



wwPDB X-ray Structure Validation Summary Report

Jun 16, 2014 – 08:45 PM BST

PDB ID : 4V83
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 validation summary report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

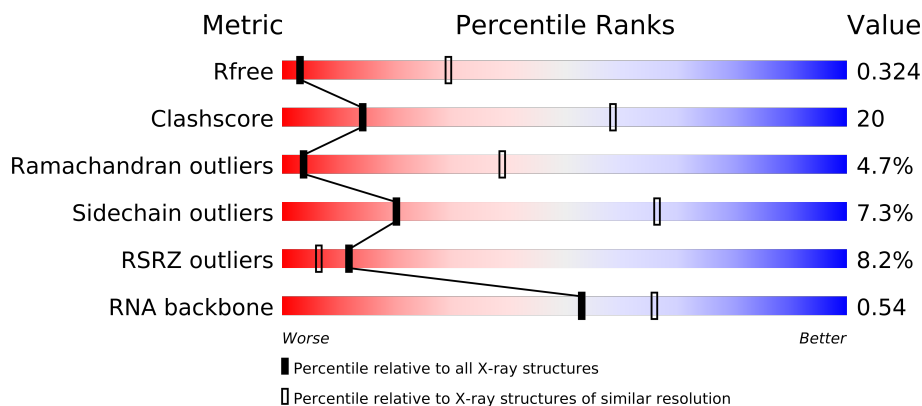
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.16 November 2013
Xtriage (Phenix) : dev-1323
EDS : stable23397
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable23397

1 Overall quality at a glance

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}	66092	1243 (3.70-3.30)
Clashscore	79885	1039 (3.66-3.34)
Ramachandran outliers	78287	1000 (3.66-3.34)
Sidechain outliers	78261	1000 (3.66-3.34)
RSRZ outliers	66119	1243 (3.70-3.30)
RNA backbone	1838	1007 (4.22-2.76)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	AA	1506	
1	CA	1506	
2	AB	234	
2	CB	234	
3	AC	206	
3	CC	206	
4	AD	208	
4	CD	208	
5	AE	151	
5	CE	151	
6	AF	101	

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Mol	Chain	Length	Quality of chain
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	
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	


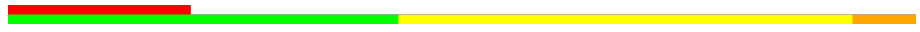







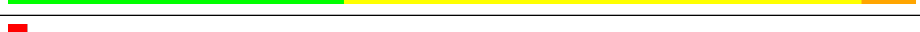

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Mol	Chain	Length	Quality of chain
27	DE	202	
28	BF	181	
28	DF	181	
29	BG	159	
29	DG	159	
30	BH	145	
30	DH	145	
31	BI	65	
31	DI	65	
32	BJ	137	
32	DJ	137	
33	BK	122	
33	DK	122	
34	BL	146	
34	DL	146	
35	BM	136	
35	DM	136	
36	BN	117	
36	DN	117	
37	BO	98	
37	DO	98	
38	BP	137	
38	DP	137	
39	BQ	116	
39	DQ	116	
40	BR	101	
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	

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

2 Entry composition

There are 55 unique types of molecules in this entry. The entry contains 283641 atoms, of which 0 are hydrogen and 0 are deuterium.

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 (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
54	DC	3	Total	Mg	0	0
			3	3		
54	DX	3	Total	Mg	0	0
			3	3		
54	B4	1	Total	Mg	0	0
			1	1		
54	BA	781	Total	Mg	0	0
			781	781		
54	AK	2	Total	Mg	0	0
			2	2		
54	DQ	2	Total	Mg	0	0
			2	2		
54	AB	3	Total	Mg	0	0
			3	3		
54	DF	2	Total	Mg	0	0
			2	2		
54	CV	7	Total	Mg	0	0
			7	7		
54	DL	3	Total	Mg	0	0
			3	3		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
54	BE	2	Total 2	Mg 2	0	0
54	DU	1	Total 1	Mg 1	0	0
54	DY	2	Total 2	Mg 2	0	0
54	AN	1	Total 1	Mg 1	0	0
54	BP	2	Total 2	Mg 2	0	0
54	CN	1	Total 1	Mg 1	0	0
54	BI	1	Total 1	Mg 1	0	0
54	AS	1	Total 1	Mg 1	0	0
54	CA	372	Total 372	Mg 372	0	0
54	B5	1	Total 1	Mg 1	0	0
54	BB	27	Total 27	Mg 27	0	0
54	BT	2	Total 2	Mg 2	0	0
54	DO	1	Total 1	Mg 1	0	0
54	AE	5	Total 5	Mg 5	0	0
54	BM	3	Total 3	Mg 3	0	0
54	CF	2	Total 2	Mg 2	0	0
54	D3	1	Total 1	Mg 1	0	0
54	BF	1	Total 1	Mg 1	0	0
54	AV	8	Total 8	Mg 8	0	0
54	BX	2	Total 2	Mg 2	0	0
54	DA	964	Total 964	Mg 964	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
54	B2	3	Total 3	Mg 3	0	0
54	AA	279	Total 279	Mg 279	0	0
54	CQ	2	Total 2	Mg 2	0	0
54	BJ	3	Total 3	Mg 3	0	0
54	DV	4	Total 4	Mg 4	0	0
54	BC	3	Total 3	Mg 3	0	0
54	AM	1	Total 1	Mg 1	0	0
54	BU	2	Total 2	Mg 2	0	0
54	CC	8	Total 8	Mg 8	0	0
54	AD	3	Total 3	Mg 3	0	0
54	BN	2	Total 2	Mg 2	0	0
54	CM	2	Total 2	Mg 2	0	0
54	DS	2	Total 2	Mg 2	0	0
54	DM	1	Total 1	Mg 1	0	0
54	AI	1	Total 1	Mg 1	0	0
54	BY	3	Total 3	Mg 3	0	0
54	DE	3	Total 3	Mg 3	0	0
54	B3	1	Total 1	Mg 1	0	0
54	DG	3	Total 3	Mg 3	0	0
54	BR	1	Total 1	Mg 1	0	0
54	DK	3	Total 3	Mg 3	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
54	D4	4	Total 4	Mg 4	0	0
54	BK	1	Total 1	Mg 1	0	0
54	CE	5	Total 5	Mg 5	0	0
54	DW	1	Total 1	Mg 1	0	0
54	D5	3	Total 3	Mg 3	0	0
54	DD	6	Total 6	Mg 6	0	0
54	D2	3	Total 3	Mg 3	0	0
54	AL	2	Total 2	Mg 2	0	0
54	BV	3	Total 3	Mg 3	0	0
54	AG	2	Total 2	Mg 2	0	0
54	BO	1	Total 1	Mg 1	0	0
54	AQ	3	Total 3	Mg 3	0	0
54	D1	1	Total 1	Mg 1	0	0
54	DI	1	Total 1	Mg 1	0	0
54	AH	1	Total 1	Mg 1	0	0
54	DJ	6	Total 6	Mg 6	0	0
54	CO	4	Total 4	Mg 4	0	0
54	AC	2	Total 2	Mg 2	0	0
54	BS	1	Total 1	Mg 1	0	0
54	DB	43	Total 43	Mg 43	0	0
54	CB	3	Total 3	Mg 3	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
54	CD	3	Total 3	Mg 3	0	0
54	DN	1	Total 1	Mg 1	0	0
54	AT	2	Total 2	Mg 2	0	0
54	CL	6	Total 6	Mg 6	0	0
54	DP	2	Total 2	Mg 2	0	0
54	AO	3	Total 3	Mg 3	0	0
54	BW	1	Total 1	Mg 1	0	0
54	CG	3	Total 3	Mg 3	0	0
54	CK	1	Total 1	Mg 1	0	0
54	AF	1	Total 1	Mg 1	0	0
54	BH	1	Total 1	Mg 1	0	0

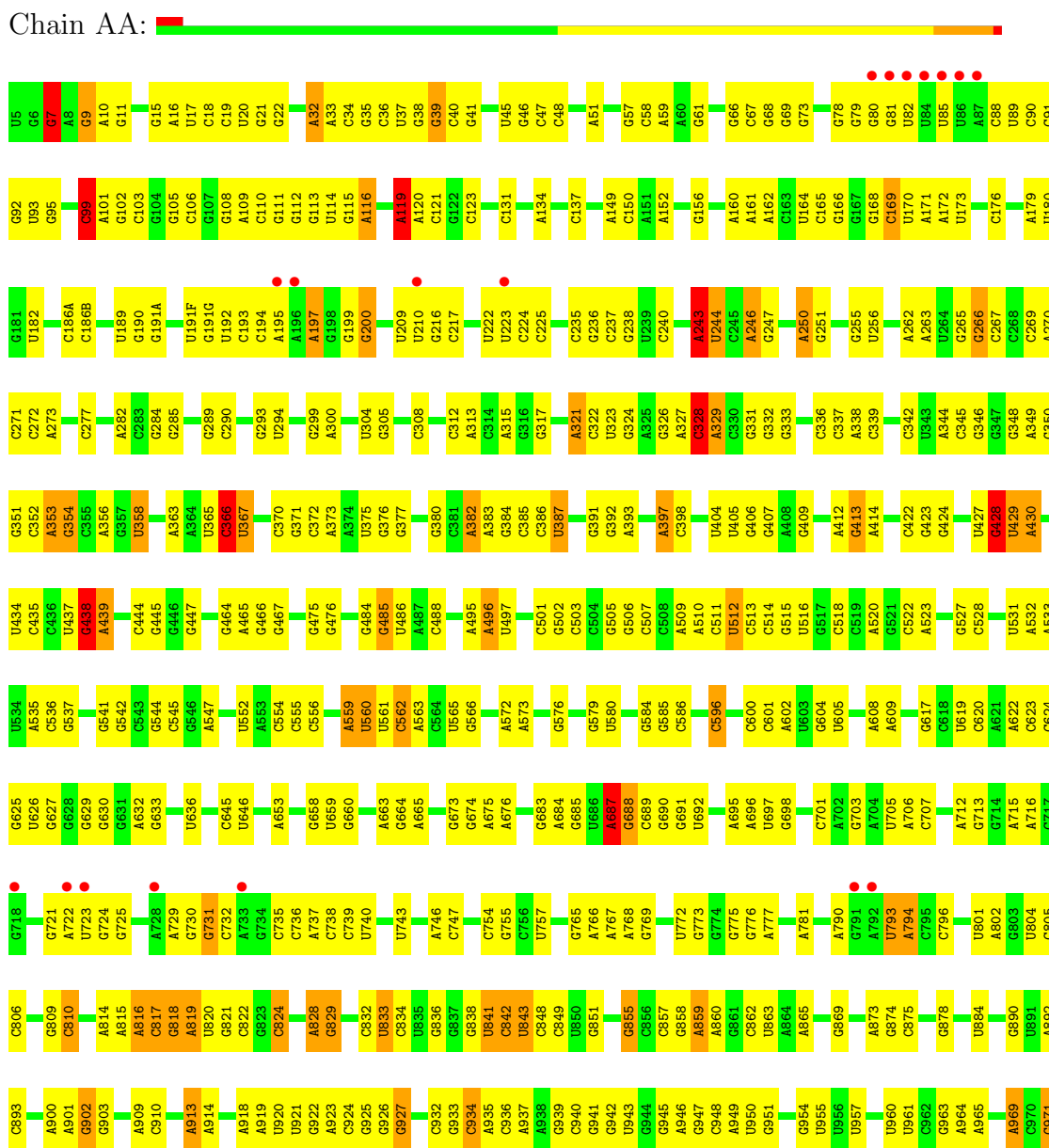
- Molecule 55 is ZINC ION (three-letter code: ZN) (formula: Zn).

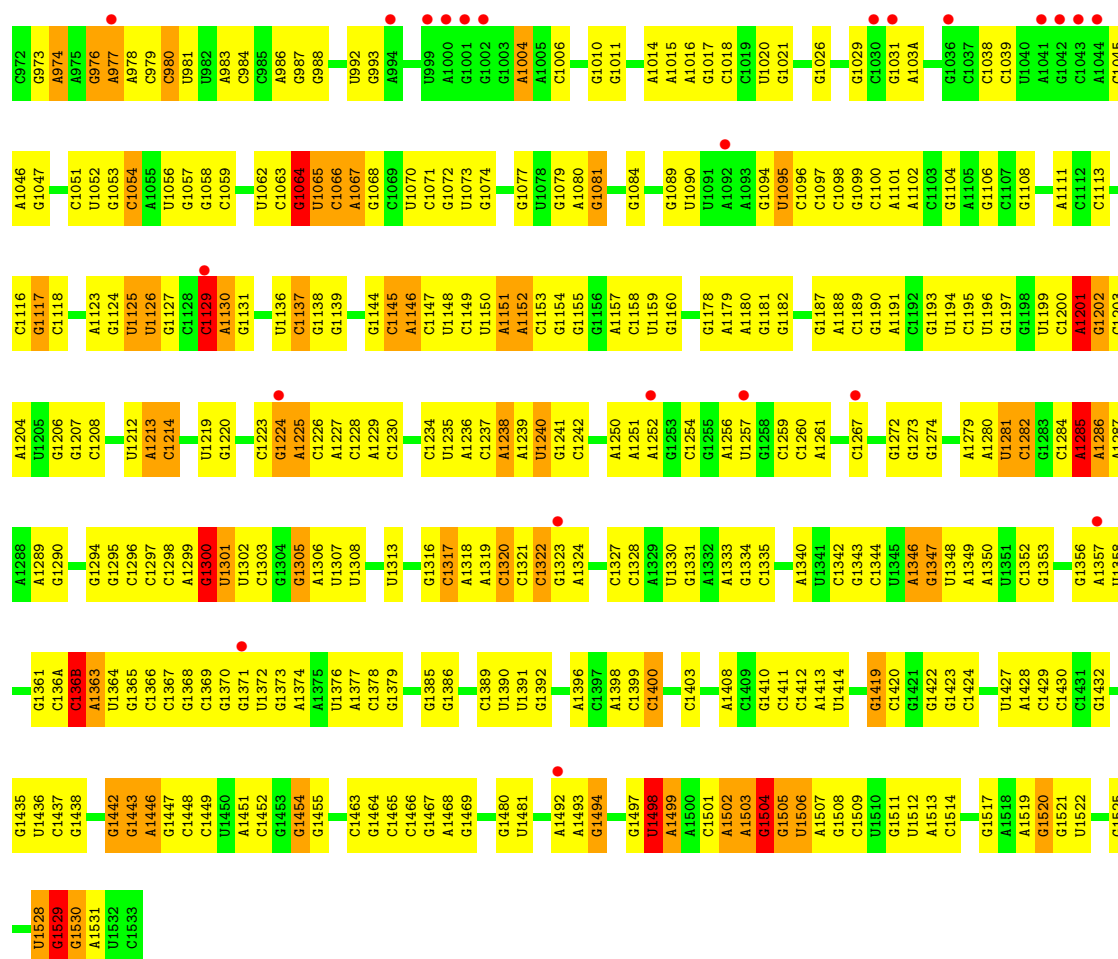
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
55	CN	1	Total 1	Zn 1	0	0
55	AD	1	Total 1	Zn 1	0	0
55	CD	1	Total 1	Zn 1	0	0
55	AN	1	Total 1	Zn 1	0	0

3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

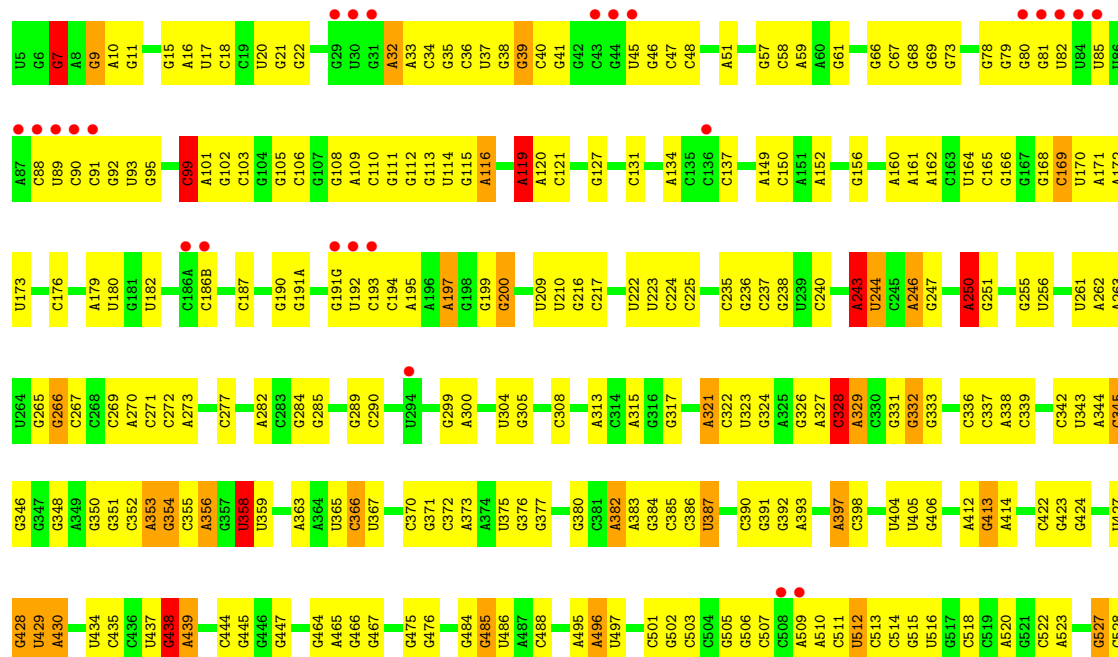
- Molecule 1: ribosomal RNA 16S

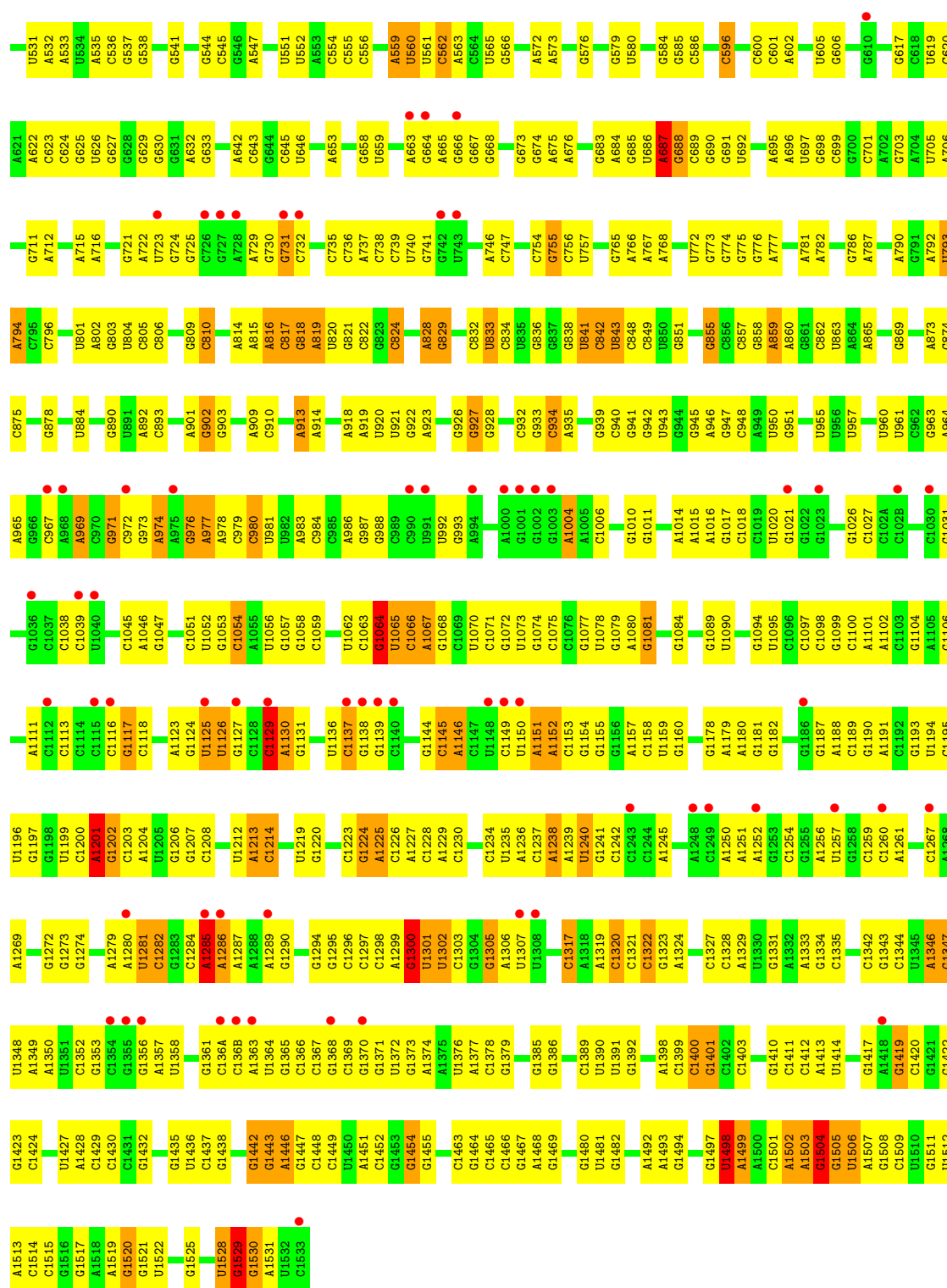




• Molecule 1: ribosomal RNA 16S

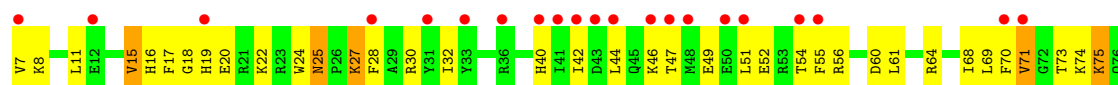
Chain CA:

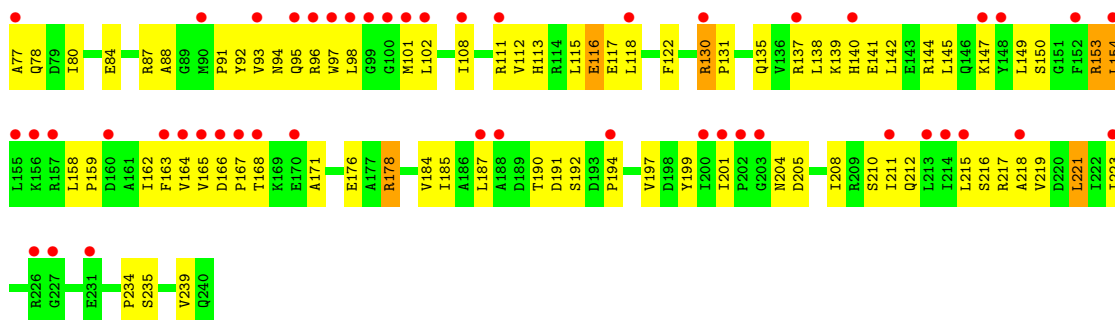




● Molecule 2: 30S ribosomal protein S2

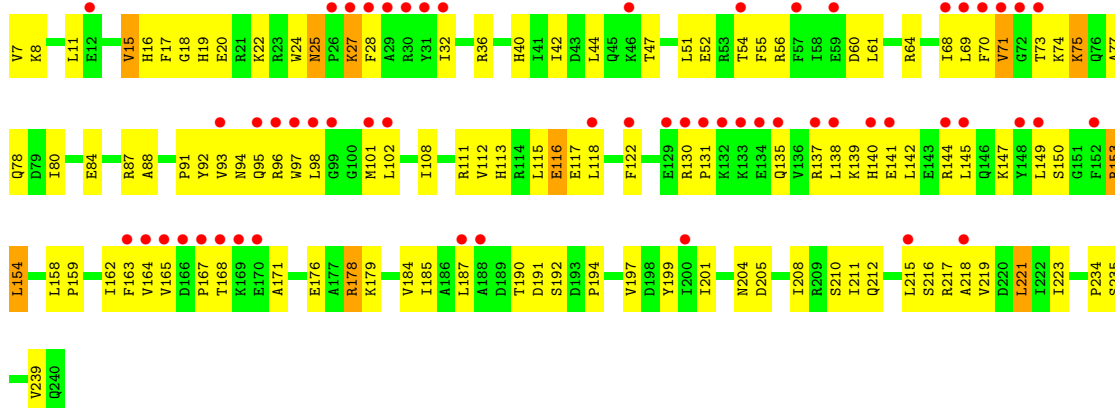
Chain AB:





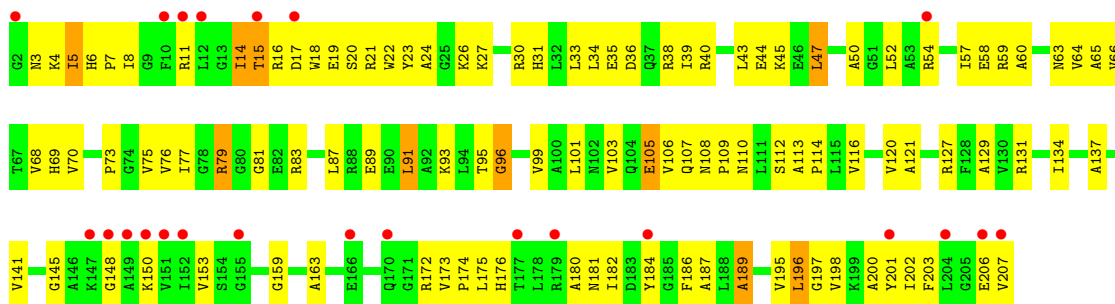
• Molecule 2: 30S ribosomal protein S2

Chain CB:



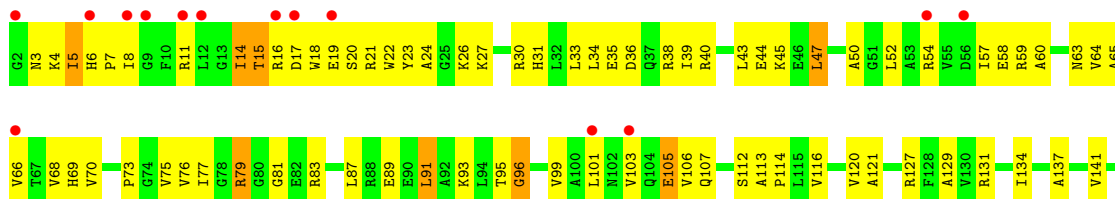
• Molecule 3: 30S ribosomal protein S3

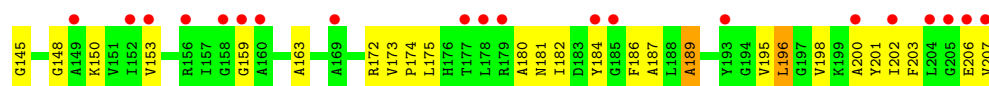
Chain AC:



• Molecule 3: 30S ribosomal protein S3

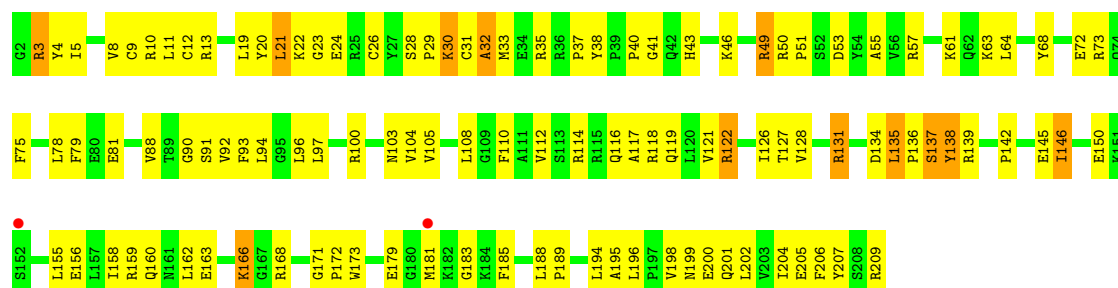
Chain CC:





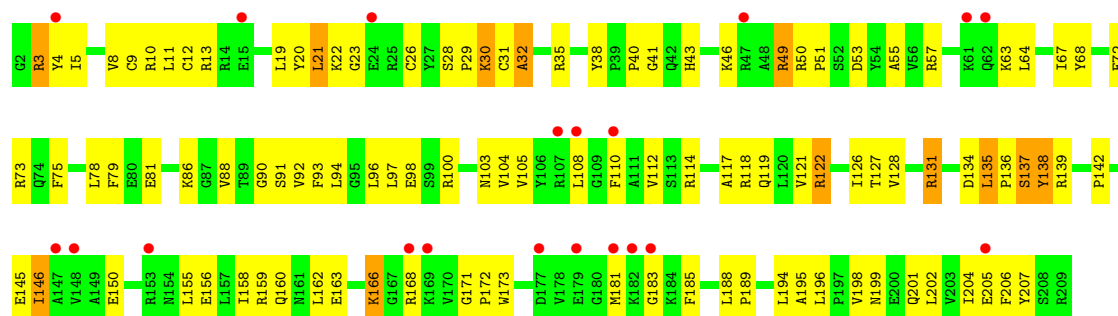
• Molecule 4: 30S ribosomal protein S4

Chain AD:



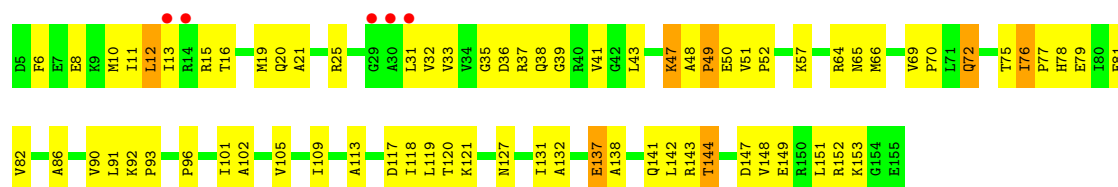
• Molecule 4: 30S ribosomal protein S4

Chain CD:



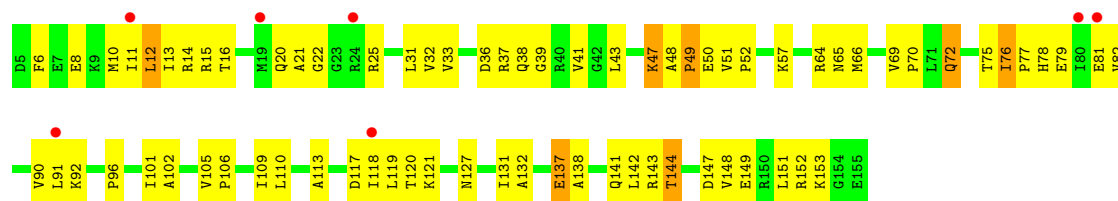
• Molecule 5: 30S ribosomal protein S5

Chain AE:



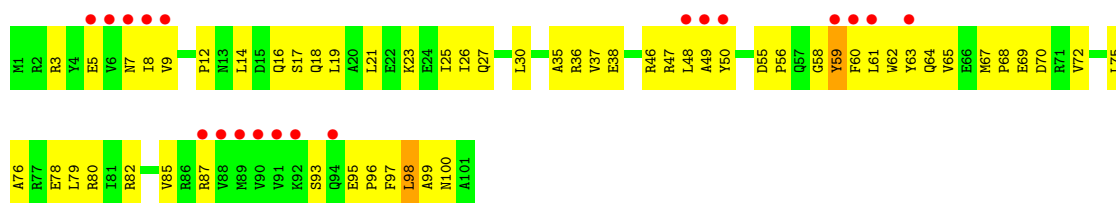
• Molecule 5: 30S ribosomal protein S5

Chain CE:



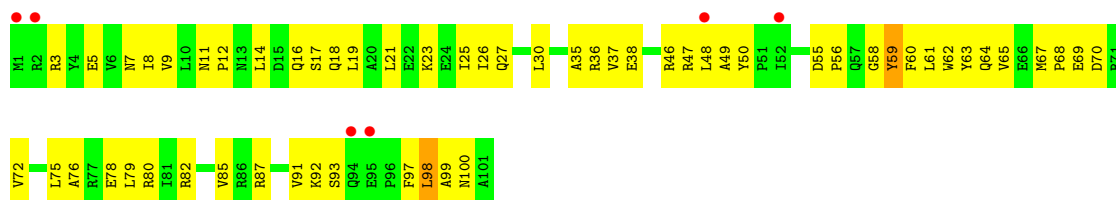
• Molecule 6: 30S ribosomal protein S6

Chain AF:



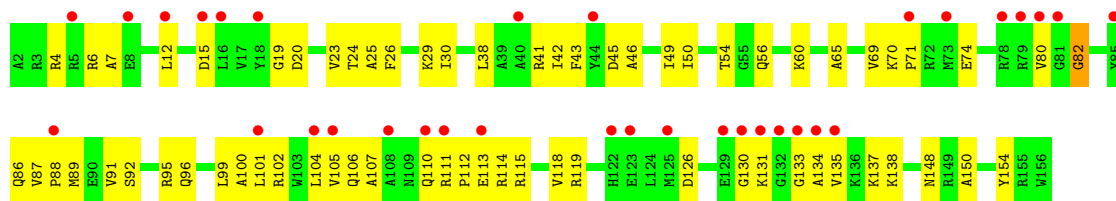
• Molecule 6: 30S ribosomal protein S6

Chain CF:



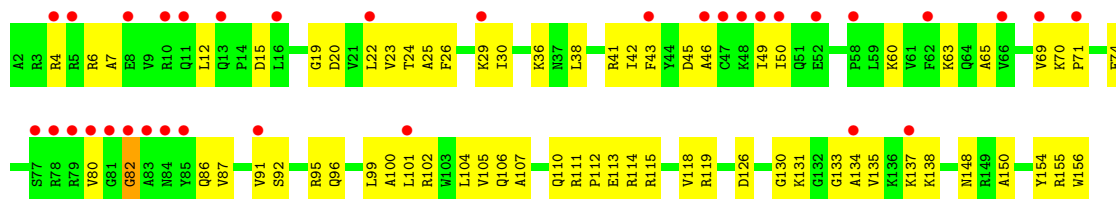
• Molecule 7: 30S ribosomal protein S7

Chain AG:



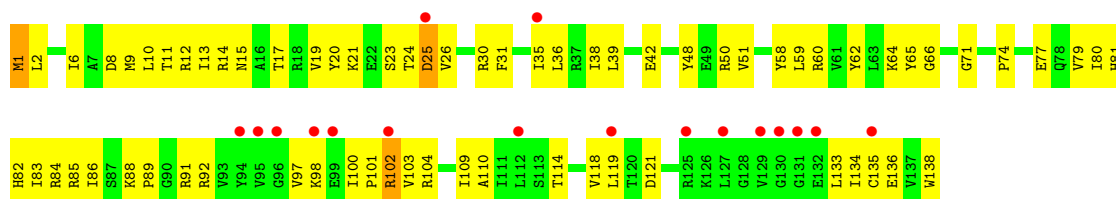
• Molecule 7: 30S ribosomal protein S7

Chain CG:



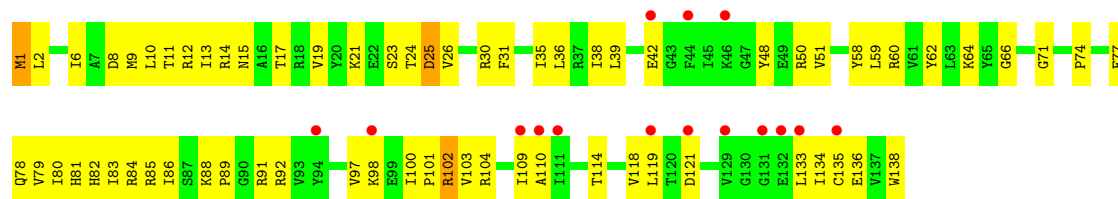
• Molecule 8: 30S ribosomal protein S8

Chain AH:



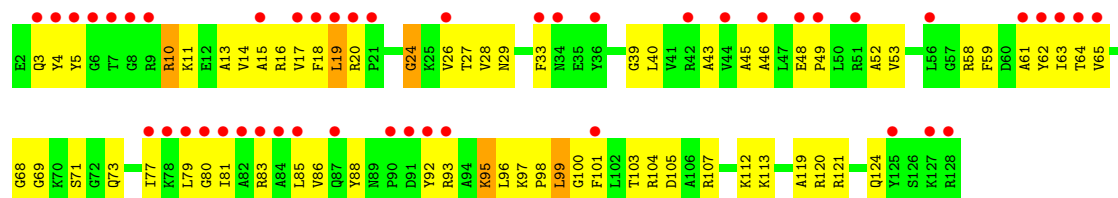
• Molecule 8: 30S ribosomal protein S8

Chain CH:



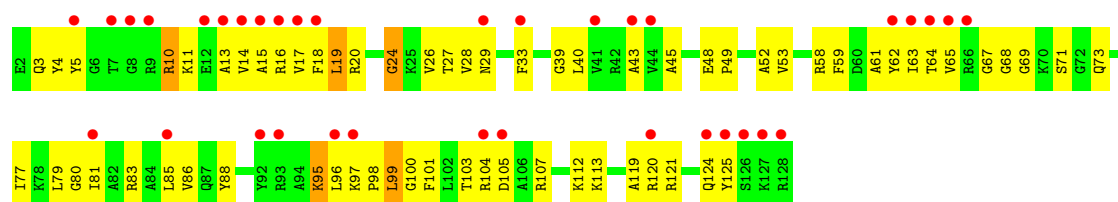
• Molecule 9: 30S ribosomal protein S9

Chain AI:



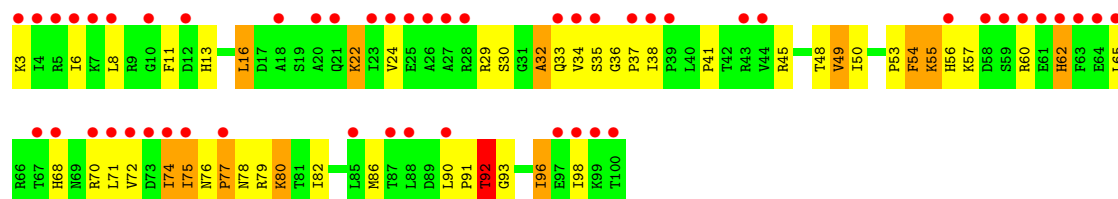
• Molecule 9: 30S ribosomal protein S9

Chain CI:



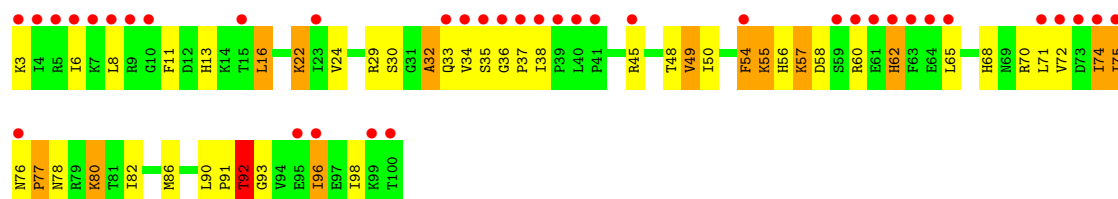
• Molecule 10: 30S ribosomal protein S10

Chain AJ:



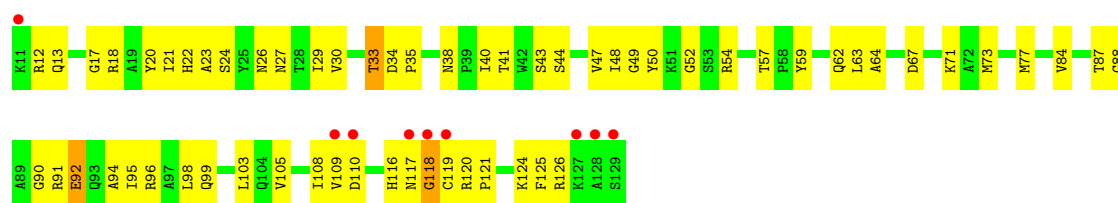
• Molecule 10: 30S ribosomal protein S10

Chain CJ:



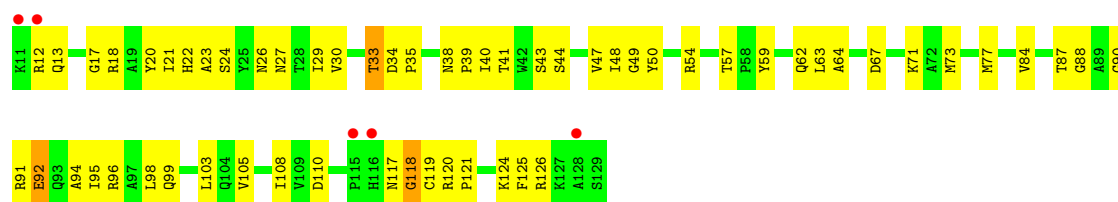
• Molecule 11: 30S ribosomal protein S11

Chain AK:



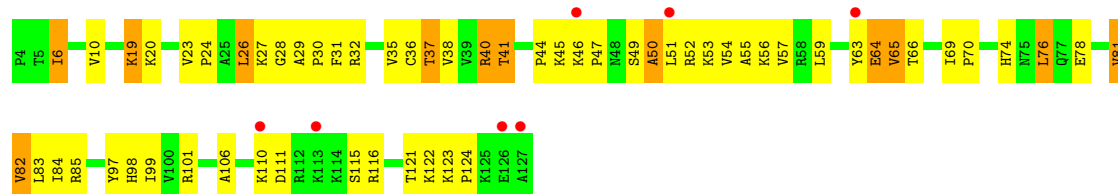
• Molecule 11: 30S ribosomal protein S11

Chain CK:



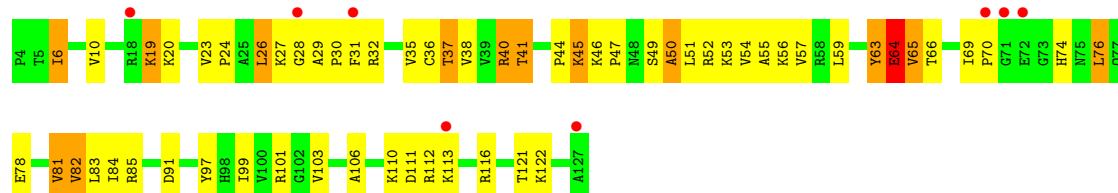
• Molecule 12: 30S ribosomal protein S12

Chain AL:



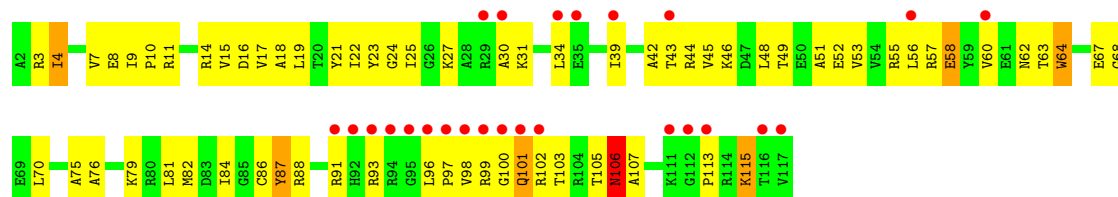
• Molecule 12: 30S ribosomal protein S12

Chain CL:



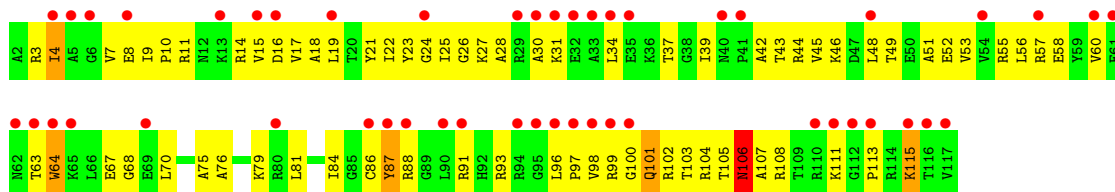
• Molecule 13: 30S ribosomal protein S13

Chain AM:



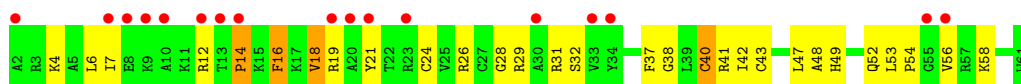
• Molecule 13: 30S ribosomal protein S13

Chain CM:



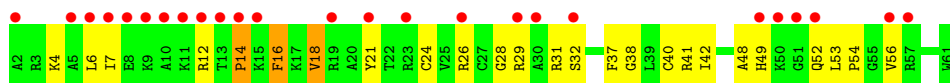
- Molecule 14: 30S ribosomal protein S14 type Z

Chain AN:



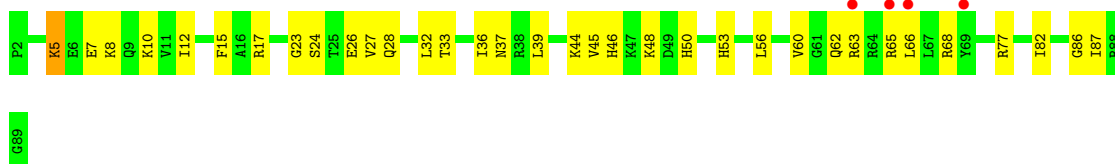
- Molecule 14: 30S ribosomal protein S14 type Z

Chain CN:



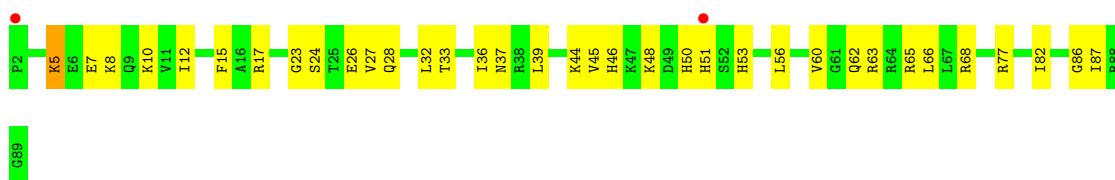
- Molecule 15: 30S ribosomal protein S15

Chain AO:



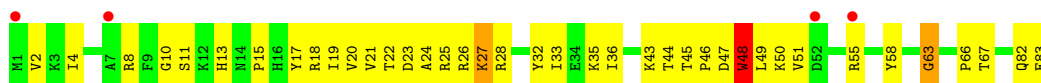
- Molecule 15: 30S ribosomal protein S15

Chain CO:



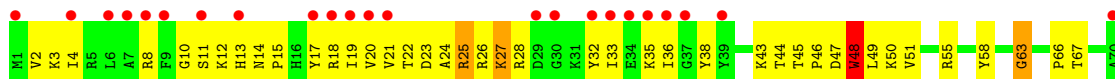
- Molecule 16: 30S ribosomal protein S16

Chain AP:



- Molecule 16: 30S ribosomal protein S16

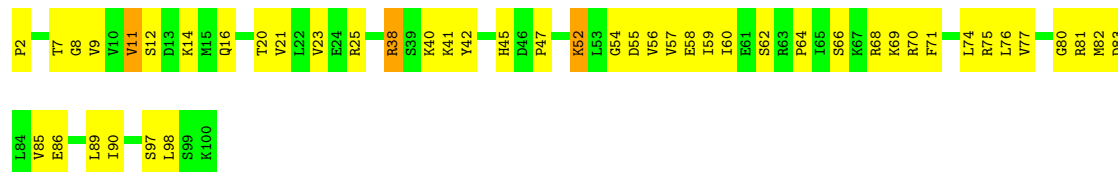
Chain CP:





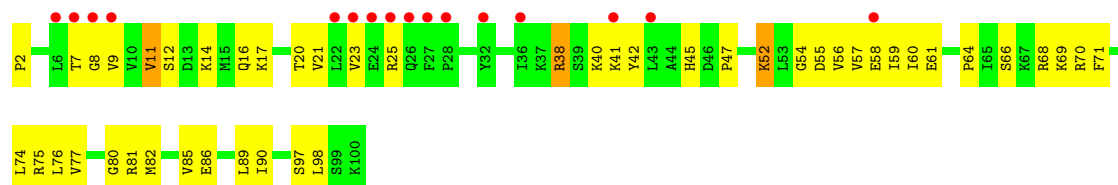
- Molecule 17: 30S ribosomal protein S17

Chain AQ:



- Molecule 17: 30S ribosomal protein S17

Chain CQ:



- Molecule 18: 30S ribosomal protein S18

Chain AR:



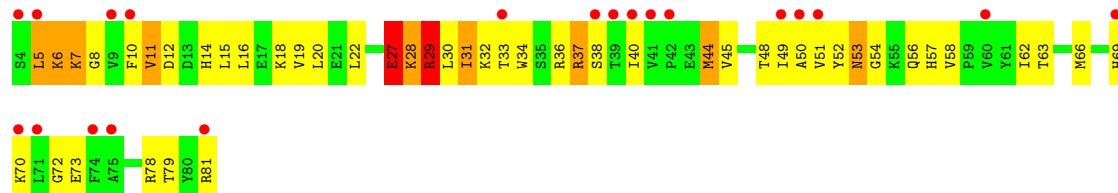
- Molecule 18: 30S ribosomal protein S18

Chain CR:



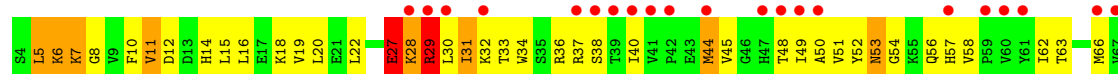
- Molecule 19: 30S ribosomal protein S19

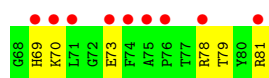
Chain AS:



- Molecule 19: 30S ribosomal protein S19

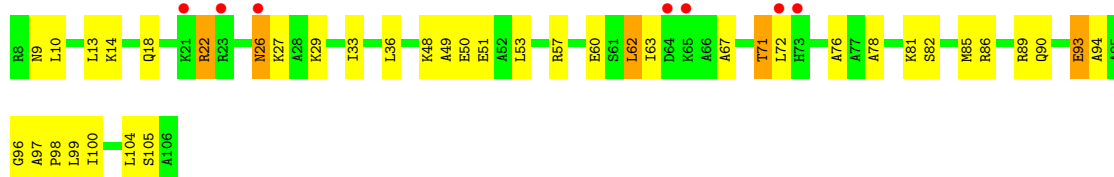
Chain CS:





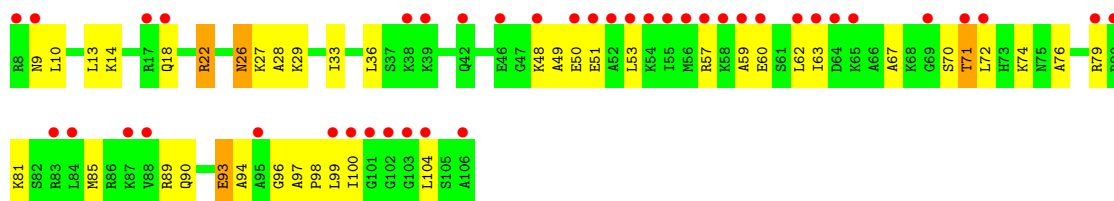
- Molecule 20: 30S ribosomal protein S20

Chain AT:



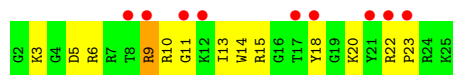
- Molecule 20: 30S ribosomal protein S20

Chain CT:



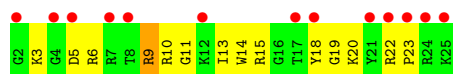
- Molecule 21: 30S ribosomal protein Thx

Chain AU:



- Molecule 21: 30S ribosomal protein Thx

Chain CU:



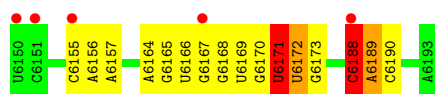
- Molecule 22: domain 3 of PSIC IGR IRES RNA

Chain AV:

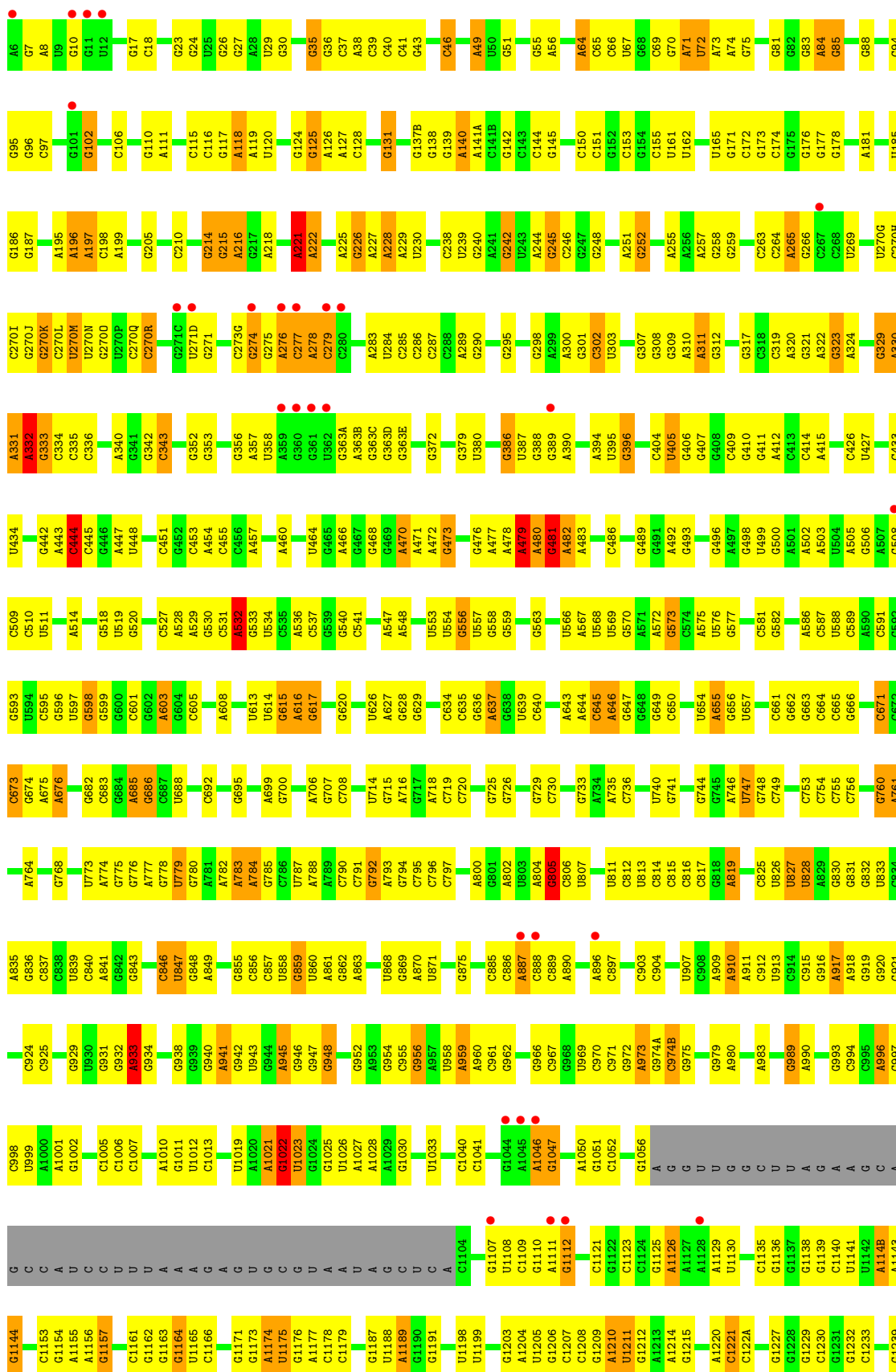


- Molecule 22: domain 3 of PSIC IGR IRES RNA

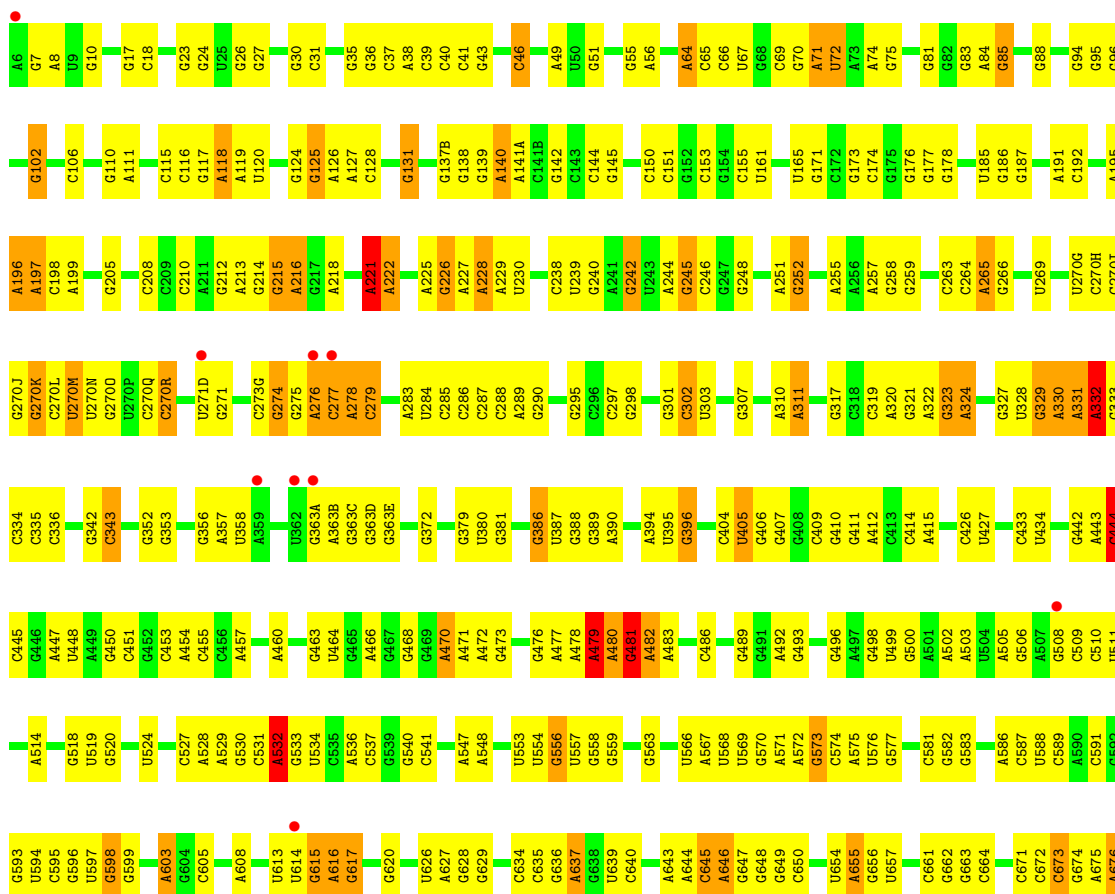
Chain CV:



- Molecule 23: 23S ribosomal RNA

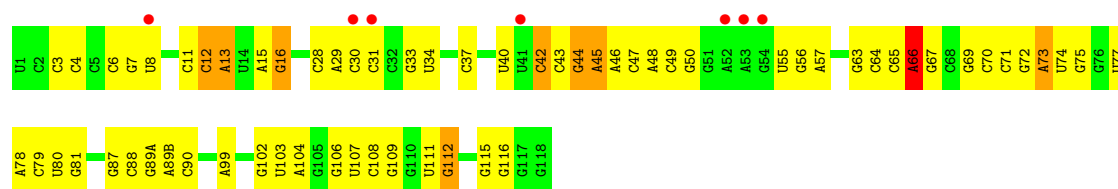






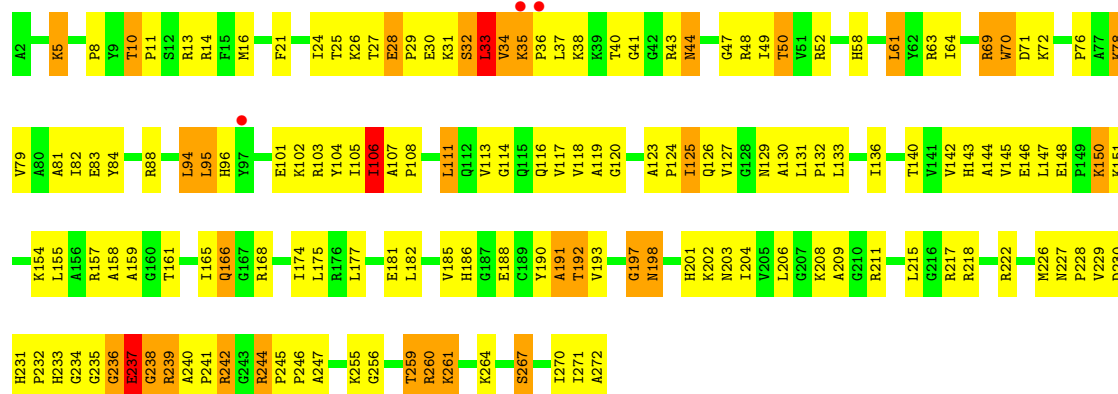
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G1984	A1887	A1786	A1677	C1585	U1497	G1413	A1336	U1249	G1163	U	C1005	G929	C838	G769
G1989	C1887	C1790	G1678	A1586	C1498	G1414	G1337	U1250	U1165	U	C1006	G930	U839	U773
C1990	A1888	A1791	U1679	C1588	U1502	G1416	U1341	G1251	C1166	A	C1007	G931	C840	G775
U1991	A1889	U1680	G1681	C1589	U1503	G1417	U1342	G1252	G1170	A	A1010	G932	G842	A774
G1992	G1899	G1682	G1683	C1590	C1504	G1418	G1343	A1253	G1171	A	A1011	A833	G843	G776
U1993	A1900	C1683	C1684	G1591	C1505	A1419	G1344	U1254	G1172	G	G1012	G938	C846	A777
U1995	A1901	C1684	C1684	C1592	C1506	U1420	G1345	G1256	U1173	A	U1012	G939	U847	G778
C1996	C1902	U1798	C1684	A1508	A1509	G1427	G1348	G1257	U1174	G	C1013	G940	U848	U779
G1997	G1903	G1594	C1684	A1509	A1510	A1428	A1349	C1257	U1175	U	U1019	A941	A849	G780
G1998	U1688	G1595	U1688	A1510	A1511	C1429	A1350	G1258	G1176	G	A1020	G942	C850	A781
C1999	A1689	C1596	A1690	A1511	A1512	G1430	U1352	A1259	G1177	C	A1021	G943	U851	A782
G2004	A1913	C1691	U1692	C1599	U1516	C1431	U1353	G1260	C1178	G	U1022	G944	C855	A783
C2005	C1914	U1693	U1693	C1600	G1517	C1432	A1354	U1267	C1179	U	G1023	A945	C856	A784
G2010	U1915	C1694	C1694	G1601	C1518	U1433	G1355	G1268	C1180	A	G1024	G946	C857	G785
U2011	A1916	G1695	G1695	U1602	G1519	A1434	G1356	C1270	C1185	U	G1025	G947	C858	G786
G2012	U1917	A1809	G1696	A1603	G1526	G1435	U1357	G1271	G1186	A	U1026	G948	U858	U787
A2013	A1810	A1810	C1697	C1604	G1527	G1436	G1358	U1272	G1187	G	A1027	G954	C859	C790
A2014	U1918	G1697	G1697	C1607	G1528	C1437	A1359	A1273	U1188	C	A1028	C955	U860	C791
A2015	A1919	A1698	A1698	A1608	A1529	U1438	A1360	A1274	A1189	U	A1029	G956	A861	G792
C2019	C1920	G1699	A1700	A1609	A1529	G1444	G1361	A1276	G1191	A	G1030	A957	C862	A793
A2020	U1926	A1610	C1532	A1609	C1532	G1444	A1365	A1276	G1191	C	U1033	U958	A863	G794
A2021	G1816	C1611	C1612	A1610	C1532	C1445	A1365	A1284	U1198	C	C104	A859	U868	C795
G1929	C1817	C1611	C1612	C1612	U1535	C1446	G1368	G1285	U1199	C	C1040	A860	C869	C796
U2022	U1818	C1612	C1612	A1536	C1536	G1447	G1369	G1285	U1199	C	C1041	A861	A870	C797
G2023	U1931	A1614	G1537	G1538	C1537	G1448	G1369	C1289	C1201	C	A1046	G962	U871	A800
G2024	A1932	C1615	G1538	A1498	G1538	A1498	A1373	C1290	U1205	C	G1047	G966	C885	G801
C2025	G1933	C1615	G1538	A1498	G1538	G1449	G1374	C1291	U1206	C	A1047	G967	C886	A802
C2026	G1933	C1616	G1540	A1450	G1540	C1450	A1378	U1292	C1207	C	A1050	G968	A887	G803
G2027	A1936	C1617	U1541	C1451	U1541	G1451	A1378	U1292	C1207	C	A1050	G968	C888	A804
U2028	A1937	C1618	G1542	A1454	G1542	C1454	A1379	U1292	C1207	C	G1051	G969	C889	G805
G2029	A1938	G1620	G1542	A1454	G1542	U1454	G1380	U1300	C1208	C	G1052	C970	C890	C806
A2030	U1939	G1620	G1542	A1454	G1542	G1455	G1380	A1301	U1210	C	G1056	G971	A890	U807
A2031	C1830	A1632	A1545	G1455	C1544	G1455	A1384	A1301	U1211	C	A1056	G972	A896	
C2032	C1831	G1633	A1546	G1461	A1546	G1461	G1385	A1308	G1212	C	A	A973	C896	U811
A2033	C1832	A1634	C1548	C1462	C1548	C1462	G1386	G1309	A1213	C	G	G974A	C897	C812
U2034	U1833	A1634	C1548	C1463	C1548	G1463	C1387	G1310	A1214	C	G	G975	C903	U813
G2035	G1954	C1640	C1559	C1464	C1559	G1464	G1388	G1311	G1215	C	U	G979	C904	C814
C2036	U1955	C1640	C1559	G1465	C1559	G1465	G1389	U1312	G1136	C	U	G979	C904	C815
G2037	U1956	C1640	C1559	G1466	C1559	G1466	U1390	U1312	G1136	C	U	G979	C904	C816
C2038	C1838	G1647	G1563	C1467	C1563	C1467	U1391	U1314	C1221	C	G	A880	U907	C817
C2039	G1839	C1648	C1564	C1467	C1564	C1467	U1391	U1314	C1221	C	C	A880	C908	C818
C2040	A1847	G1649	C1565	G1478	C1565	G1478	A1395	U1316	G1225	C	U	A983	A909	C819
U2041	U1847	G1649	C1565	G1478	C1565	G1478	A1395	U1316	G1225	C	U	A983	A910	A819
A2042	A1759	C1652	A1567	G1483	A1567	G1483	C1399	C1318	G1226	C	A	G989	A911	C825
C2043	U1850	G1653	A1568	G1484	A1568	G1484	G1400	U1142	G1227	C	G	A990	C912	U826
G2049	C1852	A1655	A1569	G1485	A1569	G1485	G1401	G1228	G1229	C	A	C991	U913	U827
C2050	G1855	C1656	C1574	G1486	C1574	G1486	C1402	G1229	G1229	C	A	C992	G914	U828
A2051	C1657	C1658	C1575	A1487	C1575	G1487	C1403	G1230	G1231	C	G	G993	C915	U829
G2052	U1772	C1658	C1576	G1488	C1576	G1488	C1404	G1232	G1232	C	C	C994	C916	A830
C2053	G1773	C1658	C1577	U1489	C1577	U1489	U1405	C1233	C1233	C	A	C995	A917	C831
G2055	U1776	A1688	U1578	A1490	C1578	A1490	U1406	C1233	C1233	C	G	A996	A918	C832
C2056	U1777	A1689	U1579	C1497	C1579	C1497	G1407	C1233	C1233	C	C	G997	G919	C833
A2057	U1778	A1580	A1580	C1498	C1580	C1498	C1408	A1331	G1239	C	A	C998	G920	U834
A2058	A1871	C1673	A1581	C1499	A1581	C1499	C1408	A1332	U1240	C	U	A1000	G921	C835
A2059	A1872	C1674	C1582	A1495	C1582	A1495	C1411	G1334	A1242	C	C	A1001	C924	G836





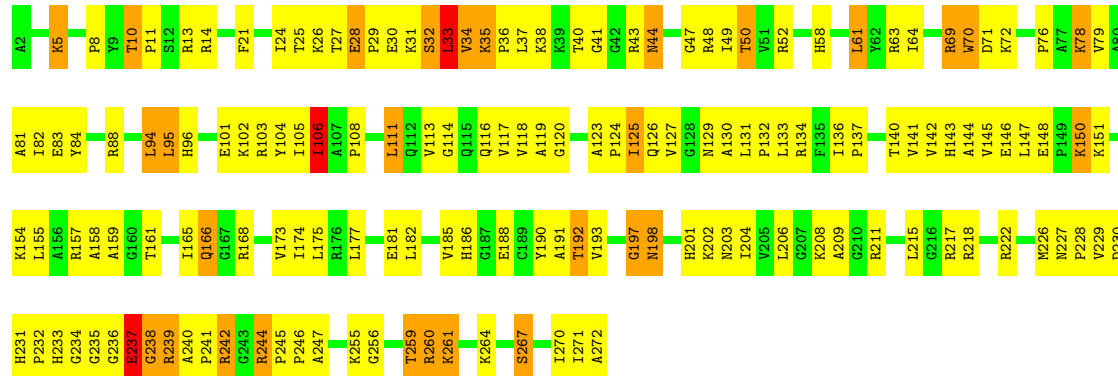
• Molecule 25: 50S ribosomal protein L2

Chain BC:



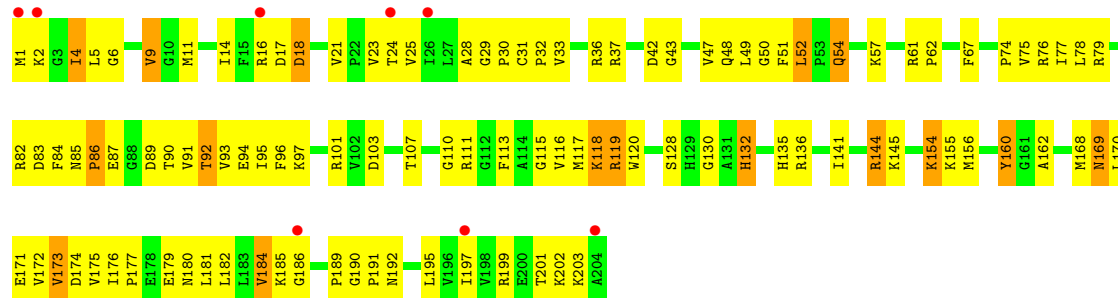
• Molecule 25: 50S ribosomal protein L2

Chain DC:



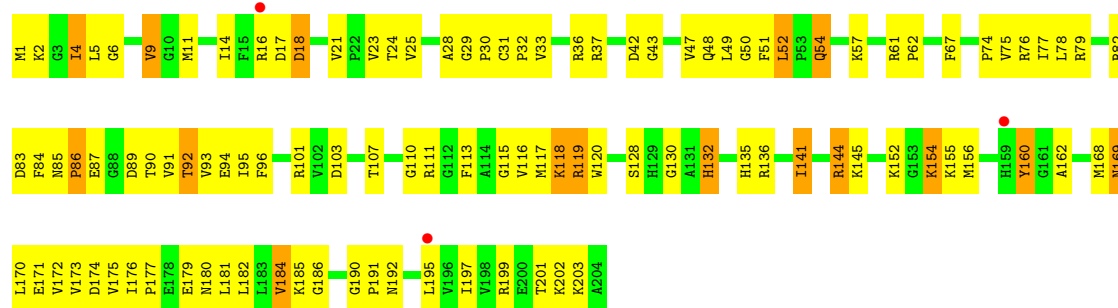
• Molecule 26: 50S ribosomal protein L3

Chain BD:



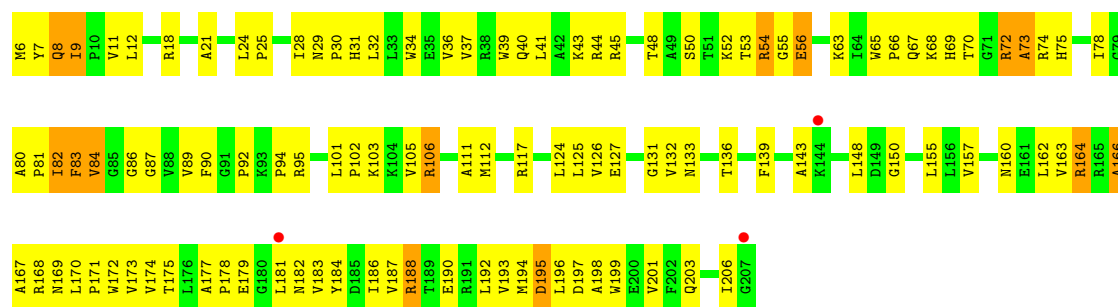
• Molecule 26: 50S ribosomal protein L3

Chain DD:



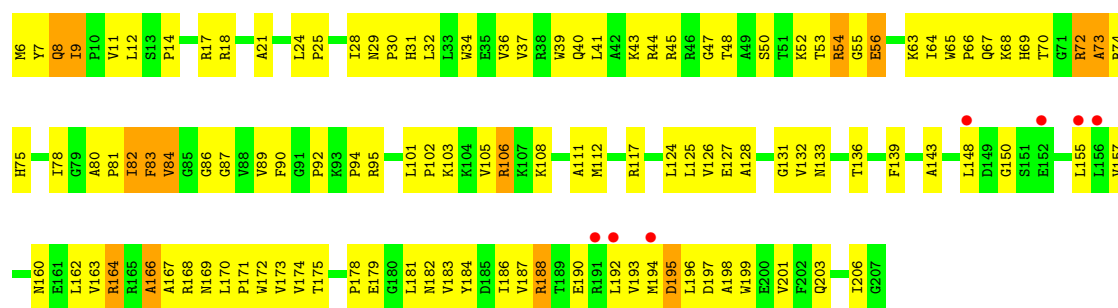
- Molecule 27: 50S ribosomal protein L4

Chain BE:



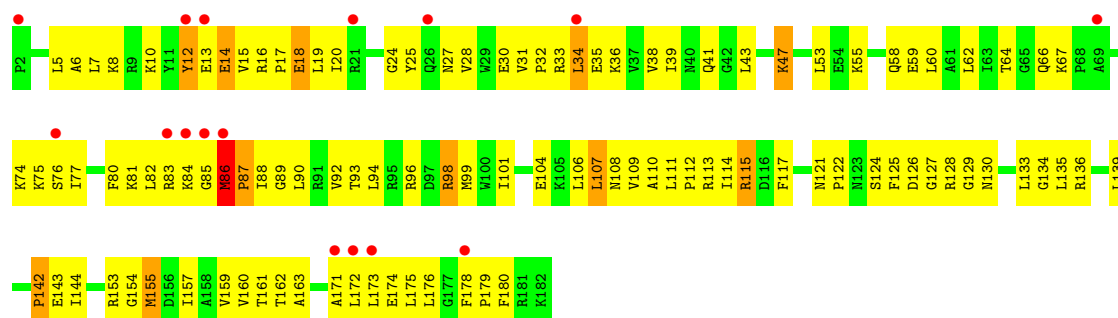
- Molecule 27: 50S ribosomal protein L4

Chain DE:



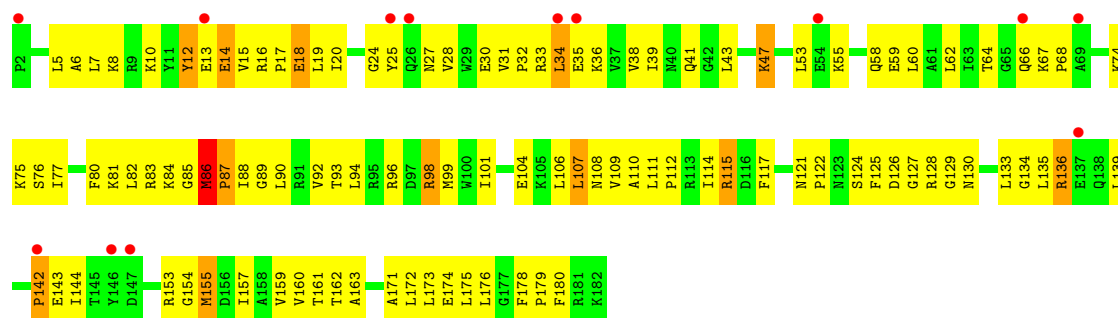
- Molecule 28: 50S ribosomal protein L5

Chain BF:



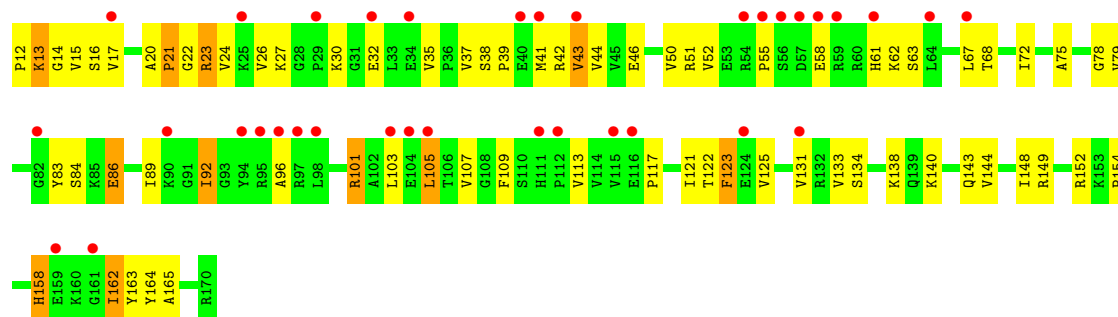
- Molecule 28: 50S ribosomal protein L5

Chain DF:



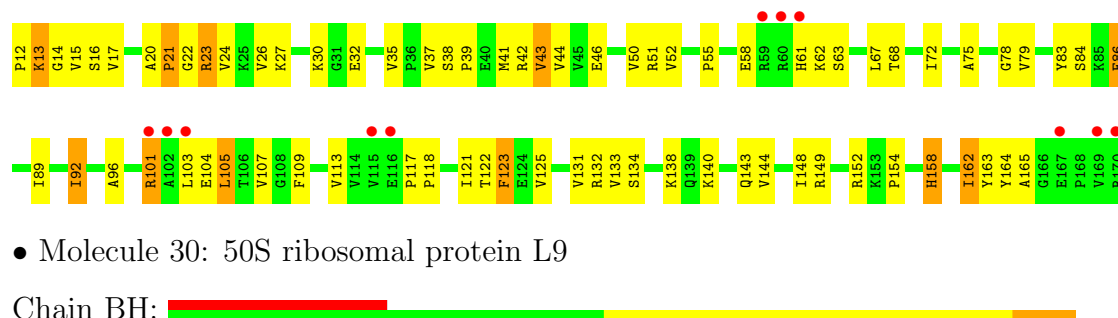
- Molecule 29: 50S ribosomal protein L6

Chain BG:



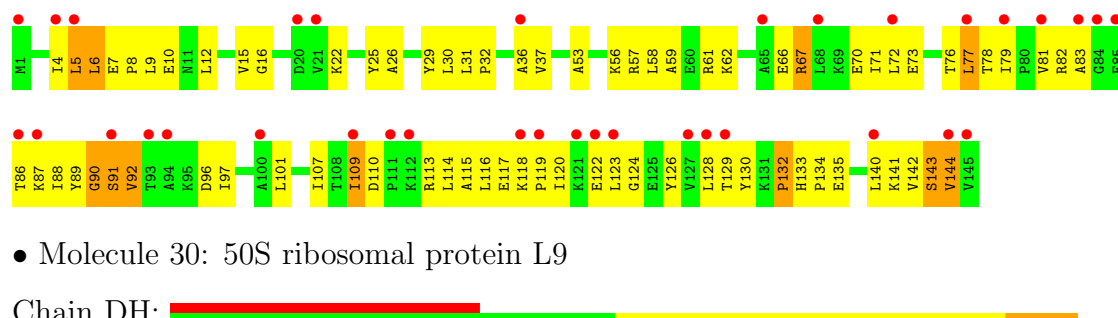
- Molecule 29: 50S ribosomal protein L6

Chain DG:



- Molecule 30: 50S ribosomal protein L9

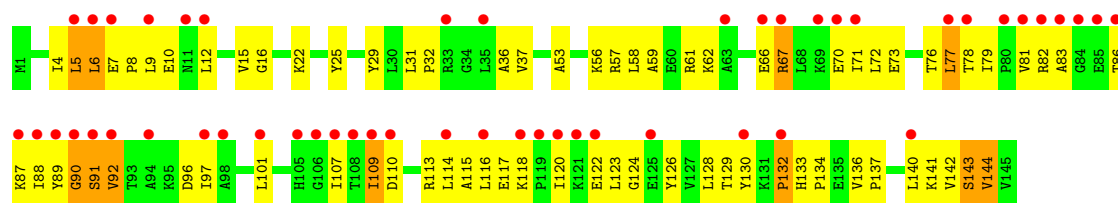
Chain BH:



- Molecule 30: 50S ribosomal protein L9

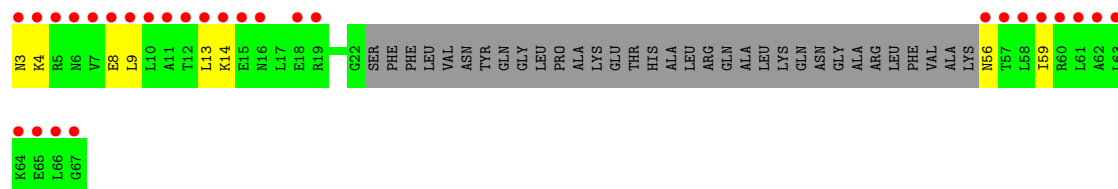
Chain DH:





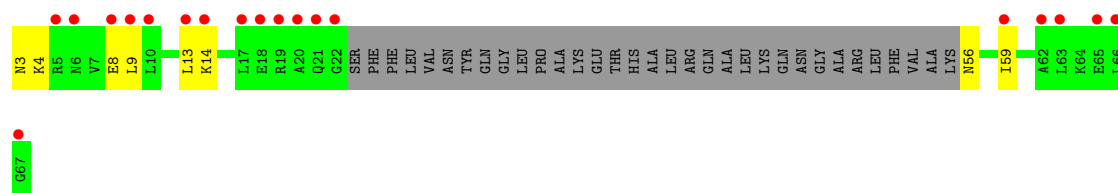
• Molecule 31: 50S ribosomal protein L10

Chain BI:



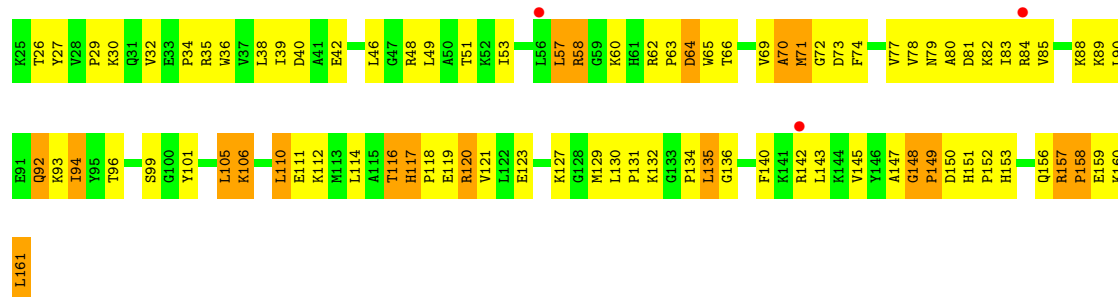
• Molecule 31: 50S ribosomal protein L10

Chain DI:



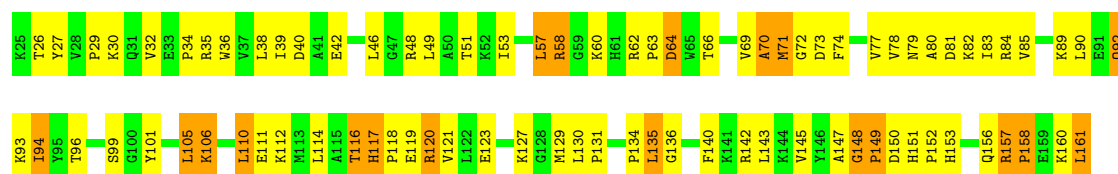
• Molecule 32: 50S ribosomal protein L13

Chain BJ:



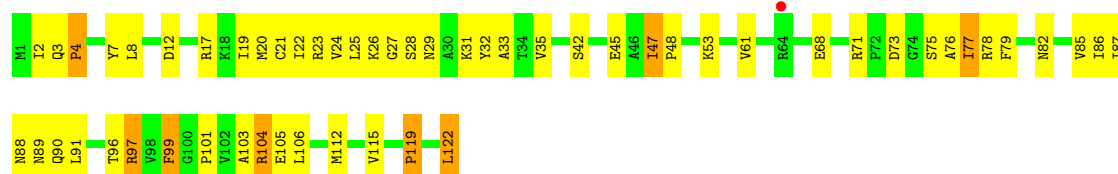
• Molecule 32: 50S ribosomal protein L13

Chain DJ:



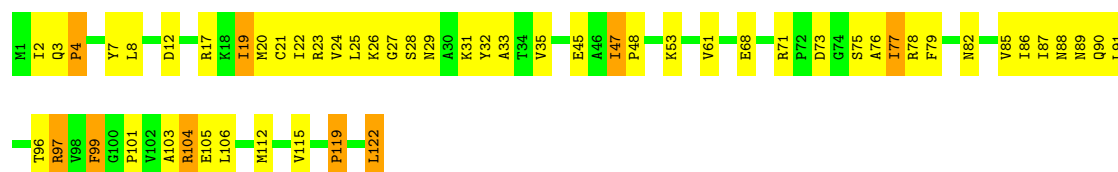
• Molecule 33: 50S ribosomal protein L14

Chain BK:



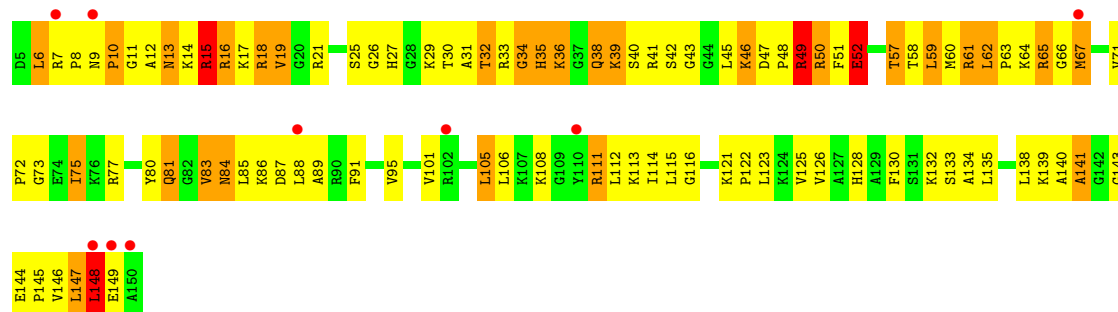
• Molecule 33: 50S ribosomal protein L14

Chain DK:



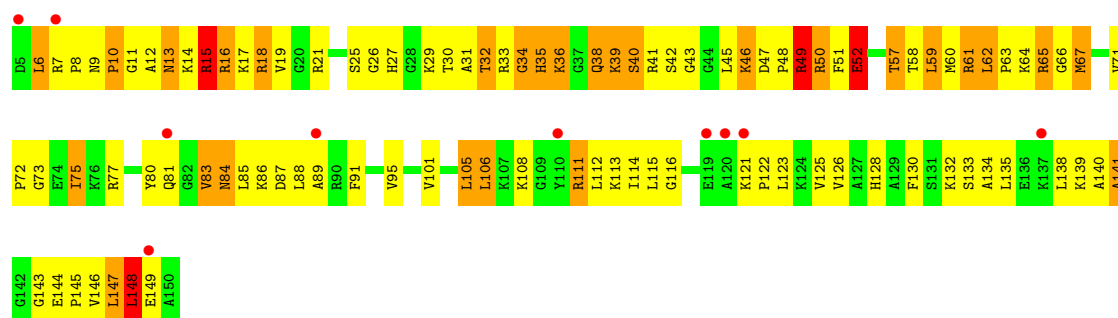
• Molecule 34: 50S ribosomal protein L15

Chain BL:



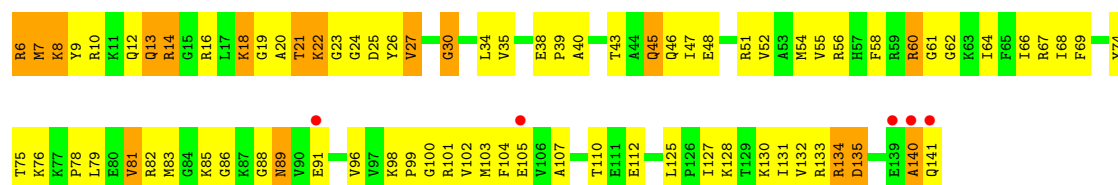
• Molecule 34: 50S ribosomal protein L15

Chain DL:



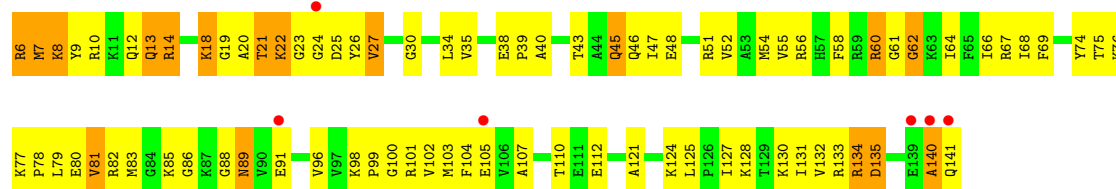
• Molecule 35: 50S ribosomal protein L16

Chain BM:



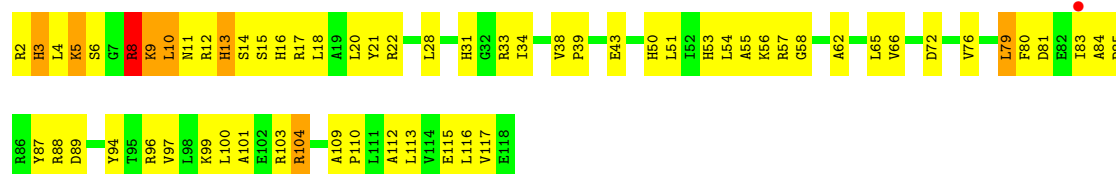
- Molecule 35: 50S ribosomal protein L16

Chain DM:



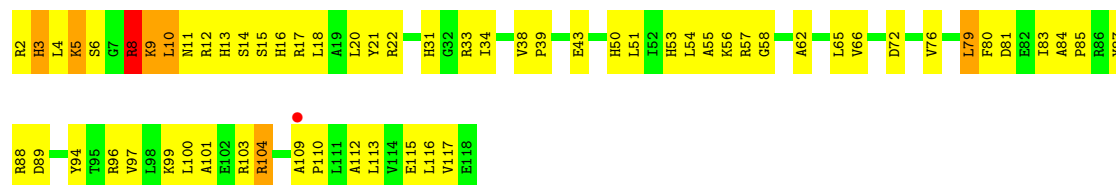
- Molecule 36: 50S ribosomal protein L17

Chain BN:



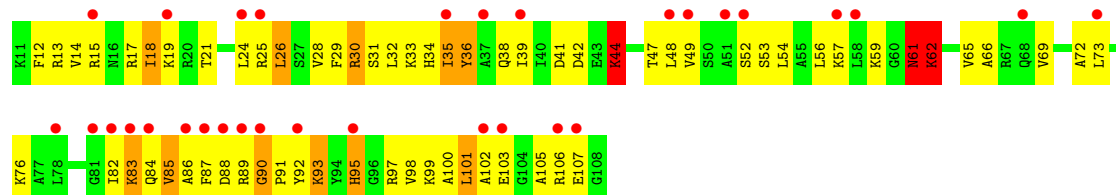
- Molecule 36: 50S ribosomal protein L17

Chain DN:



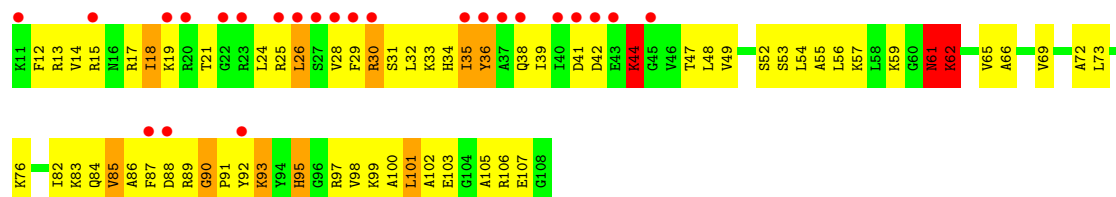
- Molecule 37: 50S ribosomal protein L18

Chain BO:



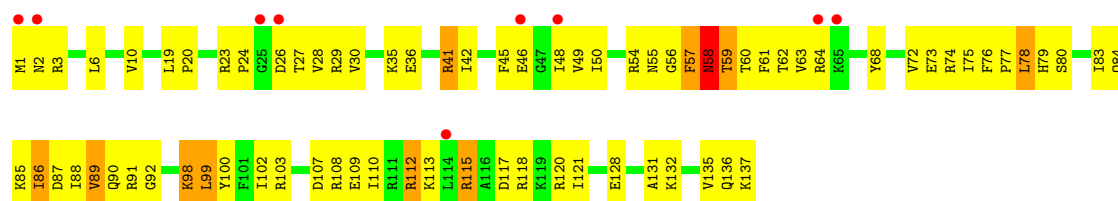
- Molecule 37: 50S ribosomal protein L18

Chain DO:



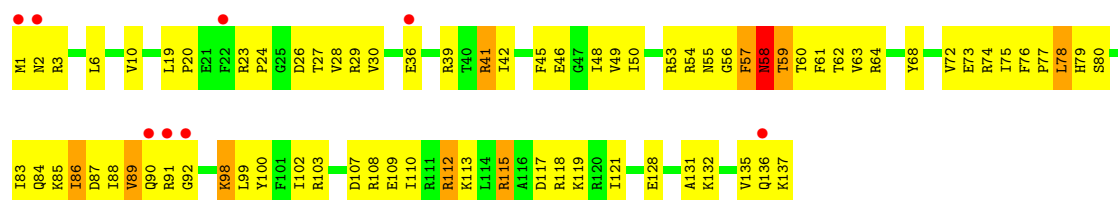
- Molecule 38: 50S ribosomal protein L19

Chain BP:



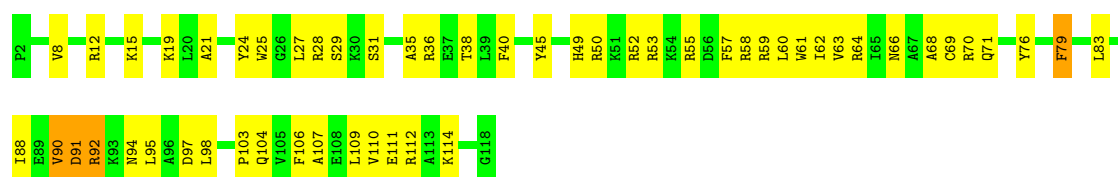
• Molecule 38: 50S ribosomal protein L19

Chain DP:



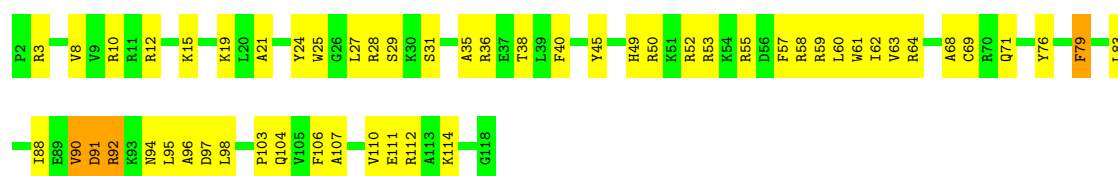
• Molecule 39: 50S ribosomal protein L20

Chain BQ:



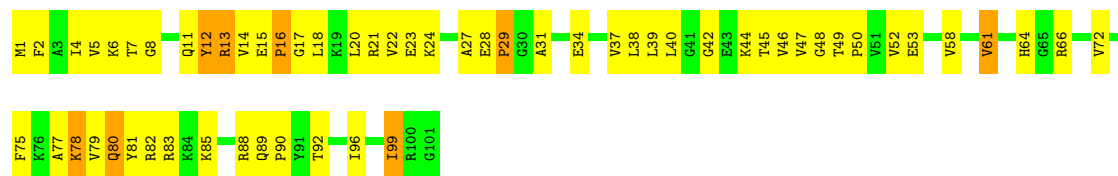
• Molecule 39: 50S ribosomal protein L20

Chain DQ:



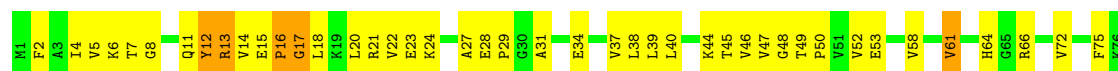
• Molecule 40: 50S ribosomal protein L21

Chain BR:



• Molecule 40: 50S ribosomal protein L21

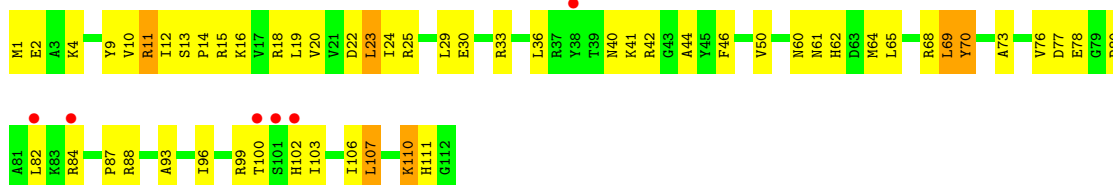
Chain DR:





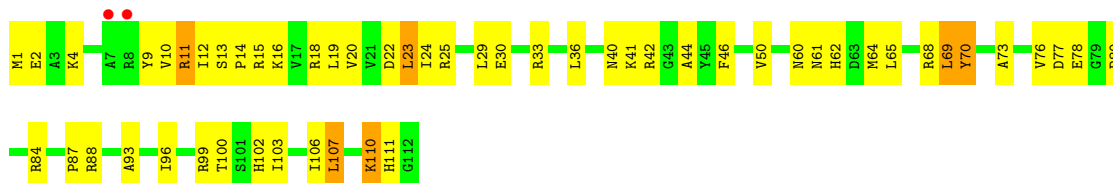
- Molecule 41: 50S ribosomal protein L22

Chain BS:



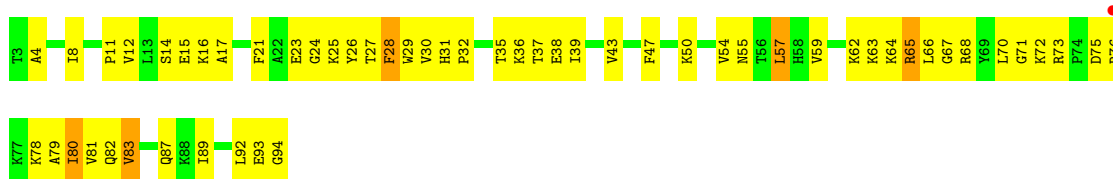
- Molecule 41: 50S ribosomal protein L22

Chain DS:



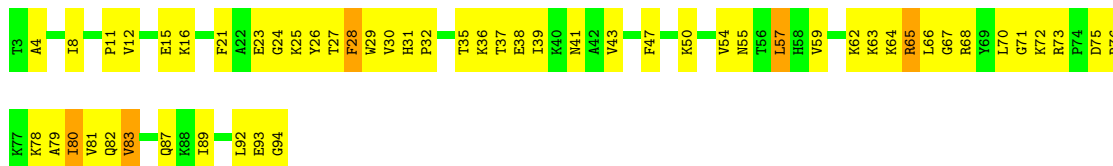
- Molecule 42: 50S ribosomal protein L23

Chain BT:



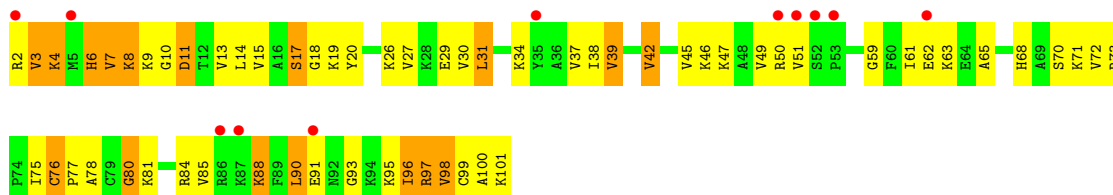
- Molecule 42: 50S ribosomal protein L23

Chain DT:



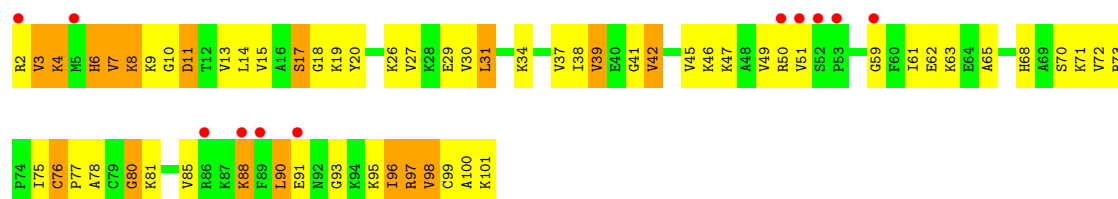
- Molecule 43: 50S ribosomal protein L24

Chain BU:



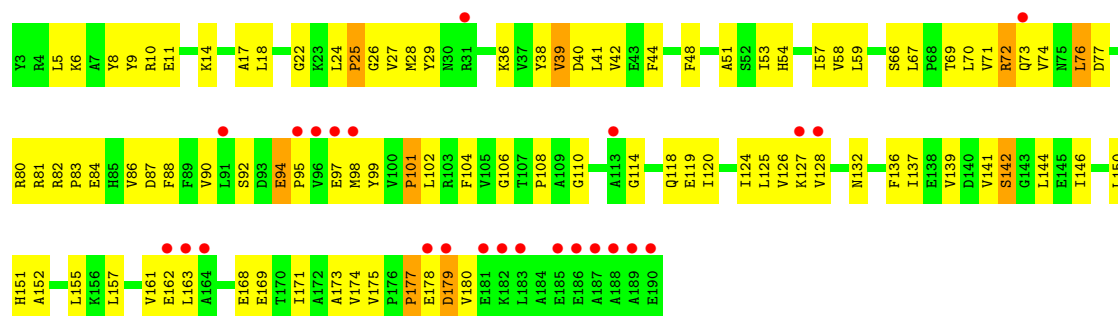
- Molecule 43: 50S ribosomal protein L24

Chain DU:



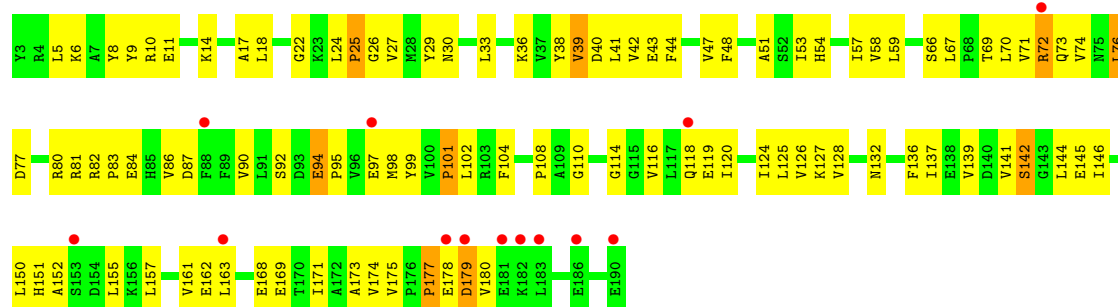
- Molecule 44: 50S ribosomal protein L25

Chain BV:



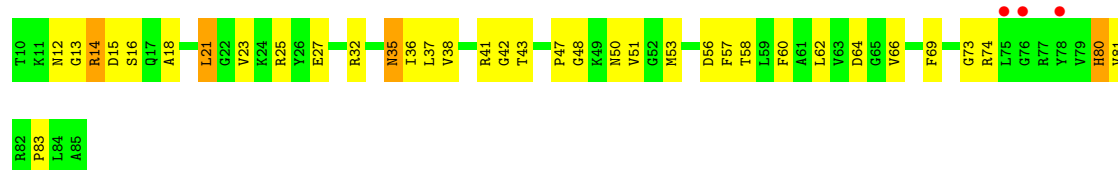
- Molecule 44: 50S ribosomal protein L25

Chain DV:



- Molecule 45: 50S ribosomal protein L27

Chain BW:



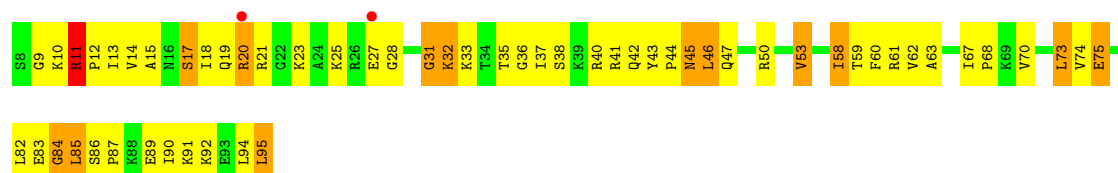
- Molecule 45: 50S ribosomal protein L27

Chain DW:



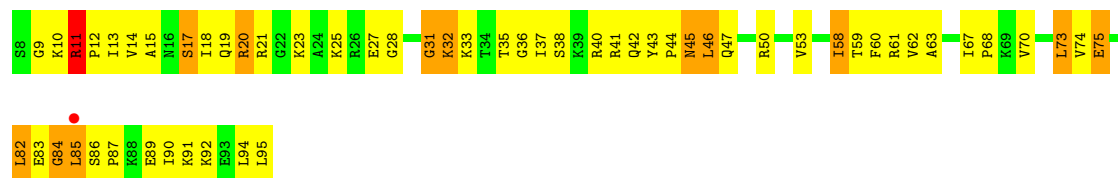
- Molecule 46: 50S ribosomal protein L28

Chain BX:



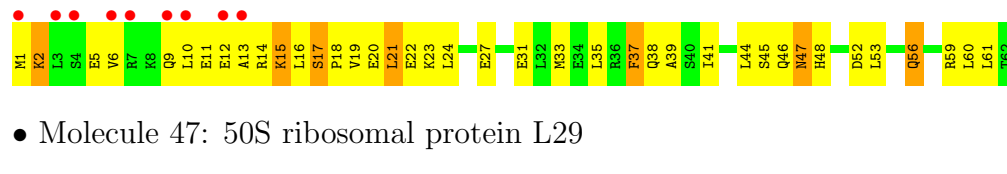
- Molecule 46: 50S ribosomal protein L28

Chain DX:



- Molecule 47: 50S ribosomal protein L29

Chain BY:



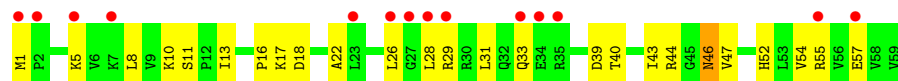
- Molecule 47: 50S ribosomal protein L29

Chain DY:



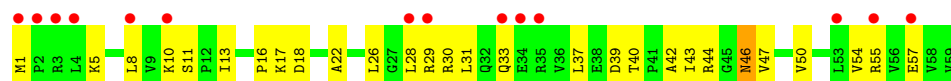
- Molecule 48: 50S ribosomal protein L30

Chain BZ:

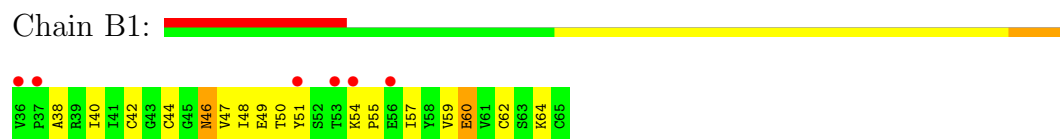


- Molecule 48: 50S ribosomal protein L30

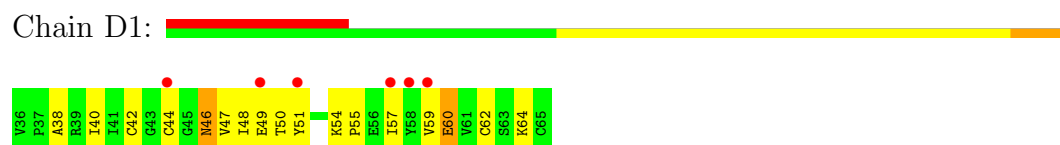
Chain DZ:



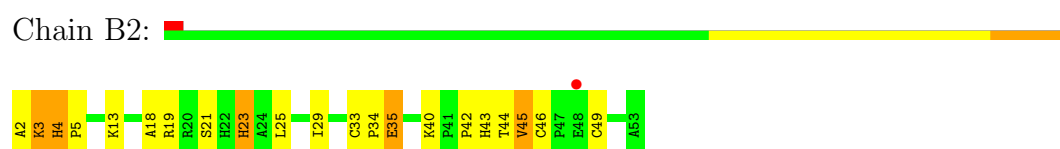
- Molecule 49: 50S ribosomal protein L31



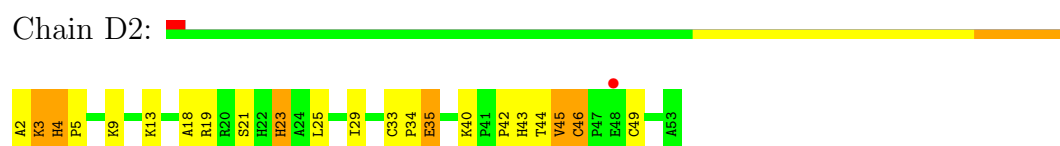
- Molecule 49: 50S ribosomal protein L31



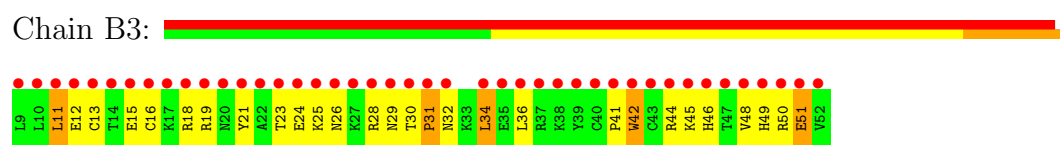
- Molecule 50: 50S ribosomal protein L32



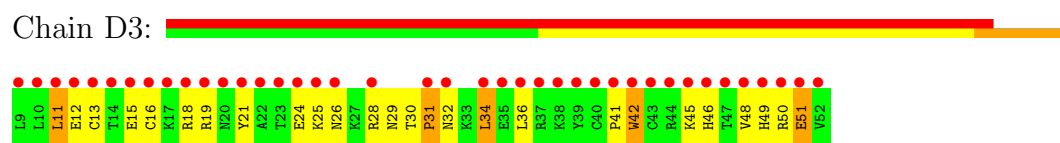
- Molecule 50: 50S ribosomal protein L32



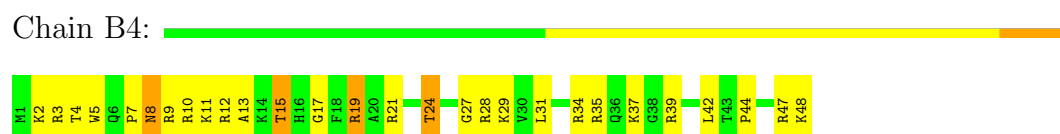
- Molecule 51: 50S ribosomal protein L33



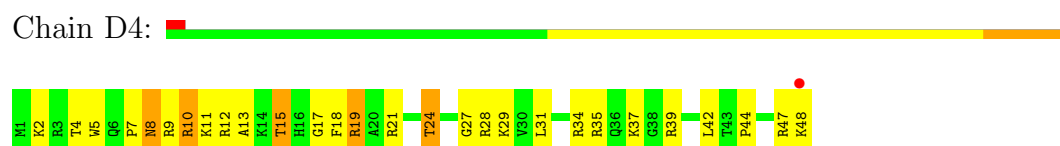
- Molecule 51: 50S ribosomal protein L33



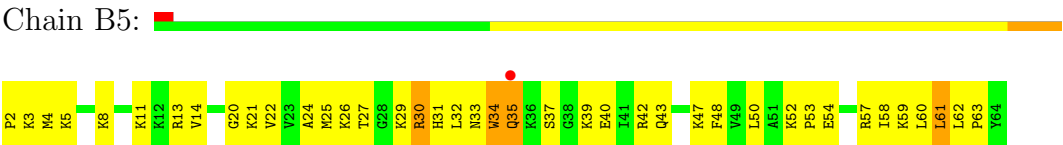
- Molecule 52: 50S ribosomal protein L34



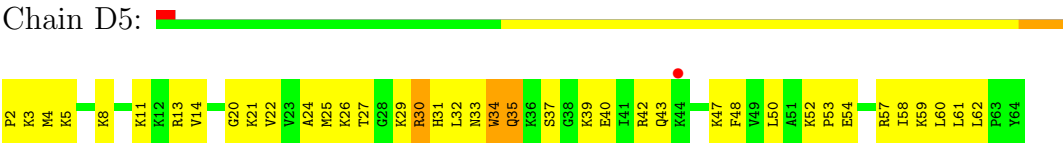
- Molecule 52: 50S ribosomal protein L34



● 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 60.01 – 3.49	Depositor EDS
% Data completeness (in resolution range)	99.9 (50.00-3.50) 99.6 (60.01-3.49)	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 (phenix.refine: 1.5_2)	Depositor
R, R_{free}	0.233 , 0.264 0.302 , 0.324	Depositor DCC
R_{free} test set	6611 reflections (0.89%)	DCC
Wilson B-factor (Å ²)	106.2	Xtriage
Anisotropy	0.163	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.24 , 69.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.38$, $\langle L^2 \rangle = 0.21$	Xtriage
Outliers	1 of 746568 reflections (0.000%)	Xtriage
F_o, F_c correlation	0.91	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.

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	0.45	0/36238	0.90	34/56561 (0.1%)
1	CA	0.44	0/36238	0.90	34/56561 (0.1%)
2	AB	0.21	0/1936	0.38	0/2609
2	CB	0.21	0/1936	0.38	0/2609
3	AC	0.21	0/1637	0.37	0/2205
3	CC	0.21	0/1637	0.37	0/2205
4	AD	0.24	0/1733	0.40	0/2318
4	CD	0.23	0/1733	0.39	0/2318
5	AE	0.24	0/1172	0.41	0/1576
5	CE	0.23	0/1172	0.40	0/1576
6	AF	0.23	0/856	0.42	0/1154
6	CF	0.23	0/856	0.43	0/1154
7	AG	0.21	0/1276	0.36	0/1709
7	CG	0.22	0/1276	0.36	0/1709
8	AH	0.23	0/1136	0.41	0/1527
8	CH	0.22	0/1136	0.41	0/1527
9	AI	0.22	0/1029	0.38	0/1378
9	CI	0.22	0/1029	0.38	0/1378
10	AJ	0.21	0/808	0.39	0/1085
10	CJ	0.21	0/808	0.39	0/1085
11	AK	0.23	0/900	0.40	0/1213
11	CK	0.23	0/900	0.40	0/1213
12	AL	0.25	0/987	0.46	0/1320
12	CL	0.24	0/987	0.46	0/1320
13	AM	0.24	0/939	0.41	0/1258
13	CM	0.24	0/939	0.41	0/1258
14	AN	0.23	0/501	0.37	0/664
14	CN	0.22	0/501	0.37	0/664
15	AO	0.24	0/745	0.38	0/992
15	CO	0.24	0/745	0.38	0/992
16	AP	0.36	1/717 (0.1%)	0.44	0/963
16	CP	0.44	1/717 (0.1%)	0.45	0/963

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	AQ	0.24	0/837	0.41	0/1117
17	CQ	0.23	0/837	0.40	0/1117
18	AR	0.24	0/579	0.42	0/768
18	CR	0.23	0/579	0.42	0/768
19	AS	0.20	0/643	0.37	0/865
19	CS	0.21	0/643	0.37	0/865
20	AT	0.23	0/764	0.39	0/1006
20	CT	0.22	0/764	0.39	0/1006
21	AU	0.20	0/213	0.37	0/277
21	CU	0.19	0/213	0.37	0/277
22	AV	0.43	0/821	0.86	2/1275 (0.2%)
22	CV	0.44	0/821	0.86	2/1275 (0.2%)
23	BA	0.51	0/66575	1.03	115/103930 (0.1%)
23	DA	0.54	0/66575	1.04	119/103930 (0.1%)
24	BB	0.44	0/2853	0.92	1/4451 (0.0%)
24	DB	0.44	0/2853	0.93	2/4451 (0.0%)
25	BC	0.33	0/2155	0.51	0/2905
25	DC	0.34	0/2155	0.52	0/2905
26	BD	0.27	0/1597	0.48	0/2153
26	DD	0.27	0/1597	0.48	0/2153
27	BE	0.29	0/1622	0.46	0/2194
27	DE	0.31	0/1622	0.47	0/2194
28	BF	0.23	0/1500	0.42	0/2017
28	DF	0.23	0/1500	0.42	0/2017
29	BG	0.22	0/1246	0.42	0/1682
29	DG	0.24	0/1246	0.43	0/1682
30	BH	0.29	0/1148	0.46	0/1552
30	DH	0.31	0/1148	0.47	0/1552
31	BI	0.21	0/252	0.38	0/333
31	DI	0.22	0/252	0.38	0/333
32	BJ	0.26	0/1124	0.47	0/1515
32	DJ	0.27	0/1124	0.47	0/1515
33	BK	0.27	0/942	0.48	0/1268
33	DK	0.28	0/942	0.49	0/1268
34	BL	0.30	0/1131	0.56	0/1504
34	DL	0.32	0/1131	0.57	0/1504
35	BM	0.30	0/1099	0.49	0/1468
35	DM	0.30	0/1099	0.50	0/1468
36	BN	0.26	0/974	0.45	0/1302
36	DN	0.27	0/974	0.45	0/1302
37	BO	0.23	0/779	0.42	0/1036
37	DO	0.24	0/779	0.42	0/1036
38	BP	0.27	0/1158	0.44	0/1544

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
38	DP	0.27	0/1158	0.44	0/1544
39	BQ	0.29	0/970	0.46	0/1290
39	DQ	0.31	0/970	0.47	0/1290
40	BR	0.27	0/790	0.45	0/1057
40	DR	0.29	0/790	0.46	0/1057
41	BS	0.31	0/902	0.51	0/1209
41	DS	0.30	0/902	0.50	0/1209
42	BT	0.30	0/740	0.49	0/993
42	DT	0.33	0/740	0.50	0/993
43	BU	0.25	0/789	0.44	0/1051
43	DU	0.26	0/789	0.45	0/1051
44	BV	0.23	0/1524	0.44	0/2068
44	DV	0.23	0/1524	0.45	0/2068
45	BW	0.26	0/613	0.43	0/816
45	DW	0.27	0/613	0.43	0/816
46	BX	0.30	0/702	0.56	0/932
46	DX	0.31	0/702	0.57	0/932
47	BY	0.29	0/523	0.52	0/690
47	DY	0.31	0/523	0.54	0/690
48	BZ	0.23	0/473	0.41	0/634
48	DZ	0.24	0/473	0.41	0/634
49	B1	0.20	0/229	0.38	0/309
49	D1	0.20	0/229	0.38	0/309
50	B2	0.28	0/419	0.51	0/567
50	D2	0.28	0/419	0.51	0/567
51	B3	0.21	0/388	0.40	0/518
51	D3	0.21	0/388	0.40	0/518
52	B4	0.34	0/427	0.52	0/561
52	D4	0.38	0/427	0.53	0/561
53	B5	0.31	0/516	0.50	0/679
53	D5	0.32	0/516	0.51	0/679
All	All	0.44	2/305254 (0.0%)	0.87	309/456136 (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

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	CP	48	TRP	CG-CD1	7.51	1.47	1.36
16	AP	48	TRP	CG-CD1	6.09	1.45	1.36

The worst 5 of 309 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	BA	945	A	C1'-O4'-C4'	-10.48	101.52	109.90
23	BA	1786	A	C1'-O4'-C4'	-10.25	101.70	109.90
23	DA	676	A	C1'-O4'-C4'	-9.79	102.07	109.90
23	DA	1786	A	C1'-O4'-C4'	-9.78	102.07	109.90
23	DA	945	A	C1'-O4'-C4'	-9.73	102.11	109.90

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 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	AA	32372	0	16339	682	0
1	CA	32372	0	16339	694	0
2	AB	1901	0	1951	103	0
2	CB	1901	0	1951	103	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	AC	1613	0	1677	95	0
3	CC	1613	0	1677	95	0
4	AD	1703	0	1764	100	0
4	CD	1703	0	1765	92	0
5	AE	1156	0	1213	68	0
5	CE	1156	0	1213	66	0
6	AF	843	0	857	46	0
6	CF	843	0	857	46	0
7	AG	1257	0	1296	60	0
7	CG	1257	0	1296	62	0
8	AH	1116	0	1177	57	0
8	CH	1116	0	1177	59	0
9	AI	1011	0	1043	62	0
9	CI	1011	0	1043	58	0
10	AJ	795	0	840	59	0
10	CJ	795	0	840	59	0
11	AK	885	0	904	56	0
11	CK	885	0	904	50	0
12	AL	971	0	1057	60	0
12	CL	971	0	1057	66	0
13	AM	929	0	987	66	0
13	CM	929	0	987	64	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	29	0
16	AP	701	0	720	30	0
16	CP	701	0	720	38	0
17	AQ	824	0	893	42	0
17	CQ	824	0	893	44	0
18	AR	574	0	644	30	0
18	CR	574	0	644	32	0
19	AS	630	0	652	59	0
19	CS	630	0	652	54	0
20	AT	762	0	859	32	0
20	CT	762	0	859	31	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	18	0
23	BA	59442	0	29966	1292	0
23	DA	59442	0	29966	1295	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
24	BB	2551	0	1295	53	0
24	DB	2551	0	1295	53	0
25	BC	2105	0	2182	202	0
25	DC	2105	0	2182	214	0
26	BD	1564	0	1629	117	0
26	DD	1564	0	1629	112	0
27	BE	1587	0	1632	107	0
27	DE	1587	0	1632	106	0
28	BF	1475	0	1537	109	0
28	DF	1475	0	1537	109	0
29	BG	1223	0	1282	64	0
29	DG	1223	0	1282	66	0
30	BH	1133	0	1220	83	0
30	DH	1133	0	1220	80	0
31	BI	254	0	275	8	0
31	DI	254	0	275	8	0
32	BJ	1097	0	1168	82	0
32	DJ	1097	0	1168	83	0
33	BK	932	0	994	54	0
33	DK	932	0	994	56	0
34	BL	1114	0	1187	167	0
34	DL	1114	0	1187	169	0
35	BM	1079	0	1127	96	0
35	DM	1079	0	1127	99	0
36	BN	960	0	1021	73	0
36	DN	960	0	1021	71	0
37	BO	771	0	832	67	0
37	DO	771	0	832	70	0
38	BP	1144	0	1211	69	0
38	DP	1144	0	1211	74	0
39	BQ	953	0	1013	71	0
39	DQ	953	0	1013	71	0
40	BR	779	0	852	76	0
40	DR	779	0	852	73	0
41	BS	891	0	951	50	0
41	DS	891	0	951	52	0
42	BT	726	0	778	58	0
42	DT	726	0	778	59	0
43	BU	776	0	870	78	0
43	DU	776	0	870	76	0
44	BV	1492	0	1513	94	0
44	DV	1492	0	1513	92	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
45	BW	605	0	628	36	0
45	DW	605	0	628	38	0
46	BX	695	0	764	69	0
46	DX	695	0	764	68	0
47	BY	521	0	575	45	0
47	DY	521	0	575	45	0
48	BZ	468	0	523	20	0
48	DZ	468	0	523	24	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	30	0
52	D4	419	0	467	32	0
53	B5	508	0	576	54	0
53	D5	508	0	576	55	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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
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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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
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	9280	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 20.

The worst 5 of 9280 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(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

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	AB	232/234 (99%)	194 (84%)	32 (14%)	6 (3%)	8	57
2	CB	232/234 (99%)	194 (84%)	32 (14%)	6 (3%)	8	57
3	AC	204/206 (99%)	153 (75%)	38 (19%)	13 (6%)	2	29
3	CC	204/206 (99%)	154 (76%)	37 (18%)	13 (6%)	2	29
4	AD	206/208 (99%)	172 (84%)	26 (13%)	8 (4%)	5	45
4	CD	206/208 (99%)	172 (84%)	25 (12%)	9 (4%)	4	41
5	AE	149/151 (99%)	123 (83%)	22 (15%)	4 (3%)	8	56
5	CE	149/151 (99%)	126 (85%)	19 (13%)	4 (3%)	8	56
6	AF	99/101 (98%)	90 (91%)	8 (8%)	1 (1%)	22	78
6	CF	99/101 (98%)	90 (91%)	8 (8%)	1 (1%)	22	78
7	AG	153/155 (99%)	132 (86%)	18 (12%)	3 (2%)	11	63
7	CG	153/155 (99%)	133 (87%)	17 (11%)	3 (2%)	11	63
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%)	9	59
9	CI	125/127 (98%)	101 (81%)	21 (17%)	3 (2%)	9	59
10	AJ	96/98 (98%)	78 (81%)	12 (12%)	6 (6%)	2	29
10	CJ	96/98 (98%)	78 (81%)	12 (12%)	6 (6%)	2	29
11	AK	117/119 (98%)	97 (83%)	16 (14%)	4 (3%)	6	50
11	CK	117/119 (98%)	97 (83%)	16 (14%)	4 (3%)	6	50
12	AL	122/124 (98%)	94 (77%)	22 (18%)	6 (5%)	3	37
12	CL	122/124 (98%)	94 (77%)	22 (18%)	6 (5%)	3	37
13	AM	114/116 (98%)	94 (82%)	16 (14%)	4 (4%)	6	50
13	CM	114/116 (98%)	94 (82%)	16 (14%)	4 (4%)	6	50
14	AN	58/60 (97%)	50 (86%)	5 (9%)	3 (5%)	3	35

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
14	CN	58/60 (97%)	50 (86%)	5 (9%)	3 (5%)	3	35
15	AO	86/88 (98%)	77 (90%)	7 (8%)	2 (2%)	10	60
15	CO	86/88 (98%)	77 (90%)	7 (8%)	2 (2%)	10	60
16	AP	81/83 (98%)	65 (80%)	14 (17%)	2 (2%)	9	57
16	CP	81/83 (98%)	65 (80%)	13 (16%)	3 (4%)	5	48
17	AQ	97/99 (98%)	81 (84%)	15 (16%)	1 (1%)	22	78
17	CQ	97/99 (98%)	81 (84%)	15 (16%)	1 (1%)	22	78
18	AR	68/70 (97%)	53 (78%)	13 (19%)	2 (3%)	7	54
18	CR	68/70 (97%)	53 (78%)	12 (18%)	3 (4%)	4	41
19	AS	76/78 (97%)	57 (75%)	14 (18%)	5 (7%)	2	28
19	CS	76/78 (97%)	57 (75%)	14 (18%)	5 (7%)	2	28
20	AT	97/99 (98%)	82 (84%)	12 (12%)	3 (3%)	7	53
20	CT	97/99 (98%)	82 (84%)	12 (12%)	3 (3%)	7	53
21	AU	22/24 (92%)	17 (77%)	4 (18%)	1 (4%)	4	40
21	CU	22/24 (92%)	17 (77%)	4 (18%)	1 (4%)	4	40
25	BC	269/271 (99%)	220 (82%)	31 (12%)	18 (7%)	2	28
25	DC	269/271 (99%)	218 (81%)	33 (12%)	18 (7%)	2	28
26	BD	202/204 (99%)	168 (83%)	26 (13%)	8 (4%)	5	44
26	DD	202/204 (99%)	167 (83%)	29 (14%)	6 (3%)	7	53
27	BE	200/202 (99%)	165 (82%)	28 (14%)	7 (4%)	6	50
27	DE	200/202 (99%)	165 (82%)	28 (14%)	7 (4%)	6	50
28	BF	179/181 (99%)	134 (75%)	37 (21%)	8 (4%)	4	40
28	DF	179/181 (99%)	133 (74%)	37 (21%)	9 (5%)	3	37
29	BG	157/159 (99%)	126 (80%)	27 (17%)	4 (2%)	9	57
29	DG	157/159 (99%)	125 (80%)	28 (18%)	4 (2%)	9	57
30	BH	143/145 (99%)	109 (76%)	28 (20%)	6 (4%)	4	43
30	DH	143/145 (99%)	109 (76%)	28 (20%)	6 (4%)	4	43
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%)	2	32
32	DJ	135/137 (98%)	108 (80%)	19 (14%)	8 (6%)	2	32

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
33	BK	120/122 (98%)	105 (88%)	8 (7%)	7 (6%)	3	32
33	DK	120/122 (98%)	107 (89%)	6 (5%)	7 (6%)	3	32
34	BL	144/146 (99%)	94 (65%)	35 (24%)	15 (10%)	1	14
34	DL	144/146 (99%)	92 (64%)	37 (26%)	15 (10%)	1	14
35	BM	134/136 (98%)	98 (73%)	22 (16%)	14 (10%)	1	14
35	DM	134/136 (98%)	97 (72%)	24 (18%)	13 (10%)	1	16
36	BN	115/117 (98%)	97 (84%)	13 (11%)	5 (4%)	4	42
36	DN	115/117 (98%)	97 (84%)	14 (12%)	4 (4%)	6	50
37	BO	96/98 (98%)	65 (68%)	18 (19%)	13 (14%)	0	8
37	DO	96/98 (98%)	65 (68%)	18 (19%)	13 (14%)	0	8
38	BP	135/137 (98%)	99 (73%)	30 (22%)	6 (4%)	4	41
38	DP	135/137 (98%)	99 (73%)	30 (22%)	6 (4%)	4	41
39	BQ	114/116 (98%)	99 (87%)	13 (11%)	2 (2%)	13	65
39	DQ	114/116 (98%)	99 (87%)	13 (11%)	2 (2%)	13	65
40	BR	99/101 (98%)	71 (72%)	19 (19%)	9 (9%)	1	18
40	DR	99/101 (98%)	71 (72%)	19 (19%)	9 (9%)	1	18
41	BS	110/112 (98%)	94 (86%)	14 (13%)	2 (2%)	13	65
41	DS	110/112 (98%)	94 (86%)	14 (13%)	2 (2%)	13	65
42	BT	90/92 (98%)	82 (91%)	7 (8%)	1 (1%)	21	77
42	DT	90/92 (98%)	82 (91%)	7 (8%)	1 (1%)	21	77
43	BU	98/100 (98%)	65 (66%)	22 (22%)	11 (11%)	1	13
43	DU	98/100 (98%)	63 (64%)	23 (24%)	12 (12%)	1	11
44	BV	186/188 (99%)	140 (75%)	36 (19%)	10 (5%)	3	35
44	DV	186/188 (99%)	140 (75%)	36 (19%)	10 (5%)	3	35
45	BW	74/76 (97%)	59 (80%)	12 (16%)	3 (4%)	4	44
45	DW	74/76 (97%)	57 (77%)	14 (19%)	3 (4%)	4	44
46	BX	86/88 (98%)	57 (66%)	20 (23%)	9 (10%)	1	14
46	DX	86/88 (98%)	57 (66%)	20 (23%)	9 (10%)	1	14
47	BY	60/62 (97%)	48 (80%)	9 (15%)	3 (5%)	3	37
47	DY	60/62 (97%)	49 (82%)	8 (13%)	3 (5%)	3	37
48	BZ	57/59 (97%)	51 (90%)	5 (9%)	1 (2%)	13	65

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
48	DZ	57/59 (97%)	51 (90%)	5 (9%)	1 (2%)	13	65
49	B1	28/30 (93%)	15 (54%)	10 (36%)	3 (11%)	1	13
49	D1	28/30 (93%)	15 (54%)	10 (36%)	3 (11%)	1	13
50	B2	50/52 (96%)	39 (78%)	8 (16%)	3 (6%)	2	31
50	D2	50/52 (96%)	40 (80%)	6 (12%)	4 (8%)	1	21
51	B3	42/44 (96%)	35 (83%)	2 (5%)	5 (12%)	1	11
51	D3	42/44 (96%)	35 (83%)	2 (5%)	5 (12%)	1	11
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%)	1	21
53	D5	61/63 (97%)	44 (72%)	13 (21%)	4 (7%)	2	28
All	All	11192/11458 (98%)	8966 (80%)	1699 (15%)	527 (5%)	4	39

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%)	192 (95%)	10 (5%)	34	79
2	CB	202/202 (100%)	192 (95%)	10 (5%)	34	79
3	AC	160/160 (100%)	154 (96%)	6 (4%)	44	85
3	CC	160/160 (100%)	154 (96%)	6 (4%)	44	85
4	AD	180/180 (100%)	168 (93%)	12 (7%)	23	70
4	CD	180/180 (100%)	167 (93%)	13 (7%)	21	67

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	AE	116/116 (100%)	108 (93%)	8 (7%)	22	69
5	CE	116/116 (100%)	108 (93%)	8 (7%)	22	69
6	AF	90/90 (100%)	85 (94%)	5 (6%)	30	76
6	CF	90/90 (100%)	85 (94%)	5 (6%)	30	76
7	AG	126/126 (100%)	126 (100%)	0	100	100
7	CG	126/126 (100%)	126 (100%)	0	100	100
8	AH	119/119 (100%)	114 (96%)	5 (4%)	40	84
8	CH	119/119 (100%)	114 (96%)	5 (4%)	40	84
9	AI	98/98 (100%)	92 (94%)	6 (6%)	26	73
9	CI	98/98 (100%)	92 (94%)	6 (6%)	26	73
10	AJ	88/88 (100%)	79 (90%)	9 (10%)	11	48
10	CJ	88/88 (100%)	79 (90%)	9 (10%)	11	48
11	AK	90/90 (100%)	86 (96%)	4 (4%)	39	83
11	CK	90/90 (100%)	86 (96%)	4 (4%)	39	83
12	AL	104/104 (100%)	94 (90%)	10 (10%)	12	51
12	CL	104/104 (100%)	94 (90%)	10 (10%)	12	51
13	AM	94/94 (100%)	88 (94%)	6 (6%)	25	72
13	CM	94/94 (100%)	88 (94%)	6 (6%)	25	72
14	AN	49/49 (100%)	47 (96%)	2 (4%)	41	84
14	CN	49/49 (100%)	48 (98%)	1 (2%)	68	93
15	AO	79/79 (100%)	75 (95%)	4 (5%)	33	79
15	CO	79/79 (100%)	75 (95%)	4 (5%)	33	79
16	AP	72/72 (100%)	67 (93%)	5 (7%)	22	69
16	CP	72/72 (100%)	68 (94%)	4 (6%)	30	76
17	AQ	94/94 (100%)	92 (98%)	2 (2%)	66	92
17	CQ	94/94 (100%)	92 (98%)	2 (2%)	66	92
18	AR	61/61 (100%)	59 (97%)	2 (3%)	50	88
18	CR	61/61 (100%)	59 (97%)	2 (3%)	50	88
19	AS	69/69 (100%)	60 (87%)	9 (13%)	6	33
19	CS	69/69 (100%)	60 (87%)	9 (13%)	6	33
20	AT	76/76 (100%)	71 (93%)	5 (7%)	24	71

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
20	CT	76/76 (100%)	71 (93%)	5 (7%)	24	71
21	AU	19/19 (100%)	18 (95%)	1 (5%)	32	78
21	CU	19/19 (100%)	18 (95%)	1 (5%)	32	78
25	BC	213/213 (100%)	192 (90%)	21 (10%)	11	49
25	DC	213/213 (100%)	192 (90%)	21 (10%)	11	49
26	BD	165/165 (100%)	149 (90%)	16 (10%)	12	50
26	DD	165/165 (100%)	149 (90%)	16 (10%)	12	50
27	BE	161/161 (100%)	148 (92%)	13 (8%)	17	61
27	DE	161/161 (100%)	147 (91%)	14 (9%)	15	57
28	BF	155/155 (100%)	144 (93%)	11 (7%)	21	67
28	DF	155/155 (100%)	144 (93%)	11 (7%)	21	67
29	BG	132/132 (100%)	123 (93%)	9 (7%)	22	70
29	DG	132/132 (100%)	123 (93%)	9 (7%)	22	70
30	BH	122/122 (100%)	115 (94%)	7 (6%)	29	76
30	DH	122/122 (100%)	115 (94%)	7 (6%)	29	76
31	BI	27/53 (51%)	26 (96%)	1 (4%)	45	86
31	DI	27/53 (51%)	26 (96%)	1 (4%)	45	86
32	BJ	116/116 (100%)	103 (89%)	13 (11%)	9	41
32	DJ	116/116 (100%)	103 (89%)	13 (11%)	9	41
33	BK	100/100 (100%)	92 (92%)	8 (8%)	17	61
33	DK	100/100 (100%)	92 (92%)	8 (8%)	17	61
34	BL	112/112 (100%)	87 (78%)	25 (22%)	1	8
34	DL	112/112 (100%)	87 (78%)	25 (22%)	1	8
35	BM	106/106 (100%)	98 (92%)	8 (8%)	19	65
35	DM	106/106 (100%)	98 (92%)	8 (8%)	19	65
36	BN	100/100 (100%)	94 (94%)	6 (6%)	27	74
36	DN	100/100 (100%)	94 (94%)	6 (6%)	27	74
37	BO	77/77 (100%)	68 (88%)	9 (12%)	8	38
37	DO	77/77 (100%)	68 (88%)	9 (12%)	8	38
38	BP	121/121 (100%)	109 (90%)	12 (10%)	11	49
38	DP	121/121 (100%)	110 (91%)	11 (9%)	14	54

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
39	BQ	92/92 (100%)	88 (96%)	4 (4%)	40	84
39	DQ	92/92 (100%)	88 (96%)	4 (4%)	40	84
40	BR	82/82 (100%)	77 (94%)	5 (6%)	26	73
40	DR	82/82 (100%)	77 (94%)	5 (6%)	26	73
41	BS	91/91 (100%)	85 (93%)	6 (7%)	24	71
41	DS	91/91 (100%)	85 (93%)	6 (7%)	24	71
42	BT	74/74 (100%)	67 (90%)	7 (10%)	12	51
42	DT	74/74 (100%)	67 (90%)	7 (10%)	12	51
43	BU	84/84 (100%)	78 (93%)	6 (7%)	21	67
43	DU	84/84 (100%)	78 (93%)	6 (7%)	21	67
44	BV	163/163 (100%)	159 (98%)	4 (2%)	60	91
44	DV	163/163 (100%)	159 (98%)	4 (2%)	60	91
45	BW	61/61 (100%)	55 (90%)	6 (10%)	12	50
45	DW	61/61 (100%)	55 (90%)	6 (10%)	12	50
46	BX	73/73 (100%)	61 (84%)	12 (16%)	3	20
46	DX	73/73 (100%)	61 (84%)	12 (16%)	3	20
47	BY	58/58 (100%)	51 (88%)	7 (12%)	7	36
47	DY	58/58 (100%)	51 (88%)	7 (12%)	7	36
48	BZ	51/51 (100%)	49 (96%)	2 (4%)	43	85
48	DZ	51/51 (100%)	49 (96%)	2 (4%)	43	85
49	B1	27/27 (100%)	24 (89%)	3 (11%)	9	42
49	D1	27/27 (100%)	24 (89%)	3 (11%)	9	42
50	B2	45/45 (100%)	43 (96%)	2 (4%)	39	83
50	D2	45/45 (100%)	43 (96%)	2 (4%)	39	83
51	B3	43/43 (100%)	39 (91%)	4 (9%)	13	53
51	D3	43/43 (100%)	39 (91%)	4 (9%)	13	53
52	B4	41/41 (100%)	34 (83%)	7 (17%)	3	18
52	D4	41/41 (100%)	34 (83%)	7 (17%)	3	18
53	B5	53/53 (100%)	51 (96%)	2 (4%)	44	85
53	D5	53/53 (100%)	51 (96%)	2 (4%)	44	85
All	All	9462/9514 (100%)	8769 (93%)	693 (7%)	20	66

5 of 693 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
46	BX	45	ASN
6	CF	98	LEU
43	DU	8	LYS
47	BY	37	PHE
2	CB	116	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 257 such sidechains are listed below:

Mol	Chain	Res	Type
46	BX	19	GLN
5	CE	78	HIS
43	DU	6	HIS
46	BX	66	HIS
53	B5	33	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	AA	1505/1506 (99%)	204 (13%)	35 (2%)
1	CA	1505/1506 (99%)	205 (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%)	410 (14%)	69 (2%)
23	DA	2757/2879 (95%)	407 (14%)	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%)	1262 (14%)	215 (2%)

5 of 1262 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	AA	9	G
1	AA	22	G
1	AA	32	A
1	AA	39	G
1	AA	41	G

5 of 215 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
23	BA	2468	G
1	CA	496	A
23	DA	2098	U
23	BA	2585	U
1	CA	119	A

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

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.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	AA	1506/1506 (100%)	0.03	41 (2%) 52 24	66, 119, 257, 429	0
1	CA	1506/1506 (100%)	0.28	92 (6%) 21 9	75, 164, 286, 403	0
2	AB	234/234 (100%)	1.45	69 (29%) 1 1	88, 178, 260, 354	0
2	CB	234/234 (100%)	1.22	57 (24%) 1 2	106, 202, 279, 372	0
3	AC	206/206 (100%)	0.61	23 (11%) 6 4	83, 165, 233, 293	0
3	CC	206/206 (100%)	0.91	34 (16%) 2 2	124, 198, 272, 337	0
4	AD	208/208 (100%)	0.21	2 (0%) 79 47	45, 119, 180, 228	0
4	CD	208/208 (100%)	0.73	20 (9%) 8 5	96, 186, 253, 314	0
5	AE	151/151 (100%)	0.28	5 (3%) 44 20	71, 118, 191, 293	0
5	CE	151/151 (100%)	0.54	7 (4%) 31 14	72, 165, 223, 282	0
6	AF	101/101 (100%)	0.72	19 (18%) 2 2	87, 160, 207, 278	0
6	CF	101/101 (100%)	0.27	6 (5%) 22 9	60, 130, 195, 271	0
7	AG	155/155 (100%)	1.32	33 (21%) 1 2	134, 201, 260, 328	0
7	CG	155/155 (100%)	1.26	34 (21%) 1 2	124, 213, 271, 320	0
8	AH	138/138 (100%)	0.67	17 (12%) 5 3	60, 122, 190, 265	0
8	CH	138/138 (100%)	0.76	15 (10%) 6 4	101, 171, 217, 257	0
9	AI	127/127 (100%)	1.66	47 (37%) 1 1	119, 228, 303, 333	0
9	CI	127/127 (100%)	1.48	35 (27%) 1 2	148, 229, 297, 370	0
10	AJ	98/98 (100%)	2.17	51 (52%) 0 1	113, 203, 294, 334	0
10	CJ	98/98 (100%)	1.89	38 (38%) 1 1	133, 232, 290, 339	0
11	AK	119/119 (100%)	0.13	9 (7%) 14 7	66, 136, 219, 274	0
11	CK	119/119 (100%)	0.40	5 (4%) 35 14	87, 145, 207, 287	0
12	AL	124/124 (100%)	0.73	7 (5%) 24 10	56, 108, 182, 328	0
12	CL	124/124 (100%)	0.55	8 (6%) 18 8	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%)	1.07	25 (21%) 1 2	129, 216, 277, 325	0
13	CM	116/116 (100%)	1.85	48 (41%) 1 1	119, 238, 307, 372	0
14	AN	60/60 (100%)	1.49	17 (28%) 1 1	94, 178, 243, 278	0
14	CN	60/60 (100%)	1.97	25 (41%) 1 1	110, 207, 261, 344	0
15	AO	88/88 (100%)	0.36	4 (4%) 32 14	73, 127, 187, 281	0
15	CO	88/88 (100%)	0.40	2 (2%) 57 27	73, 138, 201, 244	0
16	AP	83/83 (100%)	0.48	4 (4%) 29 13	67, 109, 175, 245	0
16	CP	83/83 (100%)	1.14	23 (27%) 1 1	128, 171, 247, 277	0
17	AQ	99/99 (100%)	0.17	0 100 100	63, 112, 169, 222	0
17	CQ	99/99 (100%)	0.87	16 (16%) 2 2	99, 155, 196, 228	0
18	AR	70/70 (100%)	1.39	19 (27%) 1 2	82, 149, 241, 325	0
18	CR	70/70 (100%)	0.78	5 (7%) 16 7	76, 145, 204, 232	0
19	AS	78/78 (100%)	1.39	20 (25%) 1 2	133, 212, 274, 295	0
19	CS	78/78 (100%)	1.92	30 (38%) 1 1	173, 235, 302, 347	0
20	AT	99/99 (100%)	0.68	7 (7%) 16 7	65, 131, 220, 241	0
20	CT	99/99 (100%)	2.08	41 (41%) 1 1	103, 178, 284, 301	0
21	AU	24/24 (100%)	2.25	9 (37%) 1 1	122, 220, 292, 333	0
21	CU	24/24 (100%)	2.27	13 (54%) 0 1	173, 236, 317, 346	0
22	AV	35/35 (100%)	1.32	8 (22%) 1 2	96, 223, 325, 366	0
22	CV	35/35 (100%)	1.09	5 (14%) 3 3	117, 192, 362, 386	0
23	BA	2760/2879 (95%)	-0.09	69 (2%) 54 25	38, 86, 205, 371	0
23	DA	2760/2879 (95%)	-0.18	40 (1%) 72 38	33, 77, 196, 377	0
24	BB	119/119 (100%)	-0.09	0 100 100	83, 149, 196, 251	0
24	DB	119/119 (100%)	0.05	7 (5%) 22 9	87, 132, 198, 274	0
25	BC	271/271 (100%)	0.23	3 (1%) 77 44	24, 81, 150, 209	0
25	DC	271/271 (100%)	-0.04	0 100 100	26, 72, 144, 220	0
26	BD	204/204 (100%)	0.39	8 (3%) 37 16	45, 96, 173, 331	0
26	DD	204/204 (100%)	0.21	3 (1%) 70 36	36, 90, 189, 305	0
27	BE	202/202 (100%)	0.33	3 (1%) 70 36	32, 94, 172, 311	0
27	DE	202/202 (100%)	0.37	7 (3%) 42 19	20, 85, 182, 249	0
28	BF	181/181 (100%)	0.60	16 (8%) 10 6	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%)	0.66	13 (7%) 15 7	109, 198, 281, 324	0
29	BG	159/159 (100%)	1.13	35 (22%) 1 2	102, 192, 269, 331	0
29	DG	159/159 (100%)	0.47	11 (6%) 17 7	61, 117, 190, 269	0
30	BH	145/145 (100%)	1.50	35 (24%) 1 2	60, 224, 376, 453	0
30	DH	145/145 (100%)	1.69	50 (34%) 1 1	60, 210, 372, 482	0
31	BI	32/65 (49%)	5.04	28 (87%) 0 0	163, 256, 325, 352	0
31	DI	32/65 (49%)	2.57	19 (59%) 0 1	176, 235, 294, 325	0
32	BJ	137/137 (100%)	0.53	3 (2%) 59 28	58, 105, 182, 221	0
32	DJ	137/137 (100%)	0.26	0 100 100	55, 101, 170, 219	0
33	BK	122/122 (100%)	0.04	1 (0%) 83 53	48, 90, 142, 194	0
33	DK	122/122 (100%)	0.09	0 100 100	41, 90, 153, 251	0
34	BL	146/146 (100%)	0.69	9 (6%) 20 9	40, 114, 204, 306	0
34	DL	146/146 (100%)	0.62	10 (6%) 17 8	27, 111, 207, 324	0
35	BM	136/136 (100%)	0.34	5 (3%) 39 17	57, 110, 205, 344	0
35	DM	136/136 (100%)	0.64	6 (4%) 33 14	46, 106, 199, 388	0
36	BN	117/117 (100%)	0.44	1 (0%) 81 51	44, 92, 166, 282	0
36	DN	117/117 (100%)	0.28	1 (0%) 81 51	41, 89, 173, 285	0
37	BO	98/98 (100%)	1.56	31 (31%) 1 1	89, 155, 230, 299	0
37	DO	98/98 (100%)	0.88	24 (24%) 1 2	80, 148, 221, 299	0
38	BP	137/137 (100%)	0.58	9 (6%) 18 8	52, 115, 216, 248	0
38	DP	137/137 (100%)	0.51	8 (5%) 22 9	60, 119, 249, 299	0
39	BQ	116/116 (100%)	0.10	0 100 100	43, 88, 163, 244	0
39	DQ	116/116 (100%)	0.08	0 100 100	34, 84, 154, 205	0
40	BR	101/101 (100%)	0.10	0 100 100	55, 134, 187, 294	0
40	DR	101/101 (100%)	0.06	0 100 100	52, 132, 197, 321	0
41	BS	112/112 (100%)	0.72	6 (5%) 25 10	45, 78, 151, 250	0
41	DS	112/112 (100%)	0.35	2 (1%) 65 33	40, 72, 166, 277	0
42	BT	92/92 (100%)	0.41	1 (1%) 77 44	57, 107, 174, 204	0
42	DT	92/92 (100%)	0.29	0 100 100	41, 78, 161, 204	0
43	BU	100/100 (100%)	0.64	11 (11%) 6 4	59, 139, 289, 344	0
43	DU	100/100 (100%)	0.83	11 (11%) 6 4	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%)	0.78	24 (12%) 4 3	80, 160, 224, 277	0
44	DV	188/188 (100%)	0.51	13 (6%) 17 7	67, 154, 220, 254	0
45	BW	76/76 (100%)	0.24	3 (3%) 37 16	61, 101, 160, 258	0
45	DW	76/76 (100%)	0.39	2 (2%) 53 24	54, 101, 167, 254	0
46	BX	88/88 (100%)	0.28	2 (2%) 57 27	50, 106, 191, 346	0
46	DX	88/88 (100%)	0.16	1 (1%) 77 44	31, 83, 196, 340	0
47	BY	62/62 (100%)	0.56	9 (14%) 3 3	61, 141, 244, 287	0
47	DY	62/62 (100%)	0.57	5 (8%) 12 6	45, 99, 224, 304	0
48	BZ	59/59 (100%)	1.54	14 (23%) 1 2	47, 102, 174, 342	0
48	DZ	59/59 (100%)	1.49	14 (23%) 1 2	45, 102, 189, 335	0
49	B1	30/30 (100%)	1.25	6 (20%) 2 2	161, 244, 282, 323	0
49	D1	30/30 (100%)	1.52	6 (20%) 2 2	187, 262, 306, 326	0
50	B2	52/52 (100%)	0.13	1 (1%) 64 32	36, 93, 189, 273	0
50	D2	52/52 (100%)	-0.13	1 (1%) 64 32	24, 93, 214, 262	0
51	B3	44/44 (100%)	5.41	43 (97%) 0 0	151, 254, 304, 322	0
51	D3	44/44 (100%)	6.04	40 (90%) 0 0	191, 247, 298, 313	0
52	B4	48/48 (100%)	0.41	0 100 100	43, 66, 132, 297	0
52	D4	48/48 (100%)	0.00	1 (2%) 60 29	23, 45, 122, 217	0
53	B5	63/63 (100%)	0.22	1 (1%) 68 35	47, 94, 171, 222	0
53	D5	63/63 (100%)	0.57	1 (1%) 68 35	43, 92, 170, 209	0
All	All	20232/20536 (98%)	0.42	1668 (8%) 12 6	20, 120, 258, 482	0

The worst 5 of 1668 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	AA	85	U	21.8
1	AA	82	U	16.2
1	AA	84	U	15.6
30	DH	90	GLY	14.1
51	B3	39	TYR	13.7

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 carbohydrates in this entry.

6.4 Ligands

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	RSR	LLDF	B-factors(Å ²)	Q<0.9
54	MG	DA	3698	1/1	0.67	-	61,61,61,61	0
54	MG	DA	3303	1/1	0.29	-	67,67,67,67	0
54	MG	BA	3555	1/1	0.33	-	66,66,66,66	0
54	MG	AA	1720	1/1	1.04	-	101,101,101,101	0
54	MG	BA	3417	1/1	0.16	-	65,65,65,65	0
54	MG	DA	3278	1/1	0.79	-	99,99,99,99	0
54	MG	CA	1604	1/1	0.49	-	43,43,43,43	0
54	MG	DA	3113	1/1	0.21	-	66,66,66,66	0
54	MG	DA	3166	1/1	0.08	-	73,73,73,73	0
54	MG	DA	3496	1/1	0.46	-	95,95,95,95	0
54	MG	CA	1711	1/1	0.50	-	76,76,76,76	0
54	MG	DA	3242	1/1	0.12	-	59,59,59,59	0
54	MG	AA	1690	1/1	0.34	-	88,88,88,88	0
54	MG	BA	2940	1/1	0.34	-	30,30,30,30	0
54	MG	DA	2929	1/1	0.48	-	21,21,21,21	0
54	MG	BV	203	1/1	0.09	-	104,104,104,104	0
54	MG	DA	3421	1/1	0.13	-	63,63,63,63	0
54	MG	DA	3379	1/1	0.05	-	78,78,78,78	0
54	MG	BA	3672	1/1	0.31	-	92,92,92,92	0
54	MG	CA	1634	1/1	0.41	-	78,78,78,78	0
54	MG	AK	202	1/1	0.10	-	101,101,101,101	0
54	MG	DA	3820	1/1	0.99	-	59,59,59,59	0
54	MG	DA	3332	1/1	0.78	-	88,88,88,88	0
54	MG	AA	1760	1/1	0.58	-	88,88,88,88	0
54	MG	BA	3072	1/1	0.41	-	57,57,57,57	0
54	MG	BA	3399	1/1	0.40	-	104,104,104,104	0
54	MG	BA	3602	1/1	0.57	-	98,98,98,98	0
54	MG	CA	1652	1/1	0.14	-	87,87,87,87	0
54	MG	DA	3508	1/1	0.16	-	70,70,70,70	0
54	MG	BA	3633	1/1	0.55	-	88,88,88,88	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
54	MG	BA	3590	1/1	0.39	-	119,119,119,119	0
54	MG	AA	1762	1/1	0.58	-	91,91,91,91	0
54	MG	CA	1699	1/1	0.13	-	76,76,76,76	0
54	MG	CO	104	1/1	0.27	-	99,99,99,99	0
54	MG	BA	3318	1/1	0.52	-	73,73,73,73	0
54	MG	DA	3177	1/1	0.61	-	46,46,46,46	0
54	MG	BA	2931	1/1	0.40	-	49,49,49,49	0
54	MG	CA	1864	1/1	0.17	-	90,90,90,90	0
54	MG	AA	1855	1/1	0.21	-	81,81,81,81	0
54	MG	CA	1654	1/1	0.30	-	78,78,78,78	0
54	MG	AA	1608	1/1	0.32	-	46,46,46,46	0
54	MG	CA	1621	1/1	0.19	-	67,67,67,67	0
54	MG	DB	226	1/1	0.11	-	73,73,73,73	0
54	MG	CA	1972	1/1	0.19	-	67,67,67,67	0
54	MG	CA	1815	1/1	0.48	-	97,97,97,97	0
54	MG	CA	1720	1/1	0.25	-	69,69,69,69	0
54	MG	BA	3287	1/1	0.48	-	83,83,83,83	0
54	MG	DA	3482	1/1	0.19	-	69,69,69,69	0
54	MG	BA	3370	1/1	0.26	-	76,76,76,76	0
54	MG	DA	3604	1/1	0.26	-	103,103,103,103	0
54	MG	BA	2973	1/1	0.17	-	60,60,60,60	0
54	MG	BA	3571	1/1	0.17	-	74,74,74,74	0
54	MG	DA	3274	1/1	0.15	-	116,116,116,116	0
54	MG	DA	3637	1/1	0.49	-	15,15,15,15	0
54	MG	BA	2974	1/1	0.40	-	81,81,81,81	0
54	MG	BA	3304	1/1	0.44	-	100,100,100,100	0
54	MG	DA	3079	1/1	0.35	-	51,51,51,51	0
54	MG	BA	3156	1/1	0.48	-	70,70,70,70	0
54	MG	CA	1639	1/1	0.34	-	59,59,59,59	0
54	MG	BA	2965	1/1	0.28	-	51,51,51,51	0
54	MG	DA	3161	1/1	0.48	-	70,70,70,70	0
54	MG	DA	2940	1/1	0.55	-	31,31,31,31	0
54	MG	AA	1672	1/1	0.68	-	78,78,78,78	0
54	MG	DJ	205	1/1	0.46	-	91,91,91,91	0
54	MG	BA	3112	1/1	0.28	-	65,65,65,65	0
54	MG	AK	201	1/1	0.35	-	101,101,101,101	0
54	MG	AA	1776	1/1	0.38	-	108,108,108,108	0
54	MG	BA	3078	1/1	0.28	-	104,104,104,104	0
54	MG	DA	3413	1/1	0.22	-	60,60,60,60	0
54	MG	DA	3485	1/1	0.37	-	119,119,119,119	0
54	MG	DA	3520	1/1	0.20	-	133,133,133,133	0
54	MG	DA	3101	1/1	0.53	-	75,75,75,75	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
54	MG	DA	3388	1/1	0.31	-	51,51,51,51	0
54	MG	BB	205	1/1	0.20	-	108,108,108,108	0
54	MG	AA	1691	1/1	0.13	-	69,69,69,69	0
54	MG	DA	3826	1/1	0.19	-	100,100,100,100	0
54	MG	CA	1603	1/1	0.52	-	48,48,48,48	0
54	MG	BA	2996	1/1	0.26	-	125,125,125,125	0
54	MG	DA	3569	1/1	0.44	-	36,36,36,36	0
54	MG	BA	3463	1/1	0.44	-	54,54,54,54	0
54	MG	DA	3063	1/1	0.74	-	126,126,126,126	0
54	MG	AA	1696	1/1	0.05	-	120,120,120,120	0
54	MG	DA	3517	1/1	0.20	-	102,102,102,102	0
54	MG	DA	3481	1/1	0.28	-	77,77,77,77	0
54	MG	CA	1659	1/1	0.29	-	100,100,100,100	0
54	MG	BA	3570	1/1	0.53	-	67,67,67,67	0
54	MG	DA	3390	1/1	0.72	-	72,72,72,72	0
54	MG	BA	3643	1/1	0.96	-	92,92,92,92	0
54	MG	DA	3472	1/1	0.42	-	95,95,95,95	0
54	MG	CA	1627	1/1	1.08	-	99,99,99,99	0
54	MG	BA	3196	1/1	0.94	-	80,80,80,80	0
54	MG	AA	1813	1/1	0.08	-	76,76,76,76	0
54	MG	BA	3408	1/1	0.72	-	86,86,86,86	0
54	MG	BA	3517	1/1	0.45	-	87,87,87,87	0
54	MG	BA	2906	1/1	0.49	-	24,24,24,24	0
54	MG	BA	3250	1/1	0.24	-	67,67,67,67	0
54	MG	AA	1821	1/1	0.55	-	91,91,91,91	0
54	MG	BA	3131	1/1	0.18	-	47,47,47,47	0
54	MG	AA	1775	1/1	0.11	-	105,105,105,105	0
54	MG	DA	3149	1/1	0.21	-	60,60,60,60	0
54	MG	BA	3519	1/1	0.15	-	50,50,50,50	0
54	MG	DA	3731	1/1	0.25	-	60,60,60,60	0
54	MG	DA	3550	1/1	0.11	-	65,65,65,65	0
54	MG	DA	3840	1/1	0.31	-	81,81,81,81	0
54	MG	CA	1647	1/1	0.36	-	94,94,94,94	0
54	MG	DA	2921	1/1	0.13	-	32,32,32,32	0
54	MG	BA	3369	1/1	0.41	-	108,108,108,108	0
54	MG	CF	201	1/1	0.30	-	131,131,131,131	0
54	MG	CA	1715	1/1	0.41	-	107,107,107,107	0
54	MG	CA	1752	1/1	0.40	-	71,71,71,71	0
54	MG	DA	3439	1/1	0.35	-	52,52,52,52	0
54	MG	AA	1810	1/1	0.44	-	86,86,86,86	0
54	MG	CA	1683	1/1	0.31	-	72,72,72,72	0
54	MG	DA	3384	1/1	0.31	-	84,84,84,84	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
54	MG	DJ	206	1/1	0.14	-	135,135,135,135	0
54	MG	DD	305	1/1	0.43	-	52,52,52,52	0
54	MG	DA	2945	1/1	0.60	-	29,29,29,29	0
54	MG	CA	1952	1/1	0.27	-	88,88,88,88	0
54	MG	BA	3423	1/1	0.22	-	72,72,72,72	0
54	MG	DA	3525	1/1	0.72	-	73,73,73,73	0
54	MG	DA	3174	1/1	0.19	-	66,66,66,66	0
54	MG	DA	3257	1/1	0.14	-	48,48,48,48	0
54	MG	DA	3361	1/1	0.16	-	69,69,69,69	0
54	MG	AA	1670	1/1	0.15	-	93,93,93,93	0
54	MG	CA	1613	1/1	0.66	-	68,68,68,68	0
54	MG	DA	3434	1/1	0.27	-	89,89,89,89	0
54	MG	AA	1644	1/1	0.14	-	62,62,62,62	0
54	MG	DA	3493	1/1	0.59	-	59,59,59,59	0
54	MG	DA	3705	1/1	0.08	-	86,86,86,86	0
54	MG	CA	1822	1/1	0.34	-	93,93,93,93	0
54	MG	BA	3529	1/1	0.33	-	79,79,79,79	0
54	MG	DA	3665	1/1	0.97	-	137,137,137,137	0
54	MG	AA	1741	1/1	0.42	-	112,112,112,112	0
54	MG	BA	3497	1/1	0.28	-	61,61,61,61	0
54	MG	AB	302	1/1	0.27	-	57,57,57,57	0
54	MG	BA	3617	1/1	0.18	-	96,96,96,96	0
54	MG	BA	3591	1/1	0.20	-	99,99,99,99	0
54	MG	BA	3409	1/1	0.26	-	51,51,51,51	0
54	MG	BA	3561	1/1	0.13	-	75,75,75,75	0
54	MG	BA	3346	1/1	0.15	-	136,136,136,136	0
54	MG	DA	3549	1/1	0.37	-	115,115,115,115	0
54	MG	DA	3513	1/1	0.28	-	30,30,30,30	0
54	MG	DA	3229	1/1	0.14	-	59,59,59,59	0
54	MG	BA	3455	1/1	0.33	-	32,32,32,32	0
54	MG	DA	3306	1/1	0.19	-	152,152,152,152	0
54	MG	CA	1863	1/1	0.16	-	125,125,125,125	0
54	MG	DA	3582	1/1	0.24	-	85,85,85,85	0
54	MG	DA	3418	1/1	0.24	-	65,65,65,65	0
54	MG	BA	3502	1/1	0.12	-	81,81,81,81	0
54	MG	AA	1648	1/1	0.46	-	90,90,90,90	0
54	MG	BA	3407	1/1	0.31	-	79,79,79,79	0
54	MG	DA	3083	1/1	0.28	-	120,120,120,120	0
54	MG	DA	3264	1/1	0.12	-	78,78,78,78	0
54	MG	AV	6202	1/1	0.08	-	97,97,97,97	0
54	MG	DA	2903	1/1	0.25	-	16,16,16,16	0
54	MG	DA	3556	1/1	0.14	-	110,110,110,110	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
54	MG	DA	3397	1/1	1.03	-	124,124,124,124	0
54	MG	DA	3040	1/1	0.30	-	76,76,76,76	0
54	MG	DA	3054	1/1	0.97	-	72,72,72,72	0
54	MG	DA	3056	1/1	0.27	-	25,25,25,25	0
54	MG	AA	1689	1/1	0.60	-	75,75,75,75	0
54	MG	BA	3243	1/1	0.55	-	85,85,85,85	0
54	MG	DA	3236	1/1	0.20	-	75,75,75,75	0
54	MG	DA	2967	1/1	0.27	-	34,34,34,34	0
54	MG	AA	1692	1/1	0.15	-	89,89,89,89	0
54	MG	DD	302	1/1	0.19	-	61,61,61,61	0
54	MG	DB	208	1/1	0.16	-	86,86,86,86	0
54	MG	CA	1934	1/1	0.14	-	80,80,80,80	0
54	MG	AA	1816	1/1	0.97	-	89,89,89,89	0
54	MG	CA	1734	1/1	0.95	-	90,90,90,90	0
54	MG	BA	3282	1/1	0.61	-	98,98,98,98	0
54	MG	BA	3665	1/1	0.30	-	123,123,123,123	0
54	MG	DA	3824	1/1	0.22	-	113,113,113,113	0
54	MG	CB	301	1/1	0.22	-	115,115,115,115	0
54	MG	DA	3186	1/1	0.47	-	82,82,82,82	0
54	MG	DA	3603	1/1	0.66	-	64,64,64,64	0
54	MG	DA	3147	1/1	0.52	-	86,86,86,86	0
54	MG	BA	3312	1/1	0.53	-	71,71,71,71	0
54	MG	CA	1774	1/1	0.41	-	79,79,79,79	0
54	MG	BA	3302	1/1	0.48	-	84,84,84,84	0
54	MG	CA	1913	1/1	0.20	-	109,109,109,109	0
54	MG	BA	3609	1/1	0.19	-	65,65,65,65	0
54	MG	DA	3530	1/1	0.31	-	71,71,71,71	0
54	MG	DA	2995	1/1	0.22	-	26,26,26,26	0
54	MG	DA	3038	1/1	0.43	-	44,44,44,44	0
54	MG	BA	3522	1/1	0.21	-	54,54,54,54	0
54	MG	BA	3668	1/1	0.56	-	97,97,97,97	0
54	MG	DA	3494	1/1	0.36	-	63,63,63,63	0
54	MG	DA	3488	1/1	0.33	-	102,102,102,102	0
54	MG	DA	3324	1/1	0.17	-	95,95,95,95	0
54	MG	AA	1792	1/1	0.12	-	101,101,101,101	0
54	MG	BA	3155	1/1	1.01	-	99,99,99,99	0
54	MG	DA	2913	1/1	0.69	-	21,21,21,21	0
54	MG	AA	1654	1/1	0.32	-	99,99,99,99	0
54	MG	AV	6208	1/1	0.23	-	79,79,79,79	0
54	MG	CE	203	1/1	0.14	-	79,79,79,79	0
54	MG	DB	204	1/1	0.29	-	56,56,56,56	0
54	MG	DA	3201	1/1	0.05	-	46,46,46,46	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
54	MG	BA	3231	1/1	0.36	-	64,64,64,64	0
54	MG	DA	3845	1/1	0.28	-	94,94,94,94	0
54	MG	AA	1789	1/1	0.39	-	106,106,106,106	0
54	MG	BA	2959	1/1	0.28	-	40,40,40,40	0
54	MG	BA	3292	1/1	0.23	-	71,71,71,71	0
54	MG	DB	218	1/1	0.09	-	113,113,113,113	0
54	MG	AA	1602	1/1	0.90	-	45,45,45,45	0
54	MG	DB	222	1/1	0.17	-	137,137,137,137	0
54	MG	CV	6201	1/1	0.10	-	95,95,95,95	0
54	MG	CA	1851	1/1	0.45	-	103,103,103,103	0
54	MG	DA	3420	1/1	0.29	-	110,110,110,110	0
54	MG	DA	3857	1/1	0.18	-	98,98,98,98	0
54	MG	DA	3571	1/1	0.85	-	72,72,72,72	0
54	MG	DA	3829	1/1	0.11	-	96,96,96,96	0
54	MG	AT	201	1/1	0.08	-	103,103,103,103	0
54	MG	DA	3551	1/1	0.23	-	80,80,80,80	0
54	MG	AA	1808	1/1	0.26	-	97,97,97,97	0
54	MG	AA	1735	1/1	0.09	-	68,68,68,68	0
54	MG	BA	2998	1/1	0.10	-	75,75,75,75	0
54	MG	DA	3048	1/1	0.46	-	51,51,51,51	0
54	MG	BA	3007	1/1	0.10	-	98,98,98,98	0
54	MG	AA	1675	1/1	0.23	-	82,82,82,82	0
54	MG	DA	3438	1/1	0.20	-	54,54,54,54	0
54	MG	CA	1882	1/1	0.11	-	135,135,135,135	0
54	MG	DI	101	1/1	0.29	-	104,104,104,104	0
54	MG	BA	2989	1/1	0.32	-	50,50,50,50	0
54	MG	DA	3222	1/1	0.52	-	112,112,112,112	0
54	MG	DA	3398	1/1	0.17	-	80,80,80,80	0
54	MG	BA	3315	1/1	0.18	-	84,84,84,84	0
54	MG	DA	3626	1/1	0.20	-	106,106,106,106	0
54	MG	DA	3555	1/1	0.51	-	61,61,61,61	0
54	MG	BB	227	1/1	0.27	-	80,80,80,80	0
54	MG	DA	3495	1/1	0.29	-	111,111,111,111	0
54	MG	CA	1616	1/1	0.21	-	94,94,94,94	0
54	MG	CA	1785	1/1	0.27	-	76,76,76,76	0
54	MG	CA	1650	1/1	0.32	-	111,111,111,111	0
54	MG	AA	1746	1/1	0.06	-	86,86,86,86	0
54	MG	DA	3012	1/1	0.27	-	48,48,48,48	0
54	MG	AA	1638	1/1	0.24	-	89,89,89,89	0
54	MG	DP	201	1/1	0.28	-	72,72,72,72	0
54	MG	AA	1863	1/1	0.12	-	119,119,119,119	0
54	MG	BA	2968	1/1	0.58	-	47,47,47,47	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
54	MG	DK	202	1/1	0.28	-	69,69,69,69	0
54	MG	CA	1839	1/1	0.31	-	92,92,92,92	0
54	MG	BA	2995	1/1	0.81	-	57,57,57,57	0
54	MG	AA	1744	1/1	0.23	-	96,96,96,96	0
54	MG	AA	1656	1/1	0.58	-	86,86,86,86	0
54	MG	BA	3629	1/1	0.32	-	86,86,86,86	0
54	MG	CA	1921	1/1	0.23	-	97,97,97,97	0
54	MG	DA	3082	1/1	0.41	-	68,68,68,68	0
54	MG	DA	3529	1/1	0.23	-	61,61,61,61	0
54	MG	DA	2907	1/1	0.56	-	17,17,17,17	0
54	MG	BJ	203	1/1	0.20	-	89,89,89,89	0
54	MG	DA	3738	1/1	0.23	-	91,91,91,91	0
54	MG	CA	1631	1/1	0.56	-	82,82,82,82	0
54	MG	BA	3050	1/1	0.59	-	57,57,57,57	0
54	MG	BA	3424	1/1	0.35	-	115,115,115,115	0
54	MG	BA	3391	1/1	0.28	-	93,93,93,93	0
54	MG	DA	3410	1/1	0.33	-	48,48,48,48	0
54	MG	DA	3686	1/1	0.22	-	52,52,52,52	0
54	MG	DA	3025	1/1	0.81	-	80,80,80,80	0
54	MG	BA	3337	1/1	0.17	-	77,77,77,77	0
54	MG	DA	3258	1/1	0.28	-	67,67,67,67	0
54	MG	BA	3624	1/1	0.11	-	82,82,82,82	0
54	MG	DB	217	1/1	0.14	-	93,93,93,93	0
54	MG	BA	3188	1/1	0.19	-	103,103,103,103	0
54	MG	DC	303	1/1	0.83	-	80,80,80,80	0
54	MG	DA	3298	1/1	1.03	-	72,72,72,72	0
54	MG	BA	3382	1/1	0.12	-	85,85,85,85	0
54	MG	BA	3241	1/1	0.21	-	69,69,69,69	0
54	MG	AA	1715	1/1	0.22	-	58,58,58,58	0
54	MG	DA	3199	1/1	0.09	-	108,108,108,108	0
54	MG	DB	243	1/1	0.29	-	101,101,101,101	0
54	MG	BA	3211	1/1	0.49	-	100,100,100,100	0
54	MG	DA	3444	1/1	0.32	-	72,72,72,72	0
54	MG	BA	3096	1/1	0.31	-	76,76,76,76	0
54	MG	CA	1856	1/1	1.31	-	118,118,118,118	0
54	MG	BA	3599	1/1	0.25	-	94,94,94,94	0
54	MG	BA	2988	1/1	0.25	-	40,40,40,40	0
54	MG	AH	201	1/1	0.26	-	78,78,78,78	0
54	MG	DA	3790	1/1	0.42	-	63,63,63,63	0
54	MG	BA	3137	1/1	0.45	-	90,90,90,90	0
54	MG	AA	1850	1/1	0.61	-	70,70,70,70	0
54	MG	DA	3210	1/1	0.22	-	92,92,92,92	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
54	MG	DE	302	1/1	0.39	-	83,83,83,83	0
54	MG	DA	2916	1/1	0.44	-	15,15,15,15	0
54	MG	DA	3144	1/1	0.48	-	69,69,69,69	0
54	MG	BE	302	1/1	0.38	-	93,93,93,93	0
54	MG	BA	3626	1/1	0.46	-	64,64,64,64	0
54	MG	DA	3377	1/1	0.42	-	107,107,107,107	0
54	MG	BA	2910	1/1	0.37	-	17,17,17,17	0
54	MG	DA	3100	1/1	0.17	-	78,78,78,78	0
54	MG	CA	1898	1/1	0.94	-	87,87,87,87	0
54	MG	CC	306	1/1	0.62	-	117,117,117,117	0
54	MG	DA	3608	1/1	0.34	-	128,128,128,128	0
54	MG	DA	3645	1/1	0.24	-	23,23,23,23	0
54	MG	DA	3308	1/1	0.14	-	83,83,83,83	0
54	MG	DA	3690	1/1	0.44	-	70,70,70,70	0
54	MG	DA	3030	1/1	0.36	-	73,73,73,73	0
54	MG	DA	3061	1/1	0.32	-	55,55,55,55	0
54	MG	BA	3265	1/1	0.15	-	53,53,53,53	0
54	MG	CA	1744	1/1	0.22	-	80,80,80,80	0
54	MG	DY	102	1/1	0.33	-	69,69,69,69	0
54	MG	DA	3323	1/1	1.16	-	78,78,78,78	0
54	MG	DA	3616	1/1	0.51	-	103,103,103,103	0
54	MG	CA	1814	1/1	0.23	-	47,47,47,47	0
54	MG	DA	3652	1/1	0.62	-	66,66,66,66	0
54	MG	BA	2942	1/1	0.22	-	19,19,19,19	0
54	MG	BA	3133	1/1	0.42	-	86,86,86,86	0
54	MG	BA	3190	1/1	0.29	-	72,72,72,72	0
54	MG	BA	3237	1/1	0.34	-	64,64,64,64	0
54	MG	CA	1708	1/1	0.12	-	60,60,60,60	0
54	MG	DA	3827	1/1	0.27	-	103,103,103,103	0
54	MG	CA	1795	1/1	0.19	-	131,131,131,131	0
54	MG	BA	3192	1/1	0.62	-	110,110,110,110	0
54	MG	BA	3041	1/1	0.48	-	62,62,62,62	0
54	MG	CE	201	1/1	0.14	-	117,117,117,117	0
54	MG	DA	3598	1/1	0.17	-	108,108,108,108	0
54	MG	CA	1813	1/1	0.23	-	107,107,107,107	0
54	MG	BA	2980	1/1	0.18	-	51,51,51,51	0
54	MG	DA	3407	1/1	0.17	-	108,108,108,108	0
54	MG	DA	3117	1/1	0.17	-	31,31,31,31	0
54	MG	DA	2919	1/1	0.33	-	12,12,12,12	0
54	MG	AA	1745	1/1	0.44	-	119,119,119,119	0
54	MG	AA	1737	1/1	0.33	-	111,111,111,111	0
54	MG	DA	2979	1/1	0.20	-	16,16,16,16	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
54	MG	BA	3560	1/1	0.63	-	74,74,74,74	0
54	MG	CA	1824	1/1	0.22	-	123,123,123,123	0
54	MG	BA	3134	1/1	0.45	-	90,90,90,90	0
54	MG	AA	1661	1/1	0.17	-	51,51,51,51	0
54	MG	BA	3206	1/1	0.16	-	96,96,96,96	0
54	MG	DA	2973	1/1	0.36	-	50,50,50,50	0
54	MG	CA	1601	1/1	0.39	-	60,60,60,60	0
54	MG	CA	1946	1/1	0.11	-	137,137,137,137	0
54	MG	BA	3079	1/1	0.11	-	73,73,73,73	0
54	MG	BA	3254	1/1	0.29	-	68,68,68,68	0
54	MG	BA	3274	1/1	0.79	-	98,98,98,98	0
54	MG	DA	3414	1/1	0.32	-	55,55,55,55	0
54	MG	AA	1653	1/1	0.13	-	102,102,102,102	0
54	MG	BA	2933	1/1	0.26	-	36,36,36,36	0
54	MG	CA	1758	1/1	0.25	-	77,77,77,77	0
54	MG	CM	201	1/1	1.00	-	85,85,85,85	0
54	MG	BA	3343	1/1	0.35	-	87,87,87,87	0
54	MG	BB	226	1/1	0.71	-	98,98,98,98	0
54	MG	DA	3096	1/1	0.54	-	59,59,59,59	0
54	MG	DA	2968	1/1	0.61	-	36,36,36,36	0
54	MG	BA	3491	1/1	0.42	-	79,79,79,79	0
54	MG	AA	1812	1/1	0.84	-	81,81,81,81	0
54	MG	DA	3221	1/1	0.31	-	73,73,73,73	0
54	MG	DB	241	1/1	0.14	-	90,90,90,90	0
54	MG	DA	3293	1/1	0.22	-	66,66,66,66	0
54	MG	BA	3073	1/1	0.36	-	63,63,63,63	0
54	MG	DA	3764	1/1	0.36	-	80,80,80,80	0
54	MG	DA	3593	1/1	0.30	-	125,125,125,125	0
54	MG	DA	3132	1/1	0.52	-	62,62,62,62	0
54	MG	CC	301	1/1	0.14	-	93,93,93,93	0
54	MG	BA	2912	1/1	0.57	-	19,19,19,19	0
54	MG	DA	3066	1/1	0.30	-	114,114,114,114	0
54	MG	DA	3400	1/1	0.12	-	127,127,127,127	0
54	MG	DA	3516	1/1	0.32	-	73,73,73,73	0
54	MG	BA	3500	1/1	0.33	-	72,72,72,72	0
54	MG	DA	3799	1/1	0.31	-	96,96,96,96	0
54	MG	DA	3256	1/1	0.39	-	65,65,65,65	0
54	MG	CO	102	1/1	0.51	-	103,103,103,103	0
54	MG	DA	3514	1/1	0.14	-	68,68,68,68	0
54	MG	BA	3085	1/1	0.50	-	53,53,53,53	0
54	MG	DA	3157	1/1	0.26	-	33,33,33,33	0
54	MG	DA	3114	1/1	0.38	-	66,66,66,66	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
54	MG	DA	3528	1/1	0.09	-	87,87,87,87	0
54	MG	AA	1632	1/1	0.34	-	65,65,65,65	0
54	MG	BA	3120	1/1	0.16	-	85,85,85,85	0
54	MG	AA	1664	1/1	0.45	-	80,80,80,80	0
54	MG	CA	1924	1/1	0.21	-	116,116,116,116	0
54	MG	DA	2961	1/1	0.47	-	58,58,58,58	0
54	MG	DA	3629	1/1	0.48	-	89,89,89,89	0
54	MG	DA	3045	1/1	0.57	-	39,39,39,39	0
54	MG	BA	3009	1/1	0.41	-	73,73,73,73	0
54	MG	BA	3499	1/1	0.31	-	66,66,66,66	0
54	MG	BA	3204	1/1	0.58	-	68,68,68,68	0
54	MG	BV	201	1/1	0.27	-	98,98,98,98	0
54	MG	AA	1772	1/1	0.18	-	111,111,111,111	0
54	MG	BA	3459	1/1	0.36	-	30,30,30,30	0
54	MG	DA	3021	1/1	1.24	-	68,68,68,68	0
54	MG	DA	2949	1/1	0.38	-	52,52,52,52	0
54	MG	BA	3059	1/1	0.63	-	48,48,48,48	0
54	MG	DA	3678	1/1	0.24	-	58,58,58,58	0
54	MG	CA	1674	1/1	0.66	-	70,70,70,70	0
54	MG	DA	3014	1/1	0.33	-	52,52,52,52	0
54	MG	BA	3645	1/1	0.22	-	69,69,69,69	0
55	ZN	CN	101	1/1	0.23	-	244,244,244,244	0
54	MG	D4	104	1/1	0.26	-	76,76,76,76	0
54	MG	DA	3713	1/1	0.72	-	96,96,96,96	0
54	MG	BA	3550	1/1	0.22	-	79,79,79,79	0
54	MG	DA	3272	1/1	0.55	-	87,87,87,87	0
54	MG	BA	3277	1/1	0.30	-	110,110,110,110	0
54	MG	CA	1673	1/1	0.38	-	61,61,61,61	0
54	MG	DA	3247	1/1	0.07	-	92,92,92,92	0
54	MG	DA	3671	1/1	1.11	-	69,69,69,69	0
54	MG	BA	3046	1/1	0.42	-	65,65,65,65	0
54	MG	BA	3220	1/1	0.37	-	79,79,79,79	0
54	MG	DA	3241	1/1	0.12	-	76,76,76,76	0
54	MG	BA	3620	1/1	0.53	-	88,88,88,88	0
54	MG	DA	3784	1/1	0.09	-	108,108,108,108	0
54	MG	CD	303	1/1	0.23	-	76,76,76,76	0
54	MG	DG	202	1/1	0.13	-	102,102,102,102	0
54	MG	BA	3557	1/1	0.36	-	67,67,67,67	0
54	MG	DA	3260	1/1	1.20	-	90,90,90,90	0
54	MG	BA	3030	1/1	0.22	-	61,61,61,61	0
54	MG	DA	3103	1/1	0.93	-	58,58,58,58	0
54	MG	DA	3382	1/1	0.40	-	92,92,92,92	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
54	MG	CC	307	1/1	0.15	-	108,108,108,108	0
54	MG	DA	3609	1/1	0.47	-	113,113,113,113	0
54	MG	DA	3262	1/1	0.52	-	73,73,73,73	0
54	MG	DA	3426	1/1	0.26	-	96,96,96,96	0
54	MG	BA	3178	1/1	0.22	-	74,74,74,74	0
54	MG	DA	2974	1/1	0.27	-	60,60,60,60	0
54	MG	DA	3475	1/1	0.55	-	120,120,120,120	0
54	MG	CA	1703	1/1	0.26	-	113,113,113,113	0
54	MG	BA	3143	1/1	0.12	-	48,48,48,48	0
54	MG	DA	3823	1/1	0.58	-	84,84,84,84	0
54	MG	BA	3027	1/1	0.27	-	72,72,72,72	0
54	MG	BF	201	1/1	0.10	-	122,122,122,122	0
54	MG	CA	1767	1/1	0.35	-	72,72,72,72	0
54	MG	AA	1767	1/1	0.16	-	118,118,118,118	0
54	MG	DA	3509	1/1	0.22	-	148,148,148,148	0
54	MG	BA	3234	1/1	0.43	-	73,73,73,73	0
54	MG	AA	1829	1/1	0.13	-	64,64,64,64	0
54	MG	BA	2943	1/1	0.19	-	34,34,34,34	0
54	MG	BA	3642	1/1	0.21	-	98,98,98,98	0
54	MG	BA	3056	1/1	0.18	-	31,31,31,31	0
54	MG	DA	3098	1/1	0.30	-	46,46,46,46	0
54	MG	CA	1615	1/1	0.21	-	70,70,70,70	0
54	MG	BA	3648	1/1	0.28	-	63,63,63,63	0
54	MG	BA	3533	1/1	0.21	-	83,83,83,83	0
54	MG	DA	3007	1/1	0.34	-	44,44,44,44	0
54	MG	CA	1762	1/1	0.17	-	114,114,114,114	0
54	MG	BA	2945	1/1	0.31	-	56,56,56,56	0
54	MG	CA	1775	1/1	0.17	-	64,64,64,64	0
54	MG	BA	3163	1/1	0.54	-	87,87,87,87	0
54	MG	CA	1681	1/1	0.20	-	66,66,66,66	0
54	MG	BA	3457	1/1	0.37	-	48,48,48,48	0
54	MG	BA	3402	1/1	0.38	-	90,90,90,90	0
54	MG	DA	3297	1/1	0.60	-	76,76,76,76	0
54	MG	DA	3109	1/1	0.40	-	88,88,88,88	0
54	MG	BA	3087	1/1	1.46	-	84,84,84,84	0
54	MG	BA	2917	1/1	0.27	-	6,6,6,6	0
54	MG	AA	1857	1/1	0.15	-	103,103,103,103	0
54	MG	BA	3487	1/1	0.44	-	90,90,90,90	0
54	MG	AA	1639	1/1	0.66	-	54,54,54,54	0
54	MG	CA	1638	1/1	0.06	-	101,101,101,101	0
54	MG	DA	3527	1/1	0.17	-	104,104,104,104	0
54	MG	BA	3191	1/1	1.12	-	90,90,90,90	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
54	MG	DA	3554	1/1	0.24	-	136,136,136,136	0
54	MG	BA	3169	1/1	0.29	-	43,43,43,43	0
54	MG	AA	1612	1/1	0.56	-	39,39,39,39	0
54	MG	DA	3696	1/1	0.14	-	82,82,82,82	0
54	MG	DA	3544	1/1	0.28	-	53,53,53,53	0
54	MG	DA	2928	1/1	0.47	-	31,31,31,31	0
54	MG	CA	1845	1/1	1.84	-	100,100,100,100	0
54	MG	CA	1838	1/1	0.15	-	94,94,94,94	0
54	MG	CA	1626	1/1	0.56	-	68,68,68,68	0
54	MG	BA	2985	1/1	0.54	-	43,43,43,43	0
54	MG	DA	3785	1/1	0.22	-	109,109,109,109	0
54	MG	AE	203	1/1	0.19	-	91,91,91,91	0
54	MG	BA	3146	1/1	0.05	-	99,99,99,99	0
54	MG	DA	3039	1/1	0.16	-	70,70,70,70	0
54	MG	DA	3432	1/1	0.23	-	84,84,84,84	0
54	MG	CA	1859	1/1	0.23	-	93,93,93,93	0
54	MG	AE	201	1/1	0.14	-	123,123,123,123	0
54	MG	DA	3381	1/1	0.19	-	49,49,49,49	0
54	MG	DA	3756	1/1	0.56	-	80,80,80,80	0
54	MG	DA	3205	1/1	0.61	-	97,97,97,97	0
54	MG	DA	3170	1/1	0.51	-	56,56,56,56	0
54	MG	DA	3852	1/1	0.21	-	80,80,80,80	0
54	MG	BA	3310	1/1	0.45	-	109,109,109,109	0
54	MG	BA	3434	1/1	0.24	-	19,19,19,19	0
54	MG	AA	1843	1/1	1.10	-	126,126,126,126	0
54	MG	BA	2964	1/1	0.37	-	43,43,43,43	0
54	MG	DA	3111	1/1	0.16	-	84,84,84,84	0
54	MG	AA	1668	1/1	0.19	-	77,77,77,77	0
54	MG	DA	3036	1/1	0.24	-	72,72,72,72	0
54	MG	CA	1870	1/1	0.21	-	94,94,94,94	0
54	MG	BA	3210	1/1	0.07	-	86,86,86,86	0
54	MG	BA	3631	1/1	0.13	-	85,85,85,85	0
54	MG	DA	3301	1/1	0.52	-	87,87,87,87	0
54	MG	DA	3279	1/1	0.33	-	38,38,38,38	0
54	MG	DA	3422	1/1	0.67	-	62,62,62,62	0
54	MG	DA	3195	1/1	0.28	-	83,83,83,83	0
54	MG	DB	227	1/1	0.14	-	104,104,104,104	0
54	MG	BA	3505	1/1	0.30	-	81,81,81,81	0
54	MG	DA	3224	1/1	0.35	-	55,55,55,55	0
54	MG	BA	3589	1/1	0.29	-	105,105,105,105	0
54	MG	DA	3461	1/1	0.47	-	88,88,88,88	0
54	MG	BA	3125	1/1	0.24	-	78,78,78,78	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
54	MG	DV	203	1/1	0.14	-	128,128,128,128	0
54	MG	CA	1755	1/1	0.27	-	69,69,69,69	0
54	MG	DA	3649	1/1	1.12	-	50,50,50,50	0
54	MG	BA	3151	1/1	0.46	-	70,70,70,70	0
54	MG	DA	3072	1/1	0.86	-	80,80,80,80	0
54	MG	CA	1894	1/1	0.46	-	97,97,97,97	0
54	MG	BA	3581	1/1	0.12	-	127,127,127,127	0
54	MG	BA	2956	1/1	0.64	-	49,49,49,49	0
54	MG	DA	3748	1/1	0.29	-	61,61,61,61	0
54	MG	DA	3707	1/1	0.19	-	54,54,54,54	0
54	MG	CA	1784	1/1	0.26	-	94,94,94,94	0
54	MG	DA	3126	1/1	0.36	-	64,64,64,64	0
54	MG	CA	1857	1/1	0.38	-	76,76,76,76	0
54	MG	DA	3490	1/1	0.20	-	70,70,70,70	0
54	MG	DA	3252	1/1	0.06	-	52,52,52,52	0
54	MG	CA	1869	1/1	0.09	-	96,96,96,96	0
54	MG	BA	2977	1/1	0.44	-	69,69,69,69	0
54	MG	DA	3546	1/1	0.21	-	56,56,56,56	0
54	MG	BA	3468	1/1	0.58	-	57,57,57,57	0
54	MG	DA	3492	1/1	0.13	-	102,102,102,102	0
54	MG	D5	103	1/1	0.47	-	71,71,71,71	0
54	MG	BA	2949	1/1	0.23	-	65,65,65,65	0
54	MG	BA	3364	1/1	0.27	-	107,107,107,107	0
54	MG	DA	3619	1/1	0.83	-	83,83,83,83	0
54	MG	DA	3566	1/1	0.28	-	91,91,91,91	0
54	MG	CA	1630	1/1	0.22	-	49,49,49,49	0
54	MG	DA	3442	1/1	0.66	-	71,71,71,71	0
54	MG	DA	3300	1/1	0.23	-	46,46,46,46	0
54	MG	BA	3044	1/1	0.35	-	39,39,39,39	0
54	MG	CA	1906	1/1	0.28	-	80,80,80,80	0
54	MG	CA	1657	1/1	0.17	-	60,60,60,60	0
54	MG	DQ	201	1/1	0.21	-	57,57,57,57	0
54	MG	BA	3319	1/1	0.10	-	79,79,79,79	0
54	MG	DA	3365	1/1	0.39	-	83,83,83,83	0
54	MG	AA	1852	1/1	0.79	-	84,84,84,84	0
54	MG	CA	1832	1/1	0.11	-	92,92,92,92	0
54	MG	CA	1821	1/1	0.35	-	96,96,96,96	0
54	MG	BA	2915	1/1	0.36	-	20,20,20,20	0
54	MG	CA	1748	1/1	0.21	-	115,115,115,115	0
54	MG	CA	1609	1/1	0.30	-	66,66,66,66	0
54	MG	DA	3702	1/1	0.54	-	74,74,74,74	0
54	MG	BA	3413	1/1	0.39	-	65,65,65,65	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
54	MG	BA	3064	1/1	0.40	-	61,61,61,61	0
54	MG	BA	3053	1/1	0.45	-	69,69,69,69	0
54	MG	BA	3065	1/1	0.12	-	59,59,59,59	0
54	MG	DA	3590	1/1	0.51	-	47,47,47,47	0
54	MG	DA	2924	1/1	0.52	-	68,68,68,68	0
54	MG	B2	103	1/1	0.08	-	75,75,75,75	0
54	MG	BA	3541	1/1	0.79	-	89,89,89,89	0
54	MG	CA	1881	1/1	0.35	-	74,74,74,74	0
54	MG	DA	3158	1/1	0.38	-	42,42,42,42	0
54	MG	AS	101	1/1	0.11	-	106,106,106,106	0
54	MG	BA	3127	1/1	0.92	-	61,61,61,61	0
54	MG	DA	3577	1/1	0.31	-	73,73,73,73	0
54	MG	DA	3089	1/1	0.34	-	71,71,71,71	0
54	MG	AV	6207	1/1	0.13	-	78,78,78,78	0
54	MG	BA	3623	1/1	0.59	-	64,64,64,64	0
54	MG	CA	1729	1/1	0.22	-	58,58,58,58	0
54	MG	CA	1899	1/1	0.10	-	98,98,98,98	0
54	MG	BA	2928	1/1	0.48	-	28,28,28,28	0
54	MG	CQ	202	1/1	0.16	-	79,79,79,79	0
54	MG	DA	3664	1/1	1.53	-	109,109,109,109	0
54	MG	DA	2963	1/1	0.13	-	32,32,32,32	0
54	MG	BM	203	1/1	0.33	-	90,90,90,90	0
54	MG	BA	3677	1/1	0.28	-	72,72,72,72	0
54	MG	CA	1797	1/1	0.26	-	133,133,133,133	0
54	MG	DA	3653	1/1	0.51	-	51,51,51,51	0
54	MG	BA	3233	1/1	0.46	-	97,97,97,97	0
54	MG	CA	1823	1/1	0.12	-	61,61,61,61	0
54	MG	CA	1671	1/1	0.25	-	51,51,51,51	0
54	MG	BA	3426	1/1	0.34	-	87,87,87,87	0
54	MG	CA	1937	1/1	0.22	-	100,100,100,100	0
54	MG	DA	2976	1/1	1.41	-	68,68,68,68	0
54	MG	DA	3119	1/1	0.17	-	74,74,74,74	0
54	MG	BA	3166	1/1	0.94	-	86,86,86,86	0
54	MG	BA	3460	1/1	0.30	-	47,47,47,47	0
54	MG	CA	1642	1/1	0.14	-	79,79,79,79	0
54	MG	DA	3165	1/1	0.17	-	59,59,59,59	0
54	MG	DB	225	1/1	0.23	-	72,72,72,72	0
54	MG	AA	1748	1/1	0.33	-	56,56,56,56	0
54	MG	DA	3500	1/1	0.24	-	108,108,108,108	0
54	MG	AA	1779	1/1	0.56	-	108,108,108,108	0
54	MG	AA	1609	1/1	0.39	-	26,26,26,26	0
54	MG	DP	202	1/1	0.09	-	90,90,90,90	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
54	MG	BA	3205	1/1	0.39	-	70,70,70,70	0
54	MG	DA	3437	1/1	0.56	-	120,120,120,120	0
54	MG	DA	3374	1/1	0.17	-	80,80,80,80	0
54	MG	DA	3218	1/1	0.10	-	79,79,79,79	0
54	MG	CA	1684	1/1	0.46	-	63,63,63,63	0
54	MG	BA	3039	1/1	0.12	-	54,54,54,54	0
54	MG	BA	3636	1/1	0.74	-	76,76,76,76	0
54	MG	DA	3787	1/1	1.26	-	114,114,114,114	0
54	MG	BA	3320	1/1	0.36	-	71,71,71,71	0
54	MG	DA	3310	1/1	0.30	-	54,54,54,54	0
54	MG	DA	3156	1/1	0.22	-	52,52,52,52	0
54	MG	CA	1707	1/1	0.18	-	102,102,102,102	0
54	MG	BA	3341	1/1	0.64	-	125,125,125,125	0
54	MG	BA	3218	1/1	0.21	-	55,55,55,55	0
54	MG	BB	218	1/1	0.42	-	79,79,79,79	0
54	MG	DA	3369	1/1	0.09	-	99,99,99,99	0
54	MG	BA	3164	1/1	0.33	-	75,75,75,75	0
54	MG	BA	3026	1/1	0.19	-	68,68,68,68	0
54	MG	BA	3216	1/1	0.17	-	87,87,87,87	0
54	MG	DA	3244	1/1	0.56	-	85,85,85,85	0
54	MG	DA	3836	1/1	0.63	-	135,135,135,135	0
54	MG	AA	1607	1/1	0.62	-	46,46,46,46	0
54	MG	DA	3121	1/1	0.26	-	38,38,38,38	0
54	MG	BA	3470	1/1	0.49	-	71,71,71,71	0
54	MG	BA	2926	1/1	0.71	-	50,50,50,50	0
54	MG	DA	3179	1/1	0.66	-	105,105,105,105	0
54	MG	BA	3058	1/1	0.57	-	78,78,78,78	0
54	MG	DJ	204	1/1	0.41	-	32,32,32,32	0
54	MG	DA	3484	1/1	0.30	-	21,21,21,21	0
54	MG	CA	1816	1/1	0.47	-	107,107,107,107	0
54	MG	AA	1811	1/1	0.19	-	61,61,61,61	0
54	MG	BA	3136	1/1	0.37	-	64,64,64,64	0
54	MG	DA	3521	1/1	0.37	-	101,101,101,101	0
54	MG	BA	3305	1/1	0.10	-	87,87,87,87	0
54	MG	DA	3849	1/1	0.13	-	89,89,89,89	0
54	MG	CA	1901	1/1	0.39	-	76,76,76,76	0
54	MG	DA	3069	1/1	0.43	-	61,61,61,61	0
54	MG	CA	1837	1/1	0.64	-	83,83,83,83	0
54	MG	DV	204	1/1	0.33	-	96,96,96,96	0
54	MG	DA	3071	1/1	0.12	-	49,49,49,49	0
54	MG	BA	3016	1/1	0.48	-	54,54,54,54	0
54	MG	BA	3595	1/1	0.30	-	108,108,108,108	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
54	MG	DA	3295	1/1	0.45	-	107,107,107,107	0
54	MG	DA	3591	1/1	0.21	-	90,90,90,90	0
54	MG	CA	1819	1/1	0.29	-	109,109,109,109	0
54	MG	AA	1613	1/1	0.61	-	55,55,55,55	0
54	MG	DD	303	1/1	0.16	-	70,70,70,70	0
54	MG	BA	3496	1/1	0.27	-	67,67,67,67	0
54	MG	DA	3123	1/1	0.48	-	59,59,59,59	0
54	MG	DA	3597	1/1	0.13	-	124,124,124,124	0
54	MG	BA	3361	1/1	0.31	-	154,154,154,154	0
54	MG	CA	1709	1/1	0.08	-	107,107,107,107	0
54	MG	DA	2959	1/1	0.31	-	42,42,42,42	0
54	MG	DA	3196	1/1	0.23	-	84,84,84,84	0
54	MG	BA	3100	1/1	0.31	-	79,79,79,79	0
54	MG	BA	3322	1/1	0.34	-	71,71,71,71	0
54	MG	DA	3533	1/1	0.28	-	60,60,60,60	0
54	MG	DA	3710	1/1	0.12	-	92,92,92,92	0
54	MG	DA	3386	1/1	0.12	-	76,76,76,76	0
54	MG	CA	1829	1/1	0.14	-	89,89,89,89	0
54	MG	DA	3094	1/1	0.39	-	67,67,67,67	0
54	MG	DA	3044	1/1	0.21	-	45,45,45,45	0
54	MG	AA	1674	1/1	0.99	-	113,113,113,113	0
54	MG	AG	202	1/1	0.28	-	129,129,129,129	0
54	MG	DA	3535	1/1	0.30	-	107,107,107,107	0
54	MG	AA	1663	1/1	0.27	-	54,54,54,54	0
54	MG	BA	3456	1/1	0.26	-	64,64,64,64	0
54	MG	BA	3464	1/1	0.73	-	67,67,67,67	0
54	MG	CA	1790	1/1	0.28	-	132,132,132,132	0
54	MG	DA	3743	1/1	0.32	-	105,105,105,105	0
54	MG	DA	3636	1/1	0.45	-	12,12,12,12	0
54	MG	BA	3475	1/1	1.21	-	67,67,67,67	0
55	ZN	AD	301	1/1	0.29	-	51,51,51,51	0
54	MG	DA	3447	1/1	0.29	-	73,73,73,73	0
54	MG	DB	205	1/1	0.34	-	78,78,78,78	0
54	MG	DA	3655	1/1	0.38	-	60,60,60,60	0
54	MG	BA	2946	1/1	0.21	-	37,37,37,37	0
54	MG	DA	3479	1/1	0.38	-	130,130,130,130	0
54	MG	CA	1807	1/1	0.41	-	125,125,125,125	0
54	MG	AV	6205	1/1	0.13	-	107,107,107,107	0
54	MG	DA	3436	1/1	1.09	-	101,101,101,101	0
54	MG	BA	3057	1/1	0.15	-	64,64,64,64	0
54	MG	BP	202	1/1	0.11	-	84,84,84,84	0
54	MG	BA	2924	1/1	0.43	-	48,48,48,48	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
54	MG	CA	1670	1/1	0.53	-	106,106,106,106	0
54	MG	CA	1672	1/1	0.10	-	137,137,137,137	0
54	MG	DA	2954	1/1	0.54	-	41,41,41,41	0
54	MG	AO	101	1/1	0.11	-	115,115,115,115	0
54	MG	CA	1835	1/1	0.31	-	76,76,76,76	0
54	MG	BA	3106	1/1	0.24	-	142,142,142,142	0
54	MG	BA	2908	1/1	0.45	-	26,26,26,26	0
54	MG	DA	3052	1/1	0.27	-	50,50,50,50	0
54	MG	DA	3097	1/1	0.34	-	55,55,55,55	0
54	MG	CA	1961	1/1	0.11	-	63,63,63,63	0
54	MG	DV	202	1/1	0.33	-	115,115,115,115	0
54	MG	AA	1627	1/1	0.61	-	59,59,59,59	0
54	MG	BA	3630	1/1	0.37	-	151,151,151,151	0
54	MG	BA	3582	1/1	0.35	-	102,102,102,102	0
54	MG	CA	1624	1/1	0.45	-	94,94,94,94	0
54	MG	CA	1697	1/1	0.08	-	83,83,83,83	0
54	MG	AA	1680	1/1	0.53	-	140,140,140,140	0
54	MG	CA	1718	1/1	0.35	-	109,109,109,109	0
54	MG	AA	1650	1/1	0.25	-	92,92,92,92	0
54	MG	BA	3678	1/1	0.57	-	122,122,122,122	0
54	MG	DB	214	1/1	0.20	-	72,72,72,72	0
54	MG	AA	1739	1/1	0.33	-	81,81,81,81	0
54	MG	BB	216	1/1	0.69	-	154,154,154,154	0
54	MG	BA	3404	1/1	0.21	-	80,80,80,80	0
54	MG	BA	3362	1/1	1.16	-	130,130,130,130	0
54	MG	DA	3693	1/1	0.27	-	63,63,63,63	0
54	MG	DA	3383	1/1	0.34	-	112,112,112,112	0
54	MG	AA	1669	1/1	0.35	-	54,54,54,54	0
54	MG	AA	1611	1/1	0.42	-	55,55,55,55	0
54	MG	BA	3148	1/1	0.44	-	62,62,62,62	0
54	MG	BA	3349	1/1	0.32	-	95,95,95,95	0
54	MG	DA	3055	1/1	0.32	-	59,59,59,59	0
54	MG	AE	202	1/1	0.26	-	173,173,173,173	0
54	MG	BA	3232	1/1	0.43	-	68,68,68,68	0
54	MG	CA	1628	1/1	0.61	-	84,84,84,84	0
54	MG	DA	3357	1/1	0.48	-	169,169,169,169	0
54	MG	DB	203	1/1	0.21	-	69,69,69,69	0
54	MG	BA	3001	1/1	0.35	-	65,65,65,65	0
54	MG	DA	3349	1/1	0.15	-	116,116,116,116	0
54	MG	BA	3197	1/1	0.19	-	84,84,84,84	0
54	MG	CA	1809	1/1	0.14	-	92,92,92,92	0
54	MG	BA	3018	1/1	0.89	-	88,88,88,88	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
54	MG	DA	3265	1/1	0.68	-	138,138,138,138	0
54	MG	DA	3340	1/1	0.32	-	59,59,59,59	0
54	MG	BA	3038	1/1	0.29	-	63,63,63,63	0
54	MG	DQ	202	1/1	0.20	-	97,97,97,97	0
54	MG	DA	3800	1/1	0.47	-	95,95,95,95	0
54	MG	DA	3854	1/1	0.11	-	124,124,124,124	0
54	MG	DA	3312	1/1	0.11	-	130,130,130,130	0
54	MG	DA	3448	1/1	0.14	-	99,99,99,99	0
54	MG	DB	224	1/1	0.33	-	95,95,95,95	0
54	MG	AA	1662	1/1	0.51	-	78,78,78,78	0
54	MG	BA	3172	1/1	0.29	-	74,74,74,74	0
54	MG	BA	3045	1/1	0.48	-	94,94,94,94	0
54	MG	BA	3651	1/1	0.50	-	77,77,77,77	0
54	MG	BA	2967	1/1	0.50	-	51,51,51,51	0
54	MG	DA	3560	1/1	0.42	-	83,83,83,83	0
54	MG	DA	3099	1/1	0.17	-	49,49,49,49	0
54	MG	AA	1721	1/1	0.30	-	56,56,56,56	0
54	MG	DA	3726	1/1	0.34	-	106,106,106,106	0
54	MG	DA	3392	1/1	0.47	-	76,76,76,76	0
54	MG	DA	3537	1/1	0.61	-	101,101,101,101	0
54	MG	BA	3430	1/1	0.27	-	6,6,6,6	0
54	MG	DA	3395	1/1	0.45	-	75,75,75,75	0
54	MG	BY	103	1/1	0.25	-	95,95,95,95	0
54	MG	DA	3469	1/1	0.44	-	83,83,83,83	0
54	MG	CA	1641	1/1	0.45	-	79,79,79,79	0
54	MG	BB	223	1/1	0.28	-	94,94,94,94	0
54	MG	BA	3344	1/1	0.45	-	99,99,99,99	0
54	MG	DA	3235	1/1	0.20	-	59,59,59,59	0
54	MG	BA	3625	1/1	0.33	-	53,53,53,53	0
54	MG	BA	3383	1/1	0.28	-	66,66,66,66	0
54	MG	BA	3199	1/1	0.34	-	61,61,61,61	0
54	MG	CA	1928	1/1	0.62	-	117,117,117,117	0
54	MG	AA	1866	1/1	0.62	-	108,108,108,108	0
54	MG	BA	3179	1/1	0.14	-	79,79,79,79	0
54	MG	DA	3035	1/1	0.65	-	43,43,43,43	0
54	MG	AA	1624	1/1	0.17	-	58,58,58,58	0
54	MG	CA	1802	1/1	0.03	-	94,94,94,94	0
54	MG	BB	224	1/1	0.41	-	140,140,140,140	0
54	MG	BA	3247	1/1	0.26	-	109,109,109,109	0
54	MG	CA	1799	1/1	0.20	-	109,109,109,109	0
54	MG	DA	3403	1/1	0.39	-	56,56,56,56	0
54	MG	DA	3579	1/1	0.68	-	80,80,80,80	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
54	MG	DB	223	1/1	0.17	-	82,82,82,82	0
54	MG	DA	3068	1/1	0.50	-	64,64,64,64	0
54	MG	DA	3728	1/1	0.57	-	83,83,83,83	0
54	MG	BA	3527	1/1	0.38	-	65,65,65,65	0
54	MG	BA	3138	1/1	0.32	-	88,88,88,88	0
54	MG	BC	303	1/1	0.46	-	95,95,95,95	0
54	MG	AA	1828	1/1	0.32	-	82,82,82,82	0
54	MG	BA	3275	1/1	0.21	-	68,68,68,68	0
54	MG	DA	3172	1/1	0.17	-	88,88,88,88	0
54	MG	DA	3757	1/1	0.16	-	89,89,89,89	0
54	MG	DA	2910	1/1	0.66	-	38,38,38,38	0
54	MG	DA	3536	1/1	0.17	-	92,92,92,92	0
54	MG	DA	3458	1/1	0.09	-	95,95,95,95	0
54	MG	DL	203	1/1	0.26	-	66,66,66,66	0
54	MG	DA	3268	1/1	0.26	-	51,51,51,51	0
54	MG	DA	3819	1/1	0.56	-	130,130,130,130	0
54	MG	CA	1971	1/1	0.35	-	86,86,86,86	0
54	MG	DA	3688	1/1	0.60	-	50,50,50,50	0
54	MG	DA	3440	1/1	0.55	-	125,125,125,125	0
54	MG	DA	2983	1/1	0.40	-	52,52,52,52	0
54	MG	CC	303	1/1	0.33	-	147,147,147,147	0
54	MG	AA	1756	1/1	0.29	-	111,111,111,111	0
54	MG	DA	2915	1/1	0.46	-	49,49,49,49	0
54	MG	DA	2905	1/1	0.36	-	18,18,18,18	0
54	MG	DW	101	1/1	0.34	-	56,56,56,56	0
54	MG	BB	215	1/1	0.47	-	82,82,82,82	0
54	MG	CA	1849	1/1	0.08	-	167,167,167,167	0
54	MG	BA	2984	1/1	0.28	-	50,50,50,50	0
54	MG	DA	3163	1/1	0.35	-	113,113,113,113	0
54	MG	DA	3237	1/1	0.69	-	64,64,64,64	0
54	MG	BA	3201	1/1	0.35	-	107,107,107,107	0
54	MG	BA	3175	1/1	0.29	-	71,71,71,71	0
54	MG	AA	1614	1/1	0.27	-	68,68,68,68	0
54	MG	DA	3273	1/1	0.08	-	94,94,94,94	0
54	MG	BA	3386	1/1	0.52	-	134,134,134,134	0
54	MG	CA	1847	1/1	0.17	-	58,58,58,58	0
54	MG	DA	3669	1/1	0.49	-	61,61,61,61	0
54	MG	BA	3091	1/1	0.23	-	72,72,72,72	0
54	MG	AA	1769	1/1	0.70	-	118,118,118,118	0
54	MG	BA	3324	1/1	0.40	-	109,109,109,109	0
54	MG	DA	3592	1/1	0.11	-	114,114,114,114	0
54	MG	BA	3242	1/1	0.19	-	112,112,112,112	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
54	MG	DA	3766	1/1	0.12	-	123,123,123,123	0
54	MG	BA	3299	1/1	0.17	-	72,72,72,72	0
54	MG	DA	3612	1/1	0.14	-	74,74,74,74	0
54	MG	DA	3641	1/1	0.24	-	13,13,13,13	0
54	MG	AD	303	1/1	0.63	-	68,68,68,68	0
54	MG	BA	3195	1/1	0.79	-	91,91,91,91	0
54	MG	DA	3614	1/1	0.32	-	128,128,128,128	0
54	MG	DA	3206	1/1	0.36	-	89,89,89,89	0
54	MG	CA	1712	1/1	0.38	-	108,108,108,108	0
54	MG	DA	3212	1/1	0.47	-	75,75,75,75	0
54	MG	DA	3689	1/1	1.07	-	67,67,67,67	0
54	MG	BA	3593	1/1	0.14	-	81,81,81,81	0
54	MG	DA	3833	1/1	0.41	-	73,73,73,73	0
54	MG	CA	1732	1/1	0.96	-	78,78,78,78	0
54	MG	CA	1945	1/1	0.56	-	95,95,95,95	0
54	MG	BA	3317	1/1	0.14	-	84,84,84,84	0
54	MG	DA	3223	1/1	0.10	-	83,83,83,83	0
54	MG	CA	1663	1/1	0.31	-	128,128,128,128	0
54	MG	AF	201	1/1	0.15	-	90,90,90,90	0
54	MG	CA	1743	1/1	0.12	-	88,88,88,88	0
54	MG	DA	2980	1/1	0.37	-	12,12,12,12	0
54	MG	CA	1817	1/1	0.22	-	89,89,89,89	0
54	MG	DA	3687	1/1	0.19	-	57,57,57,57	0
54	MG	AA	1872	1/1	0.59	-	88,88,88,88	0
54	MG	AA	1631	1/1	0.50	-	76,76,76,76	0
54	MG	DA	3675	1/1	0.48	-	46,46,46,46	0
54	MG	BA	2936	1/1	0.21	-	32,32,32,32	0
54	MG	BA	3150	1/1	0.69	-	97,97,97,97	0
54	MG	BB	219	1/1	0.11	-	69,69,69,69	0
54	MG	DA	3352	1/1	0.17	-	121,121,121,121	0
54	MG	BA	3401	1/1	0.16	-	85,85,85,85	0
54	MG	AA	1783	1/1	0.21	-	123,123,123,123	0
54	MG	BA	3359	1/1	0.11	-	89,89,89,89	0
54	MG	AA	1684	1/1	0.10	-	71,71,71,71	0
54	MG	BA	3217	1/1	0.21	-	55,55,55,55	0
54	MG	CA	1792	1/1	0.34	-	93,93,93,93	0
54	MG	BA	3467	1/1	0.28	-	30,30,30,30	0
54	MG	BA	3257	1/1	0.74	-	108,108,108,108	0
54	MG	BA	3080	1/1	0.19	-	43,43,43,43	0
54	MG	CE	202	1/1	0.20	-	80,80,80,80	0
54	MG	CA	1602	1/1	0.48	-	43,43,43,43	0
54	MG	BA	3263	1/1	0.33	-	107,107,107,107	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
54	MG	DA	3769	1/1	0.39	-	90,90,90,90	0
54	MG	BA	3300	1/1	0.30	-	93,93,93,93	0
54	MG	BA	3285	1/1	0.11	-	91,91,91,91	0
54	MG	DA	3362	1/1	0.28	-	78,78,78,78	0
54	MG	DA	3709	1/1	0.64	-	75,75,75,75	0
54	MG	DA	3814	1/1	0.17	-	186,186,186,186	0
54	MG	CA	1827	1/1	0.17	-	82,82,82,82	0
54	MG	BA	3600	1/1	0.15	-	93,93,93,93	0
54	MG	DA	3405	1/1	0.94	-	67,67,67,67	0
54	MG	DB	237	1/1	0.79	-	109,109,109,109	0
54	MG	DA	3565	1/1	0.14	-	97,97,97,97	0
54	MG	BA	3566	1/1	0.46	-	72,72,72,72	0
54	MG	CA	1872	1/1	0.32	-	84,84,84,84	0
54	MG	DA	3644	1/1	0.55	-	75,75,75,75	0
54	MG	CA	1911	1/1	0.75	-	90,90,90,90	0
54	MG	BA	3347	1/1	0.14	-	77,77,77,77	0
54	MG	BA	3005	1/1	0.71	-	53,53,53,53	0
54	MG	DA	3545	1/1	0.78	-	94,94,94,94	0
54	MG	BA	3029	1/1	0.35	-	41,41,41,41	0
54	MG	BA	3587	1/1	0.28	-	77,77,77,77	0
54	MG	BA	3093	1/1	0.39	-	67,67,67,67	0
54	MG	DA	3350	1/1	0.10	-	95,95,95,95	0
54	MG	DA	2939	1/1	0.42	-	21,21,21,21	0
54	MG	BA	3598	1/1	0.09	-	100,100,100,100	0
54	MG	BA	3077	1/1	0.58	-	55,55,55,55	0
54	MG	DA	3804	1/1	0.20	-	72,72,72,72	0
54	MG	BA	2952	1/1	0.16	-	59,59,59,59	0
54	MG	DA	3245	1/1	0.74	-	100,100,100,100	0
54	MG	AA	1686	1/1	0.52	-	65,65,65,65	0
54	MG	BA	3130	1/1	0.20	-	47,47,47,47	0
54	MG	DA	3093	1/1	0.32	-	47,47,47,47	0
54	MG	AA	1766	1/1	0.42	-	106,106,106,106	0
54	MG	BA	3108	1/1	0.74	-	72,72,72,72	0
54	MG	CA	1643	1/1	0.21	-	70,70,70,70	0
54	MG	AA	1859	1/1	0.17	-	87,87,87,87	0
54	MG	BB	213	1/1	0.43	-	111,111,111,111	0
54	MG	BA	3453	1/1	0.23	-	27,27,27,27	0
54	MG	BA	2982	1/1	0.21	-	38,38,38,38	0
54	MG	DA	3406	1/1	0.20	-	59,59,59,59	0
54	MG	DA	3115	1/1	0.18	-	58,58,58,58	0
54	MG	BA	2944	1/1	0.48	-	47,47,47,47	0
54	MG	CA	1938	1/1	0.16	-	81,81,81,81	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
54	MG	AA	1719	1/1	0.31	-	66,66,66,66	0
54	MG	DA	3230	1/1	0.35	-	80,80,80,80	0
54	MG	DA	3307	1/1	0.20	-	84,84,84,84	0
54	MG	CA	1605	1/1	0.59	-	54,54,54,54	0
54	MG	BA	3094	1/1	0.32	-	63,63,63,63	0
54	MG	BA	3040	1/1	1.23	-	76,76,76,76	0
54	MG	BA	3113	1/1	0.53	-	59,59,59,59	0
54	MG	DA	2937	1/1	0.38	-	43,43,43,43	0
54	MG	DA	3553	1/1	0.12	-	91,91,91,91	0
54	MG	DA	3084	1/1	1.01	-	65,65,65,65	0
54	MG	BA	3444	1/1	0.31	-	26,26,26,26	0
54	MG	DA	3138	1/1	0.27	-	81,81,81,81	0
54	MG	BA	3111	1/1	0.70	-	64,64,64,64	0
54	MG	DK	201	1/1	0.16	-	87,87,87,87	0
54	MG	DD	304	1/1	0.86	-	94,94,94,94	0
54	MG	BA	3537	1/1	0.21	-	60,60,60,60	0
54	MG	CA	1831	1/1	0.40	-	90,90,90,90	0
54	MG	AD	304	1/1	0.48	-	113,113,113,113	0
54	MG	DA	3512	1/1	0.31	-	159,159,159,159	0
54	MG	DA	3711	1/1	0.50	-	84,84,84,84	0
54	MG	CA	1721	1/1	0.91	-	118,118,118,118	0
54	MG	BA	3255	1/1	0.56	-	101,101,101,101	0
54	MG	BA	3063	1/1	0.93	-	85,85,85,85	0
54	MG	DA	3650	1/1	0.53	-	55,55,55,55	0
54	MG	DA	3085	1/1	0.45	-	68,68,68,68	0
54	MG	DA	2956	1/1	0.47	-	44,44,44,44	0
54	MG	BA	3182	1/1	0.35	-	78,78,78,78	0
54	MG	AA	1676	1/1	0.12	-	90,90,90,90	0
54	MG	DA	3122	1/1	0.29	-	93,93,93,93	0
54	MG	CA	1860	1/1	0.19	-	68,68,68,68	0
54	MG	AA	1649	1/1	0.21	-	74,74,74,74	0
54	MG	DA	3813	1/1	0.14	-	50,50,50,50	0
54	MG	BA	3081	1/1	0.25	-	67,67,67,67	0
54	MG	DA	2947	1/1	0.50	-	37,37,37,37	0
54	MG	CA	1957	1/1	0.50	-	73,73,73,73	0
54	MG	AA	1823	1/1	0.58	-	148,148,148,148	0
54	MG	DA	3239	1/1	0.21	-	126,126,126,126	0
54	MG	AL	202	1/1	0.08	-	67,67,67,67	0
54	MG	AA	1770	1/1	0.21	-	76,76,76,76	0
54	MG	BA	3356	1/1	0.27	-	33,33,33,33	0
54	MG	AA	1797	1/1	0.43	-	72,72,72,72	0
54	MG	AA	1768	1/1	0.81	-	87,87,87,87	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
54	MG	DA	3699	1/1	0.12	-	96,96,96,96	0
54	MG	AA	1771	1/1	1.27	-	111,111,111,111	0
54	MG	DA	3542	1/1	0.27	-	65,65,65,65	0
54	MG	BA	3627	1/1	0.30	-	67,67,67,67	0
54	MG	DA	3659	1/1	1.15	-	61,61,61,61	0
54	MG	BA	2978	1/1	0.60	-	58,58,58,58	0
54	MG	CA	1907	1/1	0.82	-	87,87,87,87	0
54	MG	CA	1897	1/1	0.79	-	74,74,74,74	0
54	MG	DA	3188	1/1	0.63	-	69,69,69,69	0
54	MG	BA	3224	1/1	0.24	-	97,97,97,97	0
54	MG	BA	3543	1/1	0.25	-	76,76,76,76	0
54	MG	BA	3032	1/1	0.42	-	76,76,76,76	0
54	MG	DA	3200	1/1	0.30	-	97,97,97,97	0
54	MG	CA	1820	1/1	1.19	-	99,99,99,99	0
54	MG	BA	3416	1/1	0.13	-	83,83,83,83	0
54	MG	DK	203	1/1	0.24	-	73,73,73,73	0
54	MG	CN	102	1/1	1.02	-	134,134,134,134	0
54	MG	BA	3296	1/1	0.31	-	71,71,71,71	0
54	MG	DA	2923	1/1	0.48	-	12,12,12,12	0
54	MG	CA	1836	1/1	0.49	-	98,98,98,98	0
54	MG	BA	3574	1/1	0.21	-	62,62,62,62	0
54	MG	DA	3821	1/1	0.30	-	79,79,79,79	0
54	MG	DA	3732	1/1	0.45	-	81,81,81,81	0
54	MG	BA	3559	1/1	0.66	-	70,70,70,70	0
54	MG	DA	3253	1/1	0.23	-	70,70,70,70	0
54	MG	CA	1776	1/1	0.11	-	118,118,118,118	0
54	MG	AA	1647	1/1	0.43	-	63,63,63,63	0
54	MG	DA	3839	1/1	0.29	-	86,86,86,86	0
54	MG	BA	3279	1/1	0.06	-	85,85,85,85	0
54	MG	CA	1841	1/1	0.19	-	95,95,95,95	0
54	MG	AA	1671	1/1	0.16	-	74,74,74,74	0
54	MG	CA	1676	1/1	0.57	-	90,90,90,90	0
54	MG	BA	3601	1/1	0.18	-	76,76,76,76	0
54	MG	DS	201	1/1	0.39	-	98,98,98,98	0
54	MG	DA	2946	1/1	0.48	-	25,25,25,25	0
54	MG	AM	201	1/1	0.10	-	126,126,126,126	0
54	MG	AA	1799	1/1	0.59	-	58,58,58,58	0
54	MG	AA	1729	1/1	0.43	-	107,107,107,107	0
54	MG	AA	1750	1/1	0.42	-	128,128,128,128	0
54	MG	AA	1818	1/1	0.24	-	76,76,76,76	0
54	MG	CA	1757	1/1	0.21	-	102,102,102,102	0
54	MG	DA	3183	1/1	0.41	-	76,76,76,76	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
54	MG	DA	3611	1/1	0.69	-	74,74,74,74	0
54	MG	CA	1826	1/1	0.31	-	97,97,97,97	0
54	MG	DA	3358	1/1	0.29	-	83,83,83,83	0
54	MG	BA	3583	1/1	0.66	-	105,105,105,105	0
54	MG	BA	3354	1/1	0.54	-	123,123,123,123	0
54	MG	DA	3049	1/1	0.46	-	43,43,43,43	0
54	MG	BA	3314	1/1	0.23	-	69,69,69,69	0
54	MG	CA	1959	1/1	0.17	-	106,106,106,106	0
54	MG	DB	219	1/1	0.18	-	73,73,73,73	0
54	MG	BA	3516	1/1	0.39	-	100,100,100,100	0
54	MG	AA	1841	1/1	0.19	-	83,83,83,83	0
54	MG	AA	1848	1/1	0.45	-	77,77,77,77	0
54	MG	DA	3523	1/1	0.05	-	77,77,77,77	0
54	MG	BB	210	1/1	0.32	-	82,82,82,82	0
54	MG	DA	3348	1/1	0.10	-	83,83,83,83	0
54	MG	CA	1925	1/1	0.37	-	77,77,77,77	0
54	MG	DA	3786	1/1	0.82	-	104,104,104,104	0
54	MG	DA	3425	1/1	0.33	-	113,113,113,113	0
54	MG	DA	3474	1/1	1.33	-	81,81,81,81	0
54	MG	DA	3282	1/1	0.54	-	69,69,69,69	0
54	MG	CA	1651	1/1	0.50	-	111,111,111,111	0
54	MG	AI	201	1/1	0.22	-	70,70,70,70	0
54	MG	BA	3021	1/1	0.59	-	66,66,66,66	0
54	MG	AA	1702	1/1	0.17	-	56,56,56,56	0
54	MG	CA	1868	1/1	0.28	-	71,71,71,71	0
54	MG	BA	3610	1/1	0.73	-	80,80,80,80	0
54	MG	AA	1754	1/1	0.16	-	98,98,98,98	0
54	MG	CA	1661	1/1	0.11	-	80,80,80,80	0
54	MG	CA	1830	1/1	0.29	-	82,82,82,82	0
54	MG	AA	1725	1/1	0.21	-	93,93,93,93	0
54	MG	CA	1794	1/1	0.11	-	122,122,122,122	0
54	MG	CA	1825	1/1	0.38	-	97,97,97,97	0
54	MG	DA	2944	1/1	0.44	-	25,25,25,25	0
54	MG	DA	3487	1/1	0.28	-	66,66,66,66	0
54	MG	BA	3293	1/1	0.26	-	60,60,60,60	0
54	MG	BA	3135	1/1	0.23	-	61,61,61,61	0
54	MG	DA	3216	1/1	0.45	-	91,91,91,91	0
54	MG	BA	3451	1/1	0.90	-	47,47,47,47	0
54	MG	AA	1633	1/1	0.29	-	123,123,123,123	0
54	MG	AA	1851	1/1	0.67	-	93,93,93,93	0
54	MG	DA	3712	1/1	0.19	-	41,41,41,41	0
54	MG	BA	3538	1/1	0.35	-	75,75,75,75	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
54	MG	BA	2987	1/1	0.06	-	79,79,79,79	0
54	MG	DA	2906	1/1	0.34	-	16,16,16,16	0
54	MG	BC	301	1/1	0.78	-	60,60,60,60	0
54	MG	BA	3638	1/1	0.71	-	127,127,127,127	0
54	MG	BA	3398	1/1	0.33	-	74,74,74,74	0
54	MG	DA	3586	1/1	0.35	-	79,79,79,79	0
54	MG	CA	1874	1/1	0.37	-	76,76,76,76	0
54	MG	DA	3031	1/1	0.50	-	79,79,79,79	0
54	MG	AA	1753	1/1	0.37	-	103,103,103,103	0
54	MG	BA	3229	1/1	0.28	-	90,90,90,90	0
54	MG	DB	221	1/1	0.32	-	98,98,98,98	0
54	MG	AA	1687	1/1	0.56	-	108,108,108,108	0
54	MG	DA	3338	1/1	0.13	-	123,123,123,123	0
54	MG	DA	3783	1/1	0.16	-	63,63,63,63	0
54	MG	BA	3392	1/1	0.31	-	108,108,108,108	0
54	MG	DA	3430	1/1	0.26	-	103,103,103,103	0
54	MG	CD	302	1/1	0.13	-	74,74,74,74	0
54	MG	CA	1737	1/1	0.56	-	70,70,70,70	0
54	MG	AA	1791	1/1	0.10	-	106,106,106,106	0
54	MG	DA	3208	1/1	0.19	-	56,56,56,56	0
54	MG	BA	3515	1/1	0.38	-	54,54,54,54	0
54	MG	BA	3048	1/1	0.77	-	70,70,70,70	0
54	MG	D1	101	1/1	0.39	-	80,80,80,80	0
54	MG	AA	1681	1/1	0.50	-	65,65,65,65	0
54	MG	CA	1954	1/1	0.09	-	89,89,89,89	0
54	MG	BA	3552	1/1	0.10	-	99,99,99,99	0
54	MG	CA	1812	1/1	0.78	-	92,92,92,92	0
54	MG	DA	3578	1/1	0.35	-	96,96,96,96	0
54	MG	BA	3372	1/1	1.31	-	123,123,123,123	0
54	MG	BB	206	1/1	0.50	-	125,125,125,125	0
54	MG	BA	3389	1/1	0.42	-	66,66,66,66	0
54	MG	AD	302	1/1	0.19	-	76,76,76,76	0
54	MG	AA	1796	1/1	0.55	-	106,106,106,106	0
54	MG	BA	3680	1/1	0.67	-	97,97,97,97	0
54	MG	DA	3518	1/1	0.26	-	102,102,102,102	0
54	MG	DA	3155	1/1	0.31	-	70,70,70,70	0
54	MG	DA	3370	1/1	0.95	-	92,92,92,92	0
54	MG	BA	3298	1/1	0.21	-	126,126,126,126	0
54	MG	DA	3808	1/1	0.38	-	116,116,116,116	0
54	MG	DA	3744	1/1	0.28	-	64,64,64,64	0
54	MG	DA	3714	1/1	0.08	-	96,96,96,96	0
54	MG	BA	3200	1/1	0.25	-	93,93,93,93	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
54	MG	BA	3465	1/1	0.28	-	31,31,31,31	0
54	MG	AA	1728	1/1	0.22	-	71,71,71,71	0
54	MG	BA	2969	1/1	0.66	-	69,69,69,69	0
54	MG	BA	3284	1/1	0.22	-	95,95,95,95	0
54	MG	BA	3212	1/1	0.27	-	67,67,67,67	0
54	MG	BA	2954	1/1	0.28	-	73,73,73,73	0
54	MG	BJ	202	1/1	0.30	-	69,69,69,69	0
54	MG	DA	2926	1/1	0.40	-	25,25,25,25	0
54	MG	BA	2960	1/1	0.52	-	39,39,39,39	0
54	MG	DA	3142	1/1	0.22	-	61,61,61,61	0
54	MG	CA	1862	1/1	0.41	-	96,96,96,96	0
54	MG	BA	3436	1/1	0.55	-	38,38,38,38	0
54	MG	DA	3433	1/1	0.29	-	67,67,67,67	0
54	MG	CL	202	1/1	0.09	-	105,105,105,105	0
54	MG	BA	3115	1/1	0.50	-	76,76,76,76	0
54	MG	BA	3289	1/1	0.43	-	61,61,61,61	0
54	MG	BA	3471	1/1	0.25	-	70,70,70,70	0
54	MG	DA	3075	1/1	0.23	-	50,50,50,50	0
54	MG	DA	3661	1/1	0.64	-	98,98,98,98	0
54	MG	CA	1636	1/1	0.10	-	98,98,98,98	0
54	MG	DA	3211	1/1	0.34	-	64,64,64,64	0
54	MG	BA	3657	1/1	0.39	-	84,84,84,84	0
54	MG	CA	1690	1/1	0.21	-	65,65,65,65	0
54	MG	DA	3325	1/1	0.27	-	66,66,66,66	0
54	MG	BA	3420	1/1	0.63	-	94,94,94,94	0
54	MG	DA	3076	1/1	0.17	-	78,78,78,78	0
54	MG	CA	1808	1/1	0.11	-	98,98,98,98	0
54	MG	CA	1875	1/1	0.62	-	63,63,63,63	0
54	MG	BA	3422	1/1	0.40	-	93,93,93,93	0
54	MG	CA	1664	1/1	0.07	-	85,85,85,85	0
54	MG	DA	2993	1/1	0.34	-	47,47,47,47	0
54	MG	BA	3395	1/1	0.35	-	84,84,84,84	0
54	MG	DA	3037	1/1	0.18	-	44,44,44,44	0
54	MG	BA	3577	1/1	0.43	-	142,142,142,142	0
54	MG	AA	1706	1/1	0.53	-	78,78,78,78	0
54	MG	DB	240	1/1	0.18	-	123,123,123,123	0
54	MG	AA	1742	1/1	0.11	-	90,90,90,90	0
54	MG	BA	2986	1/1	0.69	-	54,54,54,54	0
54	MG	DA	3302	1/1	0.69	-	102,102,102,102	0
54	MG	DA	3380	1/1	0.21	-	84,84,84,84	0
54	MG	BA	3181	1/1	0.20	-	62,62,62,62	0
54	MG	DA	3393	1/1	0.54	-	77,77,77,77	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
54	MG	BA	3132	1/1	0.25	-	66,66,66,66	0
54	MG	DA	3360	1/1	0.29	-	107,107,107,107	0
54	MG	BA	3122	1/1	0.32	-	56,56,56,56	0
54	MG	CG	203	1/1	0.18	-	100,100,100,100	0
54	MG	BA	3028	1/1	1.60	-	61,61,61,61	0
54	MG	DA	2912	1/1	0.40	-	19,19,19,19	0
54	MG	BR	201	1/1	0.07	-	75,75,75,75	0
54	MG	AA	1677	1/1	0.15	-	50,50,50,50	0
54	MG	DA	3723	1/1	0.32	-	67,67,67,67	0
54	MG	DA	3682	1/1	0.28	-	59,59,59,59	0
54	MG	BA	3556	1/1	0.64	-	77,77,77,77	0
54	MG	DA	3415	1/1	0.25	-	66,66,66,66	0
54	MG	BA	3355	1/1	0.27	-	72,72,72,72	0
54	MG	DA	3343	1/1	0.30	-	97,97,97,97	0
54	MG	CB	302	1/1	0.32	-	112,112,112,112	0
54	MG	CA	1892	1/1	0.69	-	114,114,114,114	0
54	MG	BA	3283	1/1	0.26	-	100,100,100,100	0
54	MG	BA	3539	1/1	0.40	-	97,97,97,97	0
54	MG	BA	3345	1/1	0.31	-	71,71,71,71	0
54	MG	DA	3148	1/1	0.17	-	94,94,94,94	0
54	MG	CA	1722	1/1	0.27	-	116,116,116,116	0
54	MG	BA	3331	1/1	0.77	-	66,66,66,66	0
54	MG	AA	1878	1/1	0.08	-	92,92,92,92	0
54	MG	DA	3456	1/1	0.34	-	121,121,121,121	0
54	MG	CA	1923	1/1	0.53	-	74,74,74,74	0
54	MG	AA	1623	1/1	0.21	-	99,99,99,99	0
54	MG	B2	101	1/1	0.12	-	27,27,27,27	0
54	MG	BA	3565	1/1	0.25	-	104,104,104,104	0
54	MG	DA	3269	1/1	0.15	-	109,109,109,109	0
54	MG	DA	3219	1/1	0.17	-	60,60,60,60	0
54	MG	BA	3511	1/1	1.17	-	78,78,78,78	0
54	MG	AA	1819	1/1	0.47	-	73,73,73,73	0
54	MG	AA	1801	1/1	1.04	-	71,71,71,71	0
54	MG	AA	1747	1/1	0.55	-	116,116,116,116	0
54	MG	DA	3716	1/1	0.47	-	78,78,78,78	0
54	MG	BA	2925	1/1	0.27	-	12,12,12,12	0
54	MG	DA	3368	1/1	0.30	-	98,98,98,98	0
54	MG	DB	202	1/1	0.32	-	33,33,33,33	0
54	MG	DA	3794	1/1	0.18	-	104,104,104,104	0
54	MG	DA	3809	1/1	0.94	-	84,84,84,84	0
54	MG	CA	1706	1/1	0.78	-	106,106,106,106	0
54	MG	BA	2953	1/1	0.22	-	45,45,45,45	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
54	MG	DA	3411	1/1	0.58	-	68,68,68,68	0
54	MG	DA	3290	1/1	0.21	-	61,61,61,61	0
54	MG	AA	1803	1/1	0.56	-	69,69,69,69	0
54	MG	CA	1895	1/1	0.80	-	88,88,88,88	0
54	MG	DD	301	1/1	0.50	-	39,39,39,39	0
54	MG	BA	3207	1/1	0.48	-	70,70,70,70	0
54	MG	DA	3547	1/1	0.48	-	115,115,115,115	0
54	MG	DA	3112	1/1	0.33	-	91,91,91,91	0
54	MG	AA	1765	1/1	0.12	-	91,91,91,91	0
54	MG	DA	3191	1/1	0.28	-	62,62,62,62	0
54	MG	DA	3651	1/1	0.38	-	51,51,51,51	0
54	MG	AA	1794	1/1	0.13	-	112,112,112,112	0
54	MG	DA	3507	1/1	0.86	-	70,70,70,70	0
54	MG	DB	207	1/1	0.31	-	58,58,58,58	0
54	MG	DA	3576	1/1	0.45	-	99,99,99,99	0
54	MG	BA	2929	1/1	0.70	-	50,50,50,50	0
54	MG	BA	3335	1/1	0.90	-	80,80,80,80	0
54	MG	DA	3081	1/1	0.70	-	67,67,67,67	0
54	MG	AA	1635	1/1	0.24	-	37,37,37,37	0
54	MG	DA	3798	1/1	0.38	-	88,88,88,88	0
54	MG	DA	3315	1/1	0.38	-	58,58,58,58	0
54	MG	DA	3450	1/1	0.66	-	81,81,81,81	0
54	MG	DA	3642	1/1	0.52	-	52,52,52,52	0
54	MG	CA	1834	1/1	0.22	-	81,81,81,81	0
54	MG	DA	3145	1/1	0.28	-	100,100,100,100	0
54	MG	CA	1900	1/1	0.23	-	86,86,86,86	0
54	MG	DA	3133	1/1	0.20	-	114,114,114,114	0
54	MG	DF	201	1/1	0.42	-	70,70,70,70	0
54	MG	CA	1844	1/1	0.55	-	78,78,78,78	0
54	MG	DA	3822	1/1	0.12	-	70,70,70,70	0
54	MG	AA	1667	1/1	0.83	-	78,78,78,78	0
54	MG	AA	1864	1/1	0.17	-	75,75,75,75	0
54	MG	BA	3209	1/1	0.49	-	81,81,81,81	0
54	MG	BA	2951	1/1	0.85	-	53,53,53,53	0
54	MG	BA	3168	1/1	0.31	-	20,20,20,20	0
54	MG	AT	202	1/1	0.33	-	80,80,80,80	0
54	MG	BA	3472	1/1	0.47	-	65,65,65,65	0
54	MG	DA	3187	1/1	0.28	-	114,114,114,114	0
54	MG	AA	1703	1/1	0.49	-	63,63,63,63	0
54	MG	BA	3614	1/1	0.17	-	112,112,112,112	0
54	MG	DA	3841	1/1	0.39	-	80,80,80,80	0
54	MG	DA	3587	1/1	0.09	-	113,113,113,113	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
54	MG	DA	3313	1/1	0.68	-	78,78,78,78	0
54	MG	CA	1779	1/1	0.27	-	79,79,79,79	0
54	MG	BA	3521	1/1	0.23	-	88,88,88,88	0
54	MG	CA	1611	1/1	0.33	-	128,128,128,128	0
54	MG	BA	3528	1/1	0.20	-	73,73,73,73	0
54	MG	BY	101	1/1	0.33	-	42,42,42,42	0
54	MG	DA	3510	1/1	0.23	-	64,64,64,64	0
54	MG	DA	3213	1/1	0.14	-	59,59,59,59	0
54	MG	BB	214	1/1	0.65	-	84,84,84,84	0
54	MG	AA	1712	1/1	0.19	-	105,105,105,105	0
54	MG	AA	1716	1/1	0.42	-	96,96,96,96	0
54	MG	DA	2914	1/1	0.43	-	23,23,23,23	0
54	MG	CA	1618	1/1	0.64	-	84,84,84,84	0
54	MG	DA	3759	1/1	0.31	-	97,97,97,97	0
54	MG	BT	101	1/1	0.80	-	101,101,101,101	0
54	MG	DL	202	1/1	0.27	-	146,146,146,146	0
54	MG	CA	1855	1/1	0.39	-	107,107,107,107	0
54	MG	CA	1625	1/1	0.48	-	67,67,67,67	0
54	MG	DA	3670	1/1	0.67	-	83,83,83,83	0
54	MG	DA	3134	1/1	0.80	-	69,69,69,69	0
54	MG	BA	3548	1/1	0.37	-	61,61,61,61	0
54	MG	BA	3411	1/1	0.38	-	90,90,90,90	0
54	MG	AA	1655	1/1	0.69	-	58,58,58,58	0
54	MG	DA	3708	1/1	0.21	-	63,63,63,63	0
54	MG	BA	3160	1/1	0.59	-	87,87,87,87	0
54	MG	DA	3596	1/1	0.62	-	113,113,113,113	0
54	MG	CA	1914	1/1	0.10	-	97,97,97,97	0
54	MG	DA	2964	1/1	0.47	-	45,45,45,45	0
54	MG	BA	2963	1/1	0.75	-	34,34,34,34	0
54	MG	DA	3136	1/1	0.15	-	57,57,57,57	0
54	MG	DA	3697	1/1	0.41	-	92,92,92,92	0
54	MG	DA	2981	1/1	0.39	-	40,40,40,40	0
54	MG	DA	3796	1/1	0.14	-	67,67,67,67	0
54	MG	DA	3396	1/1	0.27	-	78,78,78,78	0
54	MG	BA	3603	1/1	0.23	-	86,86,86,86	0
54	MG	DA	3169	1/1	0.40	-	54,54,54,54	0
54	MG	BA	3531	1/1	0.15	-	91,91,91,91	0
54	MG	DA	3855	1/1	0.20	-	104,104,104,104	0
54	MG	BA	2962	1/1	0.36	-	54,54,54,54	0
54	MG	DA	3080	1/1	0.97	-	83,83,83,83	0
54	MG	CA	1687	1/1	0.85	-	63,63,63,63	0
54	MG	DA	3404	1/1	0.32	-	79,79,79,79	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
54	MG	DA	3285	1/1	0.60	-	65,65,65,65	0
54	MG	BA	3184	1/1	0.65	-	67,67,67,67	0
54	MG	DA	3539	1/1	0.22	-	81,81,81,81	0
54	MG	BB	220	1/1	0.28	-	75,75,75,75	0
54	MG	AA	1621	1/1	0.70	-	71,71,71,71	0
54	MG	BB	201	1/1	0.47	-	63,63,63,63	0
54	MG	DV	201	1/1	0.27	-	90,90,90,90	0
54	MG	DA	3305	1/1	0.22	-	99,99,99,99	0
54	MG	BA	3397	1/1	0.71	-	125,125,125,125	0
54	MG	BA	3554	1/1	0.99	-	90,90,90,90	0
54	MG	AA	1617	1/1	0.60	-	84,84,84,84	0
54	MG	BA	3514	1/1	0.19	-	83,83,83,83	0
54	MG	DA	3184	1/1	0.13	-	38,38,38,38	0
54	MG	DA	3078	1/1	0.56	-	48,48,48,48	0
54	MG	BA	3271	1/1	0.18	-	83,83,83,83	0
54	MG	BA	3445	1/1	0.43	-	61,61,61,61	0
54	MG	AA	1782	1/1	0.26	-	104,104,104,104	0
54	MG	DX	101	1/1	0.39	-	103,103,103,103	0
54	MG	CA	1947	1/1	0.42	-	136,136,136,136	0
54	MG	BA	3635	1/1	0.33	-	113,113,113,113	0
54	MG	BA	3326	1/1	0.24	-	82,82,82,82	0
54	MG	AA	1865	1/1	0.11	-	107,107,107,107	0
54	MG	DA	2953	1/1	0.58	-	46,46,46,46	0
54	MG	DA	3727	1/1	0.41	-	88,88,88,88	0
54	MG	DA	3760	1/1	0.31	-	97,97,97,97	0
54	MG	AA	1629	1/1	0.43	-	66,66,66,66	0
54	MG	BA	3547	1/1	0.13	-	87,87,87,87	0
54	MG	CA	1735	1/1	0.62	-	77,77,77,77	0
54	MG	DB	211	1/1	0.07	-	65,65,65,65	0
54	MG	CC	304	1/1	0.23	-	121,121,121,121	0
54	MG	DA	3326	1/1	0.25	-	81,81,81,81	0
54	MG	DA	3203	1/1	0.09	-	67,67,67,67	0
54	MG	DA	3599	1/1	0.27	-	58,58,58,58	0
54	MG	DA	3060	1/1	0.55	-	77,77,77,77	0
54	MG	DA	3328	1/1	0.51	-	85,85,85,85	0
54	MG	DA	3001	1/1	0.21	-	25,25,25,25	0
54	MG	BA	3036	1/1	1.50	-	57,57,57,57	0
54	MG	DA	3751	1/1	0.22	-	76,76,76,76	0
54	MG	BA	3586	1/1	0.25	-	97,97,97,97	0
54	MG	AA	1751	1/1	0.12	-	88,88,88,88	0
54	MG	DA	3607	1/1	0.42	-	79,79,79,79	0
54	MG	BA	3675	1/1	0.10	-	120,120,120,120	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
54	MG	CA	1724	1/1	0.68	-	124,124,124,124	0
54	MG	DA	3643	1/1	0.49	-	40,40,40,40	0
54	MG	BA	2919	1/1	0.36	-	14,14,14,14	0
54	MG	DA	3538	1/1	0.53	-	66,66,66,66	0
54	MG	BA	3185	1/1	0.53	-	85,85,85,85	0
54	MG	BA	3661	1/1	0.16	-	82,82,82,82	0
54	MG	BA	3240	1/1	0.44	-	157,157,157,157	0
54	MG	DA	3058	1/1	0.19	-	56,56,56,56	0
54	MG	DA	3445	1/1	0.16	-	137,137,137,137	0
54	MG	BA	2975	1/1	0.27	-	58,58,58,58	0
54	MG	CA	1929	1/1	0.44	-	95,95,95,95	0
54	MG	BA	3488	1/1	0.23	-	53,53,53,53	0
54	MG	AA	1763	1/1	0.05	-	121,121,121,121	0
54	MG	BA	3082	1/1	0.19	-	38,38,38,38	0
54	MG	BB	211	1/1	0.38	-	85,85,85,85	0
54	MG	CK	201	1/1	0.12	-	136,136,136,136	0
54	MG	BA	3469	1/1	0.20	-	58,58,58,58	0
54	MG	CA	1936	1/1	0.57	-	102,102,102,102	0
54	MG	CA	1698	1/1	0.17	-	123,123,123,123	0
54	MG	DA	3701	1/1	0.26	-	56,56,56,56	0
54	MG	CA	1614	1/1	0.59	-	66,66,66,66	0
54	MG	BA	3644	1/1	0.36	-	86,86,86,86	0
54	MG	BA	3594	1/1	0.17	-	129,129,129,129	0
54	MG	DB	212	1/1	0.22	-	85,85,85,85	0
54	MG	AA	1646	1/1	0.74	-	89,89,89,89	0
54	MG	BA	2907	1/1	0.40	-	15,15,15,15	0
54	MG	CA	1843	1/1	0.24	-	109,109,109,109	0
54	MG	DA	2917	1/1	0.18	-	71,71,71,71	0
54	MG	DA	3095	1/1	0.65	-	72,72,72,72	0
54	MG	BM	201	1/1	0.24	-	50,50,50,50	0
54	MG	CA	1958	1/1	0.76	-	125,125,125,125	0
54	MG	BA	3213	1/1	0.12	-	102,102,102,102	0
54	MG	DA	3672	1/1	0.28	-	80,80,80,80	0
54	MG	DA	3773	1/1	0.56	-	37,37,37,37	0
54	MG	CA	1645	1/1	0.15	-	80,80,80,80	0
54	MG	DA	3385	1/1	0.44	-	69,69,69,69	0
54	MG	CA	1876	1/1	0.21	-	69,69,69,69	0
54	MG	DA	2969	1/1	0.51	-	39,39,39,39	0
54	MG	CA	1685	1/1	0.43	-	109,109,109,109	0
54	MG	BA	3286	1/1	0.16	-	68,68,68,68	0
54	MG	BA	3501	1/1	1.78	-	105,105,105,105	0
54	MG	DA	2977	1/1	0.67	-	49,49,49,49	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
54	MG	DA	2984	1/1	0.20	-	22,22,22,22	0
54	MG	BC	302	1/1	0.45	-	82,82,82,82	0
54	MG	BA	3443	1/1	0.33	-	36,36,36,36	0
54	MG	DA	3446	1/1	0.16	-	57,57,57,57	0
54	MG	AA	1781	1/1	0.27	-	92,92,92,92	0
54	MG	DA	3342	1/1	0.88	-	112,112,112,112	0
54	MG	BA	3580	1/1	0.70	-	94,94,94,94	0
54	MG	BA	3183	1/1	0.17	-	68,68,68,68	0
54	MG	CL	201	1/1	0.09	-	99,99,99,99	0
54	MG	BA	3461	1/1	0.45	-	48,48,48,48	0
54	MG	BA	3158	1/1	1.17	-	99,99,99,99	0
54	MG	DA	3780	1/1	0.33	-	67,67,67,67	0
54	MG	CA	1669	1/1	0.18	-	76,76,76,76	0
54	MG	AA	1714	1/1	0.73	-	81,81,81,81	0
54	MG	DA	3749	1/1	0.47	-	59,59,59,59	0
54	MG	DA	3561	1/1	0.25	-	85,85,85,85	0
54	MG	BA	3126	1/1	0.27	-	60,60,60,60	0
54	MG	BA	3142	1/1	0.20	-	47,47,47,47	0
54	MG	DA	3346	1/1	0.17	-	68,68,68,68	0
54	MG	DA	3322	1/1	0.14	-	65,65,65,65	0
54	MG	DA	2920	1/1	0.28	-	14,14,14,14	0
54	MG	BX	101	1/1	0.20	-	71,71,71,71	0
54	MG	DA	3167	1/1	0.33	-	58,58,58,58	0
54	MG	BA	2916	1/1	0.47	-	37,37,37,37	0
54	MG	DA	3275	1/1	0.47	-	92,92,92,92	0
54	MG	DA	3684	1/1	0.40	-	69,69,69,69	0
54	MG	CA	1617	1/1	0.32	-	104,104,104,104	0
54	MG	CA	1926	1/1	0.24	-	76,76,76,76	0
54	MG	AA	1805	1/1	0.46	-	66,66,66,66	0
54	MG	BA	3447	1/1	0.77	-	39,39,39,39	0
54	MG	DA	3455	1/1	0.80	-	97,97,97,97	0
54	MG	DA	3763	1/1	0.22	-	57,57,57,57	0
54	MG	BB	221	1/1	0.33	-	89,89,89,89	0
54	MG	CA	1964	1/1	0.33	-	99,99,99,99	0
54	MG	DA	3042	1/1	0.24	-	81,81,81,81	0
54	MG	D2	101	1/1	1.12	-	78,78,78,78	0
54	MG	BA	3440	1/1	0.41	-	23,23,23,23	0
54	MG	DA	3788	1/1	0.31	-	92,92,92,92	0
54	MG	AA	1697	1/1	0.79	-	73,73,73,73	0
54	MG	AA	1749	1/1	0.20	-	90,90,90,90	0
54	MG	BA	3572	1/1	0.08	-	87,87,87,87	0
54	MG	AA	1800	1/1	1.08	-	69,69,69,69	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
54	MG	DA	3304	1/1	0.31	-	85,85,85,85	0
54	MG	DA	3267	1/1	0.40	-	43,43,43,43	0
54	MG	BA	3012	1/1	0.90	-	71,71,71,71	0
54	MG	CA	1887	1/1	0.22	-	75,75,75,75	0
54	MG	DA	3124	1/1	0.45	-	51,51,51,51	0
54	MG	DA	3467	1/1	0.12	-	97,97,97,97	0
54	MG	DA	3818	1/1	0.11	-	78,78,78,78	0
54	MG	DA	3330	1/1	0.50	-	100,100,100,100	0
54	MG	CB	303	1/1	0.09	-	122,122,122,122	0
54	MG	DA	2972	1/1	0.23	-	37,37,37,37	0
54	MG	BA	3659	1/1	0.29	-	68,68,68,68	0
54	MG	CA	1750	1/1	0.23	-	87,87,87,87	0
54	MG	DA	3347	1/1	0.48	-	67,67,67,67	0
54	MG	BA	3425	1/1	0.70	-	85,85,85,85	0
54	MG	DA	2952	1/1	0.46	-	25,25,25,25	0
54	MG	BA	3585	1/1	0.51	-	69,69,69,69	0
54	MG	DA	3621	1/1	0.18	-	88,88,88,88	0
54	MG	BA	3323	1/1	0.27	-	98,98,98,98	0
54	MG	BA	3545	1/1	0.46	-	59,59,59,59	0
54	MG	DA	2999	1/1	0.26	-	69,69,69,69	0
54	MG	AA	1641	1/1	0.37	-	66,66,66,66	0
54	MG	DA	3408	1/1	0.21	-	109,109,109,109	0
54	MG	AA	1835	1/1	0.20	-	158,158,158,158	0
54	MG	BA	3367	1/1	0.33	-	74,74,74,74	0
54	MG	BA	3478	1/1	0.82	-	78,78,78,78	0
54	MG	DA	3505	1/1	0.37	-	105,105,105,105	0
54	MG	DA	3795	1/1	0.50	-	80,80,80,80	0
54	MG	AA	1601	1/1	0.25	-	35,35,35,35	0
54	MG	BA	3251	1/1	0.81	-	95,95,95,95	0
54	MG	CA	1730	1/1	0.26	-	112,112,112,112	0
54	MG	BA	3141	1/1	0.56	-	91,91,91,91	0
54	MG	BA	3227	1/1	0.59	-	61,61,61,61	0
54	MG	BA	3303	1/1	0.17	-	157,157,157,157	0
54	MG	DA	2994	1/1	0.37	-	54,54,54,54	0
54	MG	CA	1777	1/1	0.27	-	98,98,98,98	0
54	MG	DA	3816	1/1	0.17	-	52,52,52,52	0
54	MG	DA	3197	1/1	0.22	-	46,46,46,46	0
54	MG	DA	2992	1/1	0.47	-	60,60,60,60	0
54	MG	DA	3453	1/1	0.48	-	87,87,87,87	0
54	MG	DA	3314	1/1	0.43	-	105,105,105,105	0
54	MG	CA	1800	1/1	0.21	-	89,89,89,89	0
54	MG	DA	3152	1/1	0.28	-	43,43,43,43	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
54	MG	DA	3231	1/1	0.56	-	81,81,81,81	0
54	MG	DA	3289	1/1	0.28	-	44,44,44,44	0
54	MG	DA	3345	1/1	0.35	-	88,88,88,88	0
54	MG	AA	1673	1/1	0.30	-	95,95,95,95	0
54	MG	BO	201	1/1	0.11	-	70,70,70,70	0
54	MG	BA	3628	1/1	0.11	-	102,102,102,102	0
54	MG	DA	2985	1/1	0.47	-	40,40,40,40	0
54	MG	AA	1758	1/1	0.57	-	69,69,69,69	0
54	MG	BA	3493	1/1	0.39	-	75,75,75,75	0
54	MG	DA	3150	1/1	0.14	-	56,56,56,56	0
54	MG	DA	3074	1/1	0.31	-	43,43,43,43	0
54	MG	DA	3771	1/1	0.34	-	58,58,58,58	0
54	MG	DA	3240	1/1	0.12	-	69,69,69,69	0
54	MG	CA	1778	1/1	0.39	-	94,94,94,94	0
54	MG	DA	3364	1/1	0.49	-	75,75,75,75	0
54	MG	AA	1778	1/1	0.28	-	113,113,113,113	0
54	MG	AA	1622	1/1	0.61	-	62,62,62,62	0
54	MG	DA	3768	1/1	0.42	-	102,102,102,102	0
54	MG	DA	3431	1/1	0.22	-	94,94,94,94	0
54	MG	DA	3777	1/1	0.31	-	90,90,90,90	0
54	MG	BA	2999	1/1	0.49	-	39,39,39,39	0
54	MG	BK	201	1/1	0.21	-	77,77,77,77	0
54	MG	BA	3479	1/1	0.36	-	69,69,69,69	0
54	MG	DA	3465	1/1	0.29	-	105,105,105,105	0
54	MG	BA	3428	1/1	0.25	-	90,90,90,90	0
54	MG	AA	1620	1/1	0.56	-	56,56,56,56	0
54	MG	DJ	202	1/1	0.31	-	126,126,126,126	0
54	MG	DA	3700	1/1	1.26	-	96,96,96,96	0
54	MG	BA	3239	1/1	0.64	-	62,62,62,62	0
54	MG	BA	3061	1/1	0.12	-	54,54,54,54	0
54	MG	DA	3753	1/1	0.38	-	79,79,79,79	0
54	MG	AA	1853	1/1	0.10	-	86,86,86,86	0
54	MG	BA	3473	1/1	1.45	-	70,70,70,70	0
54	MG	BA	3450	1/1	0.62	-	46,46,46,46	0
54	MG	DA	3633	1/1	0.30	-	83,83,83,83	0
54	MG	CV	6202	1/1	0.09	-	108,108,108,108	0
54	MG	DA	3003	1/1	0.57	-	51,51,51,51	0
54	MG	BA	3330	1/1	0.61	-	101,101,101,101	0
54	MG	BB	225	1/1	1.20	-	96,96,96,96	0
54	MG	BA	3301	1/1	0.31	-	58,58,58,58	0
54	MG	DA	2965	1/1	0.57	-	34,34,34,34	0
54	MG	DJ	201	1/1	0.34	-	61,61,61,61	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
54	MG	CA	1768	1/1	0.28	-	123,123,123,123	0
54	MG	DA	2989	1/1	0.40	-	39,39,39,39	0
54	MG	DA	3736	1/1	0.25	-	134,134,134,134	0
54	MG	AA	1817	1/1	0.74	-	84,84,84,84	0
54	MG	BA	3437	1/1	0.52	-	42,42,42,42	0
54	MG	CA	1772	1/1	0.15	-	112,112,112,112	0
54	MG	DA	3178	1/1	0.84	-	54,54,54,54	0
54	MG	DA	3129	1/1	0.62	-	93,93,93,93	0
54	MG	DA	3255	1/1	0.49	-	70,70,70,70	0
54	MG	BA	3403	1/1	0.21	-	106,106,106,106	0
54	MG	BA	2911	1/1	0.63	-	33,33,33,33	0
54	MG	BA	3655	1/1	0.23	-	92,92,92,92	0
54	MG	DA	2951	1/1	0.81	-	56,56,56,56	0
54	MG	DA	3558	1/1	0.24	-	148,148,148,148	0
54	MG	CA	1655	1/1	0.34	-	100,100,100,100	0
54	MG	DO	201	1/1	0.35	-	55,55,55,55	0
54	MG	AA	1777	1/1	0.33	-	49,49,49,49	0
54	MG	DA	3034	1/1	0.58	-	89,89,89,89	0
54	MG	BA	3489	1/1	0.19	-	73,73,73,73	0
54	MG	BA	3495	1/1	0.09	-	74,74,74,74	0
54	MG	DA	3718	1/1	0.20	-	70,70,70,70	0
54	MG	CA	1653	1/1	0.14	-	133,133,133,133	0
54	MG	DA	2971	1/1	0.67	-	38,38,38,38	0
54	MG	BA	3280	1/1	0.36	-	61,61,61,61	0
54	MG	BA	3219	1/1	0.14	-	80,80,80,80	0
54	MG	BA	3338	1/1	0.16	-	78,78,78,78	0
54	MG	BA	3248	1/1	0.52	-	82,82,82,82	0
54	MG	DA	3632	1/1	0.18	-	111,111,111,111	0
54	MG	DB	231	1/1	0.31	-	117,117,117,117	0
54	MG	DA	3220	1/1	0.16	-	98,98,98,98	0
54	MG	CA	1932	1/1	0.21	-	84,84,84,84	0
54	MG	BA	3187	1/1	0.68	-	73,73,73,73	0
54	MG	DA	3540	1/1	0.18	-	93,93,93,93	0
54	MG	CA	1956	1/1	0.22	-	85,85,85,85	0
54	MG	BA	3198	1/1	0.45	-	85,85,85,85	0
54	MG	DA	3634	1/1	1.21	-	106,106,106,106	0
54	MG	BA	3365	1/1	0.12	-	131,131,131,131	0
54	MG	DA	3595	1/1	0.20	-	61,61,61,61	0
54	MG	AN	102	1/1	0.69	-	91,91,91,91	0
54	MG	BA	3350	1/1	0.22	-	66,66,66,66	0
54	MG	BA	3062	1/1	0.61	-	79,79,79,79	0
54	MG	CA	1904	1/1	0.40	-	97,97,97,97	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
54	MG	AA	1723	1/1	0.23	-	126,126,126,126	0
54	MG	DA	2933	1/1	0.30	-	25,25,25,25	0
54	MG	CA	1632	1/1	0.57	-	59,59,59,59	0
54	MG	AA	1875	1/1	0.23	-	97,97,97,97	0
54	MG	DA	3734	1/1	0.32	-	76,76,76,76	0
54	MG	BA	3017	1/1	0.27	-	55,55,55,55	0
54	MG	DA	3681	1/1	0.27	-	78,78,78,78	0
54	MG	DA	3259	1/1	0.24	-	87,87,87,87	0
54	MG	BA	3119	1/1	0.69	-	73,73,73,73	0
54	MG	BA	2937	1/1	0.12	-	56,56,56,56	0
54	MG	AA	1733	1/1	0.16	-	89,89,89,89	0
54	MG	DA	2931	1/1	0.42	-	21,21,21,21	0
54	MG	DA	3329	1/1	0.19	-	96,96,96,96	0
54	MG	DA	3299	1/1	0.43	-	104,104,104,104	0
54	MG	CA	1828	1/1	0.42	-	88,88,88,88	0
54	MG	BA	3452	1/1	0.26	-	41,41,41,41	0
54	MG	DA	3423	1/1	0.26	-	79,79,79,79	0
54	MG	DA	3373	1/1	0.10	-	78,78,78,78	0
54	MG	DA	3102	1/1	0.31	-	50,50,50,50	0
54	MG	DA	3562	1/1	0.16	-	60,60,60,60	0
54	MG	DA	3483	1/1	0.60	-	63,63,63,63	0
54	MG	AA	1867	1/1	0.18	-	114,114,114,114	0
54	MG	BA	3400	1/1	0.47	-	83,83,83,83	0
54	MG	DA	3226	1/1	0.51	-	86,86,86,86	0
54	MG	DA	3140	1/1	0.56	-	50,50,50,50	0
54	MG	DA	3185	1/1	0.22	-	54,54,54,54	0
54	MG	AA	1701	1/1	0.30	-	84,84,84,84	0
54	MG	DA	3574	1/1	0.23	-	152,152,152,152	0
54	MG	CA	1733	1/1	0.57	-	78,78,78,78	0
54	MG	DA	3120	1/1	0.08	-	61,61,61,61	0
54	MG	DA	2943	1/1	0.26	-	5,5,5,5	0
54	MG	CA	1786	1/1	0.20	-	94,94,94,94	0
54	MG	DA	3703	1/1	0.31	-	60,60,60,60	0
54	MG	BA	3015	1/1	0.12	-	55,55,55,55	0
54	MG	CA	1930	1/1	0.25	-	89,89,89,89	0
54	MG	AA	1708	1/1	0.42	-	137,137,137,137	0
54	MG	DA	3613	1/1	0.19	-	121,121,121,121	0
54	MG	DA	3761	1/1	0.10	-	100,100,100,100	0
54	MG	CA	1677	1/1	0.40	-	93,93,93,93	0
54	MG	AA	1757	1/1	0.10	-	98,98,98,98	0
54	MG	DA	3601	1/1	0.25	-	59,59,59,59	0
54	MG	DA	3401	1/1	0.26	-	100,100,100,100	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
54	MG	DG	201	1/1	0.17	-	108,108,108,108	0
54	MG	AA	1820	1/1	1.02	-	94,94,94,94	0
54	MG	CA	1693	1/1	0.67	-	95,95,95,95	0
54	MG	D4	102	1/1	0.23	-	65,65,65,65	0
54	MG	DA	3740	1/1	0.19	-	99,99,99,99	0
54	MG	DA	3387	1/1	0.13	-	124,124,124,124	0
54	MG	DA	3283	1/1	0.34	-	71,71,71,71	0
54	MG	DA	3842	1/1	0.28	-	105,105,105,105	0
54	MG	BA	3306	1/1	0.26	-	78,78,78,78	0
54	MG	BA	3438	1/1	0.51	-	29,29,29,29	0
54	MG	DA	3217	1/1	0.31	-	59,59,59,59	0
54	MG	DA	3033	1/1	0.52	-	79,79,79,79	0
54	MG	AA	1854	1/1	0.52	-	114,114,114,114	0
54	MG	BA	3086	1/1	0.15	-	63,63,63,63	0
54	MG	BA	3378	1/1	0.49	-	80,80,80,80	0
54	MG	BA	3325	1/1	0.19	-	168,168,168,168	0
54	MG	DA	3789	1/1	0.19	-	56,56,56,56	0
54	MG	CA	1793	1/1	0.26	-	125,125,125,125	0
54	MG	DA	3460	1/1	0.50	-	86,86,86,86	0
54	MG	CA	1883	1/1	0.49	-	75,75,75,75	0
54	MG	DA	3478	1/1	0.37	-	48,48,48,48	0
54	MG	D2	102	1/1	0.08	-	42,42,42,42	0
54	MG	BA	3492	1/1	0.18	-	70,70,70,70	0
54	MG	AA	1640	1/1	0.36	-	58,58,58,58	0
54	MG	BA	2990	1/1	0.15	-	35,35,35,35	0
54	MG	DL	201	1/1	0.10	-	7,7,7,7	0
54	MG	BA	3098	1/1	0.34	-	90,90,90,90	0
54	MG	BA	3568	1/1	0.30	-	69,69,69,69	0
54	MG	BA	3619	1/1	0.15	-	145,145,145,145	0
54	MG	AA	1603	1/1	0.53	-	37,37,37,37	0
54	MG	DA	3646	1/1	0.68	-	45,45,45,45	0
54	MG	BA	3208	1/1	0.37	-	96,96,96,96	0
54	MG	DA	3321	1/1	0.91	-	110,110,110,110	0
54	MG	CA	1941	1/1	0.17	-	70,70,70,70	0
54	MG	BA	3104	1/1	0.15	-	49,49,49,49	0
54	MG	CA	1910	1/1	0.19	-	109,109,109,109	0
54	MG	AA	1858	1/1	0.19	-	86,86,86,86	0
54	MG	DA	3779	1/1	0.39	-	81,81,81,81	0
54	MG	AG	201	1/1	0.16	-	106,106,106,106	0
54	MG	AA	1732	1/1	0.12	-	104,104,104,104	0
54	MG	BA	3384	1/1	0.30	-	93,93,93,93	0
54	MG	DA	3162	1/1	0.40	-	30,30,30,30	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
54	MG	DA	3292	1/1	1.11	-	73,73,73,73	0
54	MG	DA	3261	1/1	0.29	-	57,57,57,57	0
54	MG	DA	3583	1/1	0.45	-	119,119,119,119	0
54	MG	AA	1833	1/1	0.45	-	75,75,75,75	0
54	MG	DA	3013	1/1	0.89	-	52,52,52,52	0
54	MG	DA	3584	1/1	0.55	-	130,130,130,130	0
54	MG	BU	201	1/1	0.39	-	70,70,70,70	0
54	MG	AO	103	1/1	0.12	-	111,111,111,111	0
55	ZN	CD	301	1/1	0.28	-	116,116,116,116	0
54	MG	CA	1701	1/1	0.65	-	83,83,83,83	0
54	MG	CA	1717	1/1	0.93	-	103,103,103,103	0
54	MG	BA	3226	1/1	0.35	-	59,59,59,59	0
54	MG	DA	3399	1/1	0.17	-	75,75,75,75	0
54	MG	AA	1731	1/1	0.26	-	83,83,83,83	0
54	MG	DA	3137	1/1	0.28	-	29,29,29,29	0
54	MG	DA	3207	1/1	0.29	-	43,43,43,43	0
54	MG	DA	3077	1/1	0.15	-	33,33,33,33	0
54	MG	DA	3409	1/1	0.26	-	110,110,110,110	0
54	MG	DA	2901	1/1	0.47	-	9,9,9,9	0
54	MG	AA	1610	1/1	0.37	-	29,29,29,29	0
54	MG	DA	2958	1/1	0.07	-	31,31,31,31	0
54	MG	CA	1935	1/1	0.27	-	101,101,101,101	0
54	MG	CA	1939	1/1	0.06	-	144,144,144,144	0
54	MG	BA	3410	1/1	0.53	-	112,112,112,112	0
54	MG	DA	3280	1/1	0.15	-	85,85,85,85	0
54	MG	DB	213	1/1	0.19	-	113,113,113,113	0
54	MG	DA	3834	1/1	0.18	-	60,60,60,60	0
54	MG	DA	3692	1/1	0.92	-	86,86,86,86	0
54	MG	CA	1678	1/1	0.37	-	81,81,81,81	0
54	MG	CA	1738	1/1	0.14	-	93,93,93,93	0
54	MG	BA	3637	1/1	0.20	-	105,105,105,105	0
54	MG	CA	1905	1/1	0.23	-	130,130,130,130	0
54	MG	CA	1885	1/1	0.38	-	75,75,75,75	0
54	MG	AA	1679	1/1	0.38	-	78,78,78,78	0
54	MG	AA	1786	1/1	0.57	-	119,119,119,119	0
54	MG	CA	1781	1/1	0.33	-	76,76,76,76	0
54	MG	AA	1619	1/1	0.27	-	57,57,57,57	0
54	MG	CA	1665	1/1	1.09	-	71,71,71,71	0
54	MG	DA	3277	1/1	0.27	-	59,59,59,59	0
54	MG	DA	3557	1/1	0.09	-	128,128,128,128	0
54	MG	DA	3532	1/1	0.32	-	106,106,106,106	0
54	MG	DA	2997	1/1	0.29	-	46,46,46,46	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
54	MG	DA	3762	1/1	0.82	-	103,103,103,103	0
54	MG	BA	2966	1/1	0.16	-	38,38,38,38	0
54	MG	CA	1648	1/1	0.45	-	61,61,61,61	0
54	MG	DA	3504	1/1	0.54	-	97,97,97,97	0
54	MG	DA	3600	1/1	0.07	-	86,86,86,86	0
54	MG	CA	1805	1/1	0.12	-	94,94,94,94	0
54	MG	DA	3805	1/1	0.10	-	70,70,70,70	0
54	MG	DA	2982	1/1	0.26	-	39,39,39,39	0
54	MG	CA	1608	1/1	0.37	-	121,121,121,121	0
54	MG	DA	3486	1/1	0.55	-	124,124,124,124	0
54	MG	BA	3385	1/1	0.19	-	125,125,125,125	0
54	MG	DA	3778	1/1	0.32	-	80,80,80,80	0
54	MG	BA	3103	1/1	0.93	-	74,74,74,74	0
54	MG	DA	2932	1/1	0.28	-	24,24,24,24	0
54	MG	BA	3117	1/1	0.52	-	91,91,91,91	0
54	MG	DA	3515	1/1	0.66	-	73,73,73,73	0
54	MG	CA	1656	1/1	0.07	-	78,78,78,78	0
54	MG	AA	1840	1/1	0.05	-	91,91,91,91	0
54	MG	DA	3311	1/1	0.51	-	95,95,95,95	0
54	MG	D2	103	1/1	0.51	-	56,56,56,56	0
54	MG	DA	3351	1/1	0.42	-	89,89,89,89	0
54	MG	DA	3011	1/1	0.14	-	36,36,36,36	0
54	MG	BA	3203	1/1	0.11	-	67,67,67,67	0
54	MG	DA	3341	1/1	0.24	-	75,75,75,75	0
54	MG	DA	3543	1/1	0.23	-	87,87,87,87	0
54	MG	BA	3084	1/1	0.48	-	82,82,82,82	0
54	MG	DA	3588	1/1	0.47	-	96,96,96,96	0
54	MG	CA	1833	1/1	0.25	-	79,79,79,79	0
54	MG	AA	1802	1/1	0.11	-	62,62,62,62	0
54	MG	AA	1658	1/1	0.25	-	84,84,84,84	0
54	MG	DA	3238	1/1	0.22	-	56,56,56,56	0
54	MG	DA	3454	1/1	0.39	-	81,81,81,81	0
54	MG	BA	3612	1/1	0.32	-	85,85,85,85	0
54	MG	BA	3647	1/1	0.63	-	149,149,149,149	0
54	MG	DA	3725	1/1	0.65	-	65,65,65,65	0
54	MG	CA	1726	1/1	0.31	-	49,49,49,49	0
54	MG	BA	2934	1/1	0.53	-	33,33,33,33	0
54	MG	BA	3253	1/1	0.23	-	88,88,88,88	0
54	MG	DY	101	1/1	0.29	-	12,12,12,12	0
54	MG	DB	209	1/1	0.35	-	103,103,103,103	0
54	MG	BA	3266	1/1	0.10	-	104,104,104,104	0
54	MG	BA	3615	1/1	0.25	-	93,93,93,93	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
54	MG	DA	3811	1/1	0.20	-	60,60,60,60	0
54	MG	BA	3484	1/1	0.24	-	56,56,56,56	0
54	MG	DX	102	1/1	0.11	-	91,91,91,91	0
54	MG	DA	3067	1/1	0.74	-	91,91,91,91	0
54	MG	BA	3368	1/1	0.07	-	58,58,58,58	0
54	MG	BA	3622	1/1	0.31	-	90,90,90,90	0
54	MG	CA	1951	1/1	0.22	-	87,87,87,87	0
54	MG	CA	1666	1/1	0.41	-	104,104,104,104	0
54	MG	BA	3387	1/1	0.13	-	84,84,84,84	0
54	MG	DA	3552	1/1	0.24	-	68,68,68,68	0
54	MG	AA	1752	1/1	0.24	-	94,94,94,94	0
54	MG	BA	3328	1/1	0.23	-	80,80,80,80	0
54	MG	DA	3354	1/1	0.64	-	79,79,79,79	0
54	MG	DA	3477	1/1	0.24	-	78,78,78,78	0
54	MG	DA	2986	1/1	0.62	-	41,41,41,41	0
54	MG	BA	3278	1/1	0.29	-	88,88,88,88	0
54	MG	DA	3356	1/1	0.17	-	70,70,70,70	0
54	MG	CA	1747	1/1	0.18	-	69,69,69,69	0
54	MG	BA	3249	1/1	0.26	-	36,36,36,36	0
54	MG	DA	3572	1/1	0.11	-	93,93,93,93	0
54	MG	DA	3131	1/1	0.09	-	63,63,63,63	0
54	MG	CA	1888	1/1	0.11	-	109,109,109,109	0
54	MG	DA	3317	1/1	0.29	-	96,96,96,96	0
54	MG	CA	1804	1/1	1.59	-	100,100,100,100	0
54	MG	BA	3632	1/1	0.49	-	61,61,61,61	0
54	MG	AA	1626	1/1	0.25	-	88,88,88,88	0
54	MG	BB	204	1/1	0.35	-	102,102,102,102	0
54	MG	CA	1963	1/1	0.17	-	99,99,99,99	0
54	MG	BA	3089	1/1	0.56	-	69,69,69,69	0
54	MG	DA	3462	1/1	0.42	-	83,83,83,83	0
54	MG	CA	1649	1/1	0.94	-	96,96,96,96	0
54	MG	AA	1727	1/1	0.38	-	104,104,104,104	0
54	MG	BA	3170	1/1	0.34	-	87,87,87,87	0
54	MG	BA	2902	1/1	0.51	-	12,12,12,12	0
54	MG	BA	3043	1/1	0.30	-	50,50,50,50	0
54	MG	CA	1691	1/1	0.06	-	92,92,92,92	0
54	MG	AA	1615	1/1	0.36	-	67,67,67,67	0
54	MG	DA	3679	1/1	0.24	-	50,50,50,50	0
54	MG	AA	1860	1/1	0.62	-	138,138,138,138	0
54	MG	DA	3190	1/1	0.40	-	69,69,69,69	0
54	MG	CA	1716	1/1	0.23	-	89,89,89,89	0
54	MG	BA	3336	1/1	0.58	-	87,87,87,87	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
54	MG	DA	3378	1/1	0.24	-	68,68,68,68	0
54	MG	DA	3674	1/1	0.54	-	47,47,47,47	0
54	MG	DA	3135	1/1	0.17	-	114,114,114,114	0
54	MG	DJ	203	1/1	0.78	-	84,84,84,84	0
54	MG	DA	3548	1/1	0.84	-	110,110,110,110	0
54	MG	DA	3837	1/1	0.36	-	95,95,95,95	0
54	MG	DA	3847	1/1	0.28	-	91,91,91,91	0
54	MG	DA	2975	1/1	0.24	-	50,50,50,50	0
54	MG	DA	3843	1/1	0.58	-	55,55,55,55	0
54	MG	BA	3153	1/1	0.25	-	79,79,79,79	0
54	MG	DA	3720	1/1	0.59	-	79,79,79,79	0
54	MG	AA	1717	1/1	1.55	-	103,103,103,103	0
54	MG	DA	3594	1/1	0.18	-	58,58,58,58	0
54	MG	BS	201	1/1	0.17	-	52,52,52,52	0
54	MG	DA	3164	1/1	0.22	-	83,83,83,83	0
54	MG	BA	3494	1/1	0.24	-	66,66,66,66	0
54	MG	BA	3466	1/1	0.62	-	61,61,61,61	0
54	MG	DE	301	1/1	0.24	-	32,32,32,32	0
54	MG	BA	3524	1/1	0.16	-	107,107,107,107	0
54	MG	BA	3194	1/1	0.62	-	64,64,64,64	0
54	MG	DA	3559	1/1	1.48	-	92,92,92,92	0
54	MG	BA	3054	1/1	0.17	-	65,65,65,65	0
54	MG	CA	1725	1/1	0.08	-	82,82,82,82	0
54	MG	DE	303	1/1	0.23	-	81,81,81,81	0
54	MG	DA	3281	1/1	0.23	-	62,62,62,62	0
54	MG	DA	3198	1/1	0.21	-	65,65,65,65	0
54	MG	BA	3415	1/1	0.45	-	128,128,128,128	0
54	MG	CA	1756	1/1	0.33	-	84,84,84,84	0
54	MG	AA	1784	1/1	0.38	-	89,89,89,89	0
54	MG	BA	3640	1/1	0.30	-	97,97,97,97	0
54	MG	DA	3563	1/1	0.79	-	95,95,95,95	0
54	MG	BA	3162	1/1	0.08	-	86,86,86,86	0
54	MG	AA	1804	1/1	1.51	-	80,80,80,80	0
54	MG	AA	1824	1/1	0.28	-	81,81,81,81	0
54	MG	BA	3442	1/1	0.50	-	26,26,26,26	0
54	MG	BA	3510	1/1	0.41	-	86,86,86,86	0
54	MG	BA	3352	1/1	0.31	-	80,80,80,80	0
54	MG	BA	3342	1/1	0.44	-	62,62,62,62	0
54	MG	DA	3862	1/1	0.80	-	119,119,119,119	0
54	MG	AA	1693	1/1	0.45	-	83,83,83,83	0
54	MG	DA	3581	1/1	0.12	-	68,68,68,68	0
54	MG	DA	3006	1/1	0.31	-	60,60,60,60	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
54	MG	DA	3498	1/1	0.48	-	51,51,51,51	0
54	MG	CA	1858	1/1	1.01	-	107,107,107,107	0
54	MG	BA	3264	1/1	0.13	-	87,87,87,87	0
54	MG	AA	1873	1/1	0.27	-	105,105,105,105	0
54	MG	DU	201	1/1	0.10	-	84,84,84,84	0
54	MG	DA	3181	1/1	0.17	-	96,96,96,96	0
54	MG	AA	1604	1/1	0.50	-	62,62,62,62	0
54	MG	BA	2935	1/1	0.38	-	26,26,26,26	0
54	MG	D5	102	1/1	0.28	-	59,59,59,59	0
54	MG	DA	3666	1/1	0.42	-	81,81,81,81	0
54	MG	BA	3095	1/1	0.61	-	96,96,96,96	0
54	MG	BA	3186	1/1	0.18	-	85,85,85,85	0
54	MG	BA	3244	1/1	0.23	-	79,79,79,79	0
54	MG	BA	3549	1/1	1.60	-	87,87,87,87	0
54	MG	DA	3568	1/1	0.10	-	78,78,78,78	0
54	MG	DA	3706	1/1	0.22	-	75,75,75,75	0
54	MG	BA	2909	1/1	0.50	-	16,16,16,16	0
54	MG	BA	3258	1/1	0.25	-	78,78,78,78	0
54	MG	CA	1854	1/1	0.19	-	111,111,111,111	0
54	MG	DA	3838	1/1	0.41	-	117,117,117,117	0
54	MG	CA	1840	1/1	0.31	-	76,76,76,76	0
54	MG	DA	3331	1/1	0.12	-	90,90,90,90	0
54	MG	DA	3573	1/1	0.46	-	85,85,85,85	0
54	MG	AQ	203	1/1	0.12	-	101,101,101,101	0
54	MG	AE	205	1/1	0.47	-	106,106,106,106	0
54	MG	CA	1623	1/1	0.38	-	93,93,93,93	0
54	MG	DA	3825	1/1	0.28	-	103,103,103,103	0
54	MG	BA	3071	1/1	0.13	-	71,71,71,71	0
54	MG	DA	3531	1/1	0.44	-	93,93,93,93	0
54	MG	DA	3175	1/1	0.10	-	102,102,102,102	0
54	MG	CA	1728	1/1	0.17	-	120,120,120,120	0
54	MG	DA	3228	1/1	0.38	-	54,54,54,54	0
54	MG	BB	217	1/1	0.34	-	72,72,72,72	0
54	MG	BA	3025	1/1	0.49	-	76,76,76,76	0
54	MG	DA	3466	1/1	0.06	-	117,117,117,117	0
54	MG	DA	3828	1/1	0.35	-	85,85,85,85	0
54	MG	DB	201	1/1	0.28	-	44,44,44,44	0
54	MG	BA	3110	1/1	0.38	-	72,72,72,72	0
54	MG	BA	3483	1/1	0.41	-	71,71,71,71	0
54	MG	DA	3755	1/1	0.33	-	89,89,89,89	0
54	MG	DA	3204	1/1	0.38	-	53,53,53,53	0
54	MG	AA	1755	1/1	0.16	-	98,98,98,98	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
54	MG	CA	1873	1/1	0.45	-	58,58,58,58	0
54	MG	AA	1695	1/1	0.13	-	96,96,96,96	0
54	MG	BB	212	1/1	0.23	-	107,107,107,107	0
54	MG	DA	3807	1/1	0.41	-	61,61,61,61	0
54	MG	DA	3602	1/1	0.27	-	91,91,91,91	0
54	MG	AA	1718	1/1	0.22	-	63,63,63,63	0
54	MG	CA	1944	1/1	0.32	-	66,66,66,66	0
54	MG	DA	2942	1/1	0.91	-	54,54,54,54	0
54	MG	CA	1969	1/1	0.54	-	124,124,124,124	0
54	MG	CM	202	1/1	0.60	-	164,164,164,164	0
54	MG	AA	1809	1/1	0.76	-	94,94,94,94	0
54	MG	BA	3008	1/1	0.40	-	70,70,70,70	0
54	MG	BA	3608	1/1	0.31	-	101,101,101,101	0
54	MG	BA	2918	1/1	0.55	-	43,43,43,43	0
54	MG	DA	3189	1/1	0.21	-	73,73,73,73	0
54	MG	DA	3010	1/1	0.23	-	72,72,72,72	0
54	MG	BA	3480	1/1	1.07	-	79,79,79,79	0
54	MG	DA	3564	1/1	0.15	-	77,77,77,77	0
54	MG	DA	3476	1/1	0.55	-	87,87,87,87	0
54	MG	DA	2908	1/1	0.48	-	20,20,20,20	0
54	MG	AA	1730	1/1	0.39	-	107,107,107,107	0
54	MG	CA	1731	1/1	0.13	-	76,76,76,76	0
54	MG	BA	3002	1/1	1.41	-	96,96,96,96	0
54	MG	DA	3151	1/1	0.32	-	76,76,76,76	0
54	MG	BA	2991	1/1	0.26	-	42,42,42,42	0
54	MG	BA	3429	1/1	0.36	-	79,79,79,79	0
54	MG	BA	3000	1/1	0.41	-	49,49,49,49	0
54	MG	BA	2971	1/1	0.25	-	76,76,76,76	0
54	MG	DA	3812	1/1	0.17	-	87,87,87,87	0
54	MG	BA	3551	1/1	0.28	-	95,95,95,95	0
54	MG	DA	2955	1/1	0.62	-	45,45,45,45	0
54	MG	DA	3767	1/1	0.34	-	73,73,73,73	0
54	MG	DA	3339	1/1	0.21	-	81,81,81,81	0
54	MG	DC	301	1/1	0.71	-	67,67,67,67	0
54	MG	DA	3660	1/1	0.38	-	65,65,65,65	0
54	MG	CA	1903	1/1	0.27	-	84,84,84,84	0
54	MG	DA	3861	1/1	0.24	-	90,90,90,90	0
54	MG	DA	3628	1/1	0.26	-	56,56,56,56	0
54	MG	BA	3512	1/1	0.28	-	77,77,77,77	0
54	MG	BA	3530	1/1	0.20	-	65,65,65,65	0
54	MG	DA	3355	1/1	0.47	-	76,76,76,76	0
54	MG	AA	1834	1/1	1.40	-	77,77,77,77	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
54	MG	BA	2932	1/1	0.82	-	44,44,44,44	0
54	MG	BA	3333	1/1	0.67	-	54,54,54,54	0
54	MG	BA	3165	1/1	0.16	-	73,73,73,73	0
54	MG	BA	3542	1/1	0.16	-	102,102,102,102	0
54	MG	AA	1634	1/1	0.19	-	48,48,48,48	0
54	MG	DA	3752	1/1	0.29	-	74,74,74,74	0
54	MG	DA	2962	1/1	0.21	-	37,37,37,37	0
54	MG	CA	1619	1/1	0.52	-	62,62,62,62	0
54	MG	BA	3373	1/1	0.27	-	61,61,61,61	0
54	MG	BA	3173	1/1	0.54	-	87,87,87,87	0
54	MG	AA	1826	1/1	0.41	-	75,75,75,75	0
54	MG	DA	3663	1/1	0.51	-	75,75,75,75	0
54	MG	DA	3724	1/1	0.26	-	109,109,109,109	0
54	MG	DA	3848	1/1	0.99	-	105,105,105,105	0
54	MG	DA	3337	1/1	0.35	-	88,88,88,88	0
54	MG	DA	3375	1/1	0.31	-	63,63,63,63	0
54	MG	BA	3486	1/1	0.24	-	60,60,60,60	0
54	MG	DA	3276	1/1	0.54	-	86,86,86,86	0
54	MG	DA	3027	1/1	0.30	-	53,53,53,53	0
54	MG	CA	1787	1/1	0.80	-	37,37,37,37	0
54	MG	BA	3060	1/1	1.15	-	110,110,110,110	0
54	MG	DA	3194	1/1	0.47	-	74,74,74,74	0
54	MG	DA	3271	1/1	0.41	-	99,99,99,99	0
54	MG	BA	3639	1/1	0.19	-	88,88,88,88	0
54	MG	AA	1869	1/1	0.15	-	74,74,74,74	0
54	MG	BA	3507	1/1	0.34	-	68,68,68,68	0
54	MG	CA	1746	1/1	0.24	-	141,141,141,141	0
54	MG	BA	3544	1/1	0.34	-	81,81,81,81	0
54	MG	BA	3024	1/1	0.46	-	52,52,52,52	0
54	MG	DA	3719	1/1	0.30	-	84,84,84,84	0
54	MG	BP	201	1/1	0.23	-	122,122,122,122	0
54	MG	DA	3246	1/1	0.14	-	57,57,57,57	0
54	MG	DA	3104	1/1	0.20	-	49,49,49,49	0
54	MG	DA	3023	1/1	0.13	-	23,23,23,23	0
54	MG	DA	3750	1/1	0.44	-	87,87,87,87	0
54	MG	DA	2996	1/1	0.49	-	32,32,32,32	0
54	MG	DA	3835	1/1	0.38	-	111,111,111,111	0
54	MG	CA	1739	1/1	0.13	-	102,102,102,102	0
54	MG	CC	308	1/1	0.25	-	110,110,110,110	0
54	MG	DA	3412	1/1	0.21	-	86,86,86,86	0
54	MG	AA	1618	1/1	0.57	-	71,71,71,71	0
54	MG	BA	3267	1/1	0.67	-	65,65,65,65	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
54	MG	CG	202	1/1	0.84	-	131,131,131,131	0
54	MG	DA	3657	1/1	0.75	-	57,57,57,57	0
54	MG	DA	3334	1/1	0.23	-	53,53,53,53	0
54	MG	AA	1795	1/1	0.30	-	111,111,111,111	0
54	MG	DA	3635	1/1	0.21	-	73,73,73,73	0
54	MG	CA	1637	1/1	0.12	-	98,98,98,98	0
54	MG	BA	3374	1/1	0.34	-	108,108,108,108	0
54	MG	BX	102	1/1	0.33	-	103,103,103,103	0
54	MG	DA	3695	1/1	0.37	-	76,76,76,76	0
54	MG	DA	2934	1/1	0.41	-	13,13,13,13	0
54	MG	BA	3376	1/1	0.36	-	123,123,123,123	0
54	MG	DA	3002	1/1	0.14	-	52,52,52,52	0
54	MG	CA	1922	1/1	0.08	-	127,127,127,127	0
54	MG	DA	3022	1/1	0.27	-	35,35,35,35	0
54	MG	BA	3152	1/1	0.09	-	76,76,76,76	0
54	MG	BA	3358	1/1	0.39	-	81,81,81,81	0
54	MG	AE	204	1/1	0.22	-	74,74,74,74	0
54	MG	BA	3090	1/1	0.52	-	84,84,84,84	0
54	MG	BA	3228	1/1	0.17	-	42,42,42,42	0
54	MG	AA	1764	1/1	0.46	-	99,99,99,99	0
54	MG	DA	3202	1/1	0.21	-	76,76,76,76	0
54	MG	AA	1871	1/1	0.11	-	110,110,110,110	0
54	MG	CE	204	1/1	0.35	-	109,109,109,109	0
54	MG	DD	306	1/1	0.18	-	107,107,107,107	0
54	MG	CA	1896	1/1	0.35	-	70,70,70,70	0
54	MG	BA	3562	1/1	0.24	-	40,40,40,40	0
54	MG	DA	3417	1/1	0.67	-	72,72,72,72	0
54	MG	DA	3344	1/1	0.15	-	75,75,75,75	0
54	MG	CA	1919	1/1	0.31	-	145,145,145,145	0
54	MG	DA	3363	1/1	0.18	-	74,74,74,74	0
54	MG	AA	1847	1/1	0.40	-	90,90,90,90	0
54	MG	AA	1713	1/1	0.47	-	98,98,98,98	0
54	MG	CV	6205	1/1	0.10	-	159,159,159,159	0
54	MG	CA	1754	1/1	0.89	-	121,121,121,121	0
54	MG	BA	3476	1/1	0.33	-	53,53,53,53	0
54	MG	CA	1660	1/1	0.13	-	158,158,158,158	0
54	MG	AA	1798	1/1	0.46	-	46,46,46,46	0
54	MG	DA	3107	1/1	0.13	-	50,50,50,50	0
54	MG	AO	102	1/1	0.39	-	114,114,114,114	0
54	MG	AA	1774	1/1	0.08	-	70,70,70,70	0
54	MG	DA	3624	1/1	0.36	-	92,92,92,92	0
54	MG	CA	1948	1/1	0.09	-	99,99,99,99	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
54	MG	AA	1837	1/1	0.43	-	115,115,115,115	0
54	MG	DA	3501	1/1	0.31	-	96,96,96,96	0
54	MG	CA	1629	1/1	0.36	-	93,93,93,93	0
54	MG	AA	1657	1/1	0.55	-	79,79,79,79	0
54	MG	DA	3359	1/1	0.29	-	96,96,96,96	0
54	MG	AA	1836	1/1	0.09	-	91,91,91,91	0
54	MG	AA	1736	1/1	0.20	-	112,112,112,112	0
54	MG	CA	1933	1/1	0.22	-	137,137,137,137	0
54	MG	CA	1640	1/1	1.16	-	133,133,133,133	0
54	MG	BA	3673	1/1	0.31	-	92,92,92,92	0
54	MG	DA	3435	1/1	0.25	-	97,97,97,97	0
55	ZN	AN	101	1/1	0.10	-	144,144,144,144	0
54	MG	DA	2902	1/1	0.54	-	17,17,17,17	0
54	MG	BA	3116	1/1	0.19	-	70,70,70,70	0
54	MG	BA	3118	1/1	0.16	-	95,95,95,95	0
54	MG	DA	3522	1/1	0.63	-	147,147,147,147	0
54	MG	CG	201	1/1	0.51	-	104,104,104,104	0
54	MG	DA	3182	1/1	0.29	-	63,63,63,63	0
54	MG	CA	1806	1/1	0.20	-	110,110,110,110	0
54	MG	BA	3049	1/1	0.57	-	58,58,58,58	0
54	MG	CA	1884	1/1	0.20	-	99,99,99,99	0
54	MG	CA	1705	1/1	0.50	-	122,122,122,122	0
54	MG	DA	2935	1/1	0.52	-	23,23,23,23	0
54	MG	BA	2961	1/1	0.57	-	51,51,51,51	0
54	MG	BA	3508	1/1	0.17	-	90,90,90,90	0
54	MG	DB	236	1/1	0.18	-	84,84,84,84	0
54	MG	DA	2925	1/1	0.42	-	34,34,34,34	0
54	MG	BA	3334	1/1	0.30	-	60,60,60,60	0
54	MG	AA	1660	1/1	0.30	-	122,122,122,122	0
54	MG	DA	3497	1/1	0.70	-	62,62,62,62	0
54	MG	BA	3405	1/1	0.19	-	68,68,68,68	0
54	MG	DA	3765	1/1	0.22	-	64,64,64,64	0
54	MG	DA	3775	1/1	0.15	-	98,98,98,98	0
54	MG	D5	101	1/1	0.20	-	46,46,46,46	0
54	MG	DA	3064	1/1	0.27	-	127,127,127,127	0
54	MG	BA	3124	1/1	0.11	-	87,87,87,87	0
54	MG	BA	3579	1/1	0.64	-	107,107,107,107	0
54	MG	AA	1849	1/1	0.22	-	79,79,79,79	0
54	MG	DA	3070	1/1	0.06	-	85,85,85,85	0
54	MG	BA	3353	1/1	0.44	-	85,85,85,85	0
54	MG	AA	1815	1/1	1.64	-	78,78,78,78	0
54	MG	DA	3715	1/1	0.30	-	57,57,57,57	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
54	MG	DA	3288	1/1	0.21	-	104,104,104,104	0
54	MG	DA	3139	1/1	0.15	-	40,40,40,40	0
54	MG	CA	1675	1/1	0.24	-	74,74,74,74	0
54	MG	BA	3477	1/1	0.14	-	50,50,50,50	0
54	MG	CA	1801	1/1	0.25	-	82,82,82,82	0
54	MG	BA	2923	1/1	0.50	-	13,13,13,13	0
54	MG	BB	207	1/1	0.26	-	111,111,111,111	0
54	MG	DA	3735	1/1	0.16	-	97,97,97,97	0
54	MG	BA	3037	1/1	0.25	-	62,62,62,62	0
54	MG	AB	303	1/1	0.28	-	108,108,108,108	0
54	MG	DB	228	1/1	0.29	-	88,88,88,88	0
54	MG	DB	206	1/1	0.29	-	63,63,63,63	0
54	MG	BA	3225	1/1	0.33	-	54,54,54,54	0
54	MG	DA	3782	1/1	0.56	-	67,67,67,67	0
54	MG	DA	3623	1/1	0.78	-	104,104,104,104	0
54	MG	B4	101	1/1	0.26	-	91,91,91,91	0
54	MG	DA	3721	1/1	0.72	-	88,88,88,88	0
54	MG	AC	302	1/1	0.36	-	71,71,71,71	0
54	MG	DA	3503	1/1	0.30	-	91,91,91,91	0
54	MG	DA	3160	1/1	0.45	-	53,53,53,53	0
54	MG	AA	1868	1/1	0.23	-	101,101,101,101	0
54	MG	DA	3580	1/1	0.23	-	162,162,162,162	0
54	MG	BA	3652	1/1	0.48	-	109,109,109,109	0
54	MG	CC	305	1/1	0.08	-	93,93,93,93	0
54	MG	BJ	201	1/1	0.13	-	75,75,75,75	0
54	MG	BH	201	1/1	0.23	-	107,107,107,107	0
54	MG	AA	1637	1/1	0.16	-	62,62,62,62	0
54	MG	DA	3004	1/1	0.25	-	38,38,38,38	0
54	MG	BA	3268	1/1	0.70	-	84,84,84,84	0
54	MG	DA	3631	1/1	0.07	-	73,73,73,73	0
54	MG	DA	3057	1/1	0.42	-	79,79,79,79	0
54	MG	CA	1635	1/1	0.54	-	99,99,99,99	0
54	MG	CA	1908	1/1	0.43	-	104,104,104,104	0
54	MG	BA	3597	1/1	0.27	-	56,56,56,56	0
54	MG	DA	3668	1/1	0.61	-	133,133,133,133	0
54	MG	AA	1793	1/1	0.27	-	68,68,68,68	0
54	MG	DA	3116	1/1	0.58	-	52,52,52,52	0
54	MG	BA	3161	1/1	0.31	-	64,64,64,64	0
54	MG	CA	1622	1/1	0.77	-	77,77,77,77	0
54	MG	DA	3815	1/1	0.46	-	74,74,74,74	0
54	MG	DA	3741	1/1	0.20	-	84,84,84,84	0
54	MG	BA	2930	1/1	0.43	-	47,47,47,47	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
54	MG	DB	216	1/1	0.33	-	101,101,101,101	0
54	MG	DA	3043	1/1	0.14	-	59,59,59,59	0
54	MG	DA	3570	1/1	0.45	-	90,90,90,90	0
54	MG	DA	3225	1/1	0.12	-	139,139,139,139	0
54	MG	BA	3674	1/1	0.31	-	55,55,55,55	0
54	MG	BA	3664	1/1	0.15	-	69,69,69,69	0
54	MG	BA	2955	1/1	0.35	-	63,63,63,63	0
54	MG	AV	6206	1/1	0.13	-	87,87,87,87	0
54	MG	CA	1853	1/1	0.13	-	113,113,113,113	0
54	MG	DA	2938	1/1	0.34	-	7,7,7,7	0
54	MG	BA	3396	1/1	0.20	-	108,108,108,108	0
54	MG	DA	3171	1/1	0.14	-	93,93,93,93	0
54	MG	BA	3066	1/1	1.10	-	91,91,91,91	0
54	MG	DB	242	1/1	0.09	-	113,113,113,113	0
54	MG	AQ	202	1/1	0.07	-	85,85,85,85	0
54	MG	BA	3051	1/1	0.40	-	62,62,62,62	0
54	MG	DA	3797	1/1	0.29	-	101,101,101,101	0
54	MG	DA	3733	1/1	0.46	-	84,84,84,84	0
54	MG	BA	3676	1/1	0.12	-	112,112,112,112	0
54	MG	DA	3864	1/1	0.19	-	53,53,53,53	0
54	MG	BA	3269	1/1	0.57	-	104,104,104,104	0
54	MG	DA	3168	1/1	0.75	-	67,67,67,67	0
54	MG	AA	1743	1/1	0.70	-	140,140,140,140	0
54	MG	AA	1659	1/1	0.60	-	74,74,74,74	0
54	MG	CA	1723	1/1	0.82	-	85,85,85,85	0
54	MG	AA	1630	1/1	0.36	-	81,81,81,81	0
54	MG	CA	1766	1/1	0.14	-	77,77,77,77	0
54	MG	BA	3431	1/1	0.34	-	26,26,26,26	0
54	MG	BA	3235	1/1	0.29	-	54,54,54,54	0
54	MG	DA	3294	1/1	0.20	-	36,36,36,36	0
54	MG	DA	3658	1/1	0.38	-	23,23,23,23	0
54	MG	BA	3482	1/1	0.22	-	40,40,40,40	0
54	MG	BA	3525	1/1	0.57	-	67,67,67,67	0
54	MG	DA	3830	1/1	0.32	-	125,125,125,125	0
54	MG	BA	3215	1/1	0.60	-	64,64,64,64	0
54	MG	DB	234	1/1	0.15	-	105,105,105,105	0
54	MG	BA	3261	1/1	1.64	-	92,92,92,92	0
54	MG	CA	1902	1/1	0.13	-	77,77,77,77	0
54	MG	BA	3139	1/1	0.46	-	100,100,100,100	0
54	MG	DA	3673	1/1	0.24	-	85,85,85,85	0
54	MG	DA	3534	1/1	0.33	-	83,83,83,83	0
54	MG	BA	3189	1/1	0.22	-	76,76,76,76	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
54	MG	AA	1685	1/1	0.43	-	64,64,64,64	0
54	MG	BA	3427	1/1	0.10	-	74,74,74,74	0
54	MG	CA	1931	1/1	0.10	-	99,99,99,99	0
54	MG	DA	2990	1/1	0.24	-	20,20,20,20	0
54	MG	DA	2978	1/1	0.25	-	23,23,23,23	0
54	MG	DA	3747	1/1	0.26	-	78,78,78,78	0
54	MG	DA	3615	1/1	0.31	-	99,99,99,99	0
54	MG	DA	3605	1/1	0.41	-	103,103,103,103	0
54	MG	BA	3393	1/1	0.34	-	136,136,136,136	0
54	MG	CO	103	1/1	1.08	-	203,203,203,203	0
54	MG	CA	1848	1/1	0.38	-	96,96,96,96	0
54	MG	BA	3252	1/1	0.26	-	60,60,60,60	0
54	MG	DA	3691	1/1	0.71	-	96,96,96,96	0
54	MG	BA	2922	1/1	0.51	-	38,38,38,38	0
54	MG	CA	1880	1/1	1.23	-	83,83,83,83	0
54	MG	DA	3009	1/1	0.28	-	54,54,54,54	0
54	MG	BA	3083	1/1	0.10	-	70,70,70,70	0
54	MG	CA	1970	1/1	0.08	-	98,98,98,98	0
54	MG	CC	302	1/1	0.20	-	79,79,79,79	0
54	MG	CA	1662	1/1	0.20	-	84,84,84,84	0
54	MG	DM	1400	1/1	0.65	-	106,106,106,106	0
54	MG	CA	1909	1/1	0.24	-	135,135,135,135	0
54	MG	BA	2957	1/1	0.93	-	75,75,75,75	0
54	MG	BA	3290	1/1	0.37	-	79,79,79,79	0
54	MG	DC	302	1/1	0.23	-	164,164,164,164	0
54	MG	CA	1694	1/1	0.12	-	79,79,79,79	0
54	MG	DA	3249	1/1	0.21	-	111,111,111,111	0
54	MG	BA	3490	1/1	0.10	-	67,67,67,67	0
54	MG	AA	1709	1/1	0.62	-	87,87,87,87	0
54	MG	DA	3130	1/1	0.09	-	68,68,68,68	0
54	MG	CA	1612	1/1	0.36	-	76,76,76,76	0
54	MG	DA	3019	1/1	0.31	-	48,48,48,48	0
54	MG	BB	209	1/1	0.18	-	61,61,61,61	0
54	MG	DA	3506	1/1	0.43	-	101,101,101,101	0
54	MG	CA	1667	1/1	0.26	-	77,77,77,77	0
54	MG	DA	3232	1/1	0.13	-	67,67,67,67	0
54	MG	CA	1713	1/1	0.10	-	92,92,92,92	0
54	MG	DA	3737	1/1	0.45	-	136,136,136,136	0
54	MG	D4	101	1/1	0.23	-	55,55,55,55	0
54	MG	DB	233	1/1	0.35	-	67,67,67,67	0
54	MG	AA	1740	1/1	0.12	-	76,76,76,76	0
54	MG	CA	1780	1/1	0.17	-	93,93,93,93	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
54	MG	DA	3319	1/1	0.30	-	38,38,38,38	0
54	MG	AA	1636	1/1	0.13	-	96,96,96,96	0
54	MG	BA	3076	1/1	0.51	-	68,68,68,68	0
54	MG	B3	101	1/1	0.12	-	96,96,96,96	0
54	MG	BA	3439	1/1	0.40	-	17,17,17,17	0
54	MG	BA	3419	1/1	0.29	-	67,67,67,67	0
54	MG	AA	1788	1/1	0.12	-	148,148,148,148	0
54	MG	BA	3070	1/1	0.50	-	85,85,85,85	0
54	MG	BA	3667	1/1	0.15	-	85,85,85,85	0
54	MG	BA	3097	1/1	0.36	-	57,57,57,57	0
54	MG	DA	3792	1/1	0.34	-	40,40,40,40	0
54	MG	CA	1714	1/1	0.32	-	123,123,123,123	0
54	MG	BA	3307	1/1	0.18	-	63,63,63,63	0
54	MG	DA	3470	1/1	0.23	-	127,127,127,127	0
54	MG	BA	3067	1/1	0.59	-	103,103,103,103	0
54	MG	CL	203	1/1	0.28	-	123,123,123,123	0
54	MG	BA	2913	1/1	0.59	-	27,27,27,27	0
54	MG	BA	2905	1/1	0.61	-	19,19,19,19	0
54	MG	BA	3245	1/1	0.43	-	95,95,95,95	0
54	MG	AA	1711	1/1	0.28	-	58,58,58,58	0
54	MG	BA	2981	1/1	0.31	-	56,56,56,56	0
54	MG	AA	1726	1/1	0.17	-	103,103,103,103	0
54	MG	DA	2957	1/1	0.60	-	40,40,40,40	0
54	MG	DA	3511	1/1	0.33	-	52,52,52,52	0
54	MG	BA	3055	1/1	0.53	-	78,78,78,78	0
54	MG	AA	1790	1/1	0.17	-	109,109,109,109	0
54	MG	AA	1704	1/1	0.18	-	77,77,77,77	0
54	MG	CA	1788	1/1	0.44	-	95,95,95,95	0
54	MG	BA	3222	1/1	0.24	-	86,86,86,86	0
54	MG	AA	1876	1/1	0.11	-	80,80,80,80	0
54	MG	DA	3801	1/1	0.30	-	83,83,83,83	0
54	MG	CA	1692	1/1	1.16	-	115,115,115,115	0
54	MG	DA	3449	1/1	0.21	-	79,79,79,79	0
54	MG	AA	1652	1/1	0.42	-	95,95,95,95	0
54	MG	CA	1765	1/1	0.22	-	95,95,95,95	0
54	MG	CA	1949	1/1	0.13	-	98,98,98,98	0
54	MG	DA	3853	1/1	0.28	-	114,114,114,114	0
54	MG	BA	3291	1/1	0.36	-	102,102,102,102	0
54	MG	BA	2903	1/1	0.86	-	22,22,22,22	0
54	MG	CA	1918	1/1	0.66	-	84,84,84,84	0
54	MG	DA	3176	1/1	0.25	-	50,50,50,50	0
54	MG	DB	215	1/1	0.31	-	103,103,103,103	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
54	MG	CA	1962	1/1	0.17	-	96,96,96,96	0
54	MG	DA	3502	1/1	0.54	-	93,93,93,93	0
54	MG	BA	2950	1/1	0.15	-	68,68,68,68	0
54	MG	AV	6203	1/1	0.18	-	62,62,62,62	0
54	MG	BA	2947	1/1	0.72	-	37,37,37,37	0
54	MG	DA	3856	1/1	0.39	-	86,86,86,86	0
54	MG	AA	1861	1/1	0.24	-	81,81,81,81	0
54	MG	BA	2993	1/1	0.56	-	49,49,49,49	0
54	MG	DA	3742	1/1	0.40	-	47,47,47,47	0
54	MG	BA	3167	1/1	0.72	-	87,87,87,87	0
54	MG	DA	3683	1/1	0.28	-	58,58,58,58	0
54	MG	BA	3606	1/1	0.47	-	118,118,118,118	0
54	MG	DA	3263	1/1	0.18	-	55,55,55,55	0
54	MG	B2	102	1/1	0.66	-	65,65,65,65	0
54	MG	AA	1682	1/1	0.15	-	91,91,91,91	0
54	MG	BA	3616	1/1	0.26	-	89,89,89,89	0
54	MG	DA	3024	1/1	0.36	-	58,58,58,58	0
54	MG	BA	3366	1/1	0.27	-	80,80,80,80	0
54	MG	BA	3270	1/1	0.12	-	93,93,93,93	0
54	MG	BA	3390	1/1	0.08	-	103,103,103,103	0
54	MG	DA	3567	1/1	0.79	-	87,87,87,87	0
54	MG	DA	3327	1/1	0.29	-	79,79,79,79	0
54	MG	BA	3140	1/1	0.34	-	62,62,62,62	0
54	MG	BB	222	1/1	0.23	-	112,112,112,112	0
54	MG	DA	3802	1/1	0.11	-	84,84,84,84	0
54	MG	DA	3286	1/1	0.43	-	76,76,76,76	0
54	MG	BN	202	1/1	0.29	-	78,78,78,78	0
54	MG	CV	6207	1/1	0.13	-	94,94,94,94	0
54	MG	DA	3146	1/1	0.25	-	31,31,31,31	0
54	MG	CA	1955	1/1	0.19	-	98,98,98,98	0
54	MG	BA	3596	1/1	0.20	-	71,71,71,71	0
54	MG	AA	1605	1/1	0.18	-	65,65,65,65	0
54	MG	DA	3817	1/1	0.37	-	76,76,76,76	0
54	MG	BA	2970	1/1	0.43	-	55,55,55,55	0
54	MG	CA	1610	1/1	0.46	-	90,90,90,90	0
54	MG	CE	205	1/1	0.38	-	104,104,104,104	0
54	MG	BA	3230	1/1	0.45	-	111,111,111,111	0
54	MG	DA	3015	1/1	0.29	-	33,33,33,33	0
54	MG	DB	220	1/1	0.32	-	75,75,75,75	0
54	MG	CA	1943	1/1	0.41	-	87,87,87,87	0
54	MG	AA	1773	1/1	0.10	-	97,97,97,97	0
54	MG	AA	1738	1/1	0.39	-	104,104,104,104	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
54	MG	DB	238	1/1	0.17	-	74,74,74,74	0
54	MG	DA	3008	1/1	0.20	-	50,50,50,50	0
54	MG	CA	1769	1/1	0.13	-	67,67,67,67	0
54	MG	DA	3402	1/1	0.24	-	95,95,95,95	0
54	MG	BE	301	1/1	0.18	-	75,75,75,75	0
54	MG	BA	3297	1/1	0.83	-	98,98,98,98	0
54	MG	BA	2976	1/1	0.34	-	65,65,65,65	0
54	MG	DA	3806	1/1	0.15	-	92,92,92,92	0
54	MG	BA	3607	1/1	0.83	-	62,62,62,62	0
54	MG	BA	3558	1/1	0.38	-	91,91,91,91	0
54	MG	AA	1707	1/1	0.79	-	86,86,86,86	0
54	MG	CA	1682	1/1	0.53	-	88,88,88,88	0
54	MG	BA	3441	1/1	0.33	-	35,35,35,35	0
54	MG	AA	1665	1/1	0.31	-	70,70,70,70	0
54	MG	DA	3524	1/1	0.10	-	87,87,87,87	0
54	MG	DA	3480	1/1	0.12	-	76,76,76,76	0
54	MG	DA	3776	1/1	0.22	-	172,172,172,172	0
54	MG	DA	3851	1/1	0.27	-	74,74,74,74	0
54	MG	DA	3059	1/1	0.36	-	39,39,39,39	0
54	MG	DA	3680	1/1	0.20	-	41,41,41,41	0
54	MG	BA	3340	1/1	0.34	-	85,85,85,85	0
54	MG	CA	1890	1/1	0.61	-	78,78,78,78	0
54	MG	DA	3254	1/1	0.74	-	71,71,71,71	0
54	MG	BA	3532	1/1	0.26	-	107,107,107,107	0
54	MG	DB	230	1/1	0.98	-	114,114,114,114	0
54	MG	BA	3380	1/1	0.29	-	55,55,55,55	0
54	MG	BA	3052	1/1	0.93	-	73,73,73,73	0
54	MG	DA	3234	1/1	0.34	-	64,64,64,64	0
54	MG	DB	229	1/1	0.56	-	134,134,134,134	0
54	MG	DA	3858	1/1	0.27	-	58,58,58,58	0
54	MG	AA	1785	1/1	0.98	-	117,117,117,117	0
54	MG	BA	3576	1/1	0.58	-	83,83,83,83	0
54	MG	BA	3513	1/1	0.17	-	74,74,74,74	0
54	MG	BA	3177	1/1	0.11	-	119,119,119,119	0
54	MG	BA	3654	1/1	0.28	-	122,122,122,122	0
54	MG	DA	3606	1/1	0.44	-	68,68,68,68	0
54	MG	BA	3105	1/1	0.20	-	72,72,72,72	0
54	MG	DA	3638	1/1	0.34	-	22,22,22,22	0
54	MG	DA	3193	1/1	0.41	-	86,86,86,86	0
54	MG	BA	3613	1/1	0.24	-	103,103,103,103	0
54	MG	DG	203	1/1	0.19	-	98,98,98,98	0
54	MG	B5	101	1/1	0.61	-	78,78,78,78	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
54	MG	BA	3681	1/1	0.26	-	95,95,95,95	0
54	MG	CL	204	1/1	0.23	-	86,86,86,86	0
54	MG	CA	1850	1/1	0.28	-	129,129,129,129	0
54	MG	CA	1763	1/1	0.10	-	90,90,90,90	0
54	MG	BA	3564	1/1	0.65	-	146,146,146,146	0
54	MG	DA	3860	1/1	0.15	-	78,78,78,78	0
54	MG	CA	1942	1/1	0.23	-	104,104,104,104	0
54	MG	BA	3446	1/1	0.45	-	53,53,53,53	0
54	MG	BA	3329	1/1	0.30	-	113,113,113,113	0
54	MG	BA	3327	1/1	0.76	-	86,86,86,86	0
54	MG	AA	1616	1/1	0.68	-	54,54,54,54	0
54	MG	AA	1694	1/1	0.11	-	71,71,71,71	0
54	MG	CA	1960	1/1	0.14	-	91,91,91,91	0
54	MG	BV	202	1/1	0.10	-	75,75,75,75	0
54	MG	BA	3260	1/1	0.36	-	64,64,64,64	0
54	MG	CA	1877	1/1	0.29	-	126,126,126,126	0
54	MG	AA	1879	1/1	0.26	-	119,119,119,119	0
54	MG	AA	1780	1/1	0.06	-	101,101,101,101	0
54	MG	BA	3180	1/1	0.36	-	88,88,88,88	0
54	MG	BA	2992	1/1	0.14	-	69,69,69,69	0
54	MG	DA	3336	1/1	1.00	-	70,70,70,70	0
54	MG	DA	3173	1/1	0.46	-	73,73,73,73	0
54	MG	CA	1917	1/1	0.28	-	105,105,105,105	0
54	MG	DA	3739	1/1	0.15	-	133,133,133,133	0
54	MG	BA	3592	1/1	0.40	-	79,79,79,79	0
54	MG	CA	1803	1/1	0.64	-	99,99,99,99	0
54	MG	CA	1770	1/1	0.09	-	125,125,125,125	0
54	MG	BA	3553	1/1	0.17	-	72,72,72,72	0
54	MG	BA	3421	1/1	0.32	-	80,80,80,80	0
54	MG	CA	1742	1/1	0.21	-	91,91,91,91	0
54	MG	BA	2979	1/1	0.12	-	86,86,86,86	0
54	MG	CA	1745	1/1	0.19	-	77,77,77,77	0
54	MG	BA	3653	1/1	0.32	-	82,82,82,82	0
54	MG	DA	3092	1/1	0.56	-	56,56,56,56	0
54	MG	DA	3376	1/1	0.26	-	44,44,44,44	0
54	MG	AA	1838	1/1	0.60	-	77,77,77,77	0
54	MG	BA	3294	1/1	0.27	-	89,89,89,89	0
54	MG	BA	3129	1/1	0.31	-	98,98,98,98	0
54	MG	BA	2914	1/1	0.40	-	24,24,24,24	0
54	MG	BA	3363	1/1	0.34	-	113,113,113,113	0
54	MG	DA	3617	1/1	0.29	-	59,59,59,59	0
54	MG	DA	3318	1/1	0.25	-	77,77,77,77	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
54	MG	BA	3147	1/1	0.34	-	123,123,123,123	0
54	MG	BA	3357	1/1	0.63	-	80,80,80,80	0
54	MG	BA	3377	1/1	0.27	-	68,68,68,68	0
54	MG	BA	3339	1/1	0.18	-	103,103,103,103	0
54	MG	DA	3065	1/1	0.46	-	61,61,61,61	0
54	MG	AA	1877	1/1	1.28	-	102,102,102,102	0
54	MG	BA	3246	1/1	0.38	-	164,164,164,164	0
54	MG	BA	3145	1/1	0.54	-	74,74,74,74	0
54	MG	CA	1861	1/1	0.31	-	64,64,64,64	0
54	MG	CA	1842	1/1	0.60	-	103,103,103,103	0
54	MG	DA	3704	1/1	0.91	-	68,68,68,68	0
54	MG	DA	3694	1/1	0.23	-	64,64,64,64	0
54	MG	CA	1783	1/1	0.10	-	139,139,139,139	0
54	MG	DA	2918	1/1	0.55	-	25,25,25,25	0
54	MG	BA	3567	1/1	0.20	-	126,126,126,126	0
54	MG	DA	3105	1/1	0.43	-	87,87,87,87	0
54	MG	DB	235	1/1	0.49	-	91,91,91,91	0
54	MG	DA	2927	1/1	0.24	-	18,18,18,18	0
54	MG	CA	1940	1/1	0.27	-	72,72,72,72	0
54	MG	CA	1927	1/1	0.14	-	88,88,88,88	0
54	MG	DA	3676	1/1	0.26	-	92,92,92,92	0
54	MG	BA	2904	1/1	0.32	-	40,40,40,40	0
54	MG	CA	1965	1/1	0.33	-	78,78,78,78	0
54	MG	BA	3611	1/1	0.47	-	75,75,75,75	0
54	MG	DA	2970	1/1	0.23	-	29,29,29,29	0
54	MG	BA	3433	1/1	0.70	-	21,21,21,21	0
54	MG	BA	3646	1/1	0.35	-	82,82,82,82	0
54	MG	BA	3406	1/1	0.61	-	88,88,88,88	0
54	MG	DA	3209	1/1	1.46	-	94,94,94,94	0
54	MG	DA	3831	1/1	0.35	-	66,66,66,66	0
54	MG	DA	3846	1/1	0.24	-	94,94,94,94	0
54	MG	CA	1811	1/1	0.18	-	181,181,181,181	0
54	MG	BA	3075	1/1	0.11	-	60,60,60,60	0
54	MG	BA	3256	1/1	0.20	-	105,105,105,105	0
54	MG	DA	2941	1/1	0.17	-	21,21,21,21	0
54	MG	DA	3526	1/1	0.22	-	84,84,84,84	0
54	MG	DA	3371	1/1	0.23	-	53,53,53,53	0
54	MG	BA	3485	1/1	0.77	-	72,72,72,72	0
54	MG	DA	3046	1/1	0.35	-	37,37,37,37	0
54	MG	BA	3481	1/1	0.33	-	71,71,71,71	0
54	MG	DA	3026	1/1	0.46	-	83,83,83,83	0
54	MG	BA	3031	1/1	0.59	-	80,80,80,80	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
54	MG	CA	1771	1/1	0.24	-	98,98,98,98	0
54	MG	CA	1798	1/1	0.24	-	111,111,111,111	0
54	MG	BM	202	1/1	0.24	-	85,85,85,85	0
54	MG	AA	1642	1/1	0.64	-	100,100,100,100	0
54	MG	AQ	201	1/1	0.27	-	90,90,90,90	0
54	MG	BA	3504	1/1	0.66	-	94,94,94,94	0
54	MG	AA	1699	1/1	0.30	-	57,57,57,57	0
54	MG	DA	3620	1/1	0.30	-	115,115,115,115	0
54	MG	BA	3047	1/1	0.21	-	72,72,72,72	0
54	MG	DA	2960	1/1	0.35	-	33,33,33,33	0
54	MG	BA	3159	1/1	0.63	-	59,59,59,59	0
54	MG	CA	1668	1/1	0.27	-	86,86,86,86	0
54	MG	DA	3758	1/1	0.43	-	60,60,60,60	0
54	MG	BA	3546	1/1	0.32	-	67,67,67,67	0
54	MG	BA	3014	1/1	0.08	-	45,45,45,45	0
54	MG	CA	1867	1/1	0.58	-	123,123,123,123	0
54	MG	DA	3320	1/1	0.36	-	80,80,80,80	0
54	MG	CA	1696	1/1	0.15	-	75,75,75,75	0
54	MG	CA	1749	1/1	0.10	-	77,77,77,77	0
54	MG	BA	3394	1/1	0.57	-	95,95,95,95	0
54	MG	DA	3251	1/1	0.17	-	77,77,77,77	0
54	MG	DX	103	1/1	0.26	-	60,60,60,60	0
54	MG	BA	2927	1/1	0.26	-	25,25,25,25	0
54	MG	DA	3087	1/1	0.77	-	71,71,71,71	0
54	MG	CA	1760	1/1	0.26	-	66,66,66,66	0
54	MG	AA	1688	1/1	0.46	-	140,140,140,140	0
54	MG	DA	3086	1/1	0.53	-	71,71,71,71	0
54	MG	BA	3414	1/1	1.70	-	137,137,137,137	0
54	MG	DA	3032	1/1	0.76	-	80,80,80,80	0
54	MG	BA	2983	1/1	0.13	-	44,44,44,44	0
54	MG	DA	3585	1/1	0.32	-	154,154,154,154	0
54	MG	BA	3099	1/1	0.17	-	56,56,56,56	0
54	MG	AA	1839	1/1	0.48	-	69,69,69,69	0
54	MG	DA	3667	1/1	0.79	-	59,59,59,59	0
54	MG	BA	3388	1/1	0.54	-	66,66,66,66	0
54	MG	DA	3028	1/1	0.42	-	58,58,58,58	0
54	MG	BA	3649	1/1	0.10	-	67,67,67,67	0
54	MG	BA	3669	1/1	0.16	-	84,84,84,84	0
54	MG	DA	3863	1/1	0.85	-	104,104,104,104	0
54	MG	CA	1773	1/1	0.20	-	97,97,97,97	0
54	MG	CA	1912	1/1	0.21	-	138,138,138,138	0
54	MG	BA	3662	1/1	0.26	-	108,108,108,108	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
54	MG	BA	3518	1/1	0.60	-	81,81,81,81	0
54	MG	BA	3634	1/1	0.22	-	98,98,98,98	0
54	MG	DA	3499	1/1	0.36	-	87,87,87,87	0
54	MG	BA	3011	1/1	0.28	-	51,51,51,51	0
54	MG	CL	205	1/1	0.24	-	97,97,97,97	0
54	MG	CA	1878	1/1	0.39	-	82,82,82,82	0
54	MG	BA	2948	1/1	0.24	-	62,62,62,62	0
54	MG	AB	301	1/1	0.29	-	92,92,92,92	0
54	MG	BA	3144	1/1	0.15	-	148,148,148,148	0
54	MG	AA	1645	1/1	0.07	-	138,138,138,138	0
54	MG	BA	3013	1/1	0.35	-	21,21,21,21	0
54	MG	CA	1700	1/1	0.14	-	129,129,129,129	0
54	MG	DA	3287	1/1	0.08	-	104,104,104,104	0
54	MG	BA	3534	1/1	0.50	-	82,82,82,82	0
54	MG	BB	202	1/1	0.46	-	48,48,48,48	0
54	MG	AA	1856	1/1	0.46	-	58,58,58,58	0
54	MG	BA	3371	1/1	0.29	-	114,114,114,114	0
54	MG	BA	3540	1/1	0.33	-	80,80,80,80	0
54	MG	BA	3238	1/1	0.55	-	49,49,49,49	0
54	MG	AA	1625	1/1	0.27	-	53,53,53,53	0
54	MG	DA	3791	1/1	0.28	-	108,108,108,108	0
54	MG	DA	3640	1/1	0.24	-	24,24,24,24	0
54	MG	DA	3309	1/1	0.32	-	127,127,127,127	0
54	MG	CA	1886	1/1	0.36	-	105,105,105,105	0
54	MG	BA	3019	1/1	0.27	-	67,67,67,67	0
54	MG	DA	3622	1/1	0.32	-	45,45,45,45	0
54	MG	DA	3159	1/1	0.39	-	106,106,106,106	0
54	MG	DA	2966	1/1	0.22	-	39,39,39,39	0
54	MG	DA	3214	1/1	0.16	-	34,34,34,34	0
54	MG	BA	3656	1/1	0.25	-	107,107,107,107	0
54	MG	DA	2911	1/1	0.39	-	11,11,11,11	0
54	MG	DA	3143	1/1	0.26	-	67,67,67,67	0
54	MG	BA	3128	1/1	0.10	-	65,65,65,65	0
54	MG	AA	1845	1/1	0.07	-	71,71,71,71	0
54	MG	BA	3321	1/1	0.23	-	179,179,179,179	0
54	MG	CA	1633	1/1	0.21	-	85,85,85,85	0
54	MG	BA	3375	1/1	0.33	-	62,62,62,62	0
54	MG	BA	3462	1/1	0.64	-	80,80,80,80	0
54	MG	DA	2991	1/1	0.24	-	36,36,36,36	0
54	MG	DA	2930	1/1	0.54	-	34,34,34,34	0
54	MG	DA	3471	1/1	0.20	-	104,104,104,104	0
54	MG	DA	3648	1/1	0.50	-	60,60,60,60	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
54	MG	DS	202	1/1	0.57	-	62,62,62,62	0
54	MG	BA	3604	1/1	0.40	-	89,89,89,89	0
54	MG	AA	1710	1/1	0.55	-	84,84,84,84	0
54	MG	BA	3020	1/1	0.60	-	88,88,88,88	0
54	MG	DA	3774	1/1	0.38	-	74,74,74,74	0
54	MG	DA	3625	1/1	0.35	-	84,84,84,84	0
54	MG	DA	3451	1/1	0.46	-	80,80,80,80	0
54	MG	CA	1915	1/1	0.30	-	58,58,58,58	0
54	MG	DA	3243	1/1	0.10	-	59,59,59,59	0
54	MG	DA	3391	1/1	0.37	-	82,82,82,82	0
54	MG	BA	3498	1/1	0.81	-	67,67,67,67	0
54	MG	BA	2994	1/1	0.62	-	90,90,90,90	0
54	MG	CA	1966	1/1	0.68	-	97,97,97,97	0
54	MG	DB	239	1/1	0.14	-	107,107,107,107	0
54	MG	CA	1646	1/1	0.17	-	115,115,115,115	0
54	MG	DA	3367	1/1	0.75	-	97,97,97,97	0
54	MG	DA	3005	1/1	0.41	-	41,41,41,41	0
54	MG	AA	1643	1/1	0.18	-	63,63,63,63	0
54	MG	BA	3618	1/1	0.24	-	76,76,76,76	0
54	MG	DA	3088	1/1	0.10	-	83,83,83,83	0
54	MG	BA	2920	1/1	0.41	-	24,24,24,24	0
54	MG	AA	1606	1/1	0.54	-	62,62,62,62	0
54	MG	BA	3088	1/1	0.59	-	57,57,57,57	0
54	MG	BA	3171	1/1	0.08	-	127,127,127,127	0
54	MG	AA	1724	1/1	0.40	-	79,79,79,79	0
54	MG	DA	3464	1/1	0.17	-	133,133,133,133	0
54	MG	BA	3023	1/1	0.68	-	57,57,57,57	0
54	MG	DA	3017	1/1	0.32	-	38,38,38,38	0
54	MG	CA	1736	1/1	0.26	-	73,73,73,73	0
54	MG	DA	3463	1/1	0.42	-	69,69,69,69	0
54	MG	BA	3351	1/1	0.72	-	116,116,116,116	0
54	MG	DA	2909	1/1	0.59	-	22,22,22,22	0
54	MG	CA	1740	1/1	0.07	-	117,117,117,117	0
54	MG	BA	3663	1/1	0.29	-	89,89,89,89	0
54	MG	BA	3123	1/1	0.17	-	40,40,40,40	0
54	MG	DA	3291	1/1	0.28	-	57,57,57,57	0
54	MG	DA	3424	1/1	0.23	-	90,90,90,90	0
54	MG	BA	3520	1/1	0.99	-	95,95,95,95	0
54	MG	BA	3578	1/1	0.08	-	74,74,74,74	0
54	MG	BA	3621	1/1	0.84	-	107,107,107,107	0
54	MG	BA	2997	1/1	0.73	-	81,81,81,81	0
54	MG	BA	3526	1/1	0.19	-	66,66,66,66	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
54	MG	CA	1688	1/1	0.26	-	80,80,80,80	0
54	MG	AA	1831	1/1	0.43	-	67,67,67,67	0
54	MG	CA	1759	1/1	0.45	-	89,89,89,89	0
54	MG	DA	3296	1/1	0.19	-	70,70,70,70	0
54	MG	BA	3309	1/1	0.25	-	84,84,84,84	0
54	MG	BA	3660	1/1	0.16	-	119,119,119,119	0
54	MG	BA	2941	1/1	0.35	-	31,31,31,31	0
54	MG	BA	3535	1/1	0.28	-	95,95,95,95	0
54	MG	DA	3781	1/1	0.31	-	55,55,55,55	0
54	MG	AA	1807	1/1	0.69	-	76,76,76,76	0
54	MG	DA	3772	1/1	0.23	-	114,114,114,114	0
54	MG	AA	1628	1/1	0.44	-	86,86,86,86	0
54	MG	DA	3647	1/1	0.77	-	54,54,54,54	0
54	MG	CA	1889	1/1	0.37	-	74,74,74,74	0
54	MG	BA	3068	1/1	0.23	-	55,55,55,55	0
54	MG	AA	1761	1/1	0.10	-	68,68,68,68	0
54	MG	DA	3050	1/1	0.23	-	89,89,89,89	0
54	MG	CA	1644	1/1	0.21	-	94,94,94,94	0
54	MG	AA	1705	1/1	0.58	-	62,62,62,62	0
54	MG	BA	3679	1/1	0.32	-	75,75,75,75	0
54	MG	DA	3284	1/1	0.15	-	79,79,79,79	0
54	MG	DA	3803	1/1	0.47	-	123,123,123,123	0
54	MG	BA	3316	1/1	0.28	-	97,97,97,97	0
54	MG	DA	3029	1/1	0.43	-	74,74,74,74	0
54	MG	DA	3018	1/1	0.53	-	60,60,60,60	0
54	MG	BA	3107	1/1	0.28	-	25,25,25,25	0
54	MG	BA	3360	1/1	0.30	-	75,75,75,75	0
54	MG	DA	3575	1/1	0.35	-	85,85,85,85	0
54	MG	DA	3443	1/1	0.06	-	92,92,92,92	0
54	MG	BB	203	1/1	0.78	-	74,74,74,74	0
54	MG	AA	1832	1/1	0.34	-	66,66,66,66	0
54	MG	BA	3381	1/1	0.51	-	82,82,82,82	0
54	MG	DA	3654	1/1	0.29	-	59,59,59,59	0
54	MG	DA	3051	1/1	0.41	-	60,60,60,60	0
54	MG	AV	6201	1/1	0.68	-	67,67,67,67	0
54	MG	BA	3259	1/1	0.09	-	105,105,105,105	0
54	MG	DA	3627	1/1	0.46	-	63,63,63,63	0
54	MG	CA	1866	1/1	0.20	-	102,102,102,102	0
54	MG	BA	3671	1/1	0.30	-	100,100,100,100	0
54	MG	CA	1879	1/1	0.23	-	76,76,76,76	0
54	MG	BA	3563	1/1	0.38	-	58,58,58,58	0
54	MG	BA	3474	1/1	0.38	-	72,72,72,72	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
54	MG	BA	3569	1/1	0.14	-	116,116,116,116	0
54	MG	BA	3295	1/1	0.42	-	60,60,60,60	0
54	MG	DA	3127	1/1	0.61	-	76,76,76,76	0
54	MG	DA	3541	1/1	0.18	-	76,76,76,76	0
54	MG	BA	3412	1/1	0.17	-	49,49,49,49	0
54	MG	BA	3313	1/1	0.20	-	67,67,67,67	0
54	MG	BA	3092	1/1	0.76	-	123,123,123,123	0
54	MG	DA	3073	1/1	0.22	-	69,69,69,69	0
54	MG	DA	3832	1/1	0.35	-	77,77,77,77	0
54	MG	DA	2948	1/1	0.17	-	21,21,21,21	0
54	MG	DA	3125	1/1	0.22	-	36,36,36,36	0
54	MG	BA	3666	1/1	0.19	-	72,72,72,72	0
54	MG	DA	3366	1/1	0.42	-	73,73,73,73	0
54	MG	BA	3449	1/1	0.56	-	31,31,31,31	0
54	MG	AA	1830	1/1	0.92	-	105,105,105,105	0
54	MG	BA	3458	1/1	0.12	-	77,77,77,77	0
54	MG	DA	3746	1/1	0.08	-	94,94,94,94	0
54	MG	BA	3509	1/1	0.20	-	64,64,64,64	0
54	MG	DA	3630	1/1	0.23	-	101,101,101,101	0
54	MG	BA	3176	1/1	0.22	-	53,53,53,53	0
54	MG	BA	3276	1/1	0.07	-	67,67,67,67	0
54	MG	AA	1844	1/1	1.05	-	121,121,121,121	0
54	MG	CA	1658	1/1	0.36	-	94,94,94,94	0
54	MG	BN	201	1/1	0.32	-	49,49,49,49	0
54	MG	DA	3729	1/1	0.16	-	81,81,81,81	0
54	MG	CA	1796	1/1	0.56	-	87,87,87,87	0
54	MG	BW	101	1/1	0.25	-	57,57,57,57	0
54	MG	DA	3270	1/1	0.28	-	82,82,82,82	0
54	MG	BA	2972	1/1	0.37	-	61,61,61,61	0
54	MG	DA	3468	1/1	0.48	-	79,79,79,79	0
54	MG	DA	3047	1/1	0.43	-	74,74,74,74	0
54	MG	DA	3745	1/1	0.15	-	109,109,109,109	0
54	MG	BA	3010	1/1	0.04	-	73,73,73,73	0
54	MG	BB	208	1/1	0.09	-	67,67,67,67	0
54	MG	AA	1846	1/1	0.52	-	88,88,88,88	0
54	MG	BA	3588	1/1	0.51	-	52,52,52,52	0
54	MG	BA	3262	1/1	0.19	-	75,75,75,75	0
54	MG	CA	1607	1/1	0.19	-	62,62,62,62	0
54	MG	BA	2939	1/1	0.53	-	47,47,47,47	0
54	MG	DA	3519	1/1	0.32	-	74,74,74,74	0
54	MG	CA	1810	1/1	0.10	-	99,99,99,99	0
54	MG	DA	3000	1/1	0.18	-	23,23,23,23	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
54	MG	DA	3656	1/1	0.21	-	36,36,36,36	0
54	MG	BA	3034	1/1	0.93	-	69,69,69,69	0
54	MG	DA	3108	1/1	0.30	-	54,54,54,54	0
54	MG	DA	2998	1/1	0.33	-	36,36,36,36	0
54	MG	CA	1967	1/1	0.33	-	93,93,93,93	0
54	MG	DA	3372	1/1	0.11	-	90,90,90,90	0
54	MG	BA	3332	1/1	0.19	-	65,65,65,65	0
54	MG	CA	1620	1/1	0.27	-	51,51,51,51	0
54	MG	BA	3432	1/1	0.44	-	12,12,12,12	0
54	MG	BA	3174	1/1	0.36	-	67,67,67,67	0
54	MG	BA	3003	1/1	0.47	-	55,55,55,55	0
54	MG	DA	3770	1/1	0.14	-	79,79,79,79	0
54	MG	BA	3202	1/1	0.39	-	126,126,126,126	0
54	MG	DA	3754	1/1	0.35	-	121,121,121,121	0
54	MG	AA	1862	1/1	0.61	-	84,84,84,84	0
54	MG	BA	3435	1/1	0.39	-	29,29,29,29	0
54	MG	BA	3641	1/1	0.24	-	95,95,95,95	0
54	MG	BA	3311	1/1	0.15	-	87,87,87,87	0
54	MG	DA	3062	1/1	0.34	-	129,129,129,129	0
54	MG	BA	3288	1/1	0.51	-	113,113,113,113	0
54	MG	AA	1825	1/1	1.01	-	79,79,79,79	0
54	MG	CA	1689	1/1	0.21	-	130,130,130,130	0
54	MG	BA	3281	1/1	0.69	-	123,123,123,123	0
54	MG	DN	201	1/1	0.07	-	88,88,88,88	0
54	MG	BA	2958	1/1	0.65	-	46,46,46,46	0
54	MG	DA	3452	1/1	0.64	-	74,74,74,74	0
54	MG	CA	1791	1/1	0.82	-	93,93,93,93	0
54	MG	D3	101	1/1	0.19	-	90,90,90,90	0
54	MG	DA	3677	1/1	0.24	-	60,60,60,60	0
54	MG	DA	3459	1/1	0.17	-	61,61,61,61	0
54	MG	BA	3236	1/1	0.21	-	56,56,56,56	0
54	MG	DA	3333	1/1	0.49	-	90,90,90,90	0
54	MG	CF	202	1/1	0.20	-	83,83,83,83	0
54	MG	DA	3427	1/1	0.39	-	85,85,85,85	0
54	MG	CA	1764	1/1	0.21	-	65,65,65,65	0
54	MG	BU	202	1/1	0.24	-	74,74,74,74	0
54	MG	BA	3193	1/1	0.40	-	81,81,81,81	0
54	MG	DA	3610	1/1	0.38	-	81,81,81,81	0
54	MG	DA	3227	1/1	0.46	-	43,43,43,43	0
54	MG	DA	2950	1/1	0.25	-	33,33,33,33	0
54	MG	CL	206	1/1	0.18	-	87,87,87,87	0
54	MG	DA	2904	1/1	0.31	-	16,16,16,16	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
54	MG	BA	3221	1/1	0.38	-	141,141,141,141	0
54	MG	CA	1920	1/1	0.26	-	87,87,87,87	0
54	MG	DA	3589	1/1	0.36	-	51,51,51,51	0
54	MG	DA	3793	1/1	0.21	-	106,106,106,106	0
54	MG	AA	1700	1/1	0.40	-	114,114,114,114	0
54	MG	CA	1753	1/1	0.32	-	97,97,97,97	0
54	MG	CA	1852	1/1	0.37	-	101,101,101,101	0
54	MG	DA	3717	1/1	0.23	-	65,65,65,65	0
54	MG	BA	3223	1/1	0.28	-	76,76,76,76	0
54	MG	DA	3722	1/1	0.17	-	138,138,138,138	0
54	MG	CV	6206	1/1	0.08	-	107,107,107,107	0
54	MG	DA	2987	1/1	0.27	-	28,28,28,28	0
54	MG	AA	1806	1/1	0.38	-	65,65,65,65	0
54	MG	DB	210	1/1	0.10	-	92,92,92,92	0
54	MG	DA	3316	1/1	0.06	-	94,94,94,94	0
54	MG	BA	2921	1/1	0.29	-	17,17,17,17	0
54	MG	CA	1891	1/1	0.51	-	113,113,113,113	0
54	MG	CA	1719	1/1	0.40	-	78,78,78,78	0
54	MG	CA	1871	1/1	0.52	-	76,76,76,76	0
54	MG	BA	3454	1/1	0.27	-	41,41,41,41	0
54	MG	DA	3491	1/1	0.98	-	99,99,99,99	0
54	MG	DB	232	1/1	0.18	-	84,84,84,84	0
54	MG	CA	1818	1/1	0.41	-	91,91,91,91	0
54	MG	AA	1678	1/1	0.24	-	78,78,78,78	0
54	MG	CQ	201	1/1	0.36	-	103,103,103,103	0
54	MG	DA	3250	1/1	0.31	-	70,70,70,70	0
54	MG	AA	1874	1/1	0.12	-	87,87,87,87	0
54	MG	BA	3670	1/1	0.64	-	90,90,90,90	0
54	MG	BA	2938	1/1	0.45	-	51,51,51,51	0
54	MG	DA	3110	1/1	0.31	-	65,65,65,65	0
54	MG	BA	3102	1/1	0.40	-	72,72,72,72	0
54	MG	CA	1710	1/1	0.16	-	169,169,169,169	0
54	MG	DA	3153	1/1	0.49	-	33,33,33,33	0
54	MG	AA	1651	1/1	0.37	-	56,56,56,56	0
54	MG	DA	3730	1/1	0.29	-	61,61,61,61	0
54	MG	DA	3457	1/1	0.32	-	86,86,86,86	0
54	MG	DA	3266	1/1	0.15	-	85,85,85,85	0
54	MG	BA	3042	1/1	1.05	-	92,92,92,92	0
54	MG	DA	3128	1/1	0.43	-	85,85,85,85	0
54	MG	DA	3053	1/1	0.46	-	63,63,63,63	0
54	MG	BA	3114	1/1	0.44	-	69,69,69,69	0
54	MG	CA	1680	1/1	0.46	-	63,63,63,63	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
54	MG	BA	3149	1/1	0.37	-	65,65,65,65	0
54	MG	DA	3020	1/1	0.81	-	47,47,47,47	0
54	MG	BA	3074	1/1	0.37	-	87,87,87,87	0
54	MG	CA	1606	1/1	0.48	-	57,57,57,57	0
54	MG	AA	1666	1/1	0.54	-	93,93,93,93	0
54	MG	CA	1789	1/1	0.17	-	103,103,103,103	0
54	MG	BA	3273	1/1	0.29	-	73,73,73,73	0
54	MG	BA	3022	1/1	0.54	-	83,83,83,83	0
54	MG	CA	1727	1/1	0.19	-	76,76,76,76	0
54	MG	DA	3844	1/1	0.21	-	132,132,132,132	0
54	MG	DF	202	1/1	0.10	-	129,129,129,129	0
54	MG	BI	101	1/1	0.21	-	109,109,109,109	0
54	MG	AV	6204	1/1	0.13	-	124,124,124,124	0
54	MG	BT	102	1/1	0.27	-	66,66,66,66	0
54	MG	DA	3192	1/1	0.18	-	49,49,49,49	0
54	MG	DA	3489	1/1	0.25	-	97,97,97,97	0
54	MG	BA	2901	1/1	0.63	-	8,8,8,8	0
54	MG	CA	1916	1/1	0.51	-	118,118,118,118	0
54	MG	DA	3215	1/1	0.55	-	73,73,73,73	0
54	MG	DA	3180	1/1	0.40	-	78,78,78,78	0
54	MG	AA	1734	1/1	0.21	-	96,96,96,96	0
54	MG	AA	1722	1/1	0.53	-	53,53,53,53	0
54	MG	DA	3141	1/1	0.38	-	57,57,57,57	0
54	MG	CV	6204	1/1	0.08	-	112,112,112,112	0
54	MG	DA	3685	1/1	0.40	-	82,82,82,82	0
54	MG	BA	3605	1/1	0.41	-	69,69,69,69	0
54	MG	DA	3041	1/1	0.30	-	76,76,76,76	0
54	MG	BA	3523	1/1	1.61	-	99,99,99,99	0
54	MG	D4	103	1/1	0.24	-	73,73,73,73	0
54	MG	BA	3004	1/1	0.35	-	49,49,49,49	0
54	MG	CA	1953	1/1	0.25	-	120,120,120,120	0
54	MG	CA	1846	1/1	0.28	-	135,135,135,135	0
54	MG	DA	3016	1/1	0.21	-	47,47,47,47	0
54	MG	BA	3584	1/1	0.17	-	83,83,83,83	0
54	MG	DA	3618	1/1	0.31	-	129,129,129,129	0
54	MG	DA	3419	1/1	0.12	-	60,60,60,60	0
54	MG	AA	1698	1/1	0.06	-	88,88,88,88	0
54	MG	DA	3233	1/1	0.44	-	67,67,67,67	0
54	MG	BA	3379	1/1	0.22	-	86,86,86,86	0
54	MG	DA	3639	1/1	0.34	-	26,26,26,26	0
54	MG	DA	3353	1/1	0.29	-	105,105,105,105	0
54	MG	DA	3394	1/1	0.37	-	110,110,110,110	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
54	MG	BA	3418	1/1	0.50	-	88,88,88,88	0
54	MG	BA	3658	1/1	0.25	-	68,68,68,68	0
54	MG	CA	1782	1/1	0.07	-	80,80,80,80	0
54	MG	CA	1761	1/1	0.99	-	88,88,88,88	0
54	MG	AA	1787	1/1	0.51	-	68,68,68,68	0
54	MG	BA	3506	1/1	0.40	-	89,89,89,89	0
54	MG	DA	3416	1/1	0.20	-	101,101,101,101	0
54	MG	DA	3118	1/1	0.43	-	50,50,50,50	0
54	MG	BA	3308	1/1	0.22	-	99,99,99,99	0
54	MG	CA	1751	1/1	0.07	-	117,117,117,117	0
54	MG	DA	3850	1/1	0.45	-	52,52,52,52	0
54	MG	DA	2936	1/1	0.11	-	42,42,42,42	0
54	MG	CA	1702	1/1	0.23	-	114,114,114,114	0
54	MG	BA	3006	1/1	0.58	-	61,61,61,61	0
54	MG	CA	1741	1/1	0.26	-	100,100,100,100	0
54	MG	DA	3106	1/1	0.30	-	69,69,69,69	0
54	MG	AA	1759	1/1	0.51	-	110,110,110,110	0
54	MG	BA	3650	1/1	0.33	-	69,69,69,69	0
54	MG	BA	3033	1/1	0.41	-	77,77,77,77	0
54	MG	BA	3121	1/1	0.35	-	69,69,69,69	0
54	MG	DA	3428	1/1	0.33	-	71,71,71,71	0
54	MG	BA	3154	1/1	0.11	-	139,139,139,139	0
54	MG	DA	3859	1/1	0.24	-	55,55,55,55	0
54	MG	BA	3575	1/1	0.25	-	59,59,59,59	0
54	MG	BA	3157	1/1	0.31	-	94,94,94,94	0
54	MG	BA	3069	1/1	0.23	-	52,52,52,52	0
54	MG	AA	1814	1/1	0.20	-	82,82,82,82	0
54	MG	AA	1870	1/1	0.25	-	98,98,98,98	0
54	MG	BA	3348	1/1	0.27	-	107,107,107,107	0
54	MG	DA	3810	1/1	0.06	-	102,102,102,102	0
54	MG	BA	3573	1/1	0.16	-	58,58,58,58	0
54	MG	DA	3473	1/1	0.56	-	61,61,61,61	0
54	MG	BY	102	1/1	0.14	-	110,110,110,110	0
54	MG	DA	3441	1/1	0.17	-	60,60,60,60	0
54	MG	CA	1679	1/1	0.46	-	89,89,89,89	0
54	MG	BA	3109	1/1	0.41	-	77,77,77,77	0
54	MG	AL	201	1/1	0.34	-	109,109,109,109	0
54	MG	DA	3090	1/1	0.41	-	59,59,59,59	0
54	MG	BA	3035	1/1	0.25	-	57,57,57,57	0
54	MG	CA	1865	1/1	0.55	-	93,93,93,93	0
54	MG	CA	1968	1/1	0.11	-	87,87,87,87	0
54	MG	DA	2922	1/1	0.45	-	37,37,37,37	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
54	MG	CV	6203	1/1	0.22	-	80,80,80,80	0
54	MG	BA	3214	1/1	0.60	-	79,79,79,79	0
54	MG	BA	3503	1/1	0.74	-	90,90,90,90	0
54	MG	DA	2988	1/1	0.47	-	23,23,23,23	0
54	MG	DA	3335	1/1	0.10	-	46,46,46,46	0
54	MG	BA	3536	1/1	0.41	-	83,83,83,83	0
54	MG	CA	1950	1/1	0.38	-	107,107,107,107	0
54	MG	AA	1683	1/1	0.46	-	64,64,64,64	0
54	MG	BA	3272	1/1	0.79	-	81,81,81,81	0
54	MG	CA	1686	1/1	0.13	-	82,82,82,82	0
54	MG	DA	3154	1/1	0.36	-	50,50,50,50	0
54	MG	DA	3389	1/1	0.14	-	76,76,76,76	0
54	MG	CO	101	1/1	0.18	-	127,127,127,127	0
54	MG	AC	301	1/1	0.21	-	104,104,104,104	0
54	MG	BA	3448	1/1	0.49	-	51,51,51,51	0
54	MG	CA	1695	1/1	0.11	-	65,65,65,65	0
54	MG	DA	3091	1/1	0.40	-	127,127,127,127	0
54	MG	BA	3101	1/1	0.93	-	74,74,74,74	0
54	MG	AA	1827	1/1	0.28	-	71,71,71,71	0
54	MG	AA	1822	1/1	0.23	-	92,92,92,92	0
54	MG	DA	3429	1/1	0.20	-	79,79,79,79	0
54	MG	CA	1704	1/1	0.63	-	140,140,140,140	0
54	MG	AA	1842	1/1	0.81	-	69,69,69,69	0
54	MG	DA	3662	1/1	0.80	-	71,71,71,71	0
54	MG	CD	304	1/1	0.67	-	108,108,108,108	0
54	MG	DA	3248	1/1	0.19	-	80,80,80,80	0
54	MG	CA	1893	1/1	0.33	-	127,127,127,127	0

6.5 Other polymers ⓘ

There are no such residues in this entry.