 (11%)	20,30,33	3.12	6 (30%)
56	PSU	DY	32	56	17,21,22	1.40	2 (11%)	20,30,33	3.16	6 (30%)
56	PSU	DW	55	56	17,21,22	1.48	2 (11%)	20,30,33	3.35	6 (30%)
56	PSU	BY	32	56	17,21,22	1.40	2 (11%)	20,30,33	3.14	5 (25%)
56	5MU	BY	54	56	15,22,23	1.08	1 (6%)	16,32,35	1.87	1 (6%)
56	7MG	BW	46	56	22,26,27	1.71	4 (18%)	28,39,42	2.91	8 (28%)
56	PSU	DY	55	56	17,21,22	1.54	3 (17%)	20,30,33	3.12	6 (30%)
56	4SU	DW	8	56	14,21,22	1.27	1 (7%)	15,30,33	1.56	2 (13%)
56	PSU	DY	39	56	17,21,22	1.54	3 (17%)	20,30,33	3.28	6 (30%)
56	PSU	BW	39	56	17,21,22	1.81	3 (17%)	20,30,33	3.22	6 (30%)
56	PSU	BW	32	56	17,21,22	1.34	3 (17%)	20,30,33	3.43	7 (35%)
56	PSU	DW	32	56	17,21,22	1.30	1 (5%)	20,30,33	3.78	8 (40%)
56	5MU	DW	54	56	15,22,23	1.16	1 (6%)	16,32,35	1.88	2 (12%)
56	7MG	DY	46	56	22,26,27	1.75	4 (18%)	28,39,42	2.95	11 (39%)
56	7MG	BY	46	56	22,26,27	1.78	4 (18%)	28,39,42	2.79	9 (32%)
56	MIA	DY	37	56	18,24,32	1.08	2 (11%)	18,35,47	1.31	2 (11%)
56	MIA	BW	37	56	24,31,32	2.43	4 (16%)	26,44,47	3.24	9 (34%)
56	MIA	BY	37	56	18,24,32	1.18	2 (11%)	18,35,47	1.38	3 (16%)
56	4SU	BW	8	56	14,21,22	1.19	1 (7%)	15,30,33	1.47	2 (13%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
56	4SU	BY	8	56	-	1/5/25/26	0/2/2/2
56	5MU	DY	54	56	-	2/5/25/26	0/2/2/2
56	PSU	DW	39	56	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
56	7MG	DW	46	56	-	2/7/37/38	0/3/3/3
56	MIA	DW	37	56	-	6/11/33/34	0/3/3/3
56	5MU	BW	54	56	-	0/5/25/26	0/2/2/2
56	4SU	DY	8	56	-	1/5/25/26	0/2/2/2
56	PSU	BY	39	56	-	0/7/25/26	0/2/2/2
56	PSU	BW	55	56	-	0/7/25/26	0/2/2/2
56	PSU	BY	55	56	-	0/7/25/26	0/2/2/2
56	PSU	DY	32	56	-	0/7/25/26	0/2/2/2
56	PSU	DW	55	56	-	0/7/25/26	0/2/2/2
56	PSU	BY	32	56	-	0/7/25/26	0/2/2/2
56	5MU	BY	54	56	-	3/5/25/26	0/2/2/2
56	7MG	BW	46	56	-	0/7/37/38	0/3/3/3
56	PSU	DY	55	56	-	5/7/25/26	0/2/2/2
56	4SU	DW	8	56	-	0/5/25/26	0/2/2/2
56	PSU	DY	39	56	-	2/7/25/26	0/2/2/2
56	PSU	BW	39	56	-	0/7/25/26	0/2/2/2
56	PSU	BW	32	56	-	3/7/25/26	0/2/2/2
56	PSU	DW	32	56	-	2/7/25/26	0/2/2/2
56	5MU	DW	54	56	-	0/5/25/26	0/2/2/2
56	7MG	DY	46	56	-	2/7/37/38	0/3/3/3
56	7MG	BY	46	56	-	5/7/37/38	0/3/3/3
56	MIA	DY	37	56	-	3/3/25/34	0/3/3/3
56	MIA	BW	37	56	-	5/11/33/34	0/3/3/3
56	MIA	BY	37	56	-	2/3/25/34	0/3/3/3
56	4SU	BW	8	56	-	0/5/25/26	0/2/2/2

The worst 5 of 63 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
56	DW	37	MIA	C2-S10	-7.81	1.69	1.75
56	BW	37	MIA	C13-C14	7.79	1.54	1.32
56	DW	37	MIA	C13-C14	7.60	1.54	1.32
56	BW	37	MIA	C2-S10	-7.10	1.69	1.75
56	BW	39	PSU	C5-C1'	-5.82	1.47	1.52

The worst 5 of 153 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
56	BW	37	MIA	C11-S10-C2	-11.66	93.56	102.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
56	DW	32	PSU	N1-C2-N3	-10.73	119.90	128.43
56	BW	32	PSU	N1-C2-N3	-10.64	119.97	128.43
56	DY	46	7MG	N3-C4-N9	9.84	139.55	126.91
56	BW	46	7MG	N3-C4-N9	9.75	139.44	126.91

There are no chirality outliers.

5 of 44 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
56	BY	8	4SU	C2'-C1'-N1-C6
56	DY	54	5MU	C3'-C4'-C5'-O5'
56	DY	54	5MU	O4'-C4'-C5'-O5'
56	DW	37	MIA	C3'-C4'-C5'-O5'
56	DW	37	MIA	C12-C13-C14-C15

There are no ring outliers.

10 monomers are involved in 18 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
56	BY	8	4SU	1	0
56	DW	39	PSU	4	0
56	DW	46	7MG	2	0
56	DW	37	MIA	2	0
56	DW	55	PSU	2	0
56	DY	55	PSU	3	0
56	DW	54	5MU	1	0
56	DY	46	7MG	2	0
56	DY	37	MIA	1	0
56	BW	37	MIA	1	0

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 2058 ligands modelled in this entry, 2052 are monoatomic - leaving 6 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The

Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
62	GDP	BZ	704	58	24,30,30	1.09	3 (12%)	31,47,47	1.83	6 (19%)
60	SF4	BD	501	37	0,12,12	0.00	-	-		
62	GDP	DZ	704	58	24,30,30	1.24	2 (8%)	31,47,47	2.17	8 (25%)
61	FUA	BZ	703	-	36,40,40	1.76	6 (16%)	46,64,64	1.52	5 (10%)
60	SF4	DD	501	37	0,12,12	0.00	-	-		
61	FUA	DZ	703	-	36,40,40	1.76	6 (16%)	46,64,64	1.52	5 (10%)

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	704	58	-	4/12/32/32	0/3/3/3
60	SF4	BD	501	37	-	-	0/6/5/5
62	GDP	DZ	704	58	-	2/12/32/32	0/3/3/3
61	FUA	BZ	703	-	-	6/11/92/92	0/4/4/4
60	SF4	DD	501	37	-	-	0/6/5/5
61	FUA	DZ	703	-	-	6/11/92/92	0/4/4/4

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
61	BZ	703	FUA	C23-C22	-6.56	1.39	1.51
61	DZ	703	FUA	C23-C22	-6.51	1.40	1.51
62	DZ	704	GDP	C6-C5	4.65	1.49	1.41
61	BZ	703	FUA	C23-C24	-4.27	1.39	1.53
61	DZ	703	FUA	C23-C24	-4.25	1.39	1.53

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
62	BZ	704	GDP	C2-N3-C4	4.85	120.90	115.36
62	DZ	704	GDP	C5-C6-N1	-4.80	116.87	123.43
62	DZ	704	GDP	C6-N1-C2	4.79	123.54	115.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
62	DZ	704	GDP	C2-N3-C4	4.58	120.58	115.36
62	DZ	704	GDP	PA-O3A-PB	-4.44	117.59	132.83

There are no chirality outliers.

5 of 18 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
61	DZ	703	FUA	C13-C17-C22-C29
61	DZ	703	FUA	C17-C22-C23-C24
61	DZ	703	FUA	C29-C22-C23-C24
62	BZ	704	GDP	PA-O3A-PB-O3B
62	BZ	704	GDP	C5'-O5'-PA-O1A

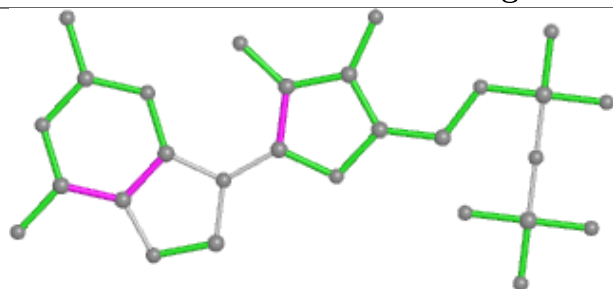
There are no ring outliers.

6 monomers are involved in 45 short contacts:

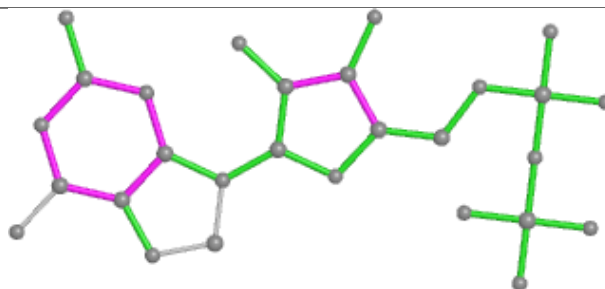
Mol	Chain	Res	Type	Clashes	Symm-Clashes
62	BZ	704	GDP	5	0
60	BD	501	SF4	1	0
62	DZ	704	GDP	9	0
61	BZ	703	FUA	11	0
60	DD	501	SF4	2	0
61	DZ	703	FUA	17	0

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.

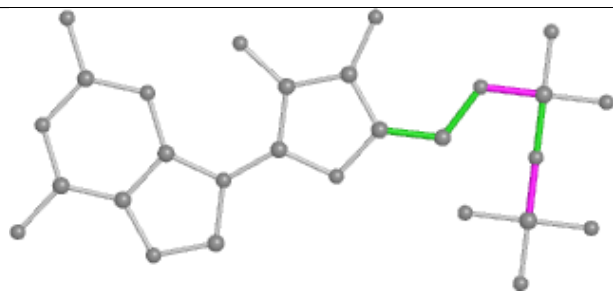
Ligand GDP BZ 704



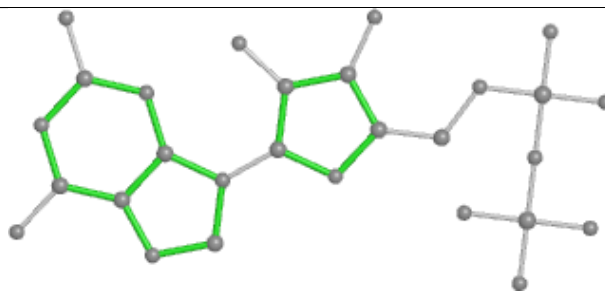
Bond lengths



Bond angles

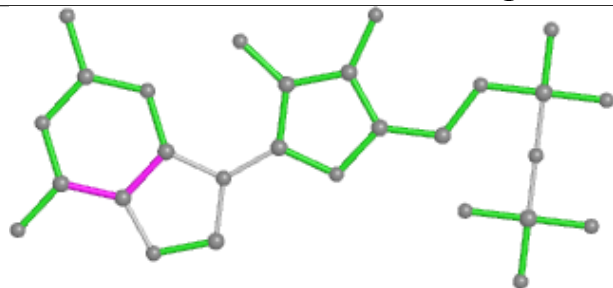


Torsions

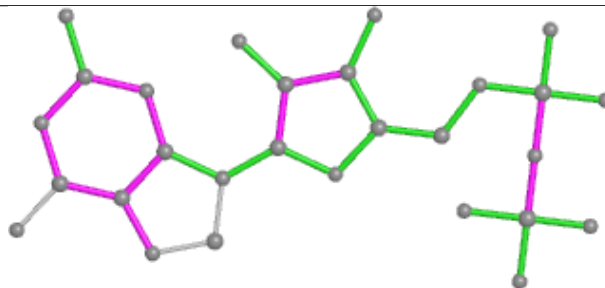


Rings

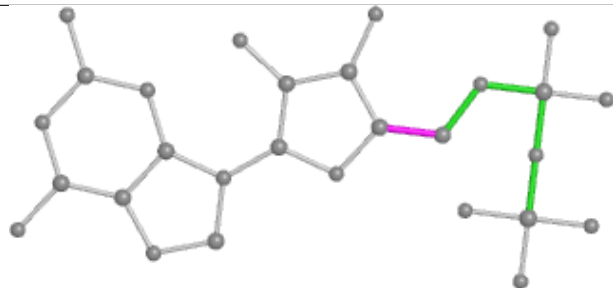
Ligand GDP DZ 704



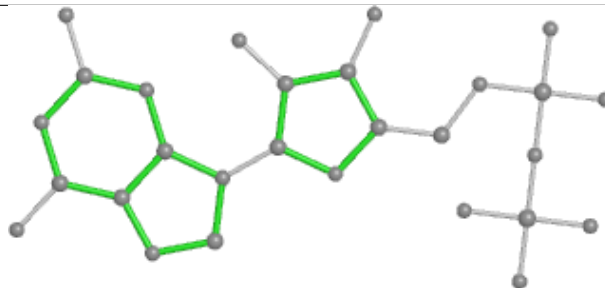
Bond lengths



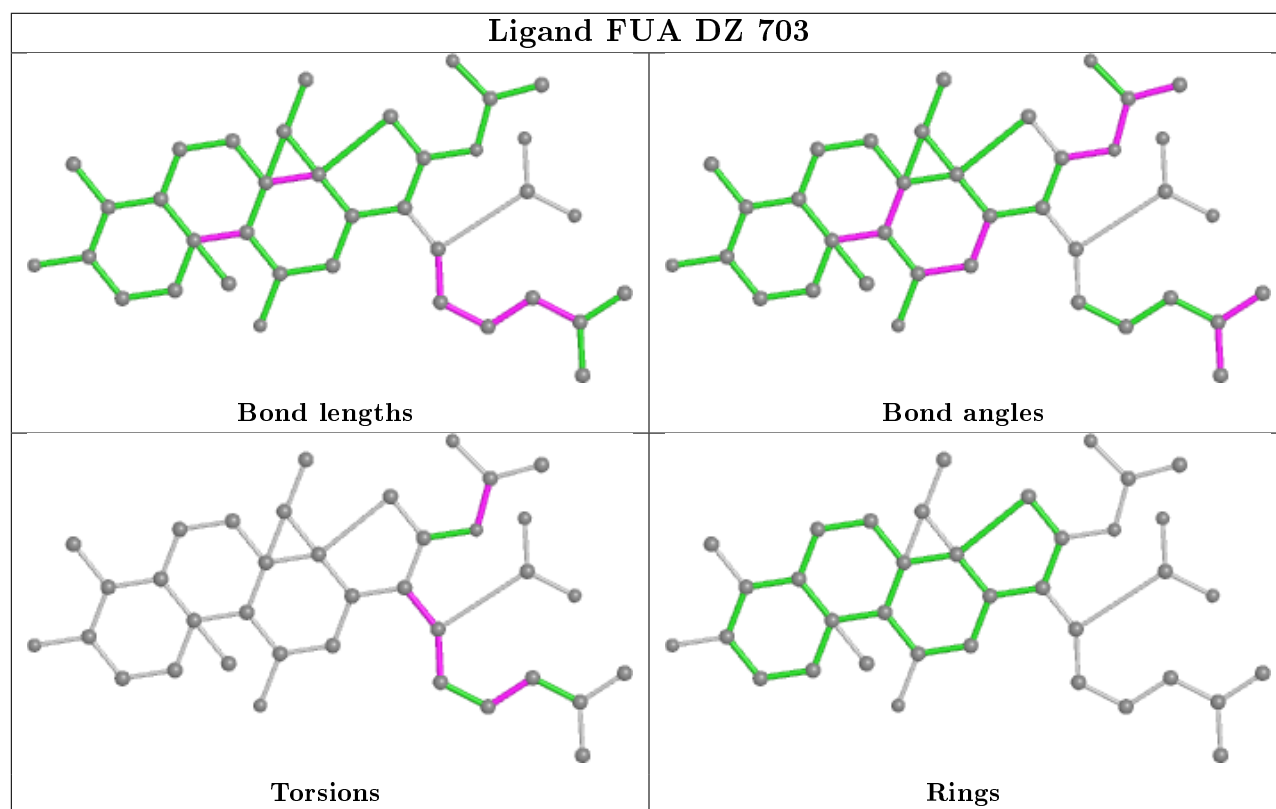
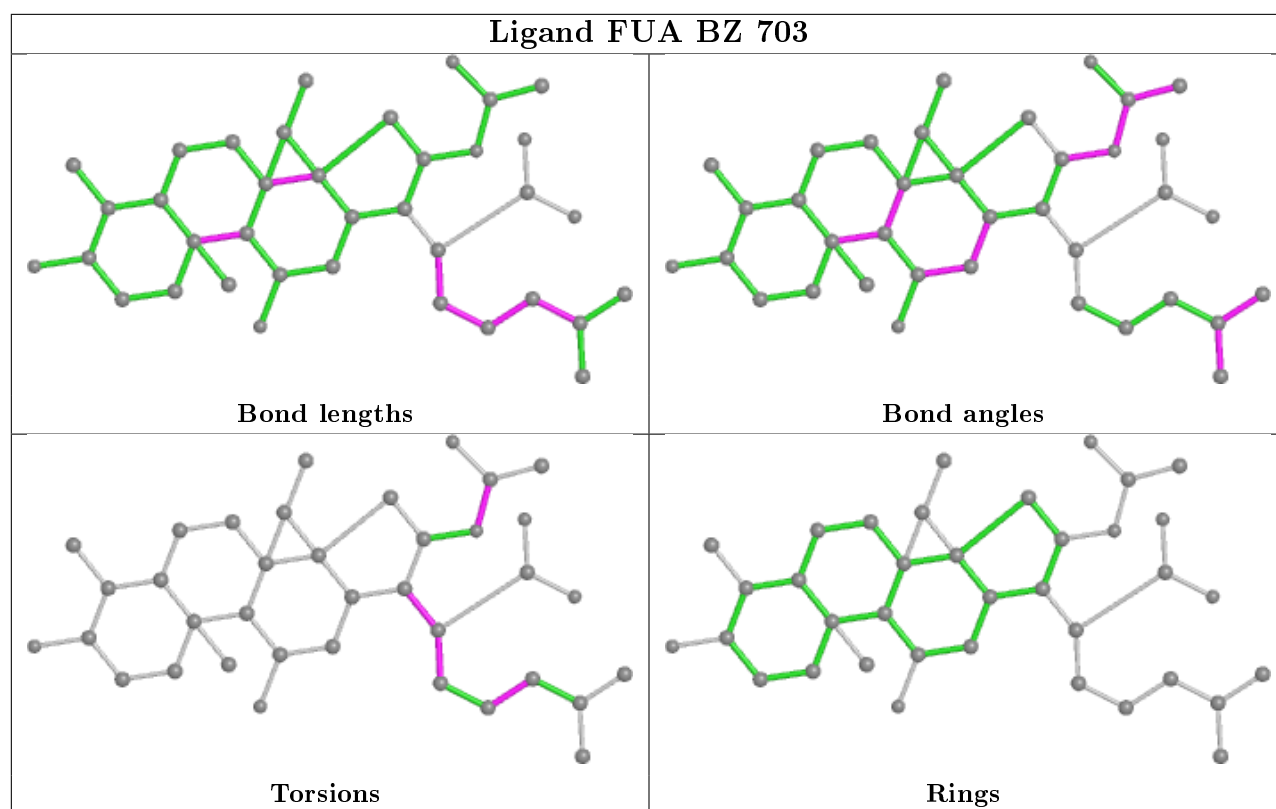
Bond angles



Torsions



Rings



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	AA	2852/2915 (97%)	0.25	110 (3%) 39 29	14, 34, 139, 364	4 (0%)
1	CA	2848/2915 (97%)	0.31	123 (4%) 35 25	27, 57, 180, 356	0
2	AB	120/121 (99%)	-0.22	0 100 100	23, 50, 73, 110	0
2	CB	120/121 (99%)	0.04	1 (0%) 86 81	64, 92, 120, 168	0
3	AC	137/228 (60%)	10.26	131 (95%) 0 0	258, 289, 307, 313	0
3	CC	137/228 (60%)	11.55	133 (97%) 0 0	281, 312, 331, 336	0
4	AD	275/276 (99%)	-0.37	2 (0%) 87 84	13, 35, 59, 137	1 (0%)
4	CD	275/276 (99%)	-0.30	2 (0%) 87 84	19, 48, 74, 130	2 (0%)
5	AE	204/206 (99%)	-0.43	0 100 100	5, 33, 57, 80	3 (1%)
5	CE	204/206 (99%)	-0.04	4 (1%) 65 56	21, 63, 107, 134	0
6	AF	203/210 (96%)	-0.32	0 100 100	10, 35, 78, 174	0
6	CF	203/210 (96%)	-0.30	0 100 100	21, 64, 107, 155	0
7	AG	181/182 (99%)	-0.00	4 (2%) 62 52	34, 78, 134, 212	1 (0%)
7	CG	181/182 (99%)	0.66	19 (10%) 6 3	73, 112, 177, 207	0
8	AH	174/180 (96%)	-0.39	1 (0%) 89 86	26, 46, 70, 112	0
8	CH	174/180 (96%)	1.24	42 (24%) 0 0	65, 112, 161, 200	0
9	AK	130/173 (75%)	0.70	16 (12%) 4 2	48, 105, 170, 232	0
9	CK	130/173 (75%)	2.54	64 (49%) 0 0	75, 162, 204, 231	0
10	AL	139/147 (94%)	3.40	91 (65%) 0 0	96, 173, 233, 253	0
10	CL	139/147 (94%)	5.80	120 (86%) 0 0	127, 196, 252, 287	1 (0%)
11	AN	140/140 (100%)	-0.42	0 100 100	14, 28, 61, 97	1 (0%)
11	CN	140/140 (100%)	0.12	3 (2%) 63 54	32, 72, 108, 150	0
12	AO	122/122 (100%)	-0.37	0 100 100	17, 37, 63, 79	1 (0%)
12	CO	122/122 (100%)	-0.25	0 100 100	36, 59, 85, 106	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	AP	149/150 (99%)	-0.11	0 100 100	11, 42, 81, 107	1 (0%)
13	CP	149/150 (99%)	0.21	3 (2%) 65 56	30, 68, 117, 137	0
14	AQ	141/141 (100%)	-0.36	0 100 100	11, 34, 54, 81	0
14	CQ	141/141 (100%)	-0.20	2 (1%) 75 70	38, 71, 101, 120	0
15	AR	118/118 (100%)	-0.39	0 100 100	16, 29, 45, 56	0
15	CR	118/118 (100%)	-0.15	0 100 100	33, 56, 90, 106	0
16	AS	110/112 (98%)	-0.26	0 100 100	29, 51, 81, 94	0
16	CS	110/112 (98%)	0.33	3 (2%) 54 44	46, 85, 120, 152	0
17	AT	131/146 (89%)	-0.33	1 (0%) 86 81	24, 41, 92, 165	0
17	CT	131/146 (89%)	-0.12	1 (0%) 86 81	43, 65, 105, 143	0
18	AU	116/118 (98%)	-0.38	0 100 100	9, 22, 38, 90	1 (0%)
18	CU	116/118 (98%)	-0.09	0 100 100	27, 65, 93, 107	0
19	AV	101/101 (100%)	-0.50	0 100 100	9, 28, 50, 75	0
19	CV	101/101 (100%)	0.13	1 (0%) 82 77	36, 80, 113, 171	0
20	AW	112/113 (99%)	-0.40	0 100 100	13, 26, 43, 112	1 (0%)
20	CW	112/113 (99%)	-0.16	0 100 100	27, 50, 81, 119	0
21	AX	95/96 (98%)	-0.34	0 100 100	16, 35, 67, 99	1 (1%)
21	CX	95/96 (98%)	-0.05	2 (2%) 63 54	38, 62, 86, 107	0
22	AY	107/110 (97%)	-0.27	1 (0%) 84 80	24, 44, 87, 161	0
22	CY	107/110 (97%)	0.45	9 (8%) 11 5	46, 76, 115, 167	0
23	AZ	185/206 (89%)	-0.41	0 100 100	29, 57, 92, 148	0
23	CZ	185/206 (89%)	0.60	18 (9%) 7 4	61, 106, 149, 213	0
24	A0	83/85 (97%)	-0.11	4 (4%) 30 21	12, 35, 83, 225	1 (1%)
24	C0	83/85 (97%)	0.71	10 (12%) 4 2	42, 66, 122, 228	0
25	A1	97/98 (98%)	-0.17	2 (2%) 63 54	19, 43, 80, 101	1 (1%)
25	C1	97/98 (98%)	-0.20	1 (1%) 82 77	31, 52, 91, 125	0
26	A2	70/72 (97%)	-0.32	1 (1%) 75 70	25, 44, 69, 123	1 (1%)
26	C2	70/72 (97%)	-0.05	2 (2%) 51 41	49, 71, 101, 117	0
27	A3	59/60 (98%)	-0.35	0 100 100	14, 30, 56, 101	1 (1%)
27	C3	59/60 (98%)	0.62	7 (11%) 4 2	46, 73, 112, 150	0
28	A4	69/71 (97%)	1.00	17 (24%) 0 0	59, 118, 206, 239	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
28	C4	69/71 (97%)	1.42	23 (33%) 0 0	81, 159, 207, 228	0
29	A5	59/60 (98%)	-0.35	0 100 100	8, 26, 40, 52	0
29	C5	59/60 (98%)	-0.12	0 100 100	27, 52, 90, 104	0
30	A6	53/54 (98%)	-0.46	0 100 100	23, 41, 55, 74	0
30	C6	53/54 (98%)	-0.36	0 100 100	41, 61, 80, 106	0
31	A7	48/49 (97%)	-0.28	1 (2%) 63 54	14, 24, 69, 134	1 (2%)
31	C7	48/49 (97%)	-0.03	2 (4%) 36 26	26, 40, 96, 119	0
32	A8	64/65 (98%)	-0.35	0 100 100	16, 29, 45, 65	1 (1%)
32	C8	64/65 (98%)	-0.13	0 100 100	37, 52, 73, 85	0
33	A9	37/37 (100%)	-0.09	0 100 100	23, 35, 57, 68	1 (2%)
33	C9	37/37 (100%)	0.87	5 (13%) 3 1	45, 79, 96, 127	0
34	BA	1495/1521 (98%)	0.42	89 (5%) 21 14	31, 85, 186, 337	0
34	DA	1501/1521 (98%)	0.51	123 (8%) 11 6	39, 90, 196, 346	0
35	BB	231/256 (90%)	0.63	29 (12%) 3 2	43, 106, 173, 223	0
35	DB	231/256 (90%)	0.78	35 (15%) 2 1	71, 125, 176, 215	0
36	BC	206/239 (86%)	1.10	40 (19%) 1 0	56, 119, 174, 197	0
36	DC	206/239 (86%)	1.37	54 (26%) 0 0	69, 136, 182, 212	0
37	BD	208/209 (99%)	0.30	9 (4%) 35 25	44, 87, 138, 196	0
37	DD	208/209 (99%)	0.19	3 (1%) 75 70	59, 87, 136, 201	0
38	BE	148/162 (91%)	-0.10	1 (0%) 87 84	35, 73, 105, 128	0
38	DE	148/162 (91%)	0.01	2 (1%) 75 70	50, 81, 117, 182	0
39	BF	100/101 (99%)	-0.17	0 100 100	56, 86, 117, 138	0
39	DF	100/101 (99%)	-0.04	2 (2%) 65 56	48, 87, 115, 134	0
40	BG	155/156 (99%)	1.17	32 (20%) 1 0	68, 113, 183, 226	0
40	DG	155/156 (99%)	1.74	45 (29%) 0 0	72, 131, 194, 222	0
41	BH	137/138 (99%)	0.05	3 (2%) 62 52	47, 73, 99, 119	0
41	DH	137/138 (99%)	0.06	1 (0%) 87 84	57, 81, 111, 140	0
42	BI	127/128 (99%)	1.85	51 (40%) 0 0	65, 125, 167, 199	0
42	DI	127/128 (99%)	2.41	68 (53%) 0 0	91, 146, 193, 216	0
43	BJ	97/105 (92%)	1.60	34 (35%) 0 0	83, 131, 186, 215	0
43	DJ	96/105 (91%)	2.16	46 (47%) 0 0	92, 151, 200, 234	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
44	BK	114/129 (88%)	0.10	0 100 100	35, 79, 125, 151	0
44	DK	114/129 (88%)	0.20	2 (1%) 68 61	52, 91, 116, 177	0
45	BL	122/132 (92%)	-0.27	0 100 100	37, 60, 78, 113	0
45	DL	122/132 (92%)	-0.12	1 (0%) 86 81	46, 72, 96, 117	0
46	BM	117/126 (92%)	1.61	36 (30%) 0 0	77, 134, 182, 211	0
46	DM	122/126 (96%)	2.06	43 (35%) 0 0	94, 151, 201, 275	0
47	BN	60/61 (98%)	1.04	12 (20%) 1 0	67, 113, 146, 168	0
47	DN	60/61 (98%)	1.83	22 (36%) 0 0	98, 137, 179, 200	0
48	BO	88/89 (98%)	-0.14	1 (1%) 80 75	36, 71, 106, 121	0
48	DO	88/89 (98%)	-0.01	1 (1%) 80 75	47, 71, 107, 153	0
49	BP	82/88 (93%)	0.40	0 100 100	49, 80, 119, 171	0
49	DP	82/88 (93%)	0.45	5 (6%) 21 13	54, 78, 111, 153	0
50	BQ	99/105 (94%)	0.03	1 (1%) 82 77	44, 73, 99, 124	0
50	DQ	99/105 (94%)	0.01	0 100 100	44, 78, 104, 119	0
51	BR	68/88 (77%)	0.33	5 (7%) 14 8	42, 81, 123, 136	0
51	DR	68/88 (77%)	0.29	1 (1%) 73 68	53, 83, 128, 145	0
52	BS	84/93 (90%)	3.19	54 (64%) 0 0	97, 145, 198, 212	0
52	DS	83/93 (89%)	3.26	51 (61%) 0 0	90, 165, 216, 226	0
53	BT	96/106 (90%)	0.18	2 (2%) 63 54	62, 85, 122, 162	0
53	DT	96/106 (90%)	0.32	3 (3%) 49 39	58, 86, 135, 157	0
54	BU	23/27 (85%)	2.31	10 (43%) 0 0	62, 119, 158, 177	0
54	DU	23/27 (85%)	2.25	12 (52%) 0 0	92, 134, 173, 189	0
55	BV	7/18 (38%)	2.72	4 (57%) 0 0	53, 88, 211, 226	0
55	DV	6/18 (33%)	2.94	4 (66%) 0 0	84, 106, 214, 225	0
56	BW	69/76 (90%)	0.82	4 (5%) 23 15	38, 72, 106, 212	0
56	BY	67/76 (88%)	8.60	66 (98%) 0 0	82, 289, 329, 354	0
56	DW	69/76 (90%)	1.11	9 (13%) 3 2	54, 98, 141, 254	0
56	DY	66/76 (86%)	9.87	66 (100%) 0 0	213, 296, 333, 355	0
57	BZ	730/758 (96%)	0.14	34 (4%) 31 22	36, 79, 135, 190	0
57	DZ	730/758 (96%)	0.60	91 (12%) 3 2	36, 102, 169, 225	0
All	All	22825/23898 (95%)	0.56	2189 (9%) 8 4	5, 71, 189, 364	25 (0%)

The worst 5 of 2189 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	AC	159	ALA	36.7
3	AC	57	GLN	34.6
3	CC	27	ALA	34.0
3	CC	68	GLY	33.6
3	CC	172	ILE	31.9

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	BY	39	20/21	0.06	1.19	316,316,316,316	0
56	PSU	BY	55	20/21	0.06	0.68	302,302,302,302	1
56	MIA	BY	37	22/30	0.06	1.34	284,284,284,284	0
56	MIA	DY	37	22/30	0.13	1.82	319,319,319,319	1
56	4SU	DY	8	20/21	0.17	0.50	275,275,275,275	0
56	PSU	DY	32	20/21	0.19	1.57	268,268,268,268	0
56	5MU	BY	54	21/22	0.23	0.83	315,315,315,315	0
56	7MG	BY	46	24/25	0.27	0.44	302,302,302,302	0
56	PSU	DY	39	20/21	0.29	1.23	284,284,284,284	0
56	4SU	BY	8	20/21	0.29	0.49	300,300,300,300	0
56	PSU	BY	32	20/21	0.35	0.89	254,254,254,254	1
56	5MU	DY	54	21/22	0.35	0.74	305,305,305,305	1
56	PSU	DY	55	20/21	0.42	0.69	246,246,246,246	0
56	7MG	DY	46	24/25	0.51	0.52	302,302,302,302	0
56	PSU	DW	55	20/21	0.79	0.22	106,106,106,106	2
56	PSU	DW	39	20/21	0.88	0.34	93,93,93,93	3
56	5MU	DW	54	21/22	0.88	0.32	114,114,114,114	1
56	PSU	BW	55	20/21	0.88	0.23	74,74,74,74	5
56	PSU	DW	32	20/21	0.89	0.21	106,106,106,106	1
56	7MG	DW	46	24/25	0.89	0.29	114,114,114,114	2
56	MIA	DW	37	29/30	0.91	0.26	94,94,94,94	0
56	PSU	BW	32	20/21	0.92	0.17	81,81,81,81	1
56	MIA	BW	37	29/30	0.93	0.26	79,79,79,79	2
56	4SU	DW	8	20/21	0.93	0.19	88,88,88,88	3
56	7MG	BW	46	24/25	0.94	0.19	63,63,63,63	5
56	5MU	BW	54	21/22	0.95	0.24	74,74,74,74	1
56	4SU	BW	8	20/21	0.95	0.15	51,51,51,51	6

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	PSU	BW	39	20/21	0.96	0.24	65,65,65,65	3

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
58	MG	CA	3046	1/1	-0.21	0.34	114,114,114,114	0
58	MG	CA	3205	1/1	0.11	0.67	105,105,105,105	0
58	MG	CA	3202	1/1	0.15	0.80	77,77,77,77	0
58	MG	AA	3192	1/1	0.19	0.63	76,76,76,76	0
58	MG	BA	1771	1/1	0.19	0.92	115,115,115,115	0
58	MG	CA	3209	1/1	0.23	0.64	93,93,93,93	0
58	MG	BZ	701	1/1	0.24	0.29	137,137,137,137	0
58	MG	CA	3071	1/1	0.30	0.48	97,97,97,97	0
58	MG	AN	3001	1/1	0.33	0.93	85,85,85,85	0
58	MG	CA	3107	1/1	0.35	0.48	108,108,108,108	0
58	MG	CA	3594	1/1	0.39	0.21	80,80,80,80	0
58	MG	DA	1700	1/1	0.40	0.27	124,124,124,124	0
58	MG	DA	1657	1/1	0.41	0.20	93,93,93,93	0
58	MG	BA	1667	1/1	0.41	0.21	89,89,89,89	0
58	MG	CA	3002	1/1	0.44	0.29	114,114,114,114	0
58	MG	AA	3244	1/1	0.45	0.27	100,100,100,100	0
58	MG	AA	3178	1/1	0.46	0.50	78,78,78,78	0
58	MG	CA	3660	1/1	0.46	0.64	101,101,101,101	0
58	MG	DA	1720	1/1	0.47	0.18	72,72,72,72	0
58	MG	CA	3527	1/1	0.48	0.13	78,78,78,78	0
58	MG	AA	3784	1/1	0.48	0.37	74,74,74,74	0
58	MG	BA	1705	1/1	0.49	0.21	92,92,92,92	0
58	MG	BA	1709	1/1	0.50	0.22	104,104,104,104	0
58	MG	AA	3610	1/1	0.50	0.18	51,51,51,51	1
58	MG	CA	3620	1/1	0.51	0.26	69,69,69,69	0
58	MG	BA	1689	1/1	0.52	0.72	91,91,91,91	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	CA	3624	1/1	0.52	0.17	104,104,104,104	0
58	MG	DJ	5001	1/1	0.53	0.47	105,105,105,105	0
58	MG	CA	3599	1/1	0.54	0.24	80,80,80,80	0
58	MG	BA	1605	1/1	0.54	0.26	67,67,67,67	0
58	MG	BA	1681	1/1	0.54	1.11	84,84,84,84	0
58	MG	DA	1623	1/1	0.55	0.13	117,117,117,117	0
58	MG	CQ	205	1/1	0.55	0.51	81,81,81,81	0
58	MG	DA	1660	1/1	0.55	0.60	90,90,90,90	0
58	MG	CA	3134	1/1	0.56	1.04	86,86,86,86	0
58	MG	AA	3739	1/1	0.56	0.49	94,94,94,94	0
58	MG	CA	3421	1/1	0.57	0.24	76,76,76,76	0
58	MG	DA	1754	1/1	0.58	0.35	81,81,81,81	0
58	MG	CA	3481	1/1	0.58	0.34	91,91,91,91	0
58	MG	DZ	701	1/1	0.58	0.59	111,111,111,111	0
58	MG	CA	3561	1/1	0.58	0.20	95,95,95,95	0
58	MG	AA	3235	1/1	0.58	0.16	64,64,64,64	0
58	MG	CA	3042	1/1	0.59	0.70	95,95,95,95	0
58	MG	CA	3093	1/1	0.60	0.59	84,84,84,84	0
58	MG	DA	1634	1/1	0.60	0.33	90,90,90,90	0
58	MG	CA	3043	1/1	0.60	0.71	102,102,102,102	0
59	ZN	C4	501	1/1	0.61	0.06	189,189,189,189	0
58	MG	AA	3766	1/1	0.61	0.19	72,72,72,72	0
58	MG	CA	3098	1/1	0.61	0.39	83,83,83,83	0
58	MG	CA	3544	1/1	0.61	0.19	81,81,81,81	0
58	MG	AA	3767	1/1	0.61	0.32	63,63,63,63	1
58	MG	DA	1672	1/1	0.62	0.46	73,73,73,73	0
58	MG	CA	3546	1/1	0.62	0.11	119,119,119,119	0
58	MG	CA	3080	1/1	0.62	0.22	87,87,87,87	0
58	MG	CA	3105	1/1	0.62	0.11	80,80,80,80	0
58	MG	CA	3241	1/1	0.62	0.53	107,107,107,107	0
58	MG	CA	3066	1/1	0.63	0.57	84,84,84,84	0
58	MG	BA	1698	1/1	0.63	0.27	74,74,74,74	0
58	MG	BA	1624	1/1	0.63	0.19	87,87,87,87	0
58	MG	AA	3613	1/1	0.63	0.12	104,104,104,104	0
58	MG	BA	1800	1/1	0.63	0.22	84,84,84,84	0
58	MG	DW	503	1/1	0.63	0.17	84,84,84,84	0
58	MG	A4	502	1/1	0.63	0.64	123,123,123,123	0
58	MG	CA	3646	1/1	0.63	0.20	95,95,95,95	0
58	MG	CA	3070	1/1	0.64	0.78	87,87,87,87	0
58	MG	BA	1805	1/1	0.65	0.18	83,83,83,83	0
58	MG	CA	3033	1/1	0.65	0.85	89,89,89,89	0
58	MG	BA	1711	1/1	0.65	0.59	71,71,71,71	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	CA	3500	1/1	0.65	0.42	64,64,64,64	0
58	MG	CA	3507	1/1	0.65	0.25	100,100,100,100	0
58	MG	CA	3101	1/1	0.66	0.14	78,78,78,78	0
58	MG	CA	3616	1/1	0.66	0.64	79,79,79,79	0
58	MG	DA	1687	1/1	0.66	0.13	100,100,100,100	0
58	MG	CA	3644	1/1	0.66	0.24	84,84,84,84	0
58	MG	DA	1673	1/1	0.66	0.35	100,100,100,100	0
58	MG	CA	3062	1/1	0.66	0.24	68,68,68,68	0
58	MG	CA	3571	1/1	0.66	0.14	65,65,65,65	0
58	MG	BA	1610	1/1	0.66	0.12	79,79,79,79	0
58	MG	AA	3445	1/1	0.66	0.22	75,75,75,75	0
58	MG	CQ	201	1/1	0.66	0.29	62,62,62,62	0
58	MG	BA	1616	1/1	0.66	0.63	134,134,134,134	0
58	MG	DA	1606	1/1	0.67	0.94	84,84,84,84	0
58	MG	AA	3735	1/1	0.67	0.23	35,35,35,35	0
58	MG	AA	3623	1/1	0.67	0.20	74,74,74,74	0
58	MG	BA	1669	1/1	0.68	0.29	73,73,73,73	0
58	MG	CA	3593	1/1	0.68	0.25	73,73,73,73	0
58	MG	BA	1734	1/1	0.68	0.39	81,81,81,81	0
58	MG	CF	301	1/1	0.68	0.40	63,63,63,63	0
58	MG	BA	1742	1/1	0.68	0.21	79,79,79,79	0
58	MG	AA	3744	1/1	0.68	0.29	86,86,86,86	0
58	MG	AA	3585	1/1	0.69	0.17	65,65,65,65	0
58	MG	BA	1603	1/1	0.69	0.22	67,67,67,67	0
58	MG	CA	3083	1/1	0.69	0.75	90,90,90,90	0
58	MG	CA	3563	1/1	0.69	0.20	91,91,91,91	0
58	MG	CA	3389	1/1	0.69	0.47	75,75,75,75	0
58	MG	CG	3001	1/1	0.69	0.31	83,83,83,83	0
58	MG	CA	3492	1/1	0.69	0.52	105,105,105,105	0
58	MG	BA	1622	1/1	0.69	1.01	75,75,75,75	0
58	MG	CA	3253	1/1	0.69	0.18	95,95,95,95	0
58	MG	CA	3393	1/1	0.69	0.08	82,82,82,82	0
58	MG	CA	3224	1/1	0.69	0.94	81,81,81,81	0
58	MG	BA	1785	1/1	0.69	0.33	87,87,87,87	0
58	MG	CA	3152	1/1	0.69	0.27	56,56,56,56	0
58	MG	AA	3760	1/1	0.69	0.20	27,27,27,27	0
58	MG	DA	1733	1/1	0.69	0.17	83,83,83,83	0
58	MG	BA	1634	1/1	0.69	0.48	100,100,100,100	0
58	MG	CA	3173	1/1	0.70	0.42	65,65,65,65	0
58	MG	AB	3017	1/1	0.70	0.17	77,77,77,77	0
58	MG	CA	3537	1/1	0.70	0.30	78,78,78,78	0
58	MG	BA	1806	1/1	0.70	0.27	81,81,81,81	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	AA	3236	1/1	0.70	0.21	57,57,57,57	0
58	MG	AA	3732	1/1	0.70	0.23	68,68,68,68	0
58	MG	CA	3618	1/1	0.70	0.34	65,65,65,65	0
58	MG	CA	3015	1/1	0.71	0.52	85,85,85,85	0
58	MG	CA	3158	1/1	0.71	0.31	70,70,70,70	0
58	MG	BA	1693	1/1	0.71	0.28	67,67,67,67	0
58	MG	AA	3246	1/1	0.71	0.40	72,72,72,72	0
58	MG	CA	3460	1/1	0.71	0.46	109,109,109,109	0
58	MG	BA	1695	1/1	0.71	0.20	98,98,98,98	0
58	MG	BA	1767	1/1	0.71	0.09	58,58,58,58	0
58	MG	BA	1630	1/1	0.71	0.29	63,63,63,63	0
58	MG	DA	1649	1/1	0.72	0.82	93,93,93,93	0
58	MG	BA	1650	1/1	0.72	0.34	72,72,72,72	0
58	MG	DA	1706	1/1	0.72	0.27	128,128,128,128	0
58	MG	CA	3246	1/1	0.72	0.49	59,59,59,59	0
58	MG	CA	3514	1/1	0.72	0.77	105,105,105,105	0
58	MG	CA	3008	1/1	0.72	0.37	100,100,100,100	0
58	MG	AA	3115	1/1	0.72	0.45	67,67,67,67	1
58	MG	DA	1663	1/1	0.72	0.21	72,72,72,72	0
58	MG	AB	3021	1/1	0.72	0.21	61,61,61,61	0
58	MG	CA	3058	1/1	0.72	0.40	77,77,77,77	0
58	MG	CA	3596	1/1	0.72	0.22	72,72,72,72	0
58	MG	DA	1678	1/1	0.72	0.36	82,82,82,82	0
58	MG	DA	1707	1/1	0.72	0.34	87,87,87,87	0
58	MG	DA	1751	1/1	0.72	0.24	81,81,81,81	0
58	MG	CA	3239	1/1	0.72	0.36	75,75,75,75	0
58	MG	CA	3590	1/1	0.72	0.17	95,95,95,95	0
58	MG	CA	3243	1/1	0.72	0.18	78,78,78,78	0
58	MG	BA	1661	1/1	0.72	0.94	82,82,82,82	0
58	MG	CA	3244	1/1	0.72	0.66	78,78,78,78	0
58	MG	AA	3136	1/1	0.72	0.20	52,52,52,52	0
58	MG	BA	1696	1/1	0.72	0.39	68,68,68,68	0
58	MG	AZ	301	1/1	0.73	0.33	98,98,98,98	0
58	MG	CA	3089	1/1	0.73	0.40	80,80,80,80	0
58	MG	CA	3140	1/1	0.73	0.58	98,98,98,98	0
58	MG	BA	1660	1/1	0.73	0.20	70,70,70,70	0
58	MG	BA	1775	1/1	0.73	0.20	75,75,75,75	0
58	MG	AA	3204	1/1	0.73	0.37	57,57,57,57	0
58	MG	AA	3638	1/1	0.73	0.39	72,72,72,72	0
58	MG	AA	3252	1/1	0.73	0.52	66,66,66,66	0
58	MG	CA	3555	1/1	0.73	0.26	83,83,83,83	0
58	MG	AA	3248	1/1	0.73	0.48	64,64,64,64	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	CB	3002	1/1	0.73	0.26	66,66,66,66	0
58	MG	AA	3640	1/1	0.73	0.43	77,77,77,77	0
58	MG	AA	3768	1/1	0.73	0.40	99,99,99,99	0
58	MG	AX	101	1/1	0.74	0.44	75,75,75,75	0
58	MG	CA	3574	1/1	0.74	0.15	72,72,72,72	0
58	MG	CA	3006	1/1	0.74	0.26	67,67,67,67	0
58	MG	BA	1715	1/1	0.74	0.21	83,83,83,83	0
58	MG	CA	3314	1/1	0.74	0.50	77,77,77,77	0
58	MG	CA	3532	1/1	0.74	0.12	79,79,79,79	0
58	MG	CA	3076	1/1	0.74	0.40	84,84,84,84	0
58	MG	CA	3335	1/1	0.74	0.18	62,62,62,62	0
58	MG	CA	3155	1/1	0.74	0.25	86,86,86,86	0
58	MG	CA	3082	1/1	0.74	0.29	70,70,70,70	0
58	MG	CA	3290	1/1	0.74	0.47	75,75,75,75	0
58	MG	CA	3295	1/1	0.74	0.20	84,84,84,84	0
58	MG	CA	3611	1/1	0.74	0.67	91,91,91,91	0
58	MG	CA	3204	1/1	0.74	0.36	74,74,74,74	0
58	MG	CA	3294	1/1	0.74	0.20	83,83,83,83	0
58	MG	BA	1618	1/1	0.74	0.29	57,57,57,57	0
58	MG	AA	3202	1/1	0.75	0.14	47,47,47,47	0
58	MG	CA	3056	1/1	0.75	0.24	85,85,85,85	0
58	MG	BA	1766	1/1	0.75	0.35	86,86,86,86	0
58	MG	AA	3272	1/1	0.75	0.46	52,52,52,52	0
58	MG	AD	309	1/1	0.75	0.31	57,57,57,57	0
58	MG	AA	3691	1/1	0.75	0.21	89,89,89,89	0
58	MG	DA	1755	1/1	0.75	0.63	86,86,86,86	0
58	MG	AA	3016	1/1	0.76	0.39	59,59,59,59	0
58	MG	AA	3112	1/1	0.76	0.60	98,98,98,98	0
58	MG	CA	3396	1/1	0.76	0.23	58,58,58,58	0
58	MG	AB	3001	1/1	0.76	0.55	87,87,87,87	0
58	MG	DA	1718	1/1	0.76	0.15	77,77,77,77	0
58	MG	AA	3260	1/1	0.76	0.38	71,71,71,71	0
58	MG	CD	301	1/1	0.76	0.45	81,81,81,81	0
58	MG	CA	3183	1/1	0.76	1.03	86,86,86,86	0
58	MG	CA	3485	1/1	0.76	0.21	83,83,83,83	0
58	MG	AA	3781	1/1	0.76	0.33	44,44,44,44	1
58	MG	BA	1708	1/1	0.76	0.18	79,79,79,79	0
58	MG	AA	3108	1/1	0.76	0.47	125,125,125,125	0
58	MG	CA	3001	1/1	0.76	0.39	73,73,73,73	0
58	MG	DA	1652	1/1	0.76	0.12	71,71,71,71	0
58	MG	CA	3180	1/1	0.76	0.47	108,108,108,108	0
58	MG	AA	3814	1/1	0.76	0.37	93,93,93,93	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	AA	3010	1/1	0.76	0.62	68,68,68,68	0
58	MG	CA	3088	1/1	0.77	0.51	75,75,75,75	0
58	MG	DA	1691	1/1	0.77	0.20	85,85,85,85	0
58	MG	AQ	201	1/1	0.77	0.49	62,62,62,62	0
58	MG	CA	3141	1/1	0.77	0.28	54,54,54,54	0
58	MG	BA	1645	1/1	0.77	0.60	61,61,61,61	0
58	MG	CA	3059	1/1	0.77	0.35	60,60,60,60	0
58	MG	CA	3304	1/1	0.77	0.11	93,93,93,93	0
58	MG	CB	3007	1/1	0.77	0.17	65,65,65,65	0
58	MG	AA	3200	1/1	0.77	0.11	91,91,91,91	0
58	MG	AA	3751	1/1	0.77	0.64	56,56,56,56	1
58	MG	AA	3537	1/1	0.77	0.14	95,95,95,95	0
58	MG	BA	1666	1/1	0.77	0.51	75,75,75,75	0
58	MG	AA	3059	1/1	0.77	0.25	51,51,51,51	0
58	MG	BA	1673	1/1	0.77	0.94	77,77,77,77	0
58	MG	CA	3583	1/1	0.77	0.31	78,78,78,78	1
58	MG	DA	1619	1/1	0.78	0.29	71,71,71,71	0
58	MG	AA	3807	1/1	0.78	0.30	62,62,62,62	1
58	MG	BA	1615	1/1	0.78	0.30	74,74,74,74	0
58	MG	CA	3236	1/1	0.78	0.43	87,87,87,87	0
58	MG	AD	305	1/1	0.78	0.40	53,53,53,53	1
58	MG	DA	1686	1/1	0.78	0.15	53,53,53,53	0
58	MG	CA	3649	1/1	0.78	0.37	85,85,85,85	0
58	MG	BA	1652	1/1	0.78	0.13	69,69,69,69	0
58	MG	CA	3573	1/1	0.78	0.20	80,80,80,80	0
58	MG	AA	3621	1/1	0.78	0.17	46,46,46,46	0
58	MG	AA	3758	1/1	0.78	0.33	81,81,81,81	0
58	MG	AA	3095	1/1	0.78	0.44	82,82,82,82	0
58	MG	CA	3174	1/1	0.78	0.51	61,61,61,61	0
58	MG	BA	1756	1/1	0.78	0.35	68,68,68,68	0
58	MG	AA	3041	1/1	0.78	0.15	75,75,75,75	0
58	MG	CA	3653	1/1	0.78	0.39	95,95,95,95	0
58	MG	AA	3672	1/1	0.78	0.35	25,25,25,25	1
58	MG	DW	502	1/1	0.78	0.11	84,84,84,84	0
58	MG	AA	3270	1/1	0.78	0.25	54,54,54,54	0
58	MG	CA	3020	1/1	0.78	0.19	63,63,63,63	0
58	MG	DA	1725	1/1	0.78	0.19	70,70,70,70	0
58	MG	CF	305	1/1	0.78	0.15	51,51,51,51	0
58	MG	AA	3710	1/1	0.79	0.26	75,75,75,75	0
58	MG	CA	3018	1/1	0.79	0.31	64,64,64,64	0
58	MG	CA	3126	1/1	0.79	0.26	93,93,93,93	0
58	MG	AB	3004	1/1	0.79	0.29	89,89,89,89	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	CA	3553	1/1	0.79	0.21	81,81,81,81	0
58	MG	BA	1716	1/1	0.79	0.17	67,67,67,67	0
58	MG	CA	3533	1/1	0.79	0.21	81,81,81,81	0
58	MG	CA	3068	1/1	0.79	0.24	57,57,57,57	0
58	MG	AA	3580	1/1	0.79	0.14	23,23,23,23	0
58	MG	AB	3006	1/1	0.79	0.30	72,72,72,72	0
58	MG	AA	3269	1/1	0.79	0.46	84,84,84,84	0
58	MG	AA	3133	1/1	0.79	0.36	69,69,69,69	0
58	MG	AA	3359	1/1	0.79	0.18	51,51,51,51	0
58	MG	DA	1614	1/1	0.79	0.77	87,87,87,87	0
58	MG	AA	3713	1/1	0.79	0.41	52,52,52,52	1
58	MG	CV	201	1/1	0.79	0.22	100,100,100,100	0
58	MG	BA	1702	1/1	0.79	0.18	89,89,89,89	0
58	MG	AA	3024	1/1	0.79	0.14	57,57,57,57	0
58	MG	CA	3524	1/1	0.80	0.09	77,77,77,77	0
58	MG	CA	3350	1/1	0.80	0.09	85,85,85,85	0
58	MG	CA	3131	1/1	0.80	0.20	62,62,62,62	0
58	MG	AA	3063	1/1	0.80	0.43	67,67,67,67	0
58	MG	DA	1627	1/1	0.80	0.22	70,70,70,70	0
58	MG	AA	3080	1/1	0.80	0.39	57,57,57,57	0
58	MG	CD	302	1/1	0.80	0.50	95,95,95,95	0
58	MG	CA	3604	1/1	0.80	0.19	69,69,69,69	0
58	MG	BA	1797	1/1	0.80	0.20	63,63,63,63	0
58	MG	AA	3078	1/1	0.80	0.28	66,66,66,66	0
58	MG	CA	3300	1/1	0.80	0.39	86,86,86,86	0
58	MG	CA	3172	1/1	0.80	0.31	83,83,83,83	0
58	MG	DA	1656	1/1	0.80	0.22	75,75,75,75	0
58	MG	AA	3447	1/1	0.80	0.17	61,61,61,61	0
58	MG	AA	3697	1/1	0.80	0.15	63,63,63,63	0
58	MG	AA	3306	1/1	0.80	0.18	47,47,47,47	0
58	MG	AE	301	1/1	0.80	0.28	69,69,69,69	0
58	MG	AA	3464	1/1	0.80	0.15	63,63,63,63	0
58	MG	CA	3603	1/1	0.80	0.24	51,51,51,51	0
58	MG	AA	3738	1/1	0.80	0.25	75,75,75,75	0
58	MG	BA	1651	1/1	0.80	0.15	102,102,102,102	0
58	MG	CA	3085	1/1	0.80	0.50	66,66,66,66	0
58	MG	CA	3013	1/1	0.80	0.30	63,63,63,63	0
58	MG	CA	3374	1/1	0.80	0.41	76,76,76,76	0
58	MG	BA	1638	1/1	0.80	0.62	78,78,78,78	0
58	MG	AA	3806	1/1	0.80	0.24	61,61,61,61	0
58	MG	CA	3598	1/1	0.80	0.10	73,73,73,73	0
58	MG	CA	3154	1/1	0.80	0.30	72,72,72,72	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	DE	202	1/1	0.80	0.12	94,94,94,94	0
58	MG	AA	3168	1/1	0.80	0.36	63,63,63,63	0
58	MG	CB	3013	1/1	0.80	0.17	98,98,98,98	0
58	MG	DF	3001	1/1	0.80	0.21	49,49,49,49	0
58	MG	A2	102	1/1	0.80	0.35	54,54,54,54	0
58	MG	AA	3268	1/1	0.80	0.12	88,88,88,88	0
58	MG	CA	3641	1/1	0.80	0.38	67,67,67,67	0
58	MG	DA	1662	1/1	0.81	0.21	64,64,64,64	0
58	MG	AA	3411	1/1	0.81	0.21	47,47,47,47	0
58	MG	CA	3117	1/1	0.81	0.30	68,68,68,68	0
58	MG	CA	3551	1/1	0.81	0.18	88,88,88,88	0
58	MG	CA	3444	1/1	0.81	0.15	91,91,91,91	0
58	MG	BA	1690	1/1	0.81	0.28	89,89,89,89	0
58	MG	AA	3308	1/1	0.81	0.13	30,30,30,30	0
58	MG	BA	1793	1/1	0.81	0.63	86,86,86,86	0
58	MG	DA	1630	1/1	0.81	0.16	61,61,61,61	0
58	MG	DA	1746	1/1	0.81	0.17	91,91,91,91	0
58	MG	AA	3015	1/1	0.81	0.47	64,64,64,64	0
58	MG	CA	3512	1/1	0.81	0.47	65,65,65,65	0
58	MG	AA	3626	1/1	0.81	0.26	74,74,74,74	0
58	MG	AD	301	1/1	0.81	0.47	70,70,70,70	0
58	MG	AA	3184	1/1	0.81	0.34	68,68,68,68	0
58	MG	AA	3834	1/1	0.81	0.21	58,58,58,58	0
58	MG	AA	3600	1/1	0.81	0.23	60,60,60,60	0
58	MG	CA	3610	1/1	0.81	0.16	98,98,98,98	0
58	MG	AA	3277	1/1	0.81	0.22	79,79,79,79	0
58	MG	AA	3656	1/1	0.81	0.20	56,56,56,56	0
58	MG	AA	3012	1/1	0.81	0.22	34,34,34,34	0
58	MG	AA	3442	1/1	0.81	0.29	49,49,49,49	0
58	MG	CA	3378	1/1	0.81	0.13	84,84,84,84	0
58	MG	DA	1762	1/1	0.81	0.08	73,73,73,73	0
58	MG	CA	3493	1/1	0.81	0.40	88,88,88,88	0
58	MG	CA	3208	1/1	0.81	0.41	84,84,84,84	0
58	MG	CA	3248	1/1	0.81	0.63	77,77,77,77	0
58	MG	CA	3186	1/1	0.81	0.33	69,69,69,69	0
58	MG	CA	3217	1/1	0.81	0.30	52,52,52,52	0
58	MG	CA	3116	1/1	0.81	0.40	75,75,75,75	0
58	MG	CA	3601	1/1	0.81	0.07	75,75,75,75	0
58	MG	BA	1671	1/1	0.82	0.22	75,75,75,75	0
58	MG	AA	3476	1/1	0.82	0.24	69,69,69,69	0
58	MG	BA	1811	1/1	0.82	0.31	75,75,75,75	0
58	MG	DA	1759	1/1	0.82	0.33	76,76,76,76	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	CA	3113	1/1	0.82	0.28	92,92,92,92	0
58	MG	AB	3023	1/1	0.82	0.46	76,76,76,76	0
58	MG	AA	3137	1/1	0.82	0.28	56,56,56,56	0
58	MG	DA	1612	1/1	0.82	0.38	72,72,72,72	0
58	MG	CA	3468	1/1	0.82	0.17	61,61,61,61	0
58	MG	BA	1644	1/1	0.82	0.30	75,75,75,75	0
58	MG	BA	1659	1/1	0.82	0.40	84,84,84,84	0
58	MG	AH	3002	1/1	0.82	0.70	74,74,74,74	0
58	MG	AA	3414	1/1	0.82	0.16	36,36,36,36	0
58	MG	AA	3233	1/1	0.82	0.34	55,55,55,55	0
58	MG	DA	1620	1/1	0.82	0.14	58,58,58,58	0
58	MG	BA	1772	1/1	0.82	0.18	70,70,70,70	0
58	MG	AA	3373	1/1	0.82	0.29	59,59,59,59	0
58	MG	AA	3026	1/1	0.82	0.38	86,86,86,86	0
58	MG	AA	3017	1/1	0.82	0.15	78,78,78,78	0
58	MG	A7	103	1/1	0.82	0.52	38,38,38,38	1
58	MG	AA	3835	1/1	0.82	0.61	111,111,111,111	0
58	MG	AA	3230	1/1	0.82	0.57	80,80,80,80	0
58	MG	AA	3122	1/1	0.82	0.27	54,54,54,54	0
58	MG	DA	1730	1/1	0.82	0.14	88,88,88,88	0
58	MG	CA	3509	1/1	0.82	0.18	76,76,76,76	0
58	MG	CA	3039	1/1	0.82	0.89	71,71,71,71	0
58	MG	CA	3096	1/1	0.82	0.35	68,68,68,68	0
58	MG	CA	3216	1/1	0.82	0.59	66,66,66,66	0
58	MG	AA	3151	1/1	0.82	0.20	50,50,50,50	0
58	MG	BA	1724	1/1	0.82	0.18	64,64,64,64	0
58	MG	BA	1647	1/1	0.83	0.16	75,75,75,75	0
58	MG	DA	1632	1/1	0.83	0.31	61,61,61,61	0
58	MG	CA	3503	1/1	0.83	0.17	62,62,62,62	0
58	MG	CA	3123	1/1	0.83	0.80	88,88,88,88	0
58	MG	CP	203	1/1	0.83	0.24	67,67,67,67	0
58	MG	CA	3100	1/1	0.83	0.43	79,79,79,79	0
58	MG	CA	3540	1/1	0.83	0.32	85,85,85,85	0
58	MG	AA	3245	1/1	0.83	0.74	69,69,69,69	0
58	MG	AA	3599	1/1	0.83	0.40	58,58,58,58	0
58	MG	CA	3097	1/1	0.83	0.25	80,80,80,80	0
58	MG	AA	3558	1/1	0.83	0.14	51,51,51,51	0
58	MG	CA	3642	1/1	0.83	0.97	80,80,80,80	0
58	MG	CA	3118	1/1	0.83	0.22	57,57,57,57	0
58	MG	BA	1646	1/1	0.83	0.79	75,75,75,75	0
58	MG	BA	1692	1/1	0.83	0.27	86,86,86,86	0
58	MG	CA	3111	1/1	0.83	0.14	71,71,71,71	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	CA	3081	1/1	0.83	0.15	68,68,68,68	0
58	MG	DA	1604	1/1	0.83	0.35	76,76,76,76	0
58	MG	DA	1676	1/1	0.83	0.09	78,78,78,78	0
58	MG	CA	3031	1/1	0.83	0.08	76,76,76,76	0
58	MG	CA	3528	1/1	0.83	0.41	79,79,79,79	0
58	MG	BA	1633	1/1	0.83	0.35	62,62,62,62	0
58	MG	BA	1719	1/1	0.83	0.26	80,80,80,80	0
58	MG	BD	502	1/1	0.83	0.61	82,82,82,82	0
58	MG	AA	3636	1/1	0.83	0.24	65,65,65,65	0
58	MG	AA	3018	1/1	0.83	1.35	78,78,78,78	0
58	MG	CA	3636	1/1	0.83	0.19	80,80,80,80	0
58	MG	AA	3543	1/1	0.83	0.20	52,52,52,52	1
58	MG	CA	3474	1/1	0.83	0.33	76,76,76,76	0
58	MG	CA	3447	1/1	0.83	0.42	80,80,80,80	0
58	MG	AA	3224	1/1	0.83	0.40	75,75,75,75	0
58	MG	AA	3490	1/1	0.83	0.09	50,50,50,50	0
58	MG	CA	3223	1/1	0.83	0.56	65,65,65,65	0
58	MG	AA	3755	1/1	0.83	0.40	63,63,63,63	0
58	MG	AA	3258	1/1	0.83	0.17	22,22,22,22	0
58	MG	AA	3460	1/1	0.83	0.46	72,72,72,72	0
58	MG	BV	101	1/1	0.83	0.34	110,110,110,110	0
58	MG	AA	3206	1/1	0.83	0.27	39,39,39,39	0
58	MG	AA	3283	1/1	0.83	0.55	62,62,62,62	0
58	MG	AA	3220	1/1	0.83	0.26	62,62,62,62	0
58	MG	AA	3382	1/1	0.83	0.16	36,36,36,36	1
58	MG	AA	3752	1/1	0.84	0.57	72,72,72,72	0
58	MG	AA	3165	1/1	0.84	0.41	57,57,57,57	0
58	MG	AA	3223	1/1	0.84	0.41	35,35,35,35	0
58	MG	AA	3538	1/1	0.84	0.26	61,61,61,61	1
58	MG	AA	3186	1/1	0.84	0.16	37,37,37,37	0
58	MG	CA	3073	1/1	0.84	0.56	91,91,91,91	0
58	MG	AA	3570	1/1	0.84	0.16	15,15,15,15	0
58	MG	BA	1714	1/1	0.84	0.24	88,88,88,88	0
58	MG	AA	3155	1/1	0.84	0.30	64,64,64,64	0
58	MG	CA	3272	1/1	0.84	0.47	75,75,75,75	0
58	MG	CA	3159	1/1	0.84	0.44	69,69,69,69	0
58	MG	CA	3657	1/1	0.84	0.20	67,67,67,67	0
58	MG	CA	3025	1/1	0.84	0.28	77,77,77,77	0
58	MG	CA	3622	1/1	0.84	0.23	55,55,55,55	0
58	MG	AA	3354	1/1	0.84	0.30	60,60,60,60	0
58	MG	AA	3281	1/1	0.84	0.39	61,61,61,61	0
58	MG	CA	3212	1/1	0.84	0.31	69,69,69,69	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	DA	1607	1/1	0.84	0.31	61,61,61,61	0
58	MG	CA	3607	1/1	0.84	0.28	97,97,97,97	0
58	MG	BA	1614	1/1	0.84	0.32	88,88,88,88	0
58	MG	CA	3063	1/1	0.84	0.28	53,53,53,53	0
58	MG	CA	3024	1/1	0.84	0.66	88,88,88,88	0
58	MG	CA	3645	1/1	0.84	0.14	82,82,82,82	0
58	MG	CA	3373	1/1	0.84	0.48	58,58,58,58	0
58	MG	AA	3665	1/1	0.84	0.33	85,85,85,85	0
58	MG	BA	1774	1/1	0.84	0.12	61,61,61,61	0
58	MG	AA	3085	1/1	0.84	0.31	53,53,53,53	0
58	MG	AA	3801	1/1	0.84	0.07	88,88,88,88	0
58	MG	BA	1653	1/1	0.84	0.41	78,78,78,78	0
58	MG	CA	3010	1/1	0.84	0.08	41,41,41,41	0
58	MG	AA	3273	1/1	0.84	0.32	90,90,90,90	0
58	MG	AA	3604	1/1	0.84	0.37	38,38,38,38	1
58	MG	CA	3534	1/1	0.84	0.18	79,79,79,79	0
58	MG	CP	201	1/1	0.85	0.81	65,65,65,65	0
58	MG	AA	3720	1/1	0.85	0.69	77,77,77,77	0
58	MG	DA	1701	1/1	0.85	0.27	63,63,63,63	0
58	MG	BA	1760	1/1	0.85	0.13	89,89,89,89	0
58	MG	BA	1648	1/1	0.85	0.21	37,37,37,37	0
58	MG	BA	1736	1/1	0.85	0.12	73,73,73,73	0
58	MG	CA	3147	1/1	0.85	0.35	76,76,76,76	0
58	MG	CA	3027	1/1	0.85	0.36	44,44,44,44	0
58	MG	AA	3052	1/1	0.85	0.62	65,65,65,65	0
58	MG	CA	3139	1/1	0.85	0.30	123,123,123,123	0
58	MG	A7	101	1/1	0.85	0.17	49,49,49,49	1
58	MG	CA	3405	1/1	0.85	0.23	91,91,91,91	0
58	MG	CA	3463	1/1	0.85	0.27	49,49,49,49	0
58	MG	AA	3729	1/1	0.85	0.11	38,38,38,38	0
58	MG	AA	3042	1/1	0.85	0.41	38,38,38,38	0
58	MG	AA	3765	1/1	0.85	0.35	63,63,63,63	0
58	MG	CA	3589	1/1	0.85	0.07	79,79,79,79	0
58	MG	DA	1684	1/1	0.85	0.53	72,72,72,72	0
58	MG	CA	3009	1/1	0.85	0.47	67,67,67,67	0
58	MG	CA	3663	1/1	0.85	0.40	91,91,91,91	0
58	MG	AA	3231	1/1	0.85	0.21	53,53,53,53	0
58	MG	CA	3515	1/1	0.85	0.19	79,79,79,79	0
58	MG	CQ	204	1/1	0.85	0.29	61,61,61,61	0
58	MG	AA	3208	1/1	0.85	0.31	61,61,61,61	0
58	MG	AA	3349	1/1	0.85	0.28	40,40,40,40	0
58	MG	AA	3615	1/1	0.85	0.19	35,35,35,35	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	CA	3075	1/1	0.85	0.37	71,71,71,71	0
58	MG	CA	3129	1/1	0.85	0.51	69,69,69,69	0
58	MG	AA	3261	1/1	0.85	0.35	51,51,51,51	0
58	MG	CE	304	1/1	0.85	0.72	68,68,68,68	0
58	MG	CA	3614	1/1	0.85	0.20	52,52,52,52	0
58	MG	BA	1764	1/1	0.85	0.32	63,63,63,63	0
58	MG	AA	3081	1/1	0.85	0.27	40,40,40,40	0
58	MG	BA	1668	1/1	0.85	0.25	83,83,83,83	0
58	MG	AA	3172	1/1	0.85	0.73	71,71,71,71	0
58	MG	AA	3201	1/1	0.85	0.36	65,65,65,65	0
58	MG	CA	3625	1/1	0.85	0.51	79,79,79,79	0
58	MG	CA	3632	1/1	0.85	0.16	79,79,79,79	0
58	MG	DA	1749	1/1	0.85	0.42	80,80,80,80	0
58	MG	CB	3006	1/1	0.85	0.10	83,83,83,83	0
58	MG	CA	3067	1/1	0.85	0.33	72,72,72,72	0
58	MG	BA	1642	1/1	0.85	0.41	69,69,69,69	0
58	MG	CA	3392	1/1	0.85	0.21	35,35,35,35	0
58	MG	AA	3703	1/1	0.85	0.10	76,76,76,76	0
58	MG	CA	3037	1/1	0.85	0.23	58,58,58,58	0
58	MG	AA	3205	1/1	0.85	0.44	64,64,64,64	0
58	MG	BA	1789	1/1	0.85	0.13	68,68,68,68	0
58	MG	CA	3427	1/1	0.85	0.14	55,55,55,55	0
58	MG	AA	3651	1/1	0.85	0.23	52,52,52,52	0
58	MG	BA	1700	1/1	0.85	0.23	61,61,61,61	0
58	MG	CA	3035	1/1	0.85	0.47	60,60,60,60	0
58	MG	AA	3105	1/1	0.85	0.13	81,81,81,81	0
58	MG	CA	3103	1/1	0.85	0.51	62,62,62,62	0
58	MG	CA	3578	1/1	0.85	0.26	80,80,80,80	0
58	MG	AA	3483	1/1	0.85	0.07	43,43,43,43	1
58	MG	DA	1765	1/1	0.85	0.20	95,95,95,95	0
58	MG	AA	3213	1/1	0.85	0.17	58,58,58,58	0
58	MG	CA	3570	1/1	0.86	0.20	77,77,77,77	0
58	MG	CA	3258	1/1	0.86	0.35	70,70,70,70	0
58	MG	BA	1810	1/1	0.86	0.24	66,66,66,66	0
58	MG	CA	3226	1/1	0.86	0.34	69,69,69,69	0
58	MG	DA	1750	1/1	0.86	0.16	68,68,68,68	0
58	MG	AA	3239	1/1	0.86	0.35	64,64,64,64	0
58	MG	BA	1694	1/1	0.86	0.07	80,80,80,80	0
58	MG	AA	3608	1/1	0.86	0.18	73,73,73,73	0
58	MG	CA	3328	1/1	0.86	0.25	55,55,55,55	0
58	MG	CA	3132	1/1	0.86	0.19	30,30,30,30	0
58	MG	CA	3221	1/1	0.86	0.27	54,54,54,54	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	CR	201	1/1	0.86	0.43	51,51,51,51	0
58	MG	DA	1696	1/1	0.86	0.18	91,91,91,91	0
58	MG	DA	1763	1/1	0.86	0.20	77,77,77,77	0
58	MG	CA	3278	1/1	0.86	0.14	37,37,37,37	0
58	MG	CA	3228	1/1	0.86	0.26	63,63,63,63	0
58	MG	AA	3424	1/1	0.86	0.14	65,65,65,65	0
58	MG	CA	3420	1/1	0.86	0.28	71,71,71,71	0
58	MG	CA	3523	1/1	0.86	0.31	40,40,40,40	0
58	MG	DA	1628	1/1	0.86	0.48	74,74,74,74	0
58	MG	AA	3803	1/1	0.86	0.31	62,62,62,62	0
58	MG	CA	3556	1/1	0.86	0.08	48,48,48,48	0
58	MG	BA	1662	1/1	0.86	0.17	53,53,53,53	0
58	MG	AA	3612	1/1	0.86	0.20	56,56,56,56	0
58	MG	CA	3032	1/1	0.86	0.57	67,67,67,67	0
58	MG	CA	3203	1/1	0.86	0.12	60,60,60,60	0
58	MG	DA	1692	1/1	0.86	0.15	76,76,76,76	0
58	MG	CA	3225	1/1	0.86	0.44	65,65,65,65	0
58	MG	DA	1635	1/1	0.86	0.33	65,65,65,65	0
58	MG	AA	3121	1/1	0.86	0.31	70,70,70,70	0
58	MG	AA	3323	1/1	0.86	0.12	22,22,22,22	0
58	MG	AA	3250	1/1	0.86	0.28	46,46,46,46	0
58	MG	BA	1788	1/1	0.86	0.11	75,75,75,75	0
58	MG	AA	3117	1/1	0.86	0.31	30,30,30,30	1
58	MG	CA	3654	1/1	0.86	0.37	51,51,51,51	0
58	MG	CA	3635	1/1	0.86	0.14	79,79,79,79	0
58	MG	BA	1657	1/1	0.86	0.38	73,73,73,73	0
58	MG	AA	3355	1/1	0.86	0.17	58,58,58,58	0
58	MG	CA	3398	1/1	0.86	0.10	65,65,65,65	0
58	MG	CA	3106	1/1	0.86	0.72	55,55,55,55	0
58	MG	CA	3138	1/1	0.86	0.11	63,63,63,63	0
58	MG	BA	1677	1/1	0.86	0.15	87,87,87,87	0
58	MG	AA	3362	1/1	0.86	0.46	69,69,69,69	0
58	MG	AA	3774	1/1	0.86	0.21	80,80,80,80	0
58	MG	BK	201	1/1	0.86	0.17	57,57,57,57	0
58	MG	BA	1802	1/1	0.86	0.14	68,68,68,68	1
61	FUA	BZ	703	37/37	0.86	0.27	69,69,69,69	0
58	MG	DA	1722	1/1	0.86	0.24	65,65,65,65	0
58	MG	AA	3193	1/1	0.86	0.22	62,62,62,62	0
58	MG	BA	1718	1/1	0.86	0.50	83,83,83,83	0
58	MG	AA	3701	1/1	0.86	0.47	43,43,43,43	1
58	MG	CA	3495	1/1	0.86	0.14	65,65,65,65	0
58	MG	BA	1732	1/1	0.86	0.07	71,71,71,71	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	CA	3036	1/1	0.86	0.18	44,44,44,44	0
58	MG	AA	3518	1/1	0.86	0.21	33,33,33,33	0
58	MG	AA	3128	1/1	0.86	0.27	59,59,59,59	0
58	MG	DA	1766	1/1	0.86	0.12	58,58,58,58	0
58	MG	CA	3388	1/1	0.86	0.12	83,83,83,83	0
58	MG	BM	202	1/1	0.86	0.37	65,65,65,65	0
58	MG	AA	3035	1/1	0.86	0.42	57,57,57,57	0
58	MG	DA	1603	1/1	0.86	0.28	74,74,74,74	0
58	MG	CA	3109	1/1	0.86	0.23	54,54,54,54	0
58	MG	CA	3302	1/1	0.86	0.20	68,68,68,68	0
58	MG	AA	3802	1/1	0.86	0.36	55,55,55,55	0
58	MG	CA	3585	1/1	0.86	0.19	78,78,78,78	0
58	MG	AA	3096	1/1	0.86	0.14	63,63,63,63	0
58	MG	BA	1790	1/1	0.87	0.10	72,72,72,72	0
58	MG	DA	1661	1/1	0.87	0.39	70,70,70,70	0
58	MG	CA	3469	1/1	0.87	0.11	69,69,69,69	0
58	MG	CA	3090	1/1	0.87	0.52	65,65,65,65	0
58	MG	BA	1656	1/1	0.87	0.12	90,90,90,90	0
58	MG	CA	3651	1/1	0.87	0.23	31,31,31,31	0
58	MG	CA	3536	1/1	0.87	0.12	71,71,71,71	0
58	MG	DA	1689	1/1	0.87	0.22	58,58,58,58	0
58	MG	AA	3793	1/1	0.87	0.21	28,28,28,28	0
58	MG	AA	3639	1/1	0.87	0.17	77,77,77,77	0
58	MG	CA	3235	1/1	0.87	0.58	75,75,75,75	0
58	MG	CA	3467	1/1	0.87	0.61	80,80,80,80	0
58	MG	CA	3087	1/1	0.87	0.20	67,67,67,67	0
58	MG	AA	3237	1/1	0.87	0.13	71,71,71,71	0
58	MG	AA	3161	1/1	0.87	0.48	60,60,60,60	0
58	MG	CA	3580	1/1	0.87	0.07	100,100,100,100	0
58	MG	DA	1739	1/1	0.87	0.19	79,79,79,79	0
58	MG	CA	3548	1/1	0.87	0.14	48,48,48,48	1
58	MG	CA	3406	1/1	0.87	0.12	70,70,70,70	0
58	MG	AA	3718	1/1	0.87	0.10	43,43,43,43	0
58	MG	CA	3072	1/1	0.87	0.26	56,56,56,56	0
58	MG	AA	3605	1/1	0.87	0.27	68,68,68,68	0
58	MG	DE	201	1/1	0.87	0.17	84,84,84,84	0
58	MG	DT	3001	1/1	0.87	0.51	67,67,67,67	0
58	MG	CA	3363	1/1	0.87	0.23	66,66,66,66	0
61	FUA	DZ	703	37/37	0.87	0.23	85,85,85,85	0
58	MG	A0	102	1/1	0.87	0.22	40,40,40,40	0
58	MG	AA	3279	1/1	0.87	0.34	53,53,53,53	0
58	MG	AA	3372	1/1	0.87	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
58	MG	CA	3078	1/1	0.87	0.24	47,47,47,47	0
58	MG	AD	307	1/1	0.87	0.16	37,37,37,37	0
58	MG	AA	3560	1/1	0.87	0.26	58,58,58,58	0
58	MG	CA	3286	1/1	0.87	0.21	64,64,64,64	0
58	MG	AA	3247	1/1	0.87	0.29	63,63,63,63	0
58	MG	CA	3662	1/1	0.87	0.23	55,55,55,55	0
58	MG	AA	3002	1/1	0.87	0.20	55,55,55,55	0
58	MG	BA	1748	1/1	0.87	0.29	84,84,84,84	0
58	MG	AA	3496	1/1	0.87	0.17	52,52,52,52	0
58	MG	CA	3640	1/1	0.87	0.27	59,59,59,59	0
58	MG	DA	1633	1/1	0.87	0.47	73,73,73,73	0
58	MG	AA	3596	1/1	0.87	0.23	40,40,40,40	0
58	MG	AA	3653	1/1	0.87	0.15	68,68,68,68	0
58	MG	AA	3028	1/1	0.87	0.36	51,51,51,51	1
58	MG	CA	3634	1/1	0.87	0.10	81,81,81,81	0
58	MG	BA	1739	1/1	0.87	0.14	93,93,93,93	0
58	MG	AA	3339	1/1	0.87	0.28	43,43,43,43	0
58	MG	BA	1691	1/1	0.87	0.55	74,74,74,74	0
58	MG	CQ	203	1/1	0.87	0.14	67,67,67,67	0
58	MG	CA	3168	1/1	0.87	0.51	56,56,56,56	0
58	MG	AA	3461	1/1	0.87	0.48	66,66,66,66	0
58	MG	DA	1639	1/1	0.87	0.16	75,75,75,75	0
58	MG	DA	1610	1/1	0.87	0.21	75,75,75,75	0
58	MG	BA	1678	1/1	0.87	0.25	69,69,69,69	0
58	MG	DA	1734	1/1	0.87	0.25	83,83,83,83	0
58	MG	AA	3143	1/1	0.87	0.32	47,47,47,47	0
58	MG	AA	3029	1/1	0.87	0.27	53,53,53,53	0
58	MG	AA	3265	1/1	0.87	0.49	77,77,77,77	0
58	MG	AA	3057	1/1	0.87	0.44	57,57,57,57	0
58	MG	AA	3630	1/1	0.87	0.22	71,71,71,71	0
58	MG	CA	3384	1/1	0.87	0.22	71,71,71,71	0
58	MG	AA	3065	1/1	0.87	0.52	48,48,48,48	0
58	MG	AA	3519	1/1	0.87	0.19	21,21,21,21	0
58	MG	CA	3323	1/1	0.87	0.22	67,67,67,67	0
58	MG	CA	3215	1/1	0.87	0.09	73,73,73,73	0
58	MG	CP	202	1/1	0.87	0.40	71,71,71,71	0
58	MG	AO	5001	1/1	0.87	0.18	55,55,55,55	0
58	MG	BA	1787	1/1	0.88	0.26	90,90,90,90	0
58	MG	CA	3518	1/1	0.88	0.30	86,86,86,86	0
58	MG	AA	3663	1/1	0.88	0.42	62,62,62,62	0
58	MG	AB	3003	1/1	0.88	0.23	51,51,51,51	0
58	MG	AA	3132	1/1	0.88	0.27	27,27,27,27	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	AA	3492	1/1	0.88	0.35	45,45,45,45	0
58	MG	CA	3045	1/1	0.88	0.38	67,67,67,67	0
58	MG	AA	3358	1/1	0.88	0.17	63,63,63,63	0
58	MG	AA	3422	1/1	0.88	0.11	71,71,71,71	0
58	MG	AA	3491	1/1	0.88	0.28	35,35,35,35	0
58	MG	AA	3625	1/1	0.88	0.20	60,60,60,60	0
58	MG	CA	3423	1/1	0.88	0.19	50,50,50,50	0
58	MG	AA	3263	1/1	0.88	0.73	80,80,80,80	0
58	MG	CA	3273	1/1	0.88	0.17	69,69,69,69	0
58	MG	AA	3633	1/1	0.88	0.24	48,48,48,48	1
58	MG	BA	1710	1/1	0.88	0.67	73,73,73,73	0
58	MG	BA	1757	1/1	0.88	0.28	65,65,65,65	0
58	MG	CA	3340	1/1	0.88	0.21	48,48,48,48	0
58	MG	AA	3257	1/1	0.88	0.17	14,14,14,14	0
58	MG	AA	3147	1/1	0.88	0.25	69,69,69,69	0
58	MG	CA	3034	1/1	0.88	0.53	101,101,101,101	0
58	MG	BA	1707	1/1	0.88	0.25	50,50,50,50	0
58	MG	CA	3348	1/1	0.88	0.27	54,54,54,54	0
58	MG	AA	3360	1/1	0.88	0.12	114,114,114,114	0
58	MG	AA	3679	1/1	0.88	0.27	65,65,65,65	0
58	MG	AA	3704	1/1	0.88	0.24	59,59,59,59	0
58	MG	AA	3364	1/1	0.88	0.32	81,81,81,81	0
58	MG	BA	1780	1/1	0.88	0.20	81,81,81,81	0
58	MG	AA	3771	1/1	0.88	0.24	31,31,31,31	1
58	MG	CA	3621	1/1	0.88	0.29	73,73,73,73	0
58	MG	DA	1677	1/1	0.88	0.13	74,74,74,74	0
58	MG	CA	3112	1/1	0.88	0.24	61,61,61,61	0
58	MG	AD	302	1/1	0.88	0.37	19,19,19,19	0
58	MG	CA	3004	1/1	0.88	0.41	64,64,64,64	0
58	MG	A9	502	1/1	0.88	0.26	60,60,60,60	0
58	MG	CA	3125	1/1	0.88	0.48	73,73,73,73	0
58	MG	CA	3480	1/1	0.88	0.28	55,55,55,55	0
58	MG	CA	3267	1/1	0.88	0.17	56,56,56,56	0
58	MG	AA	3148	1/1	0.88	0.33	68,68,68,68	0
58	MG	AA	3249	1/1	0.88	0.33	24,24,24,24	1
58	MG	BA	1625	1/1	0.88	0.32	57,57,57,57	0
58	MG	AA	3060	1/1	0.88	0.66	65,65,65,65	0
58	MG	CA	3418	1/1	0.88	0.27	41,41,41,41	0
58	MG	BA	1745	1/1	0.88	0.41	66,66,66,66	0
58	MG	AA	3390	1/1	0.88	0.22	35,35,35,35	0
58	MG	BA	1784	1/1	0.88	0.21	60,60,60,60	0
58	MG	AA	3743	1/1	0.88	0.24	80,80,80,80	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	CA	3579	1/1	0.88	0.18	51,51,51,51	0
58	MG	BA	1744	1/1	0.88	0.10	37,37,37,37	0
58	MG	AA	3294	1/1	0.88	0.23	66,66,66,66	0
58	MG	AA	3696	1/1	0.88	0.15	69,69,69,69	0
58	MG	DA	1608	1/1	0.88	0.08	47,47,47,47	0
58	MG	AA	3099	1/1	0.88	0.13	62,62,62,62	0
58	MG	BA	1687	1/1	0.88	0.33	72,72,72,72	0
58	MG	AA	3481	1/1	0.88	0.15	51,51,51,51	0
58	MG	BA	1704	1/1	0.88	0.22	61,61,61,61	0
58	MG	CA	3292	1/1	0.88	0.08	73,73,73,73	0
58	MG	AA	3163	1/1	0.88	0.37	40,40,40,40	0
58	MG	CA	3325	1/1	0.88	0.10	38,38,38,38	0
58	MG	AA	3479	1/1	0.88	0.25	54,54,54,54	0
58	MG	AA	3221	1/1	0.88	0.32	56,56,56,56	0
58	MG	AA	3565	1/1	0.88	0.28	29,29,29,29	0
58	MG	AA	3571	1/1	0.88	0.15	48,48,48,48	0
58	MG	AA	3547	1/1	0.88	0.10	31,31,31,31	0
58	MG	AD	303	1/1	0.88	0.17	63,63,63,63	0
58	MG	AA	3304	1/1	0.88	0.24	30,30,30,30	0
58	MG	AA	3280	1/1	0.88	0.33	47,47,47,47	0
58	MG	AA	3100	1/1	0.88	0.27	53,53,53,53	0
58	MG	DA	1747	1/1	0.88	0.16	70,70,70,70	0
58	MG	AA	3291	1/1	0.88	0.15	44,44,44,44	0
58	MG	AA	3109	1/1	0.88	0.21	50,50,50,50	0
58	MG	AA	3554	1/1	0.88	0.14	49,49,49,49	0
58	MG	AA	3183	1/1	0.88	0.24	35,35,35,35	1
58	MG	AA	3761	1/1	0.88	0.44	50,50,50,50	0
58	MG	AA	3727	1/1	0.88	0.14	49,49,49,49	0
58	MG	DA	1729	1/1	0.88	0.12	57,57,57,57	0
58	MG	AA	3606	1/1	0.88	0.31	61,61,61,61	0
58	MG	BM	201	1/1	0.88	0.11	57,57,57,57	0
58	MG	CA	3047	1/1	0.88	0.15	61,61,61,61	0
58	MG	DA	1624	1/1	0.88	0.13	44,44,44,44	0
58	MG	CA	3283	1/1	0.88	0.18	60,60,60,60	0
58	MG	DA	1709	1/1	0.88	0.15	72,72,72,72	0
58	MG	BA	1796	1/1	0.88	0.11	70,70,70,70	0
58	MG	AP	202	1/1	0.88	0.18	40,40,40,40	0
58	MG	BA	1746	1/1	0.89	0.18	83,83,83,83	0
58	MG	CA	3619	1/1	0.89	0.46	47,47,47,47	1
58	MG	CA	3200	1/1	0.89	0.44	54,54,54,54	0
58	MG	AA	3477	1/1	0.89	0.16	58,58,58,58	0
58	MG	CA	3557	1/1	0.89	0.10	76,76,76,76	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	AA	3561	1/1	0.89	0.25	58,58,58,58	0
58	MG	BA	1637	1/1	0.89	0.22	66,66,66,66	0
58	MG	BA	1664	1/1	0.89	0.35	59,59,59,59	0
58	MG	AV	202	1/1	0.89	0.31	55,55,55,55	1
58	MG	CA	3541	1/1	0.89	0.17	71,71,71,71	0
58	MG	AA	3437	1/1	0.89	0.24	54,54,54,54	0
58	MG	BA	1735	1/1	0.89	0.28	72,72,72,72	0
58	MG	AW	3003	1/1	0.89	0.45	52,52,52,52	0
58	MG	BA	1751	1/1	0.89	0.13	58,58,58,58	0
58	MG	BA	1672	1/1	0.89	0.25	61,61,61,61	0
58	MG	AA	3311	1/1	0.89	0.21	33,33,33,33	0
58	MG	AA	3786	1/1	0.89	0.36	59,59,59,59	0
58	MG	CA	3489	1/1	0.89	0.25	80,80,80,80	0
58	MG	AA	3662	1/1	0.89	0.21	59,59,59,59	0
58	MG	CA	3153	1/1	0.89	0.19	78,78,78,78	0
58	MG	AA	3646	1/1	0.89	0.12	58,58,58,58	0
58	MG	AA	3444	1/1	0.89	0.26	63,63,63,63	0
58	MG	AA	3255	1/1	0.89	0.36	53,53,53,53	0
58	MG	CA	3477	1/1	0.89	0.11	74,74,74,74	0
58	MG	AA	3153	1/1	0.89	0.29	59,59,59,59	0
58	MG	DA	1637	1/1	0.89	0.24	76,76,76,76	0
58	MG	AA	3356	1/1	0.89	0.18	35,35,35,35	0
58	MG	CA	3519	1/1	0.89	0.27	79,79,79,79	0
58	MG	AA	3282	1/1	0.89	0.49	40,40,40,40	0
58	MG	AA	3185	1/1	0.89	0.28	41,41,41,41	0
58	MG	AA	3174	1/1	0.89	0.31	63,63,63,63	0
58	MG	CB	3001	1/1	0.89	0.17	99,99,99,99	0
58	MG	AA	3824	1/1	0.89	0.26	45,45,45,45	0
58	MG	AA	3164	1/1	0.89	0.23	58,58,58,58	0
58	MG	AA	3345	1/1	0.89	0.10	68,68,68,68	0
58	MG	BA	1791	1/1	0.89	0.13	63,63,63,63	0
58	MG	AA	3673	1/1	0.89	0.16	67,67,67,67	0
58	MG	AA	3352	1/1	0.89	0.24	51,51,51,51	0
58	MG	BA	1627	1/1	0.89	0.24	87,87,87,87	0
58	MG	CA	3412	1/1	0.89	0.25	81,81,81,81	0
58	MG	AA	3659	1/1	0.89	0.23	14,14,14,14	0
58	MG	AA	3438	1/1	0.89	0.21	57,57,57,57	0
58	MG	AA	3753	1/1	0.89	0.17	41,41,41,41	0
58	MG	C7	101	1/1	0.89	0.65	42,42,42,42	1
58	MG	AA	3215	1/1	0.89	0.61	42,42,42,42	1
58	MG	BA	1730	1/1	0.89	0.24	78,78,78,78	0
58	MG	AW	3004	1/1	0.89	0.31	65,65,65,65	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	AA	3637	1/1	0.89	0.28	45,45,45,45	0
58	MG	A5	102	1/1	0.89	0.33	60,60,60,60	0
58	MG	CA	3538	1/1	0.89	0.07	71,71,71,71	0
58	MG	CA	3016	1/1	0.89	0.53	80,80,80,80	0
58	MG	CA	3030	1/1	0.89	0.46	57,57,57,57	1
58	MG	CA	3099	1/1	0.89	0.15	92,92,92,92	0
58	MG	CA	3220	1/1	0.89	0.24	78,78,78,78	0
58	MG	BL	201	1/1	0.89	0.24	80,80,80,80	0
58	MG	AA	3831	1/1	0.89	0.21	65,65,65,65	0
58	MG	CA	3430	1/1	0.89	0.32	53,53,53,53	0
58	MG	AA	3094	1/1	0.89	0.71	111,111,111,111	0
58	MG	A8	5001	1/1	0.89	0.34	59,59,59,59	0
58	MG	AA	3051	1/1	0.89	0.33	36,36,36,36	0
58	MG	AA	3545	1/1	0.89	0.09	51,51,51,51	1
58	MG	AA	3809	1/1	0.89	0.23	62,62,62,62	0
58	MG	CB	3008	1/1	0.89	0.13	59,59,59,59	0
58	MG	AA	3199	1/1	0.89	0.18	54,54,54,54	0
58	MG	DA	1757	1/1	0.89	0.31	75,75,75,75	0
58	MG	CA	3504	1/1	0.89	0.08	62,62,62,62	0
58	MG	AA	3126	1/1	0.89	0.41	50,50,50,50	0
58	MG	CA	3077	1/1	0.89	0.37	66,66,66,66	0
58	MG	AA	3180	1/1	0.89	0.29	94,94,94,94	0
58	MG	DA	1727	1/1	0.89	0.17	66,66,66,66	0
58	MG	AA	3573	1/1	0.89	0.14	50,50,50,50	0
58	MG	BW	503	1/1	0.89	0.14	45,45,45,45	0
58	MG	CA	3506	1/1	0.89	0.17	58,58,58,58	0
58	MG	AA	3295	1/1	0.89	0.37	47,47,47,47	0
58	MG	BA	1631	1/1	0.89	0.10	48,48,48,48	0
58	MG	CA	3054	1/1	0.89	0.13	71,71,71,71	0
58	MG	DA	1735	1/1	0.89	0.54	83,83,83,83	0
58	MG	AA	3111	1/1	0.89	0.41	48,48,48,48	0
58	MG	DA	1690	1/1	0.89	0.51	82,82,82,82	0
58	MG	BA	1649	1/1	0.89	0.23	68,68,68,68	0
58	MG	AA	3775	1/1	0.89	0.11	45,45,45,45	0
58	MG	BA	1626	1/1	0.89	0.30	75,75,75,75	0
58	MG	DA	1744	1/1	0.89	0.10	79,79,79,79	0
58	MG	CA	3568	1/1	0.89	0.20	41,41,41,41	0
58	MG	AA	3062	1/1	0.89	0.33	67,67,67,67	0
58	MG	CA	3280	1/1	0.89	0.18	30,30,30,30	0
58	MG	AA	3047	1/1	0.89	0.34	34,34,34,34	0
58	MG	BA	1665	1/1	0.89	0.35	55,55,55,55	0
58	MG	CA	3245	1/1	0.89	0.47	57,57,57,57	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	AA	3091	1/1	0.89	0.39	38,38,38,38	1
58	MG	CA	3609	1/1	0.89	0.22	76,76,76,76	0
58	MG	BA	1601	1/1	0.89	0.27	93,93,93,93	0
58	MG	BA	1801	1/1	0.89	0.45	69,69,69,69	0
58	MG	AZ	302	1/1	0.89	0.20	68,68,68,68	0
58	MG	AA	3694	1/1	0.89	0.15	45,45,45,45	0
58	MG	AA	3284	1/1	0.89	0.41	44,44,44,44	0
58	MG	CA	3255	1/1	0.89	0.46	67,67,67,67	0
58	MG	DA	1601	1/1	0.89	0.14	61,61,61,61	0
58	MG	DA	1669	1/1	0.89	0.39	84,84,84,84	0
58	MG	BA	1723	1/1	0.89	0.30	71,71,71,71	0
58	MG	CA	3121	1/1	0.89	0.14	45,45,45,45	0
58	MG	BA	1608	1/1	0.89	0.47	60,60,60,60	0
58	MG	AA	3070	1/1	0.89	0.37	60,60,60,60	0
58	MG	DA	1622	1/1	0.89	0.51	77,77,77,77	0
58	MG	CA	3199	1/1	0.90	0.35	74,74,74,74	0
58	MG	CA	3163	1/1	0.90	0.33	40,40,40,40	0
58	MG	AA	3292	1/1	0.90	0.12	74,74,74,74	0
58	MG	CA	3144	1/1	0.90	0.32	67,67,67,67	0
58	MG	AA	3101	1/1	0.90	0.35	52,52,52,52	0
58	MG	AA	3158	1/1	0.90	0.31	97,97,97,97	0
58	MG	DW	501	1/1	0.90	0.25	74,74,74,74	0
58	MG	AA	3107	1/1	0.90	0.48	76,76,76,76	0
58	MG	BA	1613	1/1	0.90	0.07	101,101,101,101	0
58	MG	CA	3386	1/1	0.90	0.26	65,65,65,65	0
58	MG	AA	3628	1/1	0.90	0.25	80,80,80,80	0
58	MG	BA	1606	1/1	0.90	0.17	74,74,74,74	0
58	MG	BA	1684	1/1	0.90	0.13	81,81,81,81	0
58	MG	BA	1682	1/1	0.90	0.11	69,69,69,69	0
58	MG	BA	1685	1/1	0.90	0.18	50,50,50,50	0
58	MG	CA	3197	1/1	0.90	0.46	64,64,64,64	0
58	MG	DA	1716	1/1	0.90	0.36	78,78,78,78	0
58	MG	BA	1725	1/1	0.90	0.11	59,59,59,59	0
58	MG	AA	3448	1/1	0.90	0.05	78,78,78,78	0
58	MG	CA	3271	1/1	0.90	0.30	57,57,57,57	0
58	MG	AA	3592	1/1	0.90	0.24	52,52,52,52	0
58	MG	DA	1617	1/1	0.90	0.10	48,48,48,48	0
58	MG	BA	1721	1/1	0.90	0.23	60,60,60,60	0
58	MG	AA	3229	1/1	0.90	0.30	43,43,43,43	0
58	MG	BA	1762	1/1	0.90	0.07	52,52,52,52	1
58	MG	CA	3014	1/1	0.90	0.44	62,62,62,62	0
58	MG	AA	3817	1/1	0.90	0.31	61,61,61,61	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	DA	1693	1/1	0.90	0.21	54,54,54,54	0
58	MG	CA	3137	1/1	0.90	0.33	73,73,73,73	0
58	MG	AA	3657	1/1	0.90	0.24	43,43,43,43	1
58	MG	BA	1640	1/1	0.90	0.19	55,55,55,55	0
58	MG	AA	3799	1/1	0.90	0.18	47,47,47,47	0
58	MG	CA	3379	1/1	0.90	0.28	65,65,65,65	0
58	MG	DA	1728	1/1	0.90	0.16	63,63,63,63	0
58	MG	AA	3058	1/1	0.90	0.19	35,35,35,35	0
58	MG	DA	1650	1/1	0.90	0.34	61,61,61,61	0
58	MG	CA	3602	1/1	0.90	0.16	66,66,66,66	0
58	MG	DA	1643	1/1	0.90	0.16	55,55,55,55	0
58	MG	BA	1632	1/1	0.90	0.29	54,54,54,54	0
58	MG	DA	1715	1/1	0.90	0.23	76,76,76,76	0
58	MG	AA	3110	1/1	0.90	0.29	79,79,79,79	0
58	MG	AA	3432	1/1	0.90	0.31	57,57,57,57	0
58	MG	DA	1732	1/1	0.90	0.34	76,76,76,76	0
58	MG	AA	3182	1/1	0.90	0.21	76,76,76,76	0
58	MG	CA	3458	1/1	0.90	0.23	49,49,49,49	0
58	MG	AA	3375	1/1	0.90	0.25	57,57,57,57	0
58	MG	CA	3482	1/1	0.90	0.21	70,70,70,70	0
58	MG	AA	3681	1/1	0.90	0.36	65,65,65,65	0
58	MG	AA	3175	1/1	0.90	0.32	51,51,51,51	0
58	MG	DA	1708	1/1	0.90	0.10	87,87,87,87	0
58	MG	AA	3310	1/1	0.90	0.25	58,58,58,58	0
58	MG	AA	3588	1/1	0.90	0.18	38,38,38,38	0
58	MG	CA	3065	1/1	0.90	0.11	52,52,52,52	0
58	MG	AA	3708	1/1	0.90	0.52	53,53,53,53	1
58	MG	AA	3176	1/1	0.90	0.30	50,50,50,50	0
58	MG	BA	1628	1/1	0.90	0.55	55,55,55,55	0
58	MG	CA	3128	1/1	0.90	0.40	71,71,71,71	0
58	MG	AW	3001	1/1	0.90	0.30	52,52,52,52	0
58	MG	AA	3757	1/1	0.90	0.12	55,55,55,55	0
58	MG	CA	3543	1/1	0.90	0.18	63,63,63,63	0
58	MG	AA	3319	1/1	0.90	0.17	69,69,69,69	0
58	MG	BA	1783	1/1	0.90	0.31	69,69,69,69	0
58	MG	DA	1653	1/1	0.90	0.18	60,60,60,60	0
58	MG	AA	3064	1/1	0.90	0.16	29,29,29,29	0
58	MG	AA	3118	1/1	0.90	0.58	64,64,64,64	0
58	MG	DA	1636	1/1	0.90	0.40	70,70,70,70	0
58	MG	BA	1798	1/1	0.90	0.15	69,69,69,69	0
58	MG	AA	3353	1/1	0.90	0.08	76,76,76,76	0
58	MG	DA	1767	1/1	0.90	0.14	74,74,74,74	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	AA	3597	1/1	0.90	0.09	63,63,63,63	0
58	MG	BA	1607	1/1	0.90	0.12	62,62,62,62	0
58	MG	CA	3142	1/1	0.90	0.25	69,69,69,69	0
58	MG	CA	3513	1/1	0.90	0.23	75,75,75,75	0
58	MG	BA	1609	1/1	0.90	0.13	69,69,69,69	0
58	MG	BA	1777	1/1	0.90	0.20	79,79,79,79	0
58	MG	C8	5001	1/1	0.90	0.35	51,51,51,51	0
58	MG	CU	201	1/1	0.90	0.58	64,64,64,64	0
58	MG	CA	3623	1/1	0.90	0.24	64,64,64,64	0
58	MG	AA	3733	1/1	0.90	0.20	68,68,68,68	0
58	MG	CA	3184	1/1	0.90	0.28	66,66,66,66	0
58	MG	AA	3222	1/1	0.90	0.31	28,28,28,28	0
58	MG	AA	3154	1/1	0.90	0.35	46,46,46,46	0
58	MG	CE	303	1/1	0.90	0.32	54,54,54,54	0
58	MG	AA	3149	1/1	0.90	0.26	62,62,62,62	0
58	MG	AA	3617	1/1	0.90	0.22	49,49,49,49	0
58	MG	DA	1638	1/1	0.90	0.30	83,83,83,83	0
58	MG	CA	3194	1/1	0.90	0.55	72,72,72,72	0
58	MG	CA	3439	1/1	0.90	0.20	38,38,38,38	0
58	MG	AE	304	1/1	0.90	0.26	30,30,30,30	0
58	MG	AA	3242	1/1	0.90	0.27	72,72,72,72	0
58	MG	BA	1688	1/1	0.90	0.69	70,70,70,70	0
58	MG	CA	3198	1/1	0.91	0.12	37,37,37,37	0
58	MG	AA	3410	1/1	0.91	0.22	30,30,30,30	0
58	MG	AA	3721	1/1	0.91	0.21	10,10,10,10	0
58	MG	AA	3587	1/1	0.91	0.30	53,53,53,53	0
58	MG	AA	3129	1/1	0.91	0.49	66,66,66,66	1
58	MG	AA	3762	1/1	0.91	0.20	53,53,53,53	1
58	MG	AA	3759	1/1	0.91	0.28	65,65,65,65	0
58	MG	AA	3810	1/1	0.91	0.23	54,54,54,54	0
58	MG	AA	3120	1/1	0.91	0.24	46,46,46,46	0
58	MG	AF	302	1/1	0.91	0.28	41,41,41,41	0
58	MG	CA	3238	1/1	0.91	0.24	59,59,59,59	0
58	MG	BA	1763	1/1	0.91	0.26	62,62,62,62	0
58	MG	CA	3531	1/1	0.91	0.20	51,51,51,51	0
58	MG	CA	3044	1/1	0.91	0.35	52,52,52,52	0
58	MG	CA	3558	1/1	0.91	0.19	51,51,51,51	1
58	MG	CA	3441	1/1	0.91	0.34	77,77,77,77	0
58	MG	AA	3014	1/1	0.91	0.20	45,45,45,45	0
58	MG	CA	3095	1/1	0.91	0.30	64,64,64,64	0
58	MG	CA	3091	1/1	0.91	0.35	111,111,111,111	0
58	MG	AA	3652	1/1	0.91	0.27	77,77,77,77	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	AA	3649	1/1	0.91	0.13	92,92,92,92	0
58	MG	AA	3455	1/1	0.91	0.32	58,58,58,58	0
58	MG	CA	3638	1/1	0.91	0.30	55,55,55,55	0
58	MG	AA	3383	1/1	0.91	0.17	54,54,54,54	0
58	MG	AA	3731	1/1	0.91	0.19	42,42,42,42	0
58	MG	CA	3407	1/1	0.91	0.22	55,55,55,55	0
58	MG	CA	3606	1/1	0.91	0.40	65,65,65,65	0
58	MG	CA	3151	1/1	0.91	0.17	50,50,50,50	0
58	MG	BA	1655	1/1	0.91	0.30	69,69,69,69	0
58	MG	CA	3545	1/1	0.91	0.13	68,68,68,68	0
58	MG	CA	3522	1/1	0.91	0.34	56,56,56,56	0
58	MG	CB	3009	1/1	0.91	0.16	67,67,67,67	0
58	MG	CA	3242	1/1	0.91	0.12	41,41,41,41	0
58	MG	CA	3188	1/1	0.91	0.53	58,58,58,58	0
58	MG	CA	3475	1/1	0.91	0.34	55,55,55,55	0
58	MG	AW	3002	1/1	0.91	0.27	55,55,55,55	0
58	MG	AA	3511	1/1	0.91	0.20	12,12,12,12	0
58	MG	BA	1697	1/1	0.91	0.36	78,78,78,78	0
58	MG	AA	3688	1/1	0.91	0.18	25,25,25,25	1
58	MG	DA	1737	1/1	0.91	0.15	72,72,72,72	0
58	MG	DA	1613	1/1	0.91	0.24	72,72,72,72	0
58	MG	CA	3185	1/1	0.91	0.46	59,59,59,59	0
58	MG	AA	3267	1/1	0.91	0.40	63,63,63,63	0
58	MG	DA	1665	1/1	0.91	0.48	61,61,61,61	0
58	MG	AA	3088	1/1	0.91	0.31	34,34,34,34	0
58	MG	AA	3690	1/1	0.91	0.24	71,71,71,71	0
58	MG	DA	1671	1/1	0.91	0.57	83,83,83,83	0
58	MG	AA	3750	1/1	0.91	0.12	24,24,24,24	0
58	MG	CA	3052	1/1	0.91	0.41	69,69,69,69	0
58	MG	CA	3332	1/1	0.91	0.21	42,42,42,42	0
58	MG	DA	1694	1/1	0.91	0.27	60,60,60,60	0
58	MG	AA	3216	1/1	0.91	0.20	51,51,51,51	0
58	MG	CA	3130	1/1	0.91	0.66	73,73,73,73	0
58	MG	AA	3795	1/1	0.91	0.31	68,68,68,68	1
58	MG	AA	3203	1/1	0.91	0.32	46,46,46,46	1
58	MG	AA	3113	1/1	0.91	0.31	64,64,64,64	0
58	MG	CA	3038	1/1	0.91	0.36	48,48,48,48	0
58	MG	CA	3647	1/1	0.91	0.08	66,66,66,66	0
58	MG	AA	3034	1/1	0.91	0.28	57,57,57,57	0
58	MG	CA	3343	1/1	0.91	0.13	36,36,36,36	0
58	MG	CA	3195	1/1	0.91	0.14	60,60,60,60	0
58	MG	CA	3661	1/1	0.91	0.26	74,74,74,74	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	AA	3446	1/1	0.91	0.49	61,61,61,61	0
58	MG	AA	3788	1/1	0.91	0.27	58,58,58,58	1
58	MG	CA	3189	1/1	0.91	0.09	68,68,68,68	0
58	MG	CA	3317	1/1	0.91	0.12	44,44,44,44	0
58	MG	CA	3630	1/1	0.91	0.11	63,63,63,63	0
58	MG	AA	3660	1/1	0.91	0.21	70,70,70,70	0
58	MG	AA	3007	1/1	0.91	0.16	21,21,21,21	0
58	MG	AA	3264	1/1	0.91	0.08	62,62,62,62	0
58	MG	AA	3093	1/1	0.91	0.27	27,27,27,27	1
58	MG	CA	3351	1/1	0.91	0.14	46,46,46,46	0
58	MG	BA	1675	1/1	0.91	0.16	57,57,57,57	0
58	MG	AA	3603	1/1	0.91	0.19	63,63,63,63	0
58	MG	AA	3634	1/1	0.91	0.30	62,62,62,62	0
58	MG	AA	3334	1/1	0.91	0.21	57,57,57,57	0
58	MG	CN	5001	1/1	0.91	0.08	77,77,77,77	0
58	MG	CA	3432	1/1	0.91	0.28	61,61,61,61	0
58	MG	AA	3794	1/1	0.91	0.16	58,58,58,58	1
58	MG	CA	3488	1/1	0.91	0.10	51,51,51,51	0
58	MG	AD	306	1/1	0.91	0.15	73,73,73,73	0
58	MG	CA	3626	1/1	0.91	0.27	75,75,75,75	0
58	MG	AA	3303	1/1	0.91	0.31	56,56,56,56	0
58	MG	AA	3302	1/1	0.91	0.21	56,56,56,56	0
58	MG	CV	202	1/1	0.91	0.30	85,85,85,85	0
58	MG	CA	3190	1/1	0.91	0.38	83,83,83,83	0
58	MG	CA	3136	1/1	0.91	0.34	53,53,53,53	0
58	MG	DA	1618	1/1	0.91	0.44	65,65,65,65	0
58	MG	CA	3213	1/1	0.91	0.27	44,44,44,44	0
58	MG	AA	3089	1/1	0.91	0.30	47,47,47,47	1
58	MG	CA	3179	1/1	0.91	0.52	75,75,75,75	0
58	MG	AA	3335	1/1	0.91	0.23	41,41,41,41	0
58	MG	AA	3285	1/1	0.91	0.35	45,45,45,45	0
58	MG	AA	3480	1/1	0.91	0.09	54,54,54,54	0
58	MG	CA	3426	1/1	0.91	0.19	55,55,55,55	0
58	MG	AA	3586	1/1	0.91	0.14	62,62,62,62	0
58	MG	AA	3426	1/1	0.91	0.14	50,50,50,50	0
58	MG	CA	3060	1/1	0.91	0.40	77,77,77,77	0
58	MG	AN	3003	1/1	0.91	0.12	47,47,47,47	0
58	MG	BF	3001	1/1	0.91	0.25	74,74,74,74	0
58	MG	CA	3631	1/1	0.91	0.13	77,77,77,77	0
58	MG	CA	3233	1/1	0.91	0.43	71,71,71,71	0
58	MG	DA	1724	1/1	0.91	0.30	61,61,61,61	0
58	MG	CA	3187	1/1	0.91	0.26	37,37,37,37	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	DA	1740	1/1	0.91	0.09	81,81,81,81	0
58	MG	BA	1612	1/1	0.91	0.10	75,75,75,75	0
58	MG	BA	1754	1/1	0.91	0.10	98,98,98,98	0
58	MG	CA	3409	1/1	0.91	0.24	40,40,40,40	0
58	MG	BA	1782	1/1	0.91	0.18	50,50,50,50	0
58	MG	AA	3456	1/1	0.91	0.18	30,30,30,30	0
58	MG	CA	3122	1/1	0.91	0.21	67,67,67,67	0
58	MG	AY	502	1/1	0.91	0.29	58,58,58,58	0
58	MG	AA	3712	1/1	0.92	0.23	46,46,46,46	0
58	MG	DA	1756	1/1	0.92	0.22	68,68,68,68	0
58	MG	BA	1619	1/1	0.92	0.17	52,52,52,52	0
58	MG	CA	3487	1/1	0.92	0.20	70,70,70,70	0
58	MG	CA	3160	1/1	0.92	0.13	42,42,42,42	0
58	MG	AB	3018	1/1	0.92	0.14	84,84,84,84	0
58	MG	CA	3192	1/1	0.92	0.14	58,58,58,58	0
58	MG	AB	3010	1/1	0.92	0.17	47,47,47,47	1
58	MG	AA	3833	1/1	0.92	0.41	49,49,49,49	0
58	MG	DA	1602	1/1	0.92	0.11	80,80,80,80	0
58	MG	BA	1712	1/1	0.92	0.14	61,61,61,61	0
58	MG	CA	3434	1/1	0.92	0.18	28,28,28,28	0
58	MG	CA	3326	1/1	0.92	0.23	34,34,34,34	0
58	MG	BA	1804	1/1	0.92	0.18	67,67,67,67	0
58	MG	CA	3143	1/1	0.92	0.68	57,57,57,57	0
58	MG	BA	1629	1/1	0.92	0.46	64,64,64,64	0
58	MG	AA	3227	1/1	0.92	0.25	55,55,55,55	0
58	MG	AA	3061	1/1	0.92	0.29	27,27,27,27	0
58	MG	AA	3715	1/1	0.92	0.08	66,66,66,66	0
58	MG	AA	3232	1/1	0.92	0.26	79,79,79,79	0
58	MG	CA	3150	1/1	0.92	0.17	54,54,54,54	0
58	MG	AA	3190	1/1	0.92	0.25	45,45,45,45	0
58	MG	DA	1705	1/1	0.92	0.31	62,62,62,62	0
58	MG	AA	3278	1/1	0.92	0.18	36,36,36,36	0
58	MG	AA	3780	1/1	0.92	0.31	42,42,42,42	0
58	MG	CA	3586	1/1	0.92	0.14	69,69,69,69	0
58	MG	AA	3785	1/1	0.92	0.18	72,72,72,72	0
58	MG	BA	1809	1/1	0.92	0.21	68,68,68,68	0
58	MG	CA	3311	1/1	0.92	0.14	48,48,48,48	0
58	MG	AA	3365	1/1	0.92	0.30	57,57,57,57	0
58	MG	CE	306	1/1	0.92	0.07	67,67,67,67	0
58	MG	AA	3745	1/1	0.92	0.17	29,29,29,29	0
58	MG	CA	3375	1/1	0.92	0.31	71,71,71,71	0
58	MG	CA	3133	1/1	0.92	0.24	69,69,69,69	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	AA	3680	1/1	0.92	0.24	59,59,59,59	0
58	MG	CA	3196	1/1	0.92	0.55	64,64,64,64	0
58	MG	AA	3484	1/1	0.92	0.22	35,35,35,35	0
58	MG	BA	1727	1/1	0.92	0.09	45,45,45,45	0
58	MG	AA	3792	1/1	0.92	0.17	45,45,45,45	0
58	MG	CA	3115	1/1	0.92	0.22	76,76,76,76	0
58	MG	CA	3061	1/1	0.92	0.45	67,67,67,67	0
58	MG	AA	3056	1/1	0.92	0.24	63,63,63,63	0
58	MG	AA	3450	1/1	0.92	0.26	53,53,53,53	0
58	MG	AA	3068	1/1	0.92	0.45	65,65,65,65	0
58	MG	CA	3358	1/1	0.92	0.29	45,45,45,45	0
58	MG	DA	1659	1/1	0.92	0.08	64,64,64,64	0
58	MG	AA	3123	1/1	0.92	0.36	37,37,37,37	1
58	MG	AA	3594	1/1	0.92	0.22	43,43,43,43	0
58	MG	AA	3420	1/1	0.92	0.23	26,26,26,26	0
58	MG	DA	1721	1/1	0.92	0.12	67,67,67,67	0
58	MG	AA	3647	1/1	0.92	0.20	72,72,72,72	0
58	MG	AA	3747	1/1	0.92	0.37	58,58,58,58	0
58	MG	CA	3094	1/1	0.92	0.32	87,87,87,87	0
58	MG	CA	3108	1/1	0.92	0.17	60,60,60,60	0
58	MG	CA	3400	1/1	0.92	0.22	62,62,62,62	0
58	MG	AA	3266	1/1	0.92	0.49	50,50,50,50	0
58	MG	CA	3149	1/1	0.92	0.08	66,66,66,66	0
58	MG	AA	3430	1/1	0.92	0.14	44,44,44,44	0
58	MG	CA	3510	1/1	0.92	0.14	65,65,65,65	0
58	MG	CA	3429	1/1	0.92	0.35	74,74,74,74	0
58	MG	DA	1764	1/1	0.92	0.07	55,55,55,55	0
58	MG	AA	3531	1/1	0.92	0.29	62,62,62,62	0
58	MG	AA	3740	1/1	0.92	0.16	45,45,45,45	0
58	MG	DA	1641	1/1	0.92	0.09	77,77,77,77	0
58	MG	CA	3074	1/1	0.92	0.48	53,53,53,53	0
58	MG	AA	3022	1/1	0.92	0.15	9,9,9,9	0
58	MG	AA	3288	1/1	0.92	0.17	24,24,24,24	0
58	MG	AA	3546	1/1	0.92	0.19	32,32,32,32	0
58	MG	AA	3650	1/1	0.92	0.07	60,60,60,60	0
58	MG	AD	304	1/1	0.92	0.31	38,38,38,38	1
58	MG	AA	3219	1/1	0.92	0.28	58,58,58,58	0
58	MG	DA	1743	1/1	0.92	0.34	72,72,72,72	0
58	MG	AA	3687	1/1	0.92	0.18	45,45,45,45	0
58	MG	CA	3357	1/1	0.92	0.06	80,80,80,80	0
58	MG	AA	3728	1/1	0.92	0.20	61,61,61,61	0
58	MG	AA	3181	1/1	0.92	0.18	56,56,56,56	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	AA	3819	1/1	0.92	0.25	25,25,25,25	1
58	MG	CA	3656	1/1	0.92	0.22	61,61,61,61	0
58	MG	AA	3225	1/1	0.92	0.24	27,27,27,27	1
58	MG	CA	3581	1/1	0.92	0.14	81,81,81,81	0
58	MG	CY	502	1/1	0.92	0.16	56,56,56,56	0
58	MG	CA	3102	1/1	0.92	0.33	56,56,56,56	0
58	MG	AA	3290	1/1	0.92	0.17	63,63,63,63	0
58	MG	DA	1719	1/1	0.92	0.11	74,74,74,74	0
58	MG	AA	3726	1/1	0.92	0.19	67,67,67,67	0
58	MG	AA	3406	1/1	0.92	0.16	57,57,57,57	0
58	MG	CA	3262	1/1	0.92	0.16	61,61,61,61	0
58	MG	AA	3274	1/1	0.92	0.28	55,55,55,55	0
58	MG	DA	1625	1/1	0.92	0.54	73,73,73,73	0
58	MG	AA	3458	1/1	0.92	0.18	72,72,72,72	0
58	MG	AA	3141	1/1	0.92	0.47	40,40,40,40	0
58	MG	CA	3165	1/1	0.92	0.17	62,62,62,62	0
58	MG	AA	3418	1/1	0.92	0.24	43,43,43,43	0
58	MG	AA	3689	1/1	0.92	0.15	55,55,55,55	1
58	MG	AA	3350	1/1	0.92	0.28	31,31,31,31	0
58	MG	CA	3145	1/1	0.92	0.08	79,79,79,79	0
58	MG	AA	3812	1/1	0.92	0.21	42,42,42,42	0
58	MG	AA	3341	1/1	0.92	0.20	15,15,15,15	0
58	MG	AA	3021	1/1	0.92	0.11	40,40,40,40	0
58	MG	AA	3699	1/1	0.92	0.37	46,46,46,46	1
58	MG	AA	3079	1/1	0.92	0.10	34,34,34,34	0
58	MG	CA	3368	1/1	0.92	0.20	59,59,59,59	0
58	MG	BA	1779	1/1	0.92	0.14	46,46,46,46	1
58	MG	AA	3677	1/1	0.92	0.21	41,41,41,41	0
58	MG	CA	3419	1/1	0.92	0.10	60,60,60,60	0
58	MG	AA	3077	1/1	0.92	0.33	50,50,50,50	0
58	MG	BB	3001	1/1	0.92	0.12	75,75,75,75	0
58	MG	CA	3356	1/1	0.92	0.15	57,57,57,57	0
58	MG	BA	1623	1/1	0.92	0.24	65,65,65,65	0
58	MG	DA	1731	1/1	0.92	0.50	82,82,82,82	0
58	MG	CA	3084	1/1	0.92	0.32	59,59,59,59	1
58	MG	CA	3520	1/1	0.92	0.17	59,59,59,59	0
58	MG	AA	3211	1/1	0.92	0.59	42,42,42,42	1
58	MG	CA	3247	1/1	0.92	0.63	66,66,66,66	0
58	MG	BA	1641	1/1	0.92	0.23	71,71,71,71	0
58	MG	AA	3457	1/1	0.92	0.17	67,67,67,67	0
58	MG	AA	3238	1/1	0.92	0.34	61,61,61,61	0
58	MG	AF	304	1/1	0.92	0.31	62,62,62,62	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	CA	3240	1/1	0.92	0.15	64,64,64,64	0
58	MG	DA	1605	1/1	0.92	0.23	73,73,73,73	0
58	MG	CA	3040	1/1	0.92	0.14	66,66,66,66	0
58	MG	CA	3428	1/1	0.92	0.29	54,54,54,54	1
58	MG	AA	3309	1/1	0.92	0.20	44,44,44,44	0
58	MG	AA	3116	1/1	0.92	0.38	51,51,51,51	0
58	MG	AA	3005	1/1	0.92	0.21	62,62,62,62	0
58	MG	CA	3491	1/1	0.92	0.20	51,51,51,51	0
58	MG	AA	3139	1/1	0.92	0.09	58,58,58,58	0
58	MG	CA	3664	1/1	0.92	0.14	54,54,54,54	0
58	MG	DA	1675	1/1	0.92	0.35	74,74,74,74	0
58	MG	AA	3828	1/1	0.92	0.30	37,37,37,37	1
58	MG	CA	3438	1/1	0.92	0.15	46,46,46,46	0
58	MG	AA	3779	1/1	0.92	0.20	62,62,62,62	0
58	MG	AA	3485	1/1	0.92	0.21	14,14,14,14	0
58	MG	CA	3577	1/1	0.92	0.18	83,83,83,83	0
58	MG	AA	3822	1/1	0.92	0.55	65,65,65,65	0
58	MG	AA	3624	1/1	0.93	0.13	65,65,65,65	0
58	MG	BA	1761	1/1	0.93	0.18	55,55,55,55	0
58	MG	CA	3413	1/1	0.93	0.20	39,39,39,39	0
58	MG	BA	1808	1/1	0.93	0.14	50,50,50,50	0
58	MG	AB	3007	1/1	0.93	0.09	45,45,45,45	0
58	MG	AA	3226	1/1	0.93	0.26	56,56,56,56	0
58	MG	AA	3030	1/1	0.93	0.32	26,26,26,26	1
58	MG	AA	3674	1/1	0.93	0.24	75,75,75,75	0
58	MG	CA	3549	1/1	0.93	0.06	57,57,57,57	0
58	MG	AA	3380	1/1	0.93	0.15	15,15,15,15	0
58	MG	BA	1658	1/1	0.93	0.49	76,76,76,76	0
58	MG	AA	3487	1/1	0.93	0.17	39,39,39,39	0
58	MG	CA	3337	1/1	0.93	0.17	41,41,41,41	0
58	MG	CA	3483	1/1	0.93	0.46	69,69,69,69	0
58	MG	DA	1726	1/1	0.93	0.16	77,77,77,77	0
58	MG	AA	3271	1/1	0.93	0.34	69,69,69,69	0
58	MG	CA	3442	1/1	0.93	0.43	67,67,67,67	0
58	MG	AA	3031	1/1	0.93	0.24	10,10,10,10	1
58	MG	BA	1604	1/1	0.93	0.14	65,65,65,65	0
58	MG	AA	3808	1/1	0.93	0.19	28,28,28,28	1
58	MG	CA	3206	1/1	0.93	0.57	56,56,56,56	0
58	MG	DA	1680	1/1	0.93	0.30	62,62,62,62	0
58	MG	CA	3608	1/1	0.93	0.20	56,56,56,56	0
58	MG	CA	3461	1/1	0.93	0.18	43,43,43,43	0
58	MG	AA	3632	1/1	0.93	0.13	76,76,76,76	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	CA	3627	1/1	0.93	0.18	63,63,63,63	0
58	MG	AA	3577	1/1	0.93	0.10	32,32,32,32	0
58	MG	AA	3298	1/1	0.93	0.07	59,59,59,59	0
58	MG	AA	3489	1/1	0.93	0.08	64,64,64,64	0
58	MG	CA	3336	1/1	0.93	0.16	69,69,69,69	0
58	MG	CA	3613	1/1	0.93	0.32	74,74,74,74	0
58	MG	DA	1658	1/1	0.93	0.21	72,72,72,72	0
58	MG	DA	1642	1/1	0.93	0.19	66,66,66,66	0
58	MG	AA	3187	1/1	0.93	0.25	32,32,32,32	0
58	MG	AA	3152	1/1	0.93	0.27	71,71,71,71	0
58	MG	AA	3301	1/1	0.93	0.31	23,23,23,23	0
58	MG	BA	1733	1/1	0.93	0.15	62,62,62,62	0
58	MG	CB	3004	1/1	0.93	0.14	68,68,68,68	0
58	MG	CA	3499	1/1	0.93	0.23	83,83,83,83	0
58	MG	CA	3535	1/1	0.93	0.28	69,69,69,69	0
58	MG	AA	3451	1/1	0.93	0.23	48,48,48,48	0
58	MG	CF	303	1/1	0.93	0.40	62,62,62,62	0
58	MG	CA	3178	1/1	0.93	0.22	57,57,57,57	0
58	MG	AB	3019	1/1	0.93	0.17	65,65,65,65	0
58	MG	AA	3289	1/1	0.93	0.11	27,27,27,27	0
58	MG	AA	3773	1/1	0.93	0.36	30,30,30,30	1
58	MG	AA	3572	1/1	0.93	0.14	32,32,32,32	0
58	MG	AA	3589	1/1	0.93	0.26	21,21,21,21	1
58	MG	AA	3769	1/1	0.93	0.23	57,57,57,57	0
58	MG	AA	3363	1/1	0.93	0.33	28,28,28,28	0
58	MG	AA	3741	1/1	0.93	0.19	34,34,34,34	1
58	MG	CA	3399	1/1	0.93	0.10	75,75,75,75	0
58	MG	AA	3027	1/1	0.93	0.47	77,77,77,77	0
58	MG	AU	201	1/1	0.93	0.28	44,44,44,44	0
58	MG	CA	3316	1/1	0.93	0.17	50,50,50,50	0
58	MG	CA	3525	1/1	0.93	0.29	83,83,83,83	0
58	MG	AA	3804	1/1	0.93	0.38	68,68,68,68	0
58	MG	CA	3643	1/1	0.93	0.09	76,76,76,76	0
58	MG	CA	3362	1/1	0.93	0.18	44,44,44,44	0
58	MG	CA	3402	1/1	0.93	0.11	70,70,70,70	0
58	MG	CA	3471	1/1	0.93	0.17	45,45,45,45	0
58	MG	CA	3505	1/1	0.93	0.26	73,73,73,73	0
58	MG	DA	1629	1/1	0.93	0.38	58,58,58,58	0
58	MG	CA	3003	1/1	0.93	0.20	45,45,45,45	0
58	MG	DA	1711	1/1	0.93	0.31	45,45,45,45	0
58	MG	AA	3811	1/1	0.93	0.29	58,58,58,58	0
58	MG	AA	3695	1/1	0.93	0.50	78,78,78,78	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	DK	5001	1/1	0.93	0.29	100,100,100,100	0
58	MG	DA	1748	1/1	0.93	0.15	78,78,78,78	0
58	MG	A2	101	1/1	0.93	0.19	35,35,35,35	0
58	MG	CB	3010	1/1	0.93	0.22	55,55,55,55	0
62	GDP	DZ	704	28/28	0.93	0.17	80,80,80,80	3
58	MG	DA	1712	1/1	0.93	0.14	81,81,81,81	0
58	MG	AA	3686	1/1	0.93	0.17	73,73,73,73	0
58	MG	CA	3156	1/1	0.93	0.31	68,68,68,68	0
58	MG	CA	3306	1/1	0.93	0.11	41,41,41,41	0
58	MG	AA	3711	1/1	0.93	0.28	34,34,34,34	1
58	MG	AA	3098	1/1	0.93	0.30	58,58,58,58	0
58	MG	CA	3210	1/1	0.93	0.30	75,75,75,75	0
58	MG	AA	3579	1/1	0.93	0.13	38,38,38,38	0
58	MG	CA	3157	1/1	0.93	0.15	55,55,55,55	0
58	MG	AF	301	1/1	0.93	0.17	43,43,43,43	0
58	MG	CA	3575	1/1	0.93	0.10	43,43,43,43	1
58	MG	CA	3600	1/1	0.93	0.11	50,50,50,50	0
58	MG	AA	3551	1/1	0.93	0.22	52,52,52,52	0
58	MG	AH	3001	1/1	0.93	0.28	52,52,52,52	0
58	MG	AA	3645	1/1	0.93	0.49	79,79,79,79	0
58	MG	BA	1740	1/1	0.93	0.19	50,50,50,50	0
58	MG	BA	1773	1/1	0.93	0.24	78,78,78,78	0
58	MG	AG	202	1/1	0.93	0.14	73,73,73,73	0
58	MG	BA	1703	1/1	0.93	0.24	78,78,78,78	0
58	MG	BA	1639	1/1	0.93	0.36	49,49,49,49	0
58	MG	AA	3036	1/1	0.93	0.18	51,51,51,51	0
58	MG	CA	3403	1/1	0.93	0.08	91,91,91,91	0
58	MG	CA	3582	1/1	0.93	0.18	44,44,44,44	0
58	MG	AA	3590	1/1	0.93	0.20	69,69,69,69	0
58	MG	AA	3209	1/1	0.93	0.30	63,63,63,63	0
58	MG	CA	3191	1/1	0.93	0.28	65,65,65,65	0
58	MG	CA	3167	1/1	0.93	0.09	60,60,60,60	0
58	MG	AA	3194	1/1	0.93	0.47	44,44,44,44	0
58	MG	A0	103	1/1	0.93	0.12	37,37,37,37	0
58	MG	AA	3368	1/1	0.93	0.20	37,37,37,37	0
58	MG	CA	3470	1/1	0.93	0.32	72,72,72,72	0
58	MG	AA	3004	1/1	0.93	0.15	25,25,25,25	0
58	MG	AA	3348	1/1	0.93	0.21	32,32,32,32	0
58	MG	AA	3214	1/1	0.93	0.15	34,34,34,34	0
58	MG	CA	3605	1/1	0.93	0.26	73,73,73,73	0
58	MG	AA	3553	1/1	0.93	0.16	40,40,40,40	0
58	MG	CA	3359	1/1	0.93	0.19	42,42,42,42	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	AA	3275	1/1	0.93	0.24	47,47,47,47	1
58	MG	CA	3057	1/1	0.93	0.16	49,49,49,49	0
58	MG	CA	3230	1/1	0.93	0.41	51,51,51,51	0
58	MG	AA	3495	1/1	0.93	0.17	59,59,59,59	0
58	MG	CA	3303	1/1	0.93	0.45	54,54,54,54	0
58	MG	AA	3119	1/1	0.93	0.34	40,40,40,40	1
58	MG	AA	3813	1/1	0.93	0.57	54,54,54,54	0
58	MG	AA	3581	1/1	0.93	0.21	40,40,40,40	0
58	MG	AD	308	1/1	0.93	0.40	42,42,42,42	0
58	MG	CA	3257	1/1	0.93	0.47	57,57,57,57	0
58	MG	AA	3114	1/1	0.93	0.21	17,17,17,17	0
58	MG	AA	3087	1/1	0.93	0.25	72,72,72,72	0
58	MG	AA	3685	1/1	0.93	0.19	47,47,47,47	0
58	MG	AA	3668	1/1	0.93	0.19	40,40,40,40	0
58	MG	AA	3698	1/1	0.93	0.28	32,32,32,32	1
58	MG	DA	1697	1/1	0.93	0.30	62,62,62,62	0
58	MG	CA	3017	1/1	0.93	0.56	46,46,46,46	0
58	MG	BA	1602	1/1	0.93	0.11	53,53,53,53	0
58	MG	CA	3445	1/1	0.93	0.30	40,40,40,40	0
58	MG	AA	3443	1/1	0.93	0.20	65,65,65,65	0
58	MG	CA	3454	1/1	0.93	0.17	81,81,81,81	0
58	MG	AA	3405	1/1	0.93	0.39	46,46,46,46	0
58	MG	DA	1698	1/1	0.93	0.39	68,68,68,68	0
58	MG	AA	3441	1/1	0.93	0.18	51,51,51,51	1
58	MG	DA	1695	1/1	0.93	0.15	66,66,66,66	0
58	MG	AA	3778	1/1	0.93	0.20	54,54,54,54	0
58	MG	AA	3512	1/1	0.93	0.32	60,60,60,60	0
58	MG	CA	3324	1/1	0.93	0.31	40,40,40,40	0
58	MG	CA	3263	1/1	0.93	0.25	57,57,57,57	0
58	MG	A6	101	1/1	0.93	0.35	65,65,65,65	0
58	MG	AA	3497	1/1	0.93	0.04	46,46,46,46	0
58	MG	AA	3434	1/1	0.93	0.12	17,17,17,17	0
58	MG	CA	3347	1/1	0.93	0.12	59,59,59,59	0
58	MG	CA	3472	1/1	0.93	0.58	72,72,72,72	0
58	MG	AA	3106	1/1	0.93	0.25	52,52,52,52	0
58	MG	AA	3006	1/1	0.93	0.45	52,52,52,52	0
58	MG	CA	3005	1/1	0.93	0.22	59,59,59,59	0
58	MG	AA	3090	1/1	0.93	0.56	30,30,30,30	1
58	MG	CA	3521	1/1	0.93	0.20	61,61,61,61	0
58	MG	CA	3473	1/1	0.93	0.16	54,54,54,54	0
58	MG	CQ	202	1/1	0.93	0.65	64,64,64,64	0
58	MG	AA	3162	1/1	0.93	0.36	47,47,47,47	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	AA	3465	1/1	0.94	0.21	39,39,39,39	0
58	MG	CA	3464	1/1	0.94	0.13	46,46,46,46	0
58	MG	AA	3191	1/1	0.94	0.26	42,42,42,42	0
58	MG	AA	3159	1/1	0.94	0.22	46,46,46,46	1
58	MG	DA	1741	1/1	0.94	0.15	78,78,78,78	0
58	MG	AA	3049	1/1	0.94	0.26	52,52,52,52	0
58	MG	CA	3181	1/1	0.94	0.23	47,47,47,47	0
58	MG	CA	3146	1/1	0.94	0.23	60,60,60,60	0
58	MG	CA	3597	1/1	0.94	0.27	39,39,39,39	0
58	MG	CA	3279	1/1	0.94	0.15	34,34,34,34	0
58	MG	AA	3722	1/1	0.94	0.14	18,18,18,18	0
58	MG	AA	3631	1/1	0.94	0.29	46,46,46,46	0
58	MG	AA	3598	1/1	0.94	0.23	54,54,54,54	0
58	MG	CO	202	1/1	0.94	0.20	53,53,53,53	0
58	MG	CA	3401	1/1	0.94	0.22	69,69,69,69	0
58	MG	DA	1768	1/1	0.94	0.42	73,73,73,73	0
58	MG	AA	3602	1/1	0.94	0.26	37,37,37,37	0
58	MG	DA	1738	1/1	0.94	0.56	80,80,80,80	0
58	MG	AA	3397	1/1	0.94	0.12	15,15,15,15	0
58	MG	CW	201	1/1	0.94	0.25	39,39,39,39	0
58	MG	AA	3504	1/1	0.94	0.19	58,58,58,58	0
58	MG	CA	3414	1/1	0.94	0.20	50,50,50,50	0
58	MG	CA	3639	1/1	0.94	0.30	55,55,55,55	0
58	MG	AA	3169	1/1	0.94	0.19	39,39,39,39	0
58	MG	CA	3376	1/1	0.94	0.07	66,66,66,66	0
58	MG	BE	3001	1/1	0.94	0.11	60,60,60,60	0
58	MG	AA	3196	1/1	0.94	0.37	52,52,52,52	0
58	MG	CA	3498	1/1	0.94	0.44	68,68,68,68	0
58	MG	CA	3360	1/1	0.94	0.12	49,49,49,49	0
58	MG	CA	3250	1/1	0.94	0.15	52,52,52,52	0
58	MG	AA	3742	1/1	0.94	0.22	82,82,82,82	0
58	MG	CA	3569	1/1	0.94	0.24	79,79,79,79	0
58	MG	DA	1674	1/1	0.94	0.38	62,62,62,62	0
58	MG	AQ	203	1/1	0.94	0.42	41,41,41,41	0
58	MG	AA	3135	1/1	0.94	0.67	62,62,62,62	1
58	MG	AA	3629	1/1	0.94	0.16	61,61,61,61	0
58	MG	CA	3381	1/1	0.94	0.09	38,38,38,38	0
58	MG	CA	3497	1/1	0.94	0.30	73,73,73,73	0
58	MG	AA	3825	1/1	0.94	0.13	17,17,17,17	1
58	MG	CA	3319	1/1	0.94	0.18	67,67,67,67	0
58	MG	AB	3008	1/1	0.94	0.46	51,51,51,51	0
58	MG	AA	3025	1/1	0.94	0.37	35,35,35,35	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	DA	1664	1/1	0.94	0.14	64,64,64,64	0
58	MG	CA	3252	1/1	0.94	0.22	64,64,64,64	0
58	MG	AA	3333	1/1	0.94	0.14	66,66,66,66	0
58	MG	CA	3327	1/1	0.94	0.24	53,53,53,53	0
58	MG	CA	3269	1/1	0.94	0.12	86,86,86,86	0
58	MG	CA	3330	1/1	0.94	0.23	43,43,43,43	0
58	MG	AA	3671	1/1	0.94	0.22	58,58,58,58	0
58	MG	AA	3776	1/1	0.94	0.12	40,40,40,40	0
58	MG	AA	3130	1/1	0.94	0.25	37,37,37,37	0
58	MG	AA	3800	1/1	0.94	0.12	30,30,30,30	0
58	MG	AA	3468	1/1	0.94	0.36	52,52,52,52	0
58	MG	AA	3616	1/1	0.94	0.10	28,28,28,28	0
58	MG	CA	3124	1/1	0.94	0.25	48,48,48,48	0
58	MG	AB	3014	1/1	0.94	0.17	67,67,67,67	0
58	MG	BA	1747	1/1	0.94	0.40	68,68,68,68	0
58	MG	BA	1683	1/1	0.94	0.28	69,69,69,69	0
58	MG	AA	3618	1/1	0.94	0.16	38,38,38,38	0
58	MG	AA	3396	1/1	0.94	0.14	22,22,22,22	0
58	MG	AA	3286	1/1	0.94	0.19	52,52,52,52	0
58	MG	AA	3125	1/1	0.94	0.22	23,23,23,23	1
58	MG	DA	1666	1/1	0.94	0.16	66,66,66,66	0
58	MG	CA	3612	1/1	0.94	0.21	68,68,68,68	0
58	MG	CA	3170	1/1	0.94	0.32	47,47,47,47	0
58	MG	CA	3333	1/1	0.94	0.30	75,75,75,75	0
58	MG	BA	1663	1/1	0.94	0.09	79,79,79,79	0
58	MG	CA	3404	1/1	0.94	0.18	54,54,54,54	0
58	MG	AA	3714	1/1	0.94	0.21	56,56,56,56	0
58	MG	CA	3086	1/1	0.94	0.23	36,36,36,36	0
58	MG	AA	3505	1/1	0.94	0.17	31,31,31,31	0
58	MG	CA	3572	1/1	0.94	0.15	54,54,54,54	0
58	MG	AA	3508	1/1	0.94	0.26	49,49,49,49	0
58	MG	CA	3287	1/1	0.94	0.15	52,52,52,52	0
58	MG	AF	305	1/1	0.94	0.21	55,55,55,55	0
58	MG	DA	1609	1/1	0.94	0.28	46,46,46,46	0
58	MG	AA	3719	1/1	0.94	0.12	58,58,58,58	0
58	MG	AA	3725	1/1	0.94	0.17	39,39,39,39	0
58	MG	CB	3005	1/1	0.94	0.28	62,62,62,62	0
58	MG	DA	1758	1/1	0.94	0.15	71,71,71,71	0
58	MG	AA	3536	1/1	0.94	0.10	35,35,35,35	0
58	MG	AA	3503	1/1	0.94	0.15	64,64,64,64	0
58	MG	AA	3593	1/1	0.94	0.20	25,25,25,25	1
58	MG	AA	3142	1/1	0.94	0.19	26,26,26,26	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	CA	3298	1/1	0.94	0.16	68,68,68,68	0
58	MG	AA	3661	1/1	0.94	0.32	43,43,43,43	0
58	MG	AA	3770	1/1	0.94	0.41	37,37,37,37	0
58	MG	BA	1617	1/1	0.94	0.13	73,73,73,73	0
58	MG	BA	1674	1/1	0.94	0.05	68,68,68,68	0
58	MG	CA	3370	1/1	0.94	0.13	47,47,47,47	0
58	MG	BA	1768	1/1	0.94	0.07	75,75,75,75	0
58	MG	CA	3346	1/1	0.94	0.16	31,31,31,31	0
58	MG	AA	3370	1/1	0.94	0.27	58,58,58,58	0
58	MG	AA	3170	1/1	0.94	0.43	53,53,53,53	0
58	MG	CA	3411	1/1	0.94	0.35	61,61,61,61	0
58	MG	AA	3140	1/1	0.94	0.30	50,50,50,50	0
58	MG	AA	3550	1/1	0.94	0.21	47,47,47,47	0
58	MG	AA	3212	1/1	0.94	0.44	34,34,34,34	1
58	MG	CA	3171	1/1	0.94	0.32	55,55,55,55	0
58	MG	CA	3069	1/1	0.94	0.17	81,81,81,81	0
58	MG	CO	201	1/1	0.94	0.15	64,64,64,64	0
58	MG	AA	3462	1/1	0.94	0.43	71,71,71,71	0
58	MG	AA	3453	1/1	0.94	0.32	56,56,56,56	0
58	MG	AB	3020	1/1	0.94	0.11	55,55,55,55	0
58	MG	AA	3092	1/1	0.94	0.13	53,53,53,53	0
58	MG	AA	3054	1/1	0.94	0.13	38,38,38,38	0
58	MG	AA	3737	1/1	0.94	0.14	29,29,29,29	0
58	MG	AA	3160	1/1	0.94	0.16	57,57,57,57	0
58	MG	AA	3805	1/1	0.94	0.33	35,35,35,35	1
58	MG	AA	3253	1/1	0.94	0.28	29,29,29,29	1
58	MG	BA	1699	1/1	0.94	0.17	75,75,75,75	0
58	MG	CA	3275	1/1	0.94	0.22	42,42,42,42	0
58	MG	CA	3478	1/1	0.94	0.13	58,58,58,58	0
58	MG	AA	3072	1/1	0.94	0.13	26,26,26,26	0
58	MG	DA	1681	1/1	0.94	0.17	55,55,55,55	0
58	MG	CA	3310	1/1	0.94	0.12	48,48,48,48	0
58	MG	AA	3463	1/1	0.94	0.29	46,46,46,46	0
58	MG	AA	3019	1/1	0.94	0.28	58,58,58,58	0
58	MG	CA	3526	1/1	0.94	0.10	40,40,40,40	0
58	MG	AA	3073	1/1	0.94	0.27	58,58,58,58	0
58	MG	AA	3782	1/1	0.94	0.26	74,74,74,74	0
58	MG	DA	1685	1/1	0.94	0.35	65,65,65,65	0
58	MG	BA	1621	1/1	0.94	0.39	49,49,49,49	0
58	MG	CB	3011	1/1	0.94	0.28	53,53,53,53	0
58	MG	BA	1807	1/1	0.94	0.15	83,83,83,83	0
58	MG	AB	3009	1/1	0.94	0.08	56,56,56,56	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	AA	3381	1/1	0.94	0.26	27,27,27,27	0
58	MG	AA	3346	1/1	0.94	0.20	46,46,46,46	0
58	MG	AA	3336	1/1	0.94	0.16	54,54,54,54	0
58	MG	CA	3542	1/1	0.94	0.38	68,68,68,68	0
58	MG	CA	3567	1/1	0.94	0.19	56,56,56,56	0
58	MG	AA	3207	1/1	0.94	0.18	22,22,22,22	1
58	MG	AA	3428	1/1	0.94	0.17	35,35,35,35	0
58	MG	AA	3829	1/1	0.94	0.61	88,88,88,88	0
58	MG	BW	501	1/1	0.94	0.26	48,48,48,48	0
58	MG	AA	3083	1/1	0.94	0.23	38,38,38,38	1
58	MG	AA	3578	1/1	0.94	0.40	55,55,55,55	0
58	MG	BA	1803	1/1	0.94	0.21	64,64,64,64	0
58	MG	AA	3556	1/1	0.94	0.15	39,39,39,39	0
58	MG	BA	1670	1/1	0.94	0.21	92,92,92,92	0
58	MG	AA	3568	1/1	0.94	0.19	16,16,16,16	0
58	MG	AA	3524	1/1	0.94	0.16	28,28,28,28	0
58	MG	AA	3818	1/1	0.94	0.16	19,19,19,19	0
58	MG	AD	310	1/1	0.94	0.31	58,58,58,58	0
58	MG	CA	3331	1/1	0.94	0.34	52,52,52,52	0
58	MG	AA	3177	1/1	0.94	0.32	61,61,61,61	0
58	MG	DA	1621	1/1	0.94	0.12	44,44,44,44	0
58	MG	CA	3114	1/1	0.94	0.43	39,39,39,39	0
58	MG	DA	1626	1/1	0.94	0.49	49,49,49,49	0
58	MG	AA	3328	1/1	0.94	0.17	18,18,18,18	0
58	MG	AA	3166	1/1	0.94	0.16	31,31,31,31	0
58	MG	CA	3658	1/1	0.94	0.12	50,50,50,50	0
58	MG	AA	3542	1/1	0.95	0.15	63,63,63,63	0
58	MG	A7	102	1/1	0.95	0.09	43,43,43,43	0
58	MG	CA	3588	1/1	0.95	0.33	63,63,63,63	0
58	MG	BA	1737	1/1	0.95	0.26	63,63,63,63	0
58	MG	BA	1743	1/1	0.95	0.18	52,52,52,52	0
58	MG	AA	3452	1/1	0.95	0.14	69,69,69,69	0
58	MG	AA	3527	1/1	0.95	0.18	26,26,26,26	0
58	MG	AA	3642	1/1	0.95	0.13	49,49,49,49	0
58	MG	CA	3284	1/1	0.95	0.23	92,92,92,92	0
58	MG	CA	3479	1/1	0.95	0.21	46,46,46,46	0
58	MG	DA	1679	1/1	0.95	0.40	58,58,58,58	0
58	MG	AA	3146	1/1	0.95	0.23	33,33,33,33	1
58	MG	AA	3086	1/1	0.95	0.15	47,47,47,47	0
58	MG	AA	3033	1/1	0.95	0.23	29,29,29,29	1
58	MG	AA	3300	1/1	0.95	0.18	50,50,50,50	0
58	MG	CA	3048	1/1	0.95	0.17	86,86,86,86	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	AA	3234	1/1	0.95	0.17	30,30,30,30	1
58	MG	AA	3620	1/1	0.95	0.31	40,40,40,40	0
58	MG	AA	3548	1/1	0.95	0.15	57,57,57,57	1
58	MG	CA	3277	1/1	0.95	0.11	90,90,90,90	0
58	MG	AU	203	1/1	0.95	0.47	62,62,62,62	0
58	MG	AA	3013	1/1	0.95	0.17	35,35,35,35	0
58	MG	CA	3313	1/1	0.95	0.33	50,50,50,50	0
58	MG	CA	3022	1/1	0.95	0.20	38,38,38,38	0
58	MG	CA	3449	1/1	0.95	0.09	66,66,66,66	0
58	MG	AA	3533	1/1	0.95	0.14	22,22,22,22	0
58	MG	AA	3614	1/1	0.95	0.11	56,56,56,56	0
58	MG	CA	3041	1/1	0.95	0.26	31,31,31,31	0
58	MG	AA	3145	1/1	0.95	0.18	33,33,33,33	0
58	MG	BN	502	1/1	0.95	0.23	66,66,66,66	0
58	MG	AA	3189	1/1	0.95	0.38	40,40,40,40	0
58	MG	CA	3193	1/1	0.95	0.22	64,64,64,64	0
58	MG	AA	3429	1/1	0.95	0.20	41,41,41,41	0
58	MG	CA	3211	1/1	0.95	0.11	40,40,40,40	0
58	MG	CB	3012	1/1	0.95	0.34	76,76,76,76	0
58	MG	CA	3648	1/1	0.95	0.32	53,53,53,53	0
58	MG	CA	3380	1/1	0.95	0.19	71,71,71,71	0
58	MG	AA	3071	1/1	0.95	0.73	41,41,41,41	0
58	MG	CF	302	1/1	0.95	0.18	56,56,56,56	0
58	MG	AA	3008	1/1	0.95	0.16	19,19,19,19	0
58	MG	AA	3366	1/1	0.95	0.21	53,53,53,53	0
58	MG	CA	3268	1/1	0.95	0.30	69,69,69,69	0
58	MG	CA	3584	1/1	0.95	0.12	46,46,46,46	0
58	MG	CA	3455	1/1	0.95	0.26	47,47,47,47	0
58	MG	AA	3379	1/1	0.95	0.13	30,30,30,30	0
58	MG	CA	3344	1/1	0.95	0.07	87,87,87,87	0
58	MG	DA	1702	1/1	0.95	0.09	65,65,65,65	0
58	MG	CA	3451	1/1	0.95	0.18	63,63,63,63	0
58	MG	CA	3476	1/1	0.95	0.24	55,55,55,55	0
59	ZN	BN	501	1/1	0.95	0.05	123,123,123,123	0
58	MG	CA	3530	1/1	0.95	0.25	59,59,59,59	0
58	MG	AA	3240	1/1	0.95	0.33	30,30,30,30	0
58	MG	BA	1749	1/1	0.95	0.12	48,48,48,48	0
58	MG	BA	1799	1/1	0.95	0.20	65,65,65,65	0
58	MG	CA	3422	1/1	0.95	0.26	55,55,55,55	0
58	MG	CA	3367	1/1	0.95	0.22	65,65,65,65	0
58	MG	DA	1640	1/1	0.95	0.17	79,79,79,79	0
58	MG	DA	1736	1/1	0.95	0.12	79,79,79,79	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	AA	3486	1/1	0.95	0.15	27,27,27,27	0
58	MG	CA	3251	1/1	0.95	0.19	56,56,56,56	0
58	MG	DA	1703	1/1	0.95	0.27	74,74,74,74	0
58	MG	AA	3746	1/1	0.95	0.14	64,64,64,64	0
58	MG	AA	3241	1/1	0.95	0.20	69,69,69,69	0
58	MG	AA	3535	1/1	0.95	0.18	15,15,15,15	0
58	MG	CA	3079	1/1	0.95	0.32	57,57,57,57	0
58	MG	BA	1635	1/1	0.95	0.22	72,72,72,72	0
58	MG	CA	3218	1/1	0.95	0.49	54,54,54,54	0
58	MG	CA	3104	1/1	0.95	0.14	48,48,48,48	0
58	MG	CA	3259	1/1	0.95	0.21	47,47,47,47	0
58	MG	CA	3508	1/1	0.95	0.14	96,96,96,96	0
58	MG	AA	3797	1/1	0.95	0.26	15,15,15,15	1
58	MG	CA	3029	1/1	0.95	0.11	33,33,33,33	0
58	MG	AA	3466	1/1	0.95	0.11	63,63,63,63	0
58	MG	AA	3510	1/1	0.95	0.35	58,58,58,58	0
58	MG	CA	3161	1/1	0.95	0.19	66,66,66,66	0
58	MG	DA	1682	1/1	0.95	0.20	47,47,47,47	0
58	MG	CA	3064	1/1	0.95	0.05	43,43,43,43	0
58	MG	CA	3576	1/1	0.95	0.10	36,36,36,36	0
58	MG	CA	3019	1/1	0.95	0.14	28,28,28,28	0
58	MG	DA	1651	1/1	0.95	0.40	59,59,59,59	0
58	MG	AA	3676	1/1	0.95	0.20	66,66,66,66	0
58	MG	AA	3404	1/1	0.95	0.18	19,19,19,19	0
58	MG	CA	3214	1/1	0.95	0.18	40,40,40,40	0
58	MG	AA	3667	1/1	0.95	0.20	28,28,28,28	0
58	MG	DA	1646	1/1	0.95	0.33	62,62,62,62	0
58	MG	AA	3644	1/1	0.95	0.17	56,56,56,56	0
58	MG	AA	3156	1/1	0.95	0.34	33,33,33,33	1
58	MG	CA	3462	1/1	0.95	0.12	49,49,49,49	0
58	MG	CA	3486	1/1	0.95	0.27	69,69,69,69	0
58	MG	AA	3069	1/1	0.95	0.12	34,34,34,34	0
58	MG	DA	1683	1/1	0.95	0.35	54,54,54,54	0
58	MG	AA	3499	1/1	0.95	0.17	51,51,51,51	1
58	MG	AA	3796	1/1	0.95	0.25	50,50,50,50	0
58	MG	DA	1616	1/1	0.95	0.23	64,64,64,64	0
58	MG	CA	3511	1/1	0.95	0.11	68,68,68,68	0
58	MG	AA	3666	1/1	0.95	0.07	64,64,64,64	0
58	MG	CA	3011	1/1	0.95	0.22	47,47,47,47	0
58	MG	CE	301	1/1	0.95	0.38	66,66,66,66	0
58	MG	AA	3501	1/1	0.95	0.11	24,24,24,24	0
58	MG	CA	3436	1/1	0.95	0.10	75,75,75,75	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	AA	3816	1/1	0.95	0.30	43,43,43,43	0
58	MG	BA	1643	1/1	0.95	0.06	58,58,58,58	0
58	MG	AA	3343	1/1	0.95	0.13	65,65,65,65	0
58	MG	AA	3331	1/1	0.95	0.27	34,34,34,34	0
58	MG	DA	1647	1/1	0.95	0.33	58,58,58,58	0
58	MG	AA	3525	1/1	0.95	0.32	40,40,40,40	0
58	MG	AA	3493	1/1	0.95	0.13	30,30,30,30	1
58	MG	CA	3281	1/1	0.95	0.26	51,51,51,51	0
58	MG	AA	3293	1/1	0.95	0.19	32,32,32,32	0
58	MG	DA	1631	1/1	0.95	0.20	70,70,70,70	0
58	MG	BZ	702	1/1	0.95	0.34	46,46,46,46	0
58	MG	AA	3338	1/1	0.95	0.14	30,30,30,30	0
58	MG	CB	3003	1/1	0.95	0.12	77,77,77,77	0
58	MG	AA	3378	1/1	0.95	0.17	19,19,19,19	0
58	MG	CA	3554	1/1	0.95	0.18	67,67,67,67	0
58	MG	AA	3789	1/1	0.95	0.18	54,54,54,54	0
58	MG	CA	3433	1/1	0.95	0.16	71,71,71,71	0
58	MG	CA	3591	1/1	0.95	0.14	83,83,83,83	0
58	MG	BT	3001	1/1	0.95	0.36	62,62,62,62	0
58	MG	AA	3700	1/1	0.95	0.22	35,35,35,35	0
58	MG	BA	1759	1/1	0.95	0.13	63,63,63,63	0
58	MG	DA	1760	1/1	0.95	0.36	66,66,66,66	0
58	MG	AA	3675	1/1	0.95	0.09	38,38,38,38	0
58	MG	AA	3706	1/1	0.95	0.25	27,27,27,27	1
58	MG	AA	3500	1/1	0.95	0.11	47,47,47,47	0
58	MG	AA	3055	1/1	0.95	0.26	35,35,35,35	0
58	MG	AA	3826	1/1	0.95	0.17	20,20,20,20	0
58	MG	AA	3039	1/1	0.95	0.33	39,39,39,39	1
58	MG	CA	3592	1/1	0.95	0.59	76,76,76,76	0
58	MG	AA	3321	1/1	0.95	0.30	70,70,70,70	0
58	MG	CA	3110	1/1	0.95	0.33	63,63,63,63	0
58	MG	CA	3595	1/1	0.95	0.09	53,53,53,53	0
58	MG	BA	1706	1/1	0.95	0.41	62,62,62,62	0
58	MG	AA	3772	1/1	0.95	0.29	17,17,17,17	1
58	MG	C3	3001	1/1	0.95	0.33	69,69,69,69	0
58	MG	AA	3522	1/1	0.95	0.22	28,28,28,28	0
58	MG	BL	202	1/1	0.95	0.33	67,67,67,67	0
58	MG	CA	3431	1/1	0.95	0.28	100,100,100,100	0
58	MG	AG	201	1/1	0.95	0.10	52,52,52,52	0
58	MG	AA	3009	1/1	0.95	0.13	24,24,24,24	0
58	MG	CA	3494	1/1	0.95	0.20	63,63,63,63	0
58	MG	CA	3390	1/1	0.95	0.15	64,64,64,64	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	BA	1753	1/1	0.95	0.12	94,94,94,94	0
58	MG	AA	3515	1/1	0.95	0.17	20,20,20,20	0
58	MG	AA	3820	1/1	0.95	0.27	40,40,40,40	0
58	MG	BA	1654	1/1	0.95	0.09	54,54,54,54	0
58	MG	CA	3382	1/1	0.95	0.18	40,40,40,40	0
58	MG	CA	3169	1/1	0.95	0.27	34,34,34,34	0
58	MG	AA	3050	1/1	0.95	0.18	53,53,53,53	0
58	MG	CA	3394	1/1	0.95	0.16	55,55,55,55	0
58	MG	AA	3032	1/1	0.95	0.27	36,36,36,36	0
58	MG	AA	3044	1/1	0.95	0.20	34,34,34,34	0
58	MG	CA	3387	1/1	0.95	0.30	70,70,70,70	0
58	MG	CA	3539	1/1	0.95	0.42	73,73,73,73	0
58	MG	AA	3198	1/1	0.95	0.07	58,58,58,58	0
58	MG	CA	3446	1/1	0.95	0.18	63,63,63,63	0
58	MG	AA	3332	1/1	0.95	0.13	46,46,46,46	0
58	MG	AA	3320	1/1	0.95	0.19	24,24,24,24	0
58	MG	CA	3652	1/1	0.95	0.16	53,53,53,53	0
58	MG	AA	3296	1/1	0.95	0.12	17,17,17,17	0
58	MG	C5	101	1/1	0.95	0.63	65,65,65,65	0
58	MG	AA	3574	1/1	0.95	0.16	30,30,30,30	1
58	MG	DA	1717	1/1	0.95	0.28	52,52,52,52	0
58	MG	AA	3401	1/1	0.95	0.18	33,33,33,33	0
58	MG	CA	3465	1/1	0.95	0.33	66,66,66,66	0
58	MG	AA	3440	1/1	0.95	0.21	31,31,31,31	0
58	MG	AA	3138	1/1	0.95	0.35	50,50,50,50	0
58	MG	AA	3469	1/1	0.95	0.16	43,43,43,43	0
58	MG	AA	3104	1/1	0.95	0.16	28,28,28,28	0
58	MG	DA	1745	1/1	0.95	0.17	61,61,61,61	0
58	MG	CA	3023	1/1	0.96	0.24	46,46,46,46	0
58	MG	AA	3517	1/1	0.96	0.19	19,19,19,19	0
58	MG	CA	3249	1/1	0.96	0.18	46,46,46,46	0
59	ZN	A4	501	1/1	0.96	0.05	137,137,137,137	0
58	MG	BA	1713	1/1	0.96	0.25	55,55,55,55	0
58	MG	BW	502	1/1	0.96	0.10	53,53,53,53	0
58	MG	AA	3197	1/1	0.96	0.36	37,37,37,37	0
58	MG	AA	3297	1/1	0.96	0.30	20,20,20,20	1
58	MG	AA	3179	1/1	0.96	0.30	71,71,71,71	0
58	MG	AA	3509	1/1	0.96	0.16	49,49,49,49	0
58	MG	BA	1686	1/1	0.96	0.31	52,52,52,52	0
58	MG	CA	3164	1/1	0.96	0.39	41,41,41,41	0
58	MG	CA	3309	1/1	0.96	0.20	29,29,29,29	0
58	MG	AA	3683	1/1	0.96	0.35	67,67,67,67	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	CA	3466	1/1	0.96	0.45	57,57,57,57	0
58	MG	AA	3427	1/1	0.96	0.10	33,33,33,33	0
58	MG	AA	3218	1/1	0.96	0.16	38,38,38,38	0
58	MG	BA	1717	1/1	0.96	0.17	44,44,44,44	0
58	MG	BA	1620	1/1	0.96	0.09	37,37,37,37	0
58	MG	CA	3334	1/1	0.96	0.26	44,44,44,44	0
58	MG	AA	3716	1/1	0.96	0.17	57,57,57,57	0
58	MG	CA	3448	1/1	0.96	0.18	43,43,43,43	0
58	MG	CA	3383	1/1	0.96	0.24	44,44,44,44	0
58	MG	CA	3410	1/1	0.96	0.19	31,31,31,31	0
58	MG	AA	3436	1/1	0.96	0.33	38,38,38,38	0
58	MG	AA	3693	1/1	0.96	0.21	48,48,48,48	0
58	MG	CE	305	1/1	0.96	0.26	43,43,43,43	0
58	MG	CA	3308	1/1	0.96	0.11	41,41,41,41	0
58	MG	AA	3736	1/1	0.96	0.20	78,78,78,78	0
58	MG	AB	3016	1/1	0.96	0.16	34,34,34,34	0
58	MG	AA	3730	1/1	0.96	0.26	30,30,30,30	0
58	MG	CA	3633	1/1	0.96	0.22	68,68,68,68	0
58	MG	AA	3682	1/1	0.96	0.29	53,53,53,53	0
58	MG	CA	3312	1/1	0.96	0.13	51,51,51,51	0
58	MG	DA	1713	1/1	0.96	0.52	72,72,72,72	0
58	MG	CA	3021	1/1	0.96	0.11	29,29,29,29	0
58	MG	BA	1741	1/1	0.96	0.09	46,46,46,46	0
58	MG	BA	1792	1/1	0.96	0.18	75,75,75,75	0
58	MG	BA	1776	1/1	0.96	0.25	64,64,64,64	0
58	MG	CA	3425	1/1	0.96	0.13	53,53,53,53	0
58	MG	AA	3046	1/1	0.96	0.22	34,34,34,34	0
58	MG	AA	3475	1/1	0.96	0.13	62,62,62,62	0
58	MG	AF	303	1/1	0.96	0.35	50,50,50,50	0
58	MG	AA	3569	1/1	0.96	0.17	19,19,19,19	0
58	MG	AA	3037	1/1	0.96	0.29	45,45,45,45	0
58	MG	AA	3228	1/1	0.96	0.17	51,51,51,51	0
58	MG	CD	303	1/1	0.96	0.50	37,37,37,37	0
58	MG	CA	3166	1/1	0.96	0.38	44,44,44,44	0
58	MG	AA	3702	1/1	0.96	0.37	35,35,35,35	1
58	MG	AA	3790	1/1	0.96	0.06	49,49,49,49	0
58	MG	AA	3532	1/1	0.96	0.16	25,25,25,25	0
58	MG	CA	3650	1/1	0.96	0.27	27,27,27,27	0
58	MG	AA	3254	1/1	0.96	0.18	42,42,42,42	0
58	MG	AA	3622	1/1	0.96	0.16	45,45,45,45	0
58	MG	AA	3421	1/1	0.96	0.18	12,12,12,12	0
58	MG	AA	3763	1/1	0.96	0.35	65,65,65,65	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	AA	3167	1/1	0.96	0.13	65,65,65,65	0
58	MG	AA	3131	1/1	0.96	0.43	55,55,55,55	0
58	MG	BA	1794	1/1	0.96	0.16	77,77,77,77	0
58	MG	DA	1742	1/1	0.96	0.32	79,79,79,79	0
58	MG	CA	3659	1/1	0.96	0.11	77,77,77,77	0
58	MG	CA	3135	1/1	0.96	0.20	66,66,66,66	0
58	MG	AA	3020	1/1	0.96	0.19	25,25,25,25	0
58	MG	AA	3210	1/1	0.96	0.32	24,24,24,24	1
58	MG	AA	3471	1/1	0.96	0.25	34,34,34,34	0
58	MG	AA	3371	1/1	0.96	0.34	62,62,62,62	0
58	MG	AA	3619	1/1	0.96	0.15	42,42,42,42	0
58	MG	AR	201	1/1	0.96	0.27	32,32,32,32	0
58	MG	CA	3229	1/1	0.96	0.32	51,51,51,51	0
58	MG	AA	3392	1/1	0.96	0.16	42,42,42,42	0
58	MG	AA	3403	1/1	0.96	0.09	28,28,28,28	0
58	MG	CA	3501	1/1	0.96	0.15	45,45,45,45	1
58	MG	CA	3452	1/1	0.96	0.23	61,61,61,61	0
58	MG	DA	1704	1/1	0.96	0.07	69,69,69,69	0
58	MG	DA	1644	1/1	0.96	0.16	57,57,57,57	0
58	MG	CA	3053	1/1	0.96	0.72	58,58,58,58	0
58	MG	AA	3327	1/1	0.96	0.14	13,13,13,13	0
58	MG	CA	3276	1/1	0.96	0.29	50,50,50,50	0
58	MG	CA	3231	1/1	0.96	0.37	57,57,57,57	0
58	MG	CA	3266	1/1	0.96	0.21	69,69,69,69	0
58	MG	AA	3076	1/1	0.96	0.24	92,92,92,92	0
58	MG	AA	3584	1/1	0.96	0.08	65,65,65,65	0
58	MG	AA	3559	1/1	0.96	0.21	39,39,39,39	0
58	MG	BA	1731	1/1	0.96	0.27	63,63,63,63	0
58	MG	AA	3217	1/1	0.96	0.16	6,6,6,6	0
58	MG	CA	3222	1/1	0.96	0.25	75,75,75,75	0
58	MG	AA	3395	1/1	0.96	0.20	18,18,18,18	0
58	MG	AA	3084	1/1	0.96	0.10	32,32,32,32	0
58	MG	AA	3595	1/1	0.96	0.24	55,55,55,55	0
58	MG	CA	3120	1/1	0.96	0.50	62,62,62,62	0
58	MG	DD	502	1/1	0.96	0.61	62,62,62,62	0
58	MG	DA	1648	1/1	0.96	0.21	50,50,50,50	0
58	MG	AA	3783	1/1	0.96	0.19	54,54,54,54	0
58	MG	CA	3562	1/1	0.96	0.20	76,76,76,76	0
58	MG	CA	3261	1/1	0.96	0.17	29,29,29,29	0
58	MG	AA	3344	1/1	0.96	0.10	84,84,84,84	0
58	MG	AA	3528	1/1	0.96	0.15	28,28,28,28	0
58	MG	DA	1667	1/1	0.96	0.23	49,49,49,49	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	DA	1611	1/1	0.96	0.08	38,38,38,38	0
58	MG	CA	3566	1/1	0.96	0.13	41,41,41,41	0
58	MG	DA	1753	1/1	0.96	0.36	70,70,70,70	0
58	MG	AA	3391	1/1	0.96	0.15	45,45,45,45	0
58	MG	AA	3312	1/1	0.96	0.18	55,55,55,55	0
58	MG	CE	302	1/1	0.96	0.13	47,47,47,47	0
58	MG	AA	3367	1/1	0.96	0.16	52,52,52,52	0
58	MG	BA	1781	1/1	0.96	0.37	62,62,62,62	0
58	MG	AA	3324	1/1	0.96	0.11	33,33,33,33	0
58	MG	AB	3015	1/1	0.96	0.17	40,40,40,40	0
58	MG	DA	1655	1/1	0.96	0.42	58,58,58,58	0
58	MG	AA	3001	1/1	0.96	0.10	37,37,37,37	0
58	MG	AA	3566	1/1	0.96	0.17	27,27,27,27	0
58	MG	CA	3615	1/1	0.96	0.18	38,38,38,38	0
58	MG	CA	3207	1/1	0.96	0.14	71,71,71,71	0
58	MG	AA	3470	1/1	0.96	0.14	29,29,29,29	0
58	MG	AA	3305	1/1	0.96	0.24	55,55,55,55	0
58	MG	CA	3265	1/1	0.96	0.11	40,40,40,40	0
58	MG	AA	3415	1/1	0.96	0.07	56,56,56,56	0
58	MG	AA	3402	1/1	0.96	0.29	33,33,33,33	0
58	MG	AA	3318	1/1	0.96	0.25	51,51,51,51	1
58	MG	AA	3830	1/1	0.96	0.25	45,45,45,45	0
58	MG	AA	3748	1/1	0.96	0.27	56,56,56,56	0
58	MG	AA	3357	1/1	0.96	0.22	27,27,27,27	0
58	MG	CA	3385	1/1	0.96	0.46	64,64,64,64	0
58	MG	AA	3040	1/1	0.96	0.29	40,40,40,40	1
58	MG	AA	3506	1/1	0.96	0.27	32,32,32,32	0
58	MG	AA	3425	1/1	0.96	0.24	18,18,18,18	0
59	ZN	DN	501	1/1	0.96	0.06	129,129,129,129	0
58	MG	CA	3254	1/1	0.96	0.20	42,42,42,42	0
58	MG	CA	3547	1/1	0.96	0.14	61,61,61,61	0
58	MG	AA	3539	1/1	0.96	0.14	28,28,28,28	0
58	MG	AA	3315	1/1	0.96	0.18	34,34,34,34	0
58	MG	CA	3628	1/1	0.96	0.14	66,66,66,66	0
58	MG	CA	3516	1/1	0.96	0.11	62,62,62,62	0
58	MG	AA	3717	1/1	0.96	0.23	47,47,47,47	0
58	MG	CA	3529	1/1	0.96	0.08	57,57,57,57	0
58	MG	CA	3232	1/1	0.96	0.08	60,60,60,60	0
58	MG	CA	3285	1/1	0.96	0.37	57,57,57,57	0
58	MG	AA	3412	1/1	0.96	0.19	43,43,43,43	0
58	MG	AA	3591	1/1	0.96	0.23	65,65,65,65	0
58	MG	AA	3472	1/1	0.96	0.21	24,24,24,24	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	CA	3227	1/1	0.96	0.15	53,53,53,53	0
58	MG	CA	3366	1/1	0.96	0.22	61,61,61,61	0
58	MG	CA	3177	1/1	0.96	0.21	36,36,36,36	0
58	MG	AA	3171	1/1	0.96	0.48	25,25,25,25	1
58	MG	AA	3827	1/1	0.96	0.22	40,40,40,40	0
58	MG	AA	3756	1/1	0.96	0.17	40,40,40,40	1
58	MG	AA	3043	1/1	0.96	0.21	31,31,31,31	0
58	MG	AA	3394	1/1	0.96	0.18	27,27,27,27	0
58	MG	AB	3011	1/1	0.96	0.19	30,30,30,30	0
58	MG	AA	3124	1/1	0.96	0.58	63,63,63,63	0
58	MG	CA	3371	1/1	0.96	0.19	55,55,55,55	0
58	MG	CA	3234	1/1	0.96	0.29	54,54,54,54	0
58	MG	CA	3395	1/1	0.96	0.32	65,65,65,65	0
58	MG	CA	3424	1/1	0.96	0.17	55,55,55,55	0
58	MG	CA	3629	1/1	0.96	0.16	55,55,55,55	0
58	MG	AA	3173	1/1	0.96	0.25	60,60,60,60	0
58	MG	CA	3484	1/1	0.96	0.27	76,76,76,76	0
58	MG	AA	3575	1/1	0.96	0.11	69,69,69,69	0
58	MG	AA	3419	1/1	0.96	0.14	31,31,31,31	0
58	MG	BA	1636	1/1	0.96	0.37	64,64,64,64	0
58	MG	AA	3670	1/1	0.96	0.12	33,33,33,33	0
58	MG	AA	3369	1/1	0.96	0.24	27,27,27,27	0
58	MG	CA	3457	1/1	0.96	0.21	47,47,47,47	0
58	MG	AP	201	1/1	0.96	0.20	28,28,28,28	1
58	MG	AA	3435	1/1	0.96	0.15	20,20,20,20	0
58	MG	BA	1679	1/1	0.96	0.15	36,36,36,36	0
58	MG	CA	3365	1/1	0.97	0.20	48,48,48,48	0
58	MG	BA	1676	1/1	0.97	0.24	44,44,44,44	0
58	MG	AA	3764	1/1	0.97	0.18	55,55,55,55	0
58	MG	AV	203	1/1	0.97	0.33	38,38,38,38	0
58	MG	AE	303	1/1	0.97	0.23	41,41,41,41	0
58	MG	CA	3435	1/1	0.97	0.11	52,52,52,52	0
58	MG	DA	1723	1/1	0.97	0.30	66,66,66,66	0
58	MG	AA	3654	1/1	0.97	0.28	66,66,66,66	0
58	MG	AA	3449	1/1	0.97	0.10	15,15,15,15	0
58	MG	AV	201	1/1	0.97	0.17	38,38,38,38	0
58	MG	DA	1710	1/1	0.97	0.19	70,70,70,70	0
58	MG	AA	3314	1/1	0.97	0.20	28,28,28,28	0
58	MG	BA	1738	1/1	0.97	0.42	56,56,56,56	0
58	MG	AA	3075	1/1	0.97	0.15	9,9,9,9	0
58	MG	AA	3102	1/1	0.97	0.18	49,49,49,49	0
58	MG	AA	3678	1/1	0.97	0.23	31,31,31,31	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	DA	1688	1/1	0.97	0.20	66,66,66,66	0
58	MG	DA	1668	1/1	0.97	0.41	62,62,62,62	0
58	MG	AA	3494	1/1	0.97	0.22	50,50,50,50	0
58	MG	DA	1714	1/1	0.97	0.11	51,51,51,51	0
58	MG	BA	1765	1/1	0.97	0.10	61,61,61,61	0
58	MG	AA	3724	1/1	0.97	0.28	40,40,40,40	0
58	MG	AA	3540	1/1	0.97	0.19	29,29,29,29	0
58	MG	CA	3338	1/1	0.97	0.17	63,63,63,63	0
58	MG	CA	3552	1/1	0.97	0.13	69,69,69,69	0
58	MG	AA	3627	1/1	0.97	0.17	54,54,54,54	0
58	MG	AA	3011	1/1	0.97	0.09	40,40,40,40	0
58	MG	AA	3134	1/1	0.97	0.39	59,59,59,59	1
58	MG	AA	3607	1/1	0.97	0.08	30,30,30,30	0
58	MG	BA	1722	1/1	0.97	0.43	55,55,55,55	0
58	MG	BA	1752	1/1	0.97	0.20	48,48,48,48	0
58	MG	AA	3832	1/1	0.97	0.22	38,38,38,38	0
58	MG	CA	3291	1/1	0.97	0.11	27,27,27,27	0
58	MG	BA	1728	1/1	0.97	0.10	52,52,52,52	0
58	MG	BA	1795	1/1	0.97	0.27	69,69,69,69	0
58	MG	CA	3237	1/1	0.97	0.29	75,75,75,75	0
58	MG	CA	3377	1/1	0.97	0.18	80,80,80,80	0
58	MG	AA	3074	1/1	0.97	0.34	15,15,15,15	0
58	MG	CA	3437	1/1	0.97	0.11	48,48,48,48	0
58	MG	CA	3450	1/1	0.97	0.18	48,48,48,48	0
58	MG	AA	3601	1/1	0.97	0.38	47,47,47,47	0
58	MG	AA	3423	1/1	0.97	0.15	22,22,22,22	0
58	MG	CA	3443	1/1	0.97	0.11	36,36,36,36	0
58	MG	AA	3529	1/1	0.97	0.16	16,16,16,16	0
58	MG	AA	3549	1/1	0.97	0.08	54,54,54,54	0
58	MG	CA	3349	1/1	0.97	0.26	41,41,41,41	0
58	MG	AA	3287	1/1	0.97	0.39	47,47,47,47	0
58	MG	AA	3326	1/1	0.97	0.12	58,58,58,58	0
58	MG	DA	1654	1/1	0.97	0.10	30,30,30,30	0
58	MG	AA	3664	1/1	0.97	0.23	57,57,57,57	0
58	MG	CA	3028	1/1	0.97	0.55	35,35,35,35	1
58	MG	AA	3552	1/1	0.97	0.14	63,63,63,63	0
58	MG	CA	3361	1/1	0.97	0.31	58,58,58,58	0
58	MG	CA	3007	1/1	0.97	0.09	28,28,28,28	0
58	MG	AA	3516	1/1	0.97	0.16	18,18,18,18	0
58	MG	AA	3502	1/1	0.97	0.11	51,51,51,51	1
58	MG	CA	3055	1/1	0.97	0.50	39,39,39,39	0
58	MG	CA	3026	1/1	0.97	0.23	81,81,81,81	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	BA	1701	1/1	0.97	0.46	58,58,58,58	0
58	MG	CA	3182	1/1	0.97	0.35	27,27,27,27	0
58	MG	AA	3347	1/1	0.97	0.10	38,38,38,38	0
58	MG	AA	3313	1/1	0.97	0.12	35,35,35,35	0
58	MG	AA	3787	1/1	0.97	0.24	53,53,53,53	0
58	MG	AA	3507	1/1	0.97	0.24	14,14,14,14	0
58	MG	AA	3754	1/1	0.97	0.07	29,29,29,29	0
58	MG	CA	3315	1/1	0.97	0.16	60,60,60,60	0
58	MG	CA	3256	1/1	0.97	0.19	40,40,40,40	0
58	MG	AA	3048	1/1	0.97	0.24	34,34,34,34	0
58	MG	CA	3049	1/1	0.97	0.11	81,81,81,81	0
58	MG	AA	3067	1/1	0.97	0.38	55,55,55,55	0
58	MG	AA	3053	1/1	0.97	0.15	14,14,14,14	0
58	MG	DA	1670	1/1	0.97	0.14	75,75,75,75	0
58	MG	AA	3317	1/1	0.97	0.14	58,58,58,58	0
58	MG	AU	202	1/1	0.97	0.31	29,29,29,29	1
62	GDP	BZ	704	28/28	0.97	0.15	53,53,53,53	1
58	MG	DA	1761	1/1	0.97	0.28	66,66,66,66	0
58	MG	CA	3293	1/1	0.97	0.05	71,71,71,71	0
58	MG	CA	3288	1/1	0.97	0.25	54,54,54,54	0
58	MG	CA	3453	1/1	0.97	0.19	39,39,39,39	0
58	MG	AA	3417	1/1	0.97	0.16	25,25,25,25	0
58	MG	AA	3376	1/1	0.97	0.17	19,19,19,19	0
58	MG	AA	3256	1/1	0.97	0.15	21,21,21,21	1
58	MG	AA	3798	1/1	0.97	0.26	35,35,35,35	0
58	MG	AA	3439	1/1	0.97	0.22	17,17,17,17	0
58	MG	AA	3567	1/1	0.97	0.20	51,51,51,51	0
58	MG	CA	3459	1/1	0.97	0.18	48,48,48,48	0
58	MG	CA	3341	1/1	0.97	0.33	71,71,71,71	0
58	MG	AA	3582	1/1	0.97	0.39	66,66,66,66	0
58	MG	AA	3431	1/1	0.97	0.10	25,25,25,25	0
58	MG	CA	3550	1/1	0.97	0.17	33,33,33,33	0
58	MG	CA	3321	1/1	0.97	0.12	31,31,31,31	0
58	MG	CA	3559	1/1	0.97	0.26	52,52,52,52	1
58	MG	AA	3433	1/1	0.97	0.20	28,28,28,28	0
58	MG	CA	3051	1/1	0.97	0.42	63,63,63,63	0
58	MG	AA	3399	1/1	0.97	0.10	18,18,18,18	0
58	MG	AA	3823	1/1	0.97	0.26	37,37,37,37	1
58	MG	CA	3354	1/1	0.97	0.24	61,61,61,61	0
58	MG	AQ	202	1/1	0.97	0.21	31,31,31,31	0
58	MG	AA	3316	1/1	0.97	0.28	60,60,60,60	0
58	MG	CA	3162	1/1	0.97	0.45	46,46,46,46	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	A8	5002	1/1	0.97	0.23	31,31,31,31	0
58	MG	CA	3127	1/1	0.97	0.24	63,63,63,63	0
58	MG	AA	3669	1/1	0.97	0.06	33,33,33,33	0
58	MG	AA	3563	1/1	0.97	0.16	49,49,49,49	1
58	MG	AB	3005	1/1	0.97	0.27	69,69,69,69	0
58	MG	AA	3082	1/1	0.97	0.21	23,23,23,23	1
58	MG	AA	3648	1/1	0.97	0.17	40,40,40,40	0
58	MG	AA	3523	1/1	0.97	0.20	30,30,30,30	0
58	MG	BA	1611	1/1	0.97	0.12	31,31,31,31	0
58	MG	AA	3544	1/1	0.97	0.11	16,16,16,16	0
58	MG	AA	3576	1/1	0.97	0.26	38,38,38,38	0
58	MG	CA	3012	1/1	0.97	0.24	59,59,59,59	0
58	MG	AA	3416	1/1	0.97	0.17	30,30,30,30	0
58	MG	AA	3337	1/1	0.97	0.23	10,10,10,10	0
58	MG	AN	3002	1/1	0.97	0.16	27,27,27,27	0
58	MG	CA	3307	1/1	0.97	0.29	52,52,52,52	0
58	MG	BA	1769	1/1	0.97	0.27	63,63,63,63	0
58	MG	AA	3150	1/1	0.97	0.30	15,15,15,15	0
58	MG	CA	3260	1/1	0.97	0.23	65,65,65,65	0
58	MG	AA	3692	1/1	0.97	0.17	53,53,53,53	0
58	MG	CA	3353	1/1	0.97	0.22	48,48,48,48	0
58	MG	AA	3474	1/1	0.97	0.27	53,53,53,53	0
58	MG	CA	3416	1/1	0.97	0.17	48,48,48,48	0
58	MG	AA	3611	1/1	0.97	0.14	51,51,51,51	0
58	MG	AA	3520	1/1	0.97	0.12	38,38,38,38	0
58	MG	AA	3562	1/1	0.97	0.06	48,48,48,48	1
58	MG	CA	3355	1/1	0.97	0.11	41,41,41,41	0
58	MG	CA	3296	1/1	0.97	0.30	42,42,42,42	0
58	MG	AA	3262	1/1	0.97	0.37	70,70,70,70	0
58	MG	AA	3330	1/1	0.97	0.12	69,69,69,69	0
58	MG	AA	3351	1/1	0.97	0.13	30,30,30,30	0
58	MG	CA	3391	1/1	0.97	0.05	63,63,63,63	0
58	MG	AA	3821	1/1	0.97	0.20	41,41,41,41	1
58	MG	AA	3684	1/1	0.97	0.10	29,29,29,29	0
58	MG	AA	3526	1/1	0.97	0.16	20,20,20,20	0
58	MG	AA	3555	1/1	0.97	0.16	38,38,38,38	0
58	MG	CA	3176	1/1	0.97	0.46	50,50,50,50	0
58	MG	CA	3490	1/1	0.97	0.27	67,67,67,67	0
58	MG	AA	3325	1/1	0.97	0.10	66,66,66,66	0
58	MG	CA	3274	1/1	0.97	0.11	50,50,50,50	1
58	MG	CA	3364	1/1	0.97	0.23	29,29,29,29	0
58	MG	DA	1752	1/1	0.97	0.21	74,74,74,74	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	AA	3557	1/1	0.97	0.17	19,19,19,19	0
58	MG	BA	1729	1/1	0.97	0.17	49,49,49,49	0
58	MG	AA	3066	1/1	0.97	0.28	50,50,50,50	0
58	MG	CA	3329	1/1	0.97	0.20	29,29,29,29	0
58	MG	CA	3289	1/1	0.97	0.30	42,42,42,42	0
58	MG	BA	1680	1/1	0.98	0.11	53,53,53,53	0
58	MG	AA	3023	1/1	0.98	0.31	33,33,33,33	1
58	MG	AA	3709	1/1	0.98	0.18	29,29,29,29	1
58	MG	CA	3050	1/1	0.98	0.09	44,44,44,44	0
58	MG	BA	1726	1/1	0.98	0.29	52,52,52,52	0
58	MG	AA	3393	1/1	0.98	0.18	21,21,21,21	0
58	MG	AA	3409	1/1	0.98	0.20	45,45,45,45	0
58	MG	AA	3384	1/1	0.98	0.15	34,34,34,34	0
58	MG	AA	3707	1/1	0.98	0.24	29,29,29,29	1
58	MG	AA	3609	1/1	0.98	0.18	53,53,53,53	0
58	MG	AA	3188	1/1	0.98	0.17	13,13,13,13	0
58	MG	AA	3815	1/1	0.98	0.17	29,29,29,29	1
58	MG	AA	3459	1/1	0.98	0.18	18,18,18,18	0
58	MG	AA	3408	1/1	0.98	0.15	20,20,20,20	0
58	MG	AA	3705	1/1	0.98	0.25	24,24,24,24	1
58	MG	CA	3496	1/1	0.98	0.17	63,63,63,63	0
58	MG	CF	304	1/1	0.98	0.34	65,65,65,65	0
58	MG	AA	3385	1/1	0.98	0.13	28,28,28,28	0
58	MG	AA	3564	1/1	0.98	0.21	19,19,19,19	0
58	MG	AA	3387	1/1	0.98	0.14	17,17,17,17	0
58	MG	BA	1770	1/1	0.98	0.36	56,56,56,56	0
58	MG	AA	3322	1/1	0.98	0.13	32,32,32,32	1
58	MG	AA	3003	1/1	0.98	0.08	20,20,20,20	0
58	MG	AA	3655	1/1	0.98	0.15	61,61,61,61	0
58	MG	AA	3454	1/1	0.98	0.11	51,51,51,51	0
58	MG	CA	3342	1/1	0.98	0.17	45,45,45,45	0
58	MG	CA	3415	1/1	0.98	0.20	31,31,31,31	1
58	MG	BA	1758	1/1	0.98	0.06	57,57,57,57	0
58	MG	AA	3045	1/1	0.98	0.20	43,43,43,43	0
58	MG	AA	3641	1/1	0.98	0.21	41,41,41,41	0
58	MG	AA	3307	1/1	0.98	0.15	6,6,6,6	0
58	MG	AA	3144	1/1	0.98	0.12	40,40,40,40	0
58	MG	AA	3749	1/1	0.98	0.13	14,14,14,14	0
58	MG	AA	3400	1/1	0.98	0.35	39,39,39,39	0
58	MG	CA	3299	1/1	0.98	0.13	61,61,61,61	0
58	MG	CA	3565	1/1	0.98	0.38	51,51,51,51	0
58	MG	AA	3386	1/1	0.98	0.22	29,29,29,29	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	CA	3201	1/1	0.98	0.38	59,59,59,59	0
60	SF4	DD	501	8/8	0.98	0.10	90,90,90,90	1
58	MG	CA	3282	1/1	0.98	0.12	50,50,50,50	0
58	MG	AA	3541	1/1	0.98	0.18	43,43,43,43	0
58	MG	AA	3127	1/1	0.98	0.36	71,71,71,71	0
58	MG	CA	3270	1/1	0.98	0.19	35,35,35,35	0
58	MG	AA	3777	1/1	0.98	0.10	19,19,19,19	0
58	MG	CA	3148	1/1	0.98	0.27	65,65,65,65	0
58	MG	AA	3534	1/1	0.98	0.16	27,27,27,27	0
58	MG	A0	101	1/1	0.98	0.14	43,43,43,43	0
58	MG	AA	3723	1/1	0.98	0.19	21,21,21,21	0
58	MG	CA	3305	1/1	0.98	0.15	62,62,62,62	0
58	MG	AA	3157	1/1	0.98	0.10	34,34,34,34	0
58	MG	AA	3243	1/1	0.98	0.23	24,24,24,24	1
58	MG	AA	3482	1/1	0.98	0.14	65,65,65,65	0
58	MG	BA	1786	1/1	0.98	0.15	66,66,66,66	0
58	MG	AA	3473	1/1	0.98	0.20	15,15,15,15	0
58	MG	AA	3329	1/1	0.98	0.23	17,17,17,17	0
58	MG	CA	3119	1/1	0.98	0.31	128,128,128,128	0
58	MG	CA	3655	1/1	0.98	0.23	70,70,70,70	0
58	MG	AA	3413	1/1	0.98	0.16	20,20,20,20	0
58	MG	AA	3488	1/1	0.98	0.22	20,20,20,20	0
58	MG	AA	3259	1/1	0.98	0.32	20,20,20,20	1
58	MG	AA	3521	1/1	0.98	0.15	29,29,29,29	0
58	MG	AA	3530	1/1	0.98	0.12	53,53,53,53	0
58	MG	AA	3389	1/1	0.98	0.19	17,17,17,17	0
58	MG	CA	3408	1/1	0.98	0.12	64,64,64,64	0
58	MG	AA	3374	1/1	0.98	0.07	18,18,18,18	0
58	MG	AA	3340	1/1	0.98	0.10	59,59,59,59	0
58	MG	CA	3301	1/1	0.98	0.33	47,47,47,47	0
58	MG	AB	3013	1/1	0.98	0.18	54,54,54,54	0
58	MG	AB	3022	1/1	0.98	0.05	58,58,58,58	0
58	MG	AA	3103	1/1	0.98	0.07	15,15,15,15	0
58	MG	BA	1750	1/1	0.98	0.25	65,65,65,65	0
58	MG	AA	3195	1/1	0.98	0.18	50,50,50,50	0
58	MG	CA	3397	1/1	0.98	0.13	59,59,59,59	0
58	MG	AA	3478	1/1	0.98	0.15	40,40,40,40	0
58	MG	CA	3456	1/1	0.98	0.13	60,60,60,60	0
58	MG	CA	3637	1/1	0.98	0.34	59,59,59,59	0
58	MG	AA	3097	1/1	0.98	0.18	26,26,26,26	0
58	MG	CA	3219	1/1	0.98	0.21	31,31,31,31	0
58	MG	AA	3299	1/1	0.98	0.13	20,20,20,20	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	BA	1755	1/1	0.98	0.30	38,38,38,38	0
58	MG	CA	3264	1/1	0.98	0.17	59,59,59,59	0
58	MG	AA	3513	1/1	0.98	0.11	35,35,35,35	0
58	MG	CA	3560	1/1	0.98	0.12	36,36,36,36	0
58	MG	AA	3467	1/1	0.98	0.12	44,44,44,44	0
58	MG	BA	1778	1/1	0.98	0.07	42,42,42,42	0
58	MG	CA	3297	1/1	0.98	0.34	56,56,56,56	0
58	MG	AA	3514	1/1	0.98	0.13	18,18,18,18	0
58	MG	AA	3734	1/1	0.98	0.17	22,22,22,22	0
60	SF4	BD	501	8/8	0.98	0.09	80,80,80,80	0
59	ZN	CY	501	1/1	0.98	0.04	93,93,93,93	0
58	MG	CA	3320	1/1	0.98	0.15	30,30,30,30	0
58	MG	CA	3369	1/1	0.98	0.12	59,59,59,59	0
58	MG	CA	3417	1/1	0.98	0.21	37,37,37,37	0
58	MG	CA	3440	1/1	0.98	0.31	57,57,57,57	0
58	MG	CA	3352	1/1	0.98	0.17	68,68,68,68	0
58	MG	AB	3002	1/1	0.98	0.18	59,59,59,59	0
58	MG	AA	3361	1/1	0.98	0.14	29,29,29,29	0
58	MG	AA	3251	1/1	0.98	0.13	42,42,42,42	0
58	MG	CA	3339	1/1	0.98	0.14	34,34,34,34	0
58	MG	BA	1720	1/1	0.98	0.44	62,62,62,62	0
58	MG	AA	3407	1/1	0.98	0.12	49,49,49,49	0
58	MG	CA	3564	1/1	0.99	0.19	40,40,40,40	1
59	ZN	C5	102	1/1	0.99	0.09	68,68,68,68	0
58	MG	AE	302	1/1	0.99	0.23	18,18,18,18	0
58	MG	AA	3342	1/1	0.99	0.13	5,5,5,5	0
58	MG	AA	3791	1/1	0.99	0.25	16,16,16,16	0
58	MG	AA	3377	1/1	0.99	0.18	20,20,20,20	0
59	ZN	AY	501	1/1	0.99	0.08	65,65,65,65	0
58	MG	DA	1699	1/1	0.99	0.07	75,75,75,75	0
58	MG	CA	3587	1/1	0.99	0.12	34,34,34,34	0
58	MG	AA	3498	1/1	0.99	0.11	37,37,37,37	0
58	MG	DZ	702	1/1	0.99	0.27	57,57,57,57	0
58	MG	AA	3038	1/1	0.99	0.12	11,11,11,11	0
58	MG	DA	1615	1/1	0.99	0.53	53,53,53,53	0
58	MG	CA	3092	1/1	0.99	0.16	70,70,70,70	0
58	MG	AA	3658	1/1	0.99	0.14	62,62,62,62	0
59	ZN	C6	501	1/1	0.99	0.10	61,61,61,61	0
58	MG	AA	3643	1/1	0.99	0.17	49,49,49,49	0
59	ZN	C9	501	1/1	0.99	0.07	94,94,94,94	0
58	MG	AA	3635	1/1	0.99	0.11	23,23,23,23	0
58	MG	CA	3517	1/1	0.99	0.32	64,64,64,64	0

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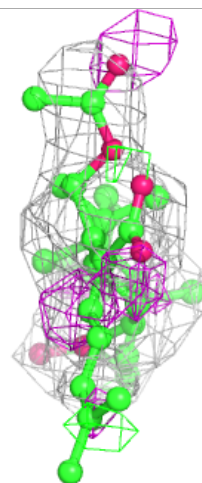
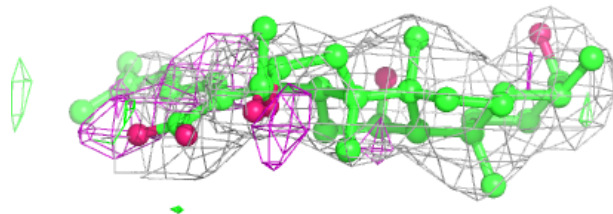
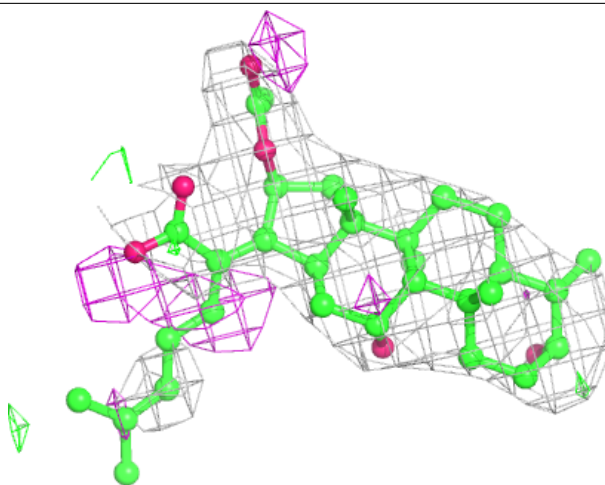
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	AA	3276	1/1	0.99	0.27	47,47,47,47	1
58	MG	CA	3175	1/1	0.99	0.28	42,42,42,42	0
58	MG	AA	3398	1/1	0.99	0.14	15,15,15,15	0
58	MG	AA	3583	1/1	0.99	0.15	13,13,13,13	0
58	MG	CA	3345	1/1	0.99	0.21	38,38,38,38	0
58	MG	AB	3012	1/1	0.99	0.21	29,29,29,29	1
58	MG	DA	1645	1/1	0.99	0.12	64,64,64,64	0
58	MG	CA	3372	1/1	0.99	0.13	42,42,42,42	0
58	MG	CA	3318	1/1	0.99	0.21	33,33,33,33	0
58	MG	CA	3322	1/1	0.99	0.27	45,45,45,45	0
58	MG	CA	3617	1/1	0.99	0.12	31,31,31,31	0
58	MG	CA	3502	1/1	0.99	0.13	70,70,70,70	0
58	MG	AA	3388	1/1	0.99	0.22	25,25,25,25	0
59	ZN	A6	102	1/1	1.00	0.11	46,46,46,46	0
59	ZN	A9	501	1/1	1.00	0.10	42,42,42,42	0
59	ZN	A5	101	1/1	1.00	0.12	36,36,36,36	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.

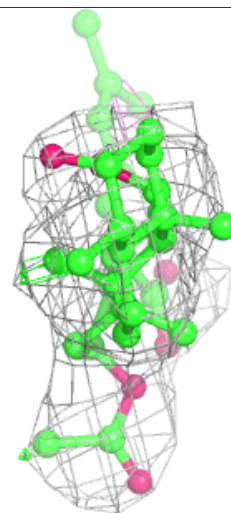
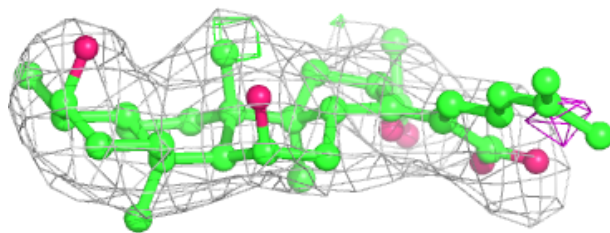
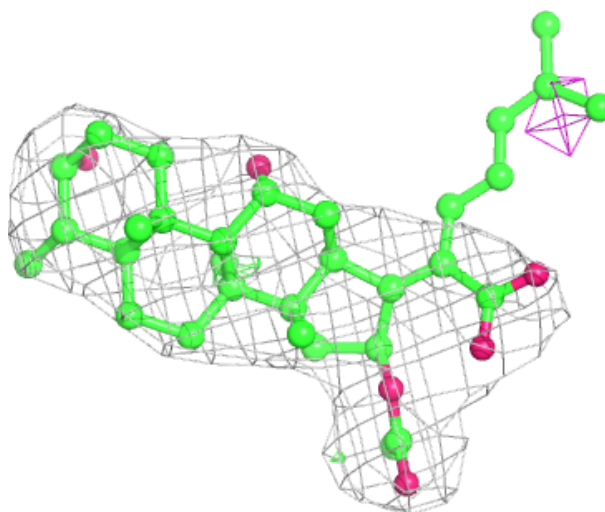
Electron density around FUA BZ 703:

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



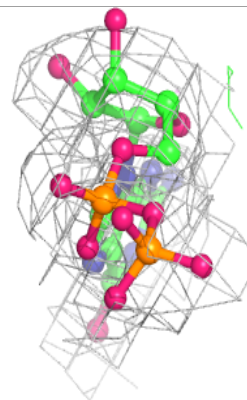
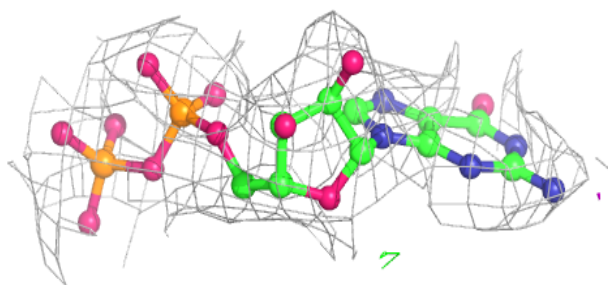
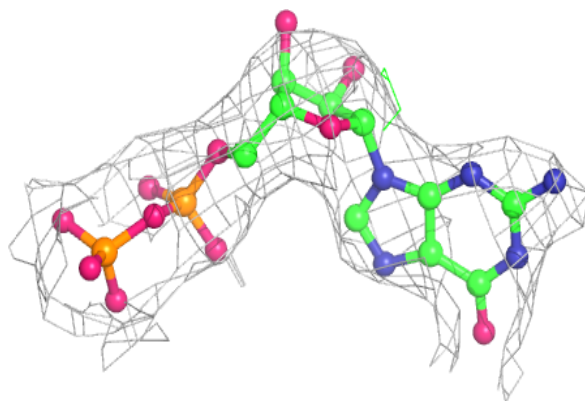
Electron density around FUA DZ 703:

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

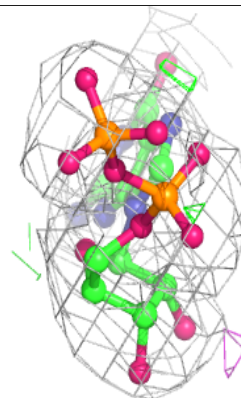
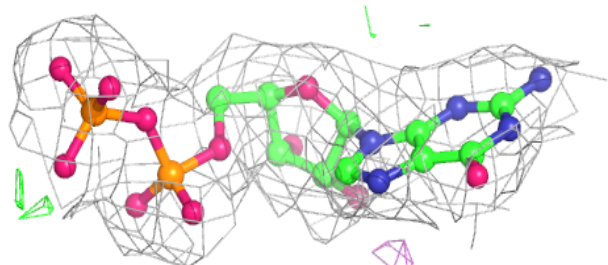
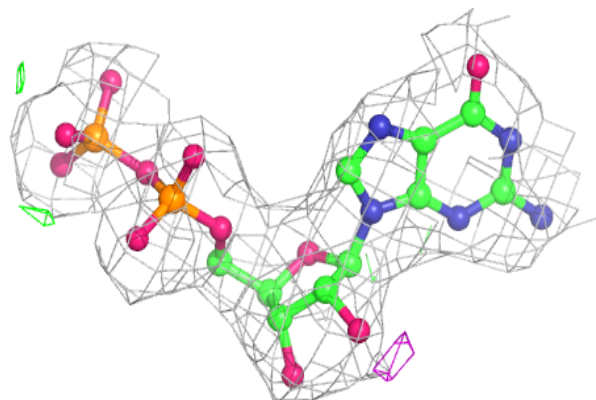


Electron density around GDP DZ 704:

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

**Electron density around GDP BZ 704:**

$2mF_o-DF_c$ (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.