



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 5, 2026 – 11:53 PM UTC

PDB ID : 4V83 / pdb_00004v83
Title : Crystal structure of a complex containing domain 3 from the PSIV IGR IRES RNA bound to the 70S ribosome.
Authors : Zhu, J.; Korostelev, A.; Costantino, D.; Noller, H.F.; Kieft, J.S.
Deposited on : 2010-12-13
Resolution : 3.50 Å(reported)

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

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A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

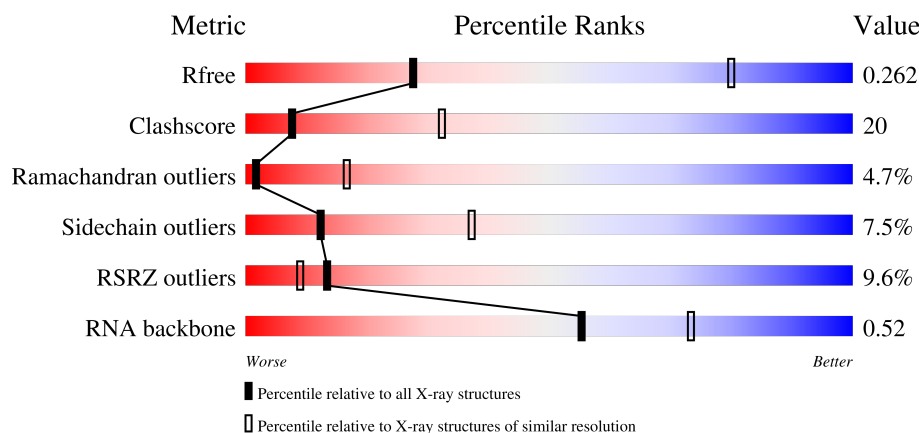
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.50 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}	180053	1085 (3.54-3.46)
Clashscore	190562	1140 (3.54-3.46)
Ramachandran outliers	187476	1113 (3.54-3.46)
Sidechain outliers	187428	1114 (3.54-3.46)
RSRZ outliers	180081	1084 (3.54-3.46)
RNA backbone	3983	1010 (3.98-3.02)

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

Mol	Chain	Length	Quality of chain
1	AA	1506	5% 47% 45% 8%
1	CA	1506	10% 47% 44% 8%
2	AB	234	8% 46% 47% 7%
2	CB	234	11% 47% 46% 7%

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Mol	Chain	Length	Quality of chain
3	AC	206	
3	CC	206	
4	AD	208	
4	CD	208	
5	AE	151	
5	CE	151	
6	AF	101	
6	CF	101	
7	AG	155	
7	CG	155	
8	AH	138	
8	CH	138	
9	AI	127	
9	CI	127	
10	AJ	98	
10	CJ	98	
11	AK	119	
11	CK	119	
12	AL	124	
12	CL	124	
13	AM	116	
13	CM	116	
14	AN	60	
14	CN	60	
15	AO	88	

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Mol	Chain	Length	Quality of chain
15	CO	88	
16	AP	83	
16	CP	83	
17	AQ	99	
17	CQ	99	
18	AR	70	
18	CR	70	
19	AS	78	
19	CS	78	
20	AT	99	
20	CT	99	
21	AU	24	
21	CU	24	
22	AV	35	
22	CV	35	
23	BA	2879	
23	DA	2879	
24	BB	119	
24	DB	119	
25	BC	271	
25	DC	271	
26	BD	204	
26	DD	204	
27	BE	202	
27	DE	202	

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Mol	Chain	Length	Quality of chain
28	BF	181	
28	DF	181	
29	BG	159	
29	DG	159	
30	BH	145	
30	DH	145	
31	BI	65	
31	DI	65	
32	BJ	137	
32	DJ	137	
33	BK	122	
33	DK	122	
34	BL	146	
34	DL	146	
35	BM	136	
35	DM	136	
36	BN	117	
36	DN	117	
37	BO	98	
37	DO	98	
38	BP	137	
38	DP	137	
39	BQ	116	
39	DQ	116	
40	BR	101	

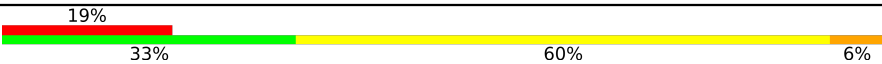
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Mol	Chain	Length	Quality of chain
40	DR	101	
41	BS	112	
41	DS	112	
42	BT	92	
42	DT	92	
43	BU	100	
43	DU	100	
44	BV	188	
44	DV	188	
45	BW	76	
45	DW	76	
46	BX	88	
46	DX	88	
47	BY	62	
47	DY	62	
48	BZ	59	
48	DZ	59	
49	B1	30	
49	D1	30	
50	B2	52	
50	D2	52	
51	B3	44	
51	D3	44	
52	B4	48	
52	D4	48	

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Mol	Chain	Length	Quality of chain
53	B5	63	
53	D5	63	

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
54	MG	AA	1687	-	-	-	X
54	MG	AA	1717	-	-	-	X
54	MG	BA	3002	-	-	-	X
54	MG	BA	3036	-	-	-	X
54	MG	BA	3040	-	-	-	X
54	MG	BA	3060	-	-	-	X
54	MG	BA	3195	-	-	-	X
54	MG	BA	3414	-	-	-	X
54	MG	BA	3501	-	-	-	X
54	MG	BA	3606	-	-	-	X
54	MG	BB	216	-	-	-	X
54	MG	CA	1627	-	-	-	X
54	MG	CA	1754	-	-	-	X
54	MG	DA	3063	-	-	-	X
54	MG	DA	3209	-	-	-	X
54	MG	DA	3367	-	-	-	X
54	MG	DA	3397	-	-	-	X
54	MG	DA	3574	-	-	-	X
54	MG	DA	3700	-	-	-	X
54	MG	DA	3786	-	-	-	X
54	MG	DL	202	-	-	-	X

2 Entry composition

There are 55 unique types of molecules in this entry. The entry contains 283641 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 ribosomal RNA 16S.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	AA	1506	Total	C	N	O	P	0	0	0
			32372	14409	5999	10459	1505			
1	CA	1506	Total	C	N	O	P	0	0	0
			32372	14409	5999	10459	1505			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	AB	234	Total	C	N	O	S	0	0	0
			1901	1213	341	342	5			
2	CB	234	Total	C	N	O	S	0	0	0
			1901	1213	341	342	5			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	AC	206	Total	C	N	O	S	0	0	0
			1613	1016	314	282	1			
3	CC	206	Total	C	N	O	S	0	0	0
			1613	1016	314	282	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	AD	208	Total	C	N	O	S	0	0	0
			1703	1066	339	291	7			
4	CD	208	Total	C	N	O	S	0	0	0
			1703	1066	339	291	7			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	AE	151	Total	C	N	O	S	0	0	0
			1156	729	218	205	4			
5	CE	151	Total	C	N	O	S	0	0	0
			1156	729	218	205	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	AF	101	Total	C	N	O	S	0	0	0
			843	531	155	154	3			
6	CF	101	Total	C	N	O	S	0	0	0
			843	531	155	154	3			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	AG	155	Total	C	N	O	S	0	0	0
			1257	781	252	218	6			
7	CG	155	Total	C	N	O	S	0	0	0
			1257	781	252	218	6			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	AH	138	Total	C	N	O	S	0	0	0
			1116	705	215	193	3			
8	CH	138	Total	C	N	O	S	0	0	0
			1116	705	215	193	3			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	AI	127	Total	C	N	O		0	0	0
			1011	639	198	174				
9	CI	127	Total	C	N	O		0	0	0
			1011	639	198	174				

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	AJ	98	Total	C	N	O	S	0	0	0
			795	499	156	139	1			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	CJ	98	Total	C	N	O	S	0	0	0
			795	499	156	139	1			

- Molecule 11 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	AK	119	Total	C	N	O	S	0	0	0
			885	549	168	165	3			
11	CK	119	Total	C	N	O	S	0	0	0
			885	549	168	165	3			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	AL	124	Total	C	N	O	S	0	0	0
			971	611	195	164	1			
12	CL	124	Total	C	N	O	S	0	0	0
			971	611	195	164	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	AM	116	Total	C	N	O	S	0	0	0
			929	574	191	162	2			
13	CM	116	Total	C	N	O	S	0	0	0
			929	574	191	162	2			

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	AO	88	Total	C	N	O	S	0	0	0
			734	459	147	126	2			
15	CO	88	Total	C	N	O	S	0	0	0
			734	459	147	126	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	AP	83	Total	C	N	O	S	0	0	0
			701	443	139	118	1			
16	CP	83	Total	C	N	O	S	0	0	0
			701	443	139	118	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	AQ	99	Total	C	N	O	S	0	0	0
			824	528	152	142	2			
17	CQ	99	Total	C	N	O	S	0	0	0
			824	528	152	142	2			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
18	AR	70	Total	C	N	O	0	0	0
			574	367	112	95			
18	CR	70	Total	C	N	O	0	0	0
			574	367	112	95			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	AS	78	Total	C	N	O	S	0	0	0
			630	403	114	111	2			
19	CS	78	Total	C	N	O	S	0	0	0
			630	403	114	111	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	AT	99	Total	C	N	O	S	0	0	0
			762	469	162	129	2			
20	CT	99	Total	C	N	O	S	0	0	0
			762	469	162	129	2			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
21	AU	24	Total	C	N	O	0	0	0
			209	128	50	31			
21	CU	24	Total	C	N	O	0	0	0
			209	128	50	31			

- Molecule 22 is a RNA chain called domain 3 of PSIC IGR IRES RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	AV	35	Total	C	N	O	P	0	0	0
			736	332	128	243	33			
22	CV	35	Total	C	N	O	P	0	0	0
			736	332	128	243	33			

- Molecule 23 is a RNA chain called 23S ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	BA	2760	Total	C	N	O	P	0	0	0
			59442	26456	11114	19113	2759			
23	DA	2760	Total	C	N	O	P	0	0	0
			59442	26456	11114	19113	2759			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
BA	1142	U	C	SEE REMARK 999	GB AE017221.1
BA	2825	U	G	SEE REMARK 999	GB AE017221.1
DA	1142	U	C	SEE REMARK 999	GB AE017221.1
DA	2825	U	G	SEE REMARK 999	GB AE017221.1

- Molecule 24 is a RNA chain called 5S ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	BB	119	Total	C	N	O	P	0	0	0
			2551	1136	471	826	118			
24	DB	119	Total	C	N	O	P	0	0	0
			2551	1136	471	826	118			

- Molecule 25 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
25	BC	271	Total	C	N	O	S	0	0	0
			2105	1329	416	357	3			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
25	DC	271	Total	C	N	O	S	0	0	0
			2105	1329	416	357	3			

- Molecule 26 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	BD	204	Total	C	N	O	S	0	0	0
			1564	988	299	271	6			
26	DD	204	Total	C	N	O	S	0	0	0
			1564	988	299	271	6			

- Molecule 27 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
27	BE	202	Total	C	N	O	S	0	0	0
			1587	1011	297	276	3			
27	DE	202	Total	C	N	O	S	0	0	0
			1587	1011	297	276	3			

- Molecule 28 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
28	BF	181	Total	C	N	O	S	0	0	0
			1475	943	268	260	4			
28	DF	181	Total	C	N	O	S	0	0	0
			1475	943	268	260	4			

- Molecule 29 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
29	BG	159	Total	C	N	O	S	0	0	0
			1223	773	228	221	1			
29	DG	159	Total	C	N	O	S	0	0	0
			1223	773	228	221	1			

- Molecule 30 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
30	BH	145	Total	C	N	O	S	0	0	0
			1133	724	200	208	1			
30	DH	145	Total	C	N	O	S	0	0	0
			1133	724	200	208	1			

- Molecule 31 is a protein called 50S ribosomal protein L10.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
31	BI	32	Total	C	N	O	0	0	0
			254	157	49	48			
31	DI	32	Total	C	N	O	0	0	0
			254	157	49	48			

- Molecule 32 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
32	BJ	137	Total	C	N	O	S	0	0	0
			1097	707	205	182	3			
32	DJ	137	Total	C	N	O	S	0	0	0
			1097	707	205	182	3			

- Molecule 33 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
33	BK	122	Total	C	N	O	S	0	0	0
			932	587	171	170	4			
33	DK	122	Total	C	N	O	S	0	0	0
			932	587	171	170	4			

- Molecule 34 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
34	BL	146	Total	C	N	O	S	0	0	0
			1114	692	227	193	2			
34	DL	146	Total	C	N	O	S	0	0	0
			1114	692	227	193	2			

- Molecule 35 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
35	BM	136	Total	C	N	O	S	0	0	0
			1079	688	204	182	5			
35	DM	136	Total	C	N	O	S	0	0	0
			1079	688	204	182	5			

- Molecule 36 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
36	BN	117	Total	C	N	O	0	0	0
			960	599	202	159			
36	DN	117	Total	C	N	O	0	0	0
			960	599	202	159			

- Molecule 37 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
37	BO	98	Total	C	N	O	0	0	0
			771	486	154	131			
37	DO	98	Total	C	N	O	0	0	0
			771	486	154	131			

- Molecule 38 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
38	BP	137	Total	C	N	O	S	0	0	0
			1144	713	234	196	1			
38	DP	137	Total	C	N	O	S	0	0	0
			1144	713	234	196	1			

- Molecule 39 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
39	BQ	116	Total	C	N	O	S	0	0	0
			953	601	201	150	1			
39	DQ	116	Total	C	N	O	S	0	0	0
			953	601	201	150	1			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
BQ	?	-	PHE	deletion	UNP Q72L76
DQ	?	-	PHE	deletion	UNP Q72L76

- Molecule 40 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
40	BR	101	Total	C	N	O	S	0	0	0
			779	501	142	135	1			
40	DR	101	Total	C	N	O	S	0	0	0
			779	501	142	135	1			

- Molecule 41 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
41	BS	112	Total	C	N	O	S	0	0	0
			891	560	175	154	2			
41	DS	112	Total	C	N	O	S	0	0	0
			891	560	175	154	2			

- Molecule 42 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
42	BT	92	Total	C	N	O		0	0	0
			726	471	131	124				
42	DT	92	Total	C	N	O		0	0	0
			726	471	131	124				

- Molecule 43 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
43	BU	100	Total	C	N	O	S	0	0	0
			776	500	148	124	4			
43	DU	100	Total	C	N	O	S	0	0	0
			776	500	148	124	4			

- Molecule 44 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
44	BV	188	Total	C	N	O	S	0	0	0
			1492	950	265	275	2			
44	DV	188	Total	C	N	O	S	0	0	0
			1492	950	265	275	2			

- Molecule 45 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
45	BW	76	Total	C	N	O	S	0	0	0
			605	376	126	102	1			
45	DW	76	Total	C	N	O	S	0	0	0
			605	376	126	102	1			

- Molecule 46 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
46	BX	88	Total	C	N	O	0	0	0
			695	435	141	119			
46	DX	88	Total	C	N	O	0	0	0
			695	435	141	119			

- Molecule 47 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
47	BY	62	Total	C	N	O	S	0	0	0
			521	325	102	92	2			
47	DY	62	Total	C	N	O	S	0	0	0
			521	325	102	92	2			

- Molecule 48 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
48	BZ	59	Total	C	N	O	S	0	0	0
			468	298	90	79	1			
48	DZ	59	Total	C	N	O	S	0	0	0
			468	298	90	79	1			

- Molecule 49 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
49	B1	30	Total	C	N	O	S	0	0	0
			226	142	36	44	4			
49	D1	30	Total	C	N	O	S	0	0	0
			226	142	36	44	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
50	B2	52	Total	C	N	O	S	0	0	0
			405	255	79	66	5			
50	D2	52	Total	C	N	O	S	0	0	0
			405	255	79	66	5			

- Molecule 51 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
51	B3	44	Total	C	N	O	S	0	0	0
			381	235	77	65	4			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
51	D3	44	Total	C	N	O	S	0	0	0
			381	235	77	65	4			

- Molecule 52 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
52	B4	48	Total	C	N	O	S	0	0	0
			419	257	104	56	2			
52	D4	48	Total	C	N	O	S	0	0	0
			419	257	104	56	2			

- Molecule 53 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
53	B5	63	Total	C	N	O	S	0	0	0
			508	326	101	79	2			
53	D5	63	Total	C	N	O	S	0	0	0
			508	326	101	79	2			

- Molecule 54 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
54	AA	279	Total	Mg	0	0
			279	279		
54	AB	3	Total	Mg	0	0
			3	3		
54	AC	2	Total	Mg	0	0
			2	2		
54	AD	3	Total	Mg	0	0
			3	3		
54	AE	5	Total	Mg	0	0
			5	5		
54	AF	1	Total	Mg	0	0
			1	1		
54	AG	2	Total	Mg	0	0
			2	2		
54	AH	1	Total	Mg	0	0
			1	1		
54	AI	1	Total	Mg	0	0
			1	1		
54	AK	2	Total	Mg	0	0
			2	2		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
54	AL	2	Total 2	Mg 2	0	0
54	AM	1	Total 1	Mg 1	0	0
54	AN	1	Total 1	Mg 1	0	0
54	AO	3	Total 3	Mg 3	0	0
54	AQ	3	Total 3	Mg 3	0	0
54	AS	1	Total 1	Mg 1	0	0
54	AT	2	Total 2	Mg 2	0	0
54	AV	8	Total 8	Mg 8	0	0
54	BA	781	Total 781	Mg 781	0	0
54	BB	27	Total 27	Mg 27	0	0
54	BC	3	Total 3	Mg 3	0	0
54	BE	2	Total 2	Mg 2	0	0
54	BF	1	Total 1	Mg 1	0	0
54	BH	1	Total 1	Mg 1	0	0
54	BI	1	Total 1	Mg 1	0	0
54	BJ	3	Total 3	Mg 3	0	0
54	BK	1	Total 1	Mg 1	0	0
54	BM	3	Total 3	Mg 3	0	0
54	BN	2	Total 2	Mg 2	0	0
54	BO	1	Total 1	Mg 1	0	0
54	BP	2	Total 2	Mg 2	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
54	BR	1	Total 1	Mg 1	0	0
54	BS	1	Total 1	Mg 1	0	0
54	BT	2	Total 2	Mg 2	0	0
54	BU	2	Total 2	Mg 2	0	0
54	BV	3	Total 3	Mg 3	0	0
54	BW	1	Total 1	Mg 1	0	0
54	BX	2	Total 2	Mg 2	0	0
54	BY	3	Total 3	Mg 3	0	0
54	B2	3	Total 3	Mg 3	0	0
54	B3	1	Total 1	Mg 1	0	0
54	B4	1	Total 1	Mg 1	0	0
54	B5	1	Total 1	Mg 1	0	0
54	CA	372	Total 372	Mg 372	0	0
54	CB	3	Total 3	Mg 3	0	0
54	CC	8	Total 8	Mg 8	0	0
54	CD	3	Total 3	Mg 3	0	0
54	CE	5	Total 5	Mg 5	0	0
54	CF	2	Total 2	Mg 2	0	0
54	CG	3	Total 3	Mg 3	0	0
54	CK	1	Total 1	Mg 1	0	0
54	CL	6	Total 6	Mg 6	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
54	CM	2	Total 2	Mg 2	0	0
54	CN	1	Total 1	Mg 1	0	0
54	CO	4	Total 4	Mg 4	0	0
54	CQ	2	Total 2	Mg 2	0	0
54	CV	7	Total 7	Mg 7	0	0
54	DA	964	Total 964	Mg 964	0	0
54	DB	43	Total 43	Mg 43	0	0
54	DC	3	Total 3	Mg 3	0	0
54	DD	6	Total 6	Mg 6	0	0
54	DE	3	Total 3	Mg 3	0	0
54	DF	2	Total 2	Mg 2	0	0
54	DG	3	Total 3	Mg 3	0	0
54	DI	1	Total 1	Mg 1	0	0
54	DJ	6	Total 6	Mg 6	0	0
54	DK	3	Total 3	Mg 3	0	0
54	DL	3	Total 3	Mg 3	0	0
54	DM	1	Total 1	Mg 1	0	0
54	DN	1	Total 1	Mg 1	0	0
54	DO	1	Total 1	Mg 1	0	0
54	DP	2	Total 2	Mg 2	0	0
54	DQ	2	Total 2	Mg 2	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
54	DS	2	Total 2	Mg 2	0	0
54	DU	1	Total 1	Mg 1	0	0
54	DV	4	Total 4	Mg 4	0	0
54	DW	1	Total 1	Mg 1	0	0
54	DX	3	Total 3	Mg 3	0	0
54	DY	2	Total 2	Mg 2	0	0
54	D1	1	Total 1	Mg 1	0	0
54	D2	3	Total 3	Mg 3	0	0
54	D3	1	Total 1	Mg 1	0	0
54	D4	4	Total 4	Mg 4	0	0
54	D5	3	Total 3	Mg 3	0	0

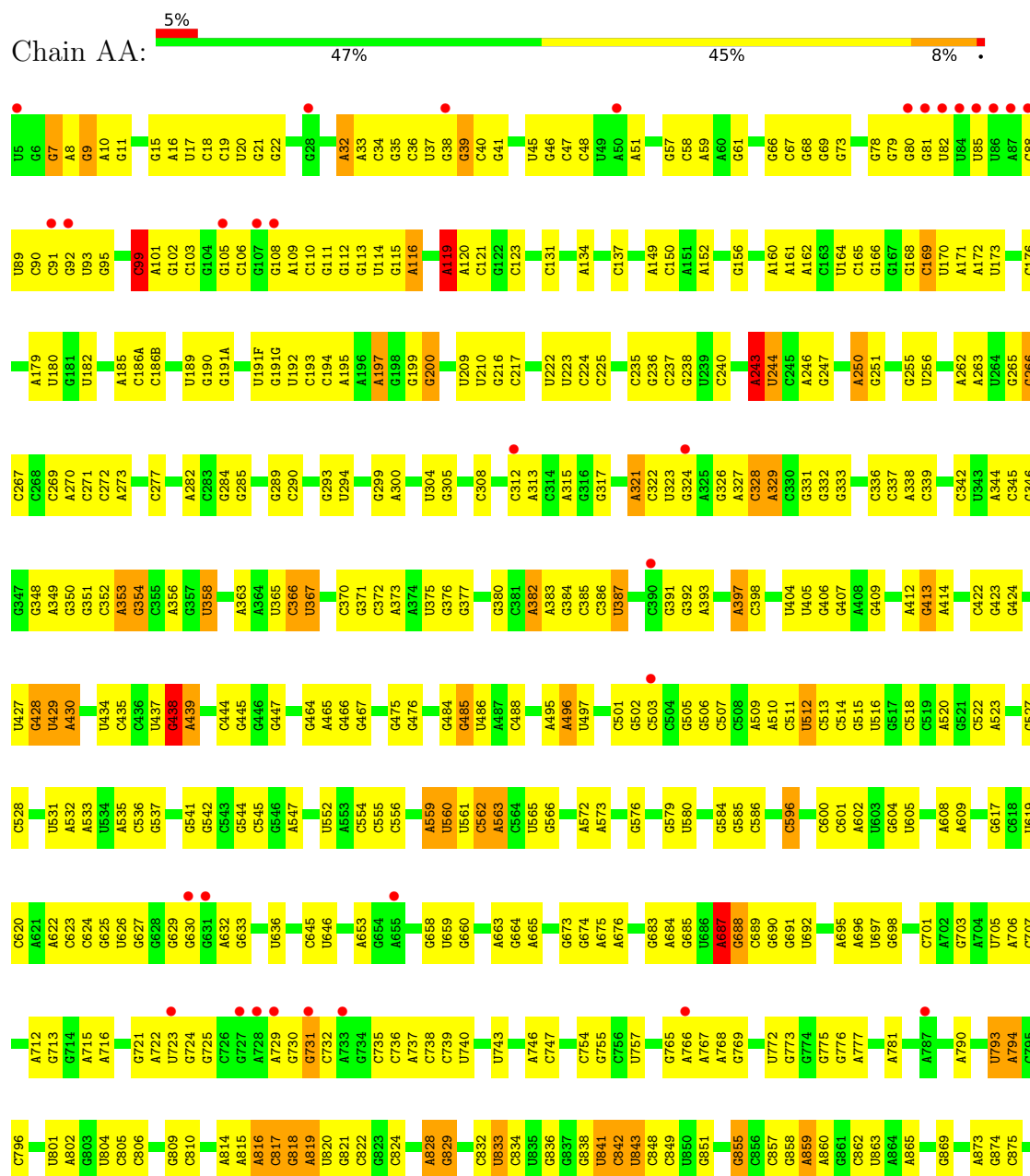
- Molecule 55 is ZINC ION (CCD ID: ZN) (formula: Zn).

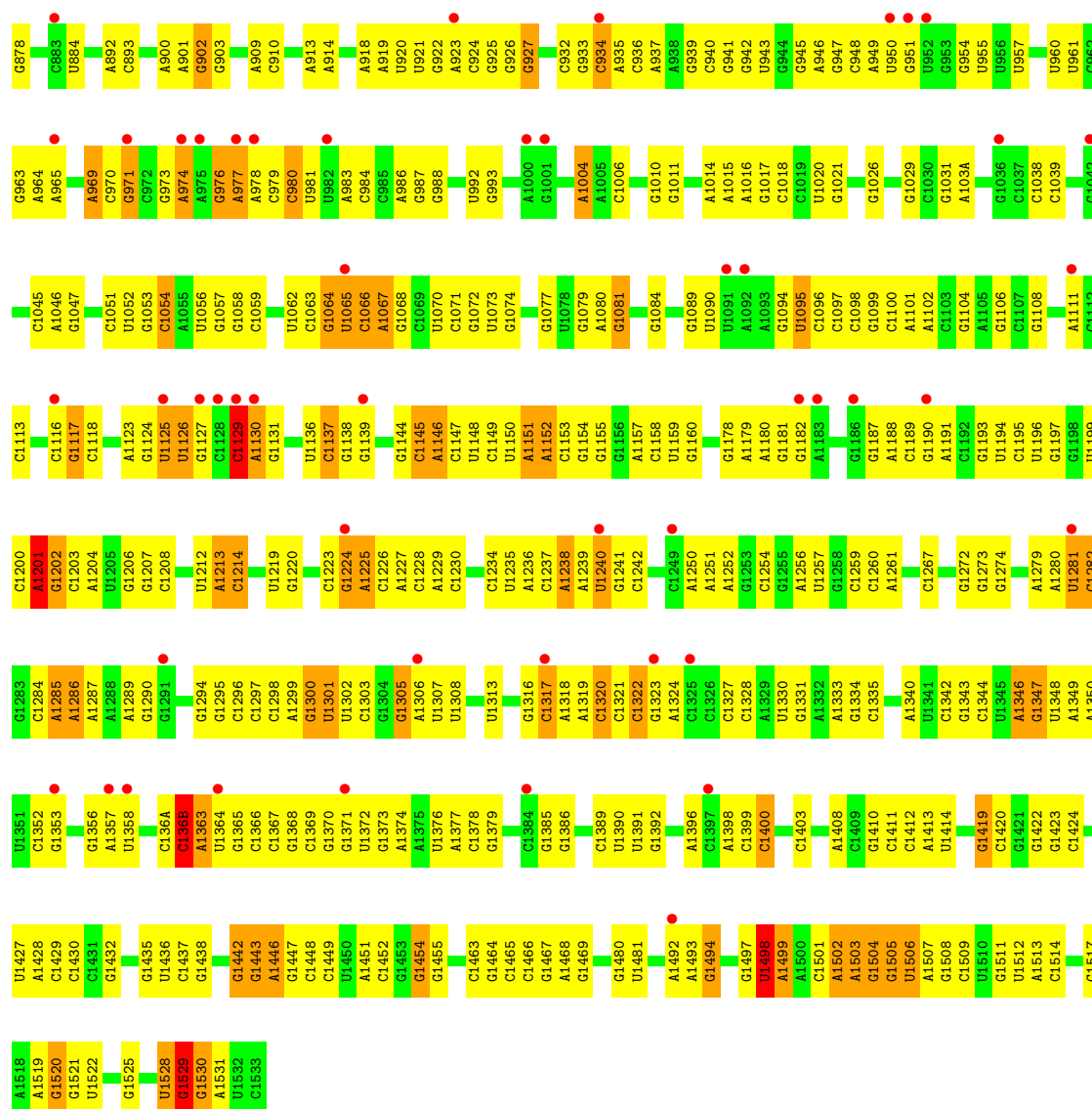
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
55	AD	1	Total 1	Zn 1	0	0
55	AN	1	Total 1	Zn 1	0	0
55	CD	1	Total 1	Zn 1	0	0
55	CN	1	Total 1	Zn 1	0	0

3 Residue-property plots

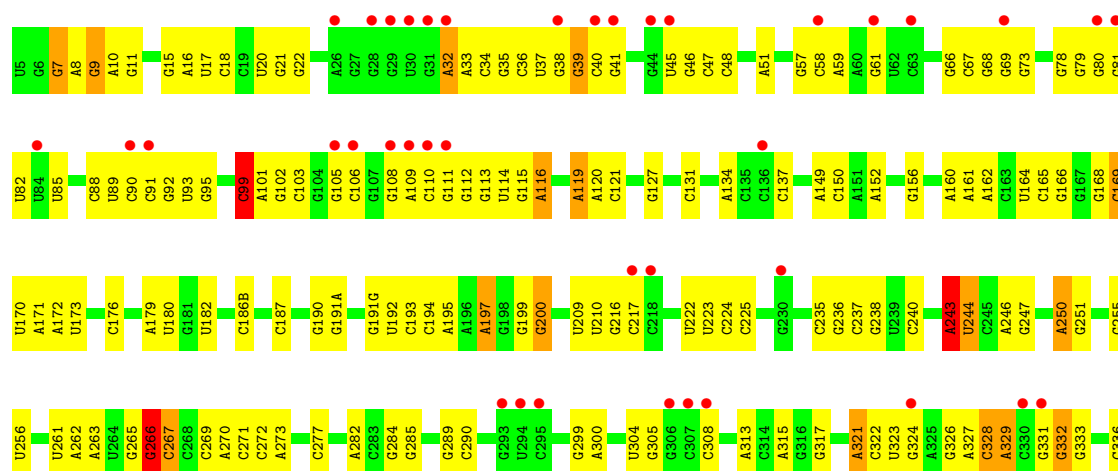
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

• Molecule 1: ribosomal RNA 16S

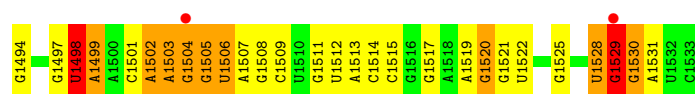




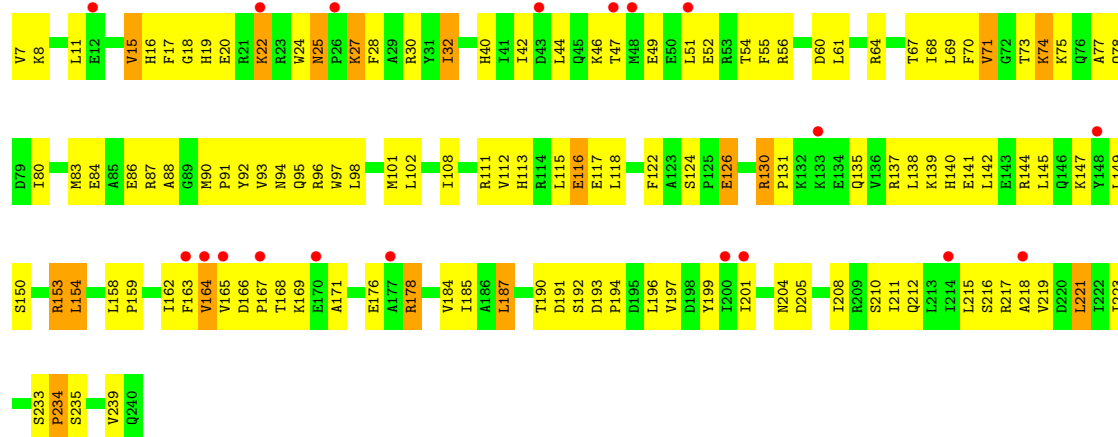
• Molecule 1: ribosomal RNA 16S



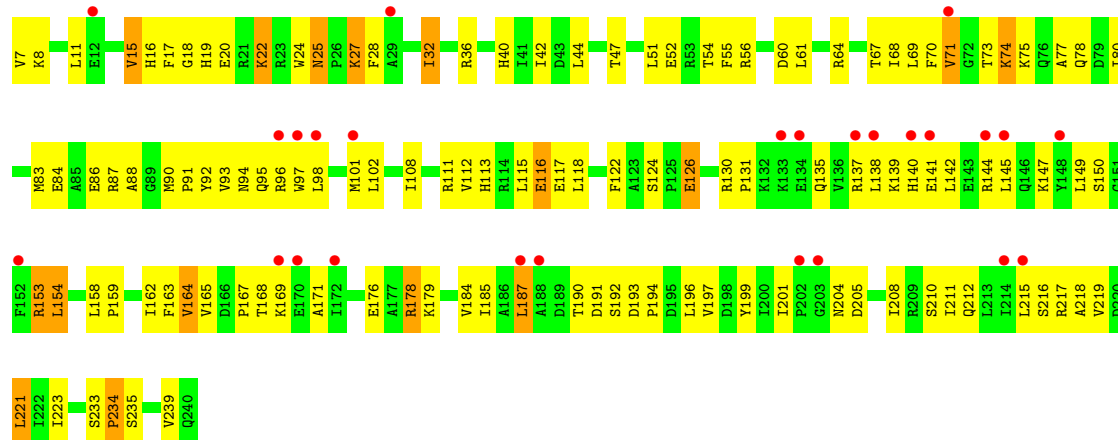




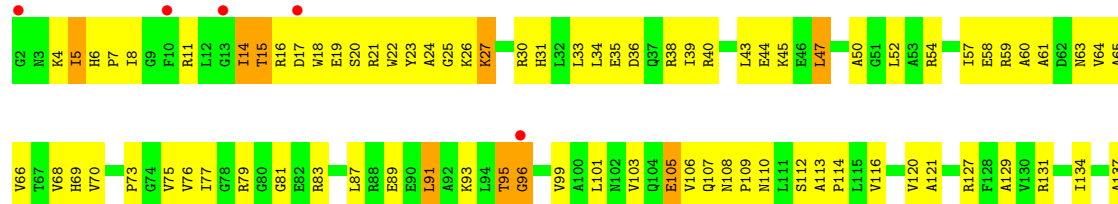
• Molecule 2: 30S ribosomal protein S2

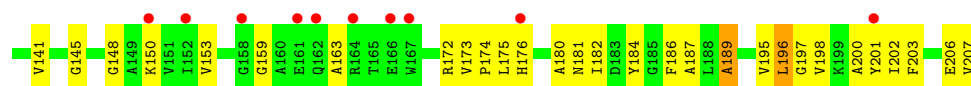


• Molecule 2: 30S ribosomal protein S2

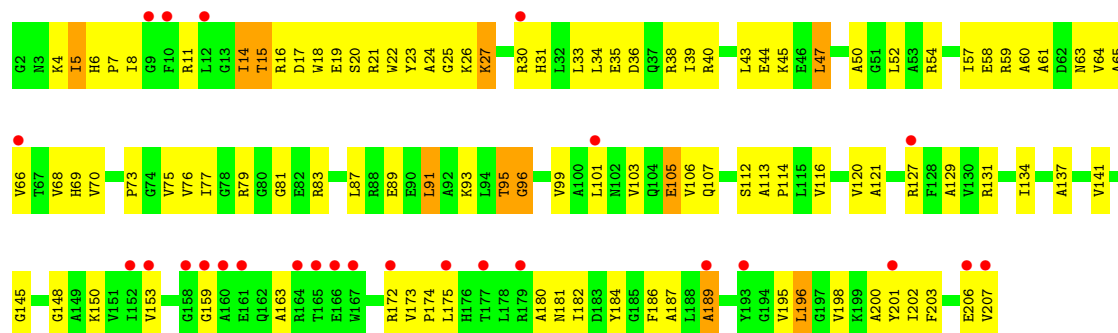


• Molecule 3: 30S ribosomal protein S3

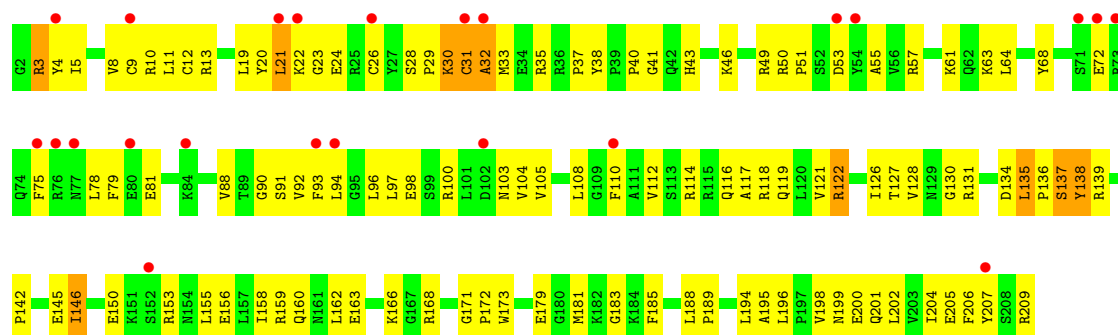




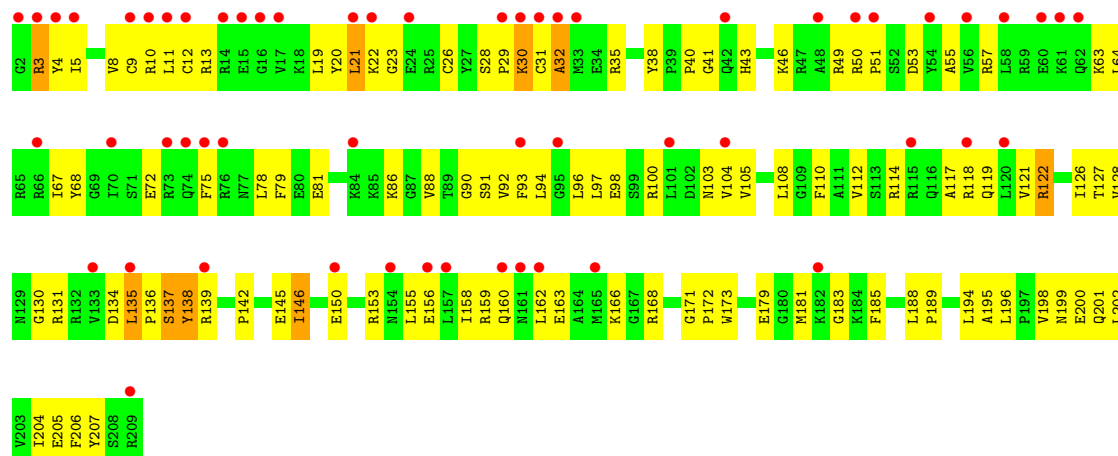
• Molecule 3: 30S ribosomal protein S3



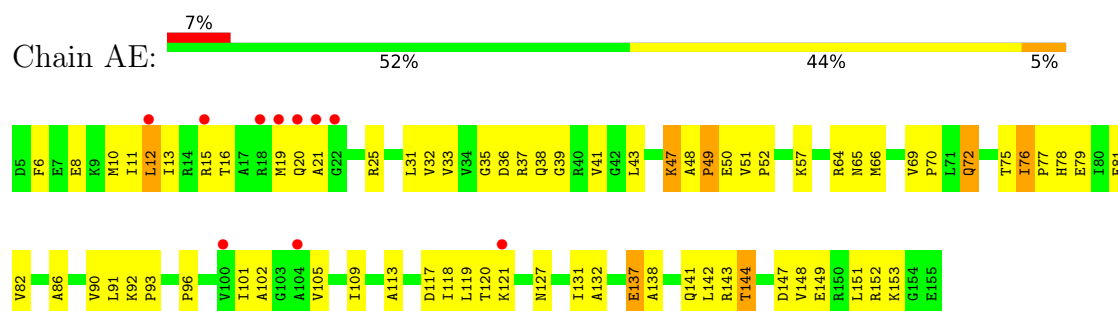
• Molecule 4: 30S ribosomal protein S4



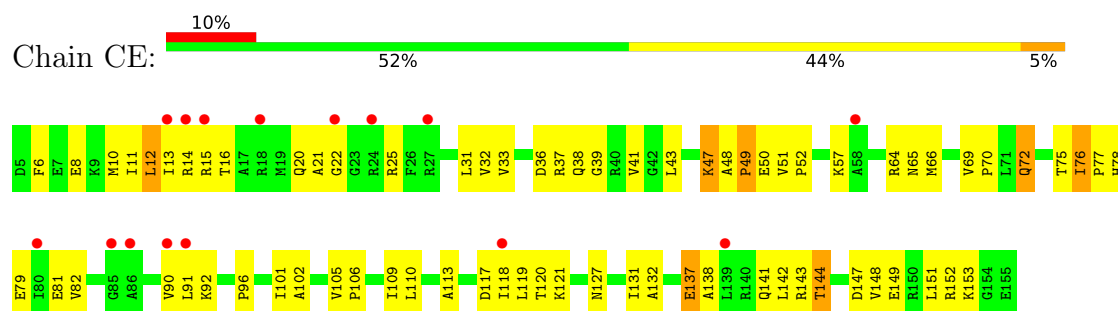
• Molecule 4: 30S ribosomal protein S4



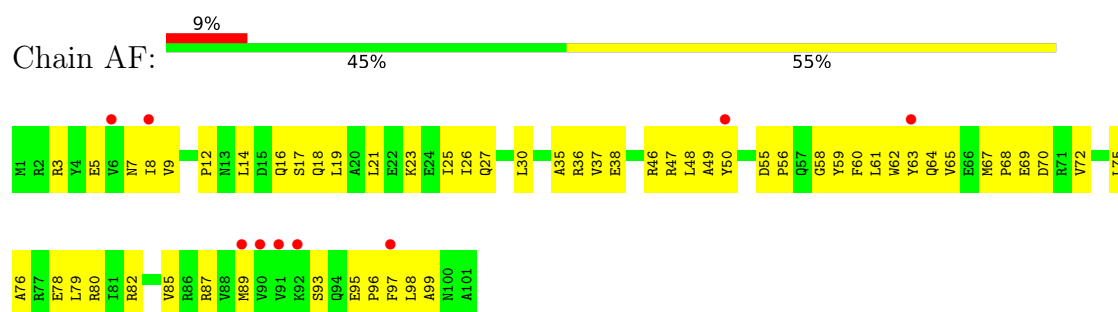
- Molecule 5: 30S ribosomal protein S5



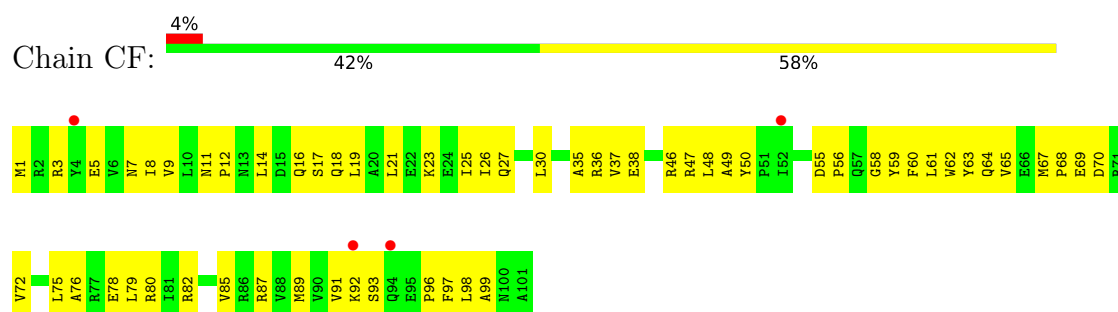
- Molecule 5: 30S ribosomal protein S5



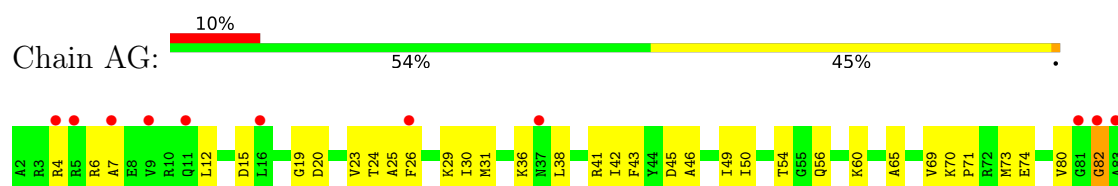
- Molecule 6: 30S ribosomal protein S6

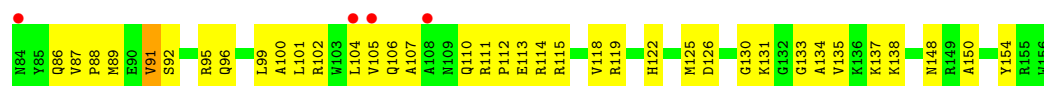


- Molecule 6: 30S ribosomal protein S6

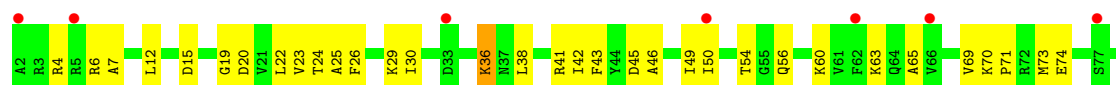


- Molecule 7: 30S ribosomal protein S7

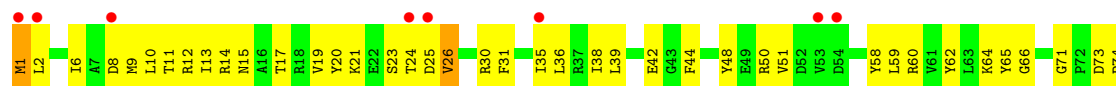




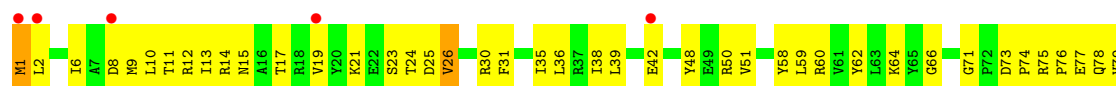
• Molecule 7: 30S ribosomal protein S7



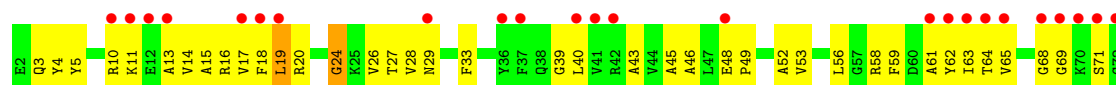
• Molecule 8: 30S ribosomal protein S8



• Molecule 8: 30S ribosomal protein S8

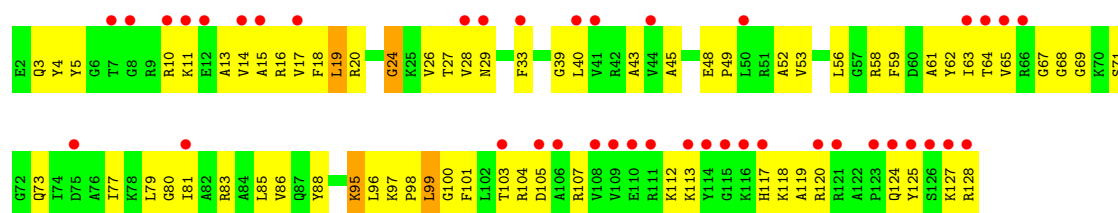


• Molecule 9: 30S ribosomal protein S9

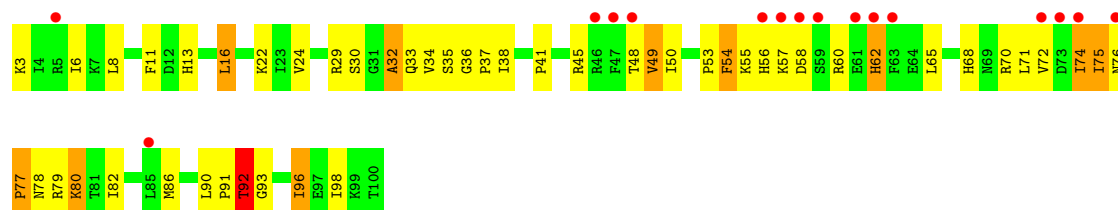


• Molecule 9: 30S ribosomal protein S9

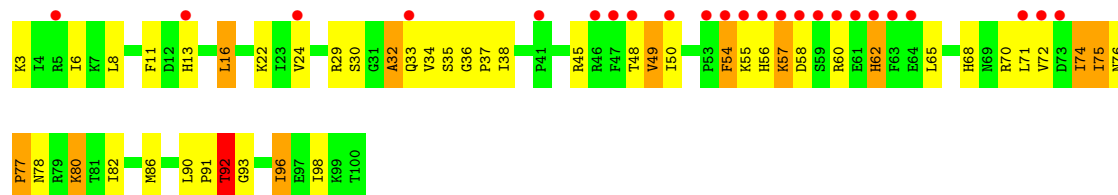




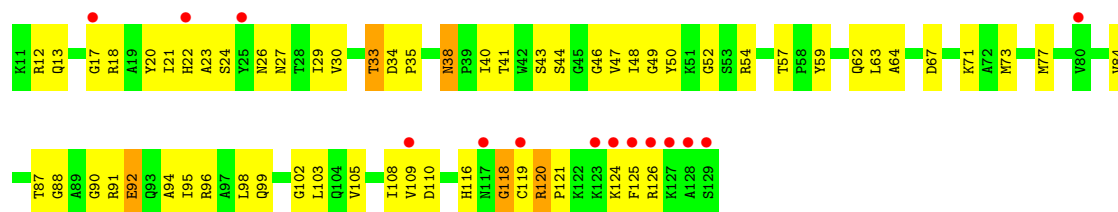
• Molecule 10: 30S ribosomal protein S10



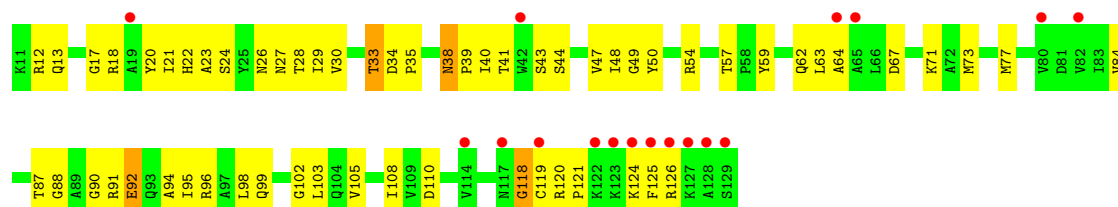
• Molecule 10: 30S ribosomal protein S10



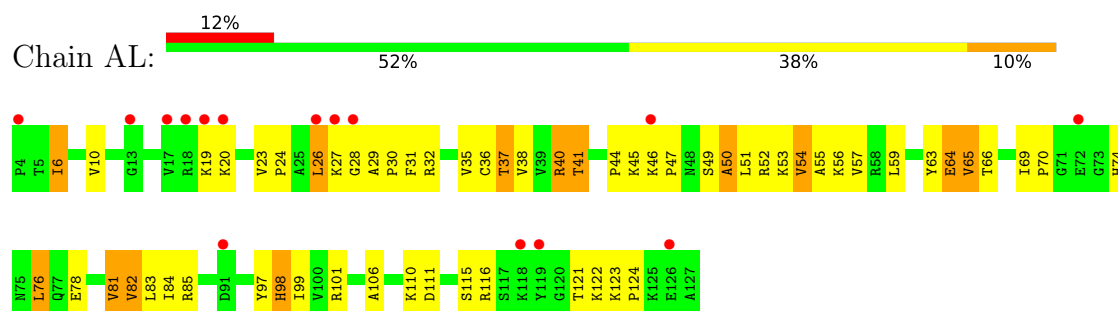
• Molecule 11: 30S ribosomal protein S11



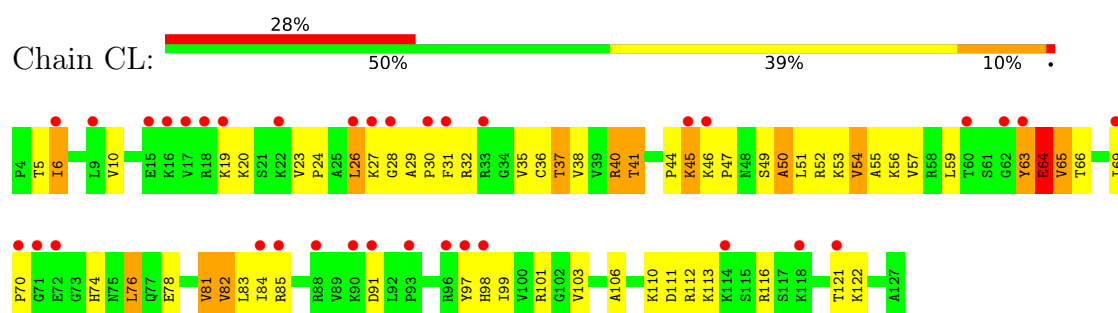
• Molecule 11: 30S ribosomal protein S11



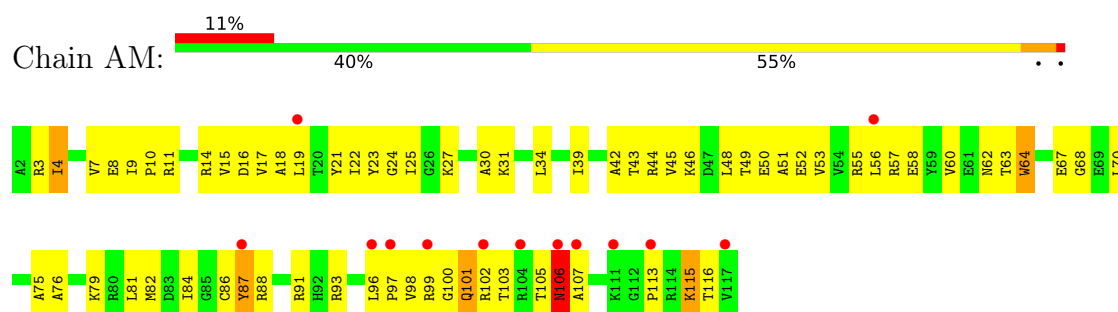
- Molecule 12: 30S ribosomal protein S12



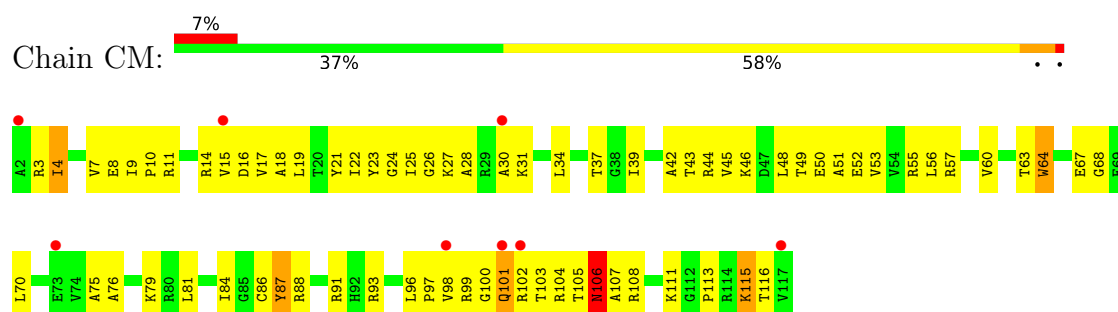
- Molecule 12: 30S ribosomal protein S12



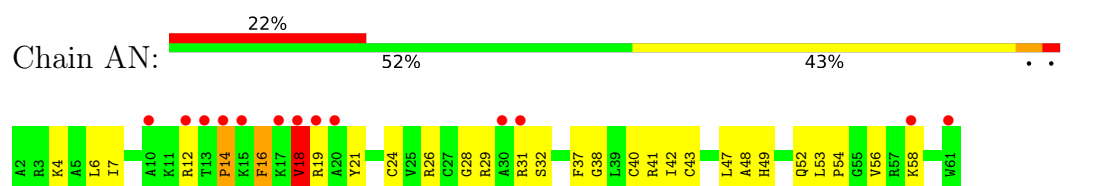
- Molecule 13: 30S ribosomal protein S13



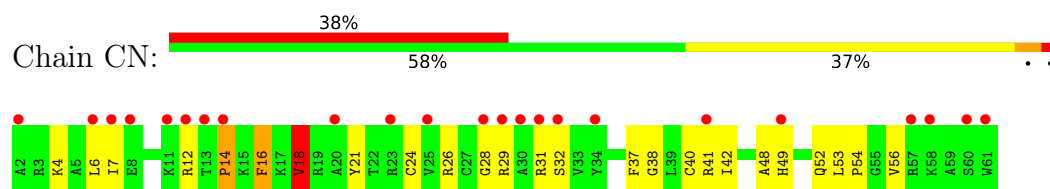
- Molecule 13: 30S ribosomal protein S13



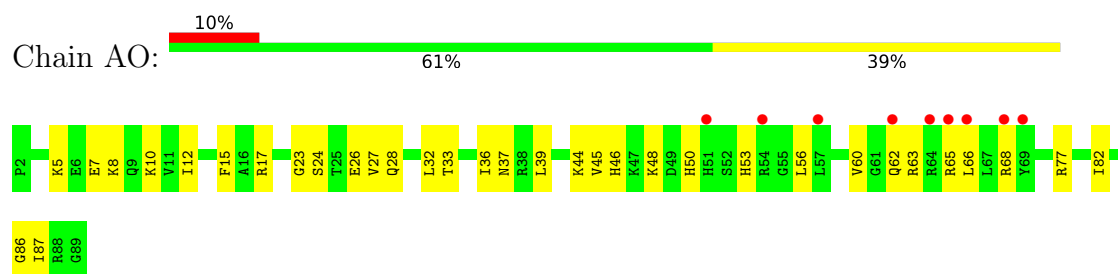
- Molecule 14: 30S ribosomal protein S14 type Z



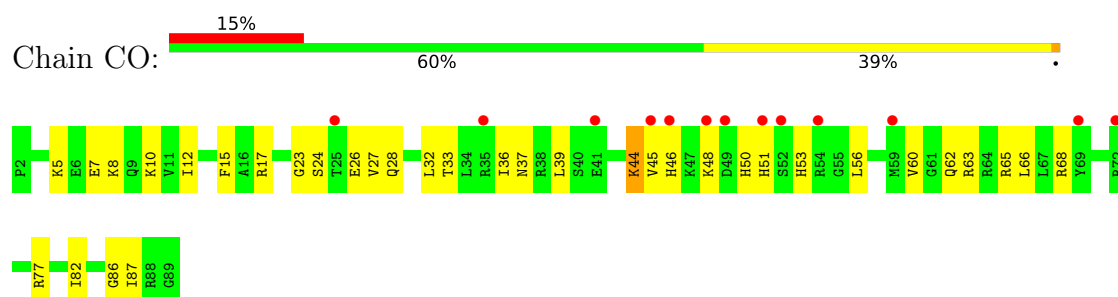
- Molecule 14: 30S ribosomal protein S14 type Z



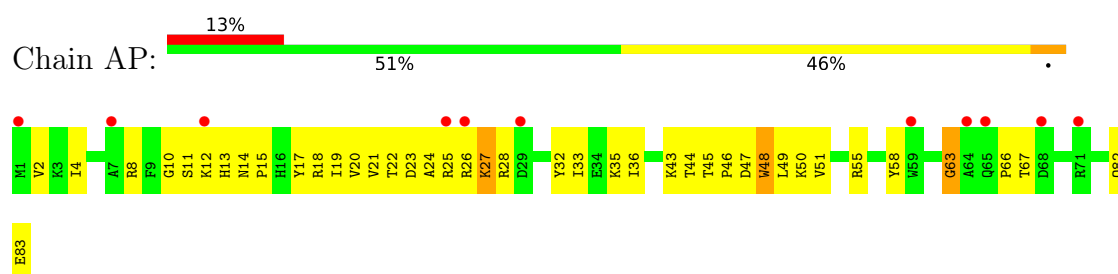
- Molecule 15: 30S ribosomal protein S15



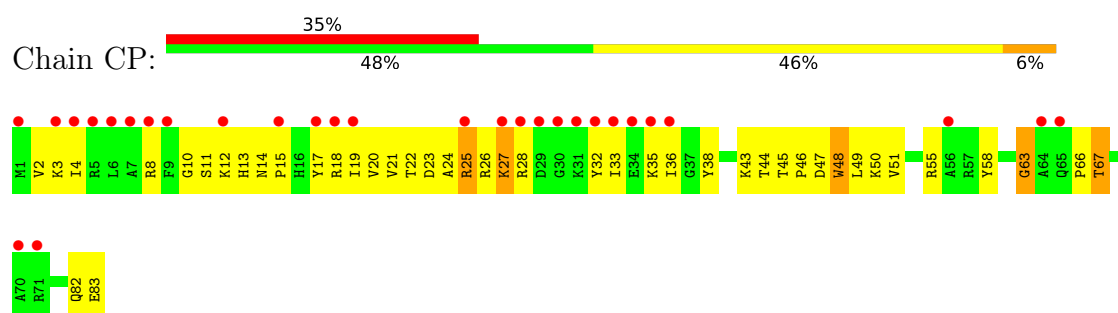
- Molecule 15: 30S ribosomal protein S15



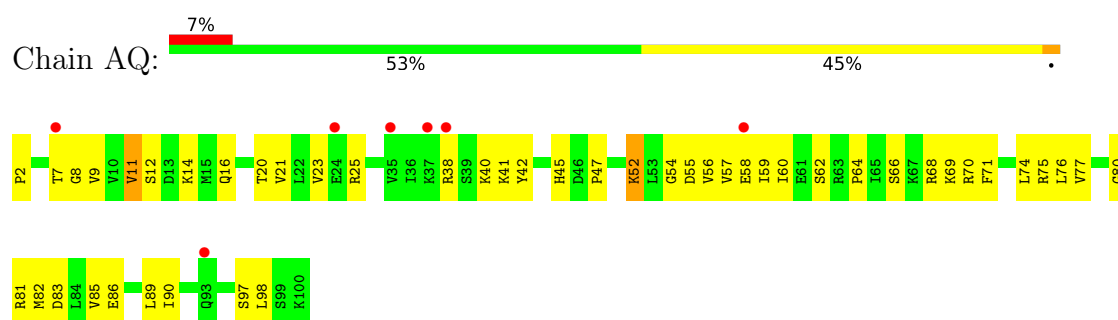
- Molecule 16: 30S ribosomal protein S16



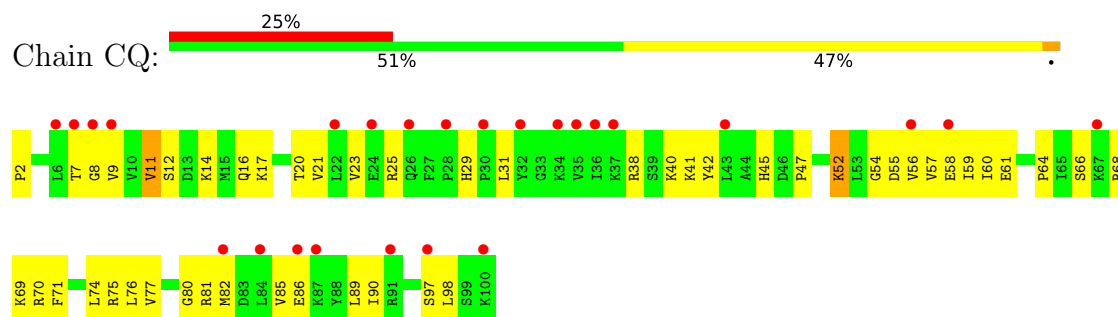
- Molecule 16: 30S ribosomal protein S16



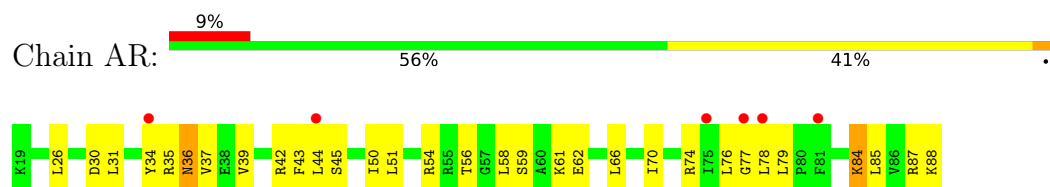
- Molecule 17: 30S ribosomal protein S17



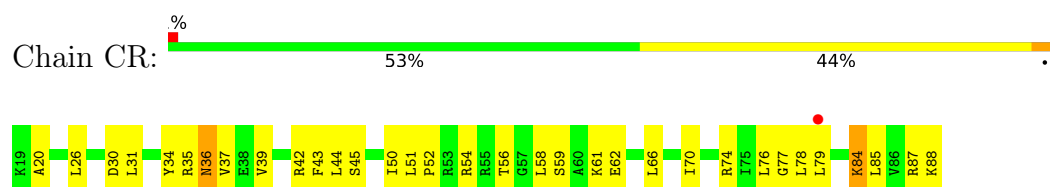
- Molecule 17: 30S ribosomal protein S17



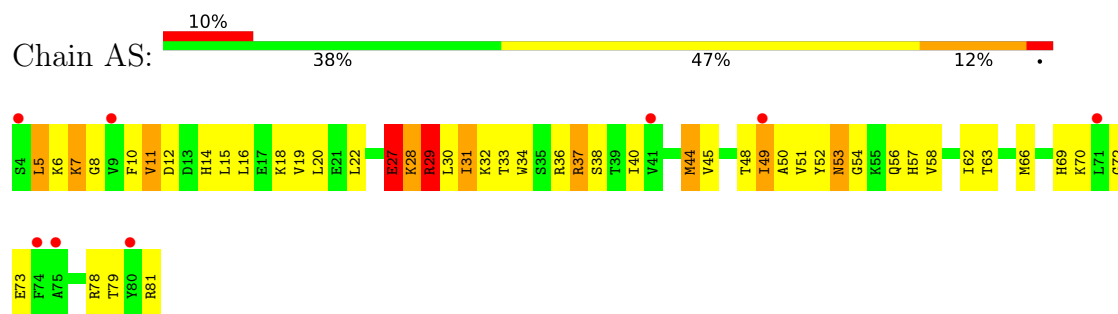
- Molecule 18: 30S ribosomal protein S18



- Molecule 18: 30S ribosomal protein S18

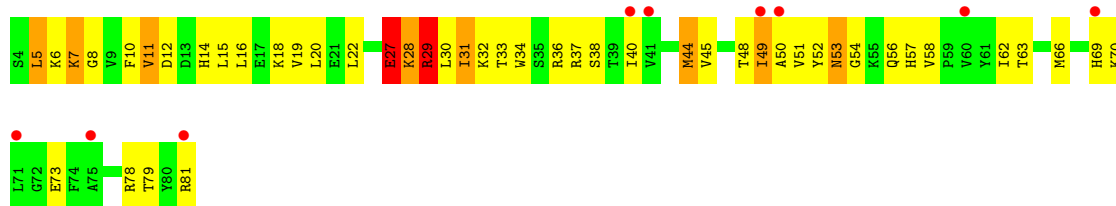


- Molecule 19: 30S ribosomal protein S19

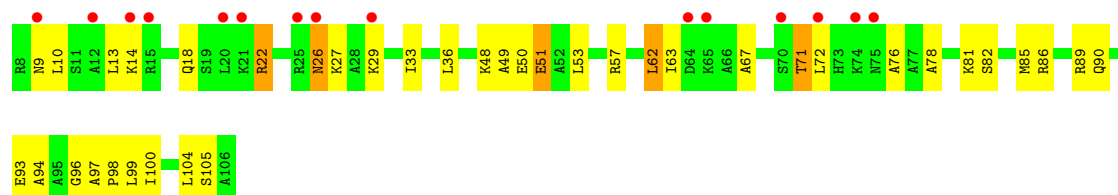


- Molecule 19: 30S ribosomal protein S19

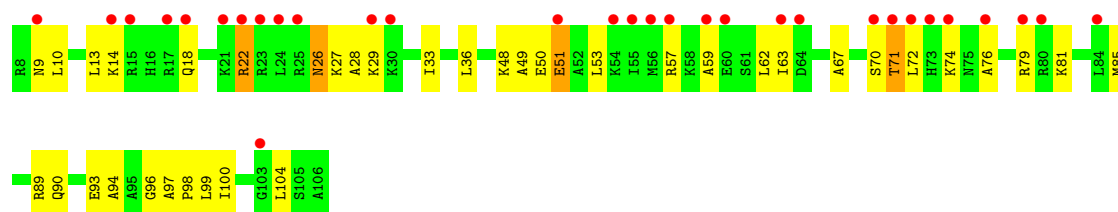




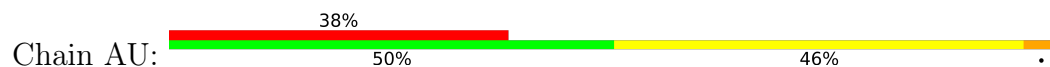
• Molecule 20: 30S ribosomal protein S20



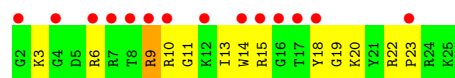
• Molecule 20: 30S ribosomal protein S20



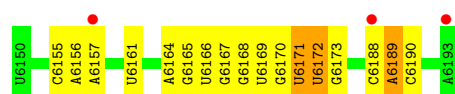
• Molecule 21: 30S ribosomal protein Thx



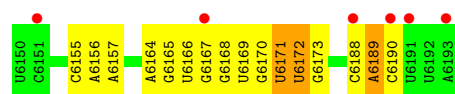
• Molecule 21: 30S ribosomal protein Thx



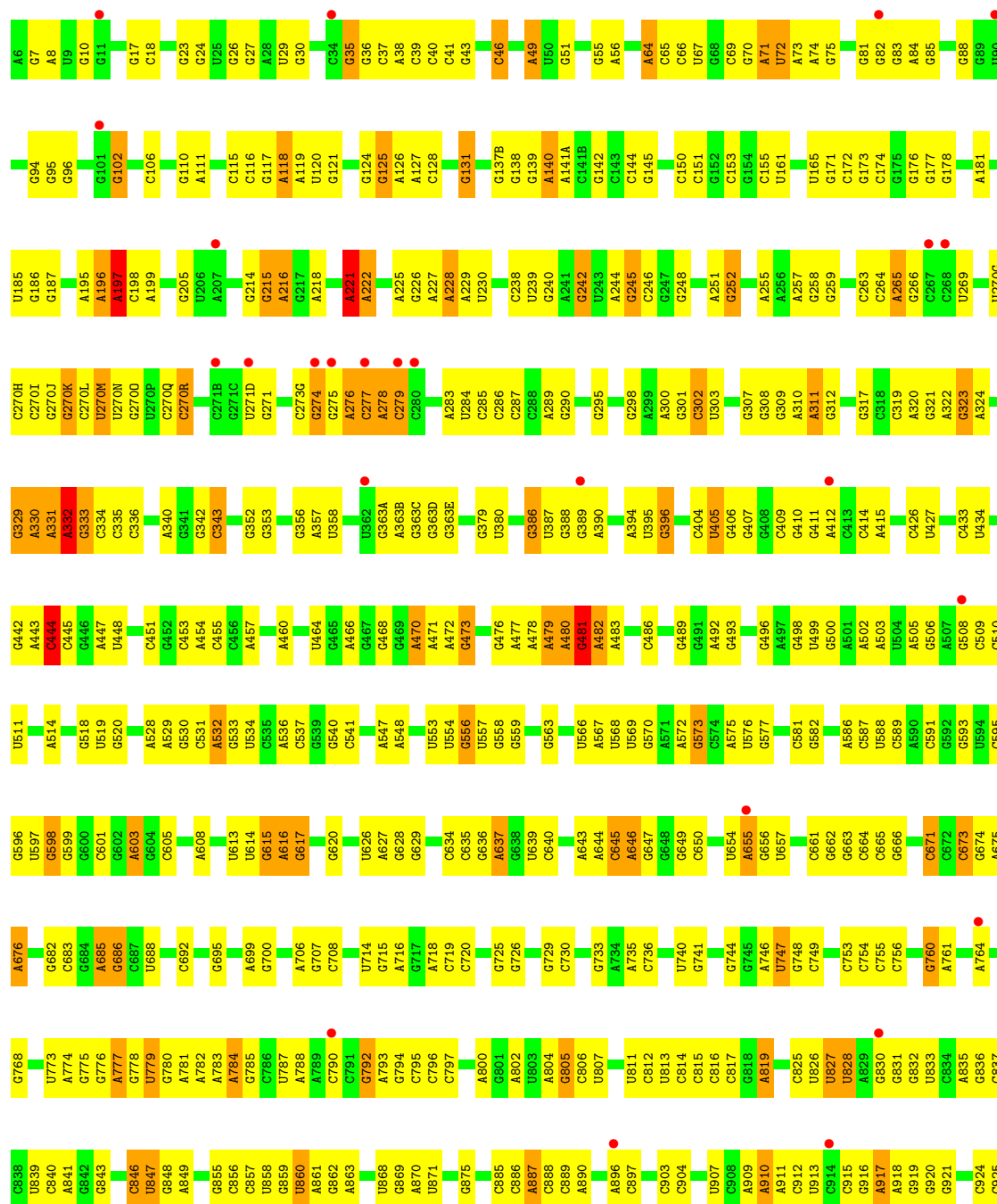
• Molecule 22: domain 3 of PSIC IGR IRES RNA



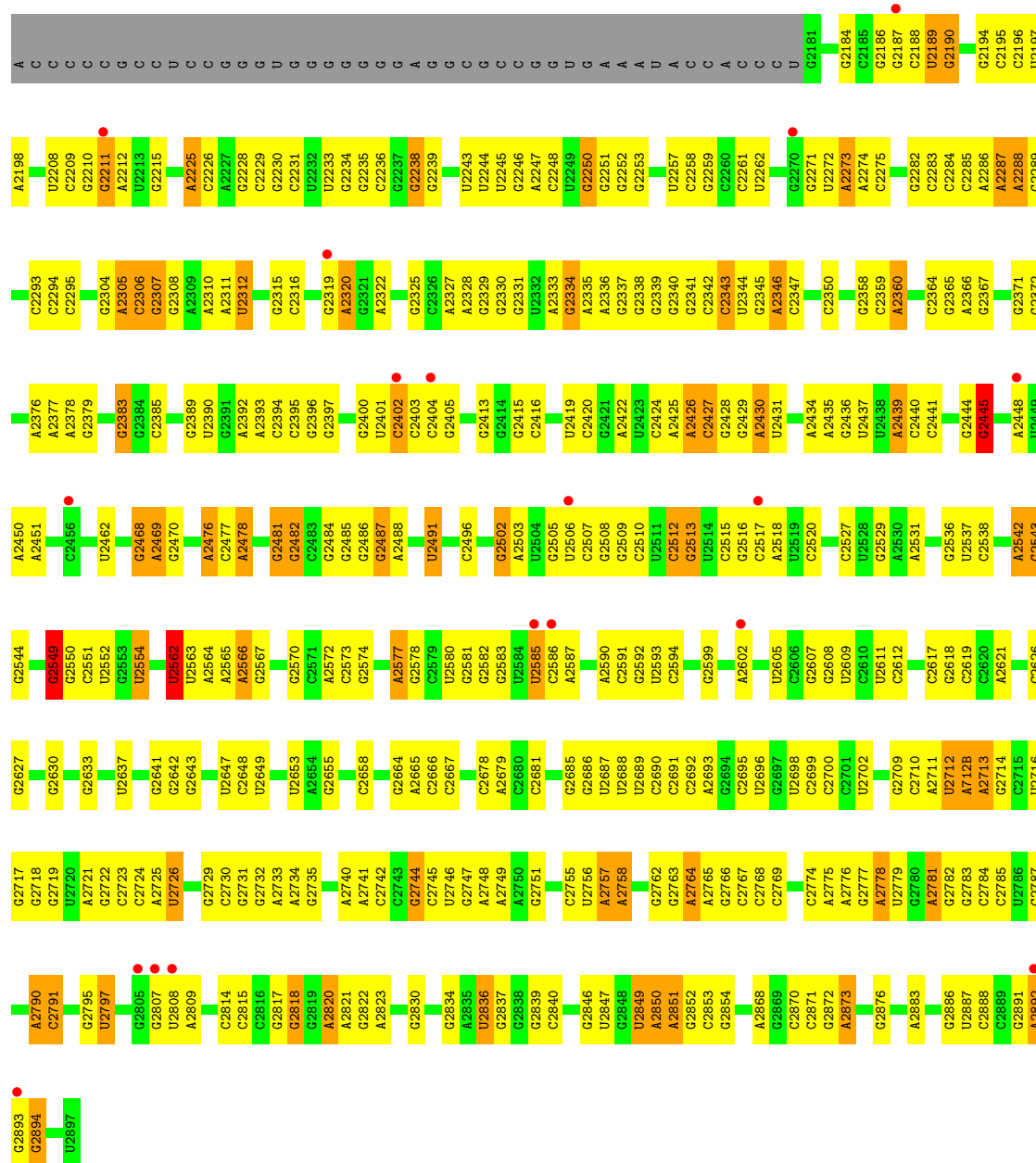
- Molecule 22: domain 3 of PSIC IGR IRES RNA



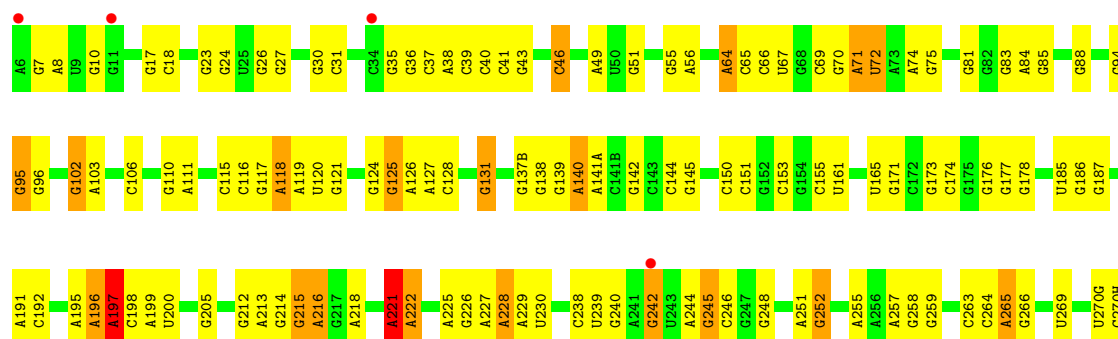
- Molecule 23: 23S ribosomal RNA



C2065	C1990	C1887	U1794	G1882	U1497	C1411	A1336	U1249	G1154	U999
C2066	U1991	C1887	C1795	C1683	C1592	A1412	G1337	G1250	A1155	A1000
G2067	C1992	C1888	C1796	C1684	C1502	G1413	U1337	U1251	C1156	A1001
U2068	U1993	A1889	U1797	U1688	U1503	U1414	U1341	G1252	C1157	G1002
G2069	C1994	C1797	U1798	U1689	C1504	U1415	A1342	A1253	C1161	C1005
C2070	U1995	G1899	U1798	A1889	C1505	G1416	G1343	A1254	G1162	C1006
A2071	U1996	A1900	G1799	U1692	C1598	C1417	G1344	U1255	G1163	U1019
U2072	C1997	C1901	C1800	U1693	A1599	G1418	C1345	U1256	G1164	A1020
U2073	G1902	G1902	A1801	C1694	G1601	A1419	G1346	G1257	U1165	A1010
U2074	G1903	C1903	A1802	G1695	U1602	U1420	G1348	C1258	G1166	G1011
U2075	G2004	A1803	A1803	G1696	U1603	U1511	A1349	U1259	G1167	U1012
C2076	G2010	G1906	C1804	G1697	A1604	A1427	C1350	G1264	G1171	C1013
C2077	U2011	C1907	A1809	G1698	C1604	C1428	C1351	A1265	G1173	G1013
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U2080	A2014	A1811	G1811	A1700	A1608	U1431	A1354	C1270	U1176	A1022
C2081	A2015	A1916	A1812	U1709	A1609	C1432	A1355	G1271	U1177	G1023
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C2083	A2019	A1918	G1816	G1717	C1611	A1434	U1356	U1273	A1179	U1025
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C2089	G2024	U1931	G1824	G1728	C1617	G1444	A1365	C1289	C1104	U1033
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C2095	A2030	U1938	A1829	G1743	A1543	G1449	C1375	U1300	G1112	G1047
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C2097	C2032	C1939	C1832	A1749	U1546	A1453	A1379	A1308	G1208	G1051
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C2099	G2034	A1952	U1833	C1751	A1558	G1461	G1380	G1310	C1122	C970
U2100	C2035	U1953	U1834	C1752	G1559	C1463	G1381	G1311	C1123	C971
C2101	C2036	C1954	C1838	A1759	G1563	G1464	A1384	G1312	G1124	G972
U2102	G2037	C1961	C1843	C1763	U1564	G1465	G1385	U1313	G1125	A973
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C2105	C2042	C1964	A1847	C1765	A1656	U1467	G1388	U1316	A1128	G975
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C2117	G2058	U1980	G1862	A1783	C1676	A1490	U1405	A1331	U1143	G993
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C2119	C2060	C1982	U1785	A1785	A1677	C1493	C1407	G1333	G1144	C995
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U2122	C2063	U1985	A1872	C1790	U1680	U1495	C1408	G1334	A1241	C998
C2123	G2064	C1986	A1872	C1790	U1680	A1495	C1408	U1335	A1242	C998
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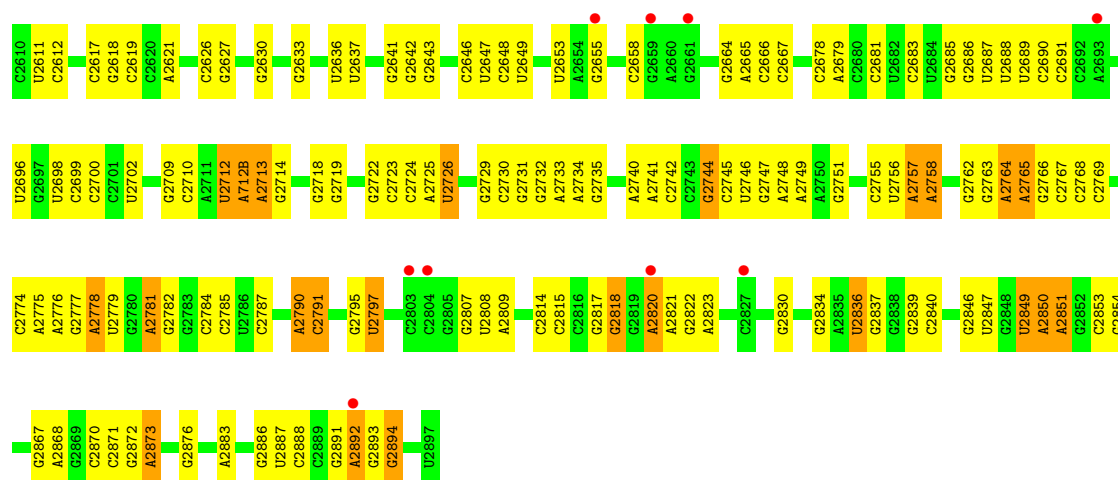


• Molecule 23: 23S ribosomal RNA

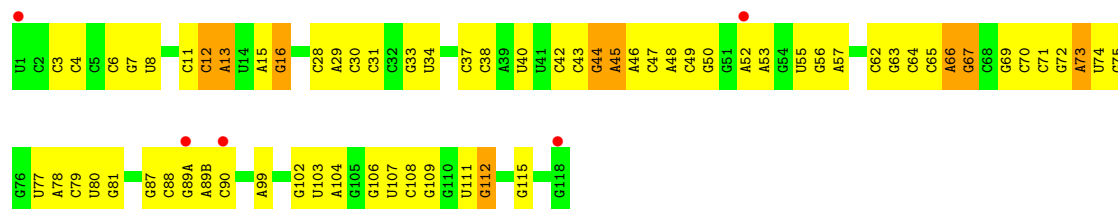
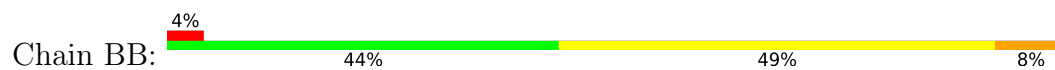


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C1005	C1006	C1007	A1010	G1011	U1012	C1013	U1019	A1020	A1021	G1022	U1023	G1024	G1025	U1026	A1027	A1028	G1029	A1030	U1033	C1040	C1041	G1044	A1045	A1046	G1047	A1050	G1051	C1052	G1056	A	G	G	U	U	G	C	U	U	A	G	A	C	A	C	A	U	C									
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A330	A331	A332	G333	C334	C335	C336	G342	C343	G352	G353	G356	A357	A359	U362	G363A	A363B	G363C	G363D	G363E	G379	U380	G381	C385	C386	U387	G388	G389	A390	A394	U395	G396	C404	U405	A406	G407	G408	C409	C410	C411	A412	C413	C414	A502	A503	C426	U427	C433	U434	C509							
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G592	G593	U594	C595	G596	U597	G598	G599	A603	G604	C605	A608	U613	U614	G615	A616	G617	G620	U626	G628	G629	C634	C635	G636	A637	G638	U639	C640	A643	A644	C645	A646	G647	G648	G649	C650	U654	A655	G656	U657	C661	G662	G663	C664	G671	C672	C673	G674	A675								
A676	G682	C683	G684	A685	G686	C687	U688	C692	G695	A699	G700	A706	G707	C708	U714	G715	C716	G717	A718	C719	C720	G725	G726	G729	C730	G733	A734	A735	C736	G744	G745	U747	G748	C749	C753	C754	C755	C756	U757	C758	G759	G760	A761	A764	G768											

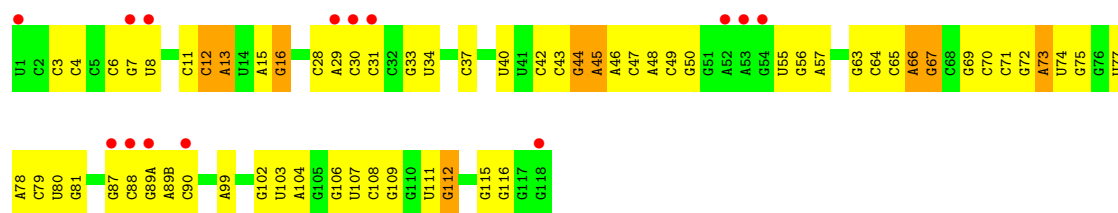




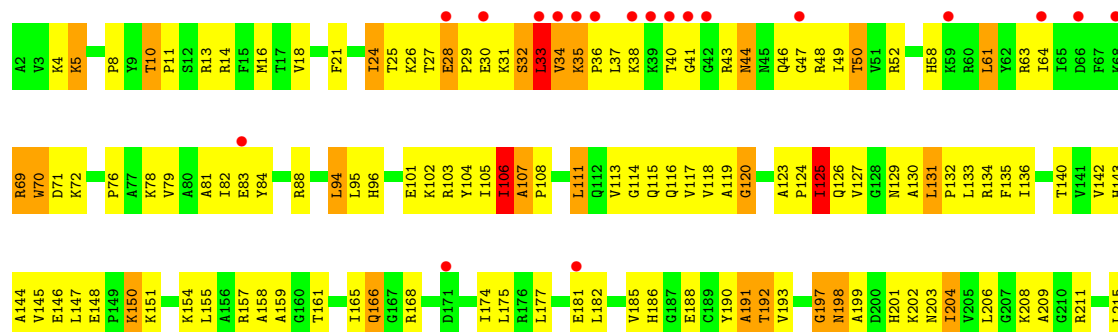
• Molecule 24: 5S ribosomal RNA

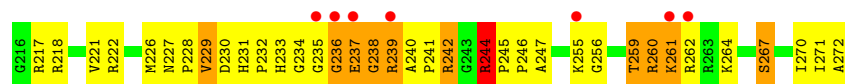


• Molecule 24: 5S ribosomal RNA

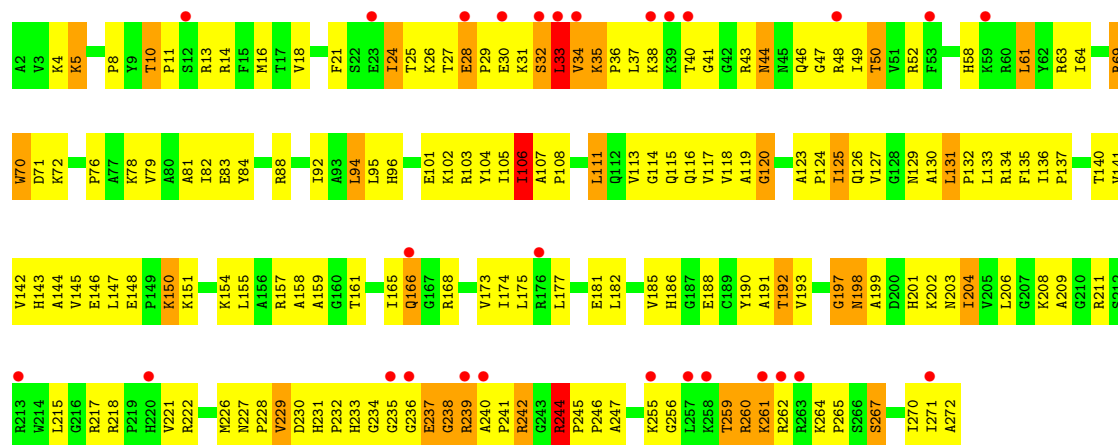


• Molecule 25: 50S ribosomal protein L2

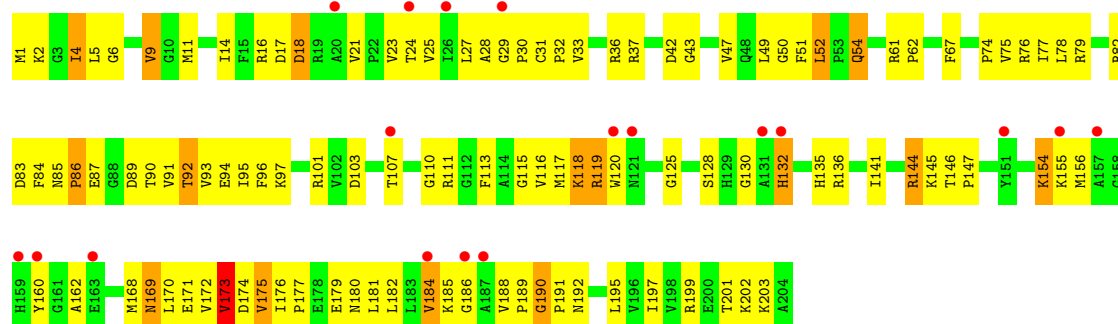




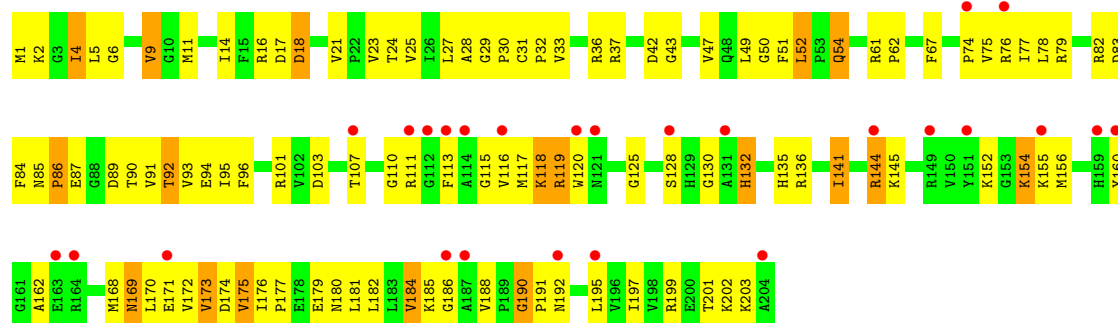
• Molecule 25: 50S ribosomal protein L2



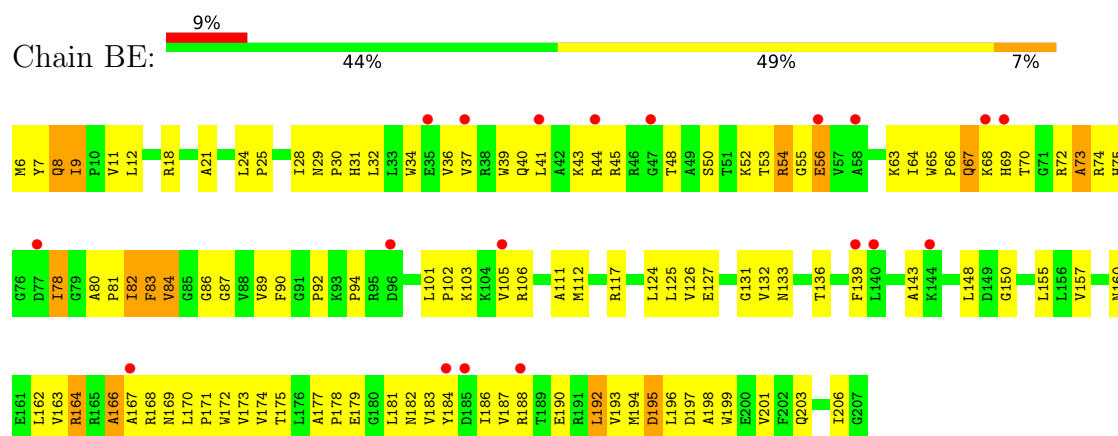
• Molecule 26: 50S ribosomal protein L3



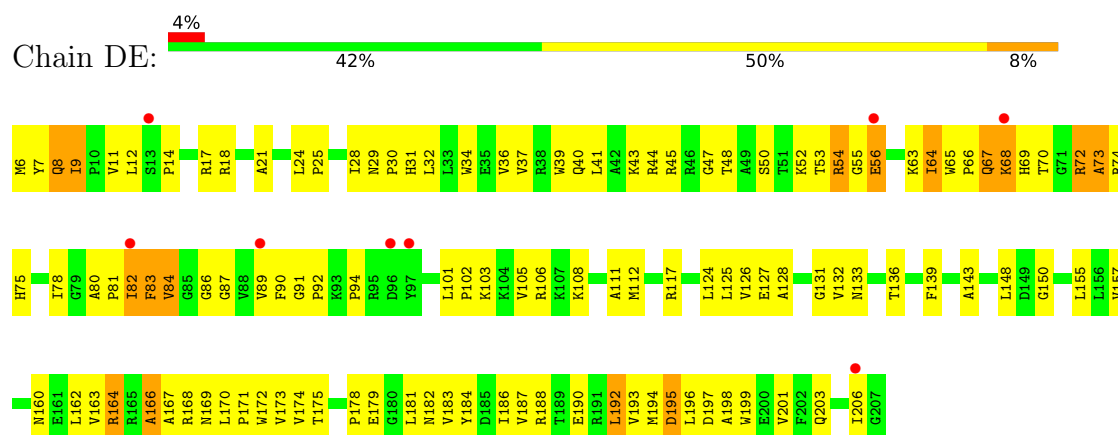
• Molecule 26: 50S ribosomal protein L3



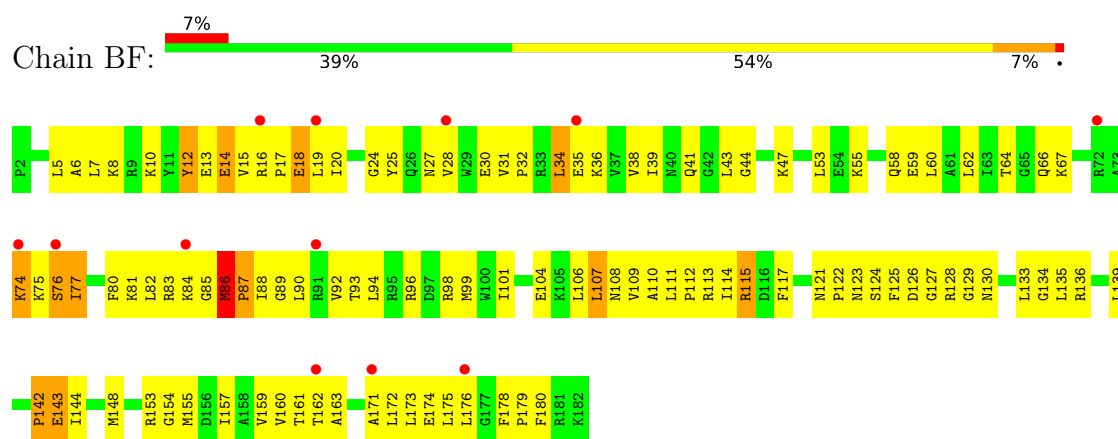
- Molecule 27: 50S ribosomal protein L4



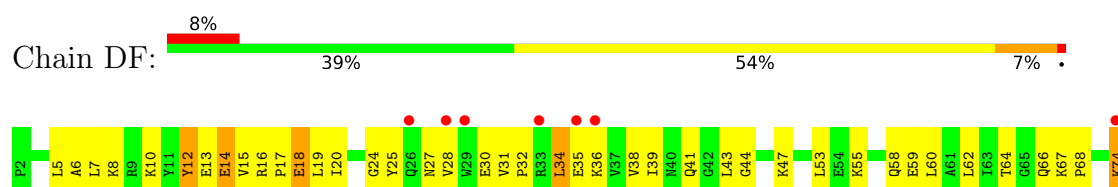
- Molecule 27: 50S ribosomal protein L4

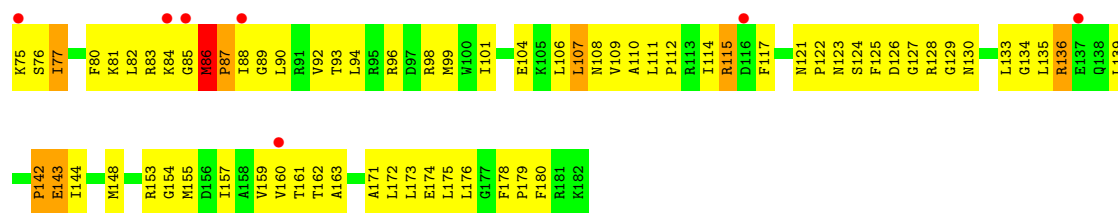


- Molecule 28: 50S ribosomal protein L5

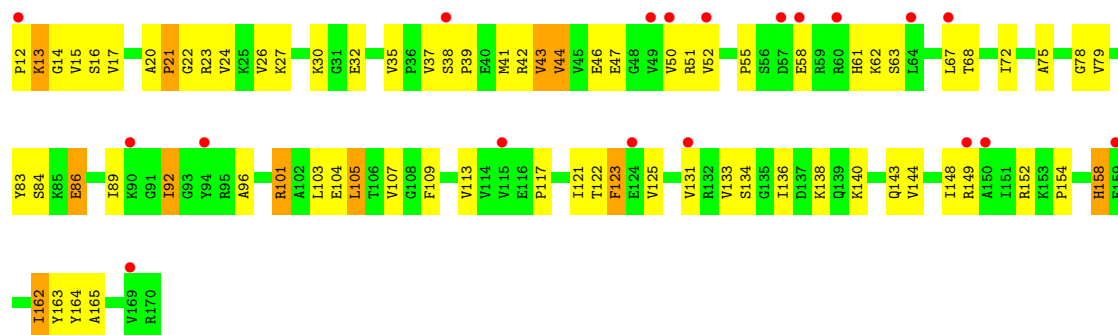


- Molecule 28: 50S ribosomal protein L5

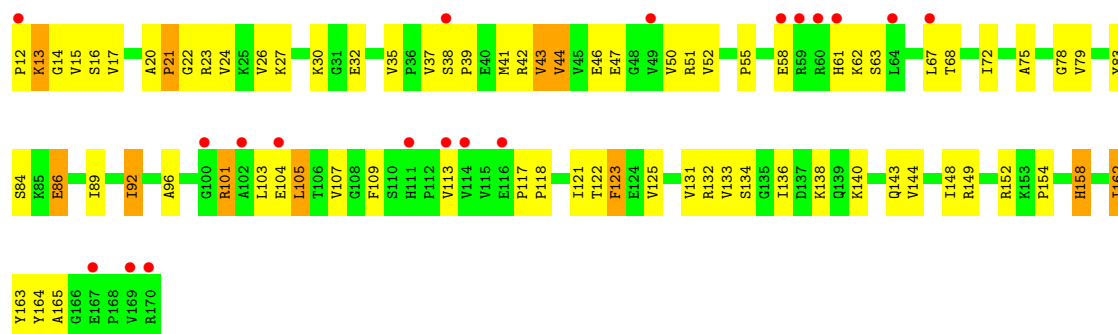




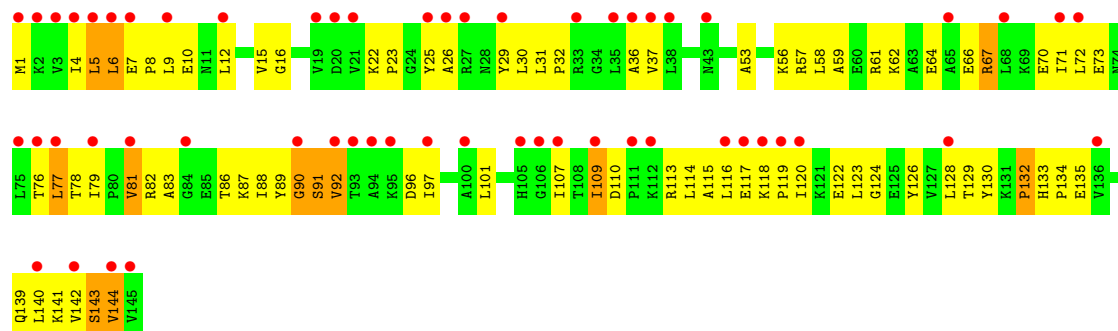
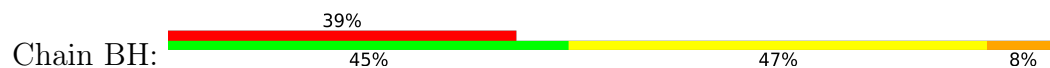
• Molecule 29: 50S ribosomal protein L6



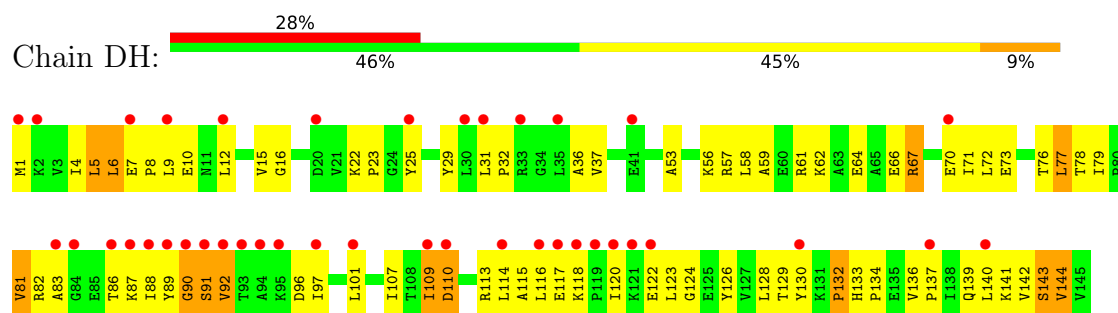
• Molecule 29: 50S ribosomal protein L6



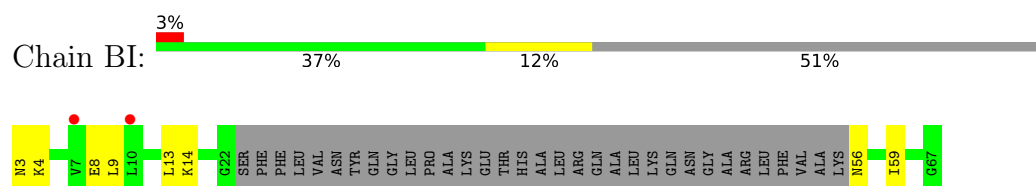
• Molecule 30: 50S ribosomal protein L9



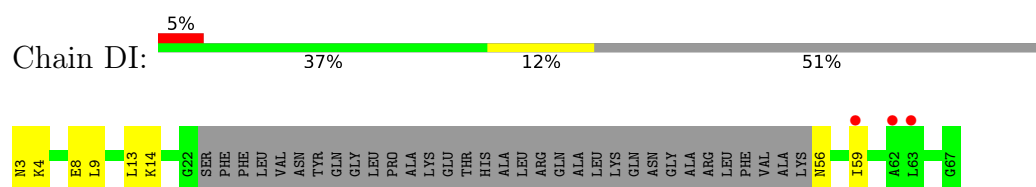
- Molecule 30: 50S ribosomal protein L9



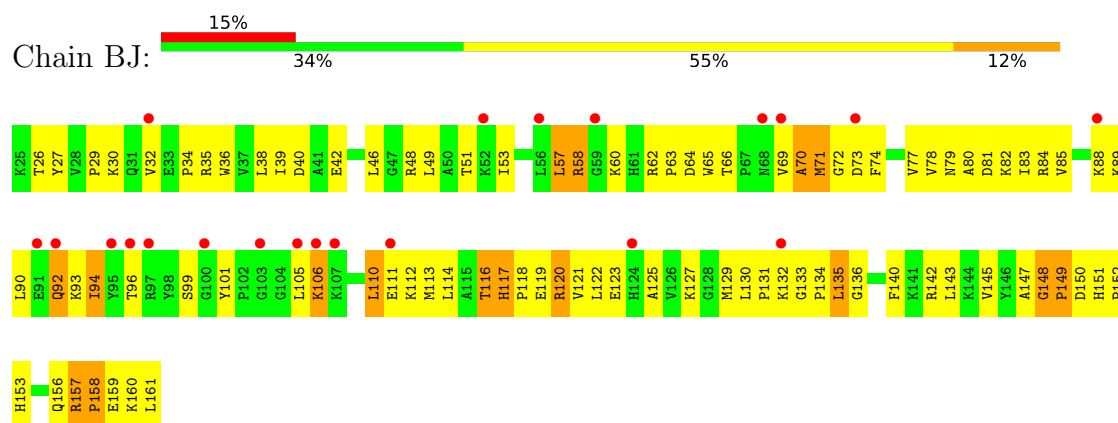
- Molecule 31: 50S ribosomal protein L10



- Molecule 31: 50S ribosomal protein L10



- Molecule 32: 50S ribosomal protein L13



- Molecule 32: 50S ribosomal protein L13



Q156
R157
P158
E159
K160
L161

• Molecule 33: 50S ribosomal protein L14

Chain BK: 4% 52% 39% 9%

M1 I2 Q3 P4 Q5 T6 Y7 L8 E9 D12 R17 K18 I19 M20 N21 C21 R104 E105 R23 R24 V24 L25 K26 K27 S28 N29 A30 K31 Y32 A33 T34 V35 V36 D37 S42 E45 A46 I47 P48 K53 V61 E68 R71 P72 D73 G74 S75 A76 R78 F79 D80 D81 N82 V85 I86 I87 N88 Q89 L91 T96 R97 F99 G100 P101 Y102 A103 E105 L106 M112 V115 P119 L122

• Molecule 33: 50S ribosomal protein L14

Chain DK: 2% 52% 39% 10%

M1 I2 Q3 P4 Q5 T6 Y7 L8 E9 D12 R17 K18 I19 M20 N21 C21 R104 E105 R23 R24 V24 L25 K26 K27 S28 N29 A30 K31 Y32 A33 T34 V35 E45 A46 I47 P48 K53 V61 E68 R71 P72 D73 G74 S75 A76 R78 F79 N82 V85 I86 I87 N88 Q89 L91 T96 R97 F99 G100 P101 Y102 A103 E105 L106 M112 V115 P119 L122

• Molecule 34: 50S ribosomal protein L15

Chain BL: 14% 32% 46% 19%

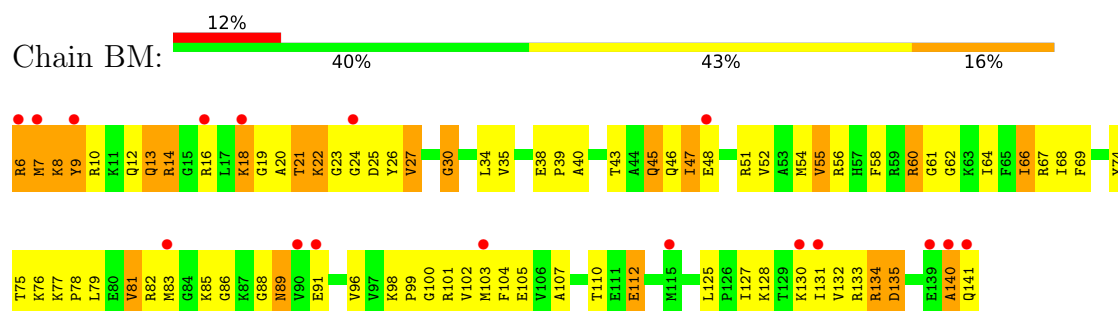
D5 L6 R7 P8 N9 P10 Q11 G12 A13 M14 R15 R16 K17 R18 R19 G20 G21 G22 S25 G26 G27 H27 G28 K29 T30 A31 T32 R33 G34 H35 K36 G37 Q38 K39 S40 R41 S42 G43 G44 L45 K46 D47 P48 R49 R50 F51 E52 G53 G54 T57 T58 L59 M60 R61 L62 P63 P64 R65 G66 M67 Q68 G69 Q70 V71 P72 G73 E74 I75 R76 R77 K78 R79 Y80 Q81 G82 N83 R84 L85 K86 D87 L88 A89 R90 F91 V95 V101 L105 L106 K107 K108 G109 R110 R111 L112 L113 I114 L115 G116 K121 P122 L123 K124 V125 G126 A127 H128 A129 F130 M131 K132 S133 A134 L135 L138 K139 A140 A141 G142 G143 E144 P145 V146 L147 L148 L149 A150

• Molecule 34: 50S ribosomal protein L15

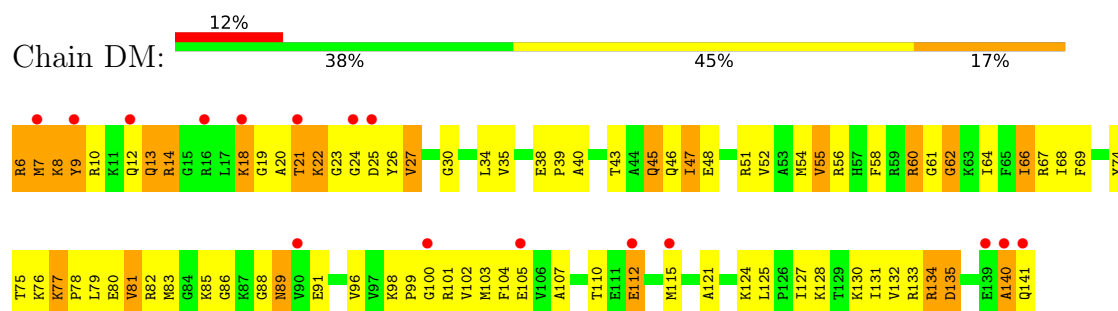
Chain DL: 21% 31% 47% 19%

P5 L6 R7 P8 N9 P10 Q11 G12 A13 M14 R15 R16 K17 R18 R19 G20 G21 G22 S25 G26 G27 H27 G28 K29 T30 A31 T32 R33 G34 H35 K36 G37 Q38 K39 S40 R41 S42 G43 G44 L45 K46 D47 P48 R49 R50 F51 E52 G53 G54 T57 T58 L59 M60 R61 L62 P63 P64 R65 G66 M67 Q68 G69 Q70 V71 P72 G73 E74 I75 R76 R77 K78 R79 Y80 Q81 G82 N83 R84 L85 K86 D87 L88 A89 R90 F91 V95 V101 L105 L106 K107 K108 G109 R110 R111 L112 L113 I114 L115 G116 K121 P122 L123 K124 V125 G126 A127 H128 A129 F130 M131 K132 S133 A134 L135 L138 K139 A140 A141 G142 G143 E144 P145 V146 L147 L148 L149 A150

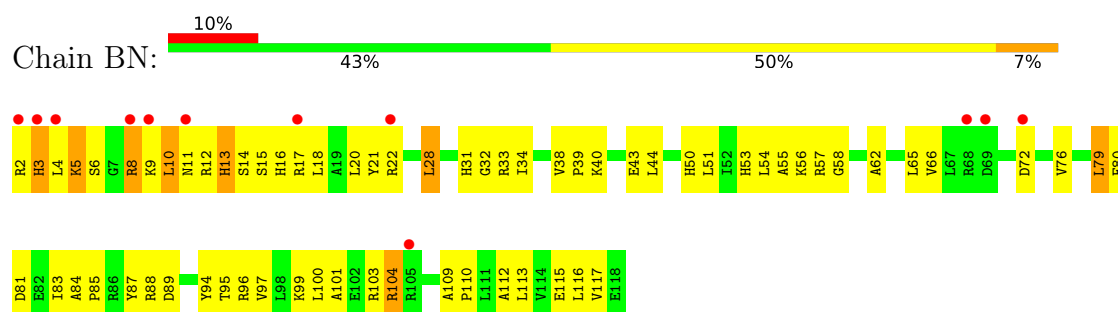
- Molecule 35: 50S ribosomal protein L16



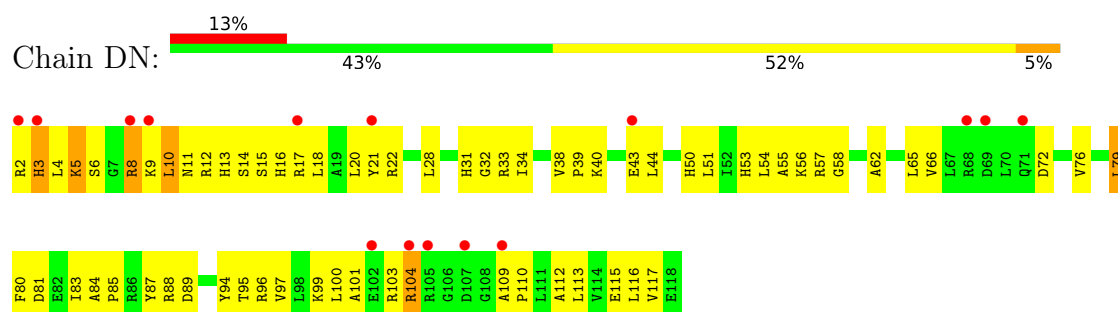
- Molecule 35: 50S ribosomal protein L16



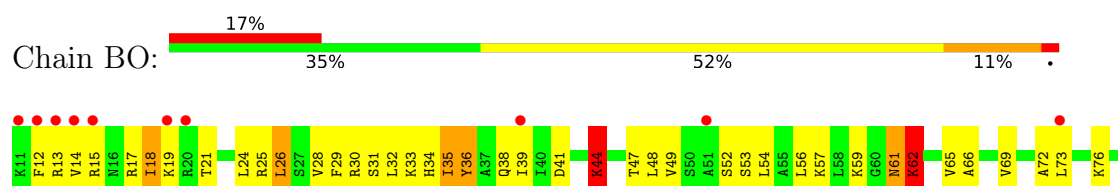
- Molecule 36: 50S ribosomal protein L17



- Molecule 36: 50S ribosomal protein L17

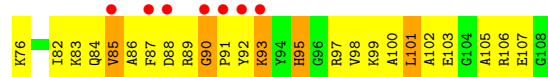
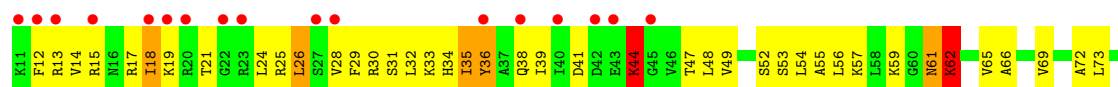


- Molecule 37: 50S ribosomal protein L18

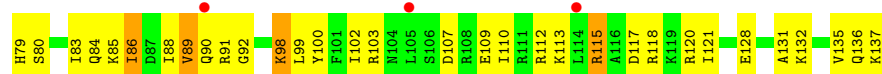
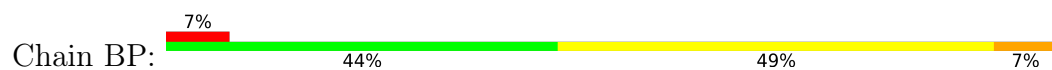




• Molecule 37: 50S ribosomal protein L18



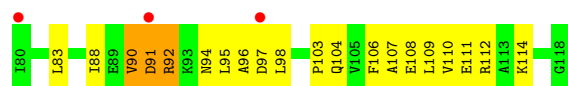
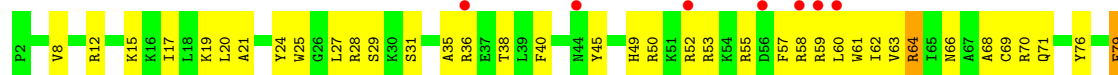
• Molecule 38: 50S ribosomal protein L19



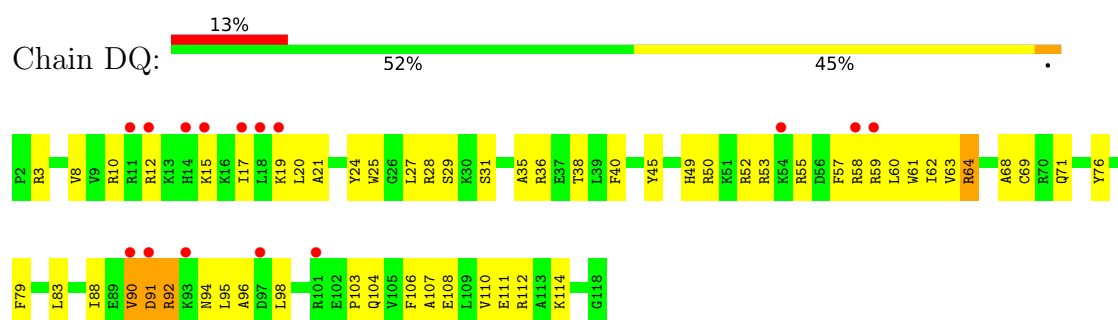
• Molecule 38: 50S ribosomal protein L19



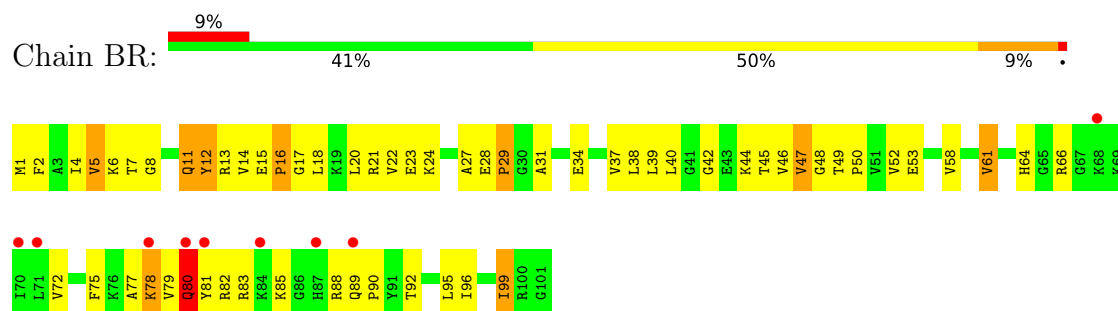
• Molecule 39: 50S ribosomal protein L20



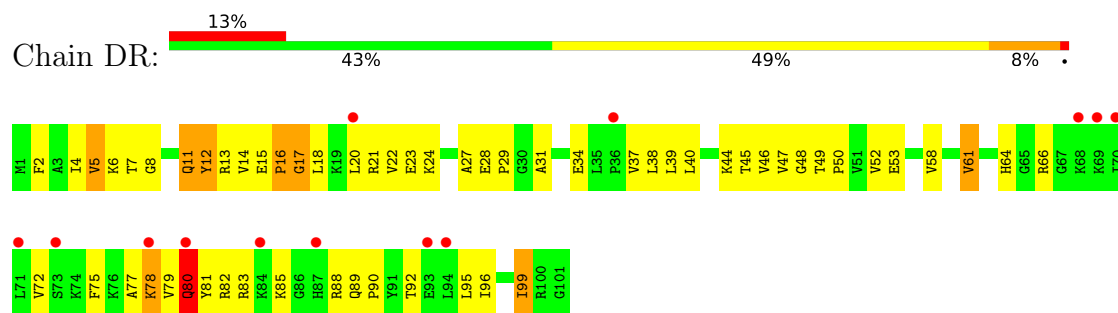
• Molecule 39: 50S ribosomal protein L20



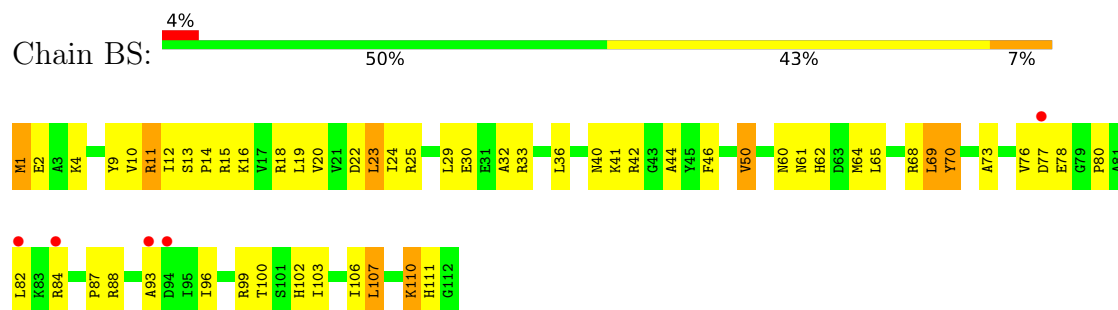
• Molecule 40: 50S ribosomal protein L21



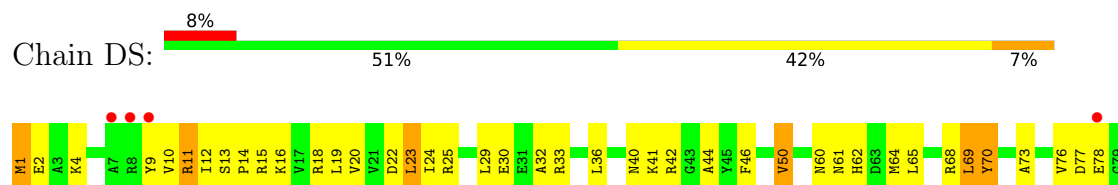
• Molecule 40: 50S ribosomal protein L21

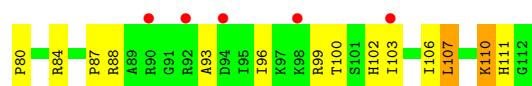


• Molecule 41: 50S ribosomal protein L22



• Molecule 41: 50S ribosomal protein L22

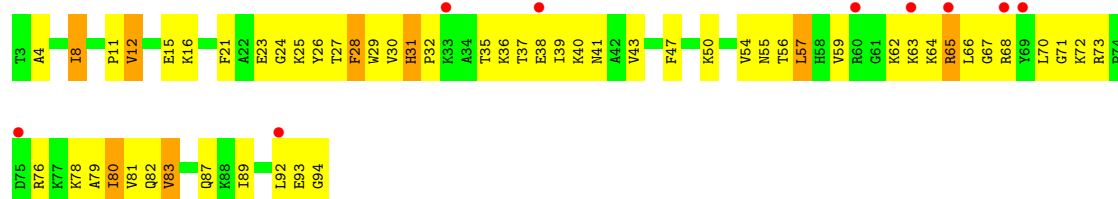
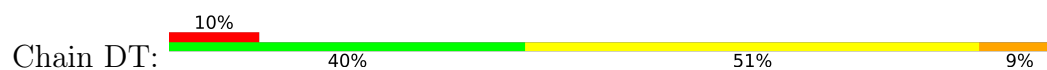




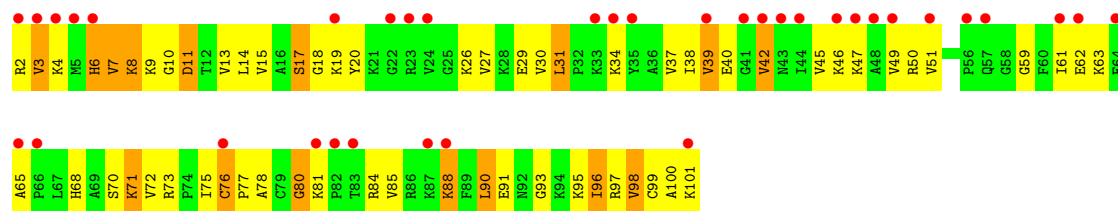
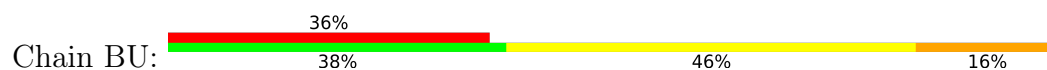
• Molecule 42: 50S ribosomal protein L23



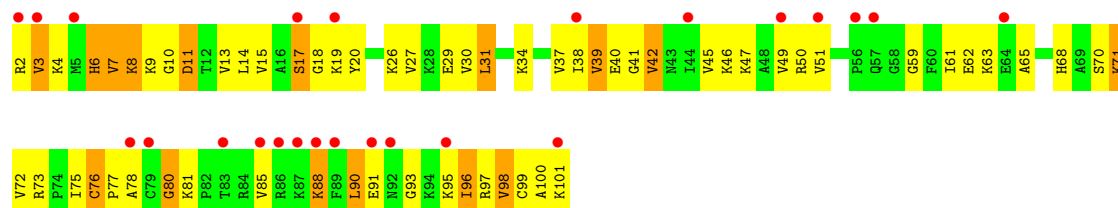
• Molecule 42: 50S ribosomal protein L23



• Molecule 43: 50S ribosomal protein L24

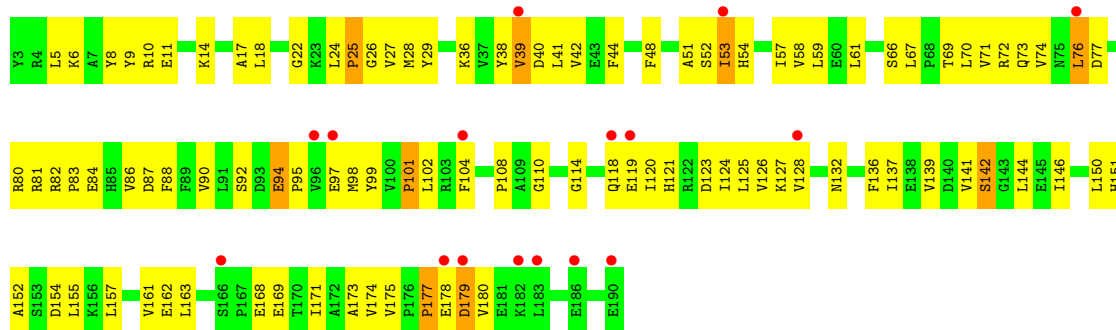


• Molecule 43: 50S ribosomal protein L24

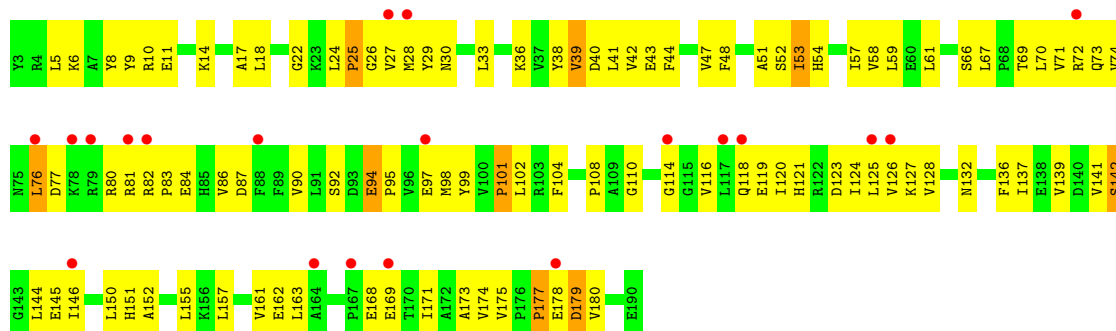


• Molecule 44: 50S ribosomal protein L25

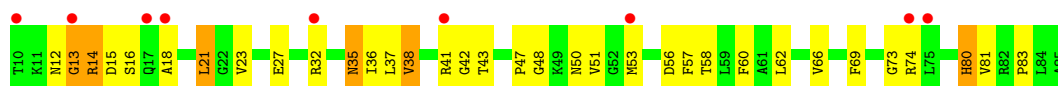




• Molecule 44: 50S ribosomal protein L25



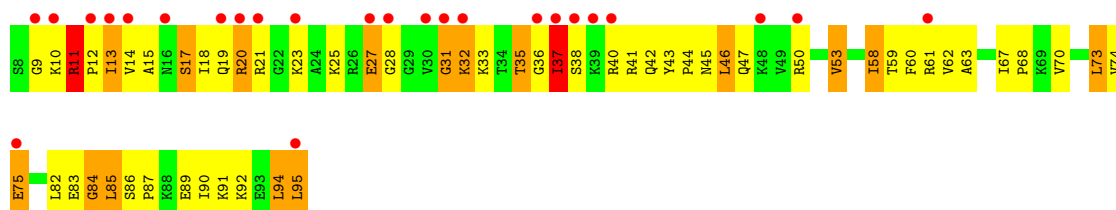
• Molecule 45: 50S ribosomal protein L27



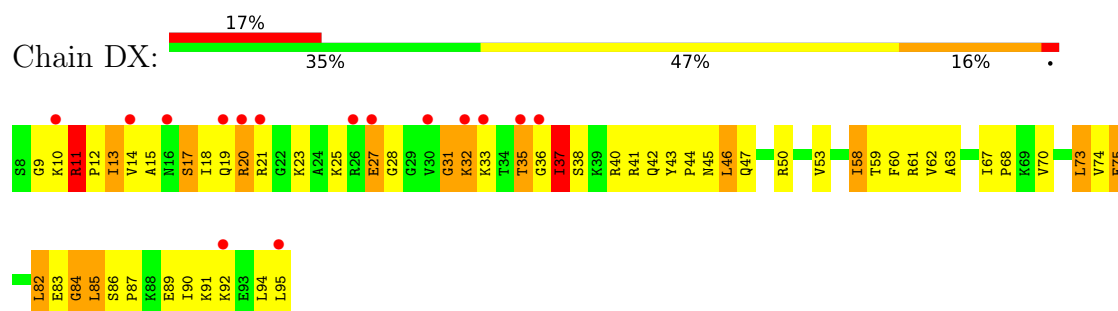
• Molecule 45: 50S ribosomal protein L27



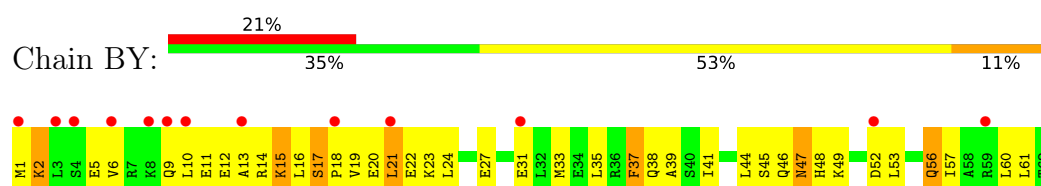
• Molecule 46: 50S ribosomal protein L28



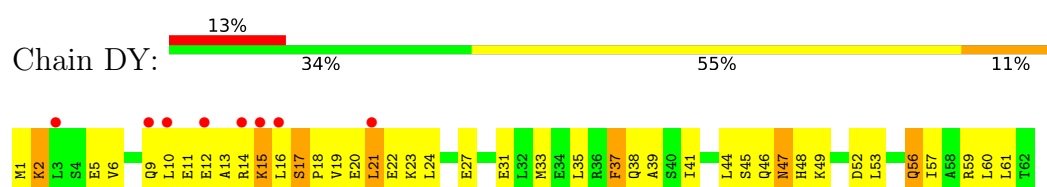
- Molecule 46: 50S ribosomal protein L28



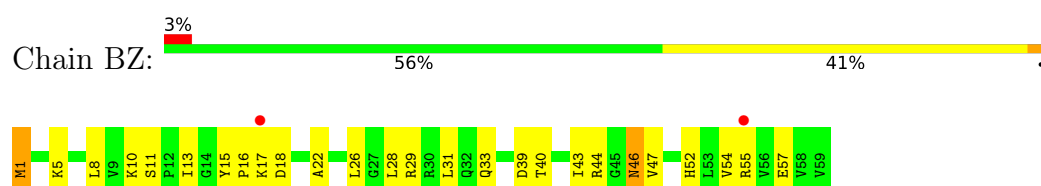
- Molecule 47: 50S ribosomal protein L29



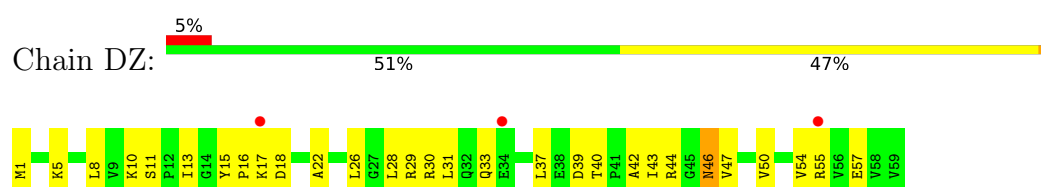
- Molecule 47: 50S ribosomal protein L29



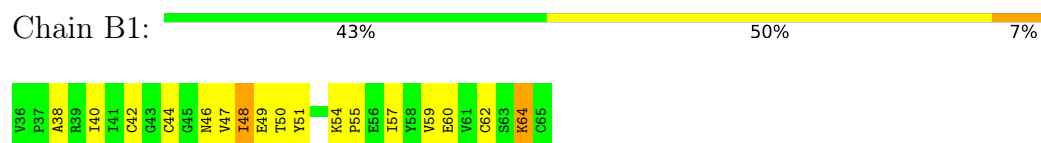
- Molecule 48: 50S ribosomal protein L30



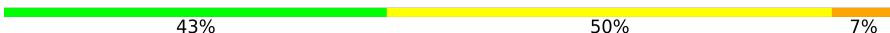
- Molecule 48: 50S ribosomal protein L30

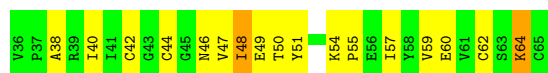


- Molecule 49: 50S ribosomal protein L31



- Molecule 49: 50S ribosomal protein L31

Chain D1:  43% 50% 7%



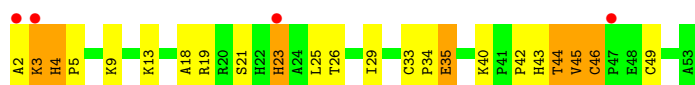
- Molecule 50: 50S ribosomal protein L32

Chain B2:  8% 58% 31% 12%



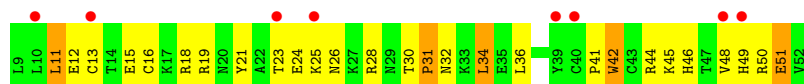
- Molecule 50: 50S ribosomal protein L32

Chain D2:  8% 56% 31% 13%



- Molecule 51: 50S ribosomal protein L33

Chain B3:  18% 39% 50% 11%



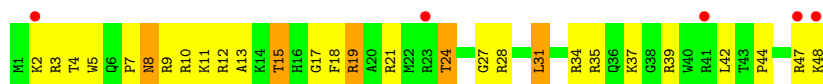
- Molecule 51: 50S ribosomal protein L33

Chain D3:  14% 43% 45% 11%



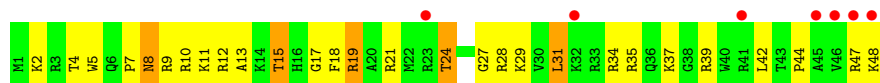
- Molecule 52: 50S ribosomal protein L34

Chain B4:  10% 42% 48% 10%

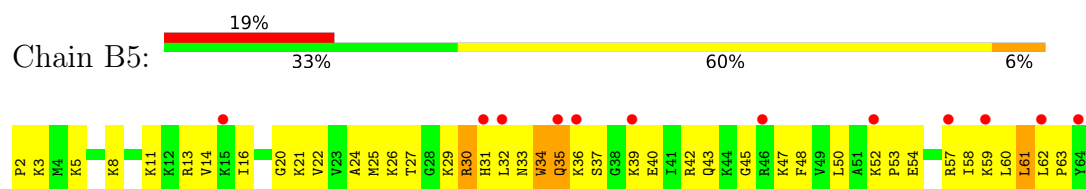


- Molecule 52: 50S ribosomal protein L34

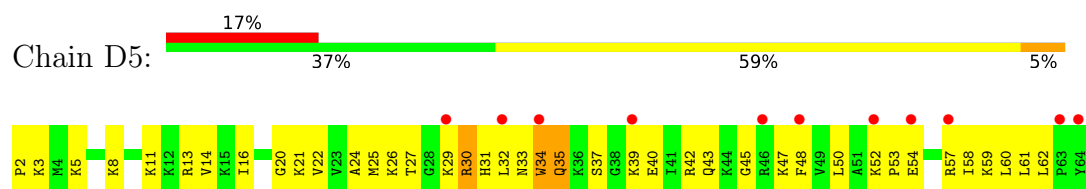
Chain D4:  15% 42% 48% 10%



● Molecule 53: 50S ribosomal protein L35



● Molecule 53: 50S ribosomal protein L35



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	211.94Å 455.59Å 618.02Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 3.50 50.00 – 3.50	Depositor EDS
% Data completeness (in resolution range)	99.9 (50.00-3.50) 99.8 (50.00-3.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.61 (at 3.49Å)	Xtriage
Refinement program	PHENIX 1.5_2, CNS	Depositor
R, R_{free}	0.233 , 0.264 0.233 , 0.262	Depositor DCC
R_{free} test set	7410 reflections (0.99%)	wwPDB-VP
Wilson B-factor (Å ²)	106.2	Xtriage
Anisotropy	0.163	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.25 , 96.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.38$, $\langle L^2 \rangle = 0.21$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	283641	wwPDB-VP
Average B, all atoms (Å ²)	127.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.63% 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: ZN, MG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	AA	0.38	0/36238	0.78	17/56561 (0.0%)
1	CA	0.38	0/36238	0.77	15/56561 (0.0%)
2	AB	0.27	0/1936	0.73	2/2609 (0.1%)
2	CB	0.26	0/1936	0.73	2/2609 (0.1%)
3	AC	0.28	0/1637	0.66	0/2205
3	CC	0.27	0/1637	0.67	0/2205
4	AD	0.31	0/1733	0.74	1/2318 (0.0%)
4	CD	0.28	0/1733	0.73	0/2318
5	AE	0.31	0/1172	0.74	0/1576
5	CE	0.29	0/1172	0.74	0/1576
6	AF	0.27	0/856	0.75	0/1154
6	CF	0.29	0/856	0.75	0/1154
7	AG	0.27	0/1276	0.69	0/1709
7	CG	0.27	0/1276	0.69	0/1709
8	AH	0.29	0/1136	0.77	1/1527 (0.1%)
8	CH	0.28	0/1136	0.77	0/1527
9	AI	0.26	0/1029	0.68	0/1378
9	CI	0.26	0/1029	0.68	0/1378
10	AJ	0.28	0/808	0.72	0/1085
10	CJ	0.28	0/808	0.72	0/1085
11	AK	0.29	0/900	0.79	4/1213 (0.3%)
11	CK	0.28	0/900	0.77	2/1213 (0.2%)
12	AL	0.33	0/987	0.82	0/1320
12	CL	0.32	0/987	0.81	0/1320
13	AM	0.31	0/939	0.74	0/1258
13	CM	0.31	0/939	0.74	0/1258
14	AN	0.31	0/501	0.68	0/664
14	CN	0.30	0/501	0.68	0/664
15	AO	0.32	0/745	0.67	0/992
15	CO	0.34	0/745	0.68	0/992
16	AP	0.36	0/717	0.69	0/963
16	CP	0.39	0/717	0.69	0/963

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	AQ	0.28	0/837	0.74	0/1117
17	CQ	0.26	0/837	0.72	0/1117
18	AR	0.27	0/579	0.72	0/768
18	CR	0.27	0/579	0.75	0/768
19	AS	0.27	0/643	0.66	0/865
19	CS	0.27	0/643	0.66	0/865
20	AT	0.31	0/764	0.69	0/1006
20	CT	0.28	0/764	0.69	0/1006
21	AU	0.26	0/213	0.63	0/277
21	CU	0.23	0/213	0.64	0/277
22	AV	0.39	0/821	0.71	0/1275
22	CV	0.38	0/821	0.72	0/1275
23	BA	0.41	0/66575	0.89	63/103930 (0.1%)
23	DA	0.43	0/66575	0.90	61/103930 (0.1%)
24	BB	0.39	0/2853	0.80	0/4451
24	DB	0.39	0/2853	0.80	0/4451
25	BC	0.42	0/2155	0.85	7/2905 (0.2%)
25	DC	0.43	0/2155	0.86	7/2905 (0.2%)
26	BD	0.34	0/1597	0.83	4/2153 (0.2%)
26	DD	0.34	0/1597	0.84	4/2153 (0.2%)
27	BE	0.38	0/1622	0.84	0/2194
27	DE	0.40	0/1622	0.84	2/2194 (0.1%)
28	BF	0.29	0/1500	0.75	3/2017 (0.1%)
28	DF	0.29	0/1500	0.75	2/2017 (0.1%)
29	BG	0.29	0/1246	0.76	1/1682 (0.1%)
29	DG	0.31	0/1246	0.76	1/1682 (0.1%)
30	BH	0.37	0/1148	0.79	0/1552
30	DH	0.39	0/1148	0.82	2/1552 (0.1%)
31	BI	0.26	0/252	0.66	0/333
31	DI	0.27	0/252	0.66	0/333
32	BJ	0.34	0/1124	0.83	2/1515 (0.1%)
32	DJ	0.35	0/1124	0.83	2/1515 (0.1%)
33	BK	0.36	0/942	0.81	0/1268
33	DK	0.36	0/942	0.82	0/1268
34	BL	0.40	0/1131	0.89	4/1504 (0.3%)
34	DL	0.42	0/1131	0.90	4/1504 (0.3%)
35	BM	0.39	0/1099	0.84	4/1468 (0.3%)
35	DM	0.40	0/1099	0.85	4/1468 (0.3%)
36	BN	0.35	0/974	0.75	0/1302
36	DN	0.34	0/974	0.74	0/1302
37	BO	0.31	0/779	0.75	0/1036
37	DO	0.31	0/779	0.76	0/1036
38	BP	0.33	0/1158	0.74	0/1544

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
38	DP	0.33	0/1158	0.74	0/1544
39	BQ	0.40	0/970	0.79	0/1290
39	DQ	0.42	0/970	0.80	0/1290
40	BR	0.33	0/790	0.73	1/1057 (0.1%)
40	DR	0.35	0/790	0.73	0/1057
41	BS	0.41	0/902	0.82	0/1209
41	DS	0.41	0/902	0.81	0/1209
42	BT	0.34	0/740	0.85	2/993 (0.2%)
42	DT	0.38	0/740	0.86	2/993 (0.2%)
43	BU	0.32	0/789	0.82	0/1051
43	DU	0.34	0/789	0.83	0/1051
44	BV	0.29	0/1524	0.77	1/2068 (0.0%)
44	DV	0.29	0/1524	0.77	1/2068 (0.0%)
45	BW	0.31	0/613	0.71	0/816
45	DW	0.31	0/613	0.71	0/816
46	BX	0.40	0/702	0.97	3/932 (0.3%)
46	DX	0.43	0/702	0.98	3/932 (0.3%)
47	BY	0.37	0/523	0.82	0/690
47	DY	0.40	0/523	0.85	0/690
48	BZ	0.32	0/473	0.80	2/634 (0.3%)
48	DZ	0.32	0/473	0.79	2/634 (0.3%)
49	B1	0.29	0/229	0.64	0/309
49	D1	0.29	0/229	0.65	0/309
50	B2	0.41	0/419	0.95	2/567 (0.4%)
50	D2	0.41	0/419	0.97	2/567 (0.4%)
51	B3	0.27	0/388	0.67	0/518
51	D3	0.27	0/388	0.67	0/518
52	B4	0.45	0/427	0.87	0/561
52	D4	0.50	0/427	0.88	0/561
53	B5	0.36	0/516	0.74	0/679
53	D5	0.39	0/516	0.76	0/679
All	All	0.39	0/305254	0.83	242/456136 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
28	BF	0	1
28	DF	0	1
34	BL	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
34	DL	0	1
All	All	0	4

There are no bond length outliers.

The worst 5 of 242 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
46	BX	35	THR	N-CA-C	10.79	122.11	108.19
46	DX	35	THR	N-CA-C	10.68	121.97	108.19
1	AA	136(B)	C	O3'-P-O5'	-8.83	90.75	104.00
23	BA	945	A	C1'-O4'-C4'	-8.18	101.52	109.70
46	BX	27	GLU	N-CA-C	8.02	118.48	107.73

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
28	BF	75	LYS	Peptide
34	BL	52	GLU	Peptide
28	DF	75	LYS	Peptide
34	DL	52	GLU	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	32372	0	16339	686	0
1	CA	32372	0	16339	697	0
2	AB	1901	0	1951	114	0
2	CB	1901	0	1951	114	0
3	AC	1613	0	1677	97	0
3	CC	1613	0	1677	97	0
4	AD	1703	0	1764	106	0
4	CD	1703	0	1765	101	0
5	AE	1156	0	1213	70	0
5	CE	1156	0	1213	67	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	AF	843	0	857	48	0
6	CF	843	0	857	50	0
7	AG	1257	0	1296	63	0
7	CG	1257	0	1296	65	0
8	AH	1116	0	1177	62	0
8	CH	1116	0	1177	62	0
9	AI	1011	0	1043	66	0
9	CI	1011	0	1043	62	0
10	AJ	795	0	840	60	0
10	CJ	795	0	840	60	0
11	AK	885	0	904	60	0
11	CK	885	0	904	53	0
12	AL	971	0	1057	60	0
12	CL	971	0	1057	66	0
13	AM	929	0	987	68	0
13	CM	929	0	987	66	0
14	AN	492	0	529	29	0
14	CN	492	0	533	26	0
15	AO	734	0	771	26	0
15	CO	734	0	771	30	0
16	AP	701	0	720	34	0
16	CP	701	0	720	42	0
17	AQ	824	0	893	44	0
17	CQ	824	0	893	48	0
18	AR	574	0	644	33	0
18	CR	574	0	644	35	0
19	AS	630	0	652	63	0
19	CS	630	0	652	58	0
20	AT	762	0	859	33	0
20	CT	762	0	859	32	0
21	AU	209	0	221	13	0
21	CU	209	0	221	14	0
22	AV	736	0	378	19	0
22	CV	736	0	378	17	0
23	BA	59442	0	29966	1290	0
23	DA	59442	0	29966	1296	0
24	BB	2551	0	1295	53	0
24	DB	2551	0	1295	53	0
25	BC	2105	0	2182	211	0
25	DC	2105	0	2182	226	0
26	BD	1564	0	1629	122	0
26	DD	1564	0	1629	116	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
27	BE	1587	0	1632	110	0
27	DE	1587	0	1632	110	0
28	BF	1475	0	1537	112	0
28	DF	1475	0	1537	113	0
29	BG	1223	0	1282	65	0
29	DG	1223	0	1282	67	0
30	BH	1133	0	1220	86	0
30	DH	1133	0	1220	83	0
31	BI	254	0	275	8	0
31	DI	254	0	275	8	0
32	BJ	1097	0	1168	85	0
32	DJ	1097	0	1168	85	0
33	BK	932	0	994	58	0
33	DK	932	0	994	61	0
34	BL	1114	0	1187	171	0
34	DL	1114	0	1187	172	0
35	BM	1079	0	1127	97	0
35	DM	1079	0	1127	103	0
36	BN	960	0	1021	80	0
36	DN	960	0	1021	78	0
37	BO	771	0	832	68	0
37	DO	771	0	832	70	0
38	BP	1144	0	1211	73	0
38	DP	1144	0	1211	78	0
39	BQ	953	0	1013	74	0
39	DQ	953	0	1013	74	0
40	BR	779	0	852	78	0
40	DR	779	0	852	75	0
41	BS	891	0	951	52	0
41	DS	891	0	951	54	0
42	BT	726	0	778	60	0
42	DT	726	0	778	60	0
43	BU	776	0	870	80	0
43	DU	776	0	870	79	0
44	BV	1492	0	1513	100	0
44	DV	1492	0	1513	97	0
45	BW	605	0	628	38	0
45	DW	605	0	628	41	0
46	BX	695	0	764	70	0
46	DX	695	0	764	69	0
47	BY	521	0	575	47	0
47	DY	521	0	575	50	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
48	BZ	468	0	523	21	0
48	DZ	468	0	523	25	0
49	B1	226	0	225	17	0
49	D1	226	0	225	17	0
50	B2	405	0	420	27	0
50	D2	405	0	420	29	0
51	B3	381	0	391	28	0
51	D3	381	0	391	26	0
52	B4	419	0	467	32	0
52	D4	419	0	467	33	0
53	B5	508	0	576	59	0
53	D5	508	0	576	58	0
54	AA	279	0	0	0	0
54	AB	3	0	0	0	0
54	AC	2	0	0	0	0
54	AD	3	0	0	0	0
54	AE	5	0	0	0	0
54	AF	1	0	0	0	0
54	AG	2	0	0	0	0
54	AH	1	0	0	0	0
54	AI	1	0	0	0	0
54	AK	2	0	0	0	0
54	AL	2	0	0	0	0
54	AM	1	0	0	0	0
54	AN	1	0	0	0	0
54	AO	3	0	0	0	0
54	AQ	3	0	0	0	0
54	AS	1	0	0	0	0
54	AT	2	0	0	0	0
54	AV	8	0	0	0	0
54	B2	3	0	0	0	0
54	B3	1	0	0	0	0
54	B4	1	0	0	0	0
54	B5	1	0	0	0	0
54	BA	781	0	0	0	0
54	BB	27	0	0	0	0
54	BC	3	0	0	0	0
54	BE	2	0	0	0	0
54	BF	1	0	0	0	0
54	BH	1	0	0	0	0
54	BI	1	0	0	0	0
54	BJ	3	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
54	BK	1	0	0	0	0
54	BM	3	0	0	0	0
54	BN	2	0	0	0	0
54	BO	1	0	0	0	0
54	BP	2	0	0	0	0
54	BR	1	0	0	0	0
54	BS	1	0	0	0	0
54	BT	2	0	0	0	0
54	BU	2	0	0	0	0
54	BV	3	0	0	0	0
54	BW	1	0	0	0	0
54	BX	2	0	0	0	0
54	BY	3	0	0	0	0
54	CA	372	0	0	0	0
54	CB	3	0	0	0	0
54	CC	8	0	0	0	0
54	CD	3	0	0	0	0
54	CE	5	0	0	0	0
54	CF	2	0	0	0	0
54	CG	3	0	0	0	0
54	CK	1	0	0	0	0
54	CL	6	0	0	0	0
54	CM	2	0	0	0	0
54	CN	1	0	0	0	0
54	CO	4	0	0	0	0
54	CQ	2	0	0	0	0
54	CV	7	0	0	0	0
54	D1	1	0	0	0	0
54	D2	3	0	0	0	0
54	D3	1	0	0	0	0
54	D4	4	0	0	0	0
54	D5	3	0	0	0	0
54	DA	964	0	0	0	0
54	DB	43	0	0	0	0
54	DC	3	0	0	0	0
54	DD	6	0	0	0	0
54	DE	3	0	0	0	0
54	DF	2	0	0	0	0
54	DG	3	0	0	0	0
54	DI	1	0	0	0	0
54	DJ	6	0	0	0	0
54	DK	3	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
54	DL	3	0	0	0	0
54	DM	1	0	0	0	0
54	DN	1	0	0	0	0
54	DO	1	0	0	0	0
54	DP	2	0	0	0	0
54	DQ	2	0	0	0	0
54	DS	2	0	0	0	0
54	DU	1	0	0	0	0
54	DV	4	0	0	0	0
54	DW	1	0	0	0	0
54	DX	3	0	0	0	0
54	DY	2	0	0	0	0
55	AD	1	0	0	0	0
55	AN	1	0	0	0	0
55	CD	1	0	0	0	0
55	CN	1	0	0	0	0
All	All	283641	0	191757	9546	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 20.

The worst 5 of 9546 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:1399:C:H4'	1:AA:1400:C:H5'	1.26	1.16
34:BL:33:ARG:HG3	34:BL:36:LYS:HD3	1.31	1.12
34:BL:128:HIS:HA	34:BL:147:LEU:HB3	1.30	1.11
23:DA:2015:A:H1'	50:D2:2:ALA:HA	1.33	1.08
34:DL:33:ARG:HG3	34:DL:36:LYS:HD3	1.33	1.08

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	AB	232/234 (99%)	194 (84%)	32 (14%)	6 (3%)	4	27
2	CB	232/234 (99%)	194 (84%)	32 (14%)	6 (3%)	4	27
3	AC	204/206 (99%)	153 (75%)	38 (19%)	13 (6%)	1	11
3	CC	204/206 (99%)	154 (76%)	37 (18%)	13 (6%)	1	11
4	AD	206/208 (99%)	172 (84%)	26 (13%)	8 (4%)	2	20
4	CD	206/208 (99%)	172 (84%)	25 (12%)	9 (4%)	2	17
5	AE	149/151 (99%)	123 (83%)	22 (15%)	4 (3%)	4	27
5	CE	149/151 (99%)	126 (85%)	19 (13%)	4 (3%)	4	27
6	AF	99/101 (98%)	90 (91%)	8 (8%)	1 (1%)	12	44
6	CF	99/101 (98%)	90 (91%)	8 (8%)	1 (1%)	12	44
7	AG	153/155 (99%)	132 (86%)	18 (12%)	3 (2%)	6	32
7	CG	153/155 (99%)	133 (87%)	17 (11%)	3 (2%)	6	32
8	AH	136/138 (99%)	119 (88%)	17 (12%)	0	100	100
8	CH	136/138 (99%)	119 (88%)	17 (12%)	0	100	100
9	AI	125/127 (98%)	102 (82%)	20 (16%)	3 (2%)	4	29
9	CI	125/127 (98%)	101 (81%)	21 (17%)	3 (2%)	4	29
10	AJ	96/98 (98%)	78 (81%)	12 (12%)	6 (6%)	1	12
10	CJ	96/98 (98%)	78 (81%)	12 (12%)	6 (6%)	1	12
11	AK	117/119 (98%)	97 (83%)	16 (14%)	4 (3%)	3	23
11	CK	117/119 (98%)	97 (83%)	16 (14%)	4 (3%)	3	23
12	AL	122/124 (98%)	94 (77%)	22 (18%)	6 (5%)	1	16
12	CL	122/124 (98%)	94 (77%)	22 (18%)	6 (5%)	1	16
13	AM	114/116 (98%)	94 (82%)	16 (14%)	4 (4%)	3	23
13	CM	114/116 (98%)	94 (82%)	16 (14%)	4 (4%)	3	23
14	AN	58/60 (97%)	50 (86%)	5 (9%)	3 (5%)	1	14
14	CN	58/60 (97%)	50 (86%)	5 (9%)	3 (5%)	1	14
15	AO	86/88 (98%)	77 (90%)	7 (8%)	2 (2%)	5	30
15	CO	86/88 (98%)	77 (90%)	7 (8%)	2 (2%)	5	30
16	AP	81/83 (98%)	65 (80%)	14 (17%)	2 (2%)	4	28
16	CP	81/83 (98%)	65 (80%)	13 (16%)	3 (4%)	2	21

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
17	AQ	97/99 (98%)	81 (84%)	15 (16%)	1 (1%)	12	44
17	CQ	97/99 (98%)	81 (84%)	15 (16%)	1 (1%)	12	44
18	AR	68/70 (97%)	53 (78%)	13 (19%)	2 (3%)	3	26
18	CR	68/70 (97%)	53 (78%)	12 (18%)	3 (4%)	2	17
19	AS	76/78 (97%)	57 (75%)	14 (18%)	5 (7%)	1	11
19	CS	76/78 (97%)	57 (75%)	14 (18%)	5 (7%)	1	11
20	AT	97/99 (98%)	82 (84%)	12 (12%)	3 (3%)	3	25
20	CT	97/99 (98%)	82 (84%)	12 (12%)	3 (3%)	3	25
21	AU	22/24 (92%)	17 (77%)	4 (18%)	1 (4%)	2	17
21	CU	22/24 (92%)	17 (77%)	4 (18%)	1 (4%)	2	17
25	BC	269/271 (99%)	220 (82%)	31 (12%)	18 (7%)	1	11
25	DC	269/271 (99%)	218 (81%)	33 (12%)	18 (7%)	1	11
26	BD	202/204 (99%)	168 (83%)	26 (13%)	8 (4%)	2	19
26	DD	202/204 (99%)	167 (83%)	29 (14%)	6 (3%)	3	25
27	BE	200/202 (99%)	165 (82%)	28 (14%)	7 (4%)	3	23
27	DE	200/202 (99%)	165 (82%)	28 (14%)	7 (4%)	3	23
28	BF	179/181 (99%)	134 (75%)	37 (21%)	8 (4%)	2	17
28	DF	179/181 (99%)	133 (74%)	37 (21%)	9 (5%)	1	15
29	BG	157/159 (99%)	126 (80%)	27 (17%)	4 (2%)	4	28
29	DG	157/159 (99%)	125 (80%)	28 (18%)	4 (2%)	4	28
30	BH	143/145 (99%)	109 (76%)	28 (20%)	6 (4%)	2	19
30	DH	143/145 (99%)	109 (76%)	28 (20%)	6 (4%)	2	19
31	BI	28/65 (43%)	27 (96%)	1 (4%)	0	100	100
31	DI	28/65 (43%)	27 (96%)	1 (4%)	0	100	100
32	BJ	135/137 (98%)	108 (80%)	19 (14%)	8 (6%)	1	12
32	DJ	135/137 (98%)	108 (80%)	19 (14%)	8 (6%)	1	12
33	BK	120/122 (98%)	105 (88%)	8 (7%)	7 (6%)	1	13
33	DK	120/122 (98%)	107 (89%)	6 (5%)	7 (6%)	1	13
34	BL	144/146 (99%)	94 (65%)	35 (24%)	15 (10%)	0	5
34	DL	144/146 (99%)	92 (64%)	37 (26%)	15 (10%)	0	5
35	BM	134/136 (98%)	98 (73%)	22 (16%)	14 (10%)	0	5

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
35	DM	134/136 (98%)	97 (72%)	24 (18%)	13 (10%)	0	6
36	BN	115/117 (98%)	97 (84%)	13 (11%)	5 (4%)	2	18
36	DN	115/117 (98%)	97 (84%)	14 (12%)	4 (4%)	3	23
37	BO	96/98 (98%)	65 (68%)	18 (19%)	13 (14%)	0	3
37	DO	96/98 (98%)	65 (68%)	18 (19%)	13 (14%)	0	3
38	BP	135/137 (98%)	99 (73%)	30 (22%)	6 (4%)	2	17
38	DP	135/137 (98%)	99 (73%)	30 (22%)	6 (4%)	2	17
39	BQ	114/116 (98%)	99 (87%)	13 (11%)	2 (2%)	6	34
39	DQ	114/116 (98%)	99 (87%)	13 (11%)	2 (2%)	6	34
40	BR	99/101 (98%)	71 (72%)	19 (19%)	9 (9%)	0	7
40	DR	99/101 (98%)	71 (72%)	19 (19%)	9 (9%)	0	7
41	BS	110/112 (98%)	94 (86%)	14 (13%)	2 (2%)	6	34
41	DS	110/112 (98%)	94 (86%)	14 (13%)	2 (2%)	6	34
42	BT	90/92 (98%)	82 (91%)	7 (8%)	1 (1%)	11	43
42	DT	90/92 (98%)	82 (91%)	7 (8%)	1 (1%)	11	43
43	BU	98/100 (98%)	65 (66%)	22 (22%)	11 (11%)	0	5
43	DU	98/100 (98%)	63 (64%)	23 (24%)	12 (12%)	0	4
44	BV	186/188 (99%)	140 (75%)	36 (19%)	10 (5%)	1	14
44	DV	186/188 (99%)	140 (75%)	36 (19%)	10 (5%)	1	14
45	BW	74/76 (97%)	59 (80%)	12 (16%)	3 (4%)	2	19
45	DW	74/76 (97%)	57 (77%)	14 (19%)	3 (4%)	2	19
46	BX	86/88 (98%)	57 (66%)	20 (23%)	9 (10%)	0	5
46	DX	86/88 (98%)	57 (66%)	20 (23%)	9 (10%)	0	5
47	BY	60/62 (97%)	48 (80%)	9 (15%)	3 (5%)	1	15
47	DY	60/62 (97%)	49 (82%)	8 (13%)	3 (5%)	1	15
48	BZ	57/59 (97%)	51 (90%)	5 (9%)	1 (2%)	6	34
48	DZ	57/59 (97%)	51 (90%)	5 (9%)	1 (2%)	6	34
49	B1	28/30 (93%)	15 (54%)	10 (36%)	3 (11%)	0	5
49	D1	28/30 (93%)	15 (54%)	10 (36%)	3 (11%)	0	5
50	B2	50/52 (96%)	39 (78%)	8 (16%)	3 (6%)	1	12
50	D2	50/52 (96%)	40 (80%)	6 (12%)	4 (8%)	1	8

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
51	B3	42/44 (96%)	35 (83%)	2 (5%)	5 (12%)	0	4
51	D3	42/44 (96%)	35 (83%)	2 (5%)	5 (12%)	0	4
52	B4	46/48 (96%)	42 (91%)	4 (9%)	0	100	100
52	D4	46/48 (96%)	41 (89%)	5 (11%)	0	100	100
53	B5	61/63 (97%)	43 (70%)	13 (21%)	5 (8%)	0	8
53	D5	61/63 (97%)	44 (72%)	13 (21%)	4 (7%)	1	11
All	All	11192/11458 (98%)	8966 (80%)	1699 (15%)	527 (5%)	2	17

5 of 527 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	AC	15	THR
4	AD	30	LYS
4	AD	137	SER
4	AD	138	TYR
4	AD	168	ARG

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	AB	202/202 (100%)	186 (92%)	16 (8%)	11	36
2	CB	202/202 (100%)	186 (92%)	16 (8%)	11	36
3	AC	160/160 (100%)	155 (97%)	5 (3%)	35	59
3	CC	160/160 (100%)	155 (97%)	5 (3%)	35	59
4	AD	180/180 (100%)	171 (95%)	9 (5%)	22	48
4	CD	180/180 (100%)	171 (95%)	9 (5%)	22	48
5	AE	116/116 (100%)	108 (93%)	8 (7%)	14	39
5	CE	116/116 (100%)	108 (93%)	8 (7%)	14	39
6	AF	90/90 (100%)	88 (98%)	2 (2%)	45	65
6	CF	90/90 (100%)	88 (98%)	2 (2%)	45	65

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
7	AG	126/126 (100%)	124 (98%)	2 (2%)	55	70
7	CG	126/126 (100%)	124 (98%)	2 (2%)	55	70
8	AH	119/119 (100%)	111 (93%)	8 (7%)	15	41
8	CH	119/119 (100%)	111 (93%)	8 (7%)	15	41
9	AI	98/98 (100%)	93 (95%)	5 (5%)	21	48
9	CI	98/98 (100%)	93 (95%)	5 (5%)	21	48
10	AJ	88/88 (100%)	81 (92%)	7 (8%)	11	35
10	CJ	88/88 (100%)	81 (92%)	7 (8%)	11	35
11	AK	90/90 (100%)	87 (97%)	3 (3%)	33	58
11	CK	90/90 (100%)	87 (97%)	3 (3%)	33	58
12	AL	104/104 (100%)	93 (89%)	11 (11%)	6	27
12	CL	104/104 (100%)	92 (88%)	12 (12%)	5	24
13	AM	94/94 (100%)	89 (95%)	5 (5%)	20	47
13	CM	94/94 (100%)	89 (95%)	5 (5%)	20	47
14	AN	49/49 (100%)	47 (96%)	2 (4%)	27	53
14	CN	49/49 (100%)	47 (96%)	2 (4%)	27	53
15	AO	79/79 (100%)	76 (96%)	3 (4%)	29	55
15	CO	79/79 (100%)	76 (96%)	3 (4%)	29	55
16	AP	72/72 (100%)	67 (93%)	5 (7%)	14	39
16	CP	72/72 (100%)	67 (93%)	5 (7%)	14	39
17	AQ	94/94 (100%)	93 (99%)	1 (1%)	65	74
17	CQ	94/94 (100%)	93 (99%)	1 (1%)	65	74
18	AR	61/61 (100%)	59 (97%)	2 (3%)	33	58
18	CR	61/61 (100%)	59 (97%)	2 (3%)	33	58
19	AS	69/69 (100%)	60 (87%)	9 (13%)	4	21
19	CS	69/69 (100%)	60 (87%)	9 (13%)	4	21
20	AT	76/76 (100%)	72 (95%)	4 (5%)	20	47
20	CT	76/76 (100%)	72 (95%)	4 (5%)	20	47
21	AU	19/19 (100%)	19 (100%)	0	100	100
21	CU	19/19 (100%)	19 (100%)	0	100	100
25	BC	213/213 (100%)	188 (88%)	25 (12%)	5	24

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
25	DC	213/213 (100%)	188 (88%)	25 (12%)	5	24
26	BD	165/165 (100%)	149 (90%)	16 (10%)	8	30
26	DD	165/165 (100%)	149 (90%)	16 (10%)	8	30
27	BE	161/161 (100%)	148 (92%)	13 (8%)	11	35
27	DE	161/161 (100%)	147 (91%)	14 (9%)	9	33
28	BF	155/155 (100%)	146 (94%)	9 (6%)	18	44
28	DF	155/155 (100%)	146 (94%)	9 (6%)	18	44
29	BG	132/132 (100%)	122 (92%)	10 (8%)	12	37
29	DG	132/132 (100%)	122 (92%)	10 (8%)	12	37
30	BH	122/122 (100%)	113 (93%)	9 (7%)	13	37
30	DH	122/122 (100%)	113 (93%)	9 (7%)	13	37
31	BI	27/53 (51%)	26 (96%)	1 (4%)	30	56
31	DI	27/53 (51%)	26 (96%)	1 (4%)	30	56
32	BJ	116/116 (100%)	105 (90%)	11 (10%)	8	31
32	DJ	116/116 (100%)	105 (90%)	11 (10%)	8	31
33	BK	100/100 (100%)	88 (88%)	12 (12%)	5	23
33	DK	100/100 (100%)	89 (89%)	11 (11%)	6	26
34	BL	112/112 (100%)	86 (77%)	26 (23%)	1	5
34	DL	112/112 (100%)	86 (77%)	26 (23%)	1	5
35	BM	106/106 (100%)	95 (90%)	11 (10%)	7	27
35	DM	106/106 (100%)	95 (90%)	11 (10%)	7	27
36	BN	100/100 (100%)	94 (94%)	6 (6%)	17	44
36	DN	100/100 (100%)	94 (94%)	6 (6%)	17	44
37	BO	77/77 (100%)	71 (92%)	6 (8%)	11	36
37	DO	77/77 (100%)	71 (92%)	6 (8%)	11	36
38	BP	121/121 (100%)	112 (93%)	9 (7%)	13	37
38	DP	121/121 (100%)	112 (93%)	9 (7%)	13	37
39	BQ	92/92 (100%)	84 (91%)	8 (9%)	9	33
39	DQ	92/92 (100%)	86 (94%)	6 (6%)	15	42
40	BR	82/82 (100%)	76 (93%)	6 (7%)	13	38
40	DR	82/82 (100%)	76 (93%)	6 (7%)	13	38

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
41	BS	91/91 (100%)	83 (91%)	8 (9%)	9	32
41	DS	91/91 (100%)	83 (91%)	8 (9%)	9	32
42	BT	74/74 (100%)	65 (88%)	9 (12%)	5	22
42	DT	74/74 (100%)	65 (88%)	9 (12%)	5	22
43	BU	84/84 (100%)	79 (94%)	5 (6%)	17	44
43	DU	84/84 (100%)	79 (94%)	5 (6%)	17	44
44	BV	163/163 (100%)	159 (98%)	4 (2%)	42	63
44	DV	163/163 (100%)	159 (98%)	4 (2%)	42	63
45	BW	61/61 (100%)	56 (92%)	5 (8%)	10	34
45	DW	61/61 (100%)	56 (92%)	5 (8%)	10	34
46	BX	73/73 (100%)	59 (81%)	14 (19%)	1	8
46	DX	73/73 (100%)	60 (82%)	13 (18%)	2	10
47	BY	58/58 (100%)	51 (88%)	7 (12%)	5	22
47	DY	58/58 (100%)	51 (88%)	7 (12%)	5	22
48	BZ	51/51 (100%)	48 (94%)	3 (6%)	18	44
48	DZ	51/51 (100%)	49 (96%)	2 (4%)	28	54
49	B1	27/27 (100%)	24 (89%)	3 (11%)	6	25
49	D1	27/27 (100%)	24 (89%)	3 (11%)	6	25
50	B2	45/45 (100%)	42 (93%)	3 (7%)	15	41
50	D2	45/45 (100%)	42 (93%)	3 (7%)	15	41
51	B3	43/43 (100%)	40 (93%)	3 (7%)	14	39
51	D3	43/43 (100%)	40 (93%)	3 (7%)	14	39
52	B4	41/41 (100%)	35 (85%)	6 (15%)	3	17
52	D4	41/41 (100%)	34 (83%)	7 (17%)	2	12
53	B5	53/53 (100%)	51 (96%)	2 (4%)	29	55
53	D5	53/53 (100%)	51 (96%)	2 (4%)	29	55
All	All	9462/9514 (100%)	8750 (92%)	712 (8%)	12	37

5 of 712 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
20	CT	51	GLU
34	DL	15	ARG

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Mol	Chain	Res	Type
25	DC	94	LEU
20	CT	26	ASN
28	DF	18	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 273 such sidechains are listed below:

Mol	Chain	Res	Type
36	DN	24	GLN
38	DP	58	ASN
46	DX	66	HIS
36	BN	13	HIS
35	BM	13	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	AA	1505/1506 (99%)	208 (13%)	35 (2%)
1	CA	1505/1506 (99%)	209 (13%)	35 (2%)
22	AV	34/35 (97%)	2 (5%)	2 (5%)
22	CV	34/35 (97%)	2 (5%)	2 (5%)
23	BA	2757/2879 (95%)	423 (15%)	69 (2%)
23	DA	2757/2879 (95%)	425 (15%)	70 (2%)
24	BB	118/119 (99%)	16 (13%)	1 (0%)
24	DB	118/119 (99%)	16 (13%)	1 (0%)
All	All	8828/9078 (97%)	1301 (14%)	215 (2%)

5 of 1301 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	AA	7	G
1	AA	8	A
1	AA	9	G
1	AA	22	G
1	AA	32	A

5 of 215 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	CA	353	A
22	CV	6188	C

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Mol	Chain	Res	Type
23	DA	2225	A
1	CA	438	G
1	CA	1145	C

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 2661 ligands modelled in this entry, 2661 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	AA	1506/1506 (100%)	0.39	81 (5%) 31 18	66, 119, 257, 429	0
1	CA	1506/1506 (100%)	0.74	155 (10%) 12 8	75, 164, 286, 403	0
2	AB	234/234 (100%)	0.59	19 (8%) 18 12	88, 178, 260, 354	0
2	CB	234/234 (100%)	0.65	26 (11%) 10 7	106, 202, 279, 372	0
3	AC	206/206 (100%)	0.60	15 (7%) 21 13	83, 165, 233, 293	0
3	CC	206/206 (100%)	0.65	26 (12%) 8 6	124, 198, 272, 337	0
4	AD	208/208 (100%)	0.69	23 (11%) 10 7	45, 119, 180, 228	0
4	CD	208/208 (100%)	1.43	57 (27%) 1 2	96, 186, 253, 314	0
5	AE	151/151 (100%)	0.44	10 (6%) 24 15	71, 118, 191, 293	0
5	CE	151/151 (100%)	0.69	15 (9%) 13 8	72, 165, 223, 282	0
6	AF	101/101 (100%)	0.63	9 (8%) 15 10	87, 160, 207, 278	0
6	CF	101/101 (100%)	0.30	4 (3%) 42 23	60, 130, 195, 271	0
7	AG	155/155 (100%)	0.63	15 (9%) 13 9	134, 201, 260, 328	0
7	CG	155/155 (100%)	0.46	9 (5%) 29 17	124, 213, 271, 320	0
8	AH	138/138 (100%)	0.54	13 (9%) 14 9	60, 122, 190, 265	0
8	CH	138/138 (100%)	0.85	15 (10%) 10 7	101, 171, 217, 257	0
9	AI	127/127 (100%)	1.66	44 (34%) 1 1	119, 228, 303, 333	0
9	CI	127/127 (100%)	1.50	41 (32%) 1 1	148, 229, 297, 370	0
10	AJ	98/98 (100%)	1.08	16 (16%) 4 4	113, 203, 294, 334	0
10	CJ	98/98 (100%)	1.20	24 (24%) 2 2	133, 232, 290, 339	0
11	AK	119/119 (100%)	0.65	14 (11%) 9 6	66, 136, 219, 274	0
11	CK	119/119 (100%)	0.73	17 (14%) 6 5	87, 145, 207, 287	0
12	AL	124/124 (100%)	0.69	15 (12%) 8 6	56, 108, 182, 328	0
12	CL	124/124 (100%)	1.67	35 (28%) 1 1	77, 139, 236, 271	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	AM	116/116 (100%)	0.64	13 (11%) 10 7	129, 216, 277, 325	0
13	CM	116/116 (100%)	0.65	8 (6%) 23 14	119, 238, 307, 372	0
14	AN	60/60 (100%)	1.35	13 (21%) 2 3	94, 178, 243, 278	0
14	CN	60/60 (100%)	1.56	23 (38%) 1 1	110, 207, 261, 344	0
15	AO	88/88 (100%)	0.63	9 (10%) 12 8	73, 127, 187, 281	0
15	CO	88/88 (100%)	0.79	13 (14%) 5 5	73, 138, 201, 244	0
16	AP	83/83 (100%)	0.85	11 (13%) 7 6	67, 109, 175, 245	0
16	CP	83/83 (100%)	1.66	29 (34%) 1 1	128, 171, 247, 277	0
17	AQ	99/99 (100%)	0.55	7 (7%) 22 14	63, 112, 169, 222	0
17	CQ	99/99 (100%)	1.34	25 (25%) 1 2	99, 155, 196, 228	0
18	AR	70/70 (100%)	0.68	6 (8%) 16 11	82, 149, 241, 325	0
18	CR	70/70 (100%)	0.32	1 (1%) 73 48	76, 145, 204, 232	0
19	AS	78/78 (100%)	0.61	8 (10%) 12 8	133, 212, 274, 295	0
19	CS	78/78 (100%)	0.81	9 (11%) 9 6	173, 235, 302, 347	0
20	AT	99/99 (100%)	0.98	15 (15%) 5 5	65, 131, 220, 241	0
20	CT	99/99 (100%)	1.56	31 (31%) 1 1	103, 178, 284, 301	0
21	AU	24/24 (100%)	2.32	9 (37%) 1 1	122, 220, 292, 333	0
21	CU	24/24 (100%)	2.47	14 (58%) 0 0	173, 236, 317, 346	0
22	AV	35/35 (100%)	0.80	3 (8%) 16 11	96, 223, 325, 366	0
22	CV	35/35 (100%)	1.10	6 (17%) 4 4	117, 192, 362, 386	0
23	BA	2760/2879 (95%)	0.02	68 (2%) 58 35	38, 86, 205, 371	0
23	DA	2760/2879 (95%)	-0.00	67 (2%) 59 35	33, 77, 196, 377	0
24	BB	119/119 (100%)	0.42	5 (4%) 40 22	83, 149, 196, 251	0
24	DB	119/119 (100%)	0.63	14 (11%) 9 6	87, 132, 198, 274	0
25	BC	271/271 (100%)	0.52	26 (9%) 13 9	24, 81, 150, 209	0
25	DC	271/271 (100%)	0.60	28 (10%) 12 8	26, 72, 144, 220	0
26	BD	204/204 (100%)	0.73	18 (8%) 15 10	45, 96, 173, 331	0
26	DD	204/204 (100%)	0.79	26 (12%) 8 6	36, 90, 189, 305	0
27	BE	202/202 (100%)	0.55	19 (9%) 14 9	32, 94, 172, 311	0
27	DE	202/202 (100%)	0.44	8 (3%) 42 23	20, 85, 182, 249	0
28	BF	181/181 (100%)	0.45	12 (6%) 24 15	107, 202, 262, 297	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å ²)	Q<0.9
28	DF	181/181 (100%)	0.51	14 (7%)	19 13	109, 198, 281, 324	0
29	BG	159/159 (100%)	0.71	19 (11%)	9 6	102, 192, 269, 331	0
29	DG	159/159 (100%)	0.73	19 (11%)	9 6	61, 117, 190, 269	0
30	BH	145/145 (100%)	1.88	56 (38%)	1 1	60, 224, 376, 453	0
30	DH	145/145 (100%)	1.63	40 (27%)	1 1	60, 210, 372, 482	0
31	BI	32/65 (49%)	0.79	2 (6%)	26 15	163, 256, 325, 352	0
31	DI	32/65 (49%)	0.74	3 (9%)	14 9	176, 235, 294, 325	0
32	BJ	137/137 (100%)	0.87	21 (15%)	5 5	58, 105, 182, 221	0
32	DJ	137/137 (100%)	0.63	10 (7%)	21 13	55, 100, 170, 219	0
33	BK	122/122 (100%)	0.24	5 (4%)	41 22	48, 90, 142, 194	0
33	DK	122/122 (100%)	0.31	2 (1%)	70 45	41, 90, 153, 251	0
34	BL	146/146 (100%)	0.91	21 (14%)	6 5	40, 114, 204, 306	0
34	DL	146/146 (100%)	1.23	30 (20%)	2 3	27, 111, 206, 324	0
35	BM	136/136 (100%)	0.80	17 (12%)	8 6	57, 110, 205, 344	0
35	DM	136/136 (100%)	0.90	16 (11%)	9 6	46, 106, 199, 388	0
36	BN	117/117 (100%)	0.71	12 (10%)	12 8	44, 92, 166, 282	0
36	DN	117/117 (100%)	0.71	15 (12%)	7 6	41, 89, 173, 285	0
37	BO	98/98 (100%)	1.06	17 (17%)	4 4	89, 155, 230, 299	0
37	DO	98/98 (100%)	1.25	24 (24%)	2 2	80, 148, 221, 299	0
38	BP	137/137 (100%)	0.60	10 (7%)	21 13	52, 115, 216, 248	0
38	DP	137/137 (100%)	0.71	19 (13%)	6 5	60, 119, 249, 299	0
39	BQ	116/116 (100%)	0.55	10 (8%)	16 11	43, 88, 163, 244	0
39	DQ	116/116 (100%)	0.78	15 (12%)	7 6	34, 84, 154, 205	0
40	BR	101/101 (100%)	0.58	9 (8%)	15 10	55, 134, 187, 294	0
40	DR	101/101 (100%)	0.78	13 (12%)	7 6	52, 132, 197, 321	0
41	BS	112/112 (100%)	0.31	5 (4%)	38 20	45, 78, 151, 250	0
41	DS	112/112 (100%)	0.31	9 (8%)	18 12	40, 72, 166, 277	0
42	BT	92/92 (100%)	0.94	15 (16%)	4 4	57, 107, 174, 204	0
42	DT	92/92 (100%)	0.47	9 (9%)	13 9	41, 78, 161, 204	0
43	BU	100/100 (100%)	1.72	36 (36%)	1 1	59, 139, 289, 344	0
43	DU	100/100 (100%)	1.20	24 (24%)	2 2	49, 119, 264, 373	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
44	BV	188/188 (100%)	0.62	16 (8%) 16 11	80, 160, 224, 277	0
44	DV	188/188 (100%)	0.57	20 (10%) 11 8	67, 154, 220, 254	0
45	BW	76/76 (100%)	0.69	9 (11%) 9 6	61, 101, 160, 258	0
45	DW	76/76 (100%)	0.90	8 (10%) 11 8	54, 101, 167, 254	0
46	BX	88/88 (100%)	1.48	25 (28%) 1 1	50, 106, 191, 346	0
46	DX	88/88 (100%)	0.95	15 (17%) 4 4	31, 83, 196, 340	0
47	BY	62/62 (100%)	1.38	13 (20%) 2 3	61, 141, 244, 287	0
47	DY	62/62 (100%)	0.74	8 (12%) 7 6	45, 99, 224, 304	0
48	BZ	59/59 (100%)	0.49	2 (3%) 48 27	47, 102, 174, 342	0
48	DZ	59/59 (100%)	0.52	3 (5%) 33 19	45, 102, 189, 335	0
49	B1	30/30 (100%)	0.04	0 100 100	161, 244, 282, 323	0
49	D1	30/30 (100%)	-0.08	0 100 100	187, 262, 306, 326	0
50	B2	52/52 (100%)	0.44	4 (7%) 19 13	36, 93, 189, 273	0
50	D2	52/52 (100%)	0.51	4 (7%) 19 13	24, 93, 214, 262	0
51	B3	44/44 (100%)	1.04	8 (18%) 3 4	151, 254, 304, 322	0
51	D3	44/44 (100%)	1.15	6 (13%) 7 5	191, 247, 298, 313	0
52	B4	48/48 (100%)	0.62	5 (10%) 11 8	43, 66, 132, 297	0
52	D4	48/48 (100%)	0.50	7 (14%) 6 5	23, 45, 122, 217	0
53	B5	63/63 (100%)	1.06	12 (19%) 3 3	47, 94, 171, 222	0
53	D5	63/63 (100%)	1.13	11 (17%) 4 4	43, 92, 170, 208	0
All	All	20232/20536 (98%)	0.55	1935 (9%) 13 9	20, 120, 258, 482	0

The worst 5 of 1935 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
35	BM	140	ALA	11.5
47	BY	3	LEU	10.9
9	AI	109	VAL	10.6
1	AA	82	U	10.5
12	CL	27	LYS	10.2

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

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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
54	MG	AA	1688	1/1	-0.11	0.22	140,140,140,140	0
54	MG	CC	303	1/1	0.08	0.16	147,147,147,147	0
54	MG	DA	3585	1/1	0.08	0.22	154,154,154,154	0
54	MG	CA	1867	1/1	0.11	0.17	123,123,123,123	0
54	MG	CA	1704	1/1	0.17	0.14	140,140,140,140	0
54	MG	AA	1680	1/1	0.22	0.24	140,140,140,140	0
54	MG	CA	1919	1/1	0.23	0.17	145,145,145,145	0
54	MG	BB	216	1/1	0.26	0.50	154,154,154,154	0
54	MG	AA	1866	1/1	0.27	0.27	108,108,108,108	0
54	MG	BA	3393	1/1	0.27	0.12	136,136,136,136	0
54	MG	CM	202	1/1	0.31	0.10	164,164,164,164	0
54	MG	DA	3836	1/1	0.32	0.10	135,135,135,135	0
54	MG	CA	1912	1/1	0.34	0.10	138,138,138,138	0
54	MG	CE	204	1/1	0.35	0.10	109,109,109,109	0
54	MG	DA	3735	1/1	0.40	0.08	97,97,97,97	0
54	MG	DA	3509	1/1	0.41	0.18	148,148,148,148	0
54	MG	AG	202	1/1	0.41	0.34	129,129,129,129	0
54	MG	BA	3106	1/1	0.42	0.12	142,142,142,142	0
54	MG	DA	3063	1/1	0.43	0.57	126,126,126,126	0
54	MG	CA	1797	1/1	0.44	0.10	133,133,133,133	0
54	MG	CA	1629	1/1	0.45	0.18	93,93,93,93	0
54	MG	AA	1674	1/1	0.45	0.33	113,113,113,113	0
54	MG	DA	3668	1/1	0.46	0.35	133,133,133,133	0
54	MG	CA	1730	1/1	0.47	0.18	112,112,112,112	0
54	MG	CA	1820	1/1	0.47	0.27	99,99,99,99	0
54	MG	CA	1958	1/1	0.48	0.34	125,125,125,125	0
54	MG	AA	1857	1/1	0.50	0.16	103,103,103,103	0
54	MG	DA	3614	1/1	0.51	0.12	128,128,128,128	0
54	MG	BA	3397	1/1	0.51	0.08	125,125,125,125	0
54	MG	BA	3372	1/1	0.51	0.28	123,123,123,123	0
54	MG	CO	104	1/1	0.51	0.09	99,99,99,99	0
54	MG	CA	1793	1/1	0.52	0.22	125,125,125,125	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
54	MG	AA	1723	1/1	0.52	0.20	126,126,126,126	0
54	MG	AA	1785	1/1	0.52	0.15	117,117,117,117	0
54	MG	AC	301	1/1	0.52	0.08	104,104,104,104	0
54	MG	CC	306	1/1	0.52	0.12	117,117,117,117	0
54	MG	BA	3202	1/1	0.53	0.17	126,126,126,126	0
54	MG	CA	1858	1/1	0.53	0.26	107,107,107,107	0
54	MG	BA	3070	1/1	0.53	0.16	85,85,85,85	0
54	MG	BJ	203	1/1	0.54	0.13	89,89,89,89	0
54	MG	BA	3614	1/1	0.54	0.10	112,112,112,112	0
54	MG	AA	1769	1/1	0.54	0.18	118,118,118,118	0
54	MG	AA	1873	1/1	0.55	0.10	105,105,105,105	0
54	MG	AA	1786	1/1	0.55	0.14	119,119,119,119	0
54	MG	BA	3303	1/1	0.55	0.13	157,157,157,157	0
54	MG	AA	1776	1/1	0.55	0.28	108,108,108,108	0
54	MG	BA	3060	1/1	0.55	0.52	110,110,110,110	0
54	MG	CA	1886	1/1	0.55	0.18	105,105,105,105	0
54	MG	AA	1633	1/1	0.55	0.26	123,123,123,123	0
54	MG	DA	3618	1/1	0.56	0.07	129,129,129,129	0
54	MG	AA	1830	1/1	0.56	0.12	105,105,105,105	0
54	MG	DA	3588	1/1	0.56	0.27	96,96,96,96	0
54	MG	CA	1660	1/1	0.56	0.15	158,158,158,158	0
54	MG	AA	1766	1/1	0.57	0.27	106,106,106,106	0
54	MG	BA	3589	1/1	0.57	0.27	105,105,105,105	0
54	MG	BA	3590	1/1	0.57	0.22	119,119,119,119	0
54	MG	DA	3775	1/1	0.57	0.10	98,98,98,98	0
54	MG	DA	3786	1/1	0.57	0.45	104,104,104,104	0
54	MG	CA	1706	1/1	0.57	0.23	106,106,106,106	0
54	MG	CA	1754	1/1	0.58	0.41	121,121,121,121	0
54	MG	CO	102	1/1	0.58	0.19	103,103,103,103	0
54	MG	AA	1687	1/1	0.58	0.55	108,108,108,108	0
54	MG	AA	1844	1/1	0.58	0.24	121,121,121,121	0
54	MG	CA	1901	1/1	0.58	0.12	76,76,76,76	0
54	MG	BA	3135	1/1	0.58	0.14	61,61,61,61	0
54	MG	DA	3830	1/1	0.58	0.24	125,125,125,125	0
54	MG	CF	201	1/1	0.58	0.09	131,131,131,131	0
54	MG	BA	3346	1/1	0.59	0.13	136,136,136,136	0
54	MG	CA	1651	1/1	0.59	0.25	111,111,111,111	0
54	MG	AA	1808	1/1	0.59	0.21	97,97,97,97	0
54	MG	BA	3594	1/1	0.59	0.14	129,129,129,129	0
54	MG	DA	3616	1/1	0.60	0.29	103,103,103,103	0
54	MG	AA	1734	1/1	0.60	0.15	96,96,96,96	0
54	MG	DA	3803	1/1	0.60	0.24	123,123,123,123	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	DA	3596	1/1	0.60	0.13	113,113,113,113	0
54	MG	DA	3066	1/1	0.60	0.25	114,114,114,114	0
54	MG	CA	1891	1/1	0.61	0.27	113,113,113,113	0
54	MG	DA	3743	1/1	0.61	0.08	105,105,105,105	0
54	MG	DA	3598	1/1	0.61	0.13	108,108,108,108	0
54	MG	AA	1717	1/1	0.61	0.43	103,103,103,103	0
54	MG	CO	101	1/1	0.61	0.20	127,127,127,127	0
54	MG	BA	3362	1/1	0.61	0.31	130,130,130,130	0
54	MG	BA	3150	1/1	0.61	0.30	97,97,97,97	0
54	MG	DV	202	1/1	0.61	0.12	115,115,115,115	0
54	MG	AA	1660	1/1	0.62	0.15	122,122,122,122	0
54	MG	AA	1843	1/1	0.62	0.27	126,126,126,126	0
54	MG	DA	3312	1/1	0.62	0.11	130,130,130,130	0
54	MG	DA	3464	1/1	0.62	0.18	133,133,133,133	0
54	MG	BA	3501	1/1	0.62	0.48	105,105,105,105	0
54	MG	BP	201	1/1	0.62	0.08	122,122,122,122	0
54	MG	CA	1917	1/1	0.62	0.23	105,105,105,105	0
54	MG	CA	1846	1/1	0.63	0.16	135,135,135,135	0
54	MG	CA	1728	1/1	0.63	0.21	120,120,120,120	0
54	MG	DA	3766	1/1	0.63	0.09	123,123,123,123	0
54	MG	DA	3772	1/1	0.63	0.22	114,114,114,114	0
54	MG	BA	3681	1/1	0.63	0.09	95,95,95,95	0
54	MG	CA	1882	1/1	0.63	0.09	135,135,135,135	0
54	MG	AV	6206	1/1	0.63	0.08	87,87,87,87	0
54	MG	BB	224	1/1	0.63	0.20	140,140,140,140	0
54	MG	AA	1879	1/1	0.63	0.10	119,119,119,119	0
54	MG	DL	202	1/1	0.63	1.23	146,146,146,146	0
54	MG	BA	3163	1/1	0.63	0.17	87,87,87,87	0
54	MG	DV	203	1/1	0.63	0.10	128,128,128,128	0
54	MG	DA	3095	1/1	0.64	0.27	72,72,72,72	0
54	MG	DA	3306	1/1	0.64	0.22	152,152,152,152	0
54	MG	BA	3462	1/1	0.64	0.30	80,80,80,80	0
54	MG	AA	1877	1/1	0.64	0.37	102,102,102,102	0
54	MG	CA	1900	1/1	0.64	0.10	86,86,86,86	0
54	MG	DA	3699	1/1	0.64	0.14	96,96,96,96	0
54	MG	CA	1789	1/1	0.64	0.17	103,103,103,103	0
54	MG	CA	1712	1/1	0.64	0.19	108,108,108,108	0
54	MG	BA	3503	1/1	0.64	0.21	90,90,90,90	0
54	MG	BA	3297	1/1	0.65	0.22	98,98,98,98	0
54	MG	DA	3353	1/1	0.65	0.26	105,105,105,105	0
54	MG	BA	3414	1/1	0.65	0.44	137,137,137,137	0
54	MG	AA	1700	1/1	0.65	0.20	114,114,114,114	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	DA	3676	1/1	0.65	0.24	92,92,92,92	0
54	MG	BA	3376	1/1	0.65	0.09	123,123,123,123	0
54	MG	DJ	202	1/1	0.65	0.07	126,126,126,126	0
54	MG	CA	1611	1/1	0.65	0.21	128,128,128,128	0
54	MG	DA	3163	1/1	0.65	0.28	113,113,113,113	0
54	MG	AA	1753	1/1	0.65	0.08	103,103,103,103	0
54	MG	DA	3829	1/1	0.66	0.11	96,96,96,96	0
54	MG	DA	3251	1/1	0.66	0.12	77,77,77,77	0
54	MG	DA	3265	1/1	0.66	0.39	138,138,138,138	0
54	MG	BA	3520	1/1	0.66	0.27	95,95,95,95	0
54	MG	AA	1712	1/1	0.66	0.10	105,105,105,105	0
54	MG	DA	3109	1/1	0.66	0.13	88,88,88,88	0
54	MG	BA	3510	1/1	0.66	0.26	86,86,86,86	0
54	MG	AA	1617	1/1	0.67	0.24	84,84,84,84	0
54	MG	CG	201	1/1	0.67	0.10	104,104,104,104	0
54	MG	AM	201	1/1	0.67	0.11	126,126,126,126	0
54	MG	BA	3155	1/1	0.67	0.26	99,99,99,99	0
54	MG	DA	3819	1/1	0.67	0.15	130,130,130,130	0
54	MG	DA	3825	1/1	0.67	0.16	103,103,103,103	0
54	MG	BA	3092	1/1	0.67	0.33	123,123,123,123	0
54	MG	AG	201	1/1	0.67	0.07	106,106,106,106	0
54	MG	BA	3259	1/1	0.67	0.08	105,105,105,105	0
54	MG	DB	237	1/1	0.67	0.16	109,109,109,109	0
54	MG	DA	3495	1/1	0.67	0.16	111,111,111,111	0
54	MG	BA	3564	1/1	0.67	0.22	146,146,146,146	0
54	MG	BA	3269	1/1	0.67	0.09	104,104,104,104	0
54	MG	BA	3288	1/1	0.67	0.19	113,113,113,113	0
54	MG	BA	3599	1/1	0.68	0.08	94,94,94,94	0
54	MG	CA	1807	1/1	0.68	0.14	125,125,125,125	0
54	MG	DA	3359	1/1	0.68	0.17	96,96,96,96	0
54	MG	DA	3387	1/1	0.68	0.14	124,124,124,124	0
54	MG	BA	3567	1/1	0.68	0.11	126,126,126,126	0
54	MG	BA	3642	1/1	0.68	0.07	98,98,98,98	0
54	MG	BA	3647	1/1	0.68	0.21	149,149,149,149	0
54	MG	DA	3222	1/1	0.68	0.27	112,112,112,112	0
54	MG	DA	3760	1/1	0.68	0.10	97,97,97,97	0
54	MG	AE	202	1/1	0.68	0.32	173,173,173,173	0
54	MG	BA	3341	1/1	0.68	0.07	125,125,125,125	0
54	MG	AA	1743	1/1	0.68	0.23	140,140,140,140	0
54	MG	CA	1818	1/1	0.69	0.06	91,91,91,91	0
54	MG	AA	1646	1/1	0.69	0.25	89,89,89,89	0
54	MG	DA	3367	1/1	0.69	0.49	97,97,97,97	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	BA	3242	1/1	0.69	0.22	112,112,112,112	0
54	MG	DA	3405	1/1	0.69	0.24	67,67,67,67	0
54	MG	DA	3432	1/1	0.69	0.12	84,84,84,84	0
54	MG	BB	225	1/1	0.69	0.37	96,96,96,96	0
54	MG	DA	3785	1/1	0.69	0.23	109,109,109,109	0
54	MG	CA	1863	1/1	0.69	0.15	125,125,125,125	0
54	MG	CA	1700	1/1	0.69	0.11	129,129,129,129	0
54	MG	DA	3145	1/1	0.69	0.21	100,100,100,100	0
54	MG	CA	1792	1/1	0.69	0.32	93,93,93,93	0
54	MG	DA	3591	1/1	0.69	0.25	90,90,90,90	0
54	MG	DA	3193	1/1	0.69	0.16	86,86,86,86	0
54	MG	AA	1759	1/1	0.69	0.11	110,110,110,110	0
54	MG	DA	3840	1/1	0.69	0.31	81,81,81,81	0
54	MG	AA	1771	1/1	0.69	0.30	111,111,111,111	0
54	MG	CG	202	1/1	0.69	0.08	131,131,131,131	0
54	MG	CA	1798	1/1	0.69	0.11	111,111,111,111	0
54	MG	BA	3040	1/1	0.69	0.42	76,76,76,76	0
54	MG	DA	3342	1/1	0.69	0.22	112,112,112,112	0
54	MG	BA	3144	1/1	0.70	0.22	148,148,148,148	0
54	MG	BA	3208	1/1	0.70	0.16	96,96,96,96	0
54	MG	DA	3740	1/1	0.70	0.14	99,99,99,99	0
54	MG	BA	3470	1/1	0.70	0.30	71,71,71,71	0
54	MG	BA	3480	1/1	0.70	0.33	79,79,79,79	0
54	MG	DA	3397	1/1	0.70	0.55	124,124,124,124	0
54	MG	BA	3606	1/1	0.70	0.63	118,118,118,118	0
54	MG	CA	1640	1/1	0.70	0.32	133,133,133,133	0
54	MG	DA	3450	1/1	0.70	0.27	81,81,81,81	0
54	MG	AA	1851	1/1	0.70	0.23	93,93,93,93	0
54	MG	BA	3634	1/1	0.70	0.14	98,98,98,98	0
54	MG	CA	1936	1/1	0.70	0.16	102,102,102,102	0
54	MG	CA	1811	1/1	0.70	0.07	181,181,181,181	0
54	MG	CA	1969	1/1	0.70	0.19	124,124,124,124	0
54	MG	DA	3210	1/1	0.70	0.27	92,92,92,92	0
54	MG	CA	1698	1/1	0.70	0.17	123,123,123,123	0
54	MG	BA	3246	1/1	0.70	0.16	164,164,164,164	0
54	MG	DB	213	1/1	0.70	0.18	113,113,113,113	0
54	MG	DB	234	1/1	0.70	0.20	105,105,105,105	0
54	MG	DA	3260	1/1	0.70	0.34	90,90,90,90	0
54	MG	AA	1670	1/1	0.70	0.08	93,93,93,93	0
54	MG	BA	2971	1/1	0.70	0.22	76,76,76,76	0
54	MG	BA	3173	1/1	0.70	0.16	87,87,87,87	0
54	MG	BA	3192	1/1	0.70	0.17	110,110,110,110	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	BA	3195	1/1	0.71	0.59	91,91,91,91	0
54	MG	CA	1928	1/1	0.71	0.11	117,117,117,117	0
54	MG	DA	3295	1/1	0.71	0.15	107,107,107,107	0
54	MG	AA	1705	1/1	0.71	0.29	62,62,62,62	0
54	MG	DD	306	1/1	0.71	0.18	107,107,107,107	0
54	MG	DA	3128	1/1	0.71	0.33	85,85,85,85	0
54	MG	DA	3664	1/1	0.71	0.39	109,109,109,109	0
54	MG	DA	3333	1/1	0.71	0.20	90,90,90,90	0
54	MG	AS	101	1/1	0.71	0.20	106,106,106,106	0
54	MG	DA	2937	1/1	0.72	0.30	43,43,43,43	0
54	MG	CA	1666	1/1	0.72	0.23	104,104,104,104	0
54	MG	AA	1815	1/1	0.72	0.26	78,78,78,78	0
54	MG	BA	3523	1/1	0.72	0.34	99,99,99,99	0
54	MG	BA	3301	1/1	0.72	0.12	58,58,58,58	0
54	MG	AA	1767	1/1	0.72	0.05	118,118,118,118	0
54	MG	CC	308	1/1	0.72	0.04	110,110,110,110	0
54	MG	CA	1898	1/1	0.72	0.23	87,87,87,87	0
54	MG	CA	1617	1/1	0.72	0.06	104,104,104,104	0
54	MG	BA	3308	1/1	0.72	0.12	99,99,99,99	0
54	MG	CA	1909	1/1	0.72	0.06	135,135,135,135	0
54	MG	DA	3437	1/1	0.72	0.11	120,120,120,120	0
54	MG	BA	3229	1/1	0.72	0.15	90,90,90,90	0
54	MG	CA	1845	1/1	0.72	0.25	100,100,100,100	0
54	MG	DG	203	1/1	0.72	0.11	98,98,98,98	0
54	MG	DA	3471	1/1	0.72	0.14	104,104,104,104	0
54	MG	BA	3171	1/1	0.72	0.12	127,127,127,127	0
54	MG	BA	3516	1/1	0.72	0.18	100,100,100,100	0
54	MG	DA	3574	1/1	0.72	0.46	152,152,152,152	0
54	MG	BA	3266	1/1	0.73	0.10	104,104,104,104	0
54	MG	BA	3652	1/1	0.73	0.06	109,109,109,109	0
54	MG	BT	102	1/1	0.73	0.13	66,66,66,66	0
54	MG	DA	3501	1/1	0.73	0.11	96,96,96,96	0
54	MG	CN	102	1/1	0.73	0.31	134,134,134,134	0
54	MG	DA	3271	1/1	0.73	0.25	99,99,99,99	0
54	MG	DA	3580	1/1	0.73	0.09	162,162,162,162	0
54	MG	CA	1608	1/1	0.73	0.27	121,121,121,121	0
54	MG	CA	1824	1/1	0.73	0.11	123,123,123,123	0
54	MG	BA	3172	1/1	0.73	0.19	74,74,74,74	0
54	MG	DA	3317	1/1	0.73	0.15	96,96,96,96	0
54	MG	BA	3478	1/1	0.73	0.31	78,78,78,78	0
54	MG	BB	221	1/1	0.73	0.09	89,89,89,89	0
54	MG	BA	3635	1/1	0.73	0.06	113,113,113,113	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	DA	3086	1/1	0.73	0.20	71,71,71,71	0
54	MG	CA	1647	1/1	0.73	0.10	94,94,94,94	0
54	MG	AA	1729	1/1	0.73	0.24	107,107,107,107	0
54	MG	BC	303	1/1	0.73	0.19	95,95,95,95	0
54	MG	BI	101	1/1	0.73	0.09	109,109,109,109	0
54	MG	CA	1897	1/1	0.73	0.22	74,74,74,74	0
54	MG	CE	205	1/1	0.73	0.16	104,104,104,104	0
54	MG	CA	1670	1/1	0.73	0.18	106,106,106,106	0
54	MG	DV	204	1/1	0.73	0.11	96,96,96,96	0
54	MG	BA	3532	1/1	0.74	0.06	107,107,107,107	0
54	MG	CA	1894	1/1	0.74	0.07	97,97,97,97	0
54	MG	BA	3055	1/1	0.74	0.19	78,78,78,78	0
54	MG	BB	222	1/1	0.74	0.18	112,112,112,112	0
54	MG	DA	3187	1/1	0.74	0.14	114,114,114,114	0
54	MG	DA	3700	1/1	0.74	0.41	96,96,96,96	0
54	MG	BA	3139	1/1	0.74	0.09	100,100,100,100	0
54	MG	DA	3205	1/1	0.74	0.32	97,97,97,97	0
54	MG	BA	3580	1/1	0.74	0.30	94,94,94,94	0
54	MG	AA	1794	1/1	0.74	0.08	112,112,112,112	0
54	MG	DA	3026	1/1	0.74	0.19	83,83,83,83	0
54	MG	AO	103	1/1	0.74	0.09	111,111,111,111	0
54	MG	BA	3025	1/1	0.74	0.24	76,76,76,76	0
54	MG	DA	3613	1/1	0.74	0.12	121,121,121,121	0
54	MG	CA	1918	1/1	0.74	0.24	84,84,84,84	0
54	MG	AA	1835	1/1	0.74	0.14	158,158,158,158	0
54	MG	BA	3676	1/1	0.75	0.10	112,112,112,112	0
54	MG	BA	3484	1/1	0.75	0.20	56,56,56,56	0
54	MG	DA	3755	1/1	0.75	0.17	89,89,89,89	0
54	MG	BA	3374	1/1	0.75	0.18	108,108,108,108	0
54	MG	AA	1730	1/1	0.75	0.24	107,107,107,107	0
54	MG	CA	1951	1/1	0.75	0.10	87,87,87,87	0
54	MG	DA	3520	1/1	0.75	0.12	133,133,133,133	0
54	MG	CA	1788	1/1	0.75	0.17	95,95,95,95	0
54	MG	BA	3066	1/1	0.75	0.38	91,91,91,91	0
54	MG	CB	303	1/1	0.75	0.05	122,122,122,122	0
54	MG	DA	3332	1/1	0.75	0.19	88,88,88,88	0
54	MG	DA	3087	1/1	0.75	0.29	71,71,71,71	0
54	MG	DA	3337	1/1	0.75	0.08	88,88,88,88	0
54	MG	CA	1790	1/1	0.75	0.10	132,132,132,132	0
54	MG	BA	3512	1/1	0.75	0.27	77,77,77,77	0
54	MG	AL	201	1/1	0.75	0.06	109,109,109,109	0
54	MG	DB	209	1/1	0.75	0.08	103,103,103,103	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	AA	1716	1/1	0.75	0.22	96,96,96,96	0
54	MG	BA	3521	1/1	0.75	0.21	88,88,88,88	0
54	MG	CA	1676	1/1	0.75	0.18	90,90,90,90	0
54	MG	DB	240	1/1	0.75	0.14	123,123,123,123	0
54	MG	DA	3665	1/1	0.75	0.37	137,137,137,137	0
54	MG	BA	3158	1/1	0.75	0.31	99,99,99,99	0
54	MG	BA	3349	1/1	0.75	0.20	95,95,95,95	0
54	MG	AA	1876	1/1	0.75	0.08	80,80,80,80	0
54	MG	DM	1400	1/1	0.75	0.29	106,106,106,106	0
54	MG	AA	1708	1/1	0.75	0.18	137,137,137,137	0
54	MG	DA	3730	1/1	0.75	0.08	61,61,61,61	0
54	MG	DA	3453	1/1	0.75	0.11	87,87,87,87	0
54	MG	CA	1723	1/1	0.76	0.33	85,85,85,85	0
54	MG	CA	1614	1/1	0.76	0.22	66,66,66,66	0
54	MG	CB	302	1/1	0.76	0.07	112,112,112,112	0
54	MG	BA	3678	1/1	0.76	0.23	122,122,122,122	0
54	MG	CA	1746	1/1	0.76	0.12	141,141,141,141	0
54	MG	CA	1877	1/1	0.76	0.22	126,126,126,126	0
54	MG	DA	3461	1/1	0.76	0.12	88,88,88,88	0
54	MG	BA	3165	1/1	0.76	0.13	73,73,73,73	0
54	MG	CA	1768	1/1	0.76	0.10	123,123,123,123	0
54	MG	CA	1635	1/1	0.76	0.10	99,99,99,99	0
54	MG	CA	1892	1/1	0.76	0.27	114,114,114,114	0
54	MG	DA	3225	1/1	0.76	0.20	139,139,139,139	0
54	MG	AA	1790	1/1	0.76	0.07	109,109,109,109	0
54	MG	BA	3608	1/1	0.76	0.11	101,101,101,101	0
54	MG	AA	1812	1/1	0.76	0.23	81,81,81,81	0
54	MG	BA	3576	1/1	0.76	0.11	83,83,83,83	0
54	MG	BA	3577	1/1	0.76	0.06	142,142,142,142	0
54	MG	DA	3304	1/1	0.76	0.08	85,85,85,85	0
54	MG	BA	3316	1/1	0.76	0.06	97,97,97,97	0
54	MG	BA	3425	1/1	0.76	0.27	85,85,85,85	0
54	MG	DB	230	1/1	0.76	0.37	114,114,114,114	0
54	MG	DA	3314	1/1	0.76	0.15	105,105,105,105	0
54	MG	CQ	201	1/1	0.76	0.08	103,103,103,103	0
54	MG	AK	201	1/1	0.76	0.30	101,101,101,101	0
54	MG	BA	3670	1/1	0.76	0.16	90,90,90,90	0
54	MG	DG	201	1/1	0.76	0.14	108,108,108,108	0
54	MG	DA	3633	1/1	0.76	0.18	83,83,83,83	0
54	MG	DA	3029	1/1	0.76	0.22	74,74,74,74	0
54	MG	BA	3675	1/1	0.76	0.14	120,120,120,120	0
54	MG	CA	1822	1/1	0.76	0.22	93,93,93,93	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	BA	3531	1/1	0.76	0.06	91,91,91,91	0
54	MG	BA	3677	1/1	0.76	0.18	72,72,72,72	0
54	MG	DA	3091	1/1	0.76	0.11	127,127,127,127	0
54	MG	CA	1815	1/1	0.77	0.18	97,97,97,97	0
54	MG	DA	3787	1/1	0.77	0.14	114,114,114,114	0
54	MG	DA	3800	1/1	0.77	0.12	95,95,95,95	0
54	MG	CA	1816	1/1	0.77	0.12	107,107,107,107	0
54	MG	BA	3243	1/1	0.77	0.14	85,85,85,85	0
54	MG	BH	201	1/1	0.77	0.07	107,107,107,107	0
54	MG	AA	1744	1/1	0.77	0.10	96,96,96,96	0
54	MG	CA	1650	1/1	0.77	0.15	111,111,111,111	0
54	MG	BA	3220	1/1	0.77	0.14	79,79,79,79	0
54	MG	BA	3348	1/1	0.77	0.22	107,107,107,107	0
54	MG	DA	3844	1/1	0.77	0.18	132,132,132,132	0
54	MG	DA	3854	1/1	0.77	0.10	124,124,124,124	0
54	MG	CA	1856	1/1	0.77	0.29	118,118,118,118	0
54	MG	BT	101	1/1	0.77	0.18	101,101,101,101	0
54	MG	CA	1668	1/1	0.77	0.11	86,86,86,86	0
54	MG	CA	1939	1/1	0.77	0.14	144,144,144,144	0
54	MG	AA	1875	1/1	0.77	0.06	97,97,97,97	0
54	MG	DA	3288	1/1	0.77	0.08	104,104,104,104	0
54	MG	BA	3487	1/1	0.77	0.12	90,90,90,90	0
54	MG	DA	3031	1/1	0.77	0.16	79,79,79,79	0
54	MG	BA	3351	1/1	0.77	0.12	116,116,116,116	0
54	MG	CA	1885	1/1	0.77	0.08	75,75,75,75	0
54	MG	AV	6205	1/1	0.77	0.09	107,107,107,107	0
54	MG	CA	1615	1/1	0.77	0.13	70,70,70,70	0
54	MG	DS	201	1/1	0.77	0.13	98,98,98,98	0
54	MG	BA	3662	1/1	0.77	0.06	108,108,108,108	0
54	MG	BA	3533	1/1	0.77	0.13	83,83,83,83	0
54	MG	CE	201	1/1	0.77	0.11	117,117,117,117	0
54	MG	AA	1804	1/1	0.78	0.34	80,80,80,80	0
54	MG	DA	3711	1/1	0.78	0.21	84,84,84,84	0
54	MG	DA	3074	1/1	0.78	0.24	43,43,43,43	0
54	MG	CA	1850	1/1	0.78	0.08	129,129,129,129	0
54	MG	AA	1666	1/1	0.78	0.25	93,93,93,93	0
54	MG	BA	3390	1/1	0.78	0.07	103,103,103,103	0
54	MG	BA	3593	1/1	0.78	0.13	81,81,81,81	0
54	MG	BA	3391	1/1	0.78	0.12	93,93,93,93	0
54	MG	DA	3426	1/1	0.78	0.16	96,96,96,96	0
54	MG	CA	1761	1/1	0.78	0.23	88,88,88,88	0
54	MG	DA	3141	1/1	0.78	0.17	57,57,57,57	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	DA	3779	1/1	0.78	0.20	81,81,81,81	0
54	MG	BA	3241	1/1	0.78	0.18	69,69,69,69	0
54	MG	BA	3604	1/1	0.78	0.09	89,89,89,89	0
54	MG	AO	101	1/1	0.78	0.12	115,115,115,115	0
54	MG	CE	202	1/1	0.78	0.06	80,80,80,80	0
54	MG	BA	2926	1/1	0.78	0.23	50,50,50,50	0
54	MG	CA	1654	1/1	0.78	0.14	78,78,78,78	0
54	MG	BA	3420	1/1	0.78	0.16	94,94,94,94	0
54	MG	CA	1895	1/1	0.78	0.18	88,88,88,88	0
54	MG	BA	2931	1/1	0.78	0.29	49,49,49,49	0
54	MG	DA	3832	1/1	0.78	0.07	77,77,77,77	0
54	MG	DA	3259	1/1	0.78	0.13	87,87,87,87	0
54	MG	DA	3837	1/1	0.78	0.07	95,95,95,95	0
54	MG	CK	201	1/1	0.78	0.10	136,136,136,136	0
54	MG	AA	1756	1/1	0.78	0.23	111,111,111,111	0
54	MG	DA	3587	1/1	0.78	0.13	113,113,113,113	0
54	MG	BA	3264	1/1	0.78	0.15	87,87,87,87	0
54	MG	DA	3286	1/1	0.78	0.10	76,76,76,76	0
54	MG	DB	222	1/1	0.78	0.19	137,137,137,137	0
54	MG	BA	3549	1/1	0.78	0.22	87,87,87,87	0
54	MG	DB	232	1/1	0.78	0.06	84,84,84,84	0
54	MG	BA	3197	1/1	0.78	0.10	84,84,84,84	0
54	MG	DA	3604	1/1	0.78	0.12	103,103,103,103	0
54	MG	DA	3299	1/1	0.78	0.18	104,104,104,104	0
54	MG	BA	3002	1/1	0.78	0.56	96,96,96,96	0
54	MG	DA	3615	1/1	0.78	0.17	99,99,99,99	0
54	MG	B5	101	1/1	0.78	0.12	78,78,78,78	0
54	MG	DI	101	1/1	0.78	0.12	104,104,104,104	0
54	MG	DA	3309	1/1	0.78	0.21	127,127,127,127	0
54	MG	CA	1705	1/1	0.78	0.15	122,122,122,122	0
54	MG	BA	3281	1/1	0.78	0.31	123,123,123,123	0
54	MG	BA	3095	1/1	0.78	0.31	96,96,96,96	0
54	MG	CA	1722	1/1	0.78	0.07	116,116,116,116	0
54	MG	DA	3036	1/1	0.78	0.29	72,72,72,72	0
54	MG	CA	1937	1/1	0.78	0.36	100,100,100,100	0
54	MG	CA	1902	1/1	0.79	0.13	77,77,77,77	0
54	MG	BA	3527	1/1	0.79	0.19	65,65,65,65	0
54	MG	BA	3027	1/1	0.79	0.29	72,72,72,72	0
54	MG	DA	3113	1/1	0.79	0.24	66,66,66,66	0
54	MG	BA	3036	1/1	0.79	0.42	57,57,57,57	0
54	MG	DA	3808	1/1	0.79	0.11	116,116,116,116	0
54	MG	CG	203	1/1	0.79	0.07	100,100,100,100	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	AA	1737	1/1	0.79	0.07	111,111,111,111	0
54	MG	CL	205	1/1	0.79	0.22	97,97,97,97	0
54	MG	BA	3628	1/1	0.79	0.08	102,102,102,102	0
54	MG	DA	3351	1/1	0.79	0.19	89,89,89,89	0
54	MG	CA	1772	1/1	0.79	0.07	112,112,112,112	0
54	MG	BA	3256	1/1	0.79	0.21	105,105,105,105	0
54	MG	DA	3209	1/1	0.79	0.44	94,94,94,94	0
54	MG	DA	3370	1/1	0.79	0.30	92,92,92,92	0
54	MG	BA	3559	1/1	0.79	0.17	70,70,70,70	0
54	MG	DA	3855	1/1	0.79	0.10	104,104,104,104	0
54	MG	DA	3216	1/1	0.79	0.17	91,91,91,91	0
54	MG	BA	3493	1/1	0.79	0.14	75,75,75,75	0
54	MG	BA	3045	1/1	0.79	0.14	94,94,94,94	0
54	MG	DA	3248	1/1	0.79	0.20	80,80,80,80	0
54	MG	DB	231	1/1	0.79	0.10	117,117,117,117	0
54	MG	DA	3435	1/1	0.79	0.23	97,97,97,97	0
54	MG	BA	3109	1/1	0.79	0.20	77,77,77,77	0
54	MG	BA	3659	1/1	0.79	0.23	68,68,68,68	0
54	MG	DB	238	1/1	0.79	0.07	74,74,74,74	0
54	MG	BA	3505	1/1	0.79	0.09	81,81,81,81	0
54	MG	BA	3211	1/1	0.79	0.25	100,100,100,100	0
54	MG	BA	3418	1/1	0.79	0.18	88,88,88,88	0
54	MG	DA	3741	1/1	0.79	0.15	84,84,84,84	0
54	MG	DA	3465	1/1	0.79	0.26	105,105,105,105	0
54	MG	AV	6204	1/1	0.79	0.16	124,124,124,124	0
54	MG	DA	3479	1/1	0.79	0.14	130,130,130,130	0
54	MG	BA	3009	1/1	0.79	0.22	73,73,73,73	0
54	MG	DA	3769	1/1	0.79	0.12	90,90,90,90	0
54	MG	BA	3233	1/1	0.79	0.24	97,97,97,97	0
54	MG	AA	1720	1/1	0.79	0.29	101,101,101,101	0
54	MG	BA	3602	1/1	0.79	0.28	98,98,98,98	0
54	MG	DW	101	1/1	0.79	0.12	56,56,56,56	0
54	MG	D5	103	1/1	0.79	0.11	71,71,71,71	0
54	MG	BA	3586	1/1	0.80	0.07	97,97,97,97	0
54	MG	BA	3240	1/1	0.80	0.24	157,157,157,157	0
54	MG	BA	2920	1/1	0.80	0.27	24,24,24,24	0
54	MG	CA	1960	1/1	0.80	0.07	91,91,91,91	0
54	MG	AA	1631	1/1	0.80	0.20	76,76,76,76	0
54	MG	DA	3420	1/1	0.80	0.11	110,110,110,110	0
54	MG	DA	3133	1/1	0.80	0.14	114,114,114,114	0
54	MG	DA	3135	1/1	0.80	0.23	114,114,114,114	0
54	MG	CA	1836	1/1	0.80	0.25	98,98,98,98	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	DA	3776	1/1	0.80	0.34	172,172,172,172	0
54	MG	CA	1841	1/1	0.80	0.10	95,95,95,95	0
54	MG	AA	1728	1/1	0.80	0.06	71,71,71,71	0
54	MG	BA	3067	1/1	0.80	0.26	103,103,103,103	0
54	MG	BA	3600	1/1	0.80	0.07	93,93,93,93	0
54	MG	DA	3797	1/1	0.80	0.06	101,101,101,101	0
54	MG	BA	3253	1/1	0.80	0.18	88,88,88,88	0
54	MG	BA	3255	1/1	0.80	0.12	101,101,101,101	0
54	MG	DA	3470	1/1	0.80	0.10	127,127,127,127	0
54	MG	AA	1846	1/1	0.80	0.14	88,88,88,88	0
54	MG	AA	1692	1/1	0.80	0.19	89,89,89,89	0
54	MG	DA	3218	1/1	0.80	0.05	79,79,79,79	0
54	MG	BA	3613	1/1	0.80	0.22	103,103,103,103	0
54	MG	DA	3504	1/1	0.80	0.23	97,97,97,97	0
54	MG	BX	102	1/1	0.80	0.22	103,103,103,103	0
54	MG	CA	1884	1/1	0.80	0.15	99,99,99,99	0
54	MG	DA	3521	1/1	0.80	0.10	101,101,101,101	0
54	MG	AO	102	1/1	0.80	0.27	114,114,114,114	0
54	MG	DA	3852	1/1	0.80	0.07	80,80,80,80	0
54	MG	CA	1748	1/1	0.80	0.10	115,115,115,115	0
54	MG	DA	3583	1/1	0.80	0.53	119,119,119,119	0
54	MG	CL	201	1/1	0.80	0.13	99,99,99,99	0
54	MG	AA	1658	1/1	0.80	0.11	84,84,84,84	0
54	MG	DA	3269	1/1	0.80	0.09	109,109,109,109	0
54	MG	AE	201	1/1	0.80	0.20	123,123,123,123	0
54	MG	CA	1766	1/1	0.80	0.11	77,77,77,77	0
54	MG	BA	3129	1/1	0.80	0.06	98,98,98,98	0
54	MG	BA	3404	1/1	0.80	0.11	80,80,80,80	0
54	MG	CA	1778	1/1	0.80	0.16	94,94,94,94	0
54	MG	BA	3413	1/1	0.80	0.17	65,65,65,65	0
54	MG	CA	1627	1/1	0.80	0.52	99,99,99,99	0
54	MG	BA	3205	1/1	0.80	0.11	70,70,70,70	0
54	MG	DE	302	1/1	0.80	0.30	83,83,83,83	0
54	MG	DA	3028	1/1	0.80	0.29	58,58,58,58	0
54	MG	BA	3537	1/1	0.80	0.08	60,60,60,60	0
54	MG	DA	3634	1/1	0.80	0.18	106,106,106,106	0
54	MG	DA	3316	1/1	0.80	0.09	94,94,94,94	0
54	MG	DJ	206	1/1	0.80	0.14	135,135,135,135	0
54	MG	AA	1834	1/1	0.80	0.26	77,77,77,77	0
54	MG	AA	1782	1/1	0.80	0.18	104,104,104,104	0
54	MG	DP	202	1/1	0.80	0.05	90,90,90,90	0
54	MG	DA	3052	1/1	0.80	0.29	50,50,50,50	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	BA	3042	1/1	0.80	0.20	92,92,92,92	0
54	MG	BA	3304	1/1	0.80	0.21	100,100,100,100	0
54	MG	AA	1874	1/1	0.80	0.14	87,87,87,87	0
54	MG	BA	3048	1/1	0.80	0.34	70,70,70,70	0
54	MG	BA	3332	1/1	0.80	0.13	65,65,65,65	0
54	MG	BA	3660	1/1	0.81	0.08	119,119,119,119	0
54	MG	DA	3215	1/1	0.81	0.23	73,73,73,73	0
54	MG	BA	3344	1/1	0.81	0.13	99,99,99,99	0
54	MG	AA	1788	1/1	0.81	0.07	148,148,148,148	0
54	MG	BA	3020	1/1	0.81	0.23	88,88,88,88	0
54	MG	DA	3223	1/1	0.81	0.09	83,83,83,83	0
54	MG	BA	3177	1/1	0.81	0.18	119,119,119,119	0
54	MG	DA	3228	1/1	0.81	0.19	54,54,54,54	0
54	MG	DA	3230	1/1	0.81	0.11	80,80,80,80	0
54	MG	BA	3186	1/1	0.81	0.14	85,85,85,85	0
54	MG	DA	3485	1/1	0.81	0.17	119,119,119,119	0
54	MG	BA	3353	1/1	0.81	0.24	85,85,85,85	0
54	MG	BA	3496	1/1	0.81	0.06	67,67,67,67	0
54	MG	BB	205	1/1	0.81	0.10	108,108,108,108	0
54	MG	DA	3814	1/1	0.81	0.49	186,186,186,186	0
54	MG	CA	1806	1/1	0.81	0.21	110,110,110,110	0
54	MG	CA	1911	1/1	0.81	0.28	90,90,90,90	0
54	MG	BB	207	1/1	0.81	0.07	111,111,111,111	0
54	MG	DA	3522	1/1	0.81	0.12	147,147,147,147	0
54	MG	DA	3559	1/1	0.81	0.34	92,92,92,92	0
54	MG	DA	3274	1/1	0.81	0.18	116,116,116,116	0
54	MG	AA	1652	1/1	0.81	0.17	95,95,95,95	0
54	MG	AA	1754	1/1	0.81	0.07	98,98,98,98	0
54	MG	AA	1795	1/1	0.81	0.06	111,111,111,111	0
54	MG	CA	1921	1/1	0.81	0.09	97,97,97,97	0
54	MG	CA	1682	1/1	0.81	0.13	88,88,88,88	0
54	MG	AA	1695	1/1	0.81	0.04	96,96,96,96	0
54	MG	DA	3862	1/1	0.81	0.18	119,119,119,119	0
54	MG	AA	1850	1/1	0.81	0.12	70,70,70,70	0
54	MG	AA	1806	1/1	0.81	0.14	65,65,65,65	0
54	MG	CA	1946	1/1	0.81	0.14	137,137,137,137	0
54	MG	AA	1781	1/1	0.81	0.20	92,92,92,92	0
54	MG	AA	1727	1/1	0.81	0.20	104,104,104,104	0
54	MG	BA	3403	1/1	0.81	0.33	106,106,106,106	0
54	MG	CA	1962	1/1	0.81	0.05	96,96,96,96	0
54	MG	CA	1718	1/1	0.81	0.06	109,109,109,109	0
54	MG	BA	3611	1/1	0.81	0.10	75,75,75,75	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	DA	3343	1/1	0.81	0.19	97,97,97,97	0
54	MG	BA	3157	1/1	0.81	0.27	94,94,94,94	0
54	MG	AA	1870	1/1	0.81	0.11	98,98,98,98	0
54	MG	CA	1859	1/1	0.81	0.08	93,93,93,93	0
54	MG	DG	202	1/1	0.81	0.10	102,102,102,102	0
54	MG	AA	1685	1/1	0.81	0.15	64,64,64,64	0
54	MG	DA	3693	1/1	0.81	0.06	63,63,63,63	0
54	MG	DA	3698	1/1	0.81	0.20	61,61,61,61	0
54	MG	BA	2996	1/1	0.81	0.15	125,125,125,125	0
54	MG	BA	3330	1/1	0.81	0.14	101,101,101,101	0
54	MG	BA	3542	1/1	0.81	0.19	102,102,102,102	0
54	MG	BA	3166	1/1	0.81	0.36	86,86,86,86	0
54	MG	DA	3734	1/1	0.81	0.12	76,76,76,76	0
54	MG	DA	3200	1/1	0.81	0.22	97,97,97,97	0
54	MG	DA	3423	1/1	0.81	0.06	79,79,79,79	0
54	MG	BA	3554	1/1	0.81	0.29	90,90,90,90	0
54	MG	AA	1690	1/1	0.81	0.33	88,88,88,88	0
54	MG	D2	101	1/1	0.81	0.39	78,78,78,78	0
54	MG	DA	3433	1/1	0.81	0.14	67,67,67,67	0
54	MG	DA	3033	1/1	0.82	0.15	79,79,79,79	0
54	MG	DA	3034	1/1	0.82	0.22	89,89,89,89	0
54	MG	BA	3283	1/1	0.82	0.10	100,100,100,100	0
54	MG	DA	3040	1/1	0.82	0.23	76,76,76,76	0
54	MG	BA	3402	1/1	0.82	0.09	90,90,90,90	0
54	MG	DA	3275	1/1	0.82	0.28	92,92,92,92	0
54	MG	BA	3284	1/1	0.82	0.13	95,95,95,95	0
54	MG	DA	3065	1/1	0.82	0.27	61,61,61,61	0
54	MG	DA	3292	1/1	0.82	0.26	73,73,73,73	0
54	MG	DA	3798	1/1	0.82	0.19	88,88,88,88	0
54	MG	CA	1762	1/1	0.82	0.15	114,114,114,114	0
54	MG	CA	1763	1/1	0.82	0.15	90,90,90,90	0
54	MG	BA	3620	1/1	0.82	0.27	88,88,88,88	0
54	MG	BA	3138	1/1	0.82	0.21	88,88,88,88	0
54	MG	CA	1770	1/1	0.82	0.07	125,125,125,125	0
54	MG	DA	3311	1/1	0.82	0.22	95,95,95,95	0
54	MG	CA	1659	1/1	0.82	0.24	100,100,100,100	0
54	MG	BA	3631	1/1	0.82	0.06	85,85,85,85	0
54	MG	BA	3167	1/1	0.82	0.24	87,87,87,87	0
54	MG	DA	3835	1/1	0.82	0.13	111,111,111,111	0
54	MG	DA	3122	1/1	0.82	0.17	93,93,93,93	0
54	MG	DA	3592	1/1	0.82	0.11	114,114,114,114	0
54	MG	DA	3318	1/1	0.82	0.10	77,77,77,77	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	DA	3320	1/1	0.82	0.20	80,80,80,80	0
54	MG	BA	2948	1/1	0.82	0.24	62,62,62,62	0
54	MG	DA	3612	1/1	0.82	0.08	74,74,74,74	0
54	MG	AT	201	1/1	0.82	0.12	103,103,103,103	0
54	MG	BA	3643	1/1	0.82	0.38	92,92,92,92	0
54	MG	CA	1680	1/1	0.82	0.20	63,63,63,63	0
54	MG	AA	1676	1/1	0.82	0.13	90,90,90,90	0
54	MG	AA	1625	1/1	0.82	0.07	53,53,53,53	0
54	MG	AA	1805	1/1	0.82	0.18	66,66,66,66	0
54	MG	CA	1703	1/1	0.82	0.09	113,113,113,113	0
54	MG	DA	3657	1/1	0.82	0.35	57,57,57,57	0
54	MG	BA	3464	1/1	0.82	0.29	67,67,67,67	0
54	MG	AA	1630	1/1	0.82	0.14	81,81,81,81	0
54	MG	DA	3377	1/1	0.82	0.22	107,107,107,107	0
54	MG	DA	3670	1/1	0.82	0.15	83,83,83,83	0
54	MG	DB	243	1/1	0.82	0.07	101,101,101,101	0
54	MG	BA	3596	1/1	0.82	0.06	71,71,71,71	0
54	MG	BA	3381	1/1	0.82	0.25	82,82,82,82	0
54	MG	CA	1717	1/1	0.82	0.11	103,103,103,103	0
54	MG	AA	1645	1/1	0.82	0.17	138,138,138,138	0
54	MG	BA	3536	1/1	0.82	0.14	83,83,83,83	0
54	MG	DA	3705	1/1	0.82	0.11	86,86,86,86	0
54	MG	CO	103	1/1	0.82	0.17	203,203,203,203	0
54	MG	CA	1832	1/1	0.82	0.09	92,92,92,92	0
54	MG	DA	3731	1/1	0.82	0.11	60,60,60,60	0
54	MG	CA	1924	1/1	0.82	0.11	116,116,116,116	0
54	MG	CA	1925	1/1	0.82	0.12	77,77,77,77	0
54	MG	BA	3335	1/1	0.82	0.27	80,80,80,80	0
54	MG	DA	3244	1/1	0.82	0.25	85,85,85,85	0
54	MG	AA	1659	1/1	0.82	0.34	74,74,74,74	0
54	MG	BA	3396	1/1	0.82	0.07	108,108,108,108	0
54	MG	DA	3255	1/1	0.82	0.17	70,70,70,70	0
54	MG	DA	3764	1/1	0.82	0.13	80,80,80,80	0
54	MG	BB	206	1/1	0.82	0.21	125,125,125,125	0
54	MG	CA	1764	1/1	0.83	0.14	65,65,65,65	0
54	MG	BA	3257	1/1	0.83	0.40	108,108,108,108	0
54	MG	DA	3762	1/1	0.83	0.11	103,103,103,103	0
54	MG	BA	3133	1/1	0.83	0.31	86,86,86,86	0
54	MG	BA	3134	1/1	0.83	0.09	90,90,90,90	0
54	MG	BA	3360	1/1	0.83	0.08	75,75,75,75	0
54	MG	DA	3468	1/1	0.83	0.13	79,79,79,79	0
54	MG	CA	1776	1/1	0.83	0.05	118,118,118,118	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	AA	1662	1/1	0.83	0.24	78,78,78,78	0
54	MG	BA	3673	1/1	0.83	0.12	92,92,92,92	0
54	MG	BA	3583	1/1	0.83	0.15	105,105,105,105	0
54	MG	DA	3489	1/1	0.83	0.12	97,97,97,97	0
54	MG	CV	6203	1/1	0.83	0.07	80,80,80,80	0
54	MG	DA	2924	1/1	0.83	0.39	68,68,68,68	0
54	MG	DA	3502	1/1	0.83	0.15	93,93,93,93	0
54	MG	CA	1655	1/1	0.83	0.15	100,100,100,100	0
54	MG	CA	1903	1/1	0.83	0.16	84,84,84,84	0
54	MG	CA	1791	1/1	0.83	0.23	93,93,93,93	0
54	MG	AA	1787	1/1	0.83	0.08	68,68,68,68	0
54	MG	DA	3278	1/1	0.83	0.34	99,99,99,99	0
54	MG	BA	3201	1/1	0.83	0.18	107,107,107,107	0
54	MG	DA	3827	1/1	0.83	0.17	103,103,103,103	0
54	MG	AA	1719	1/1	0.83	0.22	66,66,66,66	0
54	MG	BA	3502	1/1	0.83	0.10	81,81,81,81	0
54	MG	BA	3140	1/1	0.83	0.10	62,62,62,62	0
54	MG	BA	3385	1/1	0.83	0.05	125,125,125,125	0
54	MG	BA	3598	1/1	0.83	0.09	100,100,100,100	0
54	MG	AA	1809	1/1	0.83	0.23	94,94,94,94	0
54	MG	BA	3292	1/1	0.83	0.17	71,71,71,71	0
54	MG	CA	1934	1/1	0.83	0.07	80,80,80,80	0
54	MG	AA	1621	1/1	0.83	0.37	71,71,71,71	0
54	MG	AA	1653	1/1	0.83	0.10	102,102,102,102	0
54	MG	BA	3223	1/1	0.83	0.07	76,76,76,76	0
54	MG	AA	1820	1/1	0.83	0.17	94,94,94,94	0
54	MG	AA	1862	1/1	0.83	0.11	84,84,84,84	0
54	MG	DA	3106	1/1	0.83	0.10	69,69,69,69	0
54	MG	CA	1833	1/1	0.83	0.07	79,79,79,79	0
54	MG	AA	1825	1/1	0.83	0.21	79,79,79,79	0
54	MG	CA	1837	1/1	0.83	0.16	83,83,83,83	0
54	MG	BA	3410	1/1	0.83	0.07	112,112,112,112	0
54	MG	DA	3132	1/1	0.83	0.26	62,62,62,62	0
54	MG	CB	301	1/1	0.83	0.08	115,115,115,115	0
54	MG	BA	3616	1/1	0.83	0.21	89,89,89,89	0
54	MG	DA	3356	1/1	0.83	0.10	70,70,70,70	0
54	MG	DA	3666	1/1	0.83	0.14	81,81,81,81	0
54	MG	BA	3076	1/1	0.83	0.17	68,68,68,68	0
54	MG	BA	3621	1/1	0.83	0.16	107,107,107,107	0
54	MG	CA	1851	1/1	0.83	0.23	103,103,103,103	0
54	MG	DA	3678	1/1	0.83	0.14	58,58,58,58	0
54	MG	DA	3691	1/1	0.83	0.26	96,96,96,96	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	DA	3164	1/1	0.83	0.36	83,83,83,83	0
54	MG	DA	3378	1/1	0.83	0.12	68,68,68,68	0
54	MG	CA	1724	1/1	0.83	0.10	124,124,124,124	0
54	MG	BA	3026	1/1	0.83	0.06	68,68,68,68	0
54	MG	BA	3629	1/1	0.83	0.04	86,86,86,86	0
54	MG	DA	3417	1/1	0.83	0.30	72,72,72,72	0
54	MG	DQ	202	1/1	0.83	0.08	97,97,97,97	0
54	MG	AA	1656	1/1	0.83	0.06	86,86,86,86	0
54	MG	DV	201	1/1	0.83	0.05	90,90,90,90	0
54	MG	BA	3031	1/1	0.83	0.24	80,80,80,80	0
54	MG	CA	1874	1/1	0.83	0.23	76,76,76,76	0
54	MG	BA	3108	1/1	0.83	0.23	72,72,72,72	0
54	MG	BA	3552	1/1	0.83	0.09	99,99,99,99	0
54	MG	BA	3034	1/1	0.83	0.25	69,69,69,69	0
54	MG	AA	1697	1/1	0.83	0.07	73,73,73,73	0
54	MG	CA	1636	1/1	0.84	0.10	98,98,98,98	0
54	MG	AA	1864	1/1	0.84	0.09	75,75,75,75	0
54	MG	DA	3505	1/1	0.84	0.22	105,105,105,105	0
54	MG	DA	3081	1/1	0.84	0.26	67,67,67,67	0
54	MG	DA	3515	1/1	0.84	0.30	73,73,73,73	0
54	MG	DA	3516	1/1	0.84	0.10	73,73,73,73	0
54	MG	CA	1641	1/1	0.84	0.15	79,79,79,79	0
54	MG	DA	3302	1/1	0.84	0.23	102,102,102,102	0
54	MG	BA	3357	1/1	0.84	0.09	80,80,80,80	0
54	MG	BA	3422	1/1	0.84	0.11	93,93,93,93	0
54	MG	BA	3110	1/1	0.84	0.23	72,72,72,72	0
54	MG	DA	3100	1/1	0.84	0.21	78,78,78,78	0
54	MG	DA	3105	1/1	0.84	0.21	87,87,87,87	0
54	MG	BA	3445	1/1	0.84	0.30	61,61,61,61	0
54	MG	CA	1880	1/1	0.84	0.18	83,83,83,83	0
54	MG	CC	304	1/1	0.84	0.07	121,121,121,121	0
54	MG	BB	213	1/1	0.84	0.06	111,111,111,111	0
54	MG	CA	1883	1/1	0.84	0.12	75,75,75,75	0
54	MG	BA	2966	1/1	0.84	0.09	38,38,38,38	0
54	MG	AA	1865	1/1	0.84	0.13	107,107,107,107	0
54	MG	AA	1823	1/1	0.84	0.14	148,148,148,148	0
54	MG	BA	3052	1/1	0.84	0.16	73,73,73,73	0
54	MG	BA	3306	1/1	0.84	0.07	78,78,78,78	0
54	MG	DA	3349	1/1	0.84	0.10	116,116,116,116	0
54	MG	BB	226	1/1	0.84	0.33	98,98,98,98	0
54	MG	DA	3849	1/1	0.84	0.11	89,89,89,89	0
54	MG	BA	3555	1/1	0.84	0.09	66,66,66,66	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	BA	3384	1/1	0.84	0.21	93,93,93,93	0
54	MG	DA	3632	1/1	0.84	0.16	111,111,111,111	0
54	MG	DA	3856	1/1	0.84	0.08	86,86,86,86	0
54	MG	CA	1692	1/1	0.84	0.28	115,115,115,115	0
54	MG	CA	1696	1/1	0.84	0.12	75,75,75,75	0
54	MG	DA	3652	1/1	0.84	0.21	66,66,66,66	0
54	MG	DB	221	1/1	0.84	0.11	98,98,98,98	0
54	MG	BA	2997	1/1	0.84	0.26	81,81,81,81	0
54	MG	DA	3660	1/1	0.84	0.16	65,65,65,65	0
54	MG	AA	1649	1/1	0.84	0.08	74,74,74,74	0
54	MG	CA	1810	1/1	0.84	0.09	99,99,99,99	0
54	MG	CA	1904	1/1	0.84	0.17	97,97,97,97	0
54	MG	BA	3062	1/1	0.84	0.18	79,79,79,79	0
54	MG	AA	1872	1/1	0.84	0.07	88,88,88,88	0
54	MG	AE	203	1/1	0.84	0.04	91,91,91,91	0
54	MG	BV	203	1/1	0.84	0.08	104,104,104,104	0
54	MG	DD	303	1/1	0.84	0.07	70,70,70,70	0
54	MG	BA	3339	1/1	0.84	0.06	103,103,103,103	0
54	MG	DA	3226	1/1	0.84	0.14	86,86,86,86	0
54	MG	BA	3401	1/1	0.84	0.08	85,85,85,85	0
54	MG	BA	3506	1/1	0.84	0.18	89,89,89,89	0
54	MG	DA	2942	1/1	0.84	0.36	54,54,54,54	0
54	MG	AE	205	1/1	0.84	0.05	106,106,106,106	0
54	MG	AA	1796	1/1	0.84	0.14	106,106,106,106	0
54	MG	DA	3713	1/1	0.84	0.24	96,96,96,96	0
54	MG	BA	3513	1/1	0.84	0.19	74,74,74,74	0
54	MG	AA	1741	1/1	0.84	0.17	112,112,112,112	0
54	MG	CA	1622	1/1	0.84	0.34	77,77,77,77	0
54	MG	DA	3261	1/1	0.84	0.10	57,57,57,57	0
54	MG	AH	201	1/1	0.84	0.09	78,78,78,78	0
54	MG	AA	1763	1/1	0.84	0.08	121,121,121,121	0
54	MG	CA	1943	1/1	0.84	0.13	87,87,87,87	0
54	MG	DA	3047	1/1	0.84	0.30	74,74,74,74	0
54	MG	CA	1751	1/1	0.84	0.14	117,117,117,117	0
54	MG	DA	3277	1/1	0.84	0.22	59,59,59,59	0
54	MG	AA	1714	1/1	0.84	0.06	81,81,81,81	0
54	MG	CA	1955	1/1	0.84	0.18	98,98,98,98	0
54	MG	BY	101	1/1	0.85	0.23	42,42,42,42	0
54	MG	DA	3355	1/1	0.85	0.10	76,76,76,76	0
54	MG	DA	3126	1/1	0.85	0.22	64,64,64,64	0
54	MG	CA	1842	1/1	0.85	0.22	103,103,103,103	0
54	MG	CA	1843	1/1	0.85	0.15	109,109,109,109	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	CA	1844	1/1	0.85	0.11	78,78,78,78	0
54	MG	DA	3714	1/1	0.85	0.06	96,96,96,96	0
54	MG	DA	3716	1/1	0.85	0.13	78,78,78,78	0
54	MG	BA	3179	1/1	0.85	0.07	79,79,79,79	0
54	MG	CA	1721	1/1	0.85	0.14	118,118,118,118	0
54	MG	DA	3380	1/1	0.85	0.09	84,84,84,84	0
54	MG	DA	3143	1/1	0.85	0.06	67,67,67,67	0
54	MG	AA	1760	1/1	0.85	0.23	88,88,88,88	0
54	MG	DA	3155	1/1	0.85	0.07	70,70,70,70	0
54	MG	CA	1610	1/1	0.85	0.24	90,90,90,90	0
54	MG	DA	3754	1/1	0.85	0.29	121,121,121,121	0
54	MG	AA	1672	1/1	0.85	0.33	78,78,78,78	0
54	MG	CA	1613	1/1	0.85	0.12	68,68,68,68	0
54	MG	DA	3191	1/1	0.85	0.21	62,62,62,62	0
54	MG	BA	3145	1/1	0.85	0.20	74,74,74,74	0
54	MG	CA	1860	1/1	0.85	0.13	68,68,68,68	0
54	MG	DA	3768	1/1	0.85	0.28	102,102,102,102	0
54	MG	CA	1734	1/1	0.85	0.19	90,90,90,90	0
54	MG	BA	3310	1/1	0.85	0.22	109,109,109,109	0
54	MG	BA	3196	1/1	0.85	0.24	80,80,80,80	0
54	MG	CA	1750	1/1	0.85	0.09	87,87,87,87	0
54	MG	BA	3324	1/1	0.85	0.15	109,109,109,109	0
54	MG	CA	1625	1/1	0.85	0.24	67,67,67,67	0
54	MG	BA	3100	1/1	0.85	0.14	79,79,79,79	0
54	MG	AA	1620	1/1	0.85	0.26	56,56,56,56	0
54	MG	CL	202	1/1	0.85	0.11	105,105,105,105	0
54	MG	CL	203	1/1	0.85	0.20	123,123,123,123	0
54	MG	DA	3474	1/1	0.85	0.13	81,81,81,81	0
54	MG	BB	201	1/1	0.85	0.25	63,63,63,63	0
54	MG	BB	204	1/1	0.85	0.12	102,102,102,102	0
54	MG	CA	1638	1/1	0.85	0.15	101,101,101,101	0
54	MG	DA	3816	1/1	0.85	0.06	52,52,52,52	0
54	MG	DA	3245	1/1	0.85	0.48	100,100,100,100	0
54	MG	BA	3550	1/1	0.85	0.07	79,79,79,79	0
54	MG	AA	1740	1/1	0.85	0.08	76,76,76,76	0
54	MG	DA	3828	1/1	0.85	0.09	85,85,85,85	0
54	MG	CA	1645	1/1	0.85	0.09	80,80,80,80	0
54	MG	BA	3021	1/1	0.85	0.25	66,66,66,66	0
54	MG	BB	210	1/1	0.85	0.19	82,82,82,82	0
54	MG	DA	3514	1/1	0.85	0.07	68,68,68,68	0
54	MG	CA	1899	1/1	0.85	0.12	98,98,98,98	0
54	MG	CA	1784	1/1	0.85	0.10	94,94,94,94	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	DA	3838	1/1	0.85	0.21	117,117,117,117	0
54	MG	DA	3839	1/1	0.85	0.13	86,86,86,86	0
54	MG	DA	3517	1/1	0.85	0.08	102,102,102,102	0
54	MG	DA	3267	1/1	0.85	0.09	43,43,43,43	0
54	MG	BB	211	1/1	0.85	0.06	85,85,85,85	0
54	MG	DA	3270	1/1	0.85	0.19	82,82,82,82	0
54	MG	DA	3526	1/1	0.85	0.18	84,84,84,84	0
54	MG	DA	3539	1/1	0.85	0.05	81,81,81,81	0
54	MG	BB	212	1/1	0.85	0.08	107,107,107,107	0
54	MG	BA	3022	1/1	0.85	0.15	83,83,83,83	0
54	MG	BA	3618	1/1	0.85	0.13	76,76,76,76	0
54	MG	DA	3582	1/1	0.85	0.16	85,85,85,85	0
54	MG	BA	3399	1/1	0.85	0.06	104,104,104,104	0
54	MG	CA	1663	1/1	0.85	0.16	128,128,128,128	0
54	MG	DB	227	1/1	0.85	0.06	104,104,104,104	0
54	MG	DA	3280	1/1	0.85	0.25	85,85,85,85	0
54	MG	DA	3283	1/1	0.85	0.24	71,71,71,71	0
54	MG	BA	3560	1/1	0.85	0.17	74,74,74,74	0
54	MG	CA	1913	1/1	0.85	0.18	109,109,109,109	0
54	MG	DB	235	1/1	0.85	0.22	91,91,91,91	0
54	MG	BA	3114	1/1	0.85	0.17	69,69,69,69	0
54	MG	CA	1803	1/1	0.85	0.17	99,99,99,99	0
54	MG	DA	3043	1/1	0.85	0.20	59,59,59,59	0
54	MG	BA	3216	1/1	0.85	0.19	87,87,87,87	0
54	MG	AA	1648	1/1	0.85	0.22	90,90,90,90	0
54	MG	BB	227	1/1	0.85	0.19	80,80,80,80	0
54	MG	AA	1868	1/1	0.85	0.09	101,101,101,101	0
54	MG	BA	3409	1/1	0.85	0.10	51,51,51,51	0
54	MG	BA	3637	1/1	0.85	0.06	105,105,105,105	0
54	MG	AA	1821	1/1	0.85	0.27	91,91,91,91	0
54	MG	DA	3083	1/1	0.85	0.12	120,120,120,120	0
54	MG	DA	3084	1/1	0.85	0.30	65,65,65,65	0
54	MG	DA	3644	1/1	0.85	0.25	75,75,75,75	0
54	MG	AA	1847	1/1	0.85	0.18	90,90,90,90	0
54	MG	CA	1938	1/1	0.85	0.07	81,81,81,81	0
54	MG	DA	3321	1/1	0.85	0.35	110,110,110,110	0
54	MG	DA	3331	1/1	0.85	0.09	90,90,90,90	0
54	MG	AA	1693	1/1	0.85	0.26	83,83,83,83	0
54	MG	AA	1772	1/1	0.85	0.09	111,111,111,111	0
54	MG	BV	201	1/1	0.85	0.15	98,98,98,98	0
54	MG	CA	1947	1/1	0.85	0.07	136,136,136,136	0
54	MG	BA	3653	1/1	0.85	0.36	82,82,82,82	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	DA	3347	1/1	0.85	0.17	67,67,67,67	0
54	MG	CA	1711	1/1	0.85	0.12	76,76,76,76	0
54	MG	BA	3361	1/1	0.85	0.09	154,154,154,154	0
54	MG	DA	3697	1/1	0.86	0.19	92,92,92,92	0
54	MG	CA	1612	1/1	0.86	0.19	76,76,76,76	0
54	MG	BA	2956	1/1	0.86	0.33	49,49,49,49	0
54	MG	BA	3494	1/1	0.86	0.06	66,66,66,66	0
54	MG	CA	1854	1/1	0.86	0.16	111,111,111,111	0
54	MG	BA	3585	1/1	0.86	0.08	69,69,69,69	0
54	MG	DA	3383	1/1	0.86	0.09	112,112,112,112	0
54	MG	AD	304	1/1	0.86	0.05	113,113,113,113	0
54	MG	DA	3395	1/1	0.86	0.21	75,75,75,75	0
54	MG	DA	3723	1/1	0.86	0.13	67,67,67,67	0
54	MG	DA	3171	1/1	0.86	0.08	93,93,93,93	0
54	MG	CA	1618	1/1	0.86	0.22	84,84,84,84	0
54	MG	CC	307	1/1	0.86	0.04	108,108,108,108	0
54	MG	BA	3101	1/1	0.86	0.28	74,74,74,74	0
54	MG	DA	3737	1/1	0.86	0.29	136,136,136,136	0
54	MG	DA	3422	1/1	0.86	0.16	62,62,62,62	0
54	MG	DA	3195	1/1	0.86	0.07	83,83,83,83	0
54	MG	CA	1624	1/1	0.86	0.20	94,94,94,94	0
54	MG	AA	1858	1/1	0.86	0.07	86,86,86,86	0
54	MG	CA	1872	1/1	0.86	0.17	84,84,84,84	0
54	MG	BA	3230	1/1	0.86	0.24	111,111,111,111	0
54	MG	CA	1628	1/1	0.86	0.27	84,84,84,84	0
54	MG	DA	3445	1/1	0.86	0.54	137,137,137,137	0
54	MG	BA	3038	1/1	0.86	0.23	63,63,63,63	0
54	MG	BA	2981	1/1	0.86	0.20	56,56,56,56	0
54	MG	BA	3041	1/1	0.86	0.23	62,62,62,62	0
54	MG	DA	3463	1/1	0.86	0.07	69,69,69,69	0
54	MG	CA	1765	1/1	0.86	0.04	95,95,95,95	0
54	MG	BA	3320	1/1	0.86	0.08	71,71,71,71	0
54	MG	AA	1860	1/1	0.86	0.35	138,138,138,138	0
54	MG	CA	1887	1/1	0.86	0.08	75,75,75,75	0
54	MG	CA	1889	1/1	0.86	0.15	74,74,74,74	0
54	MG	CA	1890	1/1	0.86	0.31	78,78,78,78	0
54	MG	DA	3793	1/1	0.86	0.11	106,106,106,106	0
54	MG	AA	1713	1/1	0.86	0.26	98,98,98,98	0
54	MG	DA	3482	1/1	0.86	0.09	69,69,69,69	0
54	MG	CA	1771	1/1	0.86	0.10	98,98,98,98	0
54	MG	BA	3603	1/1	0.86	0.09	86,86,86,86	0
54	MG	DA	3253	1/1	0.86	0.08	70,70,70,70	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	DA	3809	1/1	0.86	0.29	84,84,84,84	0
54	MG	BA	3001	1/1	0.86	0.20	65,65,65,65	0
54	MG	BA	3605	1/1	0.86	0.10	69,69,69,69	0
54	MG	AA	1810	1/1	0.86	0.33	86,86,86,86	0
54	MG	BA	3254	1/1	0.86	0.19	68,68,68,68	0
54	MG	DA	2915	1/1	0.86	0.27	49,49,49,49	0
54	MG	DA	3266	1/1	0.86	0.06	85,85,85,85	0
54	MG	BA	3190	1/1	0.86	0.12	72,72,72,72	0
54	MG	BA	3342	1/1	0.86	0.19	62,62,62,62	0
54	MG	AA	1635	1/1	0.86	0.24	37,37,37,37	0
54	MG	DA	2953	1/1	0.86	0.27	46,46,46,46	0
54	MG	DA	3007	1/1	0.86	0.13	44,44,44,44	0
54	MG	DA	3010	1/1	0.86	0.17	72,72,72,72	0
54	MG	BA	3019	1/1	0.86	0.26	67,67,67,67	0
54	MG	DA	3531	1/1	0.86	0.35	93,93,93,93	0
54	MG	AA	1784	1/1	0.86	0.33	89,89,89,89	0
54	MG	AA	1757	1/1	0.86	0.08	98,98,98,98	0
54	MG	DA	3565	1/1	0.86	0.06	97,97,97,97	0
54	MG	DA	3573	1/1	0.86	0.20	85,85,85,85	0
54	MG	BA	3540	1/1	0.86	0.08	80,80,80,80	0
54	MG	DA	3576	1/1	0.86	0.30	99,99,99,99	0
54	MG	BA	3350	1/1	0.86	0.09	66,66,66,66	0
54	MG	DA	3857	1/1	0.86	0.08	98,98,98,98	0
54	MG	BA	3198	1/1	0.86	0.14	85,85,85,85	0
54	MG	DB	208	1/1	0.86	0.13	86,86,86,86	0
54	MG	CA	1916	1/1	0.86	0.11	118,118,118,118	0
54	MG	AB	303	1/1	0.86	0.05	108,108,108,108	0
54	MG	CA	1808	1/1	0.86	0.08	98,98,98,98	0
54	MG	CA	1685	1/1	0.86	0.13	109,109,109,109	0
54	MG	BA	3280	1/1	0.86	0.09	61,61,61,61	0
54	MG	DB	229	1/1	0.86	0.13	134,134,134,134	0
54	MG	BP	202	1/1	0.86	0.04	84,84,84,84	0
54	MG	DA	3307	1/1	0.86	0.30	84,84,84,84	0
54	MG	AA	1736	1/1	0.86	0.07	112,112,112,112	0
54	MG	BA	3468	1/1	0.86	0.29	57,57,57,57	0
54	MG	DA	3609	1/1	0.86	0.18	113,113,113,113	0
54	MG	DB	236	1/1	0.86	0.09	84,84,84,84	0
54	MG	CA	1929	1/1	0.86	0.10	95,95,95,95	0
54	MG	CA	1932	1/1	0.86	0.05	84,84,84,84	0
54	MG	DB	239	1/1	0.86	0.22	107,107,107,107	0
54	MG	BU	201	1/1	0.86	0.18	70,70,70,70	0
54	MG	AC	302	1/1	0.86	0.28	71,71,71,71	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	BA	3206	1/1	0.86	0.07	96,96,96,96	0
54	MG	CA	1825	1/1	0.86	0.21	97,97,97,97	0
54	MG	DA	3621	1/1	0.86	0.06	88,88,88,88	0
54	MG	DF	202	1/1	0.86	0.08	129,129,129,129	0
54	MG	BA	3479	1/1	0.86	0.09	69,69,69,69	0
54	MG	DA	3327	1/1	0.86	0.09	79,79,79,79	0
54	MG	CA	1710	1/1	0.86	0.07	169,169,169,169	0
54	MG	BA	3370	1/1	0.86	0.21	76,76,76,76	0
54	MG	DA	3647	1/1	0.86	0.27	54,54,54,54	0
54	MG	BA	3569	1/1	0.86	0.08	116,116,116,116	0
54	MG	CA	1949	1/1	0.86	0.10	98,98,98,98	0
54	MG	CA	1950	1/1	0.86	0.13	107,107,107,107	0
54	MG	CA	1601	1/1	0.86	0.26	60,60,60,60	0
54	MG	DA	3114	1/1	0.86	0.24	66,66,66,66	0
54	MG	DA	3348	1/1	0.86	0.06	83,83,83,83	0
54	MG	CA	1953	1/1	0.86	0.17	120,120,120,120	0
54	MG	CA	1954	1/1	0.86	0.06	89,89,89,89	0
54	MG	BA	3654	1/1	0.86	0.14	122,122,122,122	0
54	MG	CA	1719	1/1	0.86	0.12	78,78,78,78	0
54	MG	DA	3681	1/1	0.86	0.16	78,78,78,78	0
54	MG	D1	101	1/1	0.86	0.10	80,80,80,80	0
54	MG	BA	3078	1/1	0.86	0.24	104,104,104,104	0
54	MG	AN	102	1/1	0.86	0.19	91,91,91,91	0
54	MG	DA	3719	1/1	0.87	0.24	84,84,84,84	0
54	MG	BA	3548	1/1	0.87	0.08	61,61,61,61	0
54	MG	AA	1814	1/1	0.87	0.14	82,82,82,82	0
54	MG	DA	3441	1/1	0.87	0.12	60,60,60,60	0
54	MG	BA	3421	1/1	0.87	0.08	80,80,80,80	0
54	MG	CA	1888	1/1	0.87	0.08	109,109,109,109	0
54	MG	AV	6202	1/1	0.87	0.17	97,97,97,97	0
54	MG	DA	3454	1/1	0.87	0.15	81,81,81,81	0
54	MG	CL	206	1/1	0.87	0.13	87,87,87,87	0
54	MG	BA	3087	1/1	0.87	0.33	84,84,84,84	0
54	MG	BA	3272	1/1	0.87	0.24	81,81,81,81	0
54	MG	CA	1626	1/1	0.87	0.28	68,68,68,68	0
54	MG	BA	3456	1/1	0.87	0.21	64,64,64,64	0
54	MG	BA	3274	1/1	0.87	0.26	98,98,98,98	0
54	MG	AA	1878	1/1	0.87	0.12	92,92,92,92	0
54	MG	BA	3565	1/1	0.87	0.24	104,104,104,104	0
54	MG	CQ	202	1/1	0.87	0.07	79,79,79,79	0
54	MG	AA	1696	1/1	0.87	0.12	120,120,120,120	0
54	MG	BA	3282	1/1	0.87	0.09	98,98,98,98	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	DA	3774	1/1	0.87	0.06	74,74,74,74	0
54	MG	DA	3264	1/1	0.87	0.11	78,78,78,78	0
54	MG	DA	3490	1/1	0.87	0.16	70,70,70,70	0
54	MG	CA	1786	1/1	0.87	0.08	94,94,94,94	0
54	MG	DA	3781	1/1	0.87	0.11	55,55,55,55	0
54	MG	DA	3784	1/1	0.87	0.07	108,108,108,108	0
54	MG	DA	3500	1/1	0.87	0.08	108,108,108,108	0
54	MG	BA	3473	1/1	0.87	0.21	70,70,70,70	0
54	MG	BA	3475	1/1	0.87	0.23	67,67,67,67	0
54	MG	BA	3096	1/1	0.87	0.23	76,76,76,76	0
54	MG	DA	2985	1/1	0.87	0.20	40,40,40,40	0
54	MG	DA	2994	1/1	0.87	0.14	54,54,54,54	0
54	MG	DA	3512	1/1	0.87	0.25	159,159,159,159	0
54	MG	CA	1905	1/1	0.87	0.27	130,130,130,130	0
54	MG	CA	1908	1/1	0.87	0.16	104,104,104,104	0
54	MG	BA	3582	1/1	0.87	0.13	102,102,102,102	0
54	MG	AA	1852	1/1	0.87	0.05	84,84,84,84	0
54	MG	BA	3584	1/1	0.87	0.08	83,83,83,83	0
54	MG	DA	3282	1/1	0.87	0.33	69,69,69,69	0
54	MG	BA	3213	1/1	0.87	0.15	102,102,102,102	0
54	MG	DA	3523	1/1	0.87	0.05	77,77,77,77	0
54	MG	AA	1853	1/1	0.87	0.05	86,86,86,86	0
54	MG	BA	3587	1/1	0.87	0.09	77,77,77,77	0
54	MG	BA	3102	1/1	0.87	0.14	72,72,72,72	0
54	MG	DA	3541	1/1	0.87	0.06	76,76,76,76	0
54	MG	BA	3105	1/1	0.87	0.16	72,72,72,72	0
54	MG	DA	3564	1/1	0.87	0.08	77,77,77,77	0
54	MG	BA	3592	1/1	0.87	0.38	79,79,79,79	0
54	MG	BA	3378	1/1	0.87	0.13	80,80,80,80	0
54	MG	BA	3012	1/1	0.87	0.33	71,71,71,71	0
54	MG	BA	3382	1/1	0.87	0.13	85,85,85,85	0
54	MG	DA	3842	1/1	0.87	0.22	105,105,105,105	0
54	MG	DA	3578	1/1	0.87	0.04	96,96,96,96	0
54	MG	AA	1871	1/1	0.87	0.04	110,110,110,110	0
54	MG	BA	3049	1/1	0.87	0.20	58,58,58,58	0
54	MG	BA	3504	1/1	0.87	0.24	94,94,94,94	0
54	MG	CA	1686	1/1	0.87	0.17	82,82,82,82	0
54	MG	AA	1604	1/1	0.87	0.29	62,62,62,62	0
54	MG	BC	301	1/1	0.87	0.28	60,60,60,60	0
54	MG	CA	1697	1/1	0.87	0.04	83,83,83,83	0
54	MG	BA	3174	1/1	0.87	0.07	67,67,67,67	0
54	MG	CA	1945	1/1	0.87	0.12	95,95,95,95	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	BA	3507	1/1	0.87	0.13	68,68,68,68	0
54	MG	DA	3323	1/1	0.87	0.25	78,78,78,78	0
54	MG	BA	3392	1/1	0.87	0.26	108,108,108,108	0
54	MG	CA	1839	1/1	0.87	0.14	92,92,92,92	0
54	MG	DB	228	1/1	0.87	0.11	88,88,88,88	0
54	MG	BA	3315	1/1	0.87	0.08	84,84,84,84	0
54	MG	BK	201	1/1	0.87	0.21	77,77,77,77	0
54	MG	CA	1952	1/1	0.87	0.07	88,88,88,88	0
54	MG	DA	3339	1/1	0.87	0.22	81,81,81,81	0
54	MG	AA	1614	1/1	0.87	0.15	68,68,68,68	0
54	MG	DA	3118	1/1	0.87	0.18	50,50,50,50	0
54	MG	BA	2955	1/1	0.87	0.16	63,63,63,63	0
54	MG	BA	3517	1/1	0.87	0.20	87,87,87,87	0
54	MG	AA	1822	1/1	0.87	0.05	92,92,92,92	0
54	MG	DA	3635	1/1	0.87	0.10	73,73,73,73	0
54	MG	CA	1849	1/1	0.87	0.10	167,167,167,167	0
54	MG	BA	3615	1/1	0.87	0.08	93,93,93,93	0
54	MG	DA	3650	1/1	0.87	0.14	55,55,55,55	0
54	MG	DD	304	1/1	0.87	0.14	94,94,94,94	0
54	MG	BA	3400	1/1	0.87	0.08	83,83,83,83	0
54	MG	CA	1852	1/1	0.87	0.12	101,101,101,101	0
54	MG	AA	1664	1/1	0.87	0.19	80,80,80,80	0
54	MG	DA	3364	1/1	0.87	0.49	75,75,75,75	0
54	MG	BA	3191	1/1	0.87	0.35	90,90,90,90	0
54	MG	DA	3148	1/1	0.87	0.10	94,94,94,94	0
54	MG	DA	3154	1/1	0.87	0.13	50,50,50,50	0
54	MG	AA	1638	1/1	0.87	0.19	89,89,89,89	0
54	MG	BY	102	1/1	0.87	0.08	110,110,110,110	0
54	MG	B2	102	1/1	0.87	0.25	65,65,65,65	0
54	MG	BA	3627	1/1	0.87	0.12	67,67,67,67	0
54	MG	DA	3390	1/1	0.87	0.17	72,72,72,72	0
54	MG	BA	3338	1/1	0.87	0.08	78,78,78,78	0
54	MG	CD	303	1/1	0.87	0.08	76,76,76,76	0
54	MG	CA	1870	1/1	0.87	0.06	94,94,94,94	0
54	MG	BA	3137	1/1	0.87	0.08	90,90,90,90	0
54	MG	CA	1744	1/1	0.87	0.07	80,80,80,80	0
54	MG	BA	3535	1/1	0.87	0.20	95,95,95,95	0
54	MG	BA	2978	1/1	0.87	0.25	58,58,58,58	0
54	MG	BA	3075	1/1	0.87	0.06	60,60,60,60	0
54	MG	BA	3343	1/1	0.87	0.11	87,87,87,87	0
54	MG	D4	102	1/1	0.87	0.20	65,65,65,65	0
54	MG	BA	3261	1/1	0.87	0.30	92,92,92,92	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	BA	3579	1/1	0.88	0.48	107,107,107,107	0
54	MG	BA	3483	1/1	0.88	0.17	71,71,71,71	0
54	MG	DA	3434	1/1	0.88	0.19	89,89,89,89	0
54	MG	AA	1628	1/1	0.88	0.26	86,86,86,86	0
54	MG	DA	3727	1/1	0.88	0.10	88,88,88,88	0
54	MG	DA	3436	1/1	0.88	0.20	101,101,101,101	0
54	MG	AA	1683	1/1	0.88	0.19	64,64,64,64	0
54	MG	BA	3679	1/1	0.88	0.09	75,75,75,75	0
54	MG	BA	3058	1/1	0.88	0.34	78,78,78,78	0
54	MG	DA	3224	1/1	0.88	0.09	55,55,55,55	0
54	MG	DA	3452	1/1	0.88	0.12	74,74,74,74	0
54	MG	AA	1770	1/1	0.88	0.10	76,76,76,76	0
54	MG	AA	1657	1/1	0.88	0.11	79,79,79,79	0
54	MG	DA	3745	1/1	0.88	0.04	109,109,109,109	0
54	MG	DA	3753	1/1	0.88	0.11	79,79,79,79	0
54	MG	AT	202	1/1	0.88	0.30	80,80,80,80	0
54	MG	BA	3294	1/1	0.88	0.12	89,89,89,89	0
54	MG	DA	3239	1/1	0.88	0.13	126,126,126,126	0
54	MG	AD	303	1/1	0.88	0.15	68,68,68,68	0
54	MG	BA	3298	1/1	0.88	0.05	126,126,126,126	0
54	MG	BA	3018	1/1	0.88	0.26	88,88,88,88	0
54	MG	AV	6203	1/1	0.88	0.06	62,62,62,62	0
54	MG	DA	3472	1/1	0.88	0.19	95,95,95,95	0
54	MG	AA	1675	1/1	0.88	0.18	82,82,82,82	0
54	MG	CA	1658	1/1	0.88	0.06	94,94,94,94	0
54	MG	BA	3597	1/1	0.88	0.16	56,56,56,56	0
54	MG	AA	1837	1/1	0.88	0.10	115,115,115,115	0
54	MG	DA	3777	1/1	0.88	0.10	90,90,90,90	0
54	MG	DA	3488	1/1	0.88	0.22	102,102,102,102	0
54	MG	CA	1907	1/1	0.88	0.04	87,87,87,87	0
54	MG	CA	1796	1/1	0.88	0.09	87,87,87,87	0
54	MG	DA	2955	1/1	0.88	0.32	45,45,45,45	0
54	MG	DA	2976	1/1	0.88	0.34	68,68,68,68	0
54	MG	AA	1838	1/1	0.88	0.13	77,77,77,77	0
54	MG	BA	3023	1/1	0.88	0.20	57,57,57,57	0
54	MG	AA	1774	1/1	0.88	0.10	70,70,70,70	0
54	MG	CA	1669	1/1	0.88	0.06	76,76,76,76	0
54	MG	DA	3025	1/1	0.88	0.25	80,80,80,80	0
54	MG	BA	3237	1/1	0.88	0.11	64,64,64,64	0
54	MG	DA	3276	1/1	0.88	0.35	86,86,86,86	0
54	MG	CA	1672	1/1	0.88	0.13	137,137,137,137	0
54	MG	BA	3318	1/1	0.88	0.18	73,73,73,73	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	AA	1642	1/1	0.88	0.19	100,100,100,100	0
54	MG	CA	1812	1/1	0.88	0.22	92,92,92,92	0
54	MG	BC	302	1/1	0.88	0.08	82,82,82,82	0
54	MG	DA	3285	1/1	0.88	0.09	65,65,65,65	0
54	MG	CA	1684	1/1	0.88	0.11	63,63,63,63	0
54	MG	BA	3098	1/1	0.88	0.17	90,90,90,90	0
54	MG	DA	3041	1/1	0.88	0.23	76,76,76,76	0
54	MG	DA	3537	1/1	0.88	0.16	101,101,101,101	0
54	MG	CA	1819	1/1	0.88	0.07	109,109,109,109	0
54	MG	DA	3046	1/1	0.88	0.14	37,37,37,37	0
54	MG	DA	3544	1/1	0.88	0.28	53,53,53,53	0
54	MG	AA	1845	1/1	0.88	0.04	71,71,71,71	0
54	MG	CA	1821	1/1	0.88	0.06	96,96,96,96	0
54	MG	DA	3305	1/1	0.88	0.20	99,99,99,99	0
54	MG	BA	3407	1/1	0.88	0.23	79,79,79,79	0
54	MG	AA	1778	1/1	0.88	0.15	113,113,113,113	0
54	MG	AA	1779	1/1	0.88	0.22	108,108,108,108	0
54	MG	CA	1829	1/1	0.88	0.05	89,89,89,89	0
54	MG	BA	3103	1/1	0.88	0.31	74,74,74,74	0
54	MG	AA	1818	1/1	0.88	0.07	76,76,76,76	0
54	MG	AA	1755	1/1	0.88	0.06	98,98,98,98	0
54	MG	BA	3185	1/1	0.88	0.25	85,85,85,85	0
54	MG	CA	1948	1/1	0.88	0.05	99,99,99,99	0
54	MG	BA	2970	1/1	0.88	0.14	55,55,55,55	0
54	MG	BA	3624	1/1	0.88	0.08	82,82,82,82	0
54	MG	DB	212	1/1	0.88	0.13	85,85,85,85	0
54	MG	BA	3188	1/1	0.88	0.10	103,103,103,103	0
54	MG	DB	220	1/1	0.88	0.07	75,75,75,75	0
54	MG	BX	101	1/1	0.88	0.07	71,71,71,71	0
54	MG	BA	3189	1/1	0.88	0.11	76,76,76,76	0
54	MG	DB	226	1/1	0.88	0.03	73,73,73,73	0
54	MG	DA	3602	1/1	0.88	0.22	91,91,91,91	0
54	MG	BA	3426	1/1	0.88	0.16	87,87,87,87	0
54	MG	DA	3605	1/1	0.88	0.25	103,103,103,103	0
54	MG	BA	3262	1/1	0.88	0.09	75,75,75,75	0
54	MG	CA	1956	1/1	0.88	0.07	85,85,85,85	0
54	MG	AA	1797	1/1	0.88	0.17	72,72,72,72	0
54	MG	BA	2972	1/1	0.88	0.20	61,61,61,61	0
54	MG	BA	3268	1/1	0.88	0.26	84,84,84,84	0
54	MG	CA	1967	1/1	0.88	0.12	93,93,93,93	0
54	MG	DA	3129	1/1	0.88	0.22	93,93,93,93	0
54	MG	AA	1803	1/1	0.88	0.20	69,69,69,69	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	CA	1971	1/1	0.88	0.08	86,86,86,86	0
54	MG	DA	3134	1/1	0.88	0.24	69,69,69,69	0
54	MG	BA	3270	1/1	0.88	0.04	93,93,93,93	0
54	MG	BA	3128	1/1	0.88	0.16	65,65,65,65	0
54	MG	BA	3566	1/1	0.88	0.14	72,72,72,72	0
54	MG	DA	3144	1/1	0.88	0.15	69,69,69,69	0
54	MG	CA	1732	1/1	0.88	0.17	78,78,78,78	0
54	MG	DE	303	1/1	0.88	0.11	81,81,81,81	0
54	MG	DA	3368	1/1	0.88	0.14	98,98,98,98	0
54	MG	AA	1854	1/1	0.88	0.14	114,114,114,114	0
54	MG	CA	1740	1/1	0.88	0.08	117,117,117,117	0
54	MG	BA	2984	1/1	0.88	0.11	50,50,50,50	0
54	MG	DA	3159	1/1	0.88	0.36	106,106,106,106	0
54	MG	BA	3656	1/1	0.88	0.08	107,107,107,107	0
54	MG	DA	3667	1/1	0.88	0.37	59,59,59,59	0
54	MG	DA	3386	1/1	0.88	0.07	76,76,76,76	0
54	MG	BA	3570	1/1	0.88	0.11	67,67,67,67	0
54	MG	DA	3169	1/1	0.88	0.19	54,54,54,54	0
54	MG	DA	3393	1/1	0.88	0.11	77,77,77,77	0
54	MG	DA	3394	1/1	0.88	0.35	110,110,110,110	0
54	MG	BA	3572	1/1	0.88	0.04	87,87,87,87	0
54	MG	CA	1875	1/1	0.88	0.19	63,63,63,63	0
54	MG	CA	1621	1/1	0.88	0.18	67,67,67,67	0
54	MG	DA	3407	1/1	0.88	0.05	108,108,108,108	0
54	MG	CA	1752	1/1	0.88	0.17	71,71,71,71	0
54	MG	DX	101	1/1	0.88	0.64	103,103,103,103	0
54	MG	BA	3363	1/1	0.88	0.09	113,113,113,113	0
54	MG	CA	1756	1/1	0.88	0.14	84,84,84,84	0
54	MG	D3	101	1/1	0.88	0.07	90,90,90,90	0
54	MG	BA	3365	1/1	0.88	0.09	131,131,131,131	0
54	MG	BA	3578	1/1	0.88	0.04	74,74,74,74	0
55	ZN	CN	101	1/1	0.88	0.11	244,244,244,244	0
54	MG	CA	1906	1/1	0.89	0.07	80,80,80,80	0
54	MG	DA	3430	1/1	0.89	0.08	103,103,103,103	0
54	MG	CV	6204	1/1	0.89	0.09	112,112,112,112	0
54	MG	CA	1804	1/1	0.89	0.13	100,100,100,100	0
54	MG	AA	1632	1/1	0.89	0.29	65,65,65,65	0
54	MG	BA	3515	1/1	0.89	0.12	54,54,54,54	0
54	MG	AA	1643	1/1	0.89	0.22	63,63,63,63	0
54	MG	DA	2949	1/1	0.89	0.21	52,52,52,52	0
54	MG	BA	3394	1/1	0.89	0.08	95,95,95,95	0
54	MG	DA	3442	1/1	0.89	0.14	71,71,71,71	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	BA	2976	1/1	0.89	0.15	65,65,65,65	0
54	MG	AA	1745	1/1	0.89	0.27	119,119,119,119	0
54	MG	BA	3322	1/1	0.89	0.23	71,71,71,71	0
54	MG	BA	3612	1/1	0.89	0.17	85,85,85,85	0
54	MG	BA	3526	1/1	0.89	0.05	66,66,66,66	0
54	MG	DA	3250	1/1	0.89	0.07	70,70,70,70	0
54	MG	BM	201	1/1	0.89	0.13	50,50,50,50	0
54	MG	DA	3021	1/1	0.89	0.39	68,68,68,68	0
54	MG	AQ	203	1/1	0.89	0.04	101,101,101,101	0
54	MG	BA	3326	1/1	0.89	0.26	82,82,82,82	0
54	MG	AA	1750	1/1	0.89	0.10	128,128,128,128	0
54	MG	DA	3759	1/1	0.89	0.07	97,97,97,97	0
54	MG	BA	3331	1/1	0.89	0.22	66,66,66,66	0
54	MG	DA	3030	1/1	0.89	0.13	73,73,73,73	0
54	MG	BA	3182	1/1	0.89	0.18	78,78,78,78	0
54	MG	DA	3477	1/1	0.89	0.18	78,78,78,78	0
54	MG	BU	202	1/1	0.89	0.06	74,74,74,74	0
54	MG	CA	1831	1/1	0.89	0.09	90,90,90,90	0
54	MG	BA	3406	1/1	0.89	0.17	88,88,88,88	0
54	MG	DA	3486	1/1	0.89	0.24	124,124,124,124	0
54	MG	BA	2992	1/1	0.89	0.17	69,69,69,69	0
54	MG	BA	3120	1/1	0.89	0.09	85,85,85,85	0
54	MG	BA	3126	1/1	0.89	0.09	60,60,60,60	0
54	MG	DA	3492	1/1	0.89	0.10	102,102,102,102	0
54	MG	DA	3494	1/1	0.89	0.10	63,63,63,63	0
54	MG	AD	302	1/1	0.89	0.06	76,76,76,76	0
54	MG	AA	1842	1/1	0.89	0.06	69,69,69,69	0
54	MG	AV	6201	1/1	0.89	0.07	67,67,67,67	0
54	MG	DA	3062	1/1	0.89	0.14	129,129,129,129	0
54	MG	AA	1751	1/1	0.89	0.10	88,88,88,88	0
54	MG	BA	3636	1/1	0.89	0.08	76,76,76,76	0
54	MG	BA	3193	1/1	0.89	0.21	81,81,81,81	0
54	MG	AA	1867	1/1	0.89	0.06	114,114,114,114	0
54	MG	DA	3076	1/1	0.89	0.19	78,78,78,78	0
54	MG	BA	3556	1/1	0.89	0.30	77,77,77,77	0
54	MG	AA	1673	1/1	0.89	0.07	95,95,95,95	0
54	MG	AA	1816	1/1	0.89	0.21	89,89,89,89	0
54	MG	DA	3297	1/1	0.89	0.18	76,76,76,76	0
54	MG	DA	3298	1/1	0.89	0.34	72,72,72,72	0
54	MG	DA	3822	1/1	0.89	0.04	70,70,70,70	0
54	MG	AA	1817	1/1	0.89	0.21	84,84,84,84	0
54	MG	DA	3301	1/1	0.89	0.21	87,87,87,87	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	BA	3352	1/1	0.89	0.10	80,80,80,80	0
54	MG	DA	3090	1/1	0.89	0.09	59,59,59,59	0
54	MG	DA	3532	1/1	0.89	0.12	106,106,106,106	0
54	MG	BA	3199	1/1	0.89	0.11	61,61,61,61	0
54	MG	DA	3094	1/1	0.89	0.23	67,67,67,67	0
54	MG	BA	3657	1/1	0.89	0.18	84,84,84,84	0
54	MG	BA	3354	1/1	0.89	0.10	123,123,123,123	0
54	MG	DA	3549	1/1	0.89	0.20	115,115,115,115	0
54	MG	DA	3552	1/1	0.89	0.07	68,68,68,68	0
54	MG	BA	2904	1/1	0.89	0.27	40,40,40,40	0
54	MG	CA	1968	1/1	0.89	0.08	87,87,87,87	0
54	MG	BA	3661	1/1	0.89	0.10	82,82,82,82	0
54	MG	DA	3571	1/1	0.89	0.12	72,72,72,72	0
54	MG	DA	3572	1/1	0.89	0.12	93,93,93,93	0
54	MG	DA	3112	1/1	0.89	0.16	91,91,91,91	0
54	MG	CA	1864	1/1	0.89	0.15	90,90,90,90	0
54	MG	AF	201	1/1	0.89	0.05	90,90,90,90	0
54	MG	DA	3577	1/1	0.89	0.19	73,73,73,73	0
54	MG	DA	3115	1/1	0.89	0.15	58,58,58,58	0
54	MG	DA	3864	1/1	0.89	0.18	53,53,53,53	0
54	MG	BA	3471	1/1	0.89	0.14	70,70,70,70	0
54	MG	DA	3121	1/1	0.89	0.13	38,38,38,38	0
54	MG	CA	1758	1/1	0.89	0.07	77,77,77,77	0
54	MG	BA	3203	1/1	0.89	0.08	67,67,67,67	0
54	MG	AA	1624	1/1	0.89	0.12	58,58,58,58	0
54	MG	BA	3146	1/1	0.89	0.08	99,99,99,99	0
54	MG	DA	3336	1/1	0.89	0.14	70,70,70,70	0
54	MG	DB	223	1/1	0.89	0.05	82,82,82,82	0
54	MG	DA	3131	1/1	0.89	0.12	63,63,63,63	0
54	MG	BA	3364	1/1	0.89	0.07	107,107,107,107	0
54	MG	DA	3597	1/1	0.89	0.06	124,124,124,124	0
54	MG	AA	1665	1/1	0.89	0.08	70,70,70,70	0
54	MG	BA	3366	1/1	0.89	0.12	80,80,80,80	0
54	MG	BA	3210	1/1	0.89	0.10	86,86,86,86	0
54	MG	DA	3138	1/1	0.89	0.11	81,81,81,81	0
54	MG	BA	3371	1/1	0.89	0.22	114,114,114,114	0
54	MG	BB	202	1/1	0.89	0.18	48,48,48,48	0
54	MG	CA	1646	1/1	0.89	0.15	115,115,115,115	0
54	MG	BA	3154	1/1	0.89	0.15	139,139,139,139	0
54	MG	BA	2944	1/1	0.89	0.31	47,47,47,47	0
54	MG	CA	1781	1/1	0.89	0.11	76,76,76,76	0
54	MG	AA	1640	1/1	0.89	0.24	58,58,58,58	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	DA	3366	1/1	0.89	0.05	73,73,73,73	0
54	MG	BA	3499	1/1	0.89	0.21	66,66,66,66	0
54	MG	DA	3160	1/1	0.89	0.10	53,53,53,53	0
54	MG	DD	305	1/1	0.89	0.10	52,52,52,52	0
54	MG	CA	1893	1/1	0.89	0.13	127,127,127,127	0
54	MG	BA	3299	1/1	0.89	0.13	72,72,72,72	0
54	MG	DA	3638	1/1	0.89	0.30	22,22,22,22	0
54	MG	DA	3643	1/1	0.89	0.20	40,40,40,40	0
54	MG	BA	3380	1/1	0.89	0.10	55,55,55,55	0
54	MG	DA	3379	1/1	0.89	0.15	78,78,78,78	0
54	MG	CA	1896	1/1	0.89	0.07	70,70,70,70	0
54	MG	DA	3183	1/1	0.89	0.13	76,76,76,76	0
54	MG	DA	3384	1/1	0.89	0.10	84,84,84,84	0
54	MG	AA	1678	1/1	0.89	0.06	78,78,78,78	0
54	MG	DK	201	1/1	0.89	0.14	87,87,87,87	0
54	MG	DK	202	1/1	0.89	0.17	69,69,69,69	0
54	MG	BA	3028	1/1	0.89	0.39	61,61,61,61	0
54	MG	AA	1739	1/1	0.89	0.07	81,81,81,81	0
54	MG	AA	1709	1/1	0.89	0.05	87,87,87,87	0
54	MG	DQ	201	1/1	0.89	0.10	57,57,57,57	0
54	MG	DA	3197	1/1	0.89	0.08	46,46,46,46	0
54	MG	DA	3198	1/1	0.89	0.10	65,65,65,65	0
54	MG	CA	1667	1/1	0.89	0.17	77,77,77,77	0
54	MG	DA	3202	1/1	0.89	0.16	76,76,76,76	0
54	MG	BA	3388	1/1	0.89	0.21	66,66,66,66	0
54	MG	DA	3410	1/1	0.89	0.08	48,48,48,48	0
54	MG	DA	3411	1/1	0.89	0.17	68,68,68,68	0
54	MG	DA	3692	1/1	0.89	0.26	86,86,86,86	0
54	MG	DA	3207	1/1	0.89	0.15	43,43,43,43	0
54	MG	DA	3694	1/1	0.89	0.20	64,64,64,64	0
54	MG	DA	3695	1/1	0.89	0.17	76,76,76,76	0
54	MG	AA	1726	1/1	0.89	0.10	103,103,103,103	0
54	MG	CA	1800	1/1	0.89	0.14	89,89,89,89	0
54	MG	BA	3170	1/1	0.89	0.21	87,87,87,87	0
54	MG	DA	3480	1/1	0.90	0.06	76,76,76,76	0
54	MG	BA	3563	1/1	0.90	0.18	58,58,58,58	0
54	MG	BA	3033	1/1	0.90	0.32	77,77,77,77	0
54	MG	BA	2979	1/1	0.90	0.13	86,86,86,86	0
54	MG	BA	2916	1/1	0.90	0.31	37,37,37,37	0
54	MG	DA	3747	1/1	0.90	0.05	78,78,78,78	0
54	MG	DA	3748	1/1	0.90	0.10	61,61,61,61	0
54	MG	DA	3752	1/1	0.90	0.17	74,74,74,74	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	DA	3088	1/1	0.90	0.09	83,83,83,83	0
54	MG	DA	3089	1/1	0.90	0.22	71,71,71,71	0
54	MG	AA	1780	1/1	0.90	0.06	101,101,101,101	0
54	MG	B4	101	1/1	0.90	0.18	91,91,91,91	0
54	MG	BA	3232	1/1	0.90	0.16	68,68,68,68	0
54	MG	DA	3761	1/1	0.90	0.05	100,100,100,100	0
54	MG	DA	3289	1/1	0.90	0.10	44,44,44,44	0
54	MG	BA	2987	1/1	0.90	0.09	79,79,79,79	0
54	MG	CA	1857	1/1	0.90	0.23	76,76,76,76	0
54	MG	DA	3767	1/1	0.90	0.06	73,73,73,73	0
54	MG	DA	3101	1/1	0.90	0.28	75,75,75,75	0
54	MG	DA	3103	1/1	0.90	0.10	58,58,58,58	0
54	MG	AA	1636	1/1	0.90	0.06	96,96,96,96	0
54	MG	DA	3510	1/1	0.90	0.12	64,64,64,64	0
54	MG	AA	1749	1/1	0.90	0.08	90,90,90,90	0
54	MG	DA	3108	1/1	0.90	0.21	54,54,54,54	0
54	MG	CA	1743	1/1	0.90	0.09	88,88,88,88	0
54	MG	BA	3655	1/1	0.90	0.08	92,92,92,92	0
54	MG	BA	3043	1/1	0.90	0.06	50,50,50,50	0
54	MG	CC	301	1/1	0.90	0.05	93,93,93,93	0
54	MG	DA	3308	1/1	0.90	0.16	83,83,83,83	0
54	MG	BA	2932	1/1	0.90	0.25	44,44,44,44	0
54	MG	BA	3389	1/1	0.90	0.10	66,66,66,66	0
54	MG	BA	3500	1/1	0.90	0.09	72,72,72,72	0
54	MG	BA	3046	1/1	0.90	0.15	65,65,65,65	0
54	MG	BA	3245	1/1	0.90	0.28	95,95,95,95	0
54	MG	DA	3799	1/1	0.90	0.15	96,96,96,96	0
54	MG	DA	3536	1/1	0.90	0.13	92,92,92,92	0
54	MG	DA	3801	1/1	0.90	0.04	83,83,83,83	0
54	MG	CA	1755	1/1	0.90	0.07	69,69,69,69	0
54	MG	DA	3806	1/1	0.90	0.07	92,92,92,92	0
54	MG	CD	304	1/1	0.90	0.07	108,108,108,108	0
54	MG	CA	1619	1/1	0.90	0.17	62,62,62,62	0
54	MG	BA	3668	1/1	0.90	0.17	97,97,97,97	0
54	MG	BA	2939	1/1	0.90	0.20	47,47,47,47	0
54	MG	DA	3817	1/1	0.90	0.11	76,76,76,76	0
54	MG	BA	3248	1/1	0.90	0.21	82,82,82,82	0
54	MG	DA	3328	1/1	0.90	0.31	85,85,85,85	0
54	MG	DA	3824	1/1	0.90	0.42	113,113,113,113	0
54	MG	BA	3113	1/1	0.90	0.19	59,59,59,59	0
54	MG	AA	1661	1/1	0.90	0.05	51,51,51,51	0
54	MG	AA	1602	1/1	0.90	0.30	45,45,45,45	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	BA	3122	1/1	0.90	0.15	56,56,56,56	0
54	MG	BA	2951	1/1	0.90	0.35	53,53,53,53	0
54	MG	BA	3258	1/1	0.90	0.11	78,78,78,78	0
54	MG	AA	1762	1/1	0.90	0.24	91,91,91,91	0
54	MG	BA	3595	1/1	0.90	0.05	108,108,108,108	0
54	MG	BB	203	1/1	0.90	0.28	74,74,74,74	0
54	MG	DA	3156	1/1	0.90	0.20	52,52,52,52	0
54	MG	DA	3158	1/1	0.90	0.17	42,42,42,42	0
54	MG	AI	201	1/1	0.90	0.07	70,70,70,70	0
54	MG	CA	1643	1/1	0.90	0.08	70,70,70,70	0
54	MG	BA	2962	1/1	0.90	0.19	54,54,54,54	0
54	MG	DA	3845	1/1	0.90	0.14	94,94,94,94	0
54	MG	DA	3846	1/1	0.90	0.10	94,94,94,94	0
54	MG	BA	3518	1/1	0.90	0.05	81,81,81,81	0
54	MG	DA	3850	1/1	0.90	0.08	52,52,52,52	0
54	MG	DA	3851	1/1	0.90	0.09	74,74,74,74	0
54	MG	DA	3357	1/1	0.90	0.35	169,169,169,169	0
54	MG	DA	3166	1/1	0.90	0.09	73,73,73,73	0
54	MG	DA	3168	1/1	0.90	0.27	67,67,67,67	0
54	MG	BA	3263	1/1	0.90	0.16	107,107,107,107	0
54	MG	AA	1742	1/1	0.90	0.05	90,90,90,90	0
54	MG	DA	3860	1/1	0.90	0.03	78,78,78,78	0
54	MG	DA	3178	1/1	0.90	0.33	54,54,54,54	0
54	MG	DA	3181	1/1	0.90	0.13	96,96,96,96	0
54	MG	BA	3601	1/1	0.90	0.10	76,76,76,76	0
54	MG	BA	3347	1/1	0.90	0.05	77,77,77,77	0
54	MG	BA	2968	1/1	0.90	0.18	47,47,47,47	0
54	MG	BB	214	1/1	0.90	0.10	84,84,84,84	0
54	MG	AA	1626	1/1	0.90	0.23	88,88,88,88	0
54	MG	BB	219	1/1	0.90	0.06	69,69,69,69	0
54	MG	DA	2922	1/1	0.90	0.24	37,37,37,37	0
54	MG	DA	3199	1/1	0.90	0.09	108,108,108,108	0
54	MG	BB	220	1/1	0.90	0.09	75,75,75,75	0
54	MG	CA	1799	1/1	0.90	0.03	109,109,109,109	0
54	MG	BA	3071	1/1	0.90	0.05	71,71,71,71	0
54	MG	BA	3415	1/1	0.90	0.10	128,128,128,128	0
54	MG	BB	223	1/1	0.90	0.15	94,94,94,94	0
54	MG	DA	3404	1/1	0.90	0.11	79,79,79,79	0
54	MG	BA	3073	1/1	0.90	0.10	63,63,63,63	0
54	MG	DB	233	1/1	0.90	0.13	67,67,67,67	0
54	MG	AL	202	1/1	0.90	0.09	67,67,67,67	0
54	MG	DA	3408	1/1	0.90	0.36	109,109,109,109	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	DA	3409	1/1	0.90	0.38	110,110,110,110	0
54	MG	AA	1807	1/1	0.90	0.28	76,76,76,76	0
54	MG	CA	1675	1/1	0.90	0.09	74,74,74,74	0
54	MG	DA	3005	1/1	0.90	0.15	41,41,41,41	0
54	MG	BA	3279	1/1	0.90	0.11	85,85,85,85	0
54	MG	DA	3421	1/1	0.90	0.07	63,63,63,63	0
54	MG	DC	303	1/1	0.90	0.14	80,80,80,80	0
54	MG	DD	301	1/1	0.90	0.22	39,39,39,39	0
54	MG	CA	1679	1/1	0.90	0.18	89,89,89,89	0
54	MG	AA	1789	1/1	0.90	0.13	106,106,106,106	0
54	MG	CA	1922	1/1	0.90	0.11	127,127,127,127	0
54	MG	DA	3227	1/1	0.90	0.10	43,43,43,43	0
54	MG	DA	3675	1/1	0.90	0.11	46,46,46,46	0
54	MG	BA	3086	1/1	0.90	0.13	63,63,63,63	0
54	MG	BA	2977	1/1	0.90	0.38	69,69,69,69	0
54	MG	BF	201	1/1	0.90	0.10	122,122,122,122	0
54	MG	DA	3682	1/1	0.90	0.23	59,59,59,59	0
54	MG	DA	3241	1/1	0.90	0.07	76,76,76,76	0
54	MG	BA	3617	1/1	0.90	0.09	96,96,96,96	0
54	MG	BA	3088	1/1	0.90	0.15	57,57,57,57	0
54	MG	DJ	204	1/1	0.90	0.09	32,32,32,32	0
54	MG	BJ	201	1/1	0.90	0.05	75,75,75,75	0
54	MG	CA	1935	1/1	0.90	0.12	101,101,101,101	0
54	MG	BA	3459	1/1	0.90	0.19	30,30,30,30	0
54	MG	DA	3038	1/1	0.90	0.23	44,44,44,44	0
54	MG	AA	1738	1/1	0.90	0.29	104,104,104,104	0
54	MG	DO	201	1/1	0.90	0.17	55,55,55,55	0
54	MG	CA	1699	1/1	0.90	0.04	76,76,76,76	0
54	MG	DA	3702	1/1	0.90	0.15	74,74,74,74	0
54	MG	BA	3623	1/1	0.90	0.16	64,64,64,64	0
54	MG	DA	3708	1/1	0.90	0.17	63,63,63,63	0
54	MG	CA	1942	1/1	0.90	0.08	104,104,104,104	0
54	MG	DA	3262	1/1	0.90	0.17	73,73,73,73	0
54	MG	BA	3093	1/1	0.90	0.17	67,67,67,67	0
54	MG	BA	3626	1/1	0.90	0.08	64,64,64,64	0
54	MG	BA	3094	1/1	0.90	0.13	63,63,63,63	0
54	MG	DA	3721	1/1	0.90	0.19	88,88,88,88	0
54	MG	BA	3214	1/1	0.90	0.23	79,79,79,79	0
54	MG	BA	3215	1/1	0.90	0.26	64,64,64,64	0
54	MG	BA	3630	1/1	0.90	0.10	151,151,151,151	0
54	MG	BA	3032	1/1	0.90	0.22	76,76,76,76	0
54	MG	BV	202	1/1	0.90	0.09	75,75,75,75	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	BA	3561	1/1	0.90	0.07	75,75,75,75	0
54	MG	BA	2938	1/1	0.91	0.17	51,51,51,51	0
54	MG	BA	3287	1/1	0.91	0.14	83,83,83,83	0
54	MG	AA	1792	1/1	0.91	0.04	101,101,101,101	0
54	MG	CC	302	1/1	0.91	0.05	79,79,79,79	0
54	MG	BA	3291	1/1	0.91	0.12	102,102,102,102	0
54	MG	BA	3672	1/1	0.91	0.17	92,92,92,92	0
54	MG	BA	3543	1/1	0.91	0.17	76,76,76,76	0
54	MG	CA	1774	1/1	0.91	0.04	79,79,79,79	0
54	MG	DA	3746	1/1	0.91	0.06	94,94,94,94	0
54	MG	BA	3545	1/1	0.91	0.17	59,59,59,59	0
54	MG	AA	1699	1/1	0.91	0.07	57,57,57,57	0
54	MG	DA	3750	1/1	0.91	0.14	87,87,87,87	0
54	MG	AA	1869	1/1	0.91	0.08	74,74,74,74	0
54	MG	CA	1783	1/1	0.91	0.10	139,139,139,139	0
54	MG	AA	1856	1/1	0.91	0.07	58,58,58,58	0
54	MG	AA	1824	1/1	0.91	0.16	81,81,81,81	0
54	MG	CA	1787	1/1	0.91	0.24	37,37,37,37	0
54	MG	DA	3503	1/1	0.91	0.05	91,91,91,91	0
54	MG	BA	3485	1/1	0.91	0.20	72,72,72,72	0
54	MG	CF	202	1/1	0.91	0.05	83,83,83,83	0
54	MG	DA	3506	1/1	0.91	0.19	101,101,101,101	0
54	MG	DA	3507	1/1	0.91	0.23	70,70,70,70	0
54	MG	AA	1611	1/1	0.91	0.20	55,55,55,55	0
54	MG	BA	3111	1/1	0.91	0.21	64,64,64,64	0
54	MG	DA	3511	1/1	0.91	0.17	52,52,52,52	0
54	MG	CA	1688	1/1	0.91	0.17	80,80,80,80	0
54	MG	BA	3557	1/1	0.91	0.13	67,67,67,67	0
54	MG	CA	1694	1/1	0.91	0.06	79,79,79,79	0
54	MG	CA	1795	1/1	0.91	0.08	131,131,131,131	0
54	MG	BA	3558	1/1	0.91	0.04	91,91,91,91	0
54	MG	BA	2961	1/1	0.91	0.24	51,51,51,51	0
54	MG	DA	3780	1/1	0.91	0.12	67,67,67,67	0
54	MG	BA	3495	1/1	0.91	0.10	74,74,74,74	0
54	MG	CM	201	1/1	0.91	0.11	85,85,85,85	0
54	MG	DA	3142	1/1	0.91	0.16	61,61,61,61	0
54	MG	DA	3524	1/1	0.91	0.05	87,87,87,87	0
54	MG	BA	3037	1/1	0.91	0.14	62,62,62,62	0
54	MG	BA	3359	1/1	0.91	0.04	89,89,89,89	0
54	MG	DA	3794	1/1	0.91	0.09	104,104,104,104	0
54	MG	CA	1801	1/1	0.91	0.13	82,82,82,82	0
54	MG	DA	3535	1/1	0.91	0.24	107,107,107,107	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	BA	3169	1/1	0.91	0.17	43,43,43,43	0
54	MG	DA	3150	1/1	0.91	0.12	56,56,56,56	0
54	MG	DA	3329	1/1	0.91	0.07	96,96,96,96	0
54	MG	DA	3540	1/1	0.91	0.06	93,93,93,93	0
54	MG	DA	3151	1/1	0.91	0.29	76,76,76,76	0
54	MG	DA	3152	1/1	0.91	0.20	43,43,43,43	0
54	MG	DA	3545	1/1	0.91	0.19	94,94,94,94	0
54	MG	AA	1703	1/1	0.91	0.22	63,63,63,63	0
54	MG	DA	3550	1/1	0.91	0.05	65,65,65,65	0
54	MG	BA	3083	1/1	0.91	0.11	70,70,70,70	0
54	MG	BA	3313	1/1	0.91	0.06	67,67,67,67	0
54	MG	DA	3561	1/1	0.91	0.22	85,85,85,85	0
54	MG	CA	1709	1/1	0.91	0.06	107,107,107,107	0
54	MG	DA	3341	1/1	0.91	0.15	75,75,75,75	0
54	MG	DA	3569	1/1	0.91	0.25	36,36,36,36	0
54	MG	BA	3084	1/1	0.91	0.30	82,82,82,82	0
54	MG	BB	217	1/1	0.91	0.07	72,72,72,72	0
54	MG	BA	3005	1/1	0.91	0.16	53,53,53,53	0
54	MG	DA	2917	1/1	0.91	0.22	71,71,71,71	0
54	MG	DA	2918	1/1	0.91	0.27	25,25,25,25	0
54	MG	DA	3167	1/1	0.91	0.10	58,58,58,58	0
54	MG	CA	1813	1/1	0.91	0.04	107,107,107,107	0
54	MG	CA	1713	1/1	0.91	0.09	92,92,92,92	0
54	MG	DA	2929	1/1	0.91	0.18	21,21,21,21	0
54	MG	DA	3174	1/1	0.91	0.22	66,66,66,66	0
54	MG	CA	1714	1/1	0.91	0.06	123,123,123,123	0
54	MG	DA	3360	1/1	0.91	0.18	107,107,107,107	0
54	MG	CA	1715	1/1	0.91	0.10	107,107,107,107	0
54	MG	DA	3590	1/1	0.91	0.12	47,47,47,47	0
54	MG	BA	2963	1/1	0.91	0.11	34,34,34,34	0
54	MG	DA	3186	1/1	0.91	0.19	82,82,82,82	0
54	MG	BA	3132	1/1	0.91	0.18	66,66,66,66	0
54	MG	BA	3509	1/1	0.91	0.07	64,64,64,64	0
54	MG	DA	3853	1/1	0.91	0.17	114,114,114,114	0
54	MG	DA	2969	1/1	0.91	0.26	39,39,39,39	0
54	MG	BA	3416	1/1	0.91	0.04	83,83,83,83	0
54	MG	AA	1861	1/1	0.91	0.08	81,81,81,81	0
54	MG	DA	2987	1/1	0.91	0.19	28,28,28,28	0
54	MG	DA	3606	1/1	0.91	0.09	68,68,68,68	0
54	MG	DA	2993	1/1	0.91	0.20	47,47,47,47	0
54	MG	CA	1926	1/1	0.91	0.08	76,76,76,76	0
54	MG	DA	3003	1/1	0.91	0.24	51,51,51,51	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	CA	1634	1/1	0.91	0.06	78,78,78,78	0
54	MG	BA	3217	1/1	0.91	0.08	55,55,55,55	0
54	MG	DA	3208	1/1	0.91	0.10	56,56,56,56	0
54	MG	DB	215	1/1	0.91	0.07	103,103,103,103	0
54	MG	CA	1930	1/1	0.91	0.07	89,89,89,89	0
54	MG	DA	3013	1/1	0.91	0.13	52,52,52,52	0
54	MG	CA	1830	1/1	0.91	0.07	82,82,82,82	0
54	MG	DA	3400	1/1	0.91	0.13	127,127,127,127	0
54	MG	DB	224	1/1	0.91	0.10	95,95,95,95	0
54	MG	DA	3402	1/1	0.91	0.07	95,95,95,95	0
54	MG	DA	3024	1/1	0.91	0.15	58,58,58,58	0
54	MG	BA	3373	1/1	0.91	0.09	61,61,61,61	0
54	MG	CA	1637	1/1	0.91	0.07	98,98,98,98	0
54	MG	BA	3219	1/1	0.91	0.10	80,80,80,80	0
54	MG	BA	3640	1/1	0.91	0.10	97,97,97,97	0
54	MG	DA	3648	1/1	0.91	0.34	60,60,60,60	0
54	MG	CA	1735	1/1	0.91	0.06	77,77,77,77	0
54	MG	CA	1838	1/1	0.91	0.09	94,94,94,94	0
54	MG	DA	3653	1/1	0.91	0.23	51,51,51,51	0
54	MG	DA	3412	1/1	0.91	0.10	86,86,86,86	0
54	MG	DA	3032	1/1	0.91	0.28	80,80,80,80	0
54	MG	DA	3661	1/1	0.91	0.31	98,98,98,98	0
54	MG	CA	1941	1/1	0.91	0.05	70,70,70,70	0
54	MG	CA	1737	1/1	0.91	0.07	70,70,70,70	0
54	MG	DB	242	1/1	0.91	0.07	113,113,113,113	0
54	MG	DA	3233	1/1	0.91	0.06	67,67,67,67	0
54	MG	DC	302	1/1	0.91	0.26	164,164,164,164	0
54	MG	DA	3237	1/1	0.91	0.25	64,64,64,64	0
54	MG	CA	1738	1/1	0.91	0.04	93,93,93,93	0
54	MG	DA	3669	1/1	0.91	0.07	61,61,61,61	0
54	MG	BA	3017	1/1	0.91	0.09	55,55,55,55	0
54	MG	DA	3671	1/1	0.91	0.30	69,69,69,69	0
54	MG	CA	1741	1/1	0.91	0.09	100,100,100,100	0
54	MG	CA	1642	1/1	0.91	0.07	79,79,79,79	0
54	MG	DA	3677	1/1	0.91	0.38	60,60,60,60	0
54	MG	DF	201	1/1	0.91	0.12	70,70,70,70	0
54	MG	DA	3247	1/1	0.91	0.12	92,92,92,92	0
54	MG	BA	2906	1/1	0.91	0.22	24,24,24,24	0
54	MG	CA	1644	1/1	0.91	0.10	94,94,94,94	0
54	MG	DA	3685	1/1	0.91	0.17	82,82,82,82	0
54	MG	BA	3437	1/1	0.91	0.26	42,42,42,42	0
54	MG	BA	3648	1/1	0.91	0.11	63,63,63,63	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	AA	1773	1/1	0.91	0.10	97,97,97,97	0
54	MG	DA	3443	1/1	0.91	0.07	92,92,92,92	0
54	MG	AA	1863	1/1	0.91	0.07	119,119,119,119	0
54	MG	DA	3446	1/1	0.91	0.08	57,57,57,57	0
54	MG	CA	1853	1/1	0.91	0.04	113,113,113,113	0
54	MG	CA	1753	1/1	0.91	0.13	97,97,97,97	0
54	MG	AA	1819	1/1	0.91	0.17	73,73,73,73	0
54	MG	DA	3075	1/1	0.91	0.10	50,50,50,50	0
54	MG	DA	3456	1/1	0.91	0.47	121,121,121,121	0
54	MG	DA	3458	1/1	0.91	0.14	95,95,95,95	0
54	MG	BA	3383	1/1	0.91	0.08	66,66,66,66	0
54	MG	AA	1710	1/1	0.91	0.25	84,84,84,84	0
54	MG	BN	201	1/1	0.91	0.12	49,49,49,49	0
54	MG	CA	1964	1/1	0.91	0.16	99,99,99,99	0
54	MG	CA	1759	1/1	0.91	0.11	89,89,89,89	0
54	MG	BA	3466	1/1	0.91	0.18	61,61,61,61	0
54	MG	AA	1748	1/1	0.91	0.09	56,56,56,56	0
54	MG	DY	102	1/1	0.91	0.16	69,69,69,69	0
54	MG	DA	3725	1/1	0.91	0.12	65,65,65,65	0
54	MG	DA	3726	1/1	0.91	0.28	106,106,106,106	0
54	MG	CA	1661	1/1	0.91	0.06	80,80,80,80	0
54	MG	DA	3728	1/1	0.91	0.19	83,83,83,83	0
54	MG	DA	3729	1/1	0.91	0.10	81,81,81,81	0
54	MG	BA	2937	1/1	0.91	0.07	56,56,56,56	0
54	MG	AA	1655	1/1	0.92	0.22	58,58,58,58	0
54	MG	DA	3712	1/1	0.92	0.07	41,41,41,41	0
54	MG	BA	3267	1/1	0.92	0.05	65,65,65,65	0
54	MG	DA	3447	1/1	0.92	0.14	73,73,73,73	0
54	MG	DA	3715	1/1	0.92	0.14	57,57,57,57	0
54	MG	DA	3000	1/1	0.92	0.11	23,23,23,23	0
54	MG	BA	3419	1/1	0.92	0.10	67,67,67,67	0
54	MG	DA	3720	1/1	0.92	0.16	79,79,79,79	0
54	MG	AA	1629	1/1	0.92	0.27	66,66,66,66	0
54	MG	BA	3538	1/1	0.92	0.17	75,75,75,75	0
54	MG	DA	3008	1/1	0.92	0.18	50,50,50,50	0
54	MG	AA	1829	1/1	0.92	0.09	64,64,64,64	0
54	MG	BJ	202	1/1	0.92	0.12	69,69,69,69	0
54	MG	DA	3020	1/1	0.92	0.15	47,47,47,47	0
54	MG	DA	3238	1/1	0.92	0.13	56,56,56,56	0
54	MG	CA	1689	1/1	0.92	0.19	130,130,130,130	0
54	MG	DA	3467	1/1	0.92	0.10	97,97,97,97	0
54	MG	DA	3732	1/1	0.92	0.38	81,81,81,81	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	CA	1927	1/1	0.92	0.06	88,88,88,88	0
54	MG	BA	3077	1/1	0.92	0.26	55,55,55,55	0
54	MG	AA	1791	1/1	0.92	0.04	106,106,106,106	0
54	MG	DA	3739	1/1	0.92	0.30	133,133,133,133	0
54	MG	BA	3544	1/1	0.92	0.10	81,81,81,81	0
54	MG	CA	1931	1/1	0.92	0.04	99,99,99,99	0
54	MG	DA	3475	1/1	0.92	0.16	120,120,120,120	0
54	MG	AA	1722	1/1	0.92	0.22	53,53,53,53	0
54	MG	CA	1933	1/1	0.92	0.04	137,137,137,137	0
54	MG	BA	3275	1/1	0.92	0.15	68,68,68,68	0
54	MG	BA	3278	1/1	0.92	0.09	88,88,88,88	0
54	MG	DA	3749	1/1	0.92	0.12	59,59,59,59	0
54	MG	BA	3446	1/1	0.92	0.24	53,53,53,53	0
54	MG	DA	3751	1/1	0.92	0.29	76,76,76,76	0
54	MG	BA	3450	1/1	0.92	0.35	46,46,46,46	0
54	MG	BA	2908	1/1	0.92	0.20	26,26,26,26	0
54	MG	DA	3039	1/1	0.92	0.17	70,70,70,70	0
54	MG	BA	2913	1/1	0.92	0.26	27,27,27,27	0
54	MG	DA	3757	1/1	0.92	0.12	89,89,89,89	0
54	MG	DA	3491	1/1	0.92	0.09	99,99,99,99	0
54	MG	CA	1940	1/1	0.92	0.09	72,72,72,72	0
54	MG	BA	3461	1/1	0.92	0.24	48,48,48,48	0
54	MG	DA	3045	1/1	0.92	0.25	39,39,39,39	0
54	MG	BA	3638	1/1	0.92	0.35	127,127,127,127	0
54	MG	BA	3207	1/1	0.92	0.05	70,70,70,70	0
54	MG	DA	3051	1/1	0.92	0.23	60,60,60,60	0
54	MG	BA	3641	1/1	0.92	0.05	95,95,95,95	0
54	MG	DA	3053	1/1	0.92	0.14	63,63,63,63	0
54	MG	DA	3771	1/1	0.92	0.10	58,58,58,58	0
54	MG	DA	3054	1/1	0.92	0.39	72,72,72,72	0
54	MG	AK	202	1/1	0.92	0.07	101,101,101,101	0
54	MG	AA	1813	1/1	0.92	0.06	76,76,76,76	0
54	MG	DA	3508	1/1	0.92	0.09	70,70,70,70	0
54	MG	DA	3064	1/1	0.92	0.20	127,127,127,127	0
54	MG	BA	3646	1/1	0.92	0.08	82,82,82,82	0
54	MG	B2	101	1/1	0.92	0.05	27,27,27,27	0
54	MG	DA	3068	1/1	0.92	0.12	64,64,64,64	0
54	MG	DA	3072	1/1	0.92	0.14	80,80,80,80	0
54	MG	CA	1835	1/1	0.92	0.07	76,76,76,76	0
54	MG	BA	3089	1/1	0.92	0.23	69,69,69,69	0
54	MG	BA	3091	1/1	0.92	0.15	72,72,72,72	0
54	MG	DA	3294	1/1	0.92	0.07	36,36,36,36	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	BA	3649	1/1	0.92	0.11	67,67,67,67	0
54	MG	BA	3650	1/1	0.92	0.12	69,69,69,69	0
54	MG	BA	3369	1/1	0.92	0.10	108,108,108,108	0
54	MG	BA	3151	1/1	0.92	0.20	70,70,70,70	0
54	MG	BA	3153	1/1	0.92	0.06	79,79,79,79	0
54	MG	DA	3529	1/1	0.92	0.08	61,61,61,61	0
54	MG	CA	1959	1/1	0.92	0.04	106,106,106,106	0
54	MG	AA	1859	1/1	0.92	0.04	87,87,87,87	0
54	MG	DA	3807	1/1	0.92	0.20	61,61,61,61	0
54	MG	BA	2983	1/1	0.92	0.08	44,44,44,44	0
54	MG	CA	1963	1/1	0.92	0.07	99,99,99,99	0
54	MG	DA	3813	1/1	0.92	0.05	50,50,50,50	0
54	MG	BA	2929	1/1	0.92	0.38	50,50,50,50	0
54	MG	DA	3538	1/1	0.92	0.15	66,66,66,66	0
54	MG	CA	1848	1/1	0.92	0.10	96,96,96,96	0
54	MG	BA	3481	1/1	0.92	0.25	71,71,71,71	0
54	MG	DA	3821	1/1	0.92	0.14	79,79,79,79	0
54	MG	BA	2985	1/1	0.92	0.18	43,43,43,43	0
54	MG	DA	3823	1/1	0.92	0.14	84,84,84,84	0
54	MG	BA	3574	1/1	0.92	0.12	62,62,62,62	0
54	MG	BA	3222	1/1	0.92	0.05	86,86,86,86	0
54	MG	DA	3826	1/1	0.92	0.10	100,100,100,100	0
54	MG	BA	3666	1/1	0.92	0.16	72,72,72,72	0
54	MG	BA	3667	1/1	0.92	0.11	85,85,85,85	0
54	MG	BA	3379	1/1	0.92	0.09	86,86,86,86	0
54	MG	BA	3160	1/1	0.92	0.19	87,87,87,87	0
54	MG	DA	3831	1/1	0.92	0.07	66,66,66,66	0
54	MG	BA	3489	1/1	0.92	0.16	73,73,73,73	0
54	MG	AA	1647	1/1	0.92	0.14	63,63,63,63	0
54	MG	BA	3674	1/1	0.92	0.15	55,55,55,55	0
54	MG	DA	3567	1/1	0.92	0.09	87,87,87,87	0
54	MG	BA	3581	1/1	0.92	0.16	127,127,127,127	0
54	MG	DA	3570	1/1	0.92	0.20	90,90,90,90	0
54	MG	CA	1632	1/1	0.92	0.15	59,59,59,59	0
54	MG	CA	1633	1/1	0.92	0.13	85,85,85,85	0
54	MG	DA	3123	1/1	0.92	0.15	59,59,59,59	0
54	MG	CA	1868	1/1	0.92	0.06	71,71,71,71	0
54	MG	DA	3127	1/1	0.92	0.10	76,76,76,76	0
54	MG	AA	1668	1/1	0.92	0.22	77,77,77,77	0
54	MG	BA	2994	1/1	0.92	0.36	90,90,90,90	0
54	MG	CA	1873	1/1	0.92	0.09	58,58,58,58	0
54	MG	AA	1839	1/1	0.92	0.09	69,69,69,69	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	CA	1757	1/1	0.92	0.10	102,102,102,102	0
54	MG	AA	1841	1/1	0.92	0.11	83,83,83,83	0
54	MG	CA	1878	1/1	0.92	0.11	82,82,82,82	0
54	MG	CA	1879	1/1	0.92	0.07	76,76,76,76	0
54	MG	DA	3350	1/1	0.92	0.08	95,95,95,95	0
54	MG	BA	3047	1/1	0.92	0.11	72,72,72,72	0
54	MG	DA	3861	1/1	0.92	0.07	90,90,90,90	0
54	MG	CA	1760	1/1	0.92	0.15	66,66,66,66	0
54	MG	AA	1752	1/1	0.92	0.07	94,94,94,94	0
54	MG	AQ	202	1/1	0.92	0.11	85,85,85,85	0
54	MG	AA	1768	1/1	0.92	0.05	87,87,87,87	0
54	MG	DA	3599	1/1	0.92	0.14	58,58,58,58	0
54	MG	CL	204	1/1	0.92	0.14	86,86,86,86	0
54	MG	AA	1801	1/1	0.92	0.16	71,71,71,71	0
54	MG	DB	216	1/1	0.92	0.06	101,101,101,101	0
54	MG	DB	218	1/1	0.92	0.05	113,113,113,113	0
54	MG	AA	1702	1/1	0.92	0.12	56,56,56,56	0
54	MG	BA	3247	1/1	0.92	0.09	109,109,109,109	0
54	MG	AA	1694	1/1	0.92	0.14	71,71,71,71	0
54	MG	DA	3610	1/1	0.92	0.18	81,81,81,81	0
54	MG	DA	3611	1/1	0.92	0.17	74,74,74,74	0
54	MG	CA	1769	1/1	0.92	0.16	67,67,67,67	0
54	MG	DA	3369	1/1	0.92	0.09	99,99,99,99	0
54	MG	BA	3112	1/1	0.92	0.17	65,65,65,65	0
54	MG	BA	2957	1/1	0.92	0.43	75,75,75,75	0
54	MG	BA	2958	1/1	0.92	0.29	46,46,46,46	0
54	MG	BA	3333	1/1	0.92	0.16	54,54,54,54	0
54	MG	DA	3161	1/1	0.92	0.20	70,70,70,70	0
54	MG	DA	3382	1/1	0.92	0.06	92,92,92,92	0
54	MG	BA	3116	1/1	0.92	0.19	70,70,70,70	0
54	MG	CA	1777	1/1	0.92	0.17	98,98,98,98	0
54	MG	CV	6201	1/1	0.92	0.07	95,95,95,95	0
54	MG	DA	3637	1/1	0.92	0.23	15,15,15,15	0
54	MG	CV	6202	1/1	0.92	0.10	108,108,108,108	0
54	MG	BA	3117	1/1	0.92	0.18	91,91,91,91	0
54	MG	DA	3391	1/1	0.92	0.19	82,82,82,82	0
54	MG	CA	1780	1/1	0.92	0.04	93,93,93,93	0
54	MG	BA	3118	1/1	0.92	0.07	95,95,95,95	0
54	MG	DA	3649	1/1	0.92	0.41	50,50,50,50	0
54	MG	BB	218	1/1	0.92	0.20	79,79,79,79	0
54	MG	DA	3651	1/1	0.92	0.19	51,51,51,51	0
54	MG	DA	3177	1/1	0.92	0.20	46,46,46,46	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	DA	3398	1/1	0.92	0.24	80,80,80,80	0
54	MG	DA	3655	1/1	0.92	0.20	60,60,60,60	0
54	MG	AA	1608	1/1	0.92	0.12	46,46,46,46	0
54	MG	DA	3659	1/1	0.92	0.31	61,61,61,61	0
54	MG	DA	3180	1/1	0.92	0.09	78,78,78,78	0
54	MG	CA	1662	1/1	0.92	0.14	84,84,84,84	0
54	MG	BA	3068	1/1	0.92	0.14	55,55,55,55	0
54	MG	DA	2925	1/1	0.92	0.32	34,34,34,34	0
54	MG	DA	2926	1/1	0.92	0.26	25,25,25,25	0
54	MG	DA	3188	1/1	0.92	0.22	69,69,69,69	0
54	MG	DA	3189	1/1	0.92	0.20	73,73,73,73	0
54	MG	DA	2928	1/1	0.92	0.36	31,31,31,31	0
54	MG	CA	1665	1/1	0.92	0.17	71,71,71,71	0
54	MG	DA	3413	1/1	0.92	0.13	60,60,60,60	0
54	MG	DA	3673	1/1	0.92	0.24	85,85,85,85	0
54	MG	DA	2935	1/1	0.92	0.23	23,23,23,23	0
54	MG	DA	2936	1/1	0.92	0.16	42,42,42,42	0
54	MG	DL	203	1/1	0.92	0.13	66,66,66,66	0
54	MG	BA	3408	1/1	0.92	0.07	86,86,86,86	0
54	MG	BA	3522	1/1	0.92	0.14	54,54,54,54	0
54	MG	DA	2945	1/1	0.92	0.17	29,29,29,29	0
54	MG	DA	3424	1/1	0.92	0.05	90,90,90,90	0
54	MG	DA	3425	1/1	0.92	0.08	113,113,113,113	0
54	MG	DA	3689	1/1	0.92	0.16	67,67,67,67	0
54	MG	DA	3690	1/1	0.92	0.21	70,70,70,70	0
54	MG	AA	1706	1/1	0.92	0.16	78,78,78,78	0
54	MG	DA	3427	1/1	0.92	0.19	85,85,85,85	0
54	MG	BA	3524	1/1	0.92	0.07	107,107,107,107	0
54	MG	AA	1732	1/1	0.92	0.04	104,104,104,104	0
54	MG	BA	3345	1/1	0.92	0.17	71,71,71,71	0
54	MG	DA	2971	1/1	0.92	0.23	38,38,38,38	0
54	MG	CA	1673	1/1	0.92	0.04	61,61,61,61	0
54	MG	DA	3211	1/1	0.92	0.17	64,64,64,64	0
54	MG	DA	3212	1/1	0.92	0.19	75,75,75,75	0
54	MG	BA	3072	1/1	0.92	0.10	57,57,57,57	0
54	MG	D5	101	1/1	0.92	0.05	46,46,46,46	0
54	MG	BA	3265	1/1	0.92	0.11	53,53,53,53	0
54	MG	DA	2989	1/1	0.92	0.05	39,39,39,39	0
54	MG	DA	3736	1/1	0.93	0.33	134,134,134,134	0
54	MG	BA	3051	1/1	0.93	0.19	62,62,62,62	0
54	MG	BA	3367	1/1	0.93	0.06	74,74,74,74	0
54	MG	CA	1794	1/1	0.93	0.12	122,122,122,122	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	BR	201	1/1	0.93	0.03	75,75,75,75	0
54	MG	BA	3368	1/1	0.93	0.04	58,58,58,58	0
54	MG	BA	3010	1/1	0.93	0.08	73,73,73,73	0
54	MG	BA	3104	1/1	0.93	0.08	49,49,49,49	0
54	MG	DA	2902	1/1	0.93	0.27	17,17,17,17	0
54	MG	DA	2907	1/1	0.93	0.28	17,17,17,17	0
54	MG	DA	2910	1/1	0.93	0.21	38,38,38,38	0
54	MG	DA	2914	1/1	0.93	0.20	23,23,23,23	0
54	MG	DA	3315	1/1	0.93	0.21	58,58,58,58	0
54	MG	DA	3518	1/1	0.93	0.06	102,102,102,102	0
54	MG	CA	1690	1/1	0.93	0.05	65,65,65,65	0
54	MG	AA	1733	1/1	0.93	0.08	89,89,89,89	0
54	MG	CA	1693	1/1	0.93	0.09	95,95,95,95	0
54	MG	DA	3756	1/1	0.93	0.27	80,80,80,80	0
54	MG	BA	2911	1/1	0.93	0.24	33,33,33,33	0
54	MG	AA	1848	1/1	0.93	0.16	77,77,77,77	0
54	MG	BA	2914	1/1	0.93	0.27	24,24,24,24	0
54	MG	DA	3528	1/1	0.93	0.05	87,87,87,87	0
54	MG	BA	3231	1/1	0.93	0.09	64,64,64,64	0
54	MG	BA	3377	1/1	0.93	0.06	68,68,68,68	0
54	MG	BA	3064	1/1	0.93	0.09	61,61,61,61	0
54	MG	DA	2930	1/1	0.93	0.20	34,34,34,34	0
54	MG	CA	1923	1/1	0.93	0.04	74,74,74,74	0
54	MG	CA	1702	1/1	0.93	0.12	114,114,114,114	0
54	MG	DA	3770	1/1	0.93	0.04	79,79,79,79	0
54	MG	DA	3334	1/1	0.93	0.04	53,53,53,53	0
54	MG	BA	3065	1/1	0.93	0.05	59,59,59,59	0
54	MG	AA	1667	1/1	0.93	0.24	78,78,78,78	0
54	MG	DA	3338	1/1	0.93	0.09	123,123,123,123	0
54	MG	DA	3543	1/1	0.93	0.04	87,87,87,87	0
54	MG	BA	3239	1/1	0.93	0.19	62,62,62,62	0
54	MG	DA	3340	1/1	0.93	0.09	59,59,59,59	0
54	MG	DA	3547	1/1	0.93	0.34	115,115,115,115	0
54	MG	B2	103	1/1	0.93	0.06	75,75,75,75	0
54	MG	DA	3782	1/1	0.93	0.09	67,67,67,67	0
54	MG	DA	2952	1/1	0.93	0.23	25,25,25,25	0
54	MG	CA	1707	1/1	0.93	0.16	102,102,102,102	0
54	MG	DA	3553	1/1	0.93	0.05	91,91,91,91	0
54	MG	DA	3554	1/1	0.93	0.26	136,136,136,136	0
54	MG	DA	3557	1/1	0.93	0.09	128,128,128,128	0
54	MG	DA	2954	1/1	0.93	0.25	41,41,41,41	0
54	MG	DA	3796	1/1	0.93	0.07	67,67,67,67	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	CA	1708	1/1	0.93	0.06	60,60,60,60	0
54	MG	DA	3563	1/1	0.93	0.16	95,95,95,95	0
54	MG	DA	2959	1/1	0.93	0.20	42,42,42,42	0
54	MG	BA	3571	1/1	0.93	0.06	74,74,74,74	0
54	MG	BA	2969	1/1	0.93	0.33	69,69,69,69	0
54	MG	DA	3802	1/1	0.93	0.07	84,84,84,84	0
54	MG	DA	2973	1/1	0.93	0.18	50,50,50,50	0
54	MG	AA	1637	1/1	0.93	0.09	62,62,62,62	0
54	MG	CA	1602	1/1	0.93	0.20	43,43,43,43	0
54	MG	CA	1607	1/1	0.93	0.07	62,62,62,62	0
54	MG	DA	3172	1/1	0.93	0.19	88,88,88,88	0
54	MG	DA	2988	1/1	0.93	0.15	23,23,23,23	0
54	MG	DA	3361	1/1	0.93	0.06	69,69,69,69	0
54	MG	CA	1828	1/1	0.93	0.09	88,88,88,88	0
54	MG	BA	3490	1/1	0.93	0.07	67,67,67,67	0
54	MG	DA	3179	1/1	0.93	0.16	105,105,105,105	0
54	MG	DA	3820	1/1	0.93	0.58	59,59,59,59	0
54	MG	BA	3314	1/1	0.93	0.23	69,69,69,69	0
54	MG	DA	2999	1/1	0.93	0.17	69,69,69,69	0
54	MG	DA	3584	1/1	0.93	0.28	130,130,130,130	0
54	MG	BA	3115	1/1	0.93	0.09	76,76,76,76	0
54	MG	DA	3371	1/1	0.93	0.06	53,53,53,53	0
54	MG	DA	3376	1/1	0.93	0.14	44,44,44,44	0
54	MG	DA	3589	1/1	0.93	0.13	51,51,51,51	0
54	MG	DA	3002	1/1	0.93	0.15	52,52,52,52	0
54	MG	BA	3386	1/1	0.93	0.40	134,134,134,134	0
54	MG	BA	2924	1/1	0.93	0.19	48,48,48,48	0
54	MG	DA	3006	1/1	0.93	0.15	60,60,60,60	0
54	MG	CA	1720	1/1	0.93	0.05	69,69,69,69	0
54	MG	BA	3497	1/1	0.93	0.06	61,61,61,61	0
54	MG	DA	3194	1/1	0.93	0.12	74,74,74,74	0
54	MG	DA	3385	1/1	0.93	0.10	69,69,69,69	0
54	MG	BA	3669	1/1	0.93	0.04	84,84,84,84	0
54	MG	BA	3498	1/1	0.93	0.11	67,67,67,67	0
54	MG	DA	3389	1/1	0.93	0.18	76,76,76,76	0
54	MG	DA	3841	1/1	0.93	0.10	80,80,80,80	0
54	MG	DA	3019	1/1	0.93	0.19	48,48,48,48	0
54	MG	BA	3671	1/1	0.93	0.09	100,100,100,100	0
54	MG	BA	3317	1/1	0.93	0.08	84,84,84,84	0
54	MG	CA	1729	1/1	0.93	0.05	58,58,58,58	0
54	MG	DA	3204	1/1	0.93	0.07	53,53,53,53	0
54	MG	BA	3244	1/1	0.93	0.07	79,79,79,79	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	DA	3206	1/1	0.93	0.16	89,89,89,89	0
54	MG	AA	1793	1/1	0.93	0.13	68,68,68,68	0
54	MG	BA	3183	1/1	0.93	0.14	68,68,68,68	0
54	MG	DA	3620	1/1	0.93	0.17	115,115,115,115	0
54	MG	BA	3323	1/1	0.93	0.15	98,98,98,98	0
54	MG	DA	3626	1/1	0.93	0.23	106,106,106,106	0
54	MG	DA	3630	1/1	0.93	0.14	101,101,101,101	0
54	MG	BA	3184	1/1	0.93	0.06	67,67,67,67	0
54	MG	DA	3406	1/1	0.93	0.06	59,59,59,59	0
54	MG	BA	2928	1/1	0.93	0.21	28,28,28,28	0
54	MG	BA	3252	1/1	0.93	0.14	60,60,60,60	0
54	MG	DB	205	1/1	0.93	0.17	78,78,78,78	0
54	MG	BA	3680	1/1	0.93	0.16	97,97,97,97	0
54	MG	AA	1682	1/1	0.93	0.18	91,91,91,91	0
54	MG	BA	3187	1/1	0.93	0.16	73,73,73,73	0
54	MG	DA	3220	1/1	0.93	0.18	98,98,98,98	0
54	MG	BA	3121	1/1	0.93	0.14	69,69,69,69	0
54	MG	DA	3416	1/1	0.93	0.05	101,101,101,101	0
54	MG	BA	3074	1/1	0.93	0.19	87,87,87,87	0
54	MG	DB	219	1/1	0.93	0.10	73,73,73,73	0
54	MG	AA	1764	1/1	0.93	0.17	99,99,99,99	0
54	MG	BA	3127	1/1	0.93	0.15	61,61,61,61	0
54	MG	BA	3029	1/1	0.93	0.17	41,41,41,41	0
54	MG	DA	3044	1/1	0.93	0.14	45,45,45,45	0
54	MG	AA	1623	1/1	0.93	0.16	99,99,99,99	0
54	MG	AA	1654	1/1	0.93	0.18	99,99,99,99	0
54	MG	DA	3231	1/1	0.93	0.20	81,81,81,81	0
54	MG	BA	3081	1/1	0.93	0.16	67,67,67,67	0
54	MG	DA	3234	1/1	0.93	0.10	64,64,64,64	0
54	MG	DA	3663	1/1	0.93	0.26	75,75,75,75	0
54	MG	DA	3048	1/1	0.93	0.16	51,51,51,51	0
54	MG	CA	1865	1/1	0.93	0.06	93,93,93,93	0
54	MG	AA	1800	1/1	0.93	0.36	69,69,69,69	0
54	MG	DA	3240	1/1	0.93	0.04	69,69,69,69	0
54	MG	AA	1840	1/1	0.93	0.04	91,91,91,91	0
54	MG	DA	3242	1/1	0.93	0.12	59,59,59,59	0
54	MG	DA	3243	1/1	0.93	0.09	59,59,59,59	0
54	MG	BA	2941	1/1	0.93	0.18	31,31,31,31	0
54	MG	BA	3200	1/1	0.93	0.20	93,93,93,93	0
54	MG	BA	3525	1/1	0.93	0.11	67,67,67,67	0
54	MG	CA	1649	1/1	0.93	0.14	96,96,96,96	0
54	MG	DA	3249	1/1	0.93	0.18	111,111,111,111	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	AA	1619	1/1	0.93	0.07	57,57,57,57	0
54	MG	DA	3679	1/1	0.93	0.08	50,50,50,50	0
54	MG	BA	2991	1/1	0.93	0.13	42,42,42,42	0
54	MG	DA	3067	1/1	0.93	0.34	91,91,91,91	0
54	MG	CD	302	1/1	0.93	0.06	74,74,74,74	0
54	MG	DA	3069	1/1	0.93	0.22	61,61,61,61	0
54	MG	DA	3071	1/1	0.93	0.11	49,49,49,49	0
54	MG	BA	3528	1/1	0.93	0.10	73,73,73,73	0
54	MG	BA	2947	1/1	0.93	0.13	37,37,37,37	0
54	MG	DA	3263	1/1	0.93	0.06	55,55,55,55	0
54	MG	CA	1657	1/1	0.93	0.05	60,60,60,60	0
54	MG	DA	3466	1/1	0.93	0.05	117,117,117,117	0
54	MG	CA	1767	1/1	0.93	0.07	72,72,72,72	0
54	MG	DA	3079	1/1	0.93	0.21	51,51,51,51	0
54	MG	CE	203	1/1	0.93	0.06	79,79,79,79	0
54	MG	AA	1616	1/1	0.93	0.24	54,54,54,54	0
54	MG	AA	1618	1/1	0.93	0.10	71,71,71,71	0
54	MG	DJ	205	1/1	0.93	0.15	91,91,91,91	0
54	MG	AA	1651	1/1	0.93	0.05	56,56,56,56	0
54	MG	DA	3706	1/1	0.93	0.12	75,75,75,75	0
54	MG	BA	3147	1/1	0.93	0.24	123,123,123,123	0
54	MG	DA	3709	1/1	0.93	0.29	75,75,75,75	0
54	MG	BA	3358	1/1	0.93	0.18	81,81,81,81	0
54	MG	BA	3427	1/1	0.93	0.04	74,74,74,74	0
54	MG	AV	6208	1/1	0.93	0.05	79,79,79,79	0
54	MG	AA	1704	1/1	0.93	0.11	77,77,77,77	0
54	MG	BA	3625	1/1	0.93	0.10	53,53,53,53	0
54	MG	CA	1779	1/1	0.93	0.09	79,79,79,79	0
54	MG	BA	3212	1/1	0.93	0.06	67,67,67,67	0
54	MG	DU	201	1/1	0.93	0.04	84,84,84,84	0
54	MG	BA	3003	1/1	0.93	0.16	55,55,55,55	0
54	MG	BA	3451	1/1	0.93	0.35	47,47,47,47	0
54	MG	BA	3455	1/1	0.93	0.16	32,32,32,32	0
54	MG	AA	1758	1/1	0.93	0.04	69,69,69,69	0
54	MG	DA	3291	1/1	0.93	0.08	57,57,57,57	0
54	MG	BA	2959	1/1	0.93	0.16	40,40,40,40	0
54	MG	DX	102	1/1	0.93	0.10	91,91,91,91	0
54	MG	DA	3496	1/1	0.93	0.18	95,95,95,95	0
54	MG	DA	3497	1/1	0.93	0.15	62,62,62,62	0
54	MG	BA	3551	1/1	0.93	0.06	95,95,95,95	0
54	MG	D2	103	1/1	0.93	0.16	56,56,56,56	0
54	MG	DA	3111	1/1	0.93	0.13	84,84,84,84	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	CA	1678	1/1	0.93	0.05	81,81,81,81	0
54	MG	DA	3733	1/1	0.93	0.18	84,84,84,84	0
54	MG	BA	3050	1/1	0.93	0.24	57,57,57,57	0
54	MG	BA	3553	1/1	0.93	0.04	72,72,72,72	0
54	MG	BA	2954	1/1	0.94	0.16	73,73,73,73	0
54	MG	B3	101	1/1	0.94	0.08	96,96,96,96	0
54	MG	DA	3313	1/1	0.94	0.10	78,78,78,78	0
54	MG	DA	3140	1/1	0.94	0.17	50,50,50,50	0
54	MG	BA	3562	1/1	0.94	0.08	40,40,40,40	0
54	MG	DA	3742	1/1	0.94	0.15	47,47,47,47	0
54	MG	BA	3312	1/1	0.94	0.29	71,71,71,71	0
54	MG	BA	3476	1/1	0.94	0.14	53,53,53,53	0
54	MG	AA	1681	1/1	0.94	0.07	65,65,65,65	0
54	MG	AA	1606	1/1	0.94	0.21	62,62,62,62	0
54	MG	DA	3147	1/1	0.94	0.16	86,86,86,86	0
54	MG	DA	3519	1/1	0.94	0.08	74,74,74,74	0
54	MG	AA	1731	1/1	0.94	0.06	83,83,83,83	0
54	MG	DA	3324	1/1	0.94	0.09	95,95,95,95	0
54	MG	DA	3325	1/1	0.94	0.16	66,66,66,66	0
54	MG	DA	3149	1/1	0.94	0.12	60,60,60,60	0
54	MG	AA	1641	1/1	0.94	0.10	66,66,66,66	0
54	MG	BA	3249	1/1	0.94	0.08	36,36,36,36	0
54	MG	DA	3527	1/1	0.94	0.14	104,104,104,104	0
54	MG	DA	2961	1/1	0.94	0.32	58,58,58,58	0
54	MG	AA	1677	1/1	0.94	0.16	50,50,50,50	0
54	MG	DA	3530	1/1	0.94	0.06	71,71,71,71	0
54	MG	AA	1761	1/1	0.94	0.06	68,68,68,68	0
54	MG	BA	3664	1/1	0.94	0.05	69,69,69,69	0
54	MG	DA	2975	1/1	0.94	0.07	50,50,50,50	0
54	MG	DA	3765	1/1	0.94	0.08	64,64,64,64	0
54	MG	CA	1827	1/1	0.94	0.06	82,82,82,82	0
54	MG	BA	3486	1/1	0.94	0.13	60,60,60,60	0
54	MG	BA	3321	1/1	0.94	0.21	179,179,179,179	0
54	MG	BA	3006	1/1	0.94	0.26	61,61,61,61	0
54	MG	BA	3007	1/1	0.94	0.07	98,98,98,98	0
54	MG	DA	3165	1/1	0.94	0.06	59,59,59,59	0
54	MG	BA	3492	1/1	0.94	0.08	70,70,70,70	0
54	MG	DA	3344	1/1	0.94	0.09	75,75,75,75	0
54	MG	BA	3008	1/1	0.94	0.16	70,70,70,70	0
54	MG	DA	2996	1/1	0.94	0.20	32,32,32,32	0
54	MG	AA	1707	1/1	0.94	0.12	86,86,86,86	0
54	MG	CA	1725	1/1	0.94	0.06	82,82,82,82	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	BA	3327	1/1	0.94	0.15	86,86,86,86	0
54	MG	DA	3352	1/1	0.94	0.07	121,121,121,121	0
54	MG	BA	3328	1/1	0.94	0.19	80,80,80,80	0
54	MG	BA	3329	1/1	0.94	0.13	113,113,113,113	0
54	MG	AA	1828	1/1	0.94	0.06	82,82,82,82	0
54	MG	DA	3560	1/1	0.94	0.24	83,83,83,83	0
54	MG	CA	1733	1/1	0.94	0.09	78,78,78,78	0
54	MG	BA	3152	1/1	0.94	0.04	76,76,76,76	0
54	MG	DA	3009	1/1	0.94	0.12	54,54,54,54	0
54	MG	CA	1631	1/1	0.94	0.12	82,82,82,82	0
54	MG	DA	3362	1/1	0.94	0.16	78,78,78,78	0
54	MG	DA	3363	1/1	0.94	0.06	74,74,74,74	0
54	MG	DA	3012	1/1	0.94	0.09	48,48,48,48	0
54	MG	CA	1736	1/1	0.94	0.17	73,73,73,73	0
54	MG	DA	3014	1/1	0.94	0.14	52,52,52,52	0
54	MG	DA	3016	1/1	0.94	0.17	47,47,47,47	0
54	MG	DA	3190	1/1	0.94	0.07	69,69,69,69	0
54	MG	DA	3804	1/1	0.94	0.14	72,72,72,72	0
54	MG	DA	3018	1/1	0.94	0.35	60,60,60,60	0
54	MG	BA	3011	1/1	0.94	0.07	51,51,51,51	0
54	MG	DA	3372	1/1	0.94	0.17	90,90,90,90	0
54	MG	DA	3579	1/1	0.94	0.27	80,80,80,80	0
54	MG	AA	1849	1/1	0.94	0.08	79,79,79,79	0
54	MG	DA	3581	1/1	0.94	0.05	68,68,68,68	0
54	MG	CA	1739	1/1	0.94	0.10	102,102,102,102	0
54	MG	AA	1650	1/1	0.94	0.08	92,92,92,92	0
54	MG	DA	3818	1/1	0.94	0.04	78,78,78,78	0
54	MG	BA	3336	1/1	0.94	0.21	87,87,87,87	0
54	MG	AA	1679	1/1	0.94	0.15	78,78,78,78	0
54	MG	CA	1961	1/1	0.94	0.08	63,63,63,63	0
54	MG	BA	3209	1/1	0.94	0.11	81,81,81,81	0
54	MG	BA	2930	1/1	0.94	0.18	47,47,47,47	0
54	MG	CA	1855	1/1	0.94	0.09	107,107,107,107	0
54	MG	BA	3405	1/1	0.94	0.03	68,68,68,68	0
54	MG	AA	1831	1/1	0.94	0.23	67,67,67,67	0
54	MG	DA	3388	1/1	0.94	0.07	51,51,51,51	0
54	MG	BA	3162	1/1	0.94	0.04	86,86,86,86	0
54	MG	CA	1970	1/1	0.94	0.08	98,98,98,98	0
54	MG	AA	1725	1/1	0.94	0.09	93,93,93,93	0
54	MG	DA	3600	1/1	0.94	0.09	86,86,86,86	0
54	MG	CA	1972	1/1	0.94	0.04	67,67,67,67	0
54	MG	BA	2975	1/1	0.94	0.15	58,58,58,58	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	DA	3213	1/1	0.94	0.06	59,59,59,59	0
54	MG	CA	1862	1/1	0.94	0.16	96,96,96,96	0
54	MG	DA	3042	1/1	0.94	0.10	81,81,81,81	0
54	MG	DA	3217	1/1	0.94	0.14	59,59,59,59	0
54	MG	BA	2934	1/1	0.94	0.22	33,33,33,33	0
54	MG	DA	3403	1/1	0.94	0.06	56,56,56,56	0
54	MG	BA	3411	1/1	0.94	0.24	90,90,90,90	0
54	MG	AA	1689	1/1	0.94	0.06	75,75,75,75	0
54	MG	CA	1866	1/1	0.94	0.14	102,102,102,102	0
54	MG	AA	1855	1/1	0.94	0.11	81,81,81,81	0
54	MG	BA	3276	1/1	0.94	0.06	67,67,67,67	0
54	MG	DA	3619	1/1	0.94	0.08	83,83,83,83	0
54	MG	CA	1869	1/1	0.94	0.04	96,96,96,96	0
54	MG	BA	3277	1/1	0.94	0.09	110,110,110,110	0
54	MG	DA	3623	1/1	0.94	0.10	104,104,104,104	0
54	MG	CA	1653	1/1	0.94	0.12	133,133,133,133	0
54	MG	DA	3628	1/1	0.94	0.14	56,56,56,56	0
54	MG	BA	3607	1/1	0.94	0.28	62,62,62,62	0
54	MG	DA	3058	1/1	0.94	0.08	56,56,56,56	0
54	MG	DA	3859	1/1	0.94	0.07	55,55,55,55	0
54	MG	BA	3218	1/1	0.94	0.06	55,55,55,55	0
54	MG	BA	3610	1/1	0.94	0.24	80,80,80,80	0
54	MG	DA	3418	1/1	0.94	0.13	65,65,65,65	0
54	MG	DA	3235	1/1	0.94	0.14	59,59,59,59	0
54	MG	CA	1876	1/1	0.94	0.13	69,69,69,69	0
54	MG	DB	207	1/1	0.94	0.15	58,58,58,58	0
54	MG	AA	1783	1/1	0.94	0.09	123,123,123,123	0
54	MG	AA	1799	1/1	0.94	0.15	58,58,58,58	0
54	MG	BA	3221	1/1	0.94	0.13	141,141,141,141	0
54	MG	BA	2982	1/1	0.94	0.06	38,38,38,38	0
54	MG	DB	214	1/1	0.94	0.10	72,72,72,72	0
54	MG	BA	3030	1/1	0.94	0.15	61,61,61,61	0
54	MG	DA	3070	1/1	0.94	0.09	85,85,85,85	0
54	MG	DB	217	1/1	0.94	0.09	93,93,93,93	0
54	MG	BA	3226	1/1	0.94	0.10	59,59,59,59	0
54	MG	CA	1664	1/1	0.94	0.07	85,85,85,85	0
54	MG	DA	3246	1/1	0.94	0.04	57,57,57,57	0
54	MG	DA	3654	1/1	0.94	0.24	59,59,59,59	0
54	MG	BA	3529	1/1	0.94	0.36	79,79,79,79	0
54	MG	BA	3119	1/1	0.94	0.09	73,73,73,73	0
54	MG	BA	3435	1/1	0.94	0.21	29,29,29,29	0
54	MG	DB	225	1/1	0.94	0.04	72,72,72,72	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	CA	1775	1/1	0.94	0.16	64,64,64,64	0
54	MG	DA	3439	1/1	0.94	0.06	52,52,52,52	0
54	MG	DA	3662	1/1	0.94	0.32	71,71,71,71	0
54	MG	DA	3080	1/1	0.94	0.22	83,83,83,83	0
54	MG	AV	6207	1/1	0.94	0.07	78,78,78,78	0
54	MG	DA	3254	1/1	0.94	0.32	71,71,71,71	0
54	MG	BA	3622	1/1	0.94	0.13	90,90,90,90	0
54	MG	BA	3438	1/1	0.94	0.17	29,29,29,29	0
54	MG	BA	3442	1/1	0.94	0.24	26,26,26,26	0
54	MG	DA	3448	1/1	0.94	0.13	99,99,99,99	0
54	MG	BA	3443	1/1	0.94	0.23	36,36,36,36	0
54	MG	DA	3451	1/1	0.94	0.21	80,80,80,80	0
54	MG	BA	3290	1/1	0.94	0.08	79,79,79,79	0
54	MG	CA	1782	1/1	0.94	0.04	80,80,80,80	0
54	MG	BA	2946	1/1	0.94	0.07	37,37,37,37	0
54	MG	CA	1677	1/1	0.94	0.28	93,93,93,93	0
54	MG	DA	3457	1/1	0.94	0.15	86,86,86,86	0
54	MG	DC	301	1/1	0.94	0.30	67,67,67,67	0
54	MG	BA	3448	1/1	0.94	0.30	51,51,51,51	0
54	MG	DA	3460	1/1	0.94	0.19	86,86,86,86	0
54	MG	AA	1644	1/1	0.94	0.08	62,62,62,62	0
54	MG	DD	302	1/1	0.94	0.11	61,61,61,61	0
54	MG	DA	3462	1/1	0.94	0.29	83,83,83,83	0
54	MG	DA	3686	1/1	0.94	0.06	52,52,52,52	0
54	MG	DA	3268	1/1	0.94	0.37	51,51,51,51	0
54	MG	DA	3099	1/1	0.94	0.12	49,49,49,49	0
54	MG	BA	3079	1/1	0.94	0.07	73,73,73,73	0
54	MG	BA	3235	1/1	0.94	0.11	54,54,54,54	0
54	MG	DA	3273	1/1	0.94	0.10	94,94,94,94	0
54	MG	CA	1683	1/1	0.94	0.04	72,72,72,72	0
54	MG	DA	3104	1/1	0.94	0.12	49,49,49,49	0
54	MG	BA	3236	1/1	0.94	0.10	56,56,56,56	0
54	MG	BA	2903	1/1	0.94	0.35	22,22,22,22	0
54	MG	DA	3107	1/1	0.94	0.06	50,50,50,50	0
54	MG	DJ	201	1/1	0.94	0.07	61,61,61,61	0
54	MG	BA	3460	1/1	0.94	0.15	47,47,47,47	0
54	MG	DJ	203	1/1	0.94	0.10	84,84,84,84	0
54	MG	DA	3701	1/1	0.94	0.08	56,56,56,56	0
54	MG	CV	6205	1/1	0.94	0.14	159,159,159,159	0
54	MG	DA	3703	1/1	0.94	0.05	60,60,60,60	0
54	MG	DA	3478	1/1	0.94	0.12	48,48,48,48	0
54	MG	DA	2901	1/1	0.94	0.25	9,9,9,9	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	DA	3707	1/1	0.94	0.10	54,54,54,54	0
54	MG	BA	2950	1/1	0.94	0.13	68,68,68,68	0
54	MG	AA	1691	1/1	0.94	0.07	69,69,69,69	0
54	MG	DA	3710	1/1	0.94	0.07	92,92,92,92	0
54	MG	DP	201	1/1	0.94	0.13	72,72,72,72	0
54	MG	BA	3639	1/1	0.94	0.09	88,88,88,88	0
54	MG	BA	3463	1/1	0.94	0.17	54,54,54,54	0
54	MG	DA	3487	1/1	0.94	0.10	66,66,66,66	0
54	MG	DA	3116	1/1	0.94	0.07	52,52,52,52	0
54	MG	BA	3131	1/1	0.94	0.11	47,47,47,47	0
54	MG	DA	3293	1/1	0.94	0.11	66,66,66,66	0
54	MG	DA	3120	1/1	0.94	0.12	61,61,61,61	0
54	MG	BA	3305	1/1	0.94	0.07	87,87,87,87	0
54	MG	DA	3493	1/1	0.94	0.08	59,59,59,59	0
54	MG	BW	101	1/1	0.94	0.09	57,57,57,57	0
54	MG	CA	1914	1/1	0.94	0.04	97,97,97,97	0
54	MG	CA	1915	1/1	0.94	0.08	58,58,58,58	0
54	MG	DX	103	1/1	0.94	0.17	60,60,60,60	0
54	MG	BA	2993	1/1	0.94	0.10	49,49,49,49	0
54	MG	BA	3645	1/1	0.94	0.08	69,69,69,69	0
54	MG	BA	3469	1/1	0.94	0.20	58,58,58,58	0
54	MG	DA	3130	1/1	0.94	0.10	68,68,68,68	0
54	MG	BA	3039	1/1	0.94	0.10	54,54,54,54	0
54	MG	D4	101	1/1	0.94	0.10	55,55,55,55	0
54	MG	BA	3375	1/1	0.94	0.20	62,62,62,62	0
54	MG	D4	104	1/1	0.94	0.18	76,76,76,76	0
54	MG	DA	2932	1/1	0.94	0.19	24,24,24,24	0
54	MG	BA	3472	1/1	0.94	0.20	65,65,65,65	0
54	MG	DA	3310	1/1	0.94	0.10	54,54,54,54	0
54	MG	DA	3117	1/1	0.95	0.08	31,31,31,31	0
54	MG	DA	2956	1/1	0.95	0.19	44,44,44,44	0
54	MG	DA	3119	1/1	0.95	0.15	74,74,74,74	0
54	MG	DA	2957	1/1	0.95	0.28	40,40,40,40	0
54	MG	BA	3573	1/1	0.95	0.06	58,58,58,58	0
54	MG	BA	3271	1/1	0.95	0.07	83,83,83,83	0
54	MG	DA	3783	1/1	0.95	0.05	63,63,63,63	0
54	MG	DA	3272	1/1	0.95	0.26	87,87,87,87	0
54	MG	DA	3429	1/1	0.95	0.06	79,79,79,79	0
54	MG	DA	2963	1/1	0.95	0.08	32,32,32,32	0
54	MG	DA	3601	1/1	0.95	0.05	59,59,59,59	0
54	MG	DA	3788	1/1	0.95	0.13	92,92,92,92	0
54	MG	DA	3790	1/1	0.95	0.14	63,63,63,63	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	DA	3791	1/1	0.95	0.08	108,108,108,108	0
54	MG	DA	3431	1/1	0.95	0.13	94,94,94,94	0
54	MG	DA	2965	1/1	0.95	0.21	34,34,34,34	0
54	MG	BA	3059	1/1	0.95	0.15	48,48,48,48	0
54	MG	BA	3441	1/1	0.95	0.15	35,35,35,35	0
54	MG	DA	3608	1/1	0.95	0.25	128,128,128,128	0
54	MG	BM	203	1/1	0.95	0.11	90,90,90,90	0
54	MG	BA	3511	1/1	0.95	0.41	78,78,78,78	0
54	MG	BO	201	1/1	0.95	0.06	70,70,70,70	0
54	MG	DA	2977	1/1	0.95	0.25	49,49,49,49	0
54	MG	DA	3440	1/1	0.95	0.10	125,125,125,125	0
54	MG	AA	1836	1/1	0.95	0.04	91,91,91,91	0
54	MG	DA	3805	1/1	0.95	0.04	70,70,70,70	0
54	MG	DA	2986	1/1	0.95	0.29	41,41,41,41	0
54	MG	BA	3097	1/1	0.95	0.10	57,57,57,57	0
54	MG	BA	2933	1/1	0.95	0.13	36,36,36,36	0
54	MG	DA	3139	1/1	0.95	0.09	40,40,40,40	0
54	MG	DA	3810	1/1	0.95	0.06	102,102,102,102	0
54	MG	BA	3651	1/1	0.95	0.07	77,77,77,77	0
54	MG	BA	3099	1/1	0.95	0.05	56,56,56,56	0
54	MG	DA	3622	1/1	0.95	0.10	45,45,45,45	0
54	MG	DA	3449	1/1	0.95	0.04	79,79,79,79	0
54	MG	BA	3063	1/1	0.95	0.42	85,85,85,85	0
54	MG	BA	3141	1/1	0.95	0.28	91,91,91,91	0
54	MG	BA	3519	1/1	0.95	0.05	50,50,50,50	0
54	MG	BA	2995	1/1	0.95	0.33	57,57,57,57	0
54	MG	AA	1613	1/1	0.95	0.24	55,55,55,55	0
54	MG	BA	3588	1/1	0.95	0.21	52,52,52,52	0
54	MG	DA	3004	1/1	0.95	0.09	38,38,38,38	0
54	MG	BA	3238	1/1	0.95	0.07	49,49,49,49	0
54	MG	DA	3303	1/1	0.95	0.07	67,67,67,67	0
54	MG	DA	3640	1/1	0.95	0.10	24,24,24,24	0
54	MG	DA	3642	1/1	0.95	0.29	52,52,52,52	0
54	MG	CA	1681	1/1	0.95	0.08	66,66,66,66	0
54	MG	BA	3337	1/1	0.95	0.09	77,77,77,77	0
54	MG	DA	3646	1/1	0.95	0.17	45,45,45,45	0
54	MG	BA	2967	1/1	0.95	0.18	51,51,51,51	0
54	MG	BA	3663	1/1	0.95	0.12	89,89,89,89	0
54	MG	BY	103	1/1	0.95	0.12	95,95,95,95	0
54	MG	DA	3011	1/1	0.95	0.11	36,36,36,36	0
54	MG	BA	2998	1/1	0.95	0.07	75,75,75,75	0
54	MG	BA	3665	1/1	0.95	0.13	123,123,123,123	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	BA	3285	1/1	0.95	0.13	91,91,91,91	0
54	MG	DA	3015	1/1	0.95	0.16	33,33,33,33	0
54	MG	BA	3148	1/1	0.95	0.10	62,62,62,62	0
54	MG	DA	3843	1/1	0.95	0.25	55,55,55,55	0
54	MG	DA	3656	1/1	0.95	0.13	36,36,36,36	0
54	MG	DA	3473	1/1	0.95	0.11	61,61,61,61	0
54	MG	AA	1686	1/1	0.95	0.04	65,65,65,65	0
54	MG	DA	3848	1/1	0.95	0.26	105,105,105,105	0
54	MG	CC	305	1/1	0.95	0.07	93,93,93,93	0
54	MG	DA	3476	1/1	0.95	0.09	87,87,87,87	0
54	MG	CA	1785	1/1	0.95	0.05	76,76,76,76	0
54	MG	BA	3289	1/1	0.95	0.11	61,61,61,61	0
54	MG	AA	1601	1/1	0.95	0.20	35,35,35,35	0
54	MG	BA	3035	1/1	0.95	0.14	57,57,57,57	0
54	MG	CA	1603	1/1	0.95	0.22	48,48,48,48	0
54	MG	CA	1604	1/1	0.95	0.21	43,43,43,43	0
54	MG	CA	1606	1/1	0.95	0.13	57,57,57,57	0
54	MG	DA	3326	1/1	0.95	0.17	81,81,81,81	0
54	MG	AA	1671	1/1	0.95	0.04	74,74,74,74	0
54	MG	CA	1701	1/1	0.95	0.16	83,83,83,83	0
54	MG	BA	3534	1/1	0.95	0.18	82,82,82,82	0
54	MG	DA	3863	1/1	0.95	0.28	104,104,104,104	0
54	MG	CA	1609	1/1	0.95	0.13	66,66,66,66	0
54	MG	DB	202	1/1	0.95	0.06	33,33,33,33	0
54	MG	DB	203	1/1	0.95	0.05	69,69,69,69	0
54	MG	DB	204	1/1	0.95	0.12	56,56,56,56	0
54	MG	DA	3182	1/1	0.95	0.07	63,63,63,63	0
54	MG	BA	3293	1/1	0.95	0.03	60,60,60,60	0
54	MG	BA	2910	1/1	0.95	0.16	17,17,17,17	0
54	MG	AA	1603	1/1	0.95	0.23	37,37,37,37	0
54	MG	DB	211	1/1	0.95	0.03	65,65,65,65	0
54	MG	BA	3474	1/1	0.95	0.19	72,72,72,72	0
54	MG	BA	3539	1/1	0.95	0.12	97,97,97,97	0
54	MG	DA	3683	1/1	0.95	0.06	58,58,58,58	0
54	MG	DA	3499	1/1	0.95	0.08	87,87,87,87	0
54	MG	BA	2973	1/1	0.95	0.13	60,60,60,60	0
54	MG	DA	3687	1/1	0.95	0.12	57,57,57,57	0
54	MG	BA	3541	1/1	0.95	0.23	89,89,89,89	0
54	MG	BA	2974	1/1	0.95	0.21	81,81,81,81	0
54	MG	CA	1805	1/1	0.95	0.11	94,94,94,94	0
54	MG	BA	3477	1/1	0.95	0.06	50,50,50,50	0
54	MG	BA	2945	1/1	0.95	0.11	56,56,56,56	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	DA	3345	1/1	0.95	0.12	88,88,88,88	0
54	MG	BA	3302	1/1	0.95	0.09	84,84,84,84	0
54	MG	CA	1623	1/1	0.95	0.07	93,93,93,93	0
54	MG	DA	3049	1/1	0.95	0.16	43,43,43,43	0
54	MG	DA	3050	1/1	0.95	0.26	89,89,89,89	0
54	MG	DA	3203	1/1	0.95	0.12	67,67,67,67	0
54	MG	CA	1716	1/1	0.95	0.13	89,89,89,89	0
54	MG	CA	1910	1/1	0.95	0.14	109,109,109,109	0
54	MG	BA	3355	1/1	0.95	0.13	72,72,72,72	0
54	MG	BA	3161	1/1	0.95	0.14	64,64,64,64	0
54	MG	DA	3057	1/1	0.95	0.13	79,79,79,79	0
54	MG	BA	2912	1/1	0.95	0.19	19,19,19,19	0
54	MG	AA	1724	1/1	0.95	0.10	79,79,79,79	0
54	MG	BB	208	1/1	0.95	0.13	67,67,67,67	0
54	MG	AA	1663	1/1	0.95	0.16	54,54,54,54	0
54	MG	BA	3619	1/1	0.95	0.19	145,145,145,145	0
54	MG	AA	1735	1/1	0.95	0.04	68,68,68,68	0
54	MG	DA	3365	1/1	0.95	0.13	83,83,83,83	0
54	MG	DB	241	1/1	0.95	0.04	90,90,90,90	0
54	MG	AA	1746	1/1	0.95	0.07	86,86,86,86	0
54	MG	CA	1920	1/1	0.95	0.07	87,87,87,87	0
54	MG	BA	3085	1/1	0.95	0.11	53,53,53,53	0
54	MG	DA	3219	1/1	0.95	0.11	60,60,60,60	0
54	MG	CV	6206	1/1	0.95	0.11	107,107,107,107	0
54	MG	BB	215	1/1	0.95	0.06	82,82,82,82	0
54	MG	BA	2923	1/1	0.95	0.24	13,13,13,13	0
54	MG	DA	3724	1/1	0.95	0.11	109,109,109,109	0
54	MG	DA	3533	1/1	0.95	0.14	60,60,60,60	0
54	MG	DA	3373	1/1	0.95	0.07	78,78,78,78	0
54	MG	DA	3374	1/1	0.95	0.06	80,80,80,80	0
54	MG	DA	3375	1/1	0.95	0.11	63,63,63,63	0
54	MG	AA	1747	1/1	0.95	0.12	116,116,116,116	0
54	MG	DA	2908	1/1	0.95	0.33	20,20,20,20	0
54	MG	AA	1715	1/1	0.95	0.07	58,58,58,58	0
54	MG	AA	1832	1/1	0.95	0.07	66,66,66,66	0
54	MG	BA	3090	1/1	0.95	0.16	84,84,84,84	0
54	MG	DA	3229	1/1	0.95	0.06	59,59,59,59	0
54	MG	DA	2916	1/1	0.95	0.17	15,15,15,15	0
54	MG	BA	3175	1/1	0.95	0.15	71,71,71,71	0
54	MG	BA	3319	1/1	0.95	0.09	79,79,79,79	0
54	MG	DA	2921	1/1	0.95	0.16	32,32,32,32	0
54	MG	CA	1834	1/1	0.95	0.06	81,81,81,81	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	DA	3236	1/1	0.95	0.09	75,75,75,75	0
54	MG	BA	3423	1/1	0.95	0.10	72,72,72,72	0
54	MG	DA	3556	1/1	0.95	0.07	110,110,110,110	0
54	MG	DA	3744	1/1	0.95	0.06	64,64,64,64	0
54	MG	BA	3424	1/1	0.95	0.15	115,115,115,115	0
54	MG	BA	3632	1/1	0.95	0.12	61,61,61,61	0
54	MG	BA	3633	1/1	0.95	0.07	88,88,88,88	0
54	MG	DA	3093	1/1	0.95	0.10	47,47,47,47	0
54	MG	DA	3562	1/1	0.95	0.08	60,60,60,60	0
54	MG	CA	1742	1/1	0.95	0.11	91,91,91,91	0
54	MG	AA	1833	1/1	0.95	0.09	75,75,75,75	0
54	MG	DA	3096	1/1	0.95	0.21	59,59,59,59	0
54	MG	DA	3566	1/1	0.95	0.34	91,91,91,91	0
54	MG	DA	3097	1/1	0.95	0.26	55,55,55,55	0
54	MG	DA	3401	1/1	0.95	0.06	100,100,100,100	0
54	MG	AA	1684	1/1	0.95	0.05	71,71,71,71	0
54	MG	DA	2933	1/1	0.95	0.23	25,25,25,25	0
54	MG	DA	3758	1/1	0.95	0.08	60,60,60,60	0
54	MG	DA	2934	1/1	0.95	0.22	13,13,13,13	0
54	MG	CA	1745	1/1	0.95	0.07	77,77,77,77	0
54	MG	BA	3057	1/1	0.95	0.08	64,64,64,64	0
54	MG	CA	1747	1/1	0.95	0.08	69,69,69,69	0
54	MG	DA	2939	1/1	0.95	0.19	21,21,21,21	0
54	MG	BA	3568	1/1	0.95	0.06	69,69,69,69	0
54	MG	BE	301	1/1	0.95	0.09	75,75,75,75	0
54	MG	BA	3428	1/1	0.95	0.07	90,90,90,90	0
54	MG	DA	2950	1/1	0.95	0.22	33,33,33,33	0
54	MG	DA	2951	1/1	0.95	0.25	56,56,56,56	0
54	MG	DA	3415	1/1	0.95	0.07	66,66,66,66	0
54	MG	D4	103	1/1	0.95	0.11	73,73,73,73	0
54	MG	CA	1944	1/1	0.95	0.14	66,66,66,66	0
54	MG	BA	3429	1/1	0.95	0.09	79,79,79,79	0
54	MG	AA	1775	1/1	0.95	0.07	105,105,105,105	0
54	MG	BA	3436	1/1	0.95	0.25	38,38,38,38	0
54	MG	DA	3639	1/1	0.96	0.09	26,26,26,26	0
54	MG	DA	3092	1/1	0.96	0.24	56,56,56,56	0
54	MG	DA	3641	1/1	0.96	0.11	13,13,13,13	0
54	MG	CA	1726	1/1	0.96	0.05	49,49,49,49	0
54	MG	DA	2967	1/1	0.96	0.07	34,34,34,34	0
54	MG	CA	1648	1/1	0.96	0.09	61,61,61,61	0
54	MG	BA	3432	1/1	0.96	0.17	12,12,12,12	0
54	MG	DA	2972	1/1	0.96	0.13	37,37,37,37	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	DA	3221	1/1	0.96	0.05	73,73,73,73	0
54	MG	BA	3433	1/1	0.96	0.20	21,21,21,21	0
54	MG	DA	2974	1/1	0.96	0.12	60,60,60,60	0
54	MG	DA	3811	1/1	0.96	0.05	60,60,60,60	0
54	MG	DA	3812	1/1	0.96	0.04	87,87,87,87	0
54	MG	CA	1809	1/1	0.96	0.04	92,92,92,92	0
54	MG	DA	3102	1/1	0.96	0.09	50,50,50,50	0
54	MG	DA	3815	1/1	0.96	0.07	74,74,74,74	0
54	MG	CA	1731	1/1	0.96	0.04	76,76,76,76	0
54	MG	AA	1798	1/1	0.96	0.18	46,46,46,46	0
54	MG	DA	2981	1/1	0.96	0.17	40,40,40,40	0
54	MG	CA	1652	1/1	0.96	0.08	87,87,87,87	0
54	MG	BA	3309	1/1	0.96	0.12	84,84,84,84	0
54	MG	BA	3514	1/1	0.96	0.15	83,83,83,83	0
54	MG	AA	1627	1/1	0.96	0.08	59,59,59,59	0
54	MG	DA	3110	1/1	0.96	0.12	65,65,65,65	0
54	MG	BA	3311	1/1	0.96	0.14	87,87,87,87	0
54	MG	DA	2992	1/1	0.96	0.12	60,60,60,60	0
54	MG	BA	3440	1/1	0.96	0.17	23,23,23,23	0
54	MG	AA	1827	1/1	0.96	0.04	71,71,71,71	0
54	MG	BA	3204	1/1	0.96	0.20	68,68,68,68	0
54	MG	DA	2997	1/1	0.96	0.13	46,46,46,46	0
54	MG	AB	302	1/1	0.96	0.09	57,57,57,57	0
54	MG	CA	1823	1/1	0.96	0.07	61,61,61,61	0
54	MG	BA	3591	1/1	0.96	0.09	99,99,99,99	0
54	MG	DA	3833	1/1	0.96	0.25	73,73,73,73	0
54	MG	DA	3834	1/1	0.96	0.05	60,60,60,60	0
54	MG	AA	1639	1/1	0.96	0.18	54,54,54,54	0
54	MG	DA	3672	1/1	0.96	0.21	80,80,80,80	0
54	MG	BA	3159	1/1	0.96	0.23	59,59,59,59	0
54	MG	BA	3004	1/1	0.96	0.13	49,49,49,49	0
54	MG	BA	3260	1/1	0.96	0.05	64,64,64,64	0
54	MG	DA	3381	1/1	0.96	0.10	49,49,49,49	0
54	MG	DA	3125	1/1	0.96	0.18	36,36,36,36	0
54	MG	BA	2915	1/1	0.96	0.14	20,20,20,20	0
54	MG	DA	3680	1/1	0.96	0.18	41,41,41,41	0
54	MG	AA	1721	1/1	0.96	0.04	56,56,56,56	0
54	MG	CA	1749	1/1	0.96	0.12	77,77,77,77	0
54	MG	DA	3252	1/1	0.96	0.03	52,52,52,52	0
54	MG	BA	2919	1/1	0.96	0.18	14,14,14,14	0
54	MG	BA	3458	1/1	0.96	0.10	77,77,77,77	0
54	MG	BA	3164	1/1	0.96	0.05	75,75,75,75	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	DA	3256	1/1	0.96	0.06	65,65,65,65	0
54	MG	DA	3258	1/1	0.96	0.20	67,67,67,67	0
54	MG	AA	1701	1/1	0.96	0.19	84,84,84,84	0
54	MG	CA	1674	1/1	0.96	0.10	70,70,70,70	0
54	MG	BA	3082	1/1	0.96	0.05	38,38,38,38	0
54	MG	DA	3534	1/1	0.96	0.12	83,83,83,83	0
54	MG	BA	3044	1/1	0.96	0.05	39,39,39,39	0
54	MG	DA	3858	1/1	0.96	0.10	58,58,58,58	0
54	MG	DA	3696	1/1	0.96	0.06	82,82,82,82	0
54	MG	DA	3136	1/1	0.96	0.10	57,57,57,57	0
54	MG	DA	3137	1/1	0.96	0.06	29,29,29,29	0
54	MG	CA	1840	1/1	0.96	0.09	76,76,76,76	0
54	MG	BA	2949	1/1	0.96	0.15	65,65,65,65	0
54	MG	BA	2922	1/1	0.96	0.30	38,38,38,38	0
54	MG	BA	3124	1/1	0.96	0.05	87,87,87,87	0
54	MG	AA	1711	1/1	0.96	0.06	58,58,58,58	0
54	MG	DA	3704	1/1	0.96	0.24	68,68,68,68	0
54	MG	BA	2952	1/1	0.96	0.11	59,59,59,59	0
54	MG	DB	206	1/1	0.96	0.15	63,63,63,63	0
54	MG	BA	3609	1/1	0.96	0.12	65,65,65,65	0
54	MG	DA	3546	1/1	0.96	0.06	56,56,56,56	0
54	MG	DA	3027	1/1	0.96	0.12	53,53,53,53	0
54	MG	DB	210	1/1	0.96	0.07	92,92,92,92	0
54	MG	DA	3548	1/1	0.96	0.20	110,110,110,110	0
54	MG	DA	3146	1/1	0.96	0.14	31,31,31,31	0
54	MG	CA	1847	1/1	0.96	0.04	58,58,58,58	0
54	MG	DA	3551	1/1	0.96	0.06	80,80,80,80	0
54	MG	BA	3273	1/1	0.96	0.06	73,73,73,73	0
54	MG	BA	3016	1/1	0.96	0.21	54,54,54,54	0
54	MG	AA	1607	1/1	0.96	0.23	46,46,46,46	0
54	MG	DA	3555	1/1	0.96	0.33	61,61,61,61	0
54	MG	DA	3717	1/1	0.96	0.13	65,65,65,65	0
54	MG	BA	3176	1/1	0.96	0.14	53,53,53,53	0
54	MG	CV	6207	1/1	0.96	0.03	94,94,94,94	0
54	MG	BA	3224	1/1	0.96	0.16	97,97,97,97	0
54	MG	DA	3722	1/1	0.96	0.18	138,138,138,138	0
54	MG	BA	3225	1/1	0.96	0.06	54,54,54,54	0
54	MG	DA	3037	1/1	0.96	0.29	44,44,44,44	0
54	MG	DA	2904	1/1	0.96	0.17	16,16,16,16	0
54	MG	DA	3287	1/1	0.96	0.12	104,104,104,104	0
54	MG	BA	2925	1/1	0.96	0.07	12,12,12,12	0
54	MG	BA	3227	1/1	0.96	0.18	61,61,61,61	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	DA	2909	1/1	0.96	0.21	22,22,22,22	0
54	MG	DA	3162	1/1	0.96	0.10	30,30,30,30	0
54	MG	DA	3568	1/1	0.96	0.07	78,78,78,78	0
54	MG	AA	1669	1/1	0.96	0.13	54,54,54,54	0
54	MG	DA	3428	1/1	0.96	0.09	71,71,71,71	0
54	MG	DA	2911	1/1	0.96	0.21	11,11,11,11	0
54	MG	DA	2913	1/1	0.96	0.20	21,21,21,21	0
54	MG	BA	3181	1/1	0.96	0.05	62,62,62,62	0
54	MG	BA	3054	1/1	0.96	0.09	65,65,65,65	0
54	MG	DA	3738	1/1	0.96	0.11	91,91,91,91	0
54	MG	DA	3575	1/1	0.96	0.29	85,85,85,85	0
54	MG	CA	1616	1/1	0.96	0.14	94,94,94,94	0
54	MG	AA	1634	1/1	0.96	0.04	48,48,48,48	0
54	MG	AA	1612	1/1	0.96	0.26	39,39,39,39	0
54	MG	BA	3286	1/1	0.96	0.08	68,68,68,68	0
54	MG	BA	3234	1/1	0.96	0.07	73,73,73,73	0
54	MG	DA	3438	1/1	0.96	0.04	54,54,54,54	0
54	MG	DA	3175	1/1	0.96	0.15	102,102,102,102	0
54	MG	DA	3176	1/1	0.96	0.08	50,50,50,50	0
54	MG	BA	3136	1/1	0.96	0.18	64,64,64,64	0
54	MG	BA	2986	1/1	0.96	0.37	54,54,54,54	0
54	MG	BA	3488	1/1	0.96	0.22	53,53,53,53	0
54	MG	DA	3055	1/1	0.96	0.18	59,59,59,59	0
54	MG	DE	301	1/1	0.96	0.06	32,32,32,32	0
54	MG	BA	2901	1/1	0.96	0.22	8,8,8,8	0
54	MG	BA	3412	1/1	0.96	0.07	49,49,49,49	0
54	MG	DA	3061	1/1	0.96	0.14	55,55,55,55	0
54	MG	DA	3184	1/1	0.96	0.07	38,38,38,38	0
54	MG	DA	3594	1/1	0.96	0.03	58,58,58,58	0
54	MG	BA	3491	1/1	0.96	0.13	79,79,79,79	0
54	MG	CA	1871	1/1	0.96	0.05	76,76,76,76	0
54	MG	BA	2988	1/1	0.96	0.14	40,40,40,40	0
54	MG	BA	3061	1/1	0.96	0.12	54,54,54,54	0
54	MG	DA	3319	1/1	0.96	0.10	38,38,38,38	0
54	MG	DA	3455	1/1	0.96	0.39	97,97,97,97	0
54	MG	BA	2989	1/1	0.96	0.17	50,50,50,50	0
54	MG	CA	1957	1/1	0.96	0.10	73,73,73,73	0
54	MG	DA	3192	1/1	0.96	0.08	49,49,49,49	0
54	MG	DA	3459	1/1	0.96	0.14	61,61,61,61	0
54	MG	BA	2990	1/1	0.96	0.07	35,35,35,35	0
54	MG	BA	3356	1/1	0.96	0.08	33,33,33,33	0
54	MG	DA	2940	1/1	0.96	0.22	31,31,31,31	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	BA	3295	1/1	0.96	0.12	60,60,60,60	0
54	MG	DA	2944	1/1	0.96	0.28	25,25,25,25	0
54	MG	BA	3296	1/1	0.96	0.04	71,71,71,71	0
54	MG	DA	2947	1/1	0.96	0.20	37,37,37,37	0
54	MG	BA	2960	1/1	0.96	0.21	39,39,39,39	0
54	MG	AA	1615	1/1	0.96	0.18	67,67,67,67	0
54	MG	DA	3778	1/1	0.96	0.08	80,80,80,80	0
54	MG	DA	3469	1/1	0.96	0.10	83,83,83,83	0
54	MG	AE	204	1/1	0.96	0.06	74,74,74,74	0
54	MG	DA	3335	1/1	0.96	0.06	46,46,46,46	0
54	MG	CA	1966	1/1	0.96	0.07	97,97,97,97	0
54	MG	AQ	201	1/1	0.96	0.05	90,90,90,90	0
54	MG	BE	302	1/1	0.96	0.15	93,93,93,93	0
54	MG	DA	3625	1/1	0.96	0.15	84,84,84,84	0
54	MG	BA	3149	1/1	0.96	0.23	65,65,65,65	0
54	MG	DA	3627	1/1	0.96	0.12	63,63,63,63	0
54	MG	BA	2964	1/1	0.96	0.21	43,43,43,43	0
54	MG	DA	3789	1/1	0.96	0.05	56,56,56,56	0
54	MG	DA	3629	1/1	0.96	0.14	89,89,89,89	0
54	MG	BA	3069	1/1	0.96	0.10	52,52,52,52	0
54	MG	DA	3792	1/1	0.96	0.14	40,40,40,40	0
54	MG	AA	1622	1/1	0.96	0.24	62,62,62,62	0
54	MG	BA	3251	1/1	0.96	0.18	95,95,95,95	0
54	MG	DA	3795	1/1	0.96	0.22	80,80,80,80	0
54	MG	BA	3430	1/1	0.96	0.14	6,6,6,6	0
54	MG	DA	3214	1/1	0.96	0.12	34,34,34,34	0
54	MG	D5	102	1/1	0.96	0.07	59,59,59,59	0
54	MG	DA	3483	1/1	0.96	0.14	63,63,63,63	0
54	MG	DA	3484	1/1	0.96	0.11	21,21,21,21	0
54	MG	BA	3482	1/1	0.97	0.05	40,40,40,40	0
54	MG	AA	1698	1/1	0.97	0.07	88,88,88,88	0
54	MG	DA	3624	1/1	0.97	0.11	92,92,92,92	0
54	MG	BA	3447	1/1	0.97	0.25	39,39,39,39	0
54	MG	DA	3414	1/1	0.97	0.22	55,55,55,55	0
54	MG	CA	1727	1/1	0.97	0.11	76,76,76,76	0
54	MG	BA	3417	1/1	0.97	0.12	65,65,65,65	0
54	MG	DA	2960	1/1	0.97	0.13	33,33,33,33	0
54	MG	BS	201	1/1	0.97	0.04	52,52,52,52	0
54	MG	DA	3631	1/1	0.97	0.04	73,73,73,73	0
54	MG	DA	2962	1/1	0.97	0.10	37,37,37,37	0
54	MG	BA	3449	1/1	0.97	0.19	31,31,31,31	0
54	MG	DA	2964	1/1	0.97	0.14	45,45,45,45	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	BA	3644	1/1	0.97	0.12	86,86,86,86	0
54	MG	DA	3525	1/1	0.97	0.11	73,73,73,73	0
54	MG	DB	201	1/1	0.97	0.11	44,44,44,44	0
54	MG	BA	3125	1/1	0.97	0.05	78,78,78,78	0
54	MG	BA	3340	1/1	0.97	0.05	85,85,85,85	0
54	MG	BA	3452	1/1	0.97	0.08	41,41,41,41	0
54	MG	DA	3232	1/1	0.97	0.05	67,67,67,67	0
54	MG	BA	3454	1/1	0.97	0.14	41,41,41,41	0
54	MG	BA	3053	1/1	0.97	0.20	69,69,69,69	0
54	MG	BA	3168	1/1	0.97	0.17	20,20,20,20	0
54	MG	BA	3530	1/1	0.97	0.10	65,65,65,65	0
54	MG	DA	3059	1/1	0.97	0.19	39,39,39,39	0
54	MG	DA	3060	1/1	0.97	0.28	77,77,77,77	0
54	MG	CA	1687	1/1	0.97	0.13	63,63,63,63	0
54	MG	BA	3457	1/1	0.97	0.21	48,48,48,48	0
54	MG	DA	3763	1/1	0.97	0.10	57,57,57,57	0
54	MG	BA	2935	1/1	0.97	0.16	26,26,26,26	0
54	MG	DA	2982	1/1	0.97	0.10	39,39,39,39	0
54	MG	DA	2983	1/1	0.97	0.22	52,52,52,52	0
54	MG	DA	2984	1/1	0.97	0.12	22,22,22,22	0
54	MG	DA	3542	1/1	0.97	0.11	65,65,65,65	0
54	MG	AA	1765	1/1	0.97	0.02	91,91,91,91	0
54	MG	CA	1691	1/1	0.97	0.07	92,92,92,92	0
54	MG	DA	3658	1/1	0.97	0.07	23,23,23,23	0
54	MG	CA	1965	1/1	0.97	0.05	78,78,78,78	0
54	MG	DA	3773	1/1	0.97	0.10	37,37,37,37	0
54	MG	DA	2905	1/1	0.97	0.13	18,18,18,18	0
54	MG	DA	3444	1/1	0.97	0.17	72,72,72,72	0
54	MG	DA	2906	1/1	0.97	0.17	16,16,16,16	0
54	MG	DA	2990	1/1	0.97	0.23	20,20,20,20	0
54	MG	DA	3073	1/1	0.97	0.14	69,69,69,69	0
54	MG	DA	2991	1/1	0.97	0.13	36,36,36,36	0
54	MG	BA	3194	1/1	0.97	0.25	64,64,64,64	0
54	MG	BA	3575	1/1	0.97	0.13	59,59,59,59	0
54	MG	DA	3078	1/1	0.97	0.04	48,48,48,48	0
54	MG	AA	1610	1/1	0.97	0.09	29,29,29,29	0
54	MG	DA	3354	1/1	0.97	0.09	79,79,79,79	0
54	MG	DA	2995	1/1	0.97	0.09	26,26,26,26	0
54	MG	DA	3558	1/1	0.97	0.12	148,148,148,148	0
54	MG	BA	3658	1/1	0.97	0.06	68,68,68,68	0
54	MG	BA	3130	1/1	0.97	0.07	47,47,47,47	0
54	MG	DA	3358	1/1	0.97	0.14	83,83,83,83	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	DA	2998	1/1	0.97	0.17	36,36,36,36	0
54	MG	DA	3173	1/1	0.97	0.13	73,73,73,73	0
54	MG	DA	3085	1/1	0.97	0.12	68,68,68,68	0
54	MG	BA	3024	1/1	0.97	0.08	52,52,52,52	0
54	MG	BA	2902	1/1	0.97	0.21	12,12,12,12	0
54	MG	BA	3465	1/1	0.97	0.13	31,31,31,31	0
54	MG	BA	2980	1/1	0.97	0.15	51,51,51,51	0
54	MG	DA	3684	1/1	0.97	0.17	69,69,69,69	0
54	MG	BA	3467	1/1	0.97	0.09	30,30,30,30	0
54	MG	BA	2940	1/1	0.97	0.10	30,30,30,30	0
54	MG	CA	1605	1/1	0.97	0.28	54,54,54,54	0
54	MG	DA	3688	1/1	0.97	0.13	50,50,50,50	0
54	MG	BA	3431	1/1	0.97	0.21	26,26,26,26	0
54	MG	BA	3156	1/1	0.97	0.14	70,70,70,70	0
54	MG	CA	1656	1/1	0.97	0.04	78,78,78,78	0
54	MG	BA	3178	1/1	0.97	0.05	74,74,74,74	0
54	MG	DA	2927	1/1	0.97	0.15	18,18,18,18	0
54	MG	BA	3547	1/1	0.97	0.19	87,87,87,87	0
54	MG	CA	1814	1/1	0.97	0.09	47,47,47,47	0
54	MG	BA	3508	1/1	0.97	0.04	90,90,90,90	0
54	MG	DA	2931	1/1	0.97	0.16	21,21,21,21	0
54	MG	DA	3281	1/1	0.97	0.05	62,62,62,62	0
54	MG	AA	1777	1/1	0.97	0.06	49,49,49,49	0
54	MG	DA	3017	1/1	0.97	0.12	38,38,38,38	0
54	MG	DA	3284	1/1	0.97	0.12	79,79,79,79	0
54	MG	DA	3481	1/1	0.97	0.14	77,77,77,77	0
54	MG	CA	1817	1/1	0.97	0.03	89,89,89,89	0
54	MG	BA	3180	1/1	0.97	0.20	88,88,88,88	0
54	MG	DA	3196	1/1	0.97	0.15	84,84,84,84	0
54	MG	DK	203	1/1	0.97	0.03	73,73,73,73	0
54	MG	AA	1802	1/1	0.97	0.10	62,62,62,62	0
54	MG	BA	2918	1/1	0.97	0.31	43,43,43,43	0
54	MG	DA	3290	1/1	0.97	0.04	61,61,61,61	0
54	MG	DN	201	1/1	0.97	0.05	88,88,88,88	0
54	MG	DA	3022	1/1	0.97	0.09	35,35,35,35	0
54	MG	DA	3595	1/1	0.97	0.09	61,61,61,61	0
54	MG	DA	3023	1/1	0.97	0.06	23,23,23,23	0
54	MG	DA	3201	1/1	0.97	0.03	46,46,46,46	0
54	MG	BA	3014	1/1	0.97	0.03	45,45,45,45	0
54	MG	DA	3392	1/1	0.97	0.15	76,76,76,76	0
54	MG	DS	202	1/1	0.97	0.22	62,62,62,62	0
54	MG	AA	1718	1/1	0.97	0.03	63,63,63,63	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	DA	3296	1/1	0.97	0.09	70,70,70,70	0
54	MG	BA	2999	1/1	0.97	0.20	39,39,39,39	0
54	MG	DA	3718	1/1	0.97	0.10	70,70,70,70	0
54	MG	DA	3603	1/1	0.97	0.40	64,64,64,64	0
54	MG	DA	3396	1/1	0.97	0.05	78,78,78,78	0
54	MG	DA	2941	1/1	0.97	0.07	21,21,21,21	0
54	MG	DA	3498	1/1	0.97	0.14	51,51,51,51	0
54	MG	AA	1811	1/1	0.97	0.04	61,61,61,61	0
54	MG	DY	101	1/1	0.97	0.17	12,12,12,12	0
54	MG	DA	3399	1/1	0.97	0.07	75,75,75,75	0
54	MG	DA	2943	1/1	0.97	0.14	5,5,5,5	0
54	MG	CA	1881	1/1	0.97	0.12	74,74,74,74	0
54	MG	D2	102	1/1	0.97	0.03	42,42,42,42	0
54	MG	BA	3444	1/1	0.97	0.14	26,26,26,26	0
54	MG	DA	2946	1/1	0.97	0.19	25,25,25,25	0
54	MG	CA	1826	1/1	0.97	0.08	97,97,97,97	0
54	MG	CA	1620	1/1	0.97	0.10	51,51,51,51	0
54	MG	DA	3035	1/1	0.97	0.14	43,43,43,43	0
54	MG	AA	1605	1/1	0.97	0.15	65,65,65,65	0
54	MG	CA	1773	1/1	0.97	0.03	97,97,97,97	0
54	MG	DA	3847	1/1	0.97	0.13	91,91,91,91	0
54	MG	CA	1671	1/1	0.97	0.11	51,51,51,51	0
55	ZN	AN	101	1/1	0.97	0.06	144,144,144,144	0
54	MG	BN	202	1/1	0.97	0.09	78,78,78,78	0
54	MG	BA	3300	1/1	0.98	0.10	93,93,93,93	0
54	MG	DA	3279	1/1	0.98	0.10	38,38,38,38	0
54	MG	BA	3387	1/1	0.98	0.11	84,84,84,84	0
54	MG	DA	3674	1/1	0.98	0.23	47,47,47,47	0
54	MG	BA	3439	1/1	0.98	0.11	17,17,17,17	0
54	MG	DA	2948	1/1	0.98	0.09	21,21,21,21	0
54	MG	BA	3143	1/1	0.98	0.04	48,48,48,48	0
54	MG	DA	3617	1/1	0.98	0.04	59,59,59,59	0
54	MG	BA	2943	1/1	0.98	0.08	34,34,34,34	0
54	MG	BA	3080	1/1	0.98	0.06	43,43,43,43	0
54	MG	BA	3013	1/1	0.98	0.04	21,21,21,21	0
54	MG	DA	3185	1/1	0.98	0.06	54,54,54,54	0
54	MG	DA	2912	1/1	0.98	0.16	19,19,19,19	0
54	MG	BA	3325	1/1	0.98	0.23	168,168,168,168	0
54	MG	DA	3001	1/1	0.98	0.06	25,25,25,25	0
54	MG	DA	3346	1/1	0.98	0.08	68,68,68,68	0
54	MG	BA	3250	1/1	0.98	0.02	67,67,67,67	0
54	MG	AA	1826	1/1	0.98	0.11	75,75,75,75	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	BA	3395	1/1	0.98	0.14	84,84,84,84	0
54	MG	BA	3307	1/1	0.98	0.04	63,63,63,63	0
54	MG	BA	3015	1/1	0.98	0.04	55,55,55,55	0
54	MG	DA	3098	1/1	0.98	0.17	46,46,46,46	0
54	MG	BA	3398	1/1	0.98	0.07	74,74,74,74	0
54	MG	BA	2953	1/1	0.98	0.14	45,45,45,45	0
54	MG	DA	2923	1/1	0.98	0.21	12,12,12,12	0
54	MG	BA	3056	1/1	0.98	0.08	31,31,31,31	0
54	MG	BA	3453	1/1	0.98	0.12	27,27,27,27	0
54	MG	DA	2966	1/1	0.98	0.18	39,39,39,39	0
54	MG	BA	2907	1/1	0.98	0.17	15,15,15,15	0
54	MG	DA	2968	1/1	0.98	0.26	36,36,36,36	0
54	MG	DA	3153	1/1	0.98	0.10	33,33,33,33	0
54	MG	AB	301	1/1	0.98	0.07	92,92,92,92	0
54	MG	DA	2970	1/1	0.98	0.11	29,29,29,29	0
54	MG	BA	3334	1/1	0.98	0.06	60,60,60,60	0
54	MG	DA	3645	1/1	0.98	0.11	23,23,23,23	0
54	MG	DA	3419	1/1	0.98	0.02	60,60,60,60	0
54	MG	DA	3257	1/1	0.98	0.05	48,48,48,48	0
54	MG	DA	3157	1/1	0.98	0.04	33,33,33,33	0
54	MG	CA	1695	1/1	0.98	0.05	65,65,65,65	0
54	MG	BA	2965	1/1	0.98	0.15	51,51,51,51	0
54	MG	CA	1630	1/1	0.98	0.09	49,49,49,49	0
54	MG	BA	2909	1/1	0.98	0.28	16,16,16,16	0
54	MG	DA	3593	1/1	0.98	0.20	125,125,125,125	0
54	MG	BA	2927	1/1	0.98	0.13	25,25,25,25	0
54	MG	CA	1802	1/1	0.98	0.04	94,94,94,94	0
54	MG	DA	2978	1/1	0.98	0.16	23,23,23,23	0
54	MG	BA	2905	1/1	0.98	0.20	19,19,19,19	0
54	MG	BB	209	1/1	0.98	0.03	61,61,61,61	0
54	MG	BA	3123	1/1	0.98	0.03	40,40,40,40	0
54	MG	DA	2938	1/1	0.98	0.11	7,7,7,7	0
54	MG	BM	202	1/1	0.98	0.06	85,85,85,85	0
54	MG	DA	3170	1/1	0.98	0.17	56,56,56,56	0
54	MG	BA	3546	1/1	0.98	0.11	67,67,67,67	0
54	MG	BA	3434	1/1	0.98	0.08	19,19,19,19	0
54	MG	DA	3124	1/1	0.98	0.10	51,51,51,51	0
54	MG	CA	1639	1/1	0.98	0.08	59,59,59,59	0
54	MG	DA	3607	1/1	0.98	0.13	79,79,79,79	0
54	MG	DA	3330	1/1	0.98	0.11	100,100,100,100	0
55	ZN	AD	301	1/1	0.98	0.17	51,51,51,51	0
54	MG	BA	2942	1/1	0.98	0.09	19,19,19,19	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	ZN	CD	301	1/1	0.98	0.23	116,116,116,116	0
54	MG	BA	3000	1/1	0.98	0.07	49,49,49,49	0
54	MG	DA	2958	1/1	0.99	0.05	31,31,31,31	0
54	MG	BA	3107	1/1	0.99	0.03	25,25,25,25	0
54	MG	DA	3056	1/1	0.99	0.01	25,25,25,25	0
54	MG	BA	3228	1/1	0.99	0.03	42,42,42,42	0
54	MG	AA	1609	1/1	0.99	0.10	26,26,26,26	0
54	MG	BA	2936	1/1	0.99	0.08	32,32,32,32	0
54	MG	BA	2921	1/1	0.99	0.13	17,17,17,17	0
54	MG	DL	201	1/1	0.99	0.06	7,7,7,7	0
54	MG	DA	2919	1/1	0.99	0.15	12,12,12,12	0
54	MG	DA	3586	1/1	0.99	0.06	79,79,79,79	0
54	MG	DA	3077	1/1	0.99	0.08	33,33,33,33	0
54	MG	DA	2920	1/1	0.99	0.12	14,14,14,14	0
54	MG	DA	3300	1/1	0.99	0.08	46,46,46,46	0
54	MG	BA	2917	1/1	0.99	0.09	6,6,6,6	0
54	MG	DA	2979	1/1	0.99	0.06	16,16,16,16	0
54	MG	DA	2980	1/1	0.99	0.16	12,12,12,12	0
54	MG	DA	3322	1/1	0.99	0.05	65,65,65,65	0
54	MG	DA	3636	1/1	0.99	0.17	12,12,12,12	0
54	MG	DA	3513	1/1	0.99	0.19	30,30,30,30	0
54	MG	DA	3082	1/1	0.99	0.12	68,68,68,68	0
54	MG	CA	1861	1/1	0.99	0.03	64,64,64,64	0
54	MG	DA	2903	1/1	0.99	0.14	16,16,16,16	0
54	MG	BA	3142	1/1	0.99	0.09	47,47,47,47	0

6.5 Other polymers [i](#)

There are no such residues in this entry.