



wwPDB X-ray Structure Validation Summary Report

Jun 16, 2014 – 09:08 PM BST

PDB ID : 4V9N
Title : Crystal structure of the 70S ribosome bound with the Q253P mutant of release factor RF2.
Authors : Santos, N.; Zhu, J.; Donohue, J.P.; Korostelev, A.A.; Noller, H.F.
Deposited on : 2013-04-26
Resolution : 3.40 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>

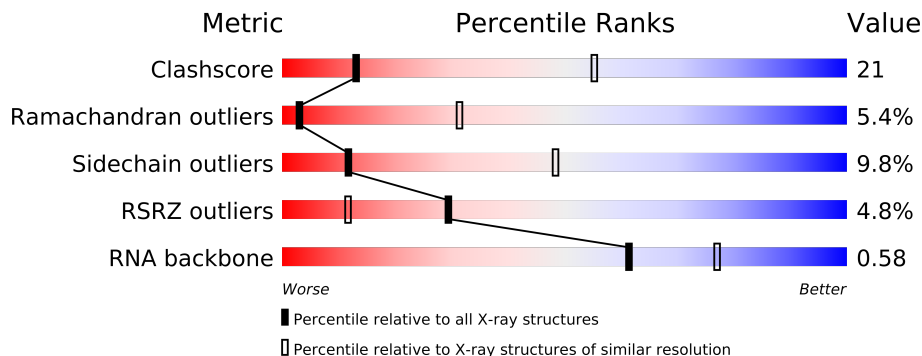
The following versions of software and data (see [references](#)) were used in the production of this report:

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 3.40 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))
Clashscore	79885	1214 (3.50-3.30)
Ramachandran outliers	78287	1177 (3.50-3.30)
Sidechain outliers	78261	1177 (3.50-3.30)
RSRZ outliers	66119	1017 (3.52-3.28)
RNA backbone	1838	1002 (4.02-2.76)

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	1504	
1	CA	1504	
2	AV	10	
2	CV	10	
3	AW	77	
3	CW	77	
4	AY	362	
4	CY	362	
5	AB	234	
5	CB	234	
6	AC	206	
6	CC	206	
7	AD	208	
7	CD	208	

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Mol	Chain	Length	Quality of chain
8	AE	151	
8	CE	151	
9	AF	101	
9	CF	101	
10	AG	155	
10	CG	155	
11	AH	138	
11	CH	138	
12	AI	127	
12	CI	127	
13	AJ	98	
13	CJ	98	
14	AK	114	
14	CK	114	
15	AL	122	
15	CL	122	
16	AM	117	
16	CM	117	
17	AN	60	
17	CN	60	
18	AO	88	
18	CO	88	
19	AP	83	
19	CP	83	
20	AQ	99	
20	CQ	99	
21	AR	70	
21	CR	70	
22	AS	78	
22	CS	78	
23	AT	99	
23	CT	99	
24	AU	24	
24	CU	24	
25	BA	2879	
25	DA	2879	
26	BB	119	
26	DB	119	
27	BD	271	
27	DD	271	
28	BE	204	
28	DE	204	

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Mol	Chain	Length	Quality of chain
29	BF	202	
29	DF	202	
30	BG	181	
30	DG	181	
31	BH	159	
31	DH	159	
32	BI	145	
32	DI	145	
33	BK	147	
33	DK	147	
34	BN	137	
34	DN	137	
35	BO	122	
35	DO	122	
36	BP	146	
36	DP	146	
37	BQ	134	
37	DQ	134	
38	BR	117	
38	DR	117	
39	BS	98	
39	DS	98	
40	BT	137	
40	DT	137	
41	BU	117	
41	DU	117	
42	BV	101	
42	DV	101	
43	BW	112	
43	DW	112	
44	BX	92	
44	DX	92	
45	BY	100	
45	DY	100	
46	BZ	187	
46	DZ	187	
47	B0	76	
47	D0	76	
48	B1	88	
48	D1	88	
49	B2	62	
49	D2	62	

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Mol	Chain	Length	Quality of chain
50	B3	59	
50	D3	59	
51	B4	30	
51	D4	30	
52	B5	52	
52	D5	52	
53	B6	44	
53	D6	44	
54	B7	48	
54	D7	48	
55	B8	63	
55	D8	63	

2 Entry composition

There are 57 unique types of molecules in this entry. The entry contains 294074 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 16S rRNA (1504-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	AA	1504	Total	C	N	O	P	0	0	0
			32332	14391	5994	10444	1503			
1	CA	1504	Total	C	N	O	P	0	0	0
			32332	14391	5994	10444	1503			

- Molecule 2 is a RNA chain called messenger RNA (5'-R(*AP*AP*UP*GP*UP*AP*G)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	AV	10	Total	C	N	O	P	0	0	0
			214	98	44	63	9			
2	CV	10	Total	C	N	O	P	0	0	0
			214	98	44	63	9			

- Molecule 3 is a RNA chain called P-site tRNA-fMet.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	AW	77	Total	C	N	O	P	0	0	0
			1640	732	297	535	76			
3	CW	77	Total	C	N	O	P	0	0	0
			1640	732	297	535	76			

- Molecule 4 is a protein called Bacterial peptide chain release factor 2 (RF-2).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	AY	362	Total	C	N	O	S	0	0	0
			2874	1794	517	555	8			
4	CY	362	Total	C	N	O	S	0	0	0
			2874	1794	517	555	8			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AY	253	PRO	GLN	ENGINEERED MUTATION	UNP Q72GJ6
CY	253	PRO	GLN	ENGINEERED MUTATION	UNP Q72GJ6

- Molecule 5 is a protein called 30S ribosomal protein S2.

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

- Molecule 6 is a protein called 30S ribosomal protein S3.

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

- Molecule 7 is a protein called 30S ribosomal protein S4.

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

- Molecule 8 is a protein called 30S ribosomal protein S5.

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

- Molecule 9 is a protein called 30S ribosomal protein S6.

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

- Molecule 10 is a protein called 30S ribosomal protein S7.

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

- Molecule 11 is a protein called 30S ribosomal protein S8.

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

- Molecule 12 is a protein called 30S ribosomal protein S9.

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

- Molecule 13 is a protein called 30S ribosomal protein S10.

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

- Molecule 14 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	AK	114	Total	C	N	O	S	0	0	0
			843	522	159	159	3			
14	CK	114	Total	C	N	O	S	0	0	0
			843	522	159	159	3			

- Molecule 15 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	AL	122	Total	C	N	O	S	0	0	0
			957	603	193	160	1			
15	CL	122	Total	C	N	O	S	0	0	0
			957	603	193	160	1			

- Molecule 16 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	AM	117	Total	C	N	O	S	0	0	0
			934	577	192	163	2			
16	CM	117	Total	C	N	O	S	0	0	0
			934	577	192	163	2			

- Molecule 17 is a protein called 30S ribosomal protein S14.

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

- Molecule 18 is a protein called 30S ribosomal protein S15.

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

- Molecule 19 is a protein called 30S ribosomal protein S16.

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

- Molecule 20 is a protein called 30S ribosomal protein S17.

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

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

- Molecule 21 is a protein called 30S ribosomal protein S18.

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

- Molecule 22 is a protein called 30S ribosomal protein S19.

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

- Molecule 23 is a protein called 30S ribosomal protein S20.

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

- Molecule 24 is a protein called 30S ribosomal protein Thx.

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

- Molecule 25 is a RNA chain called 23S ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
25	BA	2789	Total	C	N	O	P	0	0	0
			60059	26734	11225	19312	2788			
25	DA	2789	Total	C	N	O	P	0	0	0
			60059	26734	11225	19312	2788			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
BA	276	C	A	CONFLICT	GB AE017221.1
BA	277	A	C	CONFLICT	GB AE017221.1
BA	1141A	U	C	CONFLICT	GB AE017221.1
BA	2825	U	G	CONFLICT	GB AE017221.1
DA	276	C	A	CONFLICT	GB AE017221.1
DA	277	A	C	CONFLICT	GB AE017221.1
DA	1141A	U	C	CONFLICT	GB AE017221.1
DA	2825	U	G	CONFLICT	GB AE017221.1

- Molecule 26 is a RNA chain called 5S ribosomal RNA.

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

- Molecule 27 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
27	BD	271	Total	C	N	O	S	0	0	0
			2105	1329	416	357	3			
27	DD	271	Total	C	N	O	S	0	0	0
			2105	1329	416	357	3			

- Molecule 28 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
28	BE	204	Total	C	N	O	S	0	0	0
			1564	988	299	271	6			
28	DE	204	Total	C	N	O	S	0	0	0
			1564	988	299	271	6			

- Molecule 29 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
29	BF	202	Total	C	N	O	S	0	0	0
			1587	1011	297	276	3			
29	DF	202	Total	C	N	O	S	0	0	0
			1587	1011	297	276	3			

- Molecule 30 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
30	BG	181	Total	C	N	O	S	0	0	0
			1475	943	268	260	4			
30	DG	181	Total	C	N	O	S	0	0	0
			1475	943	268	260	4			

- Molecule 31 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
31	BH	159	Total	C	N	O	S	0	0	0
			1223	773	228	221	1			
31	DH	159	Total	C	N	O	S	0	0	0
			1223	773	228	221	1			

- Molecule 32 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
32	BI	145	Total	C	N	O	S	0	0	0
			1133	724	200	208	1			
32	DI	145	Total	C	N	O	S	0	0	0
			1133	724	200	208	1			

- Molecule 33 is a protein called 50S ribosomal protein L11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
33	BK	147	Total	C	N	O	S	0	0	0
			1088	692	191	199	6			
33	DK	147	Total	C	N	O	S	0	0	0
			1088	692	191	199	6			

- Molecule 34 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
34	BN	137	Total	C	N	O	S	0	0	0
			1097	707	205	182	3			
34	DN	137	Total	C	N	O	S	0	0	0
			1097	707	205	182	3			

- Molecule 35 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
35	BO	122	Total	C	N	O	S	0	0	0
			932	587	171	170	4			
35	DO	122	Total	C	N	O	S	0	0	0
			932	587	171	170	4			

- Molecule 36 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
36	BP	146	Total	C	N	O	S	0	0	0
			1114	692	227	193	2			
36	DP	146	Total	C	N	O	S	0	0	0
			1114	692	227	193	2			

- Molecule 37 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
37	BQ	134	Total	C	N	O	S	0	0	0
			1065	680	201	179	5			
37	DQ	134	Total	C	N	O	S	0	0	0
			1065	680	201	179	5			

- Molecule 38 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
38	BR	117	Total	C	N	O	0	0	0
			960	599	202	159			
38	DR	117	Total	C	N	O	0	0	0
			960	599	202	159			

- Molecule 39 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
39	BS	98	Total	C	N	O	0	0	0
			771	486	154	131			
39	DS	98	Total	C	N	O	0	0	0
			771	486	154	131			

- Molecule 40 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
40	BT	137	Total	C	N	O	S	0	0	0
			1144	713	234	196	1			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
40	DT	137	Total	C	N	O	S	0	0	0
			1144	713	234	196	1			

- Molecule 41 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
41	BU	117	Total	C	N	O	S	0	0	0
			964	610	202	151	1			
41	DU	117	Total	C	N	O	S	0	0	0
			964	610	202	151	1			

- Molecule 42 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
42	BV	101	Total	C	N	O	S	0	0	0
			779	501	142	135	1			
42	DV	101	Total	C	N	O	S	0	0	0
			779	501	142	135	1			

- Molecule 43 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
43	BW	112	Total	C	N	O	S	0	0	0
			891	560	175	154	2			
43	DW	112	Total	C	N	O	S	0	0	0
			891	560	175	154	2			

- Molecule 44 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
44	BX	92	Total	C	N	O	0	0	0
			726	471	131	124			
44	DX	92	Total	C	N	O	0	0	0
			726	471	131	124			

- Molecule 45 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
45	BY	100	Total	C	N	O	S	0	0	0
			776	500	148	124	4			
45	DY	100	Total	C	N	O	S	0	0	0
			776	500	148	124	4			

- Molecule 46 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
46	BZ	187	Total	C	N	O	S	0	0	0
			1483	945	264	272	2			
46	DZ	187	Total	C	N	O	S	0	0	0
			1483	945	264	272	2			

- Molecule 47 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
47	B0	76	Total	C	N	O	S	0	0	0
			605	376	126	102	1			
47	D0	76	Total	C	N	O	S	0	0	0
			605	376	126	102	1			

- Molecule 48 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
48	B1	88	Total	C	N	O		0	0	0
			695	435	141	119				
48	D1	88	Total	C	N	O		0	0	0
			695	435	141	119				

- Molecule 49 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
49	B2	62	Total	C	N	O	S	0	0	0
			521	325	102	92	2			
49	D2	62	Total	C	N	O	S	0	0	0
			521	325	102	92	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
50	B3	59	Total	C	N	O	S	0	0	0
			468	298	90	79	1			
50	D3	59	Total	C	N	O	S	0	0	0
			468	298	90	79	1			

- Molecule 51 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
51	B4	30	Total	C	N	O	S	0	0	0
			226	142	36	44	4			
51	D4	30	Total	C	N	O	S	0	0	0
			226	142	36	44	4			

- Molecule 52 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
52	B5	52	Total	C	N	O	S	0	0	0
			405	255	79	66	5			
52	D5	52	Total	C	N	O	S	0	0	0
			405	255	79	66	5			

- Molecule 53 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
53	B6	44	Total	C	N	O	S	0	0	0
			381	235	77	65	4			
53	D6	44	Total	C	N	O	S	0	0	0
			381	235	77	65	4			

- Molecule 54 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
54	B7	48	Total	C	N	O	S	0	0	0
			419	257	104	56	2			
54	D7	48	Total	C	N	O	S	0	0	0
			419	257	104	56	2			

- Molecule 55 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
55	B8	63	Total	C	N	O	S	0	0	0
			508	326	101	79	2			
55	D8	63	Total	C	N	O	S	0	0	0
			508	326	101	79	2			

- Molecule 56 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	BA	824	Total	Mg	0	0
			824	824		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	CA	326	Total 326	Mg 326	0	0
56	DQ	4	Total 4	Mg 4	0	0
56	DF	2	Total 2	Mg 2	0	0
56	CV	2	Total 2	Mg 2	0	0
56	B8	2	Total 2	Mg 2	0	0
56	BE	1	Total 1	Mg 1	0	0
56	AW	18	Total 18	Mg 18	0	0
56	B1	1	Total 1	Mg 1	0	0
56	CD	1	Total 1	Mg 1	0	0
56	BP	1	Total 1	Mg 1	0	0
56	CR	1	Total 1	Mg 1	0	0
56	DN	1	Total 1	Mg 1	0	0
56	CY	2	Total 2	Mg 2	0	0
56	B5	1	Total 1	Mg 1	0	0
56	BB	23	Total 23	Mg 23	0	0
56	BT	1	Total 1	Mg 1	0	0
56	BF	1	Total 1	Mg 1	0	0
56	AV	1	Total 1	Mg 1	0	0
56	BX	2	Total 2	Mg 2	0	0
56	AA	393	Total 393	Mg 393	0	0
56	D7	2	Total 2	Mg 2	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	DV	1	Total 1	Mg 1	0	0
56	DI	2	Total 2	Mg 2	0	0
56	DD	1	Total 1	Mg 1	0	0
56	CM	1	Total 1	Mg 1	0	0
56	D0	1	Total 1	Mg 1	0	0
56	BY	1	Total 1	Mg 1	0	0
56	B3	1	Total 1	Mg 1	0	0
56	DX	1	Total 1	Mg 1	0	0
56	DA	732	Total 732	Mg 732	0	0
56	DW	2	Total 2	Mg 2	0	0
56	DH	1	Total 1	Mg 1	0	0
56	AG	1	Total 1	Mg 1	0	0
56	DE	1	Total 1	Mg 1	0	0
56	AQ	1	Total 1	Mg 1	0	0
56	D1	1	Total 1	Mg 1	0	0
56	DP	2	Total 2	Mg 2	0	0
56	AC	1	Total 1	Mg 1	0	0
56	CW	16	Total 16	Mg 16	0	0
56	D5	3	Total 3	Mg 3	0	0
56	BD	1	Total 1	Mg 1	0	0
56	AT	3	Total 3	Mg 3	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	B0	2	Total 2	Mg 2	0	0
56	AO	1	Total 1	Mg 1	0	0
56	AY	3	Total 3	Mg 3	0	0
56	DB	20	Total 20	Mg 20	0	0

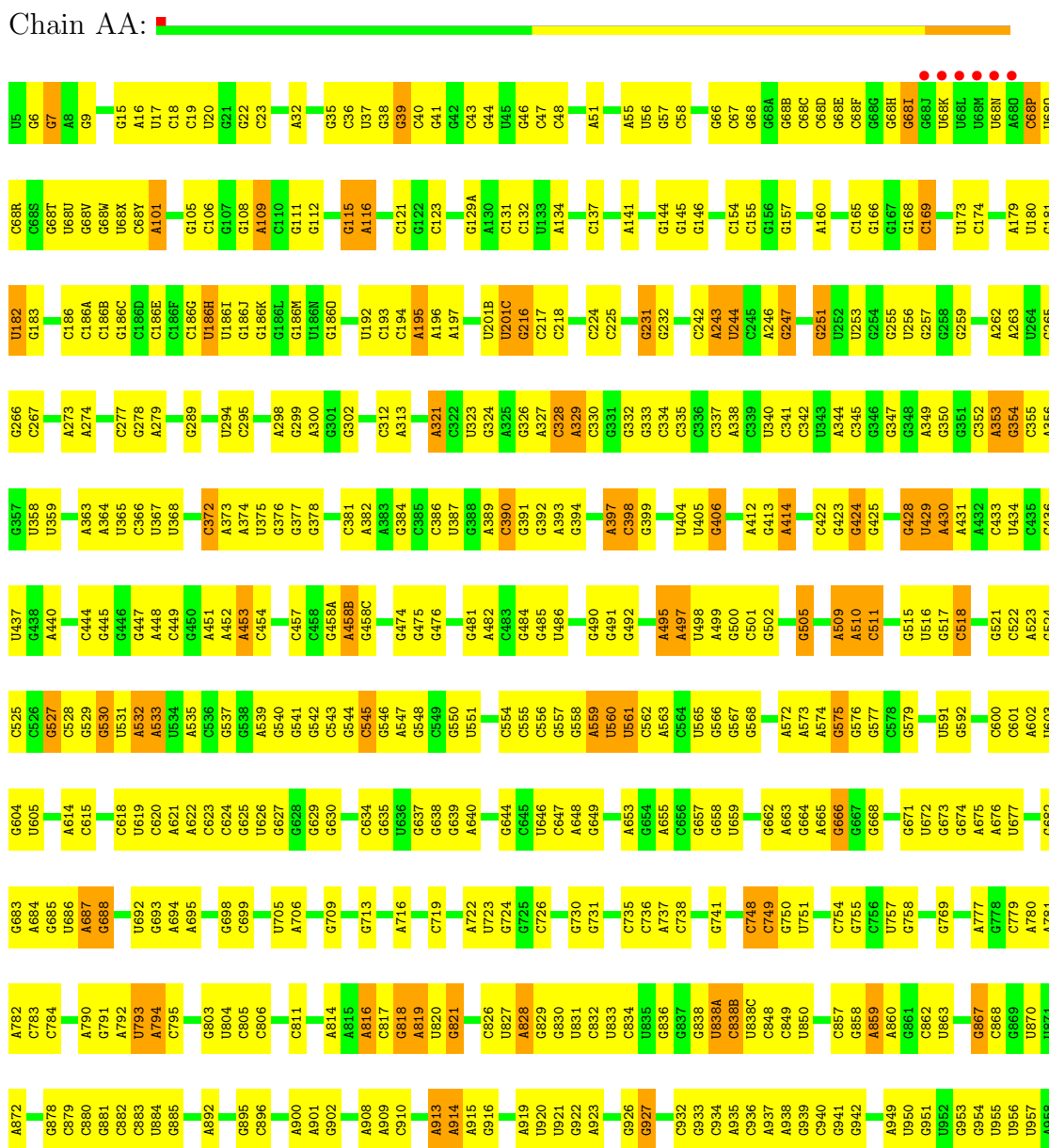
- Molecule 57 is ZINC ION (three-letter code: ZN) (formula: Zn).

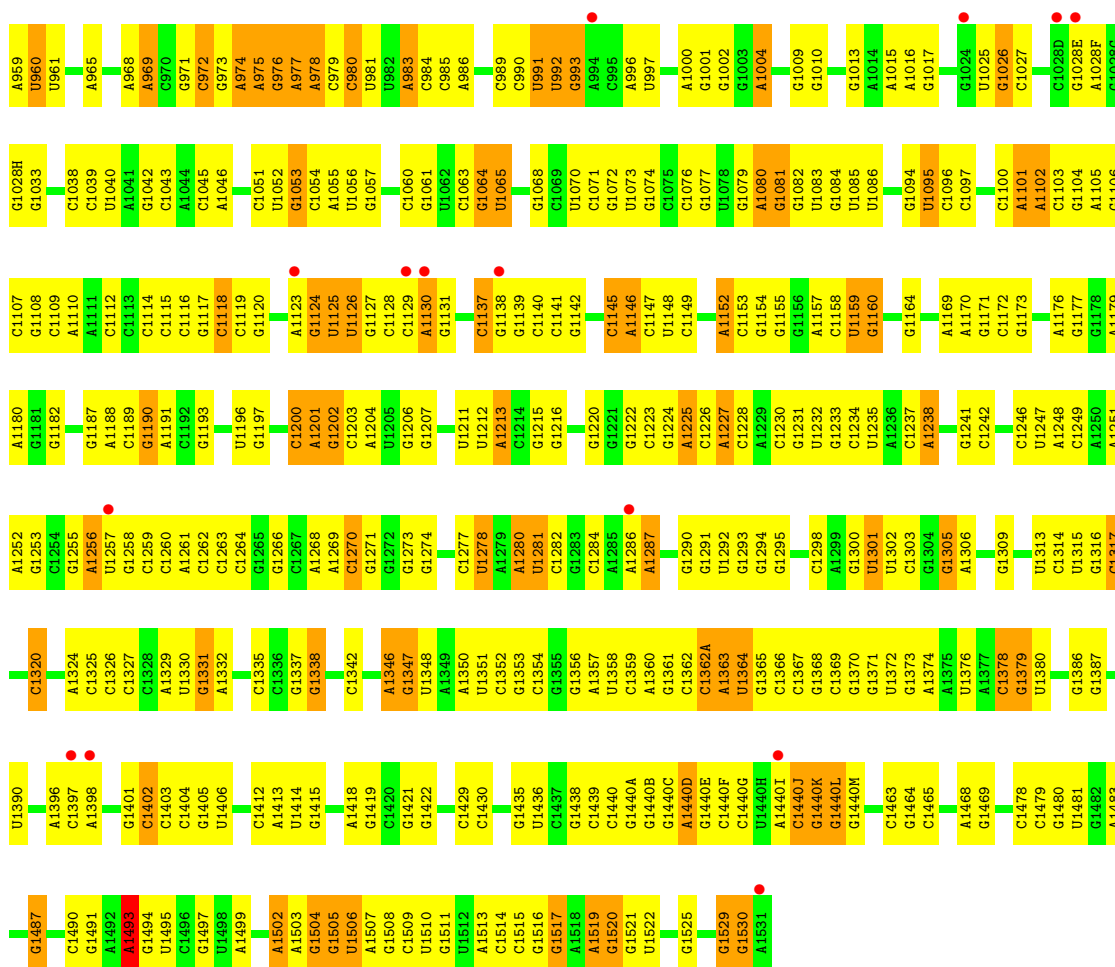
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	CN	1	Total 1	Zn 1	0	0
57	AD	1	Total 1	Zn 1	0	0
57	CD	1	Total 1	Zn 1	0	0
57	AN	1	Total 1	Zn 1	0	0

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.

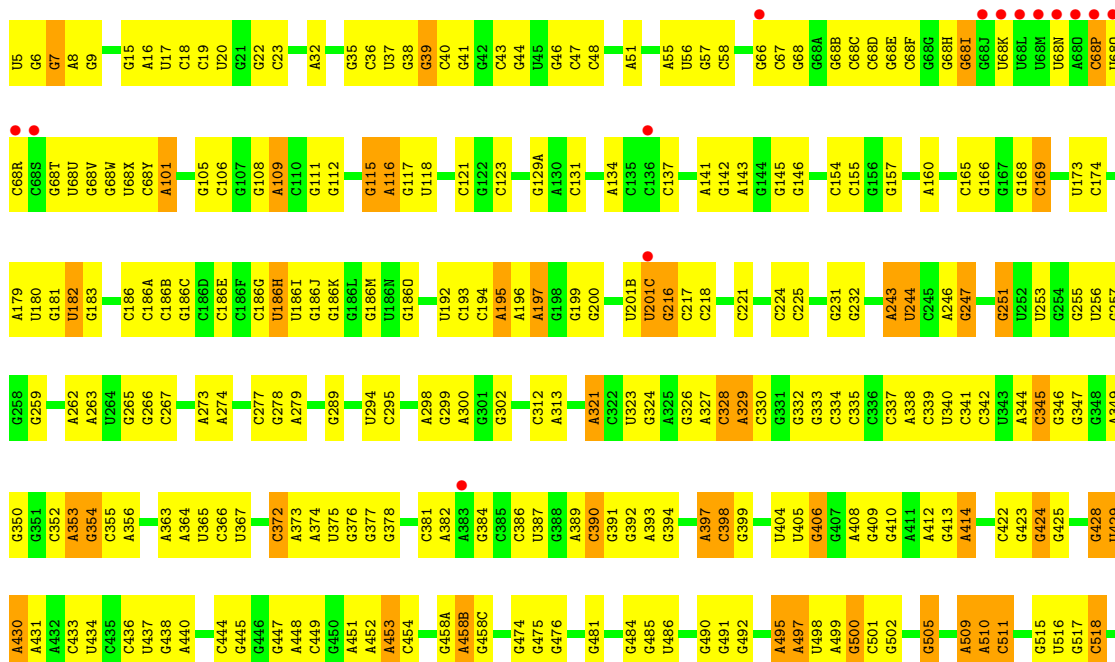
- Molecule 1: 16S rRNA (1504-MER)

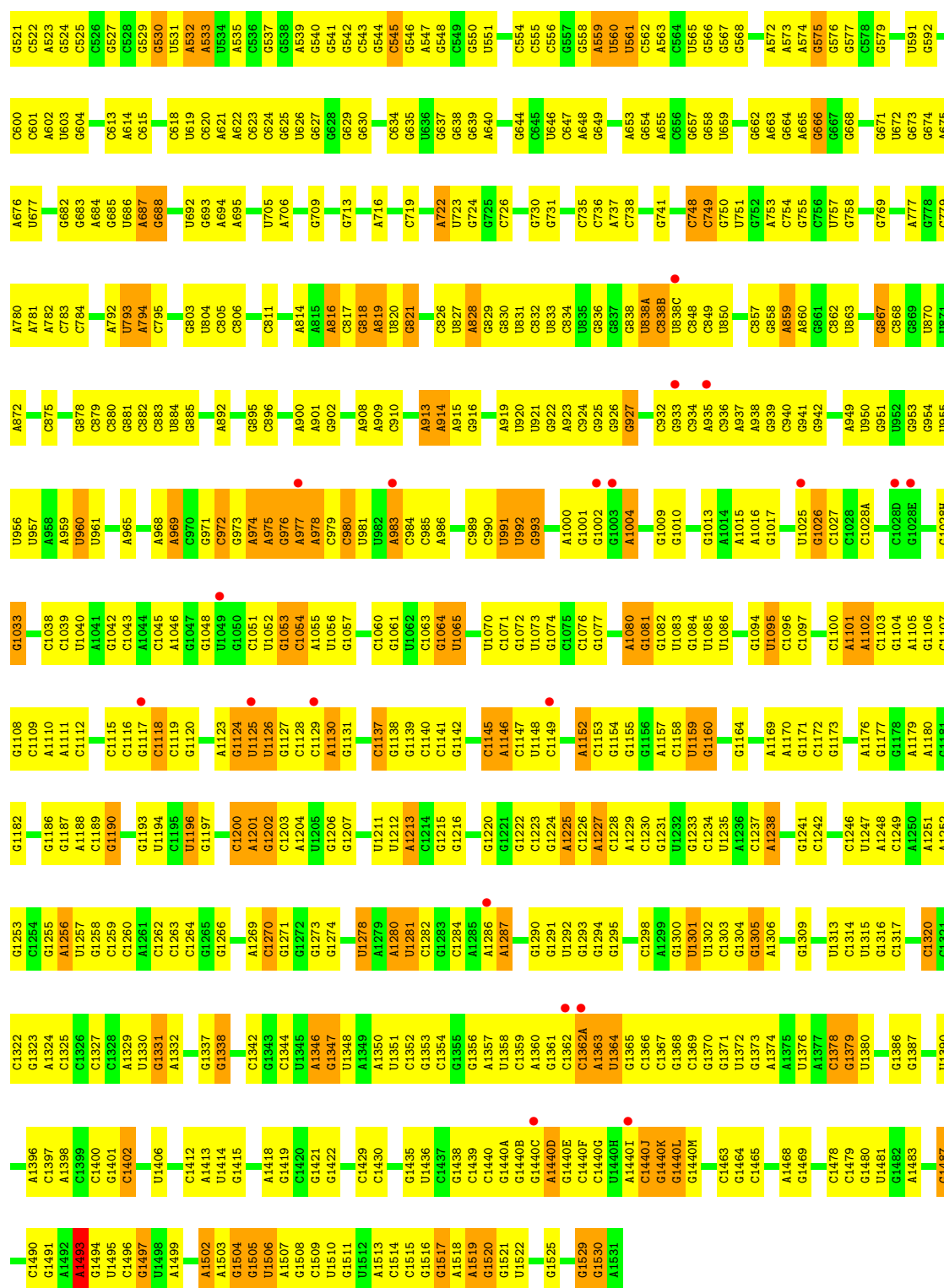




• Molecule 1: 16S rRNA (1504-MER)

Chain CA:





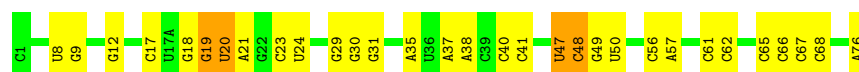
- Molecule 2: messenger RNA (5'-R(*AP*AP*UP*GP*UP*AP*G)-3')

Chain CV: 



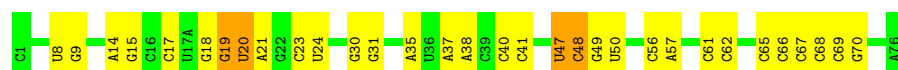
- Molecule 3: P-site tRNA-fMet

Chain AW: 



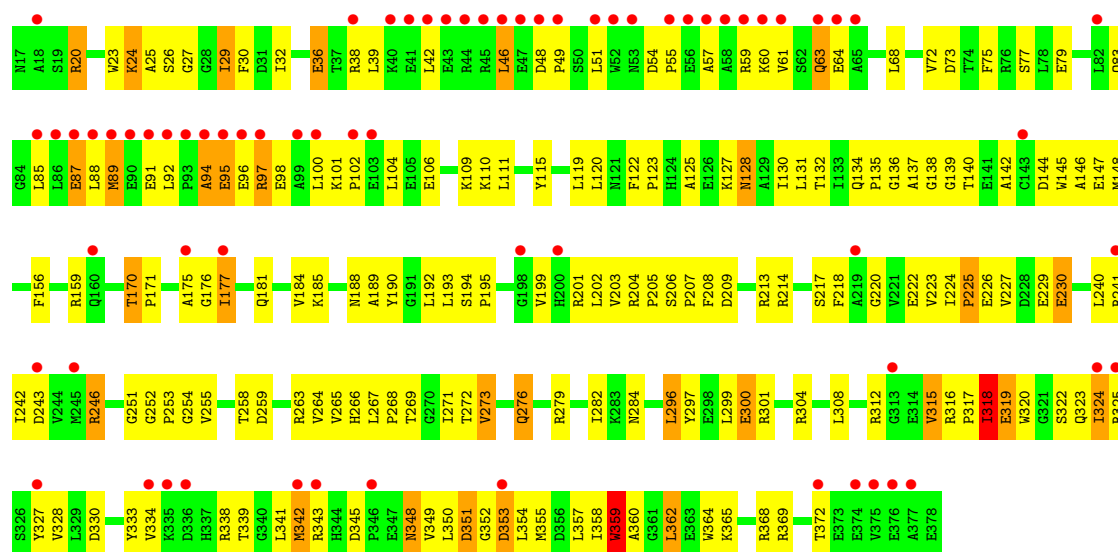
- Molecule 3: P-site tRNA-fMet

Chain CW: 



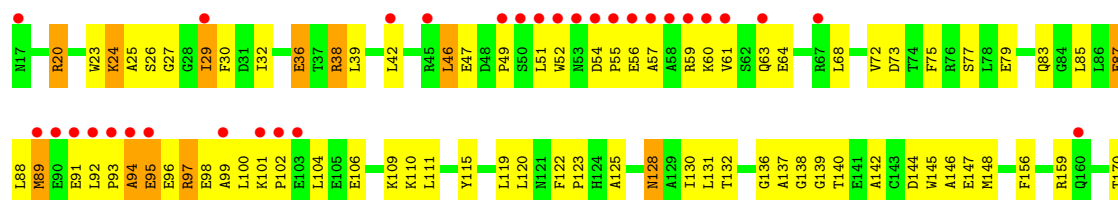
- Molecule 4: Bacterial peptide chain release factor 2 (RF-2)

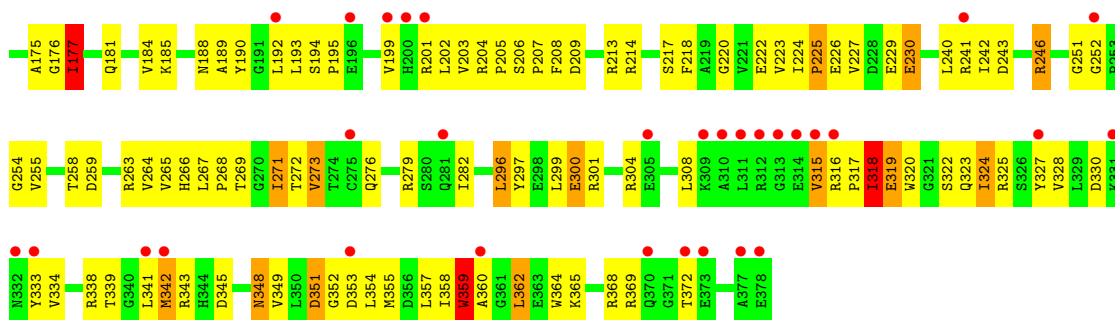
Chain AY: 



- Molecule 4: Bacterial peptide chain release factor 2 (RF-2)

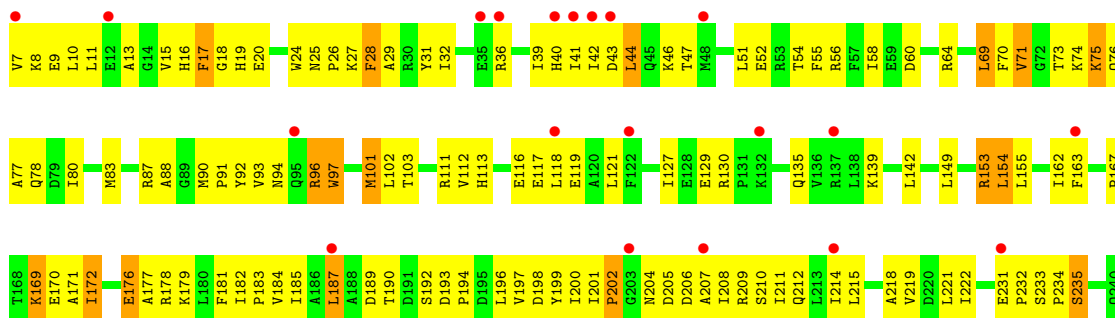
Chain CY: 





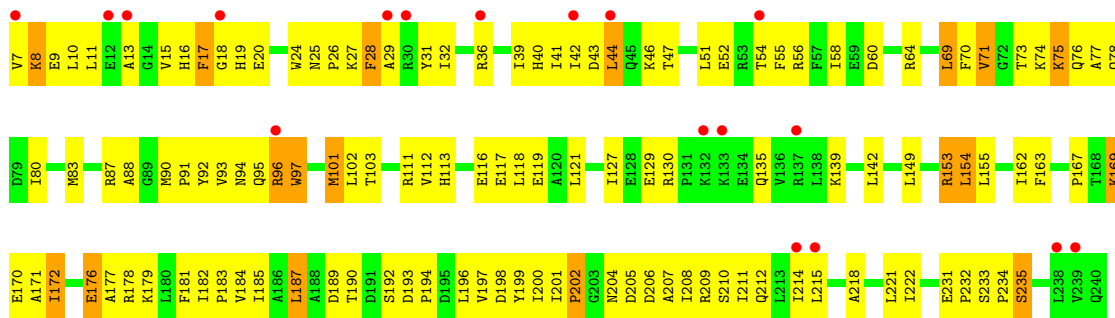
- Molecule 5: 30S ribosomal protein S2

Chain AB:



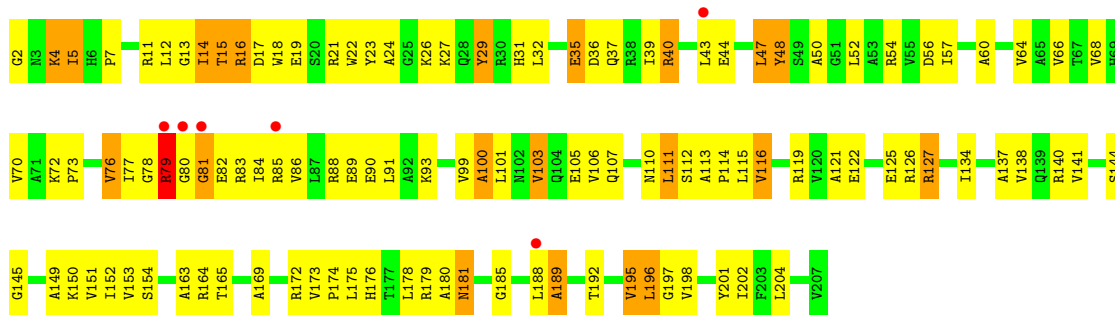
- Molecule 5: 30S ribosomal protein S2

Chain CB:



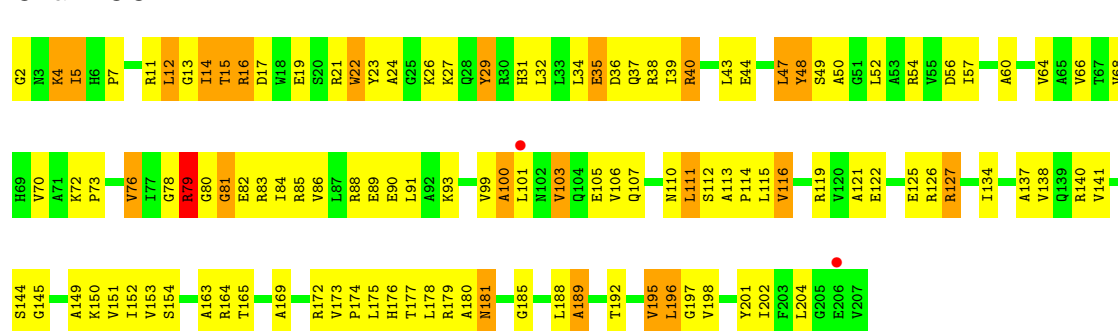
- Molecule 6: 30S ribosomal protein S3

Chain AC:



- Molecule 6: 30S ribosomal protein S3

Chain CC:



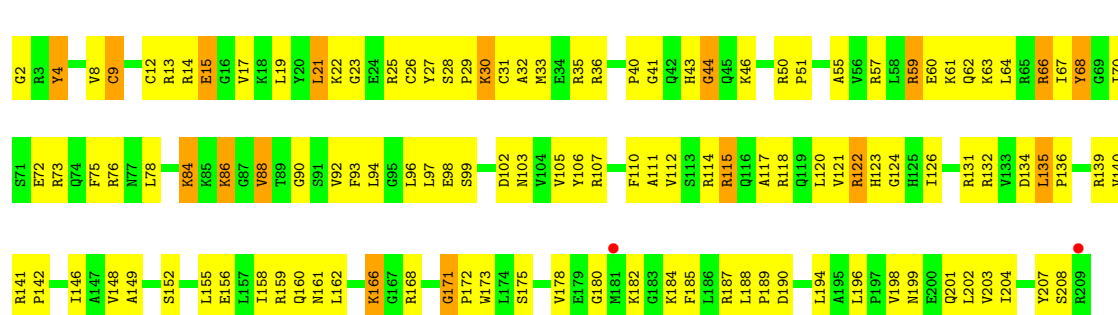
- Molecule 7: 30S ribosomal protein S4

Chain AD:



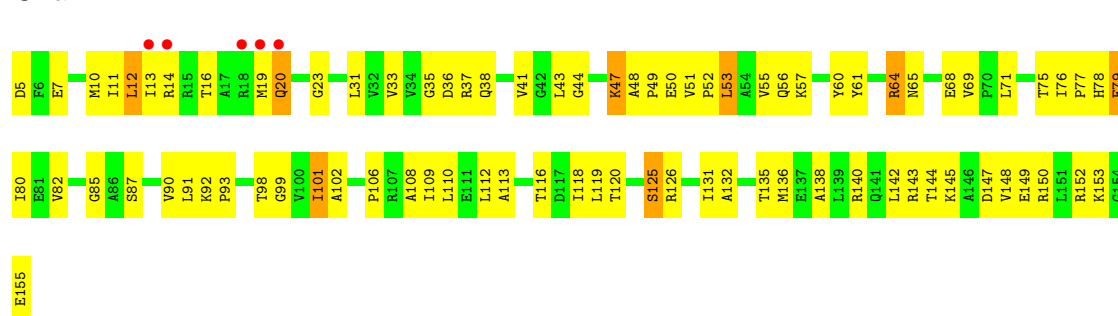
- Molecule 7: 30S ribosomal protein S4

Chain CD:



- Molecule 8: 30S ribosomal protein S5

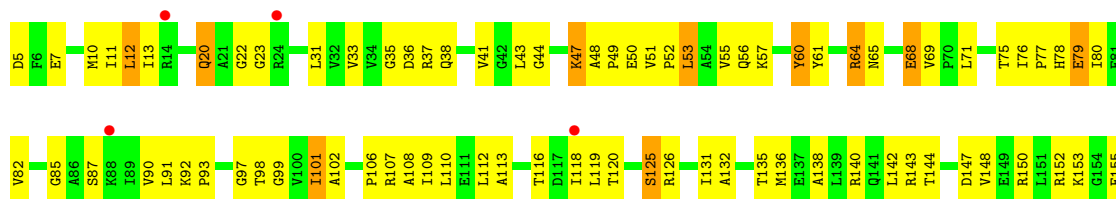
Chain AE:



- Molecule 8: 30S ribosomal protein S5

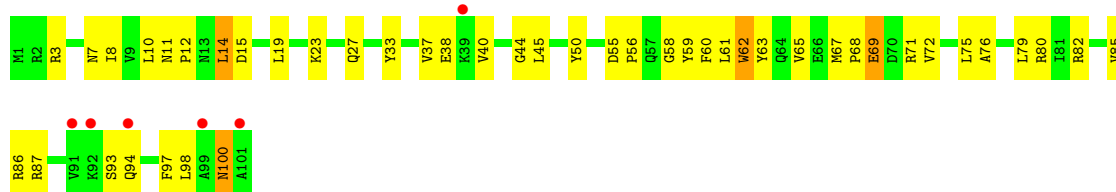
Chain CE:





• Molecule 9: 30S ribosomal protein S6

Chain AF:



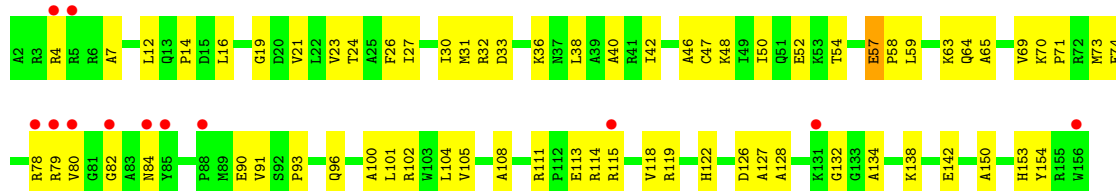
• Molecule 9: 30S ribosomal protein S6

Chain CF:



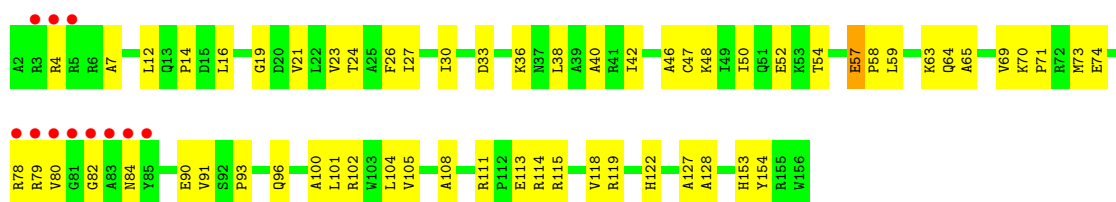
• Molecule 10: 30S ribosomal protein S7

Chain AG:



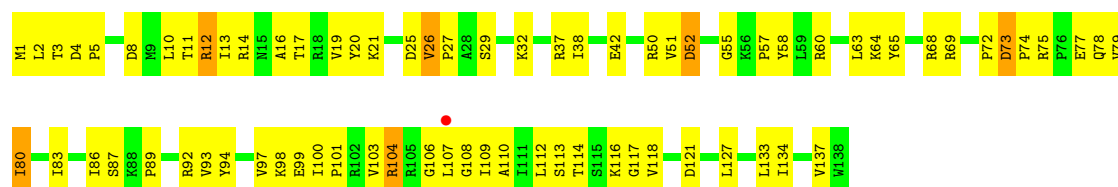
• Molecule 10: 30S ribosomal protein S7

Chain CG:



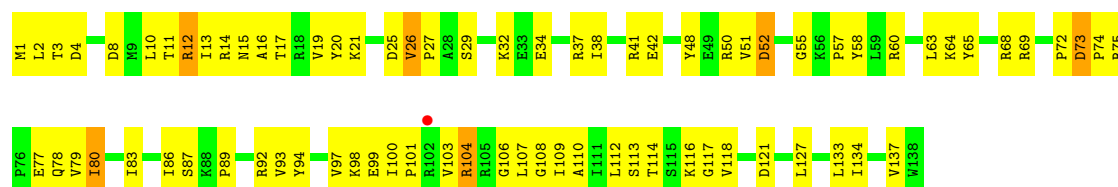
• Molecule 11: 30S ribosomal protein S8

Chain AH:



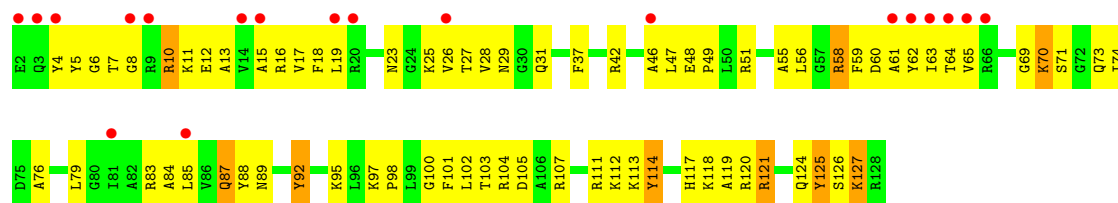
• Molecule 11: 30S ribosomal protein S8

Chain CH:



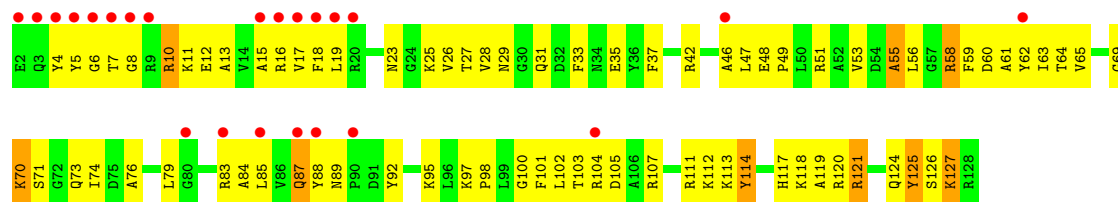
• Molecule 12: 30S ribosomal protein S9

Chain AI:



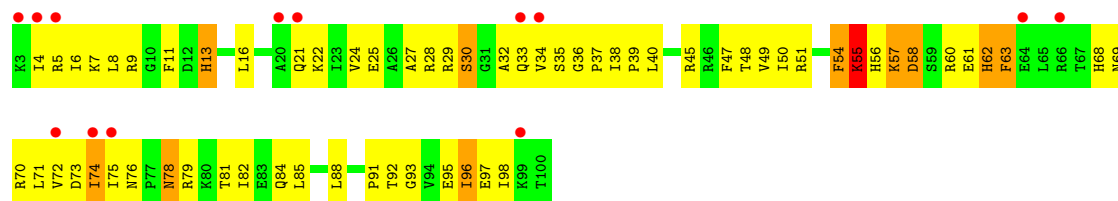
• Molecule 12: 30S ribosomal protein S9

Chain CI:



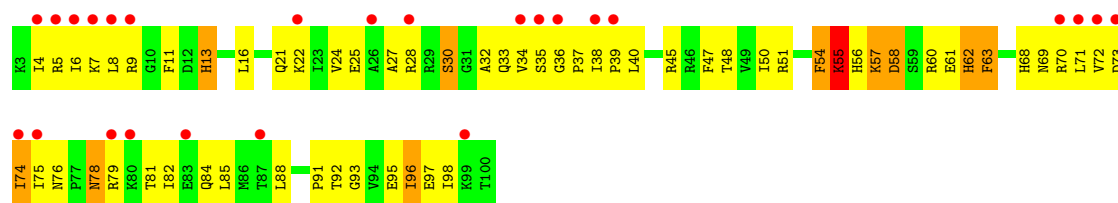
• Molecule 13: 30S ribosomal protein S10

Chain AJ:



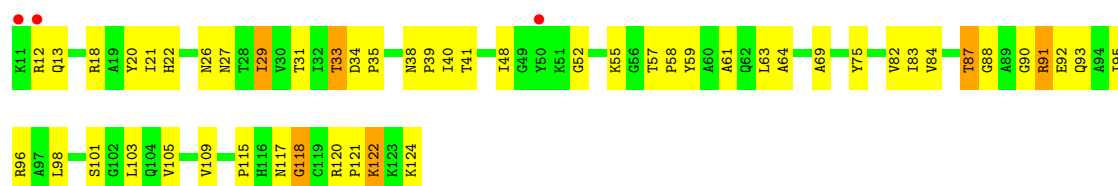
• Molecule 13: 30S ribosomal protein S10

Chain CJ:



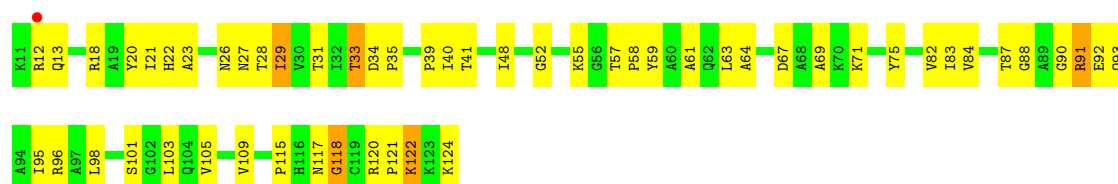
• Molecule 14: 30S ribosomal protein S11

Chain AK:



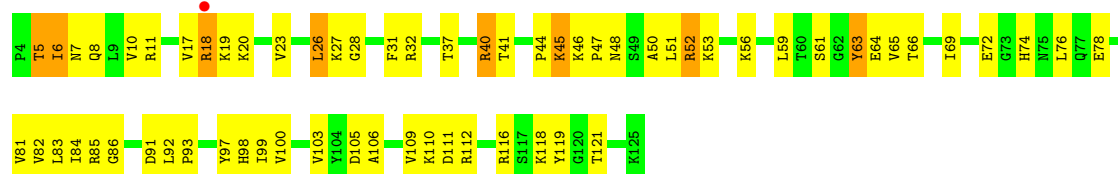
• Molecule 14: 30S ribosomal protein S11

Chain CK:



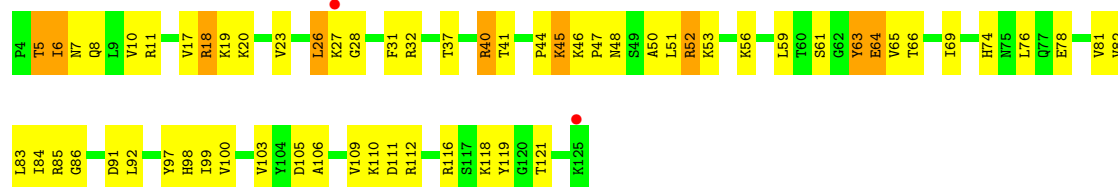
• Molecule 15: 30S ribosomal protein S12

Chain AL:



• Molecule 15: 30S ribosomal protein S12

Chain CL:



• Molecule 16: 30S ribosomal protein S13

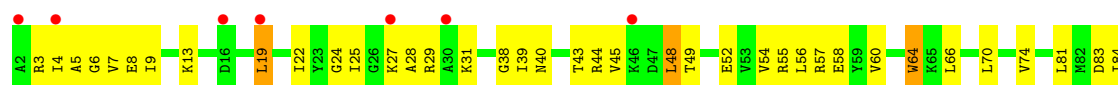
Chain AM:





- Molecule 16: 30S ribosomal protein S13

Chain CM:



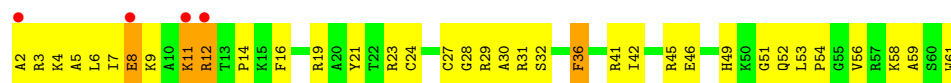
- Molecule 17: 30S ribosomal protein S14

Chain AN:



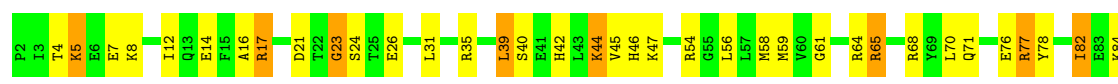
- Molecule 17: 30S ribosomal protein S14

Chain CN:



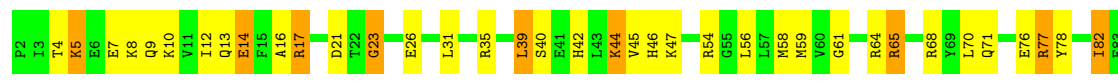
- Molecule 18: 30S ribosomal protein S15

Chain AO:



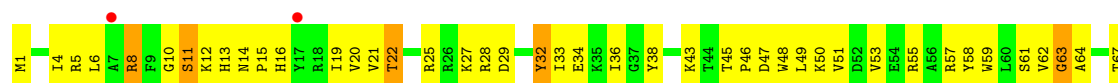
- Molecule 18: 30S ribosomal protein S15

Chain CO:



- Molecule 19: 30S ribosomal protein S16

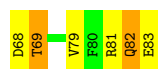
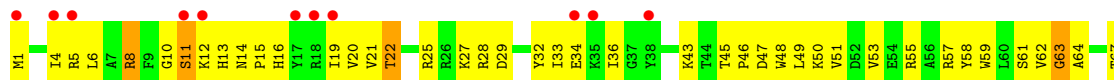
Chain AP:





- Molecule 19: 30S ribosomal protein S16

Chain CP:



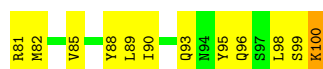
- Molecule 20: 30S ribosomal protein S17

Chain AQ:



- Molecule 20: 30S ribosomal protein S17

Chain CQ:



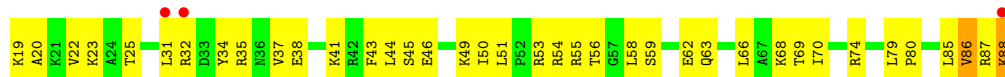
- Molecule 21: 30S ribosomal protein S18

Chain AR:



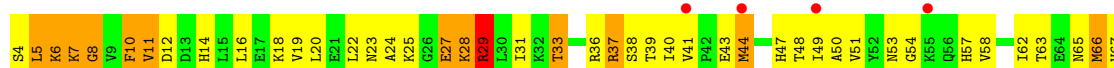
- Molecule 21: 30S ribosomal protein S18

Chain CR:



- Molecule 22: 30S ribosomal protein S19

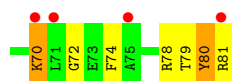
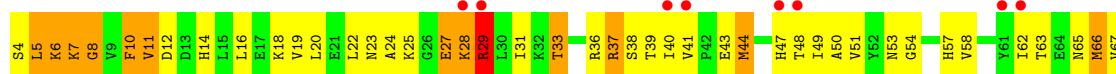
Chain AS:





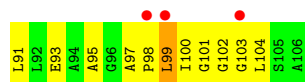
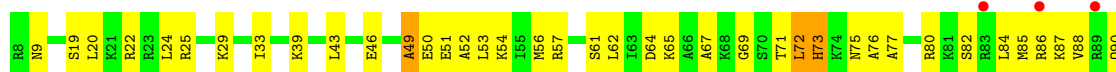
- Molecule 22: 30S ribosomal protein S19

Chain CS:



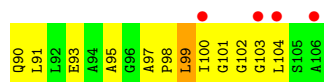
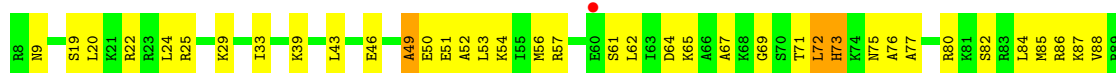
- Molecule 23: 30S ribosomal protein S20

Chain AT:



- Molecule 23: 30S ribosomal protein S20

Chain CT:



- Molecule 24: 30S ribosomal protein Thx

Chain AU:



- Molecule 24: 30S ribosomal protein Thx

Chain CU:

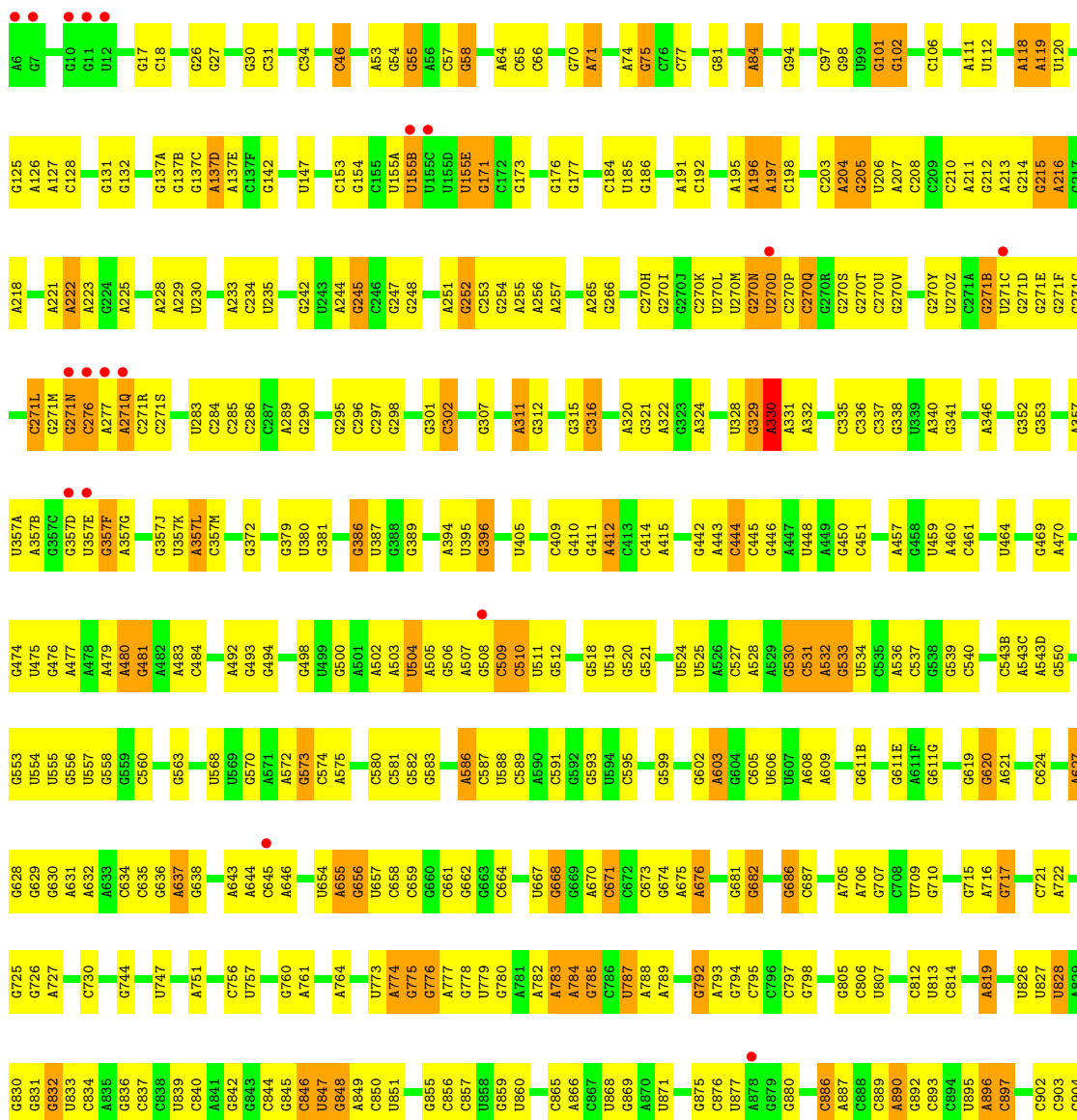


- Molecule 25: 23S ribosomal RNA

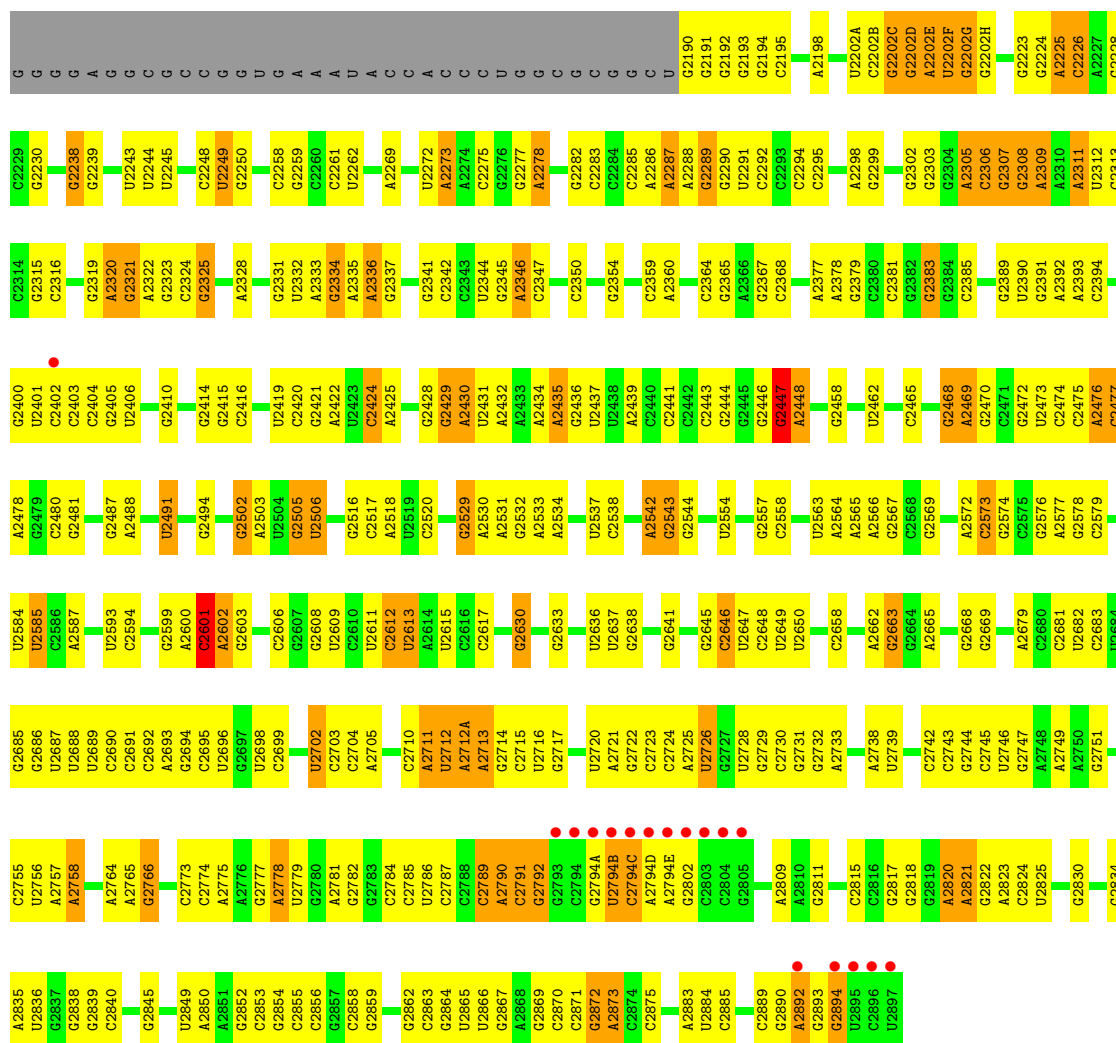
Chain BA:

G1203	A126	A1054	A980	U907	C834	G744	G629	U554	G476	U357A	G271M	A221	A127	A6
A1204	A1126	G1055	A981	C908	A835	U747	G630	U555	A477	A357B	G271N	A222	C128	G17
U1205	A1127	G956	A909	A909	C836	A631	A631	G556	A478	G357C	C276	A223	G131	C18
A1210	A1128	A1057	A983	A910	C837	A632	A632	U557	A479	G357D	A277	A224	G132	G17
U1211	A1129	G1058	A984	A911	C838	A633	A633	G558	A480	U357E	A271Q	A225	G133	G26
G1212	U1130	G985	C986	C912	C839	A634	G635	C560	G481	G357F	C271R	A226	C27	G27
		U1060	C986	U913	C840	C756	G636		A482	A357G	C271S	A228	G137A	
		U1061		C914	A841	U757	A637	G563	A483		C271T	A229	G137B	
		U1062		C915	G842		G638		A484	U357K		U230	G137C	G30
			G993	G916	G843	A761		U568		A357L		U233	A137D	C31
			A996	A917	G844	A762	A643	U569	A492	C357M		A233	G137E	C34
			G997	A918	G845		A644	G570	G493				G142	
			C998	G919	G846		A645	A571	G494					C40
			U999		U847		C645	A572					U147	C41
			A1000		G848		A646	A573	G498				U148	
			G1001		A849			G574	U499				G153	
			A1002		C950		U654	A575	G500				G154	C46
			G1003		G851		A655	A501	G501				G155	A53
			C1004		G852		U656	A502	A502				G156	G54
			U1005				U657	A503	U504				U155A	G55
			C1006				U658	A504	A505				U155B	G56
							U659	A506	G506				G172	G58
							U660	A507	A507				G173	A84
							U661	A508	G508				G174	C65
							U662	A509	U509				G175	C66
							U663	A510	C510				G176	A71
							U664	A511	U511				G177	A74
							U665	A512	G512				G178	G75
							U666	A513	C513				G179	G76
							U667	A514	C514				G180	G77
							U668	A515	A415				G181	A74
							U669	A516	U448				G182	G75
							U670	A517	U449				G183	G76
							U671	A518	U450				G184	G77
							U672	A519	U451				G185	A71
							U673	A520	U452				G186	A74
							U674	A521	U453				G187	G75
							U675	A522	U454				G188	G76
							U676	A523	U455				G189	C77
							U677	A524	U456				G190	G81
							U678	A525	U457				G191	A84
							U679	A526	U458				G192	A84
							U680	A527	U459				G193	A84
							U681	A528	U460				G194	A84
							U682	A529	U461				G195	A84
							U683	A530	U462				G196	A84
							U684	A531	U463				G197	A84
							U685	A532	U464				G198	A84
							U686	A533	U465				G199	A84
							U687	A534	U466				G200	A84
							U688	A535	U467				G201	A84
							U689	A536	U468				G202	A84
							U690	A537	U469				G203	A84
							U691	A538	U470				G204	A84
							U692	A539	U471				G205	A84
							U693	A540	U472				G206	A84
							U694	A541	U473				G207	A84
							U695	A542	U474				G208	A84
							U696	A543	U475				G209	A84
							U697	A544	U476				G210	A84
							U698	A545	U477				G211	A84
							U699	A546	U478				G212	A84
							U700	A547	U479				G213	A84
							U701	A548	U480				G214	A84
							U702	A549	U481				G215	A84
							U703	A550	U482				G216	A84
							U704	A551	U483				G217	A84
							U705	A552	U484				G218	A84
							U706	A553	U485				G219	A84
							U707	A554	U486				G220	A84
							U708	A555	U487				G221	A84
							U709	A556	U488				G222	A84
							U710	A557	U489				G223	A84
							U711	A558	U490				G224	A84
							U712	A559	U491				G225	A84
							U713	A560	U492				G226	A84
							U714	A561	U493				G227	A84
							U715	A562	U494				G228	A84
							U716	A563	U495				G229	A84
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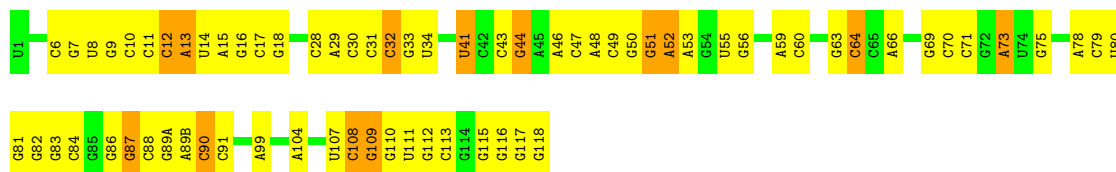


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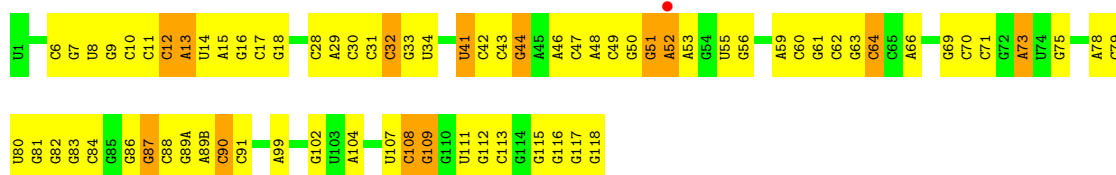
• Molecule 26: 5S ribosomal RNA

Chain BB:



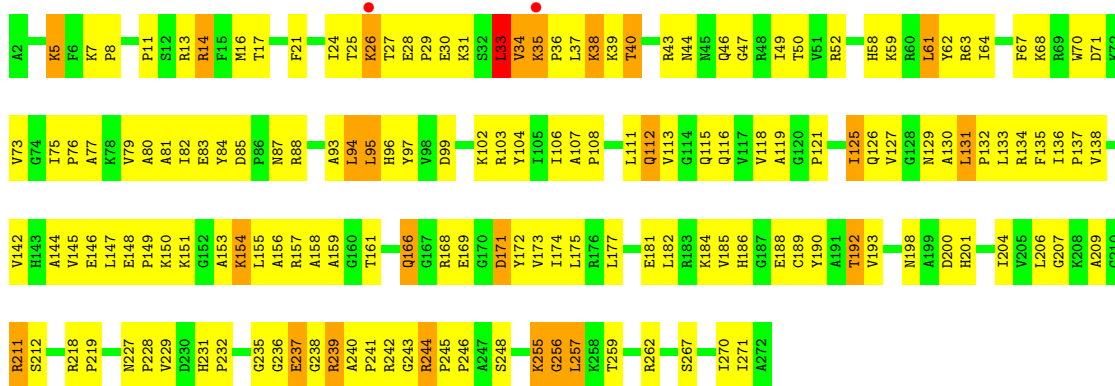
• Molecule 26: 5S ribosomal RNA

Chain DB:



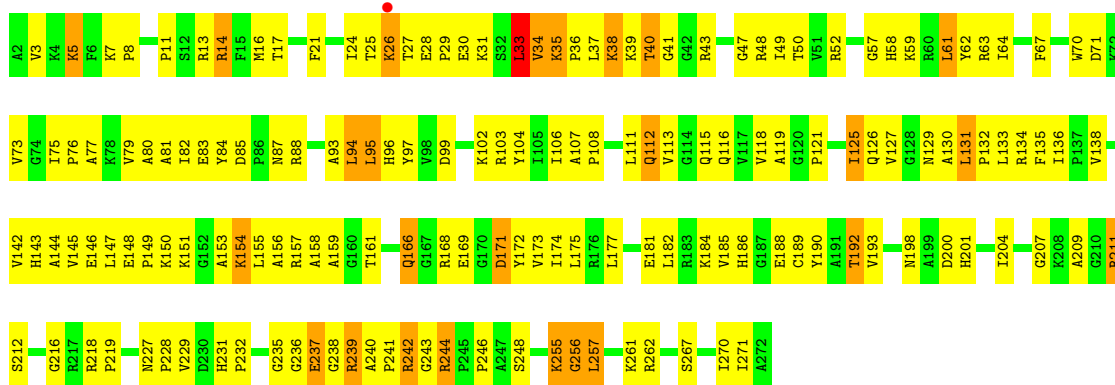
• Molecule 27: 50S ribosomal protein L2

Chain BD:



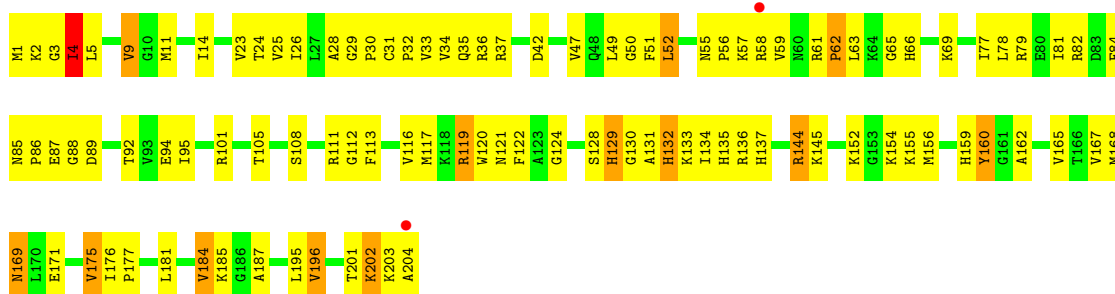
- Molecule 27: 50S ribosomal protein L2

Chain DD:



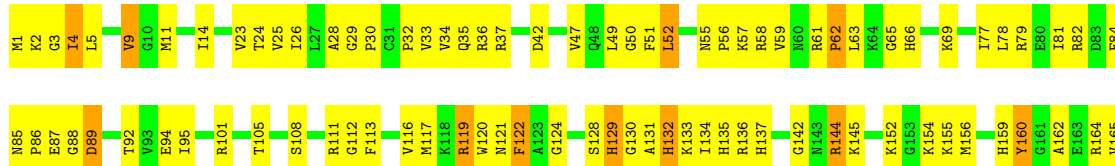
- Molecule 28: 50S ribosomal protein L3

Chain BE:



- Molecule 28: 50S ribosomal protein L3

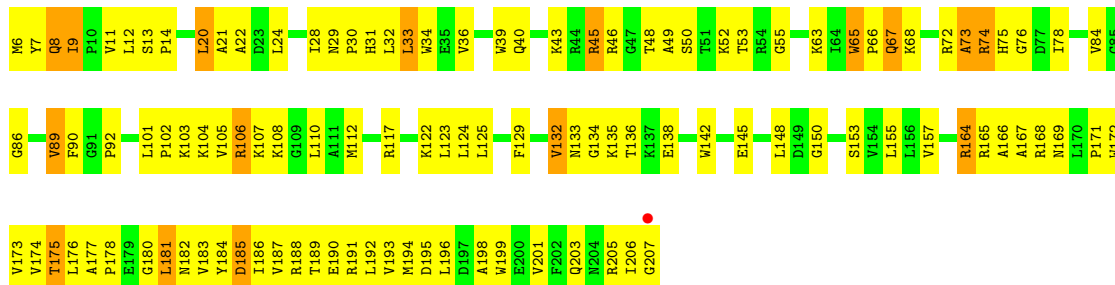
Chain DE:





- Molecule 29: 50S ribosomal protein L4

Chain BF:



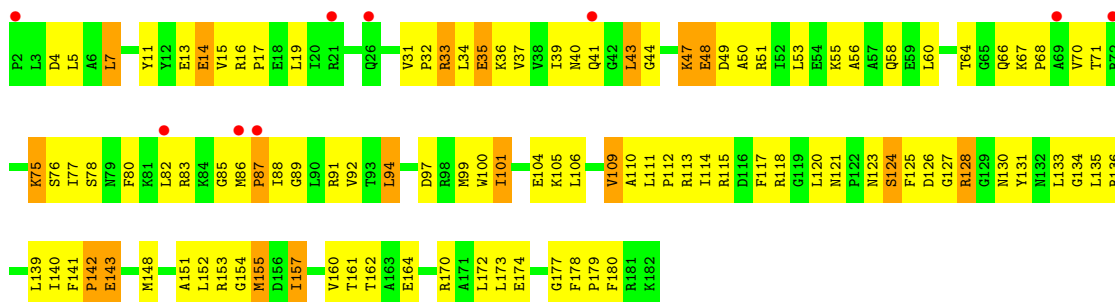
- Molecule 29: 50S ribosomal protein L4

Chain DF:



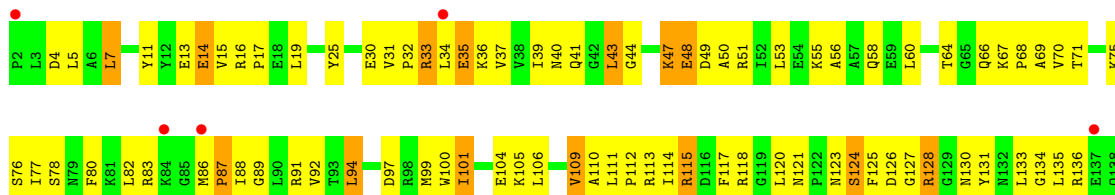
- Molecule 30: 50S ribosomal protein L5

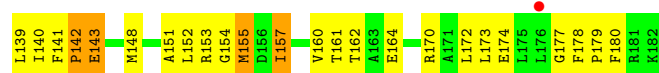
Chain BG:



- Molecule 30: 50S ribosomal protein L5

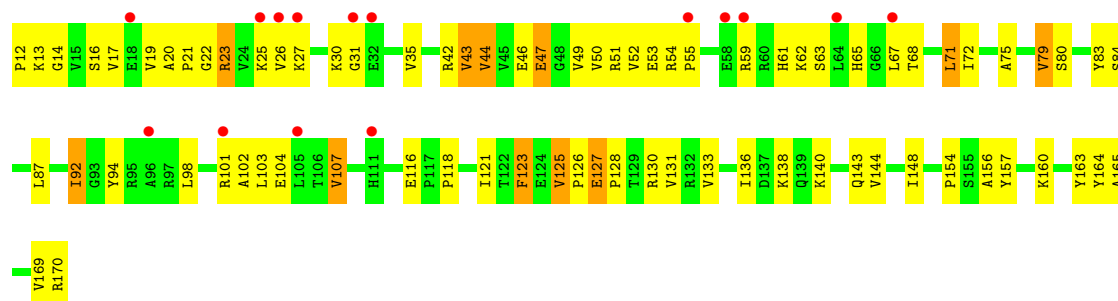
Chain DG:





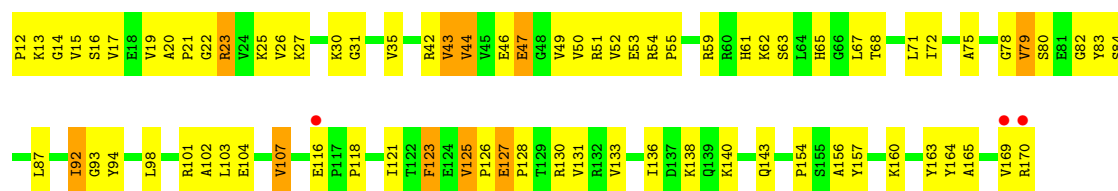
● Molecule 31: 50S ribosomal protein L6

Chain BH:



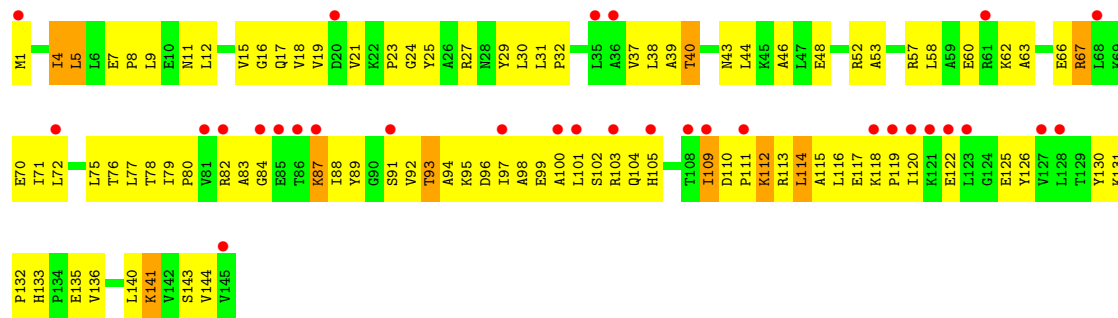
● Molecule 31: 50S ribosomal protein L6

Chain DH:



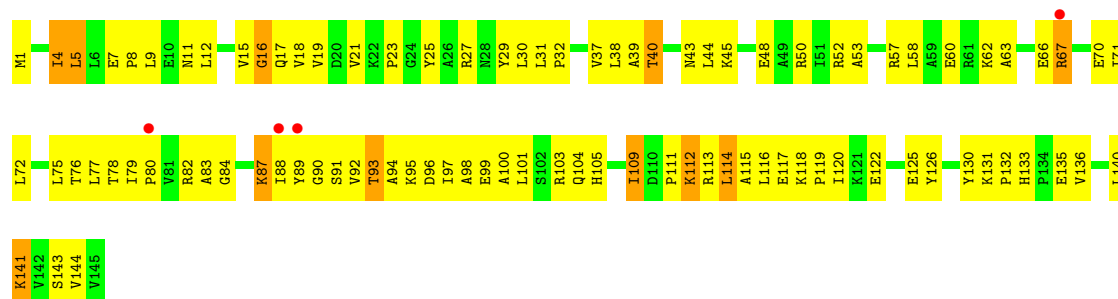
● Molecule 32: 50S ribosomal protein L9

Chain BI:



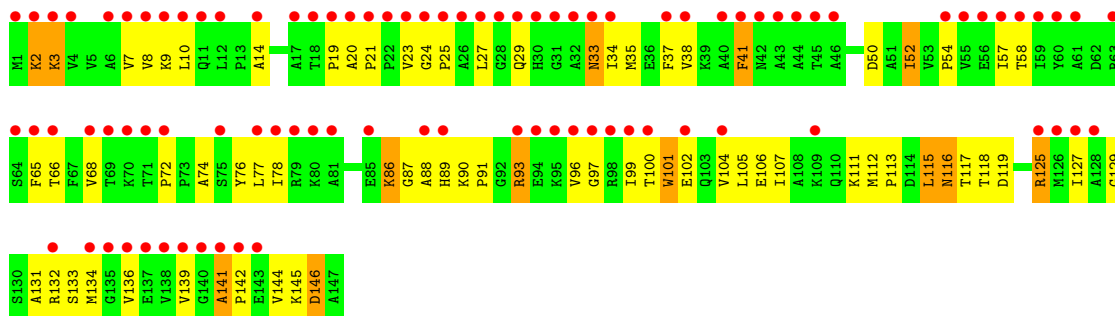
● Molecule 32: 50S ribosomal protein L9

Chain DI:



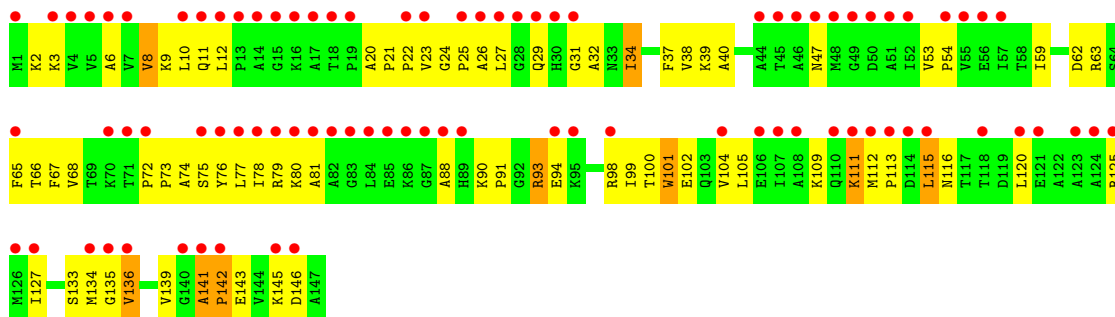
- Molecule 33: 50S ribosomal protein L11

Chain BK:



- Molecule 33: 50S ribosomal protein L11

Chain DK:



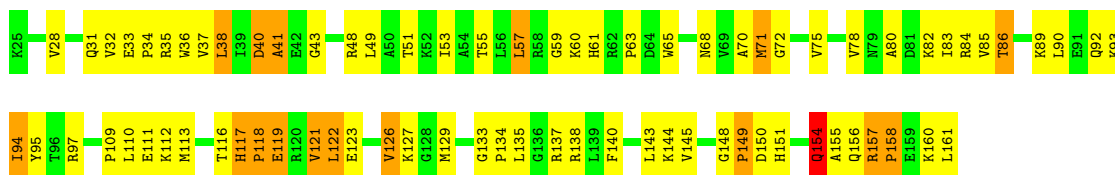
- Molecule 34: 50S ribosomal protein L13

Chain BN:



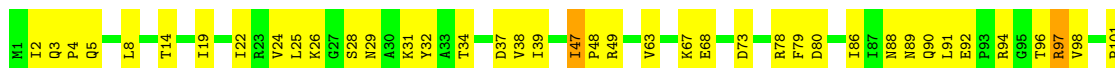
- Molecule 34: 50S ribosomal protein L13

Chain DN:



- Molecule 35: 50S ribosomal protein L14

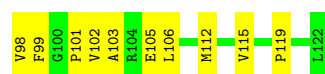
Chain BO:





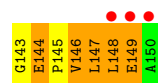
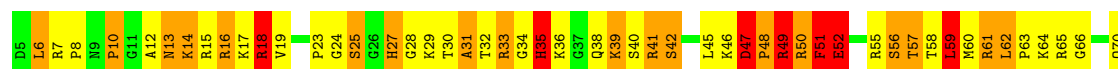
- Molecule 35: 50S ribosomal protein L14

Chain DO:



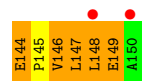
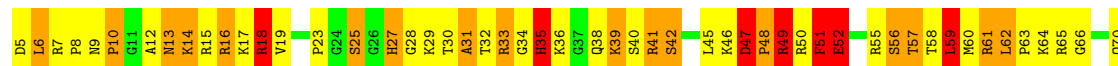
- Molecule 36: 50S ribosomal protein L15

Chain BP:



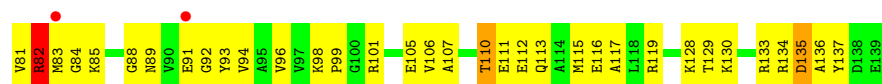
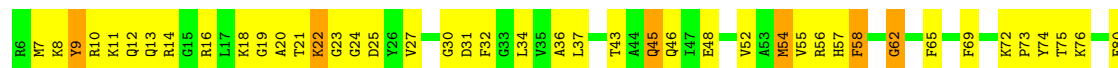
- Molecule 36: 50S ribosomal protein L15

Chain DP:



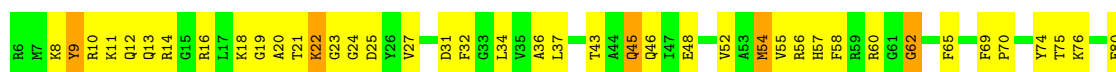
- Molecule 37: 50S ribosomal protein L16

Chain BQ:

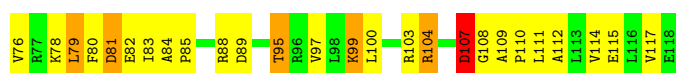


- Molecule 37: 50S ribosomal protein L16

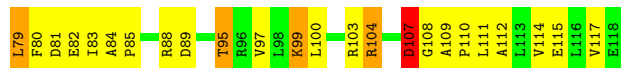
Chain DQ:



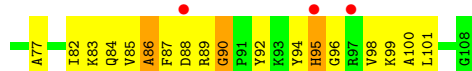
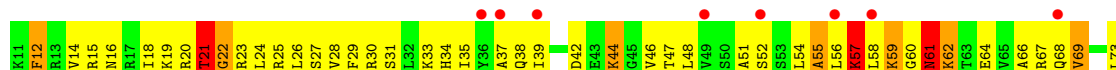
• Molecule 38: 50S ribosomal protein L17



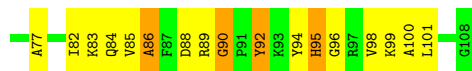
• Molecule 38: 50S ribosomal protein L17



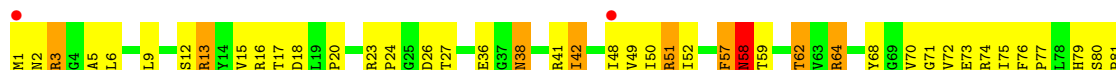
• Molecule 39: 50S ribosomal protein L18



• Molecule 39: 50S ribosomal protein L18



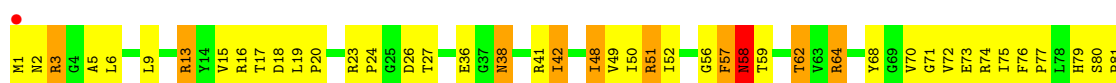
• Molecule 40: 50S ribosomal protein L19





- Molecule 40: 50S ribosomal protein L19

Chain DT:



- Molecule 41: 50S ribosomal protein L20

Chain BU:



- Molecule 41: 50S ribosomal protein L20

Chain DU:



- Molecule 42: 50S ribosomal protein L21

Chain BV:



- Molecule 42: 50S ribosomal protein L21

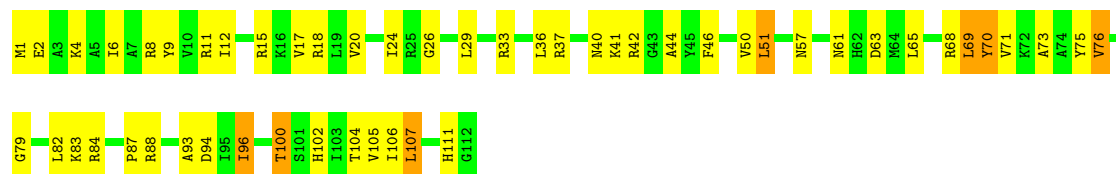
Chain DV:



- Molecule 43: 50S ribosomal protein L22

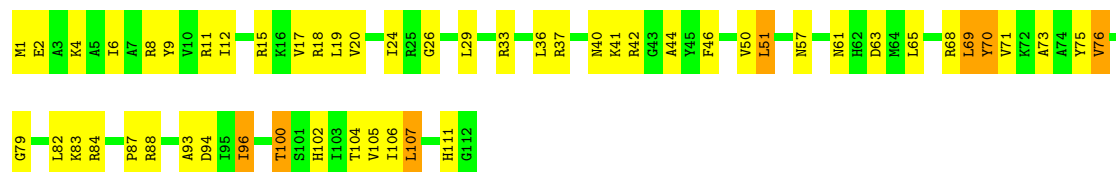


Chain BW: 



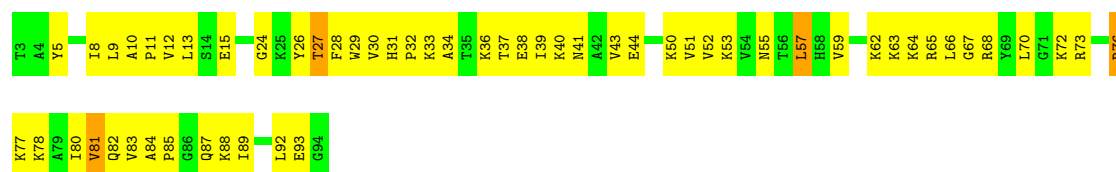
- Molecule 43: 50S ribosomal protein L22

Chain DW: 



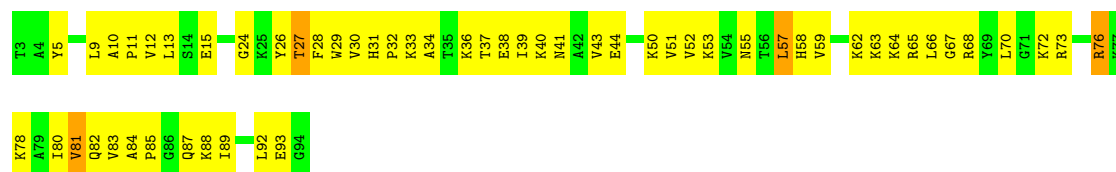
- Molecule 44: 50S ribosomal protein L23

Chain BX: 



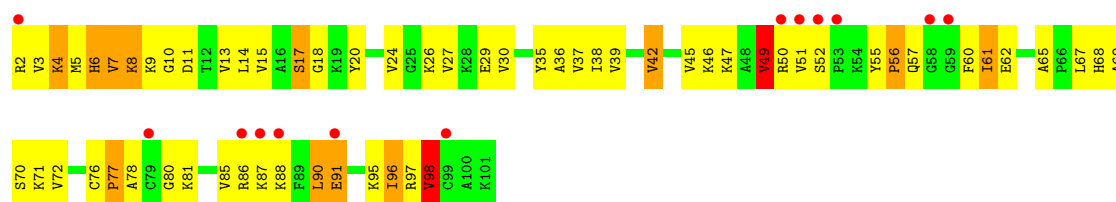
- Molecule 44: 50S ribosomal protein L23

Chain DX: 



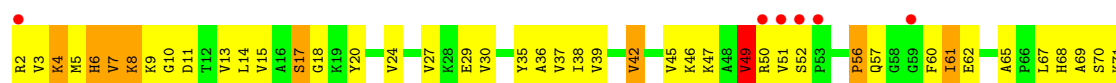
- Molecule 45: 50S ribosomal protein L24

Chain BY: 

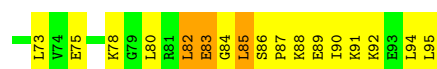


- Molecule 45: 50S ribosomal protein L24

Chain DY: 

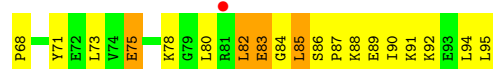
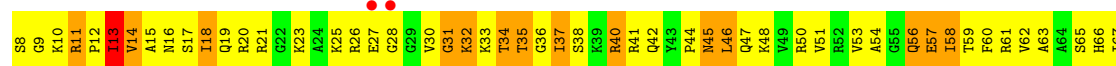






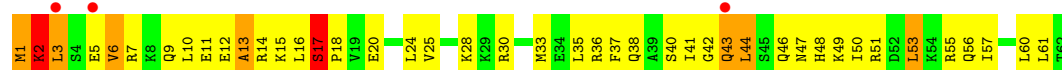
- Molecule 48: 50S ribosomal protein L28

Chain D1:



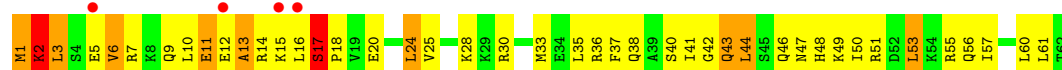
- Molecule 49: 50S ribosomal protein L29

Chain B2:



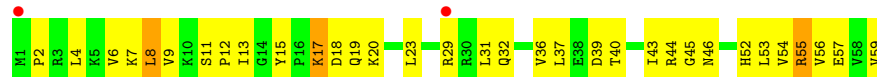
- Molecule 49: 50S ribosomal protein L29

Chain D2:



- Molecule 50: 50S ribosomal protein L30

Chain B3:



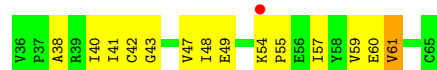
- Molecule 50: 50S ribosomal protein L30

Chain D3:



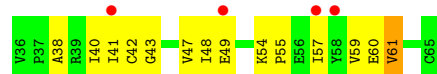
- Molecule 51: 50S ribosomal protein L31

Chain B4:



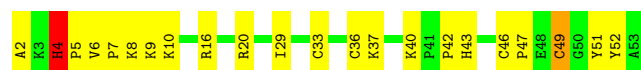
- Molecule 51: 50S ribosomal protein L31

Chain D4:



- Molecule 52: 50S ribosomal protein L32

Chain B5: 



- Molecule 52: 50S ribosomal protein L32

Chain D5: 



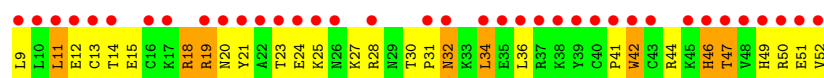
- Molecule 53: 50S ribosomal protein L33

Chain B6: 



- Molecule 53: 50S ribosomal protein L33

Chain D6: 



- Molecule 54: 50S ribosomal protein L34

Chain B7: 



- Molecule 54: 50S ribosomal protein L34

Chain D7: 



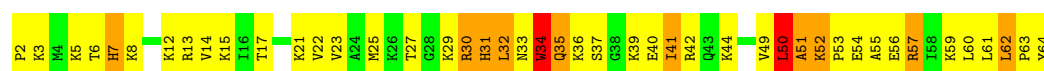
- Molecule 55: 50S ribosomal protein L35

Chain B8: 



- Molecule 55: 50S ribosomal protein L35

Chain D8: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	212.07Å 454.40Å 618.45Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.67 – 3.40 49.78 – 3.35	Depositor EDS
% Data completeness (in resolution range)	99.7 (49.67-3.40) 99.7 (49.78-3.35)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.72 (at 3.33Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.6.4_486)	Depositor
R, R_{free}	0.234 , 0.268 0.299 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å ²)	83.6	Xtriage
Anisotropy	0.218	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 61.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.26$	Xtriage
Outliers	0 of 844633 reflections	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	294074	wwPDB-VP
Average B, all atoms (Å ²)	109.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.50% 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	0.27	2/36194 (0.0%)	0.55	0/56493
1	CA	0.27	2/36194 (0.0%)	0.54	0/56493
2	AV	0.26	0/241	0.53	0/374
2	CV	0.23	0/241	0.54	0/374
3	AW	0.25	0/1832	0.52	0/2855
3	CW	0.26	0/1832	0.53	0/2855
4	AY	0.21	0/2925	0.39	0/3953
4	CY	0.21	0/2925	0.39	0/3953
5	AB	0.22	0/1936	0.40	0/2609
5	CB	0.22	0/1936	0.39	0/2609
6	AC	0.22	0/1637	0.39	0/2205
6	CC	0.22	0/1637	0.39	0/2205
7	AD	0.25	0/1733	0.44	0/2318
7	CD	0.24	0/1733	0.41	0/2318
8	AE	0.24	0/1172	0.44	0/1576
8	CE	0.24	0/1172	0.43	0/1576
9	AF	0.23	0/856	0.42	0/1154
9	CF	0.24	0/856	0.43	0/1154
10	AG	0.22	0/1276	0.37	0/1709
10	CG	0.22	0/1276	0.37	0/1709
11	AH	0.23	0/1136	0.44	0/1527
11	CH	0.22	0/1136	0.43	0/1527
12	AI	0.23	0/1029	0.40	0/1378
12	CI	0.22	0/1029	0.40	0/1378
13	AJ	0.21	0/808	0.41	0/1085
13	CJ	0.21	0/808	0.41	0/1085
14	AK	0.24	0/857	0.43	0/1157
14	CK	0.24	0/857	0.43	0/1157
15	AL	0.27	0/973	0.47	0/1301
15	CL	0.26	0/973	0.47	0/1301
16	AM	0.20	0/944	0.40	0/1265
16	CM	0.20	0/944	0.40	0/1265

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	AN	0.24	0/501	0.41	0/664
17	CN	0.25	0/501	0.39	0/664
18	AO	0.24	0/745	0.39	0/992
18	CO	0.24	0/745	0.39	0/992
19	AP	0.24	0/717	0.43	0/963
19	CP	0.22	0/717	0.43	0/963
20	AQ	0.25	0/837	0.41	0/1117
20	CQ	0.23	0/837	0.41	0/1117
21	AR	0.24	0/579	0.43	0/768
21	CR	0.24	0/579	0.43	0/768
22	AS	0.21	0/643	0.40	0/865
22	CS	0.22	0/643	0.40	0/865
23	AT	0.23	0/764	0.39	0/1006
23	CT	0.22	0/764	0.39	0/1006
24	AU	0.21	0/213	0.40	0/277
24	CU	0.21	0/213	0.41	0/277
25	BA	0.38	6/67268 (0.0%)	0.67	12/105011 (0.0%)
25	DA	0.42	6/67268 (0.0%)	0.70	21/105011 (0.0%)
26	BB	0.25	0/2853	0.55	0/4451
26	DB	0.26	0/2853	0.56	0/4451
27	BD	0.33	0/2155	0.53	0/2905
27	DD	0.35	0/2155	0.53	1/2905 (0.0%)
28	BE	0.28	0/1597	0.49	0/2153
28	DE	0.29	0/1597	0.49	0/2153
29	BF	0.29	0/1622	0.48	0/2194
29	DF	0.31	0/1622	0.48	0/2194
30	BG	0.23	0/1500	0.42	0/2017
30	DG	0.23	0/1500	0.43	0/2017
31	BH	0.22	0/1246	0.44	0/1682
31	DH	0.24	0/1246	0.45	0/1682
32	BI	0.22	0/1148	0.42	0/1552
32	DI	0.23	0/1148	0.43	0/1552
33	BK	0.21	0/1108	0.40	0/1500
33	DK	0.20	0/1108	0.39	0/1500
34	BN	0.27	0/1124	0.46	0/1515
34	DN	0.29	0/1124	0.47	0/1515
35	BO	0.28	0/942	0.47	0/1268
35	DO	0.30	0/942	0.48	0/1268
36	BP	0.34	0/1131	0.62	1/1504 (0.1%)
36	DP	0.36	0/1131	0.63	1/1504 (0.1%)
37	BQ	0.30	0/1085	0.52	0/1449
37	DQ	0.31	0/1085	0.52	0/1449
38	BR	0.28	0/974	0.48	0/1302

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
38	DR	0.29	0/974	0.49	0/1302
39	BS	0.24	0/779	0.44	0/1036
39	DS	0.25	0/779	0.44	0/1036
40	BT	0.27	0/1158	0.47	0/1544
40	DT	0.28	0/1158	0.48	0/1544
41	BU	0.31	0/982	0.47	0/1306
41	DU	0.32	0/982	0.46	0/1306
42	BV	0.28	0/790	0.49	0/1057
42	DV	0.29	0/790	0.49	0/1057
43	BW	0.30	0/902	0.47	0/1209
43	DW	0.29	0/902	0.47	0/1209
44	BX	0.30	0/740	0.46	0/993
44	DX	0.33	0/740	0.48	0/993
45	BY	0.28	0/789	0.49	0/1051
45	DY	0.30	0/789	0.49	0/1051
46	BZ	0.22	0/1515	0.42	0/2056
46	DZ	0.23	0/1515	0.42	0/2056
47	B0	0.27	0/613	0.53	0/816
47	D0	0.29	0/613	0.52	0/816
48	B1	0.34	0/702	0.59	1/932 (0.1%)
48	D1	0.36	0/702	0.61	1/932 (0.1%)
49	B2	0.27	0/523	0.50	0/690
49	D2	0.32	0/523	0.53	0/690
50	B3	0.25	0/473	0.43	0/634
50	D3	0.27	0/473	0.43	0/634
51	B4	0.24	0/229	0.40	0/309
51	D4	0.23	0/229	0.42	0/309
52	B5	0.27	0/419	0.51	0/567
52	D5	0.29	0/419	0.50	0/567
53	B6	0.21	0/388	0.41	0/518
53	D6	0.21	0/388	0.42	0/518
54	B7	0.34	0/427	0.54	0/561
54	D7	0.38	0/427	0.56	0/561
55	B8	0.32	0/516	0.49	0/679
55	D8	0.35	0/516	0.50	0/679
All	All	0.33	16/316492 (0.0%)	0.59	38/472144 (0.0%)

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
36	BP	0	1
36	DP	0	1
38	BR	0	1
38	DR	0	1
48	B1	0	1
48	D1	0	1
52	B5	0	1
All	All	0	7

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	BA	1913	A	P-OP1	-9.19	1.33	1.49
1	AA	1493	A	P-OP2	-9.00	1.33	1.49
25	BA	1912	A	P-OP2	-9.00	1.33	1.49
25	DA	1912	A	P-OP1	-8.94	1.33	1.49
1	CA	1493	A	P-OP1	-8.80	1.33	1.49

The worst 5 of 38 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	BA	2061	G	N1-C6-O6	8.50	125.00	119.90
25	DA	2447	G	N1-C6-O6	6.34	123.71	119.90
25	DA	2061	G	N1-C6-O6	6.02	123.51	119.90
25	DA	1899	G	C2-N3-C4	-6.02	108.89	111.90
25	DA	2447	G	C6-C5-N7	-5.97	126.82	130.40

There are no chirality outliers.

5 of 7 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
48	B1	26	ARG	Peptide
52	B5	4	HIS	Peptide
36	BP	51	PHE	Peptide
38	BR	10	LEU	Peptide
36	DP	51	PHE	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	32332	0	16318	783	0
1	CA	32332	0	16318	798	0
2	AV	214	0	110	7	0
2	CV	214	0	110	8	0
3	AW	1640	0	837	26	0
3	CW	1640	0	837	24	0
4	AY	2874	0	2866	173	0
4	CY	2874	0	2866	164	0
5	AB	1901	0	1951	118	0
5	CB	1901	0	1951	119	0
6	AC	1613	0	1677	100	0
6	CC	1613	0	1677	101	0
7	AD	1703	0	1764	102	0
7	CD	1703	0	1765	121	0
8	AE	1156	0	1213	80	0
8	CE	1156	0	1213	80	0
9	AF	843	0	857	36	0
9	CF	843	0	857	36	0
10	AG	1257	0	1296	46	0
10	CG	1257	0	1296	42	0
11	AH	1116	0	1177	72	0
11	CH	1116	0	1177	77	0
12	AI	1011	0	1043	69	0
12	CI	1011	0	1043	70	0
13	AJ	795	0	840	74	0
13	CJ	795	0	840	72	0
14	AK	843	0	859	39	0
14	CK	843	0	859	40	0
15	AL	957	0	1046	73	0
15	CL	957	0	1046	71	0
16	AM	934	0	992	50	0
16	CM	934	0	992	55	0
17	AN	492	0	530	47	0
17	CN	492	0	530	39	0
18	AO	734	0	771	34	0
18	CO	734	0	771	34	0
19	AP	701	0	720	51	0
19	CP	701	0	720	49	0
20	AQ	824	0	893	38	0
20	CQ	824	0	893	40	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
21	AR	574	0	644	37	0
21	CR	574	0	644	39	0
22	AS	630	0	652	55	0
22	CS	630	0	652	56	0
23	AT	762	0	859	38	0
23	CT	762	0	859	40	0
24	AU	209	0	221	16	0
24	CU	209	0	221	17	0
25	BA	60059	0	30274	1273	0
25	DA	60059	0	30274	1280	0
26	BB	2551	0	1295	81	0
26	DB	2551	0	1295	83	0
27	BD	2105	0	2182	176	0
27	DD	2105	0	2182	179	0
28	BE	1564	0	1629	122	0
28	DE	1564	0	1629	123	0
29	BF	1587	0	1632	100	0
29	DF	1587	0	1632	108	0
30	BG	1475	0	1537	110	0
30	DG	1475	0	1537	114	0
31	BH	1223	0	1282	76	0
31	DH	1223	0	1282	77	0
32	BI	1133	0	1220	100	0
32	DI	1133	0	1220	110	0
33	BK	1088	0	1138	58	0
33	DK	1088	0	1138	61	0
34	BN	1097	0	1168	80	0
34	DN	1097	0	1168	74	0
35	BO	932	0	994	45	0
35	DO	932	0	994	46	0
36	BP	1114	0	1187	184	0
36	DP	1114	0	1187	194	0
37	BQ	1065	0	1114	82	0
37	DQ	1065	0	1114	83	0
38	BR	960	0	1021	84	0
38	DR	960	0	1021	77	0
39	BS	771	0	832	60	0
39	DS	771	0	832	60	0
40	BT	1144	0	1211	76	0
40	DT	1144	0	1211	74	0
41	BU	964	0	1022	83	0
41	DU	964	0	1022	78	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
42	BV	779	0	852	83	0
42	DV	779	0	852	79	0
43	BW	891	0	951	58	0
43	DW	891	0	951	61	0
44	BX	726	0	778	64	0
44	DX	726	0	778	65	0
45	BY	776	0	870	80	0
45	DY	776	0	870	81	0
46	BZ	1483	0	1507	89	0
46	DZ	1483	0	1507	89	0
47	B0	605	0	628	36	0
47	D0	605	0	628	32	0
48	B1	695	0	764	67	0
48	D1	695	0	764	77	0
49	B2	521	0	575	52	0
49	D2	521	0	575	56	0
50	B3	468	0	523	27	0
50	D3	468	0	523	24	0
51	B4	226	0	227	13	0
51	D4	226	0	225	15	0
52	B5	405	0	420	27	0
52	D5	405	0	420	31	0
53	B6	381	0	391	28	0
53	D6	381	0	391	26	0
54	B7	419	0	467	22	0
54	D7	419	0	467	22	0
55	B8	508	0	576	58	0
55	D8	508	0	576	60	0
56	AA	393	0	0	0	0
56	AC	1	0	0	0	0
56	AG	1	0	0	0	0
56	AO	1	0	0	0	0
56	AQ	1	0	0	0	0
56	AT	3	0	0	0	0
56	AV	1	0	0	0	0
56	AW	18	0	0	0	0
56	AY	3	0	0	0	0
56	B0	2	0	0	0	0
56	B1	1	0	0	0	0
56	B3	1	0	0	0	0
56	B5	1	0	0	0	0
56	B8	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
56	BA	824	0	0	0	0
56	BB	23	0	0	0	0
56	BD	1	0	0	0	0
56	BE	1	0	0	0	0
56	BF	1	0	0	0	0
56	BP	1	0	0	0	0
56	BT	1	0	0	0	0
56	BX	2	0	0	0	0
56	BY	1	0	0	0	0
56	CA	326	0	0	0	0
56	CD	1	0	0	0	0
56	CM	1	0	0	0	0
56	CR	1	0	0	0	0
56	CV	2	0	0	0	0
56	CW	16	0	0	0	0
56	CY	2	0	0	0	0
56	D0	1	0	0	0	0
56	D1	1	0	0	0	0
56	D5	3	0	0	0	0
56	D7	2	0	0	0	0
56	DA	732	0	0	0	0
56	DB	20	0	0	0	0
56	DD	1	0	0	0	0
56	DE	1	0	0	0	0
56	DF	2	0	0	0	0
56	DH	1	0	0	0	0
56	DI	2	0	0	0	0
56	DN	1	0	0	0	0
56	DP	2	0	0	0	0
56	DQ	4	0	0	0	0
56	DV	1	0	0	0	0
56	DW	2	0	0	0	0
56	DX	1	0	0	0	0
57	AD	1	0	0	0	0
57	AN	1	0	0	0	0
57	CD	1	0	0	0	0
57	CN	1	0	0	0	0
All	All	294074	0	200805	10187	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 21.

The worst 5 of 10187 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:CA:559:A:H4'	1:CA:560:U:H3'	1.26	1.16
25:BA:1899:G:N2	25:BA:1902:C:H41	1.43	1.15
45:DY:76:CYS:SG	45:DY:77:PRO:HD2	1.91	1.11
25:DA:1899:G:N2	25:DA:1902:C:H41	1.48	1.10
1:AA:559:A:H4'	1:AA:560:U:H3'	1.26	1.09

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	
4	AY	360/362 (99%)	301 (84%)	41 (11%)	18 (5%)	3	34
4	CY	360/362 (99%)	301 (84%)	42 (12%)	17 (5%)	4	36
5	AB	232/234 (99%)	185 (80%)	37 (16%)	10 (4%)	4	40
5	CB	232/234 (99%)	184 (79%)	38 (16%)	10 (4%)	4	40
6	AC	204/206 (99%)	144 (71%)	40 (20%)	20 (10%)	1	13
6	CC	204/206 (99%)	145 (71%)	38 (19%)	21 (10%)	1	11
7	AD	206/208 (99%)	165 (80%)	32 (16%)	9 (4%)	4	39
7	CD	206/208 (99%)	166 (81%)	29 (14%)	11 (5%)	3	32
8	AE	149/151 (99%)	113 (76%)	32 (22%)	4 (3%)	8	55
8	CE	149/151 (99%)	116 (78%)	29 (20%)	4 (3%)	8	55
9	AF	99/101 (98%)	82 (83%)	16 (16%)	1 (1%)	22	78
9	CF	99/101 (98%)	82 (83%)	16 (16%)	1 (1%)	22	78
10	AG	153/155 (99%)	136 (89%)	13 (8%)	4 (3%)	8	56
10	CG	153/155 (99%)	136 (89%)	13 (8%)	4 (3%)	8	56
11	AH	136/138 (99%)	111 (82%)	23 (17%)	2 (2%)	15	68
11	CH	136/138 (99%)	113 (83%)	21 (15%)	2 (2%)	15	68
12	AI	125/127 (98%)	90 (72%)	27 (22%)	8 (6%)	2	26

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
12	CI	125/127 (98%)	90 (72%)	27 (22%)	8 (6%)	2	26
13	AJ	96/98 (98%)	72 (75%)	18 (19%)	6 (6%)	2	27
13	CJ	96/98 (98%)	72 (75%)	18 (19%)	6 (6%)	2	27
14	AK	112/114 (98%)	93 (83%)	14 (12%)	5 (4%)	4	38
14	CK	112/114 (98%)	93 (83%)	15 (13%)	4 (4%)	5	47
15	AL	120/122 (98%)	94 (78%)	21 (18%)	5 (4%)	4	41
15	CL	120/122 (98%)	93 (78%)	22 (18%)	5 (4%)	4	41
16	AM	115/117 (98%)	97 (84%)	15 (13%)	3 (3%)	8	56
16	CM	115/117 (98%)	97 (84%)	15 (13%)	3 (3%)	8	56
17	AN	58/60 (97%)	47 (81%)	9 (16%)	2 (3%)	6	49
17	CN	58/60 (97%)	43 (74%)	11 (19%)	4 (7%)	2	24
18	AO	86/88 (98%)	75 (87%)	8 (9%)	3 (4%)	6	48
18	CO	86/88 (98%)	75 (87%)	8 (9%)	3 (4%)	6	48
19	AP	81/83 (98%)	62 (76%)	16 (20%)	3 (4%)	5	46
19	CP	81/83 (98%)	61 (75%)	17 (21%)	3 (4%)	5	46
20	AQ	97/99 (98%)	82 (84%)	11 (11%)	4 (4%)	4	42
20	CQ	97/99 (98%)	83 (86%)	10 (10%)	4 (4%)	4	42
21	AR	68/70 (97%)	49 (72%)	17 (25%)	2 (3%)	7	54
21	CR	68/70 (97%)	50 (74%)	16 (24%)	2 (3%)	7	54
22	AS	76/78 (97%)	53 (70%)	15 (20%)	8 (10%)	1	11
22	CS	76/78 (97%)	53 (70%)	15 (20%)	8 (10%)	1	11
23	AT	97/99 (98%)	75 (77%)	14 (14%)	8 (8%)	1	19
23	CT	97/99 (98%)	75 (77%)	14 (14%)	8 (8%)	1	19
24	AU	22/24 (92%)	13 (59%)	7 (32%)	2 (9%)	1	15
24	CU	22/24 (92%)	13 (59%)	7 (32%)	2 (9%)	1	15
27	BD	269/271 (99%)	227 (84%)	29 (11%)	13 (5%)	4	36
27	DD	269/271 (99%)	227 (84%)	29 (11%)	13 (5%)	4	36
28	BE	202/204 (99%)	167 (83%)	26 (13%)	9 (4%)	4	38
28	DE	202/204 (99%)	165 (82%)	27 (13%)	10 (5%)	3	34
29	BF	200/202 (99%)	172 (86%)	21 (10%)	7 (4%)	6	48
29	DF	200/202 (99%)	171 (86%)	24 (12%)	5 (2%)	9	57

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
30	BG	179/181 (99%)	141 (79%)	28 (16%)	10 (6%)	3	30
30	DG	179/181 (99%)	141 (79%)	28 (16%)	10 (6%)	3	30
31	BH	157/159 (99%)	130 (83%)	19 (12%)	8 (5%)	3	33
31	DH	157/159 (99%)	131 (83%)	18 (12%)	8 (5%)	3	33
32	BI	143/145 (99%)	113 (79%)	25 (18%)	5 (4%)	6	48
32	DI	143/145 (99%)	115 (80%)	23 (16%)	5 (4%)	6	48
33	BK	145/147 (99%)	99 (68%)	41 (28%)	5 (3%)	6	49
33	DK	145/147 (99%)	103 (71%)	31 (21%)	11 (8%)	2	21
34	BN	135/137 (98%)	96 (71%)	29 (22%)	10 (7%)	2	22
34	DN	135/137 (98%)	96 (71%)	29 (22%)	10 (7%)	2	22
35	BO	120/122 (98%)	103 (86%)	14 (12%)	3 (2%)	9	57
35	DO	120/122 (98%)	103 (86%)	14 (12%)	3 (2%)	9	57
36	BP	144/146 (99%)	91 (63%)	32 (22%)	21 (15%)	0	5
36	DP	144/146 (99%)	93 (65%)	31 (22%)	20 (14%)	0	6
37	BQ	132/134 (98%)	104 (79%)	22 (17%)	6 (4%)	4	38
37	DQ	132/134 (98%)	105 (80%)	22 (17%)	5 (4%)	5	45
38	BR	115/117 (98%)	96 (84%)	17 (15%)	2 (2%)	14	66
38	DR	115/117 (98%)	97 (84%)	16 (14%)	2 (2%)	14	66
39	BS	96/98 (98%)	62 (65%)	20 (21%)	14 (15%)	0	5
39	DS	96/98 (98%)	60 (62%)	22 (23%)	14 (15%)	0	5
40	BT	135/137 (98%)	100 (74%)	24 (18%)	11 (8%)	1	19
40	DT	135/137 (98%)	101 (75%)	23 (17%)	11 (8%)	1	19
41	BU	115/117 (98%)	99 (86%)	13 (11%)	3 (3%)	8	56
41	DU	115/117 (98%)	101 (88%)	11 (10%)	3 (3%)	8	56
42	BV	99/101 (98%)	75 (76%)	18 (18%)	6 (6%)	2	28
42	DV	99/101 (98%)	74 (75%)	19 (19%)	6 (6%)	2	28
43	BW	110/112 (98%)	98 (89%)	12 (11%)	0	100	100
43	DW	110/112 (98%)	95 (86%)	15 (14%)	0	100	100
44	BX	90/92 (98%)	82 (91%)	7 (8%)	1 (1%)	21	76
44	DX	90/92 (98%)	81 (90%)	8 (9%)	1 (1%)	21	76
45	BY	98/100 (98%)	68 (69%)	14 (14%)	16 (16%)	0	4

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
45	DY	98/100 (98%)	68 (69%)	13 (13%)	17 (17%)	0	3
46	BZ	185/187 (99%)	158 (85%)	21 (11%)	6 (3%)	6	51
46	DZ	185/187 (99%)	158 (85%)	21 (11%)	6 (3%)	6	51
47	B0	74/76 (97%)	63 (85%)	7 (10%)	4 (5%)	3	31
47	D0	74/76 (97%)	63 (85%)	7 (10%)	4 (5%)	3	31
48	B1	86/88 (98%)	59 (69%)	14 (16%)	13 (15%)	0	4
48	D1	86/88 (98%)	59 (69%)	14 (16%)	13 (15%)	0	4
49	B2	60/62 (97%)	45 (75%)	7 (12%)	8 (13%)	0	7
49	D2	60/62 (97%)	45 (75%)	7 (12%)	8 (13%)	0	7
50	B3	57/59 (97%)	51 (90%)	5 (9%)	1 (2%)	13	65
50	D3	57/59 (97%)	51 (90%)	5 (9%)	1 (2%)	13	65
51	B4	28/30 (93%)	16 (57%)	10 (36%)	2 (7%)	2	23
51	D4	28/30 (93%)	16 (57%)	10 (36%)	2 (7%)	2	23
52	B5	50/52 (96%)	42 (84%)	5 (10%)	3 (6%)	2	28
52	D5	50/52 (96%)	42 (84%)	5 (10%)	3 (6%)	2	28
53	B6	42/44 (96%)	29 (69%)	8 (19%)	5 (12%)	1	9
53	D6	42/44 (96%)	29 (69%)	8 (19%)	5 (12%)	1	9
54	B7	46/48 (96%)	42 (91%)	4 (9%)	0	100	100
54	D7	46/48 (96%)	43 (94%)	3 (6%)	0	100	100
55	B8	61/63 (97%)	47 (77%)	7 (12%)	7 (12%)	1	9
55	D8	61/63 (97%)	47 (77%)	7 (12%)	7 (12%)	1	9
All	All	12130/12330 (98%)	9635 (79%)	1836 (15%)	659 (5%)	3	31

5 of 659 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	AY	55	PRO
4	AY	95	GLU
4	AY	175	ALA
4	AY	225	PRO
4	AY	315	VAL

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	
4	AY	305/305 (100%)	278 (91%)	27 (9%)	14	55
4	CY	305/305 (100%)	277 (91%)	28 (9%)	13	52
5	AB	202/202 (100%)	189 (94%)	13 (6%)	25	71
5	CB	202/202 (100%)	188 (93%)	14 (7%)	22	69
6	AC	160/160 (100%)	147 (92%)	13 (8%)	17	60
6	CC	160/160 (100%)	147 (92%)	13 (8%)	17	60
7	AD	180/180 (100%)	149 (83%)	31 (17%)	3	17
7	CD	180/180 (100%)	162 (90%)	18 (10%)	11	47
8	AE	116/116 (100%)	108 (93%)	8 (7%)	22	69
8	CE	116/116 (100%)	108 (93%)	8 (7%)	22	69
9	AF	90/90 (100%)	85 (94%)	5 (6%)	30	75
9	CF	90/90 (100%)	85 (94%)	5 (6%)	30	75
10	AG	126/126 (100%)	123 (98%)	3 (2%)	61	92
10	CG	126/126 (100%)	123 (98%)	3 (2%)	61	92
11	AH	119/119 (100%)	111 (93%)	8 (7%)	23	70
11	CH	119/119 (100%)	110 (92%)	9 (8%)	19	64
12	AI	98/98 (100%)	88 (90%)	10 (10%)	11	46
12	CI	98/98 (100%)	88 (90%)	10 (10%)	11	46
13	AJ	88/88 (100%)	78 (89%)	10 (11%)	8	38
13	CJ	88/88 (100%)	78 (89%)	10 (11%)	8	38
14	AK	86/86 (100%)	82 (95%)	4 (5%)	36	81
14	CK	86/86 (100%)	82 (95%)	4 (5%)	36	81
15	AL	103/103 (100%)	95 (92%)	8 (8%)	18	62
15	CL	103/103 (100%)	95 (92%)	8 (8%)	18	62
16	AM	94/94 (100%)	86 (92%)	8 (8%)	15	58
16	CM	94/94 (100%)	86 (92%)	8 (8%)	15	58
17	AN	49/49 (100%)	44 (90%)	5 (10%)	11	46

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
17	CN	49/49 (100%)	47 (96%)	2 (4%)	41	84
18	AO	79/79 (100%)	71 (90%)	8 (10%)	11	46
18	CO	79/79 (100%)	71 (90%)	8 (10%)	11	46
19	AP	72/72 (100%)	65 (90%)	7 (10%)	12	49
19	CP	72/72 (100%)	66 (92%)	6 (8%)	16	59
20	AQ	94/94 (100%)	89 (95%)	5 (5%)	32	77
20	CQ	94/94 (100%)	89 (95%)	5 (5%)	32	77
21	AR	61/61 (100%)	60 (98%)	1 (2%)	75	95
21	CR	61/61 (100%)	60 (98%)	1 (2%)	75	95
22	AS	69/69 (100%)	57 (83%)	12 (17%)	3	16
22	CS	69/69 (100%)	57 (83%)	12 (17%)	3	16
23	AT	76/76 (100%)	72 (95%)	4 (5%)	32	77
23	CT	76/76 (100%)	72 (95%)	4 (5%)	32	77
24	AU	19/19 (100%)	18 (95%)	1 (5%)	32	77
24	CU	19/19 (100%)	18 (95%)	1 (5%)	32	77
27	BD	213/213 (100%)	188 (88%)	25 (12%)	8	37
27	DD	213/213 (100%)	188 (88%)	25 (12%)	8	37
28	BE	165/165 (100%)	149 (90%)	16 (10%)	12	49
28	DE	165/165 (100%)	150 (91%)	15 (9%)	14	53
29	BF	161/161 (100%)	145 (90%)	16 (10%)	11	47
29	DF	161/161 (100%)	145 (90%)	16 (10%)	11	47
30	BG	155/155 (100%)	140 (90%)	15 (10%)	12	49
30	DG	155/155 (100%)	140 (90%)	15 (10%)	12	49
31	BH	132/132 (100%)	123 (93%)	9 (7%)	22	69
31	DH	132/132 (100%)	124 (94%)	8 (6%)	26	73
32	BI	122/122 (100%)	111 (91%)	11 (9%)	14	54
32	DI	122/122 (100%)	111 (91%)	11 (9%)	14	54
33	BK	111/111 (100%)	98 (88%)	13 (12%)	8	37
33	DK	111/111 (100%)	105 (95%)	6 (5%)	31	77
34	BN	116/116 (100%)	99 (85%)	17 (15%)	4	26
34	DN	116/116 (100%)	99 (85%)	17 (15%)	4	26

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
35	BO	100/100 (100%)	95 (95%)	5 (5%)	34	79
35	DO	100/100 (100%)	94 (94%)	6 (6%)	27	73
36	BP	112/112 (100%)	87 (78%)	25 (22%)	1	7
36	DP	112/112 (100%)	87 (78%)	25 (22%)	1	7
37	BQ	105/105 (100%)	94 (90%)	11 (10%)	10	44
37	DQ	105/105 (100%)	95 (90%)	10 (10%)	12	50
38	BR	100/100 (100%)	86 (86%)	14 (14%)	5	28
38	DR	100/100 (100%)	85 (85%)	15 (15%)	4	25
39	BS	77/77 (100%)	66 (86%)	11 (14%)	5	27
39	DS	77/77 (100%)	66 (86%)	11 (14%)	5	27
40	BT	121/121 (100%)	101 (84%)	20 (16%)	3	20
40	DT	121/121 (100%)	99 (82%)	22 (18%)	2	13
41	BU	93/93 (100%)	85 (91%)	8 (9%)	15	57
41	DU	93/93 (100%)	85 (91%)	8 (9%)	15	57
42	BV	82/82 (100%)	67 (82%)	15 (18%)	2	13
42	DV	82/82 (100%)	67 (82%)	15 (18%)	2	13
43	BW	91/91 (100%)	81 (89%)	10 (11%)	9	41
43	DW	91/91 (100%)	81 (89%)	10 (11%)	9	41
44	BX	74/74 (100%)	69 (93%)	5 (7%)	22	69
44	DX	74/74 (100%)	69 (93%)	5 (7%)	22	69
45	BY	84/84 (100%)	78 (93%)	6 (7%)	21	67
45	DY	84/84 (100%)	78 (93%)	6 (7%)	21	67
46	BZ	162/162 (100%)	153 (94%)	9 (6%)	30	75
46	DZ	162/162 (100%)	153 (94%)	9 (6%)	30	75
47	B0	61/61 (100%)	52 (85%)	9 (15%)	4	25
47	D0	61/61 (100%)	52 (85%)	9 (15%)	4	25
48	B1	73/73 (100%)	58 (80%)	15 (20%)	2	9
48	D1	73/73 (100%)	58 (80%)	15 (20%)	2	9
49	B2	58/58 (100%)	52 (90%)	6 (10%)	10	45
49	D2	58/58 (100%)	51 (88%)	7 (12%)	7	35
50	B3	51/51 (100%)	46 (90%)	5 (10%)	12	48

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
50	D3	51/51 (100%)	46 (90%)	5 (10%)	12	48
51	B4	27/27 (100%)	26 (96%)	1 (4%)	45	85
51	D4	27/27 (100%)	26 (96%)	1 (4%)	45	85
52	B5	45/45 (100%)	42 (93%)	3 (7%)	23	70
52	D5	45/45 (100%)	42 (93%)	3 (7%)	23	70
53	B6	43/43 (100%)	37 (86%)	6 (14%)	5	28
53	D6	43/43 (100%)	37 (86%)	6 (14%)	5	28
54	B7	41/41 (100%)	34 (83%)	7 (17%)	3	18
54	D7	41/41 (100%)	34 (83%)	7 (17%)	3	18
55	B8	53/53 (100%)	45 (85%)	8 (15%)	4	25
55	D8	53/53 (100%)	45 (85%)	8 (15%)	4	25
All	All	10228/10228 (100%)	9223 (90%)	1005 (10%)	12	48

5 of 1005 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
47	B0	20	ARG
6	CC	107	GLN
44	DX	81	VAL
48	B1	37	ILE
55	B8	52	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 268 such sidechains are listed below:

Mol	Chain	Res	Type
50	B3	19	GLN
7	CD	160	GLN
44	DX	87	GLN
51	B4	46	ASN
5	CB	40	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	AA	1503/1504 (99%)	216 (14%)	20 (1%)
1	CA	1503/1504 (99%)	217 (14%)	20 (1%)

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	AV	9/10 (90%)	2 (22%)	0
2	CV	9/10 (90%)	2 (22%)	0
25	BA	2787/2879 (96%)	431 (15%)	19 (0%)
25	DA	2787/2879 (96%)	432 (15%)	19 (0%)
26	BB	118/119 (99%)	15 (12%)	0
26	DB	118/119 (99%)	15 (12%)	0
3	AW	76/77 (98%)	7 (9%)	0
3	CW	76/77 (98%)	7 (9%)	0
All	All	8986/9178 (97%)	1344 (14%)	78 (0%)

5 of 1344 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	AA	7	G
1	AA	9	G
1	AA	32	A
1	AA	39	G
1	AA	41	G

5 of 78 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
25	BA	2225	A
1	CA	428	G
25	DA	1912	A
25	BA	2447	G
1	CA	115	G

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 2414 ligands modelled in this entry, 2414 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	1504/1504 (100%)	0.06	20 (1%) 74 37	46, 108, 215, 381	0
1	CA	1504/1504 (100%)	0.20	34 (2%) 57 24	48, 122, 235, 451	0
2	AV	10/10 (100%)	1.01	1 (10%) 8 4	76, 120, 198, 250	0
2	CV	10/10 (100%)	0.81	2 (20%) 2 2	74, 123, 204, 230	0
3	AW	77/77 (100%)	0.09	0 100 100	73, 106, 160, 212	0
3	CW	77/77 (100%)	0.01	0 100 100	65, 104, 140, 219	0
4	AY	362/362 (100%)	1.21	69 (19%) 2 2	72, 164, 304, 366	0
4	CY	362/362 (100%)	1.25	62 (17%) 2 2	69, 180, 326, 473	0
5	AB	234/234 (100%)	0.69	20 (8%) 11 5	84, 152, 249, 335	0
5	CB	234/234 (100%)	0.66	18 (7%) 13 6	84, 173, 267, 348	0
6	AC	206/206 (100%)	0.34	6 (2%) 49 21	69, 141, 224, 325	0
6	CC	206/206 (100%)	0.28	2 (0%) 79 44	88, 154, 252, 385	0
7	AD	208/208 (100%)	0.14	1 (0%) 88 61	46, 104, 158, 201	0
7	CD	208/208 (100%)	0.34	2 (0%) 79 44	78, 146, 224, 346	0
8	AE	151/151 (100%)	0.13	5 (3%) 44 18	61, 102, 156, 274	0
8	CE	151/151 (100%)	0.40	4 (2%) 53 21	84, 125, 202, 274	0
9	AF	101/101 (100%)	0.42	6 (5%) 22 8	92, 150, 222, 283	0
9	CF	101/101 (100%)	0.16	2 (1%) 62 28	60, 104, 157, 216	0
10	AG	155/155 (100%)	0.46	12 (7%) 13 6	81, 147, 220, 290	0
10	CG	155/155 (100%)	0.36	11 (7%) 16 6	91, 147, 209, 352	0
11	AH	138/138 (100%)	0.17	1 (0%) 84 52	58, 110, 163, 235	0
11	CH	138/138 (100%)	0.33	1 (0%) 84 52	74, 130, 191, 271	0
12	AI	127/127 (100%)	0.99	19 (14%) 3 2	94, 172, 247, 329	0
12	CI	127/127 (100%)	1.10	23 (18%) 2 2	85, 174, 242, 307	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	AJ	98/98 (100%)	0.84	13 (13%) 4 2	85, 172, 278, 357	0
13	CJ	98/98 (100%)	1.35	25 (25%) 1 2	86, 197, 311, 435	0
14	AK	114/114 (100%)	0.37	3 (2%) 53 21	59, 110, 172, 233	0
14	CK	114/114 (100%)	0.15	1 (0%) 81 47	55, 99, 165, 372	0
15	AL	122/122 (100%)	0.16	1 (0%) 83 49	44, 85, 148, 192	0
15	CL	122/122 (100%)	0.14	2 (1%) 68 32	48, 99, 149, 268	0
16	AM	117/117 (100%)	0.33	4 (3%) 43 17	81, 166, 258, 377	0
16	CM	117/117 (100%)	0.75	9 (7%) 13 6	109, 159, 244, 340	0
17	AN	60/60 (100%)	0.44	3 (5%) 28 10	72, 128, 174, 224	0
17	CN	60/60 (100%)	0.69	4 (6%) 17 7	80, 151, 191, 265	0
18	AO	88/88 (100%)	0.35	0 100 100	67, 109, 157, 188	0
18	CO	88/88 (100%)	0.11	0 100 100	58, 106, 146, 168	0
19	AP	83/83 (100%)	0.48	2 (2%) 56 24	65, 99, 135, 245	0
19	CP	83/83 (100%)	0.99	11 (13%) 4 2	78, 139, 192, 243	0
20	AQ	99/99 (100%)	0.26	0 100 100	63, 102, 157, 211	0
20	CQ	99/99 (100%)	0.45	1 (1%) 79 44	76, 116, 167, 283	0
21	AR	70/70 (100%)	1.21	14 (20%) 2 2	76, 134, 215, 266	0
21	CR	70/70 (100%)	0.54	3 (4%) 34 13	70, 112, 182, 225	0
22	AS	78/78 (100%)	0.90	7 (8%) 10 5	113, 164, 229, 318	0
22	CS	78/78 (100%)	1.00	12 (15%) 3 2	112, 174, 250, 339	0
23	AT	99/99 (100%)	0.55	6 (6%) 21 8	68, 115, 202, 272	0
23	CT	99/99 (100%)	0.50	5 (5%) 27 10	84, 134, 222, 336	0
24	AU	24/24 (100%)	2.26	14 (58%) 0 0	102, 150, 217, 233	0
24	CU	24/24 (100%)	2.54	14 (58%) 0 0	126, 169, 229, 236	0
25	BA	2789/2879 (96%)	-0.01	60 (2%) 59 25	36, 76, 211, 411	0
25	DA	2789/2879 (96%)	-0.07	72 (2%) 53 21	27, 65, 189, 401	0
26	BB	119/119 (100%)	0.17	0 100 100	63, 129, 186, 245	0
26	DB	119/119 (100%)	0.12	1 (0%) 83 49	73, 119, 167, 276	0
27	BD	271/271 (100%)	0.14	2 (0%) 84 52	31, 66, 114, 224	0
27	DD	271/271 (100%)	-0.05	1 (0%) 90 68	14, 56, 107, 221	0
28	BE	204/204 (100%)	0.22	2 (0%) 79 44	35, 82, 148, 377	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
28	DE	204/204 (100%)	0.02	0 100 100	29, 74, 138, 256	0
29	BF	202/202 (100%)	-0.04	1 (0%) 88 61	28, 81, 163, 345	0
29	DF	202/202 (100%)	0.07	1 (0%) 88 61	13, 69, 145, 300	0
30	BG	181/181 (100%)	0.65	9 (4%) 28 10	78, 147, 221, 323	0
30	DG	181/181 (100%)	0.42	6 (3%) 44 18	73, 136, 220, 288	0
31	BH	159/159 (100%)	0.84	15 (9%) 9 4	86, 172, 263, 376	0
31	DH	159/159 (100%)	0.12	3 (1%) 64 29	48, 100, 157, 286	0
32	BI	145/145 (100%)	1.32	31 (21%) 1 2	74, 188, 473, 559	0
32	DI	145/145 (100%)	0.42	4 (2%) 50 21	47, 118, 209, 462	0
33	BK	147/147 (100%)	3.14	91 (61%) 0 0	155, 266, 359, 430	0
33	DK	147/147 (100%)	2.55	86 (58%) 0 0	115, 275, 372, 435	0
34	BN	137/137 (100%)	0.18	1 (0%) 84 52	51, 89, 139, 220	0
34	DN	137/137 (100%)	0.01	0 100 100	37, 84, 149, 192	0
35	BO	122/122 (100%)	-0.11	0 100 100	44, 77, 121, 158	0
35	DO	122/122 (100%)	-0.13	0 100 100	31, 67, 117, 149	0
36	BP	146/146 (100%)	0.49	7 (4%) 29 12	27, 100, 201, 293	0
36	DP	146/146 (100%)	0.41	3 (2%) 60 27	23, 85, 172, 304	0
37	BQ	134/134 (100%)	0.27	2 (1%) 70 33	45, 86, 159, 419	0
37	DQ	134/134 (100%)	0.15	0 100 100	41, 83, 175, 469	0
38	BR	117/117 (100%)	0.12	0 100 100	37, 83, 141, 190	0
38	DR	117/117 (100%)	0.06	1 (0%) 81 47	32, 74, 137, 174	0
39	BS	98/98 (100%)	0.77	11 (11%) 6 3	61, 135, 212, 245	0
39	DS	98/98 (100%)	0.38	3 (3%) 47 19	72, 116, 180, 203	0
40	BT	137/137 (100%)	0.35	3 (2%) 59 25	54, 95, 195, 362	0
40	DT	137/137 (100%)	0.32	4 (2%) 49 21	34, 90, 194, 343	0
41	BU	117/117 (100%)	0.23	0 100 100	36, 73, 137, 173	0
41	DU	117/117 (100%)	0.31	2 (1%) 67 31	35, 74, 125, 363	0
42	BV	101/101 (100%)	0.04	0 100 100	49, 93, 159, 283	0
42	DV	101/101 (100%)	0.15	0 100 100	34, 96, 153, 283	0
43	BW	112/112 (100%)	-0.05	0 100 100	28, 66, 124, 378	0
43	DW	112/112 (100%)	-0.10	0 100 100	38, 66, 125, 210	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å ²)	Q<0.9
44	BX	92/92 (100%)	0.02	0	100	100	61, 87, 139, 179	0
44	DX	92/92 (100%)	-0.02	0	100	100	34, 66, 106, 168	0
45	BY	100/100 (100%)	0.83	13 (13%)	4	2	46, 112, 248, 418	0
45	DY	100/100 (100%)	0.69	7 (7%)	16	6	50, 92, 223, 452	0
46	BZ	187/187 (100%)	0.38	9 (4%)	29	12	75, 130, 200, 267	0
46	DZ	187/187 (100%)	0.34	6 (3%)	45	18	56, 123, 182, 260	0
47	B0	76/76 (100%)	0.24	0	100	100	54, 84, 150, 259	0
47	D0	76/76 (100%)	0.18	1 (1%)	74	37	37, 80, 115, 238	0
48	B1	88/88 (100%)	0.27	0	100	100	46, 90, 156, 264	0
48	D1	88/88 (100%)	0.18	3 (3%)	43	17	23, 69, 147, 267	0
49	B2	62/62 (100%)	0.31	3 (4%)	29	12	67, 119, 210, 257	0
49	D2	62/62 (100%)	0.34	4 (6%)	18	7	33, 75, 176, 304	0
50	B3	59/59 (100%)	0.60	2 (3%)	43	17	52, 80, 144, 224	0
50	D3	59/59 (100%)	0.32	1 (1%)	67	31	42, 81, 143, 236	0
51	B4	30/30 (100%)	0.39	1 (3%)	44	18	107, 184, 297, 335	0
51	D4	30/30 (100%)	1.01	4 (13%)	4	2	125, 215, 272, 361	0
52	B5	52/52 (100%)	0.14	0	100	100	32, 75, 181, 213	0
52	D5	52/52 (100%)	-0.10	0	100	100	20, 77, 172, 269	0
53	B6	44/44 (100%)	4.74	41 (93%)	0	0	118, 225, 304, 330	0
53	D6	44/44 (100%)	3.61	37 (84%)	0	0	136, 208, 276, 330	0
54	B7	48/48 (100%)	0.49	3 (6%)	19	8	35, 60, 131, 156	0
54	D7	48/48 (100%)	0.23	1 (2%)	60	27	19, 36, 94, 156	0
55	B8	63/63 (100%)	0.29	0	100	100	38, 78, 155, 190	0
55	D8	63/63 (100%)	0.13	0	100	100	33, 62, 142, 213	0
All	All	21328/21508 (99%)	0.30	1033 (4%)	29	12	13, 103, 238, 559	0

The worst 5 of 1033 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	AA	68(N)	U	14.9
1	AA	68(M)	U	14.2
33	DK	6	ALA	12.6
33	DK	1	MET	12.4
4	CY	91	GLU	11.9

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
56	MG	AA	1765	1/1	0.57	-	74,74,74,74	0
56	MG	BA	3246	1/1	0.41	-	47,47,47,47	0
56	MG	AA	1969	1/1	0.56	-	63,63,63,63	0
56	MG	BA	3123	1/1	0.20	-	156,156,156,156	0
56	MG	BA	3362	1/1	0.26	-	26,26,26,26	0
56	MG	DA	3486	1/1	0.32	-	62,62,62,62	0
56	MG	BA	3070	1/1	0.52	-	159,159,159,159	0
56	MG	AA	1724	1/1	0.40	-	133,133,133,133	0
56	MG	AA	1809	1/1	0.20	-	106,106,106,106	0
56	MG	CA	1655	1/1	0.23	-	65,65,65,65	0
56	MG	BA	3693	1/1	0.19	-	65,65,65,65	0
56	MG	BA	3628	1/1	0.70	-	82,82,82,82	0
56	MG	DA	3309	1/1	0.25	-	81,81,81,81	0
56	MG	BA	3243	1/1	0.20	-	149,149,149,149	0
56	MG	CA	1635	1/1	0.24	-	119,119,119,119	0
56	MG	DA	3073	1/1	0.54	-	80,80,80,80	0
56	MG	AA	1633	1/1	0.23	-	45,45,45,45	0
56	MG	AA	1756	1/1	0.10	-	87,87,87,87	0
56	MG	DA	3454	1/1	0.28	-	62,62,62,62	0
56	MG	BA	3286	1/1	0.52	-	63,63,63,63	0
56	MG	DA	3178	1/1	0.35	-	40,40,40,40	0
56	MG	DA	2914	1/1	0.39	-	97,97,97,97	0
56	MG	DA	3280	1/1	0.38	-	59,59,59,59	0
56	MG	DA	3013	1/1	0.29	-	55,55,55,55	0
56	MG	BA	3713	1/1	1.05	-	123,123,123,123	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	CA	1791	1/1	0.58	-	91,91,91,91	0
56	MG	BA	3682	1/1	0.31	-	64,64,64,64	0
56	MG	DD	301	1/1	0.20	-	62,62,62,62	0
56	MG	DA	3303	1/1	0.63	-	53,53,53,53	0
56	MG	CA	1627	1/1	0.61	-	85,85,85,85	0
56	MG	CA	1808	1/1	0.62	-	74,74,74,74	0
56	MG	AA	1898	1/1	0.23	-	70,70,70,70	0
56	MG	DA	3210	1/1	0.32	-	38,38,38,38	0
56	MG	BA	3567	1/1	0.39	-	75,75,75,75	0
56	MG	BA	3006	1/1	0.22	-	107,107,107,107	0
56	MG	AA	1870	1/1	0.38	-	73,73,73,73	0
56	MG	DA	3366	1/1	0.21	-	84,84,84,84	0
56	MG	AA	1663	1/1	0.28	-	44,44,44,44	0
56	MG	AA	1877	1/1	0.44	-	37,37,37,37	0
56	MG	AA	1950	1/1	0.42	-	102,102,102,102	0
56	MG	AA	1743	1/1	0.48	-	81,81,81,81	0
56	MG	DA	3338	1/1	0.77	-	76,76,76,76	0
56	MG	AA	1781	1/1	0.33	-	42,42,42,42	0
56	MG	BA	3625	1/1	0.30	-	117,117,117,117	0
56	MG	DA	2978	1/1	0.40	-	64,64,64,64	0
56	MG	DA	3578	1/1	0.56	-	57,57,57,57	0
56	MG	AA	1895	1/1	0.18	-	33,33,33,33	0
56	MG	AA	1790	1/1	0.46	-	53,53,53,53	0
56	MG	BA	3662	1/1	0.38	-	87,87,87,87	0
56	MG	BA	3326	1/1	0.63	-	56,56,56,56	0
56	MG	AA	1893	1/1	0.53	-	48,48,48,48	0
56	MG	BA	3386	1/1	0.18	-	39,39,39,39	0
56	MG	DA	3051	1/1	0.17	-	64,64,64,64	0
56	MG	DA	3191	1/1	0.36	-	28,28,28,28	0
56	MG	DA	3078	1/1	0.21	-	75,75,75,75	0
56	MG	DA	3169	1/1	0.31	-	33,33,33,33	0
56	MG	BA	3001	1/1	0.12	-	86,86,86,86	0
56	MG	DA	2984	1/1	0.23	-	34,34,34,34	0
56	MG	AA	1782	1/1	0.44	-	77,77,77,77	0
56	MG	AA	1860	1/1	0.31	-	62,62,62,62	0
56	MG	BA	3409	1/1	0.18	-	115,115,115,115	0
56	MG	BA	2970	1/1	0.22	-	93,93,93,93	0
56	MG	BA	3219	1/1	0.68	-	78,78,78,78	0
56	MG	DA	3187	1/1	0.27	-	32,32,32,32	0
56	MG	DA	2902	1/1	0.21	-	65,65,65,65	0
56	MG	BA	3005	1/1	0.26	-	45,45,45,45	0
56	MG	BA	2976	1/1	0.41	-	112,112,112,112	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	AA	1693	1/1	0.32	-	74,74,74,74	0
56	MG	CA	1925	1/1	0.27	-	94,94,94,94	0
56	MG	AA	1793	1/1	0.36	-	127,127,127,127	0
56	MG	BA	3508	1/1	0.30	-	67,67,67,67	0
56	MG	BA	3059	1/1	0.35	-	43,43,43,43	0
56	MG	AA	1945	1/1	0.39	-	115,115,115,115	0
56	MG	DA	3563	1/1	0.48	-	62,62,62,62	0
56	MG	AA	1696	1/1	0.24	-	96,96,96,96	0
56	MG	DA	3192	1/1	0.29	-	38,38,38,38	0
56	MG	BA	3137	1/1	0.25	-	83,83,83,83	0
56	MG	DA	3277	1/1	0.34	-	45,45,45,45	0
56	MG	CA	1813	1/1	0.41	-	99,99,99,99	0
56	MG	CA	1718	1/1	0.11	-	136,136,136,136	0
56	MG	DA	3211	1/1	0.33	-	33,33,33,33	0
56	MG	BA	3042	1/1	0.25	-	67,67,67,67	0
56	MG	BA	3401	1/1	0.43	-	28,28,28,28	0
56	MG	AA	1720	1/1	0.33	-	86,86,86,86	0
56	MG	BA	3270	1/1	0.39	-	70,70,70,70	0
56	MG	CA	1818	1/1	0.24	-	71,71,71,71	0
56	MG	DA	3024	1/1	0.23	-	65,65,65,65	0
56	MG	DA	3177	1/1	0.31	-	21,21,21,21	0
56	MG	BA	3214	1/1	0.14	-	85,85,85,85	0
56	MG	AA	1601	1/1	0.31	-	92,92,92,92	0
56	MG	BA	3254	1/1	0.16	-	93,93,93,93	0
56	MG	DA	3361	1/1	0.24	-	73,73,73,73	0
56	MG	BB	205	1/1	0.26	-	64,64,64,64	0
56	MG	BA	3667	1/1	0.30	-	52,52,52,52	0
56	MG	BA	3497	1/1	0.23	-	78,78,78,78	0
56	MG	AA	1887	1/1	0.09	-	70,70,70,70	0
56	MG	DA	3241	1/1	0.18	-	28,28,28,28	0
56	MG	BA	2951	1/1	0.16	-	50,50,50,50	0
56	MG	DA	3083	1/1	0.53	-	125,125,125,125	0
56	MG	AA	1985	1/1	0.22	-	108,108,108,108	0
56	MG	BB	213	1/1	0.33	-	93,93,93,93	0
56	MG	BA	3710	1/1	0.30	-	81,81,81,81	0
56	MG	BA	3645	1/1	0.33	-	48,48,48,48	0
56	MG	AA	1784	1/1	0.09	-	72,72,72,72	0
56	MG	CA	1826	1/1	0.25	-	73,73,73,73	0
56	MG	BA	3284	1/1	0.53	-	82,82,82,82	0
56	MG	BA	3209	1/1	0.31	-	96,96,96,96	0
56	MG	BA	3075	1/1	0.69	-	73,73,73,73	0
56	MG	BA	2904	1/1	0.24	-	48,48,48,48	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	BA	3643	1/1	0.48	-	57,57,57,57	0
56	MG	DA	3319	1/1	0.17	-	34,34,34,34	0
56	MG	BA	2947	1/1	0.43	-	52,52,52,52	0
56	MG	DA	2968	1/1	0.24	-	54,54,54,54	0
56	MG	DA	3562	1/1	0.24	-	45,45,45,45	0
56	MG	BA	3373	1/1	0.44	-	39,39,39,39	0
56	MG	CA	1724	1/1	0.30	-	108,108,108,108	0
56	MG	DA	3509	1/1	0.22	-	142,142,142,142	0
56	MG	AA	1992	1/1	0.28	-	84,84,84,84	0
56	MG	DA	3032	1/1	0.19	-	82,82,82,82	0
56	MG	AA	1678	1/1	0.13	-	101,101,101,101	0
56	MG	DA	3549	1/1	0.32	-	16,16,16,16	0
56	MG	CW	108	1/1	0.37	-	26,26,26,26	0
56	MG	DA	3162	1/1	0.17	-	23,23,23,23	0
56	MG	BA	3426	1/1	0.27	-	28,28,28,28	0
56	MG	BA	3205	1/1	0.58	-	95,95,95,95	0
56	MG	AA	1986	1/1	0.94	-	69,69,69,69	0
56	MG	CA	1664	1/1	0.28	-	78,78,78,78	0
56	MG	BA	3702	1/1	0.22	-	61,61,61,61	0
56	MG	DA	3217	1/1	0.36	-	24,24,24,24	0
56	MG	DA	3297	1/1	0.42	-	64,64,64,64	0
56	MG	AA	1789	1/1	0.17	-	63,63,63,63	0
56	MG	DA	3327	1/1	0.20	-	58,58,58,58	0
56	MG	AA	1683	1/1	0.12	-	249,249,249,249	0
56	MG	CA	1811	1/1	0.27	-	54,54,54,54	0
56	MG	AA	1754	1/1	0.66	-	72,72,72,72	0
56	MG	AA	1714	1/1	0.55	-	114,114,114,114	0
56	MG	CA	1687	1/1	0.18	-	58,58,58,58	0
57	ZN	AD	301	1/1	0.29	-	71,71,71,71	0
56	MG	B1	101	1/1	0.44	-	75,75,75,75	0
56	MG	BA	3313	1/1	0.31	-	63,63,63,63	0
56	MG	DA	3244	1/1	0.23	-	59,59,59,59	0
56	MG	DA	3289	1/1	0.26	-	45,45,45,45	0
56	MG	DA	3242	1/1	0.49	-	40,40,40,40	0
56	MG	BA	3498	1/1	0.08	-	67,67,67,67	0
56	MG	BA	3223	1/1	0.22	-	58,58,58,58	0
56	MG	AA	1744	1/1	0.37	-	103,103,103,103	0
56	MG	BA	3049	1/1	0.32	-	90,90,90,90	0
56	MG	DA	3050	1/1	0.48	-	56,56,56,56	0
56	MG	BA	3502	1/1	0.23	-	26,26,26,26	0
56	MG	BA	3315	1/1	0.21	-	17,17,17,17	0
56	MG	BA	3626	1/1	0.51	-	62,62,62,62	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	DA	3019	1/1	0.38	-	67,67,67,67	0
56	MG	AA	1956	1/1	0.36	-	110,110,110,110	0
56	MG	AA	1946	1/1	0.28	-	86,86,86,86	0
56	MG	DA	3182	1/1	0.50	-	24,24,24,24	0
56	MG	DA	2927	1/1	0.36	-	91,91,91,91	0
56	MG	DA	3030	1/1	1.36	-	78,78,78,78	0
56	MG	DA	3208	1/1	0.61	-	29,29,29,29	0
56	MG	BA	3092	1/1	0.40	-	99,99,99,99	0
56	MG	DA	3436	1/1	0.18	-	68,68,68,68	0
56	MG	DA	3201	1/1	0.32	-	25,25,25,25	0
56	MG	AA	1729	1/1	0.52	-	99,99,99,99	0
56	MG	BA	3072	1/1	0.18	-	88,88,88,88	0
56	MG	DA	3062	1/1	0.46	-	75,75,75,75	0
56	MG	BA	2987	1/1	0.48	-	79,79,79,79	0
56	MG	DA	3086	1/1	1.05	-	120,120,120,120	0
56	MG	AA	1806	1/1	0.41	-	111,111,111,111	0
56	MG	DA	2934	1/1	0.39	-	76,76,76,76	0
56	MG	BA	2949	1/1	0.42	-	70,70,70,70	0
56	MG	BA	3510	1/1	0.34	-	86,86,86,86	0
56	MG	DA	3038	1/1	0.29	-	77,77,77,77	0
56	MG	DA	3616	1/1	0.23	-	65,65,65,65	0
56	MG	BA	3098	1/1	0.70	-	94,94,94,94	0
56	MG	AA	1606	1/1	0.10	-	77,77,77,77	0
56	MG	DA	3057	1/1	0.10	-	107,107,107,107	0
56	MG	AA	1935	1/1	0.19	-	39,39,39,39	0
56	MG	DA	3257	1/1	0.27	-	90,90,90,90	0
56	MG	DA	3375	1/1	0.55	-	78,78,78,78	0
56	MG	DA	3153	1/1	0.46	-	22,22,22,22	0
56	MG	DA	3112	1/1	0.26	-	141,141,141,141	0
56	MG	DA	3582	1/1	0.38	-	95,95,95,95	0
56	MG	DA	3437	1/1	0.11	-	59,59,59,59	0
56	MG	BA	3479	1/1	0.54	-	59,59,59,59	0
56	MG	BA	3444	1/1	0.48	-	65,65,65,65	0
56	MG	BA	3193	1/1	0.33	-	79,79,79,79	0
56	MG	CA	1656	1/1	0.39	-	52,52,52,52	0
56	MG	BA	3336	1/1	0.32	-	31,31,31,31	0
56	MG	DA	3334	1/1	0.37	-	72,72,72,72	0
56	MG	DA	3595	1/1	0.43	-	106,106,106,106	0
56	MG	DA	3333	1/1	0.11	-	47,47,47,47	0
56	MG	AA	1920	1/1	0.14	-	71,71,71,71	0
56	MG	BA	3306	1/1	0.40	-	68,68,68,68	0
56	MG	DA	3325	1/1	0.51	-	46,46,46,46	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	DA	3104	1/1	0.36	-	70,70,70,70	0
56	MG	AA	1976	1/1	0.08	-	60,60,60,60	0
56	MG	BA	3562	1/1	0.29	-	45,45,45,45	0
56	MG	BA	3288	1/1	0.22	-	71,71,71,71	0
56	MG	BA	3430	1/1	0.25	-	47,47,47,47	0
56	MG	BA	2930	1/1	0.53	-	89,89,89,89	0
56	MG	BA	3697	1/1	0.11	-	64,64,64,64	0
56	MG	BA	2978	1/1	0.66	-	72,72,72,72	0
56	MG	CA	1854	1/1	0.44	-	98,98,98,98	0
56	MG	AA	1682	1/1	0.89	-	124,124,124,124	0
56	MG	BB	221	1/1	0.12	-	65,65,65,65	0
56	MG	BA	3030	1/1	0.45	-	64,64,64,64	0
56	MG	BA	3091	1/1	0.20	-	125,125,125,125	0
56	MG	AA	1635	1/1	0.36	-	106,106,106,106	0
56	MG	BA	3089	1/1	0.54	-	72,72,72,72	0
56	MG	DA	3431	1/1	0.27	-	74,74,74,74	0
56	MG	BA	3269	1/1	0.34	-	66,66,66,66	0
56	MG	AT	203	1/1	1.91	-	99,99,99,99	0
56	MG	BA	3147	1/1	0.46	-	88,88,88,88	0
56	MG	AA	1888	1/1	0.44	-	49,49,49,49	0
56	MG	AA	1649	1/1	0.91	-	110,110,110,110	0
56	MG	BA	3073	1/1	0.61	-	124,124,124,124	0
56	MG	AA	1609	1/1	0.24	-	46,46,46,46	0
56	MG	CA	1716	1/1	0.21	-	86,86,86,86	0
56	MG	DA	2979	1/1	0.45	-	81,81,81,81	0
56	MG	CA	1842	1/1	0.95	-	137,137,137,137	0
56	MG	DA	3145	1/1	0.28	-	39,39,39,39	0
56	MG	DA	3545	1/1	0.21	-	91,91,91,91	0
56	MG	CW	111	1/1	0.20	-	82,82,82,82	0
56	MG	BA	3719	1/1	0.09	-	125,125,125,125	0
56	MG	DA	3035	1/1	0.34	-	71,71,71,71	0
56	MG	BA	3588	1/1	0.86	-	120,120,120,120	0
56	MG	AA	1798	1/1	0.19	-	47,47,47,47	0
56	MG	AA	1667	1/1	0.27	-	53,53,53,53	0
56	MG	AW	101	1/1	0.28	-	105,105,105,105	0
56	MG	BA	3421	1/1	0.19	-	79,79,79,79	0
56	MG	BA	3706	1/1	0.34	-	102,102,102,102	0
56	MG	CA	1641	1/1	0.15	-	135,135,135,135	0
56	MG	BA	3294	1/1	0.48	-	75,75,75,75	0
56	MG	DA	3122	1/1	0.34	-	67,67,67,67	0
56	MG	BA	3152	1/1	0.14	-	72,72,72,72	0
56	MG	DA	3542	1/1	0.48	-	70,70,70,70	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	B0	102	1/1	0.32	-	68,68,68,68	0
56	MG	BA	3279	1/1	0.31	-	80,80,80,80	0
56	MG	BA	3337	1/1	0.50	-	20,20,20,20	0
56	MG	DA	3113	1/1	0.25	-	110,110,110,110	0
56	MG	DA	3476	1/1	0.30	-	73,73,73,73	0
56	MG	BA	3040	1/1	0.25	-	85,85,85,85	0
56	MG	DA	3425	1/1	0.58	-	52,52,52,52	0
56	MG	CA	1830	1/1	0.17	-	80,80,80,80	0
56	MG	AA	1896	1/1	0.77	-	77,77,77,77	0
56	MG	AA	1716	1/1	0.35	-	103,103,103,103	0
56	MG	CA	1894	1/1	0.07	-	89,89,89,89	0
56	MG	BA	3124	1/1	0.48	-	79,79,79,79	0
56	MG	BA	3120	1/1	0.57	-	62,62,62,62	0
56	MG	DA	3064	1/1	0.20	-	62,62,62,62	0
56	MG	DA	3140	1/1	0.40	-	11,11,11,11	0
56	MG	BA	3491	1/1	0.29	-	85,85,85,85	0
56	MG	BA	3169	1/1	0.08	-	64,64,64,64	0
56	MG	BA	2979	1/1	0.96	-	77,77,77,77	0
56	MG	BA	3582	1/1	0.52	-	72,72,72,72	0
56	MG	DA	3136	1/1	0.40	-	12,12,12,12	0
56	MG	DA	3453	1/1	0.20	-	85,85,85,85	0
56	MG	AA	1776	1/1	0.52	-	146,146,146,146	0
56	MG	DA	3551	1/1	0.39	-	13,13,13,13	0
56	MG	AW	113	1/1	0.36	-	96,96,96,96	0
56	MG	BY	201	1/1	0.19	-	30,30,30,30	0
56	MG	BA	3646	1/1	0.22	-	52,52,52,52	0
56	MG	CA	1657	1/1	0.20	-	95,95,95,95	0
56	MG	BA	3595	1/1	0.21	-	39,39,39,39	0
56	MG	DA	2985	1/1	0.19	-	107,107,107,107	0
56	MG	BA	3241	1/1	0.62	-	77,77,77,77	0
56	MG	CA	1704	1/1	0.67	-	88,88,88,88	0
56	MG	DA	2935	1/1	0.14	-	89,89,89,89	0
56	MG	BB	220	1/1	0.12	-	123,123,123,123	0
56	MG	DA	3382	1/1	0.35	-	49,49,49,49	0
56	MG	DA	3471	1/1	0.33	-	55,55,55,55	0
56	MG	BA	3334	1/1	0.31	-	65,65,65,65	0
56	MG	BA	3687	1/1	0.25	-	56,56,56,56	0
56	MG	DA	3406	1/1	0.17	-	62,62,62,62	0
56	MG	CA	1730	1/1	0.18	-	80,80,80,80	0
56	MG	DA	3230	1/1	0.16	-	41,41,41,41	0
56	MG	AA	1801	1/1	0.14	-	88,88,88,88	0
56	MG	CA	1741	1/1	0.29	-	104,104,104,104	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	AA	1917	1/1	0.17	-	86,86,86,86	0
56	MG	DA	3081	1/1	0.44	-	87,87,87,87	0
56	MG	BA	3388	1/1	0.57	-	22,22,22,22	0
56	MG	CA	1802	1/1	0.30	-	61,61,61,61	0
56	MG	CA	1708	1/1	0.37	-	63,63,63,63	0
56	MG	CA	1892	1/1	0.14	-	150,150,150,150	0
56	MG	BA	3576	1/1	0.38	-	97,97,97,97	0
56	MG	BA	3383	1/1	0.40	-	39,39,39,39	0
56	MG	CA	1647	1/1	0.43	-	98,98,98,98	0
56	MG	DA	3056	1/1	0.22	-	77,77,77,77	0
56	MG	DA	3054	1/1	0.59	-	93,93,93,93	0
56	MG	BA	2927	1/1	0.15	-	82,82,82,82	0
56	MG	BA	2958	1/1	0.17	-	103,103,103,103	0
56	MG	BA	3477	1/1	0.33	-	54,54,54,54	0
56	MG	CA	1880	1/1	0.82	-	118,118,118,118	0
56	MG	BB	202	1/1	0.20	-	98,98,98,98	0
56	MG	AA	1668	1/1	0.28	-	90,90,90,90	0
56	MG	CA	1736	1/1	0.41	-	193,193,193,193	0
56	MG	DA	3025	1/1	0.14	-	30,30,30,30	0
56	MG	BA	3617	1/1	0.22	-	88,88,88,88	0
56	MG	DA	3341	1/1	0.54	-	55,55,55,55	0
56	MG	BA	3189	1/1	0.46	-	105,105,105,105	0
56	MG	CA	1611	1/1	0.35	-	71,71,71,71	0
56	MG	DB	215	1/1	0.15	-	79,79,79,79	0
56	MG	BA	3584	1/1	0.47	-	96,96,96,96	0
56	MG	BA	3228	1/1	0.09	-	83,83,83,83	0
56	MG	BA	3544	1/1	0.14	-	55,55,55,55	0
56	MG	BA	3427	1/1	0.39	-	35,35,35,35	0
56	MG	BA	3201	1/1	0.32	-	71,71,71,71	0
56	MG	DA	3154	1/1	0.27	-	12,12,12,12	0
56	MG	AA	1763	1/1	0.31	-	88,88,88,88	0
56	MG	DA	3611	1/1	0.80	-	60,60,60,60	0
56	MG	CA	1793	1/1	0.25	-	114,114,114,114	0
56	MG	AW	108	1/1	0.34	-	72,72,72,72	0
56	MG	AA	1625	1/1	0.46	-	85,85,85,85	0
56	MG	AA	1648	1/1	0.25	-	61,61,61,61	0
56	MG	DA	3251	1/1	0.23	-	32,32,32,32	0
56	MG	AA	1628	1/1	0.68	-	213,213,213,213	0
56	MG	BA	3297	1/1	0.62	-	122,122,122,122	0
56	MG	BA	3515	1/1	0.34	-	58,58,58,58	0
56	MG	DA	3314	1/1	0.30	-	65,65,65,65	0
56	MG	BA	3526	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
56	MG	AA	1841	1/1	0.32	-	113,113,113,113	0
56	MG	BA	3511	1/1	0.33	-	91,91,91,91	0
56	MG	BA	3162	1/1	0.52	-	60,60,60,60	0
56	MG	DA	3167	1/1	0.17	-	13,13,13,13	0
56	MG	AA	1861	1/1	0.54	-	42,42,42,42	0
56	MG	BA	3369	1/1	0.98	-	74,74,74,74	0
56	MG	BA	3218	1/1	0.68	-	82,82,82,82	0
56	MG	BA	3668	1/1	0.17	-	71,71,71,71	0
56	MG	DQ	204	1/1	0.45	-	41,41,41,41	0
56	MG	BA	2920	1/1	0.39	-	70,70,70,70	0
56	MG	CA	1749	1/1	0.19	-	64,64,64,64	0
56	MG	CA	1698	1/1	0.25	-	100,100,100,100	0
56	MG	BA	2922	1/1	0.92	-	108,108,108,108	0
56	MG	DA	3176	1/1	0.41	-	13,13,13,13	0
56	MG	AA	1778	1/1	0.19	-	159,159,159,159	0
56	MG	BA	3233	1/1	0.28	-	55,55,55,55	0
56	MG	BA	3632	1/1	0.42	-	15,15,15,15	0
56	MG	DA	3575	1/1	0.12	-	49,49,49,49	0
56	MG	DA	3344	1/1	0.35	-	29,29,29,29	0
56	MG	BA	3130	1/1	0.43	-	82,82,82,82	0
56	MG	BA	3375	1/1	0.36	-	30,30,30,30	0
56	MG	BA	3720	1/1	0.25	-	85,85,85,85	0
56	MG	DA	3526	1/1	0.34	-	61,61,61,61	0
56	MG	BA	3148	1/1	0.14	-	111,111,111,111	0
56	MG	AA	1916	1/1	0.50	-	49,49,49,49	0
56	MG	DA	3292	1/1	0.30	-	34,34,34,34	0
56	MG	BA	3680	1/1	0.13	-	35,35,35,35	0
56	MG	AA	1760	1/1	0.21	-	172,172,172,172	0
56	MG	DA	3207	1/1	0.48	-	41,41,41,41	0
56	MG	BA	3247	1/1	0.59	-	105,105,105,105	0
56	MG	DA	3195	1/1	0.16	-	20,20,20,20	0
56	MG	CA	1915	1/1	0.66	-	67,67,67,67	0
56	MG	DA	2908	1/1	0.27	-	60,60,60,60	0
56	MG	CA	1912	1/1	0.42	-	152,152,152,152	0
56	MG	DA	2989	1/1	0.49	-	53,53,53,53	0
56	MG	BA	3382	1/1	0.60	-	51,51,51,51	0
56	MG	AA	1643	1/1	0.25	-	114,114,114,114	0
56	MG	BA	3177	1/1	0.11	-	78,78,78,78	0
56	MG	CA	1772	1/1	0.64	-	66,66,66,66	0
56	MG	CA	1662	1/1	0.55	-	90,90,90,90	0
56	MG	CA	1859	1/1	0.71	-	132,132,132,132	0
56	MG	BA	3340	1/1	0.33	-	31,31,31,31	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	DF	301	1/1	0.35	-	37,37,37,37	0
56	MG	BA	3410	1/1	0.08	-	25,25,25,25	0
56	MG	DA	3350	1/1	0.19	-	76,76,76,76	0
56	MG	AA	1943	1/1	0.13	-	45,45,45,45	0
56	MG	DA	3098	1/1	0.26	-	57,57,57,57	0
56	MG	DA	3605	1/1	0.17	-	59,59,59,59	0
56	MG	AA	1961	1/1	0.19	-	53,53,53,53	0
56	MG	BA	3298	1/1	0.22	-	101,101,101,101	0
56	MG	DA	2986	1/1	0.33	-	110,110,110,110	0
56	MG	BA	3381	1/1	0.31	-	17,17,17,17	0
56	MG	DA	3179	1/1	0.21	-	13,13,13,13	0
56	MG	B8	101	1/1	0.26	-	38,38,38,38	0
56	MG	DA	3584	1/1	0.30	-	49,49,49,49	0
56	MG	DA	3075	1/1	0.38	-	75,75,75,75	0
56	MG	BA	3610	1/1	0.65	-	95,95,95,95	0
56	MG	CA	1781	1/1	0.49	-	59,59,59,59	0
56	MG	DA	3080	1/1	0.36	-	84,84,84,84	0
56	MG	DN	201	1/1	0.17	-	56,56,56,56	0
56	MG	DA	3408	1/1	0.23	-	51,51,51,51	0
56	MG	DA	2969	1/1	0.14	-	68,68,68,68	0
56	MG	DA	3264	1/1	0.24	-	44,44,44,44	0
56	MG	BA	3114	1/1	0.19	-	119,119,119,119	0
56	MG	AA	1871	1/1	0.17	-	29,29,29,29	0
56	MG	CA	1783	1/1	0.10	-	82,82,82,82	0
56	MG	CA	1705	1/1	0.24	-	94,94,94,94	0
56	MG	DA	3060	1/1	0.24	-	77,77,77,77	0
56	MG	BA	3131	1/1	0.41	-	65,65,65,65	0
56	MG	DA	3238	1/1	0.45	-	89,89,89,89	0
56	MG	BA	3483	1/1	0.13	-	23,23,23,23	0
56	MG	BA	3547	1/1	0.19	-	43,43,43,43	0
56	MG	CA	1893	1/1	0.41	-	125,125,125,125	0
56	MG	DA	3068	1/1	0.30	-	69,69,69,69	0
56	MG	BA	2935	1/1	0.46	-	89,89,89,89	0
56	MG	BA	3603	1/1	0.12	-	88,88,88,88	0
56	MG	AA	1691	1/1	0.14	-	84,84,84,84	0
56	MG	CA	1679	1/1	0.17	-	81,81,81,81	0
56	MG	AA	1661	1/1	0.16	-	58,58,58,58	0
56	MG	DA	3488	1/1	0.07	-	70,70,70,70	0
56	MG	DA	3569	1/1	0.33	-	52,52,52,52	0
56	MG	AA	1845	1/1	0.53	-	67,67,67,67	0
56	MG	DA	3028	1/1	0.42	-	55,55,55,55	0
56	MG	CA	1726	1/1	0.25	-	80,80,80,80	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	BA	3052	1/1	0.49	-	118,118,118,118	0
56	MG	BA	3624	1/1	0.33	-	83,83,83,83	0
56	MG	BA	3377	1/1	0.51	-	56,56,56,56	0
56	MG	AA	1889	1/1	0.20	-	81,81,81,81	0
56	MG	DA	2992	1/1	0.28	-	63,63,63,63	0
56	MG	BA	3455	1/1	0.24	-	64,64,64,64	0
56	MG	BA	3069	1/1	0.19	-	69,69,69,69	0
56	MG	DA	3601	1/1	0.38	-	61,61,61,61	0
56	MG	BA	3390	1/1	0.42	-	44,44,44,44	0
56	MG	B8	102	1/1	0.26	-	39,39,39,39	0
56	MG	DE	301	1/1	0.27	-	29,29,29,29	0
56	MG	DA	2965	1/1	0.33	-	74,74,74,74	0
56	MG	BA	3387	1/1	0.21	-	49,49,49,49	0
56	MG	DA	3155	1/1	0.40	-	18,18,18,18	0
56	MG	AA	1974	1/1	0.20	-	48,48,48,48	0
56	MG	DA	3200	1/1	0.50	-	52,52,52,52	0
56	MG	DA	3301	1/1	0.29	-	52,52,52,52	0
56	MG	DA	3263	1/1	0.35	-	61,61,61,61	0
56	MG	AA	1924	1/1	0.42	-	55,55,55,55	0
56	MG	DA	2998	1/1	0.61	-	62,62,62,62	0
56	MG	BA	3714	1/1	0.10	-	94,94,94,94	0
56	MG	BA	3441	1/1	0.29	-	56,56,56,56	0
56	MG	BA	3397	1/1	0.80	-	67,67,67,67	0
56	MG	DW	202	1/1	0.25	-	50,50,50,50	0
56	MG	DA	3171	1/1	0.21	-	25,25,25,25	0
56	MG	BA	2919	1/1	0.09	-	127,127,127,127	0
56	MG	DA	3468	1/1	0.36	-	33,33,33,33	0
56	MG	DA	3499	1/1	0.19	-	98,98,98,98	0
56	MG	DA	3348	1/1	0.77	-	165,165,165,165	0
56	MG	AA	1977	1/1	0.32	-	126,126,126,126	0
56	MG	CA	1919	1/1	0.24	-	39,39,39,39	0
56	MG	DA	2996	1/1	0.26	-	65,65,65,65	0
56	MG	BA	3305	1/1	0.13	-	62,62,62,62	0
56	MG	DA	3092	1/1	1.40	-	200,200,200,200	0
56	MG	AA	1749	1/1	0.26	-	114,114,114,114	0
56	MG	CA	1620	1/1	0.26	-	74,74,74,74	0
56	MG	BA	3438	1/1	0.66	-	49,49,49,49	0
56	MG	AA	1616	1/1	0.41	-	87,87,87,87	0
56	MG	BA	3023	1/1	0.57	-	58,58,58,58	0
56	MG	BA	3136	1/1	0.65	-	205,205,205,205	0
56	MG	BA	3454	1/1	0.23	-	60,60,60,60	0
56	MG	BA	3117	1/1	0.23	-	92,92,92,92	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	BA	3601	1/1	0.16	-	50,50,50,50	0
56	MG	BA	3494	1/1	0.21	-	73,73,73,73	0
56	MG	DA	3046	1/1	0.32	-	48,48,48,48	0
56	MG	BA	2906	1/1	0.24	-	84,84,84,84	0
56	MG	DA	3248	1/1	1.20	-	66,66,66,66	0
56	MG	AA	1732	1/1	0.25	-	60,60,60,60	0
56	MG	DA	3202	1/1	0.45	-	25,25,25,25	0
56	MG	DA	3483	1/1	0.40	-	96,96,96,96	0
56	MG	DA	2951	1/1	0.18	-	78,78,78,78	0
56	MG	CA	1677	1/1	1.19	-	138,138,138,138	0
56	MG	BA	3076	1/1	0.13	-	48,48,48,48	0
56	MG	DA	3268	1/1	0.33	-	52,52,52,52	0
56	MG	DA	3541	1/1	0.73	-	70,70,70,70	0
56	MG	DA	3158	1/1	0.47	-	18,18,18,18	0
56	MG	CA	1626	1/1	0.48	-	109,109,109,109	0
56	MG	BA	3074	1/1	0.08	-	108,108,108,108	0
56	MG	DA	3189	1/1	0.53	-	27,27,27,27	0
56	MG	BA	3134	1/1	0.88	-	122,122,122,122	0
56	MG	DA	3258	1/1	0.54	-	58,58,58,58	0
56	MG	AA	1897	1/1	1.12	-	80,80,80,80	0
56	MG	BA	3295	1/1	0.61	-	97,97,97,97	0
56	MG	CA	1735	1/1	1.03	-	108,108,108,108	0
56	MG	CA	1714	1/1	0.16	-	104,104,104,104	0
56	MG	BA	3404	1/1	1.21	-	82,82,82,82	0
56	MG	DA	3003	1/1	0.44	-	59,59,59,59	0
56	MG	DI	201	1/1	0.20	-	49,49,49,49	0
56	MG	CA	1738	1/1	0.42	-	123,123,123,123	0
56	MG	DA	3497	1/1	0.22	-	61,61,61,61	0
56	MG	DA	3053	1/1	0.11	-	61,61,61,61	0
56	MG	CA	1858	1/1	0.20	-	97,97,97,97	0
56	MG	DA	3374	1/1	0.30	-	54,54,54,54	0
56	MG	AA	1697	1/1	0.22	-	148,148,148,148	0
56	MG	BA	3537	1/1	0.30	-	60,60,60,60	0
56	MG	DA	3012	1/1	0.31	-	102,102,102,102	0
56	MG	DA	3358	1/1	0.12	-	141,141,141,141	0
56	MG	BA	3557	1/1	0.14	-	97,97,97,97	0
56	MG	DA	2944	1/1	0.17	-	94,94,94,94	0
56	MG	DA	3271	1/1	0.28	-	65,65,65,65	0
56	MG	DA	3125	1/1	0.73	-	161,161,161,161	0
56	MG	CA	1888	1/1	0.18	-	67,67,67,67	0
56	MG	CA	1902	1/1	0.57	-	128,128,128,128	0
56	MG	DA	3522	1/1	0.20	-	77,77,77,77	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	AA	1964	1/1	0.15	-	84,84,84,84	0
56	MG	BA	2903	1/1	0.41	-	83,83,83,83	0
56	MG	CA	1752	1/1	0.40	-	83,83,83,83	0
56	MG	AA	1874	1/1	0.43	-	59,59,59,59	0
56	MG	CA	1658	1/1	0.47	-	93,93,93,93	0
56	MG	DA	2977	1/1	0.90	-	84,84,84,84	0
56	MG	BA	3681	1/1	0.21	-	42,42,42,42	0
56	MG	CA	1660	1/1	0.52	-	94,94,94,94	0
56	MG	BA	3195	1/1	0.17	-	97,97,97,97	0
56	MG	BF	1901	1/1	0.29	-	74,74,74,74	0
56	MG	CA	1696	1/1	0.32	-	66,66,66,66	0
56	MG	DA	3033	1/1	0.46	-	93,93,93,93	0
56	MG	DA	3006	1/1	0.37	-	66,66,66,66	0
56	MG	DA	3091	1/1	0.58	-	96,96,96,96	0
56	MG	AA	1908	1/1	0.42	-	56,56,56,56	0
56	MG	DA	3531	1/1	0.47	-	92,92,92,92	0
56	MG	BA	3318	1/1	0.18	-	93,93,93,93	0
56	MG	AA	1960	1/1	0.26	-	48,48,48,48	0
56	MG	BA	3722	1/1	0.26	-	80,80,80,80	0
56	MG	DA	3505	1/1	0.23	-	63,63,63,63	0
56	MG	AW	104	1/1	1.58	-	95,95,95,95	0
56	MG	DA	2949	1/1	0.97	-	94,94,94,94	0
56	MG	AA	1750	1/1	0.27	-	77,77,77,77	0
56	MG	BA	3574	1/1	0.38	-	70,70,70,70	0
56	MG	AA	1741	1/1	0.36	-	91,91,91,91	0
56	MG	BA	2939	1/1	0.43	-	79,79,79,79	0
56	MG	DA	3288	1/1	0.34	-	57,57,57,57	0
56	MG	DA	3538	1/1	0.13	-	70,70,70,70	0
56	MG	DA	3318	1/1	0.43	-	42,42,42,42	0
56	MG	DA	3445	1/1	0.31	-	46,46,46,46	0
56	MG	DA	3554	1/1	0.43	-	13,13,13,13	0
56	MG	AA	1847	1/1	0.32	-	209,209,209,209	0
56	MG	BA	3434	1/1	0.53	-	55,55,55,55	0
56	MG	BA	3525	1/1	0.48	-	40,40,40,40	0
56	MG	BA	3184	1/1	0.21	-	37,37,37,37	0
56	MG	BA	3321	1/1	0.25	-	50,50,50,50	0
56	MG	AA	1918	1/1	0.18	-	51,51,51,51	0
56	MG	BA	3314	1/1	0.47	-	13,13,13,13	0
56	MG	DA	3417	1/1	0.21	-	145,145,145,145	0
56	MG	BA	3395	1/1	0.78	-	107,107,107,107	0
56	MG	DA	3376	1/1	0.41	-	43,43,43,43	0
56	MG	AA	1922	1/1	0.33	-	86,86,86,86	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	DA	3559	1/1	0.60	-	51,51,51,51	0
56	MG	DA	3052	1/1	0.50	-	76,76,76,76	0
56	MG	BA	3469	1/1	0.21	-	82,82,82,82	0
56	MG	BA	3264	1/1	0.47	-	89,89,89,89	0
56	MG	BA	3093	1/1	0.43	-	55,55,55,55	0
56	MG	BB	215	1/1	0.32	-	94,94,94,94	0
56	MG	DA	3273	1/1	0.51	-	30,30,30,30	0
56	MG	BA	3633	1/1	0.47	-	12,12,12,12	0
56	MG	BA	3675	1/1	0.23	-	145,145,145,145	0
56	MG	AA	1627	1/1	0.47	-	64,64,64,64	0
56	MG	CA	1871	1/1	0.14	-	56,56,56,56	0
56	MG	DA	3416	1/1	0.17	-	60,60,60,60	0
56	MG	BA	3178	1/1	0.43	-	52,52,52,52	0
56	MG	DA	3247	1/1	0.23	-	55,55,55,55	0
56	MG	BA	3008	1/1	0.38	-	66,66,66,66	0
56	MG	BA	3331	1/1	0.76	-	121,121,121,121	0
56	MG	BA	3368	1/1	0.29	-	25,25,25,25	0
56	MG	AA	1706	1/1	0.35	-	186,186,186,186	0
56	MG	BA	3050	1/1	0.43	-	60,60,60,60	0
56	MG	CA	1777	1/1	0.26	-	98,98,98,98	0
56	MG	AA	1826	1/1	0.34	-	78,78,78,78	0
56	MG	BA	3393	1/1	0.16	-	99,99,99,99	0
56	MG	BA	2946	1/1	0.50	-	61,61,61,61	0
56	MG	BA	3256	1/1	0.60	-	91,91,91,91	0
56	MG	BA	3000	1/1	0.08	-	64,64,64,64	0
56	MG	DA	3022	1/1	0.18	-	80,80,80,80	0
56	MG	BA	3650	1/1	0.55	-	95,95,95,95	0
56	MG	BA	3078	1/1	0.82	-	117,117,117,117	0
56	MG	DA	3493	1/1	0.16	-	57,57,57,57	0
56	MG	AA	1951	1/1	0.44	-	73,73,73,73	0
56	MG	CA	1674	1/1	0.21	-	107,107,107,107	0
56	MG	BA	3452	1/1	0.69	-	53,53,53,53	0
56	MG	BA	3029	1/1	0.24	-	44,44,44,44	0
56	MG	DA	3079	1/1	0.44	-	62,62,62,62	0
56	MG	DA	3304	1/1	0.18	-	41,41,41,41	0
56	MG	CA	1845	1/1	0.22	-	60,60,60,60	0
56	MG	AA	1831	1/1	1.12	-	203,203,203,203	0
56	MG	AA	1670	1/1	0.32	-	77,77,77,77	0
56	MG	AA	1681	1/1	0.22	-	68,68,68,68	0
56	MG	DB	217	1/1	0.14	-	121,121,121,121	0
56	MG	AA	1799	1/1	0.74	-	85,85,85,85	0
56	MG	DA	3065	1/1	0.20	-	88,88,88,88	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	AA	1774	1/1	0.41	-	68,68,68,68	0
56	MG	DA	3283	1/1	0.34	-	26,26,26,26	0
56	MG	DA	3026	1/1	0.23	-	78,78,78,78	0
56	MG	AA	1762	1/1	0.34	-	95,95,95,95	0
56	MG	CA	1728	1/1	0.16	-	195,195,195,195	0
56	MG	AA	1654	1/1	0.41	-	61,61,61,61	0
56	MG	CA	1789	1/1	0.90	-	184,184,184,184	0
56	MG	BA	3493	1/1	0.25	-	61,61,61,61	0
56	MG	AA	1694	1/1	0.26	-	165,165,165,165	0
56	MG	AA	1963	1/1	0.24	-	80,80,80,80	0
56	MG	AA	1641	1/1	0.12	-	121,121,121,121	0
56	MG	DA	3254	1/1	0.30	-	50,50,50,50	0
56	MG	DA	3293	1/1	0.23	-	58,58,58,58	0
56	MG	BA	3145	1/1	0.40	-	53,53,53,53	0
56	MG	DA	3343	1/1	0.52	-	76,76,76,76	0
56	MG	DA	2937	1/1	0.67	-	104,104,104,104	0
56	MG	AA	1863	1/1	0.33	-	53,53,53,53	0
56	MG	AG	201	1/1	0.91	-	78,78,78,78	0
56	MG	BA	3573	1/1	0.28	-	81,81,81,81	0
56	MG	BA	3153	1/1	0.31	-	81,81,81,81	0
56	MG	DA	2942	1/1	0.17	-	69,69,69,69	0
56	MG	BA	3025	1/1	0.25	-	66,66,66,66	0
56	MG	BA	3676	1/1	0.46	-	181,181,181,181	0
56	MG	BA	3391	1/1	0.61	-	78,78,78,78	0
56	MG	CW	115	1/1	0.31	-	81,81,81,81	0
56	MG	CA	1688	1/1	0.25	-	45,45,45,45	0
56	MG	CA	1868	1/1	0.24	-	69,69,69,69	0
56	MG	BA	3578	1/1	0.35	-	32,32,32,32	0
56	MG	BA	3064	1/1	0.44	-	63,63,63,63	0
56	MG	BA	3212	1/1	0.37	-	109,109,109,109	0
56	MG	BA	3423	1/1	0.25	-	38,38,38,38	0
56	MG	AA	1808	1/1	0.21	-	70,70,70,70	0
56	MG	AA	1771	1/1	0.18	-	55,55,55,55	0
56	MG	DA	3219	1/1	0.31	-	42,42,42,42	0
56	MG	DA	3316	1/1	0.21	-	49,49,49,49	0
56	MG	AA	1855	1/1	0.12	-	103,103,103,103	0
56	MG	DA	3267	1/1	0.15	-	32,32,32,32	0
56	MG	DA	2903	1/1	0.45	-	77,77,77,77	0
56	MG	BA	3215	1/1	0.16	-	88,88,88,88	0
56	MG	DA	3515	1/1	0.07	-	76,76,76,76	0
56	MG	BA	3701	1/1	0.31	-	74,74,74,74	0
56	MG	DA	3286	1/1	0.32	-	42,42,42,42	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	AW	118	1/1	0.53	-	69,69,69,69	0
56	MG	DA	3066	1/1	1.31	-	90,90,90,90	0
56	MG	DA	3364	1/1	0.11	-	80,80,80,80	0
56	MG	BX	102	1/1	0.33	-	50,50,50,50	0
56	MG	DA	3379	1/1	0.24	-	54,54,54,54	0
56	MG	DA	3260	1/1	0.33	-	58,58,58,58	0
56	MG	AA	1672	1/1	0.60	-	73,73,73,73	0
56	MG	CA	1744	1/1	0.20	-	95,95,95,95	0
56	MG	BA	3487	1/1	0.35	-	51,51,51,51	0
56	MG	DA	3373	1/1	0.19	-	86,86,86,86	0
56	MG	AQ	201	1/1	0.18	-	68,68,68,68	0
56	MG	DA	3042	1/1	0.68	-	50,50,50,50	0
56	MG	BA	2959	1/1	0.73	-	81,81,81,81	0
56	MG	CA	1905	1/1	0.31	-	84,84,84,84	0
56	MG	DA	3506	1/1	0.19	-	53,53,53,53	0
56	MG	BB	216	1/1	0.69	-	109,109,109,109	0
56	MG	CA	1691	1/1	0.26	-	161,161,161,161	0
56	MG	BA	3290	1/1	0.31	-	77,77,77,77	0
56	MG	DA	3349	1/1	0.49	-	56,56,56,56	0
56	MG	CA	1675	1/1	0.52	-	75,75,75,75	0
56	MG	BA	3457	1/1	0.35	-	68,68,68,68	0
56	MG	DA	2940	1/1	0.19	-	94,94,94,94	0
56	MG	BA	3694	1/1	0.17	-	35,35,35,35	0
56	MG	BB	209	1/1	0.26	-	91,91,91,91	0
56	MG	DA	3539	1/1	0.32	-	98,98,98,98	0
56	MG	DA	3031	1/1	0.31	-	77,77,77,77	0
56	MG	AA	1891	1/1	0.17	-	67,67,67,67	0
56	MG	BA	3062	1/1	0.18	-	110,110,110,110	0
56	MG	BA	3566	1/1	0.16	-	63,63,63,63	0
56	MG	CA	1605	1/1	0.36	-	159,159,159,159	0
56	MG	DA	3313	1/1	0.40	-	12,12,12,12	0
56	MG	AW	114	1/1	0.19	-	82,82,82,82	0
56	MG	AA	1738	1/1	0.69	-	71,71,71,71	0
56	MG	CW	114	1/1	0.21	-	61,61,61,61	0
56	MG	AA	1733	1/1	0.91	-	94,94,94,94	0
56	MG	BA	3447	1/1	0.21	-	64,64,64,64	0
56	MG	BA	2995	1/1	0.23	-	92,92,92,92	0
56	MG	DA	3342	1/1	0.10	-	83,83,83,83	0
56	MG	DA	3284	1/1	0.33	-	53,53,53,53	0
56	MG	CA	1685	1/1	0.16	-	104,104,104,104	0
56	MG	BA	3104	1/1	0.16	-	120,120,120,120	0
56	MG	DA	2915	1/1	0.71	-	78,78,78,78	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	BA	2967	1/1	0.62	-	77,77,77,77	0
56	MG	DA	3110	1/1	0.25	-	63,63,63,63	0
56	MG	BA	3579	1/1	0.48	-	65,65,65,65	0
56	MG	DA	3321	1/1	0.34	-	66,66,66,66	0
56	MG	BA	3281	1/1	0.23	-	73,73,73,73	0
56	MG	DA	3419	1/1	0.22	-	54,54,54,54	0
56	MG	AA	1622	1/1	0.60	-	70,70,70,70	0
56	MG	CA	1712	1/1	0.20	-	106,106,106,106	0
56	MG	BA	3355	1/1	0.28	-	18,18,18,18	0
56	MG	AA	1792	1/1	0.34	-	84,84,84,84	0
56	MG	BA	3432	1/1	0.46	-	69,69,69,69	0
56	MG	AA	1902	1/1	0.24	-	33,33,33,33	0
56	MG	BA	3309	1/1	0.40	-	68,68,68,68	0
56	MG	DA	3452	1/1	0.31	-	73,73,73,73	0
56	MG	BA	2911	1/1	0.57	-	91,91,91,91	0
56	MG	DA	3619	1/1	0.42	-	53,53,53,53	0
56	MG	BB	219	1/1	0.32	-	33,33,33,33	0
56	MG	BA	3099	1/1	0.42	-	141,141,141,141	0
56	MG	AA	1710	1/1	0.18	-	79,79,79,79	0
56	MG	AA	1666	1/1	0.31	-	91,91,91,91	0
56	MG	BA	2923	1/1	1.17	-	85,85,85,85	0
56	MG	D1	101	1/1	0.15	-	66,66,66,66	0
56	MG	BA	2997	1/1	0.20	-	104,104,104,104	0
56	MG	AA	1655	1/1	0.51	-	80,80,80,80	0
56	MG	AA	1620	1/1	0.28	-	76,76,76,76	0
56	MG	BA	3259	1/1	0.34	-	77,77,77,77	0
56	MG	BA	2969	1/1	0.27	-	79,79,79,79	0
56	MG	CA	1923	1/1	0.15	-	77,77,77,77	0
56	MG	CA	1686	1/1	0.24	-	286,286,286,286	0
56	MG	DA	3138	1/1	0.32	-	12,12,12,12	0
56	MG	BA	3115	1/1	0.20	-	62,62,62,62	0
56	MG	BA	3716	1/1	0.08	-	80,80,80,80	0
56	MG	DA	3460	1/1	0.15	-	67,67,67,67	0
56	MG	DA	2941	1/1	0.19	-	93,93,93,93	0
56	MG	BA	3226	1/1	0.31	-	58,58,58,58	0
56	MG	AA	1862	1/1	0.77	-	212,212,212,212	0
56	MG	AA	1735	1/1	0.40	-	52,52,52,52	0
56	MG	BA	3532	1/1	0.27	-	58,58,58,58	0
56	MG	BA	3564	1/1	0.37	-	28,28,28,28	0
56	MG	DA	3059	1/1	0.29	-	82,82,82,82	0
56	MG	CA	1667	1/1	0.27	-	118,118,118,118	0
56	MG	DA	3106	1/1	0.31	-	79,79,79,79	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	DA	3049	1/1	0.63	-	52,52,52,52	0
56	MG	BB	201	1/1	0.15	-	59,59,59,59	0
56	MG	DA	3450	1/1	0.11	-	64,64,64,64	0
56	MG	DA	3604	1/1	0.41	-	58,58,58,58	0
56	MG	BA	3704	1/1	0.19	-	43,43,43,43	0
56	MG	DA	3440	1/1	0.42	-	58,58,58,58	0
56	MG	BA	3035	1/1	0.13	-	158,158,158,158	0
56	MG	AA	1660	1/1	0.27	-	105,105,105,105	0
56	MG	BA	2938	1/1	0.23	-	81,81,81,81	0
56	MG	DA	3583	1/1	0.17	-	68,68,68,68	0
56	MG	D5	101	1/1	0.21	-	71,71,71,71	0
56	MG	AA	1603	1/1	0.19	-	64,64,64,64	0
56	MG	DA	2993	1/1	0.38	-	85,85,85,85	0
56	MG	AA	1677	1/1	0.19	-	65,65,65,65	0
56	MG	BA	3034	1/1	0.23	-	36,36,36,36	0
56	MG	DA	3576	1/1	0.29	-	102,102,102,102	0
56	MG	BA	2975	1/1	0.29	-	77,77,77,77	0
56	MG	CW	101	1/1	0.39	-	96,96,96,96	0
56	MG	CA	1834	1/1	0.36	-	108,108,108,108	0
56	MG	DA	3525	1/1	0.13	-	58,58,58,58	0
56	MG	BA	3067	1/1	0.14	-	142,142,142,142	0
56	MG	DA	3492	1/1	0.24	-	61,61,61,61	0
56	MG	DA	3157	1/1	0.19	-	23,23,23,23	0
56	MG	DP	202	1/1	0.32	-	73,73,73,73	0
56	MG	DA	2930	1/1	0.56	-	86,86,86,86	0
56	MG	AA	1637	1/1	0.11	-	67,67,67,67	0
56	MG	DA	3594	1/1	0.31	-	50,50,50,50	0
56	MG	AA	1715	1/1	0.14	-	86,86,86,86	0
56	MG	BA	3160	1/1	0.33	-	51,51,51,51	0
56	MG	DV	201	1/1	0.45	-	85,85,85,85	0
56	MG	DA	3099	1/1	0.06	-	79,79,79,79	0
56	MG	AA	1900	1/1	0.31	-	213,213,213,213	0
56	MG	BA	2991	1/1	0.40	-	80,80,80,80	0
56	MG	DA	2928	1/1	0.14	-	55,55,55,55	0
56	MG	CA	1694	1/1	0.59	-	69,69,69,69	0
56	MG	DA	3510	1/1	0.75	-	69,69,69,69	0
56	MG	BA	3139	1/1	0.40	-	73,73,73,73	0
56	MG	DA	3310	1/1	0.49	-	52,52,52,52	0
56	MG	CA	1743	1/1	0.28	-	169,169,169,169	0
56	MG	DA	3299	1/1	0.39	-	38,38,38,38	0
56	MG	AA	1727	1/1	0.50	-	93,93,93,93	0
56	MG	DA	3553	1/1	0.45	-	21,21,21,21	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	DA	3082	1/1	0.10	-	67,67,67,67	0
56	MG	BA	3461	1/1	0.47	-	23,23,23,23	0
56	MG	DA	3132	1/1	0.47	-	13,13,13,13	0
56	MG	BA	3027	1/1	0.21	-	85,85,85,85	0
56	MG	BA	3200	1/1	0.81	-	63,63,63,63	0
56	MG	CY	401	1/1	0.57	-	103,103,103,103	0
56	MG	BA	3608	1/1	0.99	-	54,54,54,54	0
56	MG	DA	3523	1/1	1.03	-	76,76,76,76	0
56	MG	BA	2932	1/1	0.16	-	78,78,78,78	0
56	MG	DA	3105	1/1	0.38	-	94,94,94,94	0
56	MG	AA	1770	1/1	0.36	-	86,86,86,86	0
56	MG	BA	2955	1/1	0.24	-	45,45,45,45	0
56	MG	CA	1796	1/1	0.15	-	41,41,41,41	0
56	MG	CA	1836	1/1	0.35	-	94,94,94,94	0
56	MG	DA	3527	1/1	0.32	-	77,77,77,77	0
56	MG	DB	201	1/1	0.43	-	62,62,62,62	0
56	MG	DA	3229	1/1	0.26	-	37,37,37,37	0
56	MG	BA	3571	1/1	0.45	-	68,68,68,68	0
56	MG	BA	3225	1/1	0.31	-	96,96,96,96	0
56	MG	CA	1823	1/1	0.26	-	166,166,166,166	0
56	MG	DA	3487	1/1	0.60	-	108,108,108,108	0
56	MG	DA	3439	1/1	0.30	-	66,66,66,66	0
56	MG	CA	1874	1/1	1.31	-	89,89,89,89	0
56	MG	BA	3405	1/1	0.80	-	64,64,64,64	0
56	MG	AA	1954	1/1	0.27	-	142,142,142,142	0
56	MG	DA	3610	1/1	0.52	-	56,56,56,56	0
56	MG	BA	2977	1/1	0.25	-	72,72,72,72	0
56	MG	BA	3540	1/1	0.61	-	84,84,84,84	0
56	MG	BA	2908	1/1	0.37	-	235,235,235,235	0
56	MG	CA	1702	1/1	0.51	-	75,75,75,75	0
56	MG	CA	1729	1/1	0.23	-	139,139,139,139	0
56	MG	BA	2925	1/1	0.59	-	76,76,76,76	0
56	MG	DP	201	1/1	0.24	-	43,43,43,43	0
56	MG	BA	3384	1/1	0.14	-	71,71,71,71	0
56	MG	AA	1886	1/1	0.42	-	65,65,65,65	0
56	MG	CA	1803	1/1	0.26	-	146,146,146,146	0
56	MG	CA	1908	1/1	0.32	-	84,84,84,84	0
56	MG	BA	3289	1/1	0.22	-	83,83,83,83	0
56	MG	DA	2912	1/1	0.33	-	78,78,78,78	0
56	MG	AA	1621	1/1	0.16	-	74,74,74,74	0
56	MG	AA	1709	1/1	0.19	-	71,71,71,71	0
56	MG	BA	3011	1/1	0.57	-	82,82,82,82	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	DA	3467	1/1	0.21	-	60,60,60,60	0
56	MG	BA	3364	1/1	0.15	-	82,82,82,82	0
56	MG	B0	101	1/1	0.24	-	33,33,33,33	0
56	MG	AA	1829	1/1	1.29	-	232,232,232,232	0
56	MG	BA	3522	1/1	1.15	-	96,96,96,96	0
56	MG	BA	3019	1/1	0.18	-	109,109,109,109	0
56	MG	BA	3389	1/1	0.29	-	47,47,47,47	0
56	MG	CA	1693	1/1	0.40	-	67,67,67,67	0
56	MG	BB	214	1/1	0.29	-	68,68,68,68	0
56	MG	BA	3656	1/1	0.23	-	31,31,31,31	0
56	MG	DA	3496	1/1	0.39	-	40,40,40,40	0
56	MG	AA	1759	1/1	0.96	-	88,88,88,88	0
56	MG	AA	1652	1/1	0.22	-	98,98,98,98	0
56	MG	CA	1713	1/1	0.22	-	88,88,88,88	0
56	MG	BA	3692	1/1	0.39	-	56,56,56,56	0
56	MG	DA	2967	1/1	0.85	-	86,86,86,86	0
56	MG	BA	2926	1/1	0.55	-	80,80,80,80	0
56	MG	BA	2974	1/1	0.24	-	85,85,85,85	0
56	MG	DA	3615	1/1	0.30	-	57,57,57,57	0
56	MG	BA	2933	1/1	0.19	-	69,69,69,69	0
56	MG	AA	1968	1/1	0.91	-	86,86,86,86	0
56	MG	AT	201	1/1	0.32	-	117,117,117,117	0
56	MG	DA	3622	1/1	0.22	-	50,50,50,50	0
56	MG	DA	3212	1/1	0.51	-	42,42,42,42	0
56	MG	DA	3517	1/1	0.37	-	62,62,62,62	0
56	MG	CA	1650	1/1	0.17	-	170,170,170,170	0
56	MG	DA	3429	1/1	0.75	-	59,59,59,59	0
56	MG	BA	3110	1/1	0.30	-	72,72,72,72	0
56	MG	AA	1685	1/1	0.14	-	199,199,199,199	0
56	MG	BA	3615	1/1	0.18	-	73,73,73,73	0
56	MG	DA	3159	1/1	0.32	-	62,62,62,62	0
56	MG	BA	3439	1/1	0.35	-	59,59,59,59	0
56	MG	DA	3139	1/1	0.27	-	33,33,33,33	0
56	MG	AA	1788	1/1	0.25	-	175,175,175,175	0
56	MG	CA	1857	1/1	0.58	-	73,73,73,73	0
56	MG	BA	3450	1/1	0.83	-	83,83,83,83	0
56	MG	DA	3302	1/1	0.38	-	83,83,83,83	0
56	MG	BA	2996	1/1	0.22	-	209,209,209,209	0
56	MG	CA	1668	1/1	0.34	-	118,118,118,118	0
56	MG	AA	1794	1/1	0.11	-	151,151,151,151	0
56	MG	BA	3175	1/1	0.49	-	109,109,109,109	0
56	MG	AA	1988	1/1	0.35	-	53,53,53,53	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	DA	3331	1/1	0.25	-	93,93,93,93	0
56	MG	BA	3084	1/1	0.45	-	73,73,73,73	0
56	MG	CA	1895	1/1	0.30	-	126,126,126,126	0
56	MG	DB	218	1/1	0.49	-	111,111,111,111	0
56	MG	DA	2924	1/1	0.51	-	43,43,43,43	0
56	MG	CA	1882	1/1	0.53	-	81,81,81,81	0
56	MG	AW	102	1/1	0.32	-	94,94,94,94	0
56	MG	AA	1857	1/1	0.61	-	45,45,45,45	0
56	MG	DA	3023	1/1	0.42	-	71,71,71,71	0
56	MG	BA	3204	1/1	0.33	-	65,65,65,65	0
56	MG	AA	1905	1/1	0.20	-	59,59,59,59	0
56	MG	BA	3538	1/1	0.33	-	82,82,82,82	0
56	MG	BA	3665	1/1	0.23	-	117,117,117,117	0
56	MG	DA	3017	1/1	0.20	-	60,60,60,60	0
56	MG	BA	3670	1/1	0.29	-	79,79,79,79	0
56	MG	BA	3249	1/1	0.25	-	84,84,84,84	0
56	MG	BA	3102	1/1	0.18	-	61,61,61,61	0
56	MG	BA	3273	1/1	0.43	-	110,110,110,110	0
56	MG	CA	1775	1/1	0.26	-	47,47,47,47	0
56	MG	DA	3197	1/1	0.19	-	21,21,21,21	0
56	MG	DA	3226	1/1	0.33	-	20,20,20,20	0
56	MG	DA	3196	1/1	0.36	-	30,30,30,30	0
56	MG	CA	1692	1/1	0.28	-	62,62,62,62	0
56	MG	BA	3399	1/1	0.54	-	38,38,38,38	0
56	MG	AW	105	1/1	0.09	-	55,55,55,55	0
56	MG	DA	3630	1/1	0.15	-	76,76,76,76	0
56	MG	BA	3417	1/1	0.25	-	56,56,56,56	0
56	MG	AA	1912	1/1	0.30	-	87,87,87,87	0
56	MG	BB	207	1/1	0.15	-	84,84,84,84	0
56	MG	BA	2954	1/1	0.30	-	77,77,77,77	0
56	MG	BA	3322	1/1	0.28	-	46,46,46,46	0
56	MG	AA	1748	1/1	0.28	-	54,54,54,54	0
56	MG	DA	3354	1/1	0.49	-	33,33,33,33	0
56	MG	CA	1666	1/1	0.39	-	73,73,73,73	0
56	MG	DA	2975	1/1	0.85	-	79,79,79,79	0
56	MG	DA	3285	1/1	0.21	-	63,63,63,63	0
56	MG	DA	3520	1/1	0.69	-	93,93,93,93	0
56	MG	AA	1941	1/1	0.62	-	100,100,100,100	0
56	MG	BA	3159	1/1	0.13	-	151,151,151,151	0
56	MG	DA	3039	1/1	0.75	-	72,72,72,72	0
56	MG	BA	3348	1/1	0.41	-	25,25,25,25	0
56	MG	DA	3477	1/1	0.69	-	56,56,56,56	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	DA	3124	1/1	0.33	-	32,32,32,32	0
56	MG	AA	1719	1/1	0.13	-	92,92,92,92	0
56	MG	BA	2931	1/1	0.52	-	98,98,98,98	0
56	MG	BA	3016	1/1	0.20	-	168,168,168,168	0
56	MG	AA	1630	1/1	0.57	-	55,55,55,55	0
56	MG	DA	3585	1/1	0.26	-	66,66,66,66	0
56	MG	AA	1928	1/1	0.10	-	67,67,67,67	0
56	MG	CA	1855	1/1	0.27	-	197,197,197,197	0
56	MG	AA	1921	1/1	0.37	-	68,68,68,68	0
56	MG	BA	3291	1/1	0.35	-	94,94,94,94	0
56	MG	BA	3345	1/1	0.33	-	20,20,20,20	0
56	MG	BA	3403	1/1	0.48	-	79,79,79,79	0
56	MG	DA	3305	1/1	0.37	-	46,46,46,46	0
56	MG	DA	3118	1/1	0.15	-	61,61,61,61	0
56	MG	BB	217	1/1	0.17	-	99,99,99,99	0
56	MG	DA	3631	1/1	0.20	-	85,85,85,85	0
56	MG	DA	3369	1/1	0.66	-	86,86,86,86	0
56	MG	BA	3465	1/1	0.52	-	114,114,114,114	0
56	MG	DA	3111	1/1	0.26	-	84,84,84,84	0
56	MG	BA	3657	1/1	0.31	-	55,55,55,55	0
56	MG	DB	220	1/1	0.32	-	40,40,40,40	0
56	MG	DA	3536	1/1	0.68	-	50,50,50,50	0
56	MG	BA	3287	1/1	0.28	-	55,55,55,55	0
56	MG	DA	2988	1/1	0.21	-	85,85,85,85	0
56	MG	BA	3664	1/1	0.24	-	82,82,82,82	0
56	MG	BA	3472	1/1	0.55	-	56,56,56,56	0
56	MG	BA	3554	1/1	0.30	-	62,62,62,62	0
56	MG	BA	3507	1/1	0.29	-	56,56,56,56	0
56	MG	BA	3274	1/1	0.15	-	105,105,105,105	0
56	MG	CA	1847	1/1	0.31	-	84,84,84,84	0
56	MG	CA	1624	1/1	0.35	-	98,98,98,98	0
56	MG	DA	3224	1/1	0.20	-	40,40,40,40	0
56	MG	DA	3175	1/1	0.35	-	38,38,38,38	0
56	MG	BA	3347	1/1	0.25	-	27,27,27,27	0
56	MG	AA	1687	1/1	0.12	-	85,85,85,85	0
56	MG	AA	1838	1/1	0.26	-	56,56,56,56	0
56	MG	AA	1883	1/1	0.41	-	50,50,50,50	0
56	MG	CA	1885	1/1	0.29	-	270,270,270,270	0
56	MG	BA	3090	1/1	0.44	-	60,60,60,60	0
56	MG	DA	3470	1/1	0.27	-	81,81,81,81	0
56	MG	DA	2919	1/1	0.58	-	50,50,50,50	0
56	MG	BA	3612	1/1	0.40	-	96,96,96,96	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	DA	3323	1/1	0.15	-	42,42,42,42	0
56	MG	DA	3617	1/1	0.21	-	46,46,46,46	0
56	MG	BA	3307	1/1	0.18	-	83,83,83,83	0
56	MG	AA	1701	1/1	0.13	-	79,79,79,79	0
56	MG	DA	2936	1/1	0.47	-	82,82,82,82	0
56	MG	BA	3605	1/1	0.10	-	72,72,72,72	0
56	MG	BA	3549	1/1	0.17	-	66,66,66,66	0
56	MG	CA	1822	1/1	0.25	-	112,112,112,112	0
56	MG	BA	3534	1/1	0.17	-	32,32,32,32	0
56	MG	DA	2909	1/1	0.56	-	85,85,85,85	0
56	MG	CA	1739	1/1	0.15	-	122,122,122,122	0
56	MG	BA	3577	1/1	0.90	-	88,88,88,88	0
56	MG	DA	3586	1/1	0.63	-	133,133,133,133	0
56	MG	BA	3666	1/1	0.28	-	67,67,67,67	0
56	MG	BA	3003	1/1	0.63	-	113,113,113,113	0
56	MG	BA	3536	1/1	0.63	-	66,66,66,66	0
56	MG	DA	3557	1/1	0.21	-	16,16,16,16	0
56	MG	CA	1849	1/1	0.18	-	75,75,75,75	0
56	MG	BA	3176	1/1	0.29	-	52,52,52,52	0
56	MG	AA	1653	1/1	0.24	-	105,105,105,105	0
56	MG	DA	3233	1/1	0.36	-	62,62,62,62	0
56	MG	AA	1817	1/1	0.56	-	175,175,175,175	0
56	MG	DA	3502	1/1	1.35	-	73,73,73,73	0
56	MG	CA	1846	1/1	0.34	-	101,101,101,101	0
56	MG	AA	1753	1/1	0.46	-	72,72,72,72	0
56	MG	AA	1786	1/1	0.48	-	71,71,71,71	0
56	MG	BA	3707	1/1	0.05	-	84,84,84,84	0
56	MG	AA	1699	1/1	0.41	-	85,85,85,85	0
56	MG	BA	3699	1/1	0.33	-	70,70,70,70	0
56	MG	CA	1622	1/1	0.46	-	59,59,59,59	0
56	MG	DA	3577	1/1	0.71	-	80,80,80,80	0
56	MG	DA	3362	1/1	0.95	-	83,83,83,83	0
56	MG	DA	2955	1/1	0.27	-	30,30,30,30	0
56	MG	CA	1638	1/1	0.14	-	118,118,118,118	0
56	MG	BX	101	1/1	0.11	-	55,55,55,55	0
56	MG	BA	3690	1/1	0.12	-	66,66,66,66	0
56	MG	AA	1848	1/1	0.25	-	125,125,125,125	0
56	MG	BA	3088	1/1	0.19	-	167,167,167,167	0
56	MG	DA	2917	1/1	0.44	-	83,83,83,83	0
56	MG	BA	3081	1/1	0.19	-	79,79,79,79	0
56	MG	AA	1936	1/1	0.84	-	94,94,94,94	0
56	MG	CA	1824	1/1	0.75	-	118,118,118,118	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	DA	2995	1/1	0.17	-	65,65,65,65	0
56	MG	DA	3489	1/1	0.33	-	51,51,51,51	0
56	MG	DA	3315	1/1	0.68	-	60,60,60,60	0
56	MG	BA	3429	1/1	0.59	-	43,43,43,43	0
56	MG	DA	3014	1/1	0.19	-	54,54,54,54	0
56	MG	BA	3325	1/1	0.58	-	39,39,39,39	0
56	MG	CD	302	1/1	0.43	-	111,111,111,111	0
56	MG	AA	1890	1/1	0.15	-	124,124,124,124	0
56	MG	CA	1761	1/1	0.47	-	49,49,49,49	0
56	MG	DA	3427	1/1	1.16	-	84,84,84,84	0
56	MG	DB	202	1/1	0.07	-	51,51,51,51	0
56	MG	DA	3484	1/1	0.57	-	98,98,98,98	0
56	MG	DA	3041	1/1	0.17	-	59,59,59,59	0
56	MG	BA	2990	1/1	0.10	-	47,47,47,47	0
56	MG	BA	3051	1/1	0.32	-	32,32,32,32	0
56	MG	AA	1810	1/1	0.08	-	87,87,87,87	0
56	MG	BA	3630	1/1	0.32	-	19,19,19,19	0
56	MG	CA	1922	1/1	0.28	-	67,67,67,67	0
56	MG	AA	1772	1/1	0.44	-	94,94,94,94	0
56	MG	DA	3378	1/1	0.35	-	54,54,54,54	0
56	MG	CA	1897	1/1	0.22	-	227,227,227,227	0
56	MG	BA	3518	1/1	0.23	-	27,27,27,27	0
56	MG	DA	3387	1/1	0.27	-	39,39,39,39	0
56	MG	BA	3424	1/1	0.17	-	32,32,32,32	0
56	MG	BA	3170	1/1	0.39	-	60,60,60,60	0
56	MG	AA	1812	1/1	0.40	-	273,273,273,273	0
56	MG	CA	1615	1/1	0.63	-	110,110,110,110	0
56	MG	DA	3572	1/1	0.12	-	51,51,51,51	0
56	MG	DA	3501	1/1	0.09	-	96,96,96,96	0
56	MG	AA	1718	1/1	0.19	-	75,75,75,75	0
56	MG	AA	1640	1/1	0.13	-	102,102,102,102	0
56	MG	CA	1869	1/1	0.34	-	95,95,95,95	0
56	MG	DA	3121	1/1	0.20	-	41,41,41,41	0
56	MG	AW	112	1/1	0.59	-	82,82,82,82	0
56	MG	DQ	203	1/1	0.17	-	67,67,67,67	0
56	MG	DA	3269	1/1	0.23	-	42,42,42,42	0
56	MG	DA	2957	1/1	0.38	-	64,64,64,64	0
56	MG	CA	1640	1/1	0.32	-	78,78,78,78	0
56	MG	AA	1745	1/1	0.29	-	80,80,80,80	0
56	MG	DA	3511	1/1	0.31	-	64,64,64,64	0
56	MG	BA	3623	1/1	0.27	-	79,79,79,79	0
56	MG	CV	101	1/1	0.34	-	87,87,87,87	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	BA	3188	1/1	0.39	-	78,78,78,78	0
56	MG	DA	3548	1/1	0.41	-	85,85,85,85	0
56	MG	BA	3677	1/1	0.40	-	18,18,18,18	0
56	MG	CA	1756	1/1	0.29	-	60,60,60,60	0
56	MG	BA	2973	1/1	0.55	-	160,160,160,160	0
56	MG	AA	1827	1/1	0.34	-	98,98,98,98	0
56	MG	AA	1858	1/1	0.22	-	132,132,132,132	0
56	MG	BA	2943	1/1	1.06	-	98,98,98,98	0
56	MG	DA	3550	1/1	0.39	-	18,18,18,18	0
56	MG	DA	3446	1/1	0.15	-	59,59,59,59	0
56	MG	BA	3341	1/1	0.27	-	69,69,69,69	0
56	MG	DA	3606	1/1	0.16	-	54,54,54,54	0
56	MG	CA	1715	1/1	0.31	-	79,79,79,79	0
56	MG	AA	1611	1/1	0.24	-	109,109,109,109	0
56	MG	CA	1614	1/1	0.51	-	122,122,122,122	0
56	MG	CA	1787	1/1	0.29	-	77,77,77,77	0
56	MG	DA	3328	1/1	0.56	-	48,48,48,48	0
56	MG	DA	3415	1/1	0.42	-	46,46,46,46	0
56	MG	BA	3065	1/1	0.18	-	90,90,90,90	0
56	MG	BA	3490	1/1	0.16	-	45,45,45,45	0
56	MG	BA	3097	1/1	0.64	-	73,73,73,73	0
56	MG	BA	3054	1/1	0.33	-	91,91,91,91	0
56	MG	CA	1604	1/1	0.46	-	99,99,99,99	0
56	MG	CW	107	1/1	0.10	-	50,50,50,50	0
56	MG	DA	2904	1/1	0.55	-	71,71,71,71	0
56	MG	BA	3244	1/1	1.26	-	67,67,67,67	0
56	MG	DA	2918	1/1	0.12	-	49,49,49,49	0
56	MG	BA	3057	1/1	0.34	-	65,65,65,65	0
56	MG	AA	1638	1/1	0.74	-	132,132,132,132	0
56	MG	BA	3095	1/1	0.46	-	90,90,90,90	0
56	MG	DB	205	1/1	0.29	-	94,94,94,94	0
56	MG	CA	1725	1/1	0.98	-	78,78,78,78	0
56	MG	AA	1669	1/1	0.58	-	68,68,68,68	0
56	MG	BA	3227	1/1	0.13	-	90,90,90,90	0
56	MG	DA	3396	1/1	0.23	-	18,18,18,18	0
56	MG	AA	1702	1/1	0.83	-	97,97,97,97	0
56	MG	DA	3185	1/1	0.17	-	12,12,12,12	0
56	MG	AA	1796	1/1	0.83	-	129,129,129,129	0
56	MG	DA	3474	1/1	0.24	-	55,55,55,55	0
56	MG	BA	3158	1/1	0.26	-	150,150,150,150	0
56	MG	BA	3655	1/1	0.41	-	87,87,87,87	0
56	MG	AA	1708	1/1	0.25	-	103,103,103,103	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	CA	1853	1/1	0.13	-	52,52,52,52	0
56	MG	DA	3365	1/1	0.40	-	55,55,55,55	0
56	MG	CA	1774	1/1	0.30	-	59,59,59,59	0
56	MG	DA	3607	1/1	0.18	-	30,30,30,30	0
56	MG	DA	3130	1/1	0.62	-	69,69,69,69	0
56	MG	DA	3225	1/1	0.43	-	59,59,59,59	0
56	MG	DA	3528	1/1	0.33	-	54,54,54,54	0
56	MG	DA	3232	1/1	0.63	-	48,48,48,48	0
56	MG	BA	3581	1/1	0.55	-	94,94,94,94	0
56	MG	BA	3126	1/1	0.70	-	235,235,235,235	0
56	MG	AA	1623	1/1	0.08	-	84,84,84,84	0
56	MG	AA	1717	1/1	0.32	-	99,99,99,99	0
56	MG	BA	3535	1/1	0.32	-	68,68,68,68	0
56	MG	DA	3259	1/1	0.34	-	49,49,49,49	0
56	MG	DA	3393	1/1	0.57	-	95,95,95,95	0
56	MG	BA	3292	1/1	0.61	-	40,40,40,40	0
56	MG	AA	1734	1/1	0.22	-	66,66,66,66	0
56	MG	AA	1615	1/1	0.22	-	87,87,87,87	0
56	MG	DA	3495	1/1	0.11	-	63,63,63,63	0
56	MG	BA	3555	1/1	0.20	-	94,94,94,94	0
56	MG	BA	3172	1/1	0.25	-	62,62,62,62	0
56	MG	DA	2926	1/1	0.44	-	91,91,91,91	0
56	MG	BA	3063	1/1	0.52	-	75,75,75,75	0
56	MG	AA	1842	1/1	0.23	-	98,98,98,98	0
56	MG	BA	3569	1/1	0.50	-	87,87,87,87	0
56	MG	CA	1906	1/1	0.11	-	114,114,114,114	0
56	MG	BA	3648	1/1	0.28	-	54,54,54,54	0
56	MG	DA	3480	1/1	0.25	-	42,42,42,42	0
56	MG	BB	212	1/1	0.24	-	99,99,99,99	0
56	MG	DA	3037	1/1	0.44	-	77,77,77,77	0
56	MG	CA	1778	1/1	0.47	-	36,36,36,36	0
56	MG	DA	3504	1/1	0.28	-	68,68,68,68	0
56	MG	BA	3673	1/1	0.27	-	133,133,133,133	0
56	MG	DA	3096	1/1	0.32	-	82,82,82,82	0
56	MG	BA	3183	1/1	0.17	-	79,79,79,79	0
56	MG	BA	3194	1/1	0.37	-	91,91,91,91	0
56	MG	AA	1662	1/1	0.24	-	108,108,108,108	0
56	MG	BA	3105	1/1	0.23	-	122,122,122,122	0
56	MG	BA	3319	1/1	0.41	-	19,19,19,19	0
56	MG	DA	3423	1/1	0.19	-	35,35,35,35	0
56	MG	BA	2981	1/1	0.36	-	79,79,79,79	0
56	MG	D5	102	1/1	0.09	-	68,68,68,68	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	AA	1777	1/1	0.20	-	101,101,101,101	0
56	MG	DA	2990	1/1	0.29	-	61,61,61,61	0
56	MG	CA	1910	1/1	0.32	-	77,77,77,77	0
56	MG	AA	1645	1/1	0.36	-	82,82,82,82	0
56	MG	DA	3186	1/1	0.17	-	51,51,51,51	0
56	MG	DA	3380	1/1	0.30	-	85,85,85,85	0
56	MG	BA	3094	1/1	0.43	-	38,38,38,38	0
56	MG	AA	1899	1/1	0.15	-	89,89,89,89	0
56	MG	B5	101	1/1	0.22	-	34,34,34,34	0
56	MG	DA	3347	1/1	0.21	-	23,23,23,23	0
56	MG	CA	1602	1/1	0.22	-	112,112,112,112	0
56	MG	BA	3476	1/1	0.76	-	52,52,52,52	0
56	MG	BA	3398	1/1	0.60	-	64,64,64,64	0
56	MG	BA	3055	1/1	0.30	-	71,71,71,71	0
56	MG	BA	3111	1/1	0.14	-	96,96,96,96	0
56	MG	BA	3594	1/1	0.38	-	88,88,88,88	0
56	MG	BA	3010	1/1	0.36	-	93,93,93,93	0
56	MG	DA	3095	1/1	0.13	-	100,100,100,100	0
56	MG	CA	1697	1/1	0.69	-	50,50,50,50	0
56	MG	AA	1824	1/1	0.58	-	108,108,108,108	0
56	MG	BA	3503	1/1	0.80	-	195,195,195,195	0
56	MG	DA	3391	1/1	0.16	-	57,57,57,57	0
56	MG	BA	3548	1/1	0.71	-	88,88,88,88	0
56	MG	CA	1695	1/1	0.33	-	108,108,108,108	0
56	MG	CA	1851	1/1	0.41	-	94,94,94,94	0
56	MG	BA	2948	1/1	0.52	-	56,56,56,56	0
56	MG	AA	1978	1/1	0.29	-	129,129,129,129	0
56	MG	BA	3464	1/1	0.31	-	84,84,84,84	0
56	MG	DA	2921	1/1	0.15	-	113,113,113,113	0
56	MG	DA	3491	1/1	0.33	-	71,71,71,71	0
56	MG	DA	3552	1/1	0.50	-	19,19,19,19	0
56	MG	BA	3659	1/1	0.14	-	46,46,46,46	0
56	MG	AA	1607	1/1	0.51	-	97,97,97,97	0
56	MG	CA	1601	1/1	0.17	-	34,34,34,34	0
56	MG	AA	1865	1/1	0.51	-	98,98,98,98	0
56	MG	BA	3711	1/1	0.17	-	104,104,104,104	0
56	MG	BA	3367	1/1	0.34	-	84,84,84,84	0
56	MG	DA	3566	1/1	0.23	-	43,43,43,43	0
56	MG	AA	1650	1/1	0.14	-	93,93,93,93	0
56	MG	BA	3619	1/1	0.26	-	53,53,53,53	0
56	MG	DA	3372	1/1	0.21	-	40,40,40,40	0
56	MG	BA	2909	1/1	0.32	-	114,114,114,114	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	DA	3360	1/1	0.22	-	64,64,64,64	0
56	MG	BA	3222	1/1	0.43	-	70,70,70,70	0
56	MG	BA	3047	1/1	0.28	-	50,50,50,50	0
56	MG	BA	2956	1/1	0.14	-	42,42,42,42	0
56	MG	DA	3058	1/1	0.11	-	72,72,72,72	0
56	MG	DB	203	1/1	0.12	-	66,66,66,66	0
56	MG	BA	3022	1/1	1.01	-	168,168,168,168	0
56	MG	BA	3376	1/1	0.17	-	59,59,59,59	0
56	MG	BA	3245	1/1	0.54	-	185,185,185,185	0
56	MG	BA	3353	1/1	0.36	-	54,54,54,54	0
56	MG	AA	1647	1/1	0.18	-	34,34,34,34	0
56	MG	CA	1881	1/1	0.19	-	111,111,111,111	0
56	MG	CA	1817	1/1	0.36	-	111,111,111,111	0
56	MG	BA	3446	1/1	0.21	-	93,93,93,93	0
56	MG	DA	3456	1/1	0.17	-	116,116,116,116	0
56	MG	BA	2924	1/1	1.07	-	64,64,64,64	0
56	MG	BA	3342	1/1	0.21	-	25,25,25,25	0
56	MG	DA	3272	1/1	0.22	-	53,53,53,53	0
56	MG	AA	1882	1/1	0.44	-	32,32,32,32	0
56	MG	BA	3565	1/1	0.34	-	63,63,63,63	0
56	MG	CA	1734	1/1	0.21	-	196,196,196,196	0
56	MG	BA	3688	1/1	0.17	-	59,59,59,59	0
56	MG	CA	1665	1/1	0.55	-	94,94,94,94	0
56	MG	CA	1742	1/1	0.60	-	61,61,61,61	0
56	MG	AW	110	1/1	0.25	-	145,145,145,145	0
56	MG	BA	2915	1/1	0.26	-	102,102,102,102	0
56	MG	DA	3580	1/1	0.43	-	79,79,79,79	0
56	MG	BA	3545	1/1	0.48	-	245,245,245,245	0
56	MG	DA	3494	1/1	0.26	-	112,112,112,112	0
56	MG	DA	3443	1/1	0.20	-	45,45,45,45	0
56	MG	DX	101	1/1	0.34	-	99,99,99,99	0
56	MG	BA	3106	1/1	0.22	-	57,57,57,57	0
56	MG	DA	3114	1/1	0.16	-	81,81,81,81	0
56	MG	AA	1632	1/1	0.46	-	87,87,87,87	0
56	MG	BA	3107	1/1	0.55	-	87,87,87,87	0
56	MG	DA	3198	1/1	0.43	-	41,41,41,41	0
56	MG	BA	3500	1/1	0.47	-	72,72,72,72	0
56	MG	DA	3339	1/1	0.33	-	63,63,63,63	0
56	MG	BA	2912	1/1	0.43	-	67,67,67,67	0
56	MG	CA	1610	1/1	0.34	-	78,78,78,78	0
56	MG	DA	2932	1/1	0.11	-	59,59,59,59	0
56	MG	BA	3231	1/1	0.24	-	39,39,39,39	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	CA	1877	1/1	0.89	-	154,154,154,154	0
56	MG	DA	3560	1/1	0.40	-	55,55,55,55	0
56	MG	DA	3612	1/1	0.18	-	52,52,52,52	0
56	MG	BA	3414	1/1	0.62	-	47,47,47,47	0
56	MG	DA	3144	1/1	0.41	-	14,14,14,14	0
56	MG	DA	2956	1/1	0.32	-	59,59,59,59	0
56	MG	CA	1863	1/1	0.34	-	69,69,69,69	0
56	MG	DA	3407	1/1	0.10	-	62,62,62,62	0
56	MG	AT	202	1/1	0.40	-	100,100,100,100	0
56	MG	BA	3516	1/1	0.15	-	29,29,29,29	0
56	MG	AA	1852	1/1	0.12	-	89,89,89,89	0
56	MG	BA	2966	1/1	0.18	-	49,49,49,49	0
56	MG	BA	3166	1/1	0.37	-	70,70,70,70	0
56	MG	DA	3250	1/1	0.62	-	77,77,77,77	0
56	MG	DA	3428	1/1	0.66	-	71,71,71,71	0
56	MG	DA	2971	1/1	0.14	-	132,132,132,132	0
56	MG	CA	1617	1/1	0.42	-	69,69,69,69	0
56	MG	AW	106	1/1	0.19	-	87,87,87,87	0
56	MG	CA	1759	1/1	0.42	-	65,65,65,65	0
56	MG	CA	1903	1/1	0.27	-	73,73,73,73	0
56	MG	BB	210	1/1	0.14	-	88,88,88,88	0
56	MG	BA	3437	1/1	0.87	-	82,82,82,82	0
56	MG	DA	3279	1/1	0.23	-	29,29,29,29	0
56	MG	CA	1619	1/1	0.10	-	128,128,128,128	0
56	MG	BA	3485	1/1	0.50	-	53,53,53,53	0
56	MG	BA	3686	1/1	0.43	-	28,28,28,28	0
56	MG	BB	218	1/1	0.44	-	50,50,50,50	0
56	MG	DA	3008	1/1	0.60	-	70,70,70,70	0
56	MG	AA	1991	1/1	0.09	-	96,96,96,96	0
56	MG	CA	1699	1/1	0.56	-	152,152,152,152	0
56	MG	AA	1711	1/1	0.18	-	83,83,83,83	0
56	MG	DA	3614	1/1	0.30	-	50,50,50,50	0
56	MG	DA	3449	1/1	0.27	-	53,53,53,53	0
56	MG	DA	3306	1/1	0.53	-	48,48,48,48	0
56	MG	CA	1733	1/1	0.11	-	197,197,197,197	0
56	MG	CA	1837	1/1	0.25	-	66,66,66,66	0
56	MG	DA	3402	1/1	0.62	-	28,28,28,28	0
56	MG	CA	1890	1/1	0.25	-	59,59,59,59	0
56	MG	DA	3514	1/1	0.21	-	48,48,48,48	0
56	MG	BA	3213	1/1	0.50	-	125,125,125,125	0
56	MG	DA	3543	1/1	0.16	-	88,88,88,88	0
56	MG	BA	3678	1/1	0.29	-	20,20,20,20	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	CA	1722	1/1	0.79	-	168,168,168,168	0
56	MG	DB	210	1/1	0.27	-	82,82,82,82	0
56	MG	DA	3116	1/1	0.13	-	124,124,124,124	0
56	MG	DA	3574	1/1	0.50	-	67,67,67,67	0
56	MG	DA	3007	1/1	0.17	-	70,70,70,70	0
56	MG	DB	209	1/1	0.96	-	143,143,143,143	0
56	MG	BA	3096	1/1	0.62	-	173,173,173,173	0
56	MG	DA	3045	1/1	0.47	-	62,62,62,62	0
56	MG	DA	3370	1/1	0.45	-	66,66,66,66	0
56	MG	AA	1983	1/1	1.09	-	76,76,76,76	0
56	MG	BA	3026	1/1	0.54	-	114,114,114,114	0
56	MG	DA	3067	1/1	0.66	-	83,83,83,83	0
56	MG	DA	3252	1/1	0.36	-	42,42,42,42	0
56	MG	DA	3371	1/1	0.40	-	65,65,65,65	0
56	MG	BA	3248	1/1	0.49	-	102,102,102,102	0
56	MG	CW	103	1/1	0.09	-	57,57,57,57	0
56	MG	BA	3257	1/1	0.59	-	69,69,69,69	0
56	MG	CA	1661	1/1	0.22	-	68,68,68,68	0
56	MG	BD	301	1/1	0.20	-	15,15,15,15	0
56	MG	DA	2961	1/1	0.40	-	143,143,143,143	0
56	MG	AA	1904	1/1	0.44	-	43,43,43,43	0
56	MG	BA	3509	1/1	0.25	-	75,75,75,75	0
56	MG	DA	3308	1/1	0.87	-	72,72,72,72	0
56	MG	DA	3589	1/1	0.16	-	74,74,74,74	0
56	MG	DA	3151	1/1	0.21	-	12,12,12,12	0
56	MG	BA	3198	1/1	0.50	-	66,66,66,66	0
56	MG	DA	2938	1/1	0.38	-	71,71,71,71	0
56	MG	DA	3332	1/1	0.28	-	45,45,45,45	0
56	MG	AA	1639	1/1	0.78	-	114,114,114,114	0
56	MG	BA	3024	1/1	0.27	-	65,65,65,65	0
56	MG	BA	3602	1/1	0.46	-	117,117,117,117	0
56	MG	CA	1719	1/1	0.44	-	106,106,106,106	0
56	MG	BA	3529	1/1	0.31	-	79,79,79,79	0
56	MG	BA	3658	1/1	0.58	-	71,71,71,71	0
56	MG	AA	1869	1/1	0.57	-	34,34,34,34	0
56	MG	CA	1723	1/1	0.18	-	76,76,76,76	0
56	MG	DA	3521	1/1	0.31	-	93,93,93,93	0
56	MG	BA	2988	1/1	0.37	-	77,77,77,77	0
56	MG	BA	3085	1/1	0.50	-	116,116,116,116	0
56	MG	BA	3684	1/1	0.33	-	47,47,47,47	0
56	MG	DA	3412	1/1	0.25	-	60,60,60,60	0
56	MG	DA	3101	1/1	0.33	-	101,101,101,101	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	DA	3061	1/1	0.10	-	62,62,62,62	0
56	MG	AA	1967	1/1	0.27	-	61,61,61,61	0
56	MG	AA	1966	1/1	0.30	-	51,51,51,51	0
56	MG	AA	1915	1/1	0.15	-	50,50,50,50	0
56	MG	DA	2905	1/1	0.14	-	87,87,87,87	0
56	MG	BA	3041	1/1	0.27	-	68,68,68,68	0
56	MG	CA	1831	1/1	0.47	-	62,62,62,62	0
56	MG	AA	1736	1/1	0.55	-	83,83,83,83	0
56	MG	DA	3275	1/1	0.80	-	52,52,52,52	0
56	MG	DA	2933	1/1	0.30	-	35,35,35,35	0
56	MG	CA	1613	1/1	0.71	-	71,71,71,71	0
56	MG	BA	3400	1/1	0.21	-	37,37,37,37	0
56	MG	CA	1884	1/1	0.52	-	79,79,79,79	0
56	MG	DA	3214	1/1	0.38	-	22,22,22,22	0
56	MG	DA	3128	1/1	0.31	-	101,101,101,101	0
56	MG	DA	3618	1/1	0.23	-	69,69,69,69	0
56	MG	BA	3488	1/1	0.31	-	62,62,62,62	0
56	MG	CA	1632	1/1	0.18	-	84,84,84,84	0
56	MG	BA	3206	1/1	0.27	-	176,176,176,176	0
56	MG	AA	1608	1/1	0.73	-	108,108,108,108	0
56	MG	BA	3165	1/1	0.24	-	59,59,59,59	0
56	MG	BA	3413	1/1	0.16	-	21,21,21,21	0
56	MG	BA	3179	1/1	0.75	-	98,98,98,98	0
56	MG	BA	3366	1/1	0.48	-	31,31,31,31	0
56	MG	DA	3295	1/1	0.32	-	48,48,48,48	0
56	MG	CW	106	1/1	0.15	-	59,59,59,59	0
56	MG	DA	3043	1/1	1.31	-	77,77,77,77	0
56	MG	BA	3272	1/1	0.29	-	49,49,49,49	0
56	MG	AA	1664	1/1	0.34	-	64,64,64,64	0
56	MG	AA	1835	1/1	0.93	-	76,76,76,76	0
56	MG	BA	3642	1/1	0.37	-	34,34,34,34	0
56	MG	BA	3533	1/1	0.17	-	97,97,97,97	0
56	MG	DA	3071	1/1	0.14	-	92,92,92,92	0
56	MG	BA	3652	1/1	0.20	-	63,63,63,63	0
56	MG	DA	3529	1/1	0.30	-	70,70,70,70	0
56	MG	DA	3398	1/1	0.89	-	107,107,107,107	0
56	MG	AA	1853	1/1	0.30	-	69,69,69,69	0
56	MG	DA	3322	1/1	0.17	-	46,46,46,46	0
56	MG	AA	1910	1/1	0.65	-	68,68,68,68	0
56	MG	BA	3644	1/1	0.42	-	106,106,106,106	0
56	MG	BA	3140	1/1	0.37	-	55,55,55,55	0
56	MG	DA	3047	1/1	0.64	-	69,69,69,69	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	AA	1680	1/1	0.16	-	87,87,87,87	0
56	MG	DA	2973	1/1	0.23	-	57,57,57,57	0
56	MG	AA	1679	1/1	0.16	-	112,112,112,112	0
56	MG	DA	3204	1/1	0.18	-	35,35,35,35	0
56	MG	BA	2928	1/1	0.14	-	80,80,80,80	0
56	MG	BA	2994	1/1	0.52	-	71,71,71,71	0
56	MG	BA	3181	1/1	0.56	-	56,56,56,56	0
56	MG	CA	1918	1/1	0.19	-	107,107,107,107	0
56	MG	DA	3587	1/1	0.11	-	90,90,90,90	0
56	MG	BA	3363	1/1	0.43	-	19,19,19,19	0
56	MG	CA	1835	1/1	0.58	-	61,61,61,61	0
56	MG	BA	3304	1/1	0.32	-	167,167,167,167	0
56	MG	BA	3017	1/1	0.41	-	27,27,27,27	0
56	MG	DA	3357	1/1	0.48	-	78,78,78,78	0
56	MG	AA	1957	1/1	0.90	-	109,109,109,109	0
56	MG	DA	3209	1/1	0.23	-	17,17,17,17	0
56	MG	BA	3344	1/1	0.50	-	39,39,39,39	0
56	MG	CA	1841	1/1	0.78	-	77,77,77,77	0
56	MG	CA	1673	1/1	0.34	-	73,73,73,73	0
56	MG	DA	3090	1/1	0.25	-	47,47,47,47	0
56	MG	BP	201	1/1	0.34	-	54,54,54,54	0
56	MG	BA	3433	1/1	0.38	-	97,97,97,97	0
56	MG	CA	1689	1/1	0.27	-	52,52,52,52	0
56	MG	DA	3002	1/1	0.36	-	139,139,139,139	0
56	MG	BA	3637	1/1	0.13	-	20,20,20,20	0
56	MG	DA	3389	1/1	0.21	-	68,68,68,68	0
56	MG	AA	1813	1/1	0.29	-	134,134,134,134	0
56	MG	DA	3234	1/1	0.10	-	31,31,31,31	0
56	MG	DA	3100	1/1	0.44	-	97,97,97,97	0
56	MG	BA	3635	1/1	0.43	-	37,37,37,37	0
56	MG	BA	3674	1/1	0.30	-	55,55,55,55	0
56	MG	AA	1613	1/1	0.16	-	83,83,83,83	0
56	MG	AA	1859	1/1	0.35	-	177,177,177,177	0
57	ZN	CD	301	1/1	0.33	-	109,109,109,109	0
56	MG	DA	3444	1/1	0.25	-	55,55,55,55	0
56	MG	CA	1645	1/1	1.02	-	113,113,113,113	0
56	MG	DA	3184	1/1	0.38	-	14,14,14,14	0
56	MG	BA	3359	1/1	0.10	-	106,106,106,106	0
56	MG	BA	3649	1/1	0.28	-	104,104,104,104	0
56	MG	AW	109	1/1	0.85	-	91,91,91,91	0
56	MG	BA	3199	1/1	0.31	-	69,69,69,69	0
56	MG	BA	3467	1/1	0.14	-	103,103,103,103	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	BA	3352	1/1	0.21	-	17,17,17,17	0
56	MG	BA	3250	1/1	0.19	-	269,269,269,269	0
56	MG	BA	2901	1/1	0.90	-	123,123,123,123	0
56	MG	DA	3532	1/1	0.29	-	72,72,72,72	0
56	MG	DA	3089	1/1	0.09	-	70,70,70,70	0
56	MG	AA	1926	1/1	0.46	-	37,37,37,37	0
56	MG	DA	3590	1/1	0.57	-	74,74,74,74	0
56	MG	AA	1825	1/1	0.47	-	138,138,138,138	0
56	MG	BA	2999	1/1	0.07	-	92,92,92,92	0
56	MG	DA	3570	1/1	0.37	-	72,72,72,72	0
56	MG	CA	1678	1/1	1.68	-	128,128,128,128	0
56	MG	CA	1721	1/1	0.15	-	74,74,74,74	0
56	MG	AA	1752	1/1	0.46	-	183,183,183,183	0
56	MG	BA	3512	1/1	0.18	-	42,42,42,42	0
56	MG	AA	1757	1/1	0.33	-	74,74,74,74	0
56	MG	AA	1955	1/1	0.26	-	87,87,87,87	0
56	MG	BA	3724	1/1	0.72	-	119,119,119,119	0
56	MG	CA	1843	1/1	0.33	-	103,103,103,103	0
56	MG	DA	3117	1/1	0.28	-	72,72,72,72	0
56	MG	DA	2952	1/1	0.61	-	68,68,68,68	0
56	MG	BA	3253	1/1	0.22	-	73,73,73,73	0
56	MG	DA	3203	1/1	0.21	-	51,51,51,51	0
56	MG	DA	3473	1/1	0.26	-	51,51,51,51	0
56	MG	DA	3069	1/1	0.29	-	32,32,32,32	0
56	MG	CW	113	1/1	0.21	-	89,89,89,89	0
56	MG	DA	3568	1/1	0.42	-	65,65,65,65	0
56	MG	AA	1938	1/1	0.18	-	72,72,72,72	0
56	MG	BA	3174	1/1	0.22	-	69,69,69,69	0
56	MG	CA	1780	1/1	0.55	-	72,72,72,72	0
56	MG	CA	1763	1/1	0.19	-	46,46,46,46	0
56	MG	AA	1850	1/1	0.17	-	98,98,98,98	0
56	MG	AA	1885	1/1	0.18	-	61,61,61,61	0
56	MG	BA	3616	1/1	0.72	-	62,62,62,62	0
56	MG	DA	3190	1/1	0.15	-	25,25,25,25	0
56	MG	BA	3531	1/1	0.33	-	71,71,71,71	0
56	MG	AA	1940	1/1	0.17	-	82,82,82,82	0
56	MG	BA	3267	1/1	0.36	-	123,123,123,123	0
56	MG	BA	3207	1/1	0.25	-	65,65,65,65	0
56	MG	AA	1927	1/1	0.16	-	48,48,48,48	0
56	MG	DA	3287	1/1	0.86	-	44,44,44,44	0
56	MG	BA	3157	1/1	0.70	-	57,57,57,57	0
56	MG	DA	3466	1/1	0.25	-	90,90,90,90	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	AA	1636	1/1	0.21	-	97,97,97,97	0
56	MG	BT	201	1/1	0.24	-	63,63,63,63	0
56	MG	DA	3016	1/1	0.37	-	99,99,99,99	0
56	MG	BA	3151	1/1	0.30	-	80,80,80,80	0
56	MG	CA	1816	1/1	0.64	-	77,77,77,77	0
56	MG	CA	1637	1/1	0.35	-	53,53,53,53	0
56	MG	DA	3220	1/1	0.28	-	43,43,43,43	0
56	MG	DA	3009	1/1	0.54	-	130,130,130,130	0
56	MG	AA	1929	1/1	0.31	-	79,79,79,79	0
56	MG	DA	3626	1/1	0.38	-	117,117,117,117	0
56	MG	AA	1830	1/1	0.68	-	179,179,179,179	0
56	MG	CA	1797	1/1	0.97	-	61,61,61,61	0
56	MG	DA	3624	1/1	0.23	-	35,35,35,35	0
56	MG	CA	1618	1/1	0.48	-	49,49,49,49	0
56	MG	CA	1771	1/1	0.15	-	70,70,70,70	0
56	MG	AA	1768	1/1	0.18	-	183,183,183,183	0
56	MG	DA	3490	1/1	0.24	-	96,96,96,96	0
56	MG	DA	3401	1/1	0.35	-	81,81,81,81	0
56	MG	DA	2987	1/1	0.20	-	63,63,63,63	0
56	MG	BA	3007	1/1	0.54	-	170,170,170,170	0
56	MG	AA	1987	1/1	0.58	-	121,121,121,121	0
56	MG	AA	1815	1/1	0.36	-	74,74,74,74	0
56	MG	DA	3034	1/1	0.65	-	49,49,49,49	0
56	MG	BA	3638	1/1	0.30	-	73,73,73,73	0
56	MG	BA	3255	1/1	0.36	-	66,66,66,66	0
56	MG	BA	3621	1/1	0.45	-	106,106,106,106	0
56	MG	DA	3432	1/1	0.32	-	104,104,104,104	0
56	MG	BA	3501	1/1	0.20	-	52,52,52,52	0
56	MG	BA	3320	1/1	0.40	-	23,23,23,23	0
56	MG	DA	3282	1/1	0.41	-	42,42,42,42	0
56	MG	BA	3196	1/1	0.09	-	84,84,84,84	0
56	MG	BA	3613	1/1	0.55	-	76,76,76,76	0
56	MG	DA	2925	1/1	0.58	-	80,80,80,80	0
56	MG	DA	3392	1/1	0.12	-	38,38,38,38	0
56	MG	BA	3661	1/1	0.69	-	56,56,56,56	0
56	MG	DA	3579	1/1	0.39	-	36,36,36,36	0
56	MG	BA	2902	1/1	0.20	-	86,86,86,86	0
56	MG	AA	1807	1/1	0.24	-	45,45,45,45	0
56	MG	AA	1832	1/1	0.16	-	67,67,67,67	0
56	MG	CA	1883	1/1	0.25	-	78,78,78,78	0
56	MG	AA	1894	1/1	0.23	-	124,124,124,124	0
56	MG	AA	1958	1/1	0.28	-	72,72,72,72	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	BA	3543	1/1	0.26	-	53,53,53,53	0
56	MG	BA	3651	1/1	0.27	-	92,92,92,92	0
56	MG	BA	3167	1/1	0.37	-	60,60,60,60	0
56	MG	BA	2910	1/1	0.09	-	79,79,79,79	0
56	MG	DA	2943	1/1	0.15	-	25,25,25,25	0
56	MG	BA	2921	1/1	0.60	-	95,95,95,95	0
56	MG	DA	3411	1/1	0.67	-	59,59,59,59	0
56	MG	AA	1919	1/1	0.51	-	47,47,47,47	0
56	MG	AA	1816	1/1	0.24	-	69,69,69,69	0
56	MG	DA	3500	1/1	0.85	-	72,72,72,72	0
56	MG	BA	3459	1/1	0.21	-	80,80,80,80	0
56	MG	BA	3211	1/1	0.49	-	71,71,71,71	0
56	MG	AA	1952	1/1	0.08	-	53,53,53,53	0
56	MG	BA	3517	1/1	0.56	-	55,55,55,55	0
56	MG	DA	3556	1/1	0.25	-	19,19,19,19	0
56	MG	DA	3558	1/1	0.35	-	14,14,14,14	0
56	MG	DA	3181	1/1	0.34	-	13,13,13,13	0
56	MG	BA	3418	1/1	0.16	-	27,27,27,27	0
56	MG	BA	3285	1/1	0.21	-	66,66,66,66	0
56	MG	CA	1644	1/1	1.07	-	120,120,120,120	0
56	MG	BA	3570	1/1	0.15	-	83,83,83,83	0
56	MG	CA	1926	1/1	0.80	-	101,101,101,101	0
56	MG	CA	1754	1/1	1.33	-	162,162,162,162	0
56	MG	DA	3565	1/1	0.18	-	51,51,51,51	0
56	MG	AA	1849	1/1	0.20	-	95,95,95,95	0
56	MG	BA	3607	1/1	0.18	-	105,105,105,105	0
56	MG	DA	3368	1/1	0.14	-	83,83,83,83	0
56	MG	BA	3521	1/1	0.20	-	53,53,53,53	0
56	MG	CA	1603	1/1	0.23	-	255,255,255,255	0
56	MG	AA	1803	1/1	0.29	-	77,77,77,77	0
56	MG	DA	3571	1/1	0.99	-	70,70,70,70	0
56	MG	AA	1906	1/1	0.71	-	38,38,38,38	0
56	MG	CW	110	1/1	0.12	-	90,90,90,90	0
56	MG	BA	3357	1/1	0.20	-	64,64,64,64	0
56	MG	DA	3335	1/1	0.33	-	38,38,38,38	0
56	MG	AA	1769	1/1	0.38	-	79,79,79,79	0
56	MG	CA	1711	1/1	0.64	-	88,88,88,88	0
56	MG	DA	3537	1/1	0.34	-	62,62,62,62	0
56	MG	AA	1840	1/1	1.26	-	79,79,79,79	0
56	MG	CA	1782	1/1	0.56	-	56,56,56,56	0
56	MG	BA	2982	1/1	0.29	-	86,86,86,86	0
56	MG	AA	1674	1/1	0.27	-	126,126,126,126	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	BA	3238	1/1	0.47	-	61,61,61,61	0
56	MG	DA	2901	1/1	0.24	-	47,47,47,47	0
56	MG	BA	3239	1/1	0.43	-	99,99,99,99	0
56	MG	DA	3395	1/1	0.11	-	95,95,95,95	0
56	MG	BA	3109	1/1	0.24	-	63,63,63,63	0
56	MG	AA	1722	1/1	0.32	-	72,72,72,72	0
56	MG	BA	3346	1/1	0.12	-	111,111,111,111	0
56	MG	CA	1768	1/1	0.23	-	55,55,55,55	0
56	MG	BA	3640	1/1	0.43	-	60,60,60,60	0
56	MG	DA	3356	1/1	0.12	-	107,107,107,107	0
56	MG	DA	3336	1/1	0.15	-	51,51,51,51	0
56	MG	BA	2929	1/1	0.53	-	64,64,64,64	0
56	MG	BA	3700	1/1	0.37	-	60,60,60,60	0
56	MG	BA	3492	1/1	0.50	-	102,102,102,102	0
56	MG	CA	1864	1/1	0.40	-	157,157,157,157	0
56	MG	BA	3312	1/1	0.49	-	20,20,20,20	0
56	MG	BA	3014	1/1	0.23	-	44,44,44,44	0
56	MG	DA	3609	1/1	0.24	-	27,27,27,27	0
56	MG	AA	1965	1/1	0.12	-	37,37,37,37	0
56	MG	DA	3311	1/1	0.34	-	54,54,54,54	0
56	MG	CW	112	1/1	0.26	-	103,103,103,103	0
56	MG	DA	3001	1/1	0.56	-	79,79,79,79	0
56	MG	AA	1914	1/1	0.13	-	53,53,53,53	0
56	MG	BA	3460	1/1	0.32	-	51,51,51,51	0
56	MG	DA	2922	1/1	0.15	-	47,47,47,47	0
56	MG	BA	2971	1/1	0.91	-	89,89,89,89	0
56	MG	DA	3216	1/1	0.27	-	23,23,23,23	0
56	MG	DA	3475	1/1	0.19	-	54,54,54,54	0
56	MG	BA	3329	1/1	0.47	-	19,19,19,19	0
56	MG	D7	102	1/1	0.21	-	32,32,32,32	0
56	MG	DA	3164	1/1	0.18	-	30,30,30,30	0
56	MG	BA	3164	1/1	0.31	-	62,62,62,62	0
56	MG	DA	3326	1/1	0.40	-	47,47,47,47	0
56	MG	DA	3403	1/1	0.79	-	77,77,77,77	0
56	MG	BA	3180	1/1	0.71	-	113,113,113,113	0
56	MG	CA	1717	1/1	0.29	-	121,121,121,121	0
56	MG	BA	3308	1/1	0.15	-	88,88,88,88	0
56	MG	AA	1901	1/1	0.29	-	71,71,71,71	0
56	MG	DA	3107	1/1	0.66	-	139,139,139,139	0
56	MG	AA	1617	1/1	0.20	-	108,108,108,108	0
56	MG	BA	3083	1/1	0.20	-	69,69,69,69	0
56	MG	BA	3002	1/1	0.37	-	91,91,91,91	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	DA	3438	1/1	0.33	-	73,73,73,73	0
56	MG	BA	3356	1/1	0.30	-	43,43,43,43	0
56	MG	AA	1783	1/1	0.44	-	127,127,127,127	0
56	MG	AA	1962	1/1	0.36	-	55,55,55,55	0
56	MG	DA	2906	1/1	0.24	-	70,70,70,70	0
56	MG	CA	1770	1/1	0.29	-	39,39,39,39	0
56	MG	DA	3627	1/1	0.30	-	81,81,81,81	0
56	MG	DA	3363	1/1	0.18	-	42,42,42,42	0
56	MG	AA	1932	1/1	0.46	-	159,159,159,159	0
56	MG	AC	301	1/1	1.42	-	98,98,98,98	0
56	MG	DB	208	1/1	0.26	-	83,83,83,83	0
56	MG	AA	1673	1/1	0.21	-	104,104,104,104	0
56	MG	AA	1990	1/1	0.25	-	58,58,58,58	0
56	MG	CA	1608	1/1	0.05	-	86,86,86,86	0
56	MG	DA	3388	1/1	0.14	-	63,63,63,63	0
56	MG	DH	201	1/1	0.28	-	64,64,64,64	0
56	MG	DA	3300	1/1	0.22	-	69,69,69,69	0
56	MG	BA	3568	1/1	0.15	-	84,84,84,84	0
56	MG	CA	1651	1/1	0.37	-	95,95,95,95	0
56	MG	CA	1710	1/1	1.15	-	97,97,97,97	0
56	MG	BA	2964	1/1	0.24	-	74,74,74,74	0
56	MG	AA	1713	1/1	0.13	-	84,84,84,84	0
56	MG	CA	1794	1/1	0.35	-	60,60,60,60	0
56	MG	CA	1639	1/1	0.08	-	100,100,100,100	0
56	MG	DA	3120	1/1	0.37	-	76,76,76,76	0
56	MG	AA	1864	1/1	0.24	-	116,116,116,116	0
56	MG	BA	3108	1/1	0.40	-	61,61,61,61	0
56	MG	BA	3669	1/1	0.63	-	53,53,53,53	0
56	MG	DA	3588	1/1	0.27	-	24,24,24,24	0
56	MG	CW	104	1/1	0.36	-	87,87,87,87	0
56	MG	DA	3085	1/1	0.22	-	49,49,49,49	0
56	MG	BA	2985	1/1	0.32	-	61,61,61,61	0
56	MG	DA	3011	1/1	0.40	-	47,47,47,47	0
56	MG	CA	1680	1/1	0.87	-	77,77,77,77	0
56	MG	DA	3213	1/1	0.29	-	60,60,60,60	0
56	MG	DA	3156	1/1	0.33	-	33,33,33,33	0
56	MG	CA	1867	1/1	0.23	-	82,82,82,82	0
56	MG	CA	1757	1/1	0.46	-	43,43,43,43	0
56	MG	DA	3103	1/1	0.14	-	65,65,65,65	0
56	MG	BA	3235	1/1	0.07	-	63,63,63,63	0
56	MG	BA	3268	1/1	0.50	-	102,102,102,102	0
56	MG	BA	3190	1/1	0.33	-	49,49,49,49	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	DA	3448	1/1	0.18	-	43,43,43,43	0
56	MG	BA	3350	1/1	0.34	-	28,28,28,28	0
56	MG	CA	1870	1/1	0.09	-	73,73,73,73	0
56	MG	BA	3590	1/1	0.30	-	90,90,90,90	0
56	MG	DA	3534	1/1	0.54	-	70,70,70,70	0
56	MG	DA	3513	1/1	0.24	-	34,34,34,34	0
56	MG	CA	1776	1/1	0.69	-	125,125,125,125	0
56	MG	BA	3541	1/1	0.26	-	44,44,44,44	0
56	MG	AA	1665	1/1	0.17	-	59,59,59,59	0
56	MG	BA	3679	1/1	0.30	-	27,27,27,27	0
56	MG	BA	2937	1/1	0.23	-	71,71,71,71	0
56	MG	AA	1688	1/1	0.24	-	80,80,80,80	0
56	MG	DA	3021	1/1	0.47	-	66,66,66,66	0
56	MG	DA	3005	1/1	0.40	-	89,89,89,89	0
56	MG	DA	3441	1/1	0.38	-	46,46,46,46	0
56	MG	AA	1692	1/1	0.42	-	134,134,134,134	0
56	MG	DA	3097	1/1	0.53	-	68,68,68,68	0
56	MG	AA	1723	1/1	0.24	-	106,106,106,106	0
56	MG	BA	3618	1/1	0.52	-	79,79,79,79	0
56	MG	BA	3251	1/1	0.25	-	55,55,55,55	0
56	MG	CM	201	1/1	1.19	-	84,84,84,84	0
56	MG	DA	3599	1/1	0.32	-	14,14,14,14	0
56	MG	BA	3458	1/1	0.21	-	52,52,52,52	0
56	MG	BA	3009	1/1	0.19	-	86,86,86,86	0
56	MG	DA	3235	1/1	0.65	-	41,41,41,41	0
56	MG	BA	2961	1/1	0.20	-	83,83,83,83	0
56	MG	CA	1682	1/1	0.11	-	152,152,152,152	0
56	MG	AA	1884	1/1	0.38	-	47,47,47,47	0
56	MG	DA	2962	1/1	0.15	-	59,59,59,59	0
56	MG	AA	1873	1/1	0.24	-	110,110,110,110	0
56	MG	CA	1751	1/1	0.64	-	163,163,163,163	0
56	MG	BA	3038	1/1	0.17	-	58,58,58,58	0
56	MG	DA	2953	1/1	0.18	-	151,151,151,151	0
56	MG	BA	3156	1/1	0.51	-	74,74,74,74	0
56	MG	BE	301	1/1	0.45	-	60,60,60,60	0
56	MG	CA	1866	1/1	0.61	-	85,85,85,85	0
56	MG	CA	1875	1/1	0.90	-	267,267,267,267	0
56	MG	DA	2964	1/1	0.40	-	65,65,65,65	0
56	MG	BA	3276	1/1	0.59	-	107,107,107,107	0
56	MG	BA	3639	1/1	0.40	-	79,79,79,79	0
56	MG	DQ	201	1/1	0.19	-	49,49,49,49	0
56	MG	AA	1747	1/1	0.34	-	109,109,109,109	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	DA	3459	1/1	0.27	-	76,76,76,76	0
56	MG	BA	3592	1/1	0.26	-	132,132,132,132	0
56	MG	BA	3119	1/1	1.45	-	133,133,133,133	0
56	MG	AA	1658	1/1	0.17	-	76,76,76,76	0
56	MG	DA	3222	1/1	0.36	-	17,17,17,17	0
56	MG	AA	1624	1/1	0.46	-	45,45,45,45	0
56	MG	BA	3260	1/1	0.22	-	109,109,109,109	0
56	MG	DA	2939	1/1	0.60	-	66,66,66,66	0
56	MG	DA	3384	1/1	0.30	-	62,62,62,62	0
56	MG	BA	3514	1/1	1.23	-	80,80,80,80	0
56	MG	AA	1728	1/1	0.22	-	130,130,130,130	0
56	MG	BA	2952	1/1	0.09	-	55,55,55,55	0
56	MG	BA	3033	1/1	0.21	-	78,78,78,78	0
56	MG	BA	3580	1/1	0.47	-	60,60,60,60	0
56	MG	DA	3530	1/1	0.28	-	70,70,70,70	0
56	MG	BA	2916	1/1	0.28	-	37,37,37,37	0
56	MG	BA	3505	1/1	1.22	-	101,101,101,101	0
56	MG	DA	3383	1/1	0.42	-	51,51,51,51	0
56	MG	CA	1795	1/1	0.65	-	84,84,84,84	0
56	MG	BA	3068	1/1	0.53	-	115,115,115,115	0
56	MG	BA	3436	1/1	0.30	-	86,86,86,86	0
56	MG	AY	403	1/1	0.83	-	87,87,87,87	0
56	MG	CA	1747	1/1	1.13	-	122,122,122,122	0
56	MG	DA	3485	1/1	0.73	-	120,120,120,120	0
56	MG	BA	2907	1/1	0.34	-	129,129,129,129	0
56	MG	BA	3474	1/1	0.41	-	44,44,44,44	0
56	MG	CA	1891	1/1	0.20	-	63,63,63,63	0
56	MG	BA	3100	1/1	0.15	-	70,70,70,70	0
56	MG	AA	1971	1/1	0.17	-	60,60,60,60	0
56	MG	CA	1652	1/1	0.74	-	193,193,193,193	0
56	MG	AA	1982	1/1	0.11	-	73,73,73,73	0
56	MG	AY	402	1/1	0.18	-	40,40,40,40	0
56	MG	BA	3028	1/1	0.53	-	70,70,70,70	0
56	MG	DA	3070	1/1	0.59	-	69,69,69,69	0
56	MG	BA	3191	1/1	0.29	-	64,64,64,64	0
56	MG	AA	1980	1/1	0.52	-	76,76,76,76	0
56	MG	CA	1840	1/1	0.57	-	101,101,101,101	0
57	ZN	AN	101	1/1	0.15	-	115,115,115,115	0
56	MG	DA	3133	1/1	0.34	-	20,20,20,20	0
56	MG	BA	3695	1/1	0.10	-	95,95,95,95	0
56	MG	CA	1900	1/1	0.50	-	112,112,112,112	0
56	MG	CW	105	1/1	0.60	-	65,65,65,65	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	BA	3462	1/1	0.40	-	95,95,95,95	0
56	MG	BA	3060	1/1	0.56	-	80,80,80,80	0
56	MG	BA	3301	1/1	0.17	-	64,64,64,64	0
56	MG	DA	2999	1/1	0.19	-	102,102,102,102	0
56	MG	CA	1909	1/1	0.15	-	133,133,133,133	0
56	MG	AA	1642	1/1	0.24	-	120,120,120,120	0
56	MG	AA	1766	1/1	0.29	-	77,77,77,77	0
56	MG	BA	3103	1/1	0.39	-	89,89,89,89	0
56	MG	BA	3660	1/1	0.36	-	45,45,45,45	0
56	MG	AA	1604	1/1	0.20	-	91,91,91,91	0
56	MG	AA	1758	1/1	0.16	-	48,48,48,48	0
56	MG	BA	3563	1/1	0.68	-	83,83,83,83	0
56	MG	BA	3372	1/1	0.28	-	27,27,27,27	0
56	MG	AA	1907	1/1	0.51	-	45,45,45,45	0
56	MG	CA	1814	1/1	0.24	-	156,156,156,156	0
56	MG	DA	3240	1/1	0.13	-	35,35,35,35	0
56	MG	BA	3045	1/1	0.95	-	103,103,103,103	0
56	MG	DA	3329	1/1	0.32	-	46,46,46,46	0
56	MG	CA	1612	1/1	0.28	-	82,82,82,82	0
56	MG	BA	3698	1/1	0.33	-	55,55,55,55	0
56	MG	D5	103	1/1	0.31	-	61,61,61,61	0
56	MG	BA	3709	1/1	0.33	-	97,97,97,97	0
56	MG	AA	1949	1/1	0.14	-	60,60,60,60	0
56	MG	BA	3634	1/1	0.36	-	11,11,11,11	0
56	MG	DA	3126	1/1	0.55	-	65,65,65,65	0
56	MG	BA	3282	1/1	0.59	-	78,78,78,78	0
56	MG	BA	3449	1/1	0.35	-	49,49,49,49	0
56	MG	AY	401	1/1	0.54	-	119,119,119,119	0
56	MG	BA	3101	1/1	0.15	-	106,106,106,106	0
56	MG	DA	3547	1/1	0.44	-	70,70,70,70	0
56	MG	CA	1753	1/1	0.27	-	63,63,63,63	0
56	MG	BA	3685	1/1	1.04	-	79,79,79,79	0
56	MG	BA	3523	1/1	0.55	-	47,47,47,47	0
56	MG	CA	1700	1/1	0.98	-	180,180,180,180	0
56	MG	DA	2963	1/1	0.43	-	62,62,62,62	0
56	MG	DA	3261	1/1	0.27	-	32,32,32,32	0
56	MG	BA	3539	1/1	0.50	-	71,71,71,71	0
56	MG	DA	3561	1/1	0.17	-	16,16,16,16	0
56	MG	CA	1907	1/1	0.52	-	77,77,77,77	0
56	MG	BA	3132	1/1	0.45	-	53,53,53,53	0
56	MG	AA	1854	1/1	0.51	-	187,187,187,187	0
56	MG	BA	3161	1/1	0.41	-	73,73,73,73	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	DA	2954	1/1	0.42	-	90,90,90,90	0
56	MG	CA	1856	1/1	0.36	-	136,136,136,136	0
56	MG	BA	3265	1/1	0.23	-	114,114,114,114	0
56	MG	DA	3390	1/1	0.78	-	53,53,53,53	0
56	MG	DA	3507	1/1	0.42	-	70,70,70,70	0
56	MG	DA	3276	1/1	0.18	-	26,26,26,26	0
56	MG	BA	3354	1/1	0.33	-	38,38,38,38	0
56	MG	DA	3461	1/1	0.15	-	73,73,73,73	0
56	MG	BA	2942	1/1	0.51	-	37,37,37,37	0
56	MG	CA	1879	1/1	0.35	-	53,53,53,53	0
56	MG	BA	3263	1/1	0.41	-	66,66,66,66	0
56	MG	BA	3149	1/1	0.19	-	44,44,44,44	0
56	MG	BA	3021	1/1	0.09	-	111,111,111,111	0
56	MG	BA	3606	1/1	0.37	-	72,72,72,72	0
56	MG	DA	3270	1/1	0.65	-	69,69,69,69	0
56	MG	BA	3689	1/1	0.30	-	67,67,67,67	0
56	MG	CA	1792	1/1	0.98	-	122,122,122,122	0
56	MG	DA	3352	1/1	0.12	-	86,86,86,86	0
56	MG	AW	107	1/1	0.48	-	102,102,102,102	0
56	MG	CA	1896	1/1	0.38	-	95,95,95,95	0
56	MG	DA	2974	1/1	0.18	-	90,90,90,90	0
56	MG	DA	3165	1/1	0.48	-	25,25,25,25	0
56	MG	DA	3414	1/1	0.12	-	48,48,48,48	0
56	MG	BA	3723	1/1	0.20	-	71,71,71,71	0
56	MG	AA	1970	1/1	0.50	-	62,62,62,62	0
56	MG	BA	3324	1/1	0.32	-	15,15,15,15	0
56	MG	AA	1911	1/1	0.11	-	38,38,38,38	0
56	MG	BA	3370	1/1	0.43	-	50,50,50,50	0
56	MG	BA	3310	1/1	0.44	-	117,117,117,117	0
56	MG	BA	2941	1/1	0.33	-	87,87,87,87	0
56	MG	AA	1942	1/1	0.16	-	92,92,92,92	0
56	MG	BA	2965	1/1	0.47	-	167,167,167,167	0
56	MG	DA	3353	1/1	0.11	-	66,66,66,66	0
56	MG	CA	1671	1/1	0.33	-	92,92,92,92	0
56	MG	BA	3453	1/1	0.43	-	40,40,40,40	0
56	MG	DA	3076	1/1	0.35	-	88,88,88,88	0
56	MG	DA	2991	1/1	0.73	-	80,80,80,80	0
56	MG	AA	1787	1/1	0.30	-	79,79,79,79	0
56	MG	DA	3180	1/1	0.45	-	37,37,37,37	0
56	MG	BA	3416	1/1	0.39	-	42,42,42,42	0
56	MG	DA	3174	1/1	0.31	-	49,49,49,49	0
56	MG	BA	2986	1/1	0.41	-	45,45,45,45	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	DA	3093	1/1	0.47	-	76,76,76,76	0
56	MG	AA	1880	1/1	0.31	-	43,43,43,43	0
56	MG	CA	1706	1/1	0.23	-	88,88,88,88	0
56	MG	BA	3379	1/1	0.34	-	23,23,23,23	0
56	MG	DA	2972	1/1	0.67	-	187,187,187,187	0
56	MG	AA	1704	1/1	0.46	-	186,186,186,186	0
56	MG	DA	2981	1/1	0.56	-	105,105,105,105	0
56	MG	DI	202	1/1	0.14	-	54,54,54,54	0
56	MG	BB	206	1/1	0.23	-	188,188,188,188	0
56	MG	BA	3524	1/1	0.30	-	95,95,95,95	0
56	MG	DA	3168	1/1	0.42	-	33,33,33,33	0
56	MG	CA	1924	1/1	0.53	-	73,73,73,73	0
56	MG	CA	1631	1/1	1.27	-	119,119,119,119	0
56	MG	CA	1606	1/1	0.39	-	115,115,115,115	0
56	MG	BA	3546	1/1	0.63	-	200,200,200,200	0
56	MG	BA	2917	1/1	0.55	-	188,188,188,188	0
56	MG	BA	3647	1/1	0.32	-	88,88,88,88	0
56	MG	DA	2959	1/1	0.56	-	48,48,48,48	0
56	MG	DA	3399	1/1	0.10	-	85,85,85,85	0
56	MG	DA	3596	1/1	0.42	-	15,15,15,15	0
56	MG	BA	3258	1/1	0.65	-	67,67,67,67	0
56	MG	DA	3386	1/1	0.19	-	102,102,102,102	0
56	MG	BA	3150	1/1	0.27	-	79,79,79,79	0
56	MG	DA	3621	1/1	0.41	-	77,77,77,77	0
56	MG	AW	117	1/1	0.12	-	68,68,68,68	0
56	MG	DA	3413	1/1	0.64	-	79,79,79,79	0
56	MG	AA	1947	1/1	0.46	-	89,89,89,89	0
56	MG	DA	3593	1/1	0.14	-	70,70,70,70	0
56	MG	DA	3512	1/1	0.50	-	33,33,33,33	0
56	MG	DA	3228	1/1	0.43	-	31,31,31,31	0
56	MG	DA	3088	1/1	0.31	-	86,86,86,86	0
56	MG	CA	1623	1/1	0.14	-	43,43,43,43	0
56	MG	DB	219	1/1	0.67	-	66,66,66,66	0
56	MG	BA	3087	1/1	0.41	-	82,82,82,82	0
56	MG	AA	1612	1/1	0.67	-	87,87,87,87	0
56	MG	AA	1814	1/1	0.49	-	58,58,58,58	0
56	MG	BA	3046	1/1	0.50	-	126,126,126,126	0
56	MG	DA	3409	1/1	0.39	-	102,102,102,102	0
56	MG	AA	1820	1/1	0.34	-	166,166,166,166	0
56	MG	CY	402	1/1	0.23	-	44,44,44,44	0
56	MG	DA	3424	1/1	0.38	-	52,52,52,52	0
56	MG	DA	2982	1/1	0.23	-	44,44,44,44	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	DA	3193	1/1	0.08	-	34,34,34,34	0
56	MG	AA	1975	1/1	0.28	-	121,121,121,121	0
56	MG	CA	1832	1/1	0.17	-	65,65,65,65	0
56	MG	BA	3185	1/1	0.65	-	66,66,66,66	0
56	MG	AA	1937	1/1	0.25	-	51,51,51,51	0
56	MG	BA	3237	1/1	0.53	-	90,90,90,90	0
56	MG	BA	3271	1/1	0.23	-	68,68,68,68	0
56	MG	DA	2960	1/1	0.55	-	68,68,68,68	0
56	MG	CA	1727	1/1	0.11	-	112,112,112,112	0
56	MG	BA	3048	1/1	0.36	-	54,54,54,54	0
56	MG	CA	1676	1/1	0.21	-	88,88,88,88	0
56	MG	BA	3703	1/1	0.96	-	70,70,70,70	0
56	MG	BA	3300	1/1	0.48	-	89,89,89,89	0
56	MG	BA	3593	1/1	0.30	-	57,57,57,57	0
56	MG	CW	116	1/1	0.14	-	70,70,70,70	0
56	MG	DA	3567	1/1	0.20	-	74,74,74,74	0
56	MG	DA	3256	1/1	0.21	-	41,41,41,41	0
56	MG	CA	1670	1/1	0.32	-	61,61,61,61	0
56	MG	BA	3506	1/1	0.41	-	53,53,53,53	0
56	MG	AA	1959	1/1	0.24	-	63,63,63,63	0
56	MG	BA	3335	1/1	0.77	-	49,49,49,49	0
56	MG	CA	1765	1/1	0.25	-	38,38,38,38	0
56	MG	DA	3620	1/1	0.44	-	50,50,50,50	0
56	MG	CA	1659	1/1	0.39	-	57,57,57,57	0
56	MG	DA	3340	1/1	0.36	-	67,67,67,67	0
56	MG	BA	3071	1/1	0.24	-	52,52,52,52	0
56	MG	BA	3163	1/1	0.61	-	93,93,93,93	0
56	MG	AV	101	1/1	0.76	-	109,109,109,109	0
56	MG	BA	3585	1/1	0.42	-	87,87,87,87	0
56	MG	BA	3296	1/1	0.65	-	59,59,59,59	0
56	MG	BA	3496	1/1	0.44	-	63,63,63,63	0
56	MG	DA	3457	1/1	0.42	-	64,64,64,64	0
56	MG	BA	3018	1/1	0.15	-	59,59,59,59	0
56	MG	DA	3223	1/1	0.16	-	75,75,75,75	0
56	MG	BA	3559	1/1	0.28	-	76,76,76,76	0
56	MG	BA	3252	1/1	0.41	-	78,78,78,78	0
56	MG	DA	2916	1/1	0.49	-	57,57,57,57	0
56	MG	BA	3171	1/1	0.21	-	43,43,43,43	0
56	MG	BA	3614	1/1	0.14	-	107,107,107,107	0
56	MG	CA	1886	1/1	0.20	-	100,100,100,100	0
56	MG	BA	3552	1/1	0.23	-	29,29,29,29	0
56	MG	AA	1821	1/1	0.12	-	70,70,70,70	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	BA	3380	1/1	0.74	-	49,49,49,49	0
56	MG	DA	3426	1/1	0.45	-	63,63,63,63	0
56	MG	DA	3355	1/1	0.18	-	102,102,102,102	0
56	MG	BA	3129	1/1	0.33	-	72,72,72,72	0
56	MG	BA	3015	1/1	0.32	-	71,71,71,71	0
56	MG	BA	3142	1/1	0.52	-	67,67,67,67	0
56	MG	DA	2966	1/1	0.29	-	42,42,42,42	0
56	MG	BA	3203	1/1	0.43	-	98,98,98,98	0
56	MG	DA	3134	1/1	0.46	-	18,18,18,18	0
56	MG	BA	2960	1/1	0.42	-	74,74,74,74	0
56	MG	BA	3187	1/1	0.24	-	56,56,56,56	0
56	MG	DA	3462	1/1	0.57	-	55,55,55,55	0
56	MG	AW	115	1/1	0.41	-	111,111,111,111	0
56	MG	DA	3422	1/1	0.25	-	77,77,77,77	0
56	MG	AA	1689	1/1	0.19	-	169,169,169,169	0
56	MG	AA	1981	1/1	0.17	-	90,90,90,90	0
56	MG	BA	3080	1/1	0.24	-	112,112,112,112	0
56	MG	BA	3406	1/1	0.46	-	28,28,28,28	0
56	MG	CA	1643	1/1	0.10	-	126,126,126,126	0
56	MG	BA	3718	1/1	0.28	-	163,163,163,163	0
56	MG	BA	3480	1/1	0.29	-	77,77,77,77	0
56	MG	BA	3154	1/1	0.77	-	169,169,169,169	0
56	MG	DB	206	1/1	0.42	-	121,121,121,121	0
56	MG	BA	3236	1/1	0.43	-	132,132,132,132	0
56	MG	DA	3004	1/1	0.49	-	100,100,100,100	0
56	MG	BA	3629	1/1	0.89	-	129,129,129,129	0
56	MG	CA	1872	1/1	0.35	-	88,88,88,88	0
56	MG	CA	1815	1/1	0.24	-	80,80,80,80	0
56	MG	BA	3112	1/1	0.16	-	83,83,83,83	0
56	MG	DA	3237	1/1	0.47	-	42,42,42,42	0
56	MG	BA	3066	1/1	0.19	-	61,61,61,61	0
56	MG	DA	3434	1/1	0.36	-	61,61,61,61	0
56	MG	AO	101	1/1	0.34	-	110,110,110,110	0
56	MG	B3	101	1/1	0.42	-	26,26,26,26	0
56	MG	BA	3471	1/1	0.13	-	45,45,45,45	0
56	MG	CA	1790	1/1	0.88	-	86,86,86,86	0
56	MG	DA	3294	1/1	0.55	-	64,64,64,64	0
56	MG	DA	3143	1/1	0.47	-	19,19,19,19	0
56	MG	BA	3192	1/1	0.27	-	90,90,90,90	0
56	MG	DA	3135	1/1	0.53	-	17,17,17,17	0
56	MG	AA	1773	1/1	0.50	-	281,281,281,281	0
56	MG	AA	1984	1/1	0.26	-	42,42,42,42	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	BA	3715	1/1	0.45	-	75,75,75,75	0
56	MG	CA	1865	1/1	0.50	-	108,108,108,108	0
56	MG	BA	3082	1/1	0.20	-	119,119,119,119	0
56	MG	DB	213	1/1	0.18	-	76,76,76,76	0
56	MG	CA	1785	1/1	0.31	-	63,63,63,63	0
56	MG	AA	1876	1/1	0.39	-	123,123,123,123	0
56	MG	BA	3266	1/1	0.34	-	73,73,73,73	0
56	MG	AA	1779	1/1	0.54	-	74,74,74,74	0
56	MG	DF	302	1/1	0.23	-	25,25,25,25	0
56	MG	BA	3589	1/1	0.19	-	135,135,135,135	0
56	MG	AA	1646	1/1	0.11	-	73,73,73,73	0
56	MG	DA	3442	1/1	0.43	-	64,64,64,64	0
56	MG	BA	3317	1/1	0.39	-	16,16,16,16	0
56	MG	AA	1846	1/1	0.42	-	118,118,118,118	0
56	MG	DA	3246	1/1	0.60	-	51,51,51,51	0
56	MG	BA	3043	1/1	0.36	-	155,155,155,155	0
56	MG	DA	3123	1/1	0.64	-	72,72,72,72	0
56	MG	DA	3600	1/1	0.21	-	23,23,23,23	0
56	MG	DA	3469	1/1	0.17	-	55,55,55,55	0
56	MG	CA	1766	1/1	0.36	-	49,49,49,49	0
56	MG	CA	1758	1/1	0.21	-	40,40,40,40	0
56	MG	CA	1878	1/1	0.35	-	66,66,66,66	0
56	MG	CA	1646	1/1	0.11	-	113,113,113,113	0
56	MG	BA	3327	1/1	0.31	-	28,28,28,28	0
56	MG	BA	3489	1/1	0.21	-	54,54,54,54	0
56	MG	CA	1607	1/1	0.37	-	138,138,138,138	0
56	MG	AA	1675	1/1	0.92	-	96,96,96,96	0
56	MG	BA	3550	1/1	0.12	-	68,68,68,68	0
56	MG	BA	3138	1/1	0.28	-	82,82,82,82	0
56	MG	CA	1916	1/1	0.66	-	77,77,77,77	0
56	MG	BA	3598	1/1	0.28	-	62,62,62,62	0
56	MG	AA	1805	1/1	0.26	-	71,71,71,71	0
56	MG	AA	1631	1/1	0.76	-	76,76,76,76	0
56	MG	DA	3253	1/1	0.34	-	30,30,30,30	0
56	MG	BA	2993	1/1	0.31	-	57,57,57,57	0
56	MG	CA	1873	1/1	0.23	-	207,207,207,207	0
56	MG	DA	3160	1/1	0.56	-	45,45,45,45	0
56	MG	AA	1818	1/1	0.18	-	44,44,44,44	0
56	MG	BA	3542	1/1	0.58	-	116,116,116,116	0
56	MG	BA	3653	1/1	0.18	-	62,62,62,62	0
56	MG	BA	3182	1/1	0.48	-	70,70,70,70	0
56	MG	DA	3249	1/1	0.41	-	120,120,120,120	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	BA	3470	1/1	0.54	-	65,65,65,65	0
56	MG	DA	3048	1/1	0.56	-	49,49,49,49	0
56	MG	BA	3528	1/1	0.51	-	53,53,53,53	0
56	MG	AA	1726	1/1	0.58	-	141,141,141,141	0
56	MG	DB	207	1/1	0.12	-	87,87,87,87	0
56	MG	CA	1805	1/1	0.20	-	63,63,63,63	0
56	MG	BB	222	1/1	0.22	-	206,206,206,206	0
56	MG	DA	3044	1/1	0.39	-	87,87,87,87	0
56	MG	BA	2983	1/1	0.14	-	44,44,44,44	0
56	MG	CA	1703	1/1	0.19	-	89,89,89,89	0
56	MG	DW	201	1/1	0.54	-	76,76,76,76	0
56	MG	AA	1764	1/1	0.88	-	103,103,103,103	0
56	MG	AA	1721	1/1	0.35	-	128,128,128,128	0
56	MG	CA	1769	1/1	0.20	-	58,58,58,58	0
56	MG	AA	1953	1/1	0.38	-	51,51,51,51	0
56	MG	DA	3405	1/1	0.18	-	91,91,91,91	0
56	MG	AA	1903	1/1	0.26	-	51,51,51,51	0
56	MG	BA	3473	1/1	0.81	-	70,70,70,70	0
56	MG	CA	1904	1/1	0.26	-	80,80,80,80	0
56	MG	BA	3349	1/1	0.36	-	43,43,43,43	0
56	MG	BA	3556	1/1	0.60	-	54,54,54,54	0
56	MG	AA	1705	1/1	0.29	-	101,101,101,101	0
56	MG	BA	3230	1/1	0.82	-	103,103,103,103	0
56	MG	BA	3116	1/1	0.16	-	87,87,87,87	0
56	MG	CA	1848	1/1	0.35	-	113,113,113,113	0
56	MG	AA	1856	1/1	0.36	-	134,134,134,134	0
56	MG	BA	3133	1/1	0.30	-	48,48,48,48	0
56	MG	DA	3142	1/1	0.40	-	30,30,30,30	0
56	MG	AA	1872	1/1	0.70	-	67,67,67,67	0
56	MG	DA	3236	1/1	0.65	-	30,30,30,30	0
56	MG	CA	1914	1/1	0.23	-	96,96,96,96	0
56	MG	CA	1629	1/1	0.23	-	93,93,93,93	0
56	MG	CA	1737	1/1	0.97	-	98,98,98,98	0
56	MG	CA	1788	1/1	0.20	-	66,66,66,66	0
56	MG	DA	3320	1/1	0.12	-	78,78,78,78	0
56	MG	CA	1801	1/1	0.25	-	76,76,76,76	0
56	MG	DA	3519	1/1	1.49	-	78,78,78,78	0
56	MG	CA	1779	1/1	0.39	-	72,72,72,72	0
56	MG	DB	214	1/1	0.12	-	110,110,110,110	0
56	MG	CA	1833	1/1	0.65	-	65,65,65,65	0
56	MG	BA	3440	1/1	0.35	-	37,37,37,37	0
56	MG	DA	3137	1/1	0.29	-	23,23,23,23	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	BA	3499	1/1	0.20	-	40,40,40,40	0
56	MG	BA	3604	1/1	0.35	-	72,72,72,72	0
56	MG	AW	116	1/1	0.23	-	86,86,86,86	0
56	MG	BA	3186	1/1	0.45	-	98,98,98,98	0
56	MG	BA	3597	1/1	0.56	-	91,91,91,91	0
56	MG	AA	1742	1/1	1.38	-	197,197,197,197	0
56	MG	BA	3445	1/1	0.18	-	19,19,19,19	0
56	MG	DQ	202	1/1	0.25	-	31,31,31,31	0
56	MG	CA	1709	1/1	0.25	-	61,61,61,61	0
56	MG	CA	1755	1/1	0.84	-	120,120,120,120	0
56	MG	DA	3465	1/1	0.20	-	60,60,60,60	0
56	MG	DA	3400	1/1	0.34	-	88,88,88,88	0
56	MG	DA	3146	1/1	0.78	-	50,50,50,50	0
56	MG	BA	3475	1/1	0.61	-	55,55,55,55	0
56	MG	BA	3128	1/1	0.78	-	111,111,111,111	0
56	MG	DA	3603	1/1	0.08	-	17,17,17,17	0
56	MG	DA	3421	1/1	0.44	-	76,76,76,76	0
56	MG	CA	1616	1/1	0.43	-	61,61,61,61	0
56	MG	DA	3418	1/1	0.21	-	11,11,11,11	0
56	MG	BA	3037	1/1	0.25	-	101,101,101,101	0
56	MG	AA	1930	1/1	0.48	-	198,198,198,198	0
56	MG	BA	3323	1/1	0.26	-	47,47,47,47	0
56	MG	BA	3293	1/1	0.15	-	62,62,62,62	0
56	MG	DA	3218	1/1	0.18	-	29,29,29,29	0
56	MG	BA	3627	1/1	0.26	-	100,100,100,100	0
56	MG	DA	3015	1/1	0.51	-	91,91,91,91	0
56	MG	BA	2934	1/1	0.77	-	79,79,79,79	0
56	MG	DA	3397	1/1	0.35	-	54,54,54,54	0
56	MG	DA	3546	1/1	0.40	-	62,62,62,62	0
56	MG	DA	3055	1/1	0.12	-	75,75,75,75	0
56	MG	AA	1979	1/1	0.61	-	118,118,118,118	0
56	MG	DA	3359	1/1	0.42	-	57,57,57,57	0
56	MG	CA	1839	1/1	0.14	-	38,38,38,38	0
56	MG	DA	3194	1/1	0.09	-	28,28,28,28	0
56	MG	CA	1663	1/1	0.64	-	210,210,210,210	0
56	MG	AA	1629	1/1	0.79	-	83,83,83,83	0
56	MG	CV	102	1/1	0.67	-	78,78,78,78	0
56	MG	DA	3455	1/1	0.22	-	72,72,72,72	0
56	MG	DA	3243	1/1	0.55	-	77,77,77,77	0
56	MG	AA	1875	1/1	0.12	-	37,37,37,37	0
56	MG	DA	3307	1/1	0.13	-	82,82,82,82	0
56	MG	BA	3478	1/1	0.11	-	63,63,63,63	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	DA	3149	1/1	0.38	-	22,22,22,22	0
56	MG	BA	3412	1/1	0.85	-	58,58,58,58	0
56	MG	DA	3345	1/1	0.23	-	68,68,68,68	0
56	MG	BA	3004	1/1	0.53	-	99,99,99,99	0
56	MG	BA	3358	1/1	0.46	-	150,150,150,150	0
56	MG	BA	3442	1/1	0.37	-	79,79,79,79	0
56	MG	CA	1684	1/1	0.50	-	87,87,87,87	0
56	MG	CA	1672	1/1	0.32	-	78,78,78,78	0
56	MG	BA	3229	1/1	0.41	-	92,92,92,92	0
56	MG	AA	1804	1/1	1.65	-	108,108,108,108	0
56	MG	CA	1642	1/1	0.81	-	82,82,82,82	0
56	MG	AA	1913	1/1	0.42	-	35,35,35,35	0
56	MG	DA	2997	1/1	0.77	-	132,132,132,132	0
56	MG	AA	1626	1/1	0.09	-	91,91,91,91	0
56	MG	BA	2989	1/1	0.32	-	84,84,84,84	0
56	MG	AA	1791	1/1	0.38	-	59,59,59,59	0
56	MG	DA	3239	1/1	0.43	-	43,43,43,43	0
56	MG	BA	3520	1/1	0.44	-	51,51,51,51	0
56	MG	BA	3654	1/1	0.23	-	86,86,86,86	0
56	MG	DA	3598	1/1	0.34	-	12,12,12,12	0
56	MG	DA	3540	1/1	0.18	-	85,85,85,85	0
56	MG	DA	3508	1/1	0.32	-	37,37,37,37	0
56	MG	BA	3113	1/1	0.32	-	109,109,109,109	0
56	MG	CA	1819	1/1	0.09	-	59,59,59,59	0
56	MG	AA	1795	1/1	0.11	-	65,65,65,65	0
56	MG	BA	2984	1/1	0.45	-	40,40,40,40	0
56	MG	CA	1764	1/1	0.41	-	50,50,50,50	0
56	MG	BA	3553	1/1	0.43	-	92,92,92,92	0
56	MG	DA	3094	1/1	0.24	-	30,30,30,30	0
56	MG	DA	2910	1/1	0.11	-	90,90,90,90	0
56	MG	AA	1811	1/1	0.39	-	91,91,91,91	0
56	MG	DB	204	1/1	0.28	-	78,78,78,78	0
56	MG	AA	1690	1/1	0.48	-	174,174,174,174	0
56	MG	BA	3696	1/1	0.16	-	96,96,96,96	0
56	MG	BB	223	1/1	0.43	-	242,242,242,242	0
56	MG	CA	1889	1/1	0.07	-	92,92,92,92	0
56	MG	CA	1810	1/1	0.73	-	121,121,121,121	0
56	MG	CW	102	1/1	0.55	-	105,105,105,105	0
56	MG	CA	1636	1/1	0.89	-	56,56,56,56	0
56	MG	BA	3262	1/1	0.16	-	75,75,75,75	0
56	MG	CA	1838	1/1	0.52	-	66,66,66,66	0
56	MG	DA	3262	1/1	0.46	-	65,65,65,65	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	DA	3632	1/1	0.20	-	135,135,135,135	0
56	MG	DB	211	1/1	0.31	-	35,35,35,35	0
56	MG	AA	1618	1/1	0.30	-	104,104,104,104	0
56	MG	CA	1707	1/1	0.17	-	50,50,50,50	0
56	MG	AA	1939	1/1	0.10	-	61,61,61,61	0
56	MG	DA	2929	1/1	0.30	-	77,77,77,77	0
56	MG	DA	3430	1/1	0.16	-	80,80,80,80	0
56	MG	BA	2918	1/1	1.72	-	191,191,191,191	0
56	MG	CA	1911	1/1	1.12	-	107,107,107,107	0
56	MG	BA	3519	1/1	0.47	-	93,93,93,93	0
56	MG	AA	1868	1/1	0.26	-	49,49,49,49	0
56	MG	BA	2950	1/1	0.83	-	87,87,87,87	0
56	MG	AA	1737	1/1	0.24	-	72,72,72,72	0
56	MG	CW	109	1/1	0.10	-	49,49,49,49	0
56	MG	BA	3374	1/1	0.26	-	30,30,30,30	0
56	MG	DA	3410	1/1	0.17	-	22,22,22,22	0
56	MG	DA	3472	1/1	0.22	-	52,52,52,52	0
56	MG	BA	3611	1/1	0.24	-	67,67,67,67	0
56	MG	AA	1698	1/1	0.71	-	97,97,97,97	0
56	MG	DA	3077	1/1	0.33	-	77,77,77,77	0
56	MG	BA	3419	1/1	0.44	-	57,57,57,57	0
56	MG	BA	3717	1/1	0.17	-	100,100,100,100	0
56	MG	DA	3063	1/1	0.17	-	99,99,99,99	0
56	MG	BA	3053	1/1	0.41	-	95,95,95,95	0
56	MG	BA	3303	1/1	0.22	-	69,69,69,69	0
56	MG	CA	1683	1/1	0.58	-	62,62,62,62	0
56	MG	CA	1732	1/1	0.82	-	131,131,131,131	0
56	MG	BA	3560	1/1	0.32	-	47,47,47,47	0
56	MG	BB	203	1/1	0.35	-	78,78,78,78	0
56	MG	BA	3587	1/1	0.87	-	104,104,104,104	0
56	MG	DA	2946	1/1	0.49	-	55,55,55,55	0
56	MG	AA	1972	1/1	0.34	-	56,56,56,56	0
56	MG	CA	1821	1/1	0.24	-	56,56,56,56	0
56	MG	BA	3631	1/1	0.34	-	8,8,8,8	0
56	MG	DA	3377	1/1	0.40	-	58,58,58,58	0
56	MG	DA	3129	1/1	0.26	-	104,104,104,104	0
56	MG	BA	3012	1/1	0.82	-	91,91,91,91	0
56	MG	DA	3435	1/1	0.84	-	68,68,68,68	0
56	MG	DA	3227	1/1	0.20	-	45,45,45,45	0
56	MG	DA	3482	1/1	0.55	-	50,50,50,50	0
56	MG	DA	3591	1/1	0.14	-	129,129,129,129	0
56	MG	BA	3463	1/1	0.26	-	106,106,106,106	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	CA	1621	1/1	0.36	-	48,48,48,48	0
56	MG	AA	1819	1/1	0.91	-	84,84,84,84	0
56	MG	BA	2905	1/1	0.34	-	54,54,54,54	0
56	MG	BA	3361	1/1	0.23	-	106,106,106,106	0
56	MG	DA	3274	1/1	0.36	-	45,45,45,45	0
56	MG	BA	3422	1/1	0.52	-	42,42,42,42	0
56	MG	DA	2980	1/1	0.36	-	57,57,57,57	0
56	MG	BA	3407	1/1	0.46	-	78,78,78,78	0
56	MG	DA	3119	1/1	0.47	-	82,82,82,82	0
56	MG	AA	1909	1/1	0.18	-	65,65,65,65	0
56	MG	AA	1739	1/1	0.10	-	88,88,88,88	0
56	MG	CA	1807	1/1	0.74	-	195,195,195,195	0
56	MG	BA	3527	1/1	0.36	-	31,31,31,31	0
56	MG	DA	3564	1/1	0.59	-	25,25,25,25	0
56	MG	BA	3428	1/1	0.24	-	51,51,51,51	0
56	MG	DA	2994	1/1	0.36	-	62,62,62,62	0
56	MG	BA	3456	1/1	0.11	-	65,65,65,65	0
56	MG	CA	1767	1/1	0.54	-	50,50,50,50	0
56	MG	AA	1881	1/1	0.43	-	54,54,54,54	0
56	MG	BA	3663	1/1	0.33	-	105,105,105,105	0
56	MG	DA	2911	1/1	0.80	-	84,84,84,84	0
56	MG	BA	3299	1/1	0.65	-	102,102,102,102	0
56	MG	DA	3291	1/1	0.36	-	44,44,44,44	0
56	MG	BA	3482	1/1	1.22	-	74,74,74,74	0
56	MG	DA	3385	1/1	0.40	-	77,77,77,77	0
56	MG	CA	1681	1/1	0.54	-	136,136,136,136	0
56	MG	DA	2948	1/1	0.68	-	94,94,94,94	0
56	MG	CA	1720	1/1	0.48	-	84,84,84,84	0
56	MG	BA	3141	1/1	0.71	-	62,62,62,62	0
56	MG	CA	1921	1/1	0.24	-	108,108,108,108	0
56	MG	BA	3721	1/1	0.19	-	86,86,86,86	0
56	MG	BA	3468	1/1	0.29	-	67,67,67,67	0
56	MG	AA	1695	1/1	0.10	-	71,71,71,71	0
56	MG	AA	1993	1/1	0.36	-	73,73,73,73	0
56	MG	DA	2970	1/1	0.66	-	69,69,69,69	0
56	MG	AA	1833	1/1	0.32	-	72,72,72,72	0
56	MG	AA	1878	1/1	0.21	-	56,56,56,56	0
56	MG	DA	2950	1/1	0.19	-	61,61,61,61	0
56	MG	AA	1802	1/1	0.38	-	55,55,55,55	0
56	MG	DA	3394	1/1	0.28	-	49,49,49,49	0
56	MG	BA	3371	1/1	0.69	-	55,55,55,55	0
56	MG	DA	3087	1/1	0.80	-	52,52,52,52	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	DA	2931	1/1	0.22	-	87,87,87,87	0
56	MG	DA	3535	1/1	0.37	-	67,67,67,67	0
56	MG	BA	3378	1/1	0.38	-	30,30,30,30	0
56	MG	AA	1707	1/1	0.09	-	67,67,67,67	0
56	MG	AA	1740	1/1	0.39	-	105,105,105,105	0
56	MG	BA	2944	1/1	0.17	-	62,62,62,62	0
56	MG	BA	3125	1/1	0.24	-	106,106,106,106	0
56	MG	BB	208	1/1	0.61	-	82,82,82,82	0
56	MG	BA	3641	1/1	0.61	-	60,60,60,60	0
56	MG	DA	3161	1/1	0.20	-	10,10,10,10	0
56	MG	BA	2945	1/1	0.39	-	76,76,76,76	0
56	MG	AA	1797	1/1	0.42	-	60,60,60,60	0
56	MG	AA	1602	1/1	0.22	-	163,163,163,163	0
56	MG	BA	3220	1/1	0.24	-	58,58,58,58	0
56	MG	DA	3109	1/1	0.33	-	65,65,65,65	0
56	MG	BA	3343	1/1	0.21	-	73,73,73,73	0
56	MG	BA	3261	1/1	0.80	-	89,89,89,89	0
56	MG	CA	1630	1/1	0.14	-	177,177,177,177	0
56	MG	BA	3168	1/1	1.00	-	78,78,78,78	0
56	MG	CA	1901	1/1	0.21	-	54,54,54,54	0
56	MG	AA	1934	1/1	0.42	-	96,96,96,96	0
56	MG	CA	1812	1/1	0.52	-	75,75,75,75	0
56	MG	BA	3330	1/1	0.35	-	27,27,27,27	0
56	MG	CA	1852	1/1	0.24	-	93,93,93,93	0
56	MG	BA	2953	1/1	0.20	-	56,56,56,56	0
56	MG	DA	3166	1/1	0.26	-	25,25,25,25	0
56	MG	AA	1836	1/1	0.32	-	139,139,139,139	0
56	MG	AA	1867	1/1	1.28	-	96,96,96,96	0
56	MG	DA	3608	1/1	0.50	-	50,50,50,50	0
56	MG	DA	3337	1/1	0.29	-	51,51,51,51	0
56	MG	BA	3208	1/1	0.40	-	87,87,87,87	0
56	MG	AW	103	1/1	0.15	-	70,70,70,70	0
56	MG	AA	1834	1/1	0.25	-	178,178,178,178	0
56	MG	DA	2976	1/1	0.36	-	71,71,71,71	0
56	MG	DA	3533	1/1	0.26	-	71,71,71,71	0
56	MG	CA	1887	1/1	0.40	-	116,116,116,116	0
56	MG	DA	3170	1/1	0.10	-	12,12,12,12	0
56	MG	AA	1761	1/1	0.30	-	118,118,118,118	0
56	MG	CA	1913	1/1	0.48	-	69,69,69,69	0
56	MG	CA	1731	1/1	0.07	-	139,139,139,139	0
56	MG	DA	3278	1/1	0.28	-	83,83,83,83	0
56	MG	CA	1784	1/1	0.49	-	96,96,96,96	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	DA	3245	1/1	0.50	-	45,45,45,45	0
56	MG	DA	3312	1/1	0.17	-	61,61,61,61	0
56	MG	BA	3143	1/1	0.42	-	81,81,81,81	0
56	MG	BA	3392	1/1	0.49	-	63,63,63,63	0
56	MG	DA	3206	1/1	0.40	-	23,23,23,23	0
56	MG	DA	3324	1/1	0.47	-	13,13,13,13	0
56	MG	DA	3573	1/1	0.13	-	34,34,34,34	0
56	MG	BA	3332	1/1	0.82	-	58,58,58,58	0
56	MG	DA	3555	1/1	0.29	-	14,14,14,14	0
56	MG	BA	3622	1/1	0.98	-	68,68,68,68	0
56	MG	BB	204	1/1	0.13	-	53,53,53,53	0
56	MG	BA	3020	1/1	0.54	-	107,107,107,107	0
56	MG	BA	3031	1/1	0.47	-	255,255,255,255	0
56	MG	DA	2923	1/1	0.16	-	28,28,28,28	0
56	MG	BB	211	1/1	1.06	-	132,132,132,132	0
56	MG	BA	2992	1/1	0.66	-	73,73,73,73	0
56	MG	DA	3625	1/1	0.14	-	82,82,82,82	0
56	MG	BA	3411	1/1	0.31	-	31,31,31,31	0
56	MG	AA	1700	1/1	0.46	-	158,158,158,158	0
56	MG	DA	2947	1/1	0.38	-	192,192,192,192	0
56	MG	AA	1634	1/1	0.34	-	78,78,78,78	0
56	MG	BA	3144	1/1	0.15	-	53,53,53,53	0
56	MG	BA	3530	1/1	0.34	-	57,57,57,57	0
56	MG	BA	3451	1/1	0.50	-	83,83,83,83	0
56	MG	BA	3061	1/1	0.62	-	61,61,61,61	0
56	MG	BA	3079	1/1	0.39	-	48,48,48,48	0
56	MG	AA	1659	1/1	0.26	-	88,88,88,88	0
56	MG	BA	3596	1/1	0.39	-	140,140,140,140	0
56	MG	AA	1686	1/1	0.44	-	85,85,85,85	0
56	MG	DA	3027	1/1	0.17	-	94,94,94,94	0
56	MG	CA	1828	1/1	0.32	-	135,135,135,135	0
56	MG	BA	3481	1/1	0.14	-	59,59,59,59	0
56	MG	BA	3216	1/1	0.18	-	48,48,48,48	0
56	MG	AA	1671	1/1	0.37	-	87,87,87,87	0
56	MG	BA	3672	1/1	0.46	-	88,88,88,88	0
56	MG	CA	1850	1/1	0.39	-	93,93,93,93	0
56	MG	BA	3039	1/1	0.71	-	176,176,176,176	0
56	MG	DA	3172	1/1	0.53	-	24,24,24,24	0
56	MG	DA	3188	1/1	0.47	-	50,50,50,50	0
56	MG	AA	1703	1/1	0.47	-	64,64,64,64	0
56	MG	DA	3458	1/1	0.18	-	64,64,64,64	0
56	MG	DA	3084	1/1	0.35	-	83,83,83,83	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	DA	3221	1/1	0.26	-	38,38,38,38	0
56	MG	DA	3602	1/1	0.24	-	22,22,22,22	0
56	MG	BA	3708	1/1	0.20	-	61,61,61,61	0
56	MG	DA	3597	1/1	0.40	-	22,22,22,22	0
56	MG	AA	1843	1/1	0.23	-	124,124,124,124	0
56	MG	CA	1806	1/1	0.34	-	95,95,95,95	0
56	MG	CA	1740	1/1	0.23	-	101,101,101,101	0
56	MG	CR	101	1/1	1.45	-	182,182,182,182	0
56	MG	AA	1933	1/1	0.53	-	63,63,63,63	0
56	MG	BA	3311	1/1	0.37	-	17,17,17,17	0
56	MG	AA	1785	1/1	0.39	-	62,62,62,62	0
56	MG	BA	3551	1/1	0.25	-	52,52,52,52	0
56	MG	AA	1844	1/1	0.29	-	78,78,78,78	0
56	MG	BA	3599	1/1	0.62	-	93,93,93,93	0
56	MG	AA	1656	1/1	0.28	-	61,61,61,61	0
56	MG	BA	3278	1/1	0.66	-	115,115,115,115	0
56	MG	AA	1731	1/1	0.14	-	57,57,57,57	0
56	MG	DA	3479	1/1	0.20	-	55,55,55,55	0
56	MG	AA	1892	1/1	0.24	-	108,108,108,108	0
56	MG	AA	1839	1/1	0.41	-	88,88,88,88	0
56	MG	AA	1828	1/1	0.10	-	97,97,97,97	0
56	MG	BA	3224	1/1	0.55	-	85,85,85,85	0
56	MG	BA	2962	1/1	0.71	-	78,78,78,78	0
56	MG	CA	1917	1/1	0.31	-	123,123,123,123	0
56	MG	CA	1633	1/1	0.27	-	143,143,143,143	0
56	MG	DA	3108	1/1	0.40	-	74,74,74,74	0
56	MG	CA	1748	1/1	0.51	-	78,78,78,78	0
56	MG	BA	3122	1/1	0.14	-	89,89,89,89	0
56	MG	BA	3197	1/1	0.11	-	215,215,215,215	0
56	MG	DA	2913	1/1	0.79	-	70,70,70,70	0
56	MG	BA	3210	1/1	0.15	-	76,76,76,76	0
56	MG	DA	3330	1/1	0.38	-	36,36,36,36	0
56	MG	BA	3408	1/1	0.31	-	50,50,50,50	0
56	MG	BA	3586	1/1	0.20	-	17,17,17,17	0
56	MG	CA	1844	1/1	0.75	-	104,104,104,104	0
56	MG	BA	3365	1/1	0.30	-	14,14,14,14	0
56	MG	BA	3333	1/1	0.40	-	12,12,12,12	0
56	MG	DA	3199	1/1	0.54	-	36,36,36,36	0
56	MG	DA	3147	1/1	0.23	-	20,20,20,20	0
56	MG	BA	3146	1/1	0.33	-	57,57,57,57	0
56	MG	AA	1684	1/1	0.83	-	62,62,62,62	0
56	MG	AA	1879	1/1	0.48	-	99,99,99,99	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	DA	3281	1/1	0.14	-	48,48,48,48	0
56	MG	BA	3121	1/1	0.90	-	137,137,137,137	0
56	MG	DA	3592	1/1	0.16	-	73,73,73,73	0
56	MG	AA	1755	1/1	0.09	-	123,123,123,123	0
56	MG	AA	1866	1/1	0.10	-	118,118,118,118	0
56	MG	CA	1773	1/1	0.16	-	62,62,62,62	0
56	MG	BA	3316	1/1	0.16	-	26,26,26,26	0
56	MG	AA	1822	1/1	0.18	-	69,69,69,69	0
56	MG	CA	1809	1/1	0.90	-	117,117,117,117	0
56	MG	CA	1861	1/1	0.45	-	79,79,79,79	0
56	MG	D7	101	1/1	0.44	-	62,62,62,62	0
56	MG	CA	1669	1/1	1.77	-	118,118,118,118	0
56	MG	DA	3018	1/1	0.06	-	83,83,83,83	0
56	MG	BA	3495	1/1	0.09	-	51,51,51,51	0
56	MG	BA	3242	1/1	0.47	-	63,63,63,63	0
56	MG	BA	2957	1/1	0.54	-	71,71,71,71	0
56	MG	DA	3367	1/1	0.21	-	74,74,74,74	0
56	MG	DA	3451	1/1	0.53	-	56,56,56,56	0
56	MG	BA	3155	1/1	0.56	-	93,93,93,93	0
56	MG	DA	3000	1/1	0.17	-	68,68,68,68	0
56	MG	BA	3240	1/1	0.21	-	75,75,75,75	0
56	MG	BA	3448	1/1	0.35	-	72,72,72,72	0
56	MG	BA	3415	1/1	0.20	-	47,47,47,47	0
56	MG	BA	2968	1/1	0.22	-	46,46,46,46	0
56	MG	BA	3575	1/1	0.23	-	63,63,63,63	0
56	MG	CA	1762	1/1	0.14	-	28,28,28,28	0
56	MG	BA	3591	1/1	1.30	-	102,102,102,102	0
56	MG	DA	3544	1/1	0.42	-	73,73,73,73	0
56	MG	CA	1746	1/1	0.14	-	255,255,255,255	0
56	MG	CA	1653	1/1	0.18	-	53,53,53,53	0
56	MG	DA	2945	1/1	0.31	-	88,88,88,88	0
56	MG	DA	3629	1/1	0.27	-	67,67,67,67	0
56	MG	DA	3290	1/1	0.30	-	38,38,38,38	0
56	MG	AA	1837	1/1	0.11	-	64,64,64,64	0
56	MG	DA	3613	1/1	0.16	-	49,49,49,49	0
56	MG	BA	3302	1/1	0.68	-	63,63,63,63	0
56	MG	BA	3583	1/1	0.58	-	87,87,87,87	0
56	MG	DA	3503	1/1	0.13	-	92,92,92,92	0
56	MG	CA	1799	1/1	0.41	-	51,51,51,51	0
56	MG	BA	3484	1/1	0.32	-	104,104,104,104	0
56	MG	AW	111	1/1	0.15	-	91,91,91,91	0
56	MG	DA	3150	1/1	0.45	-	17,17,17,17	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	ZN	CN	101	1/1	0.13	-	111,111,111,111	0
56	MG	DA	3255	1/1	0.27	-	44,44,44,44	0
56	MG	DA	3029	1/1	0.28	-	73,73,73,73	0
56	MG	DA	3478	1/1	0.21	-	67,67,67,67	0
56	MG	DA	3420	1/1	0.24	-	86,86,86,86	0
56	MG	DA	3205	1/1	0.25	-	36,36,36,36	0
56	MG	BA	2972	1/1	0.40	-	122,122,122,122	0
56	MG	DA	3152	1/1	0.38	-	23,23,23,23	0
56	MG	CA	1745	1/1	0.20	-	115,115,115,115	0
56	MG	CA	1825	1/1	0.24	-	80,80,80,80	0
56	MG	CA	1876	1/1	0.29	-	127,127,127,127	0
56	MG	BA	3127	1/1	0.36	-	102,102,102,102	0
56	MG	BA	3013	1/1	0.64	-	81,81,81,81	0
56	MG	CA	1609	1/1	0.19	-	100,100,100,100	0
56	MG	AA	1610	1/1	0.19	-	65,65,65,65	0
56	MG	BA	2980	1/1	0.28	-	74,74,74,74	0
56	MG	DA	3464	1/1	0.61	-	42,42,42,42	0
56	MG	CA	1829	1/1	0.69	-	49,49,49,49	0
56	MG	BA	3221	1/1	0.26	-	77,77,77,77	0
56	MG	AA	1775	1/1	0.88	-	66,66,66,66	0
56	MG	BA	3513	1/1	0.28	-	40,40,40,40	0
56	MG	BA	3086	1/1	0.57	-	64,64,64,64	0
56	MG	CA	1920	1/1	0.12	-	138,138,138,138	0
56	MG	BA	3118	1/1	0.47	-	132,132,132,132	0
56	MG	BA	3609	1/1	0.71	-	149,149,149,149	0
56	MG	BA	3572	1/1	0.26	-	62,62,62,62	0
56	MG	AA	1605	1/1	0.15	-	142,142,142,142	0
56	MG	BA	3032	1/1	0.69	-	97,97,97,97	0
56	MG	DA	2907	1/1	0.10	-	75,75,75,75	0
56	MG	CA	1654	1/1	0.24	-	106,106,106,106	0
56	MG	DA	3072	1/1	0.68	-	94,94,94,94	0
56	MG	AA	1931	1/1	0.29	-	102,102,102,102	0
56	MG	DA	3524	1/1	0.18	-	67,67,67,67	0
56	MG	AA	1767	1/1	0.59	-	102,102,102,102	0
56	MG	BA	3600	1/1	0.83	-	73,73,73,73	0
56	MG	DA	3141	1/1	0.44	-	15,15,15,15	0
56	MG	DA	3231	1/1	0.44	-	32,32,32,32	0
56	MG	AA	1851	1/1	0.29	-	111,111,111,111	0
56	MG	AA	1923	1/1	0.12	-	72,72,72,72	0
56	MG	BA	3360	1/1	0.55	-	24,24,24,24	0
56	MG	BA	3234	1/1	0.15	-	83,83,83,83	0
56	MG	BA	3705	1/1	0.13	-	62,62,62,62	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	DA	3351	1/1	0.43	-	116,116,116,116	0
56	MG	DA	3447	1/1	0.49	-	89,89,89,89	0
56	MG	CA	1820	1/1	0.72	-	193,193,193,193	0
56	MG	BA	3217	1/1	0.21	-	65,65,65,65	0
56	MG	DA	3074	1/1	0.94	-	99,99,99,99	0
56	MG	DA	3127	1/1	0.58	-	88,88,88,88	0
56	MG	BA	3173	1/1	0.88	-	67,67,67,67	0
56	MG	CA	1628	1/1	0.17	-	86,86,86,86	0
56	MG	BA	2963	1/1	0.39	-	63,63,63,63	0
56	MG	CA	1898	1/1	0.54	-	126,126,126,126	0
56	MG	D0	101	1/1	0.29	-	42,42,42,42	0
56	MG	DA	3102	1/1	0.45	-	126,126,126,126	0
56	MG	BA	3338	1/1	0.21	-	28,28,28,28	0
56	MG	BA	3283	1/1	0.22	-	67,67,67,67	0
56	MG	BA	3058	1/1	0.35	-	60,60,60,60	0
56	MG	BA	3486	1/1	0.23	-	47,47,47,47	0
56	MG	BA	2998	1/1	0.34	-	65,65,65,65	0
56	MG	BA	3077	1/1	0.25	-	50,50,50,50	0
56	MG	DA	3518	1/1	0.47	-	63,63,63,63	0
56	MG	BA	3351	1/1	0.53	-	29,29,29,29	0
56	MG	CA	1862	1/1	0.26	-	117,117,117,117	0
56	MG	DB	216	1/1	0.13	-	51,51,51,51	0
56	MG	DA	3020	1/1	0.19	-	74,74,74,74	0
56	MG	CA	1798	1/1	0.35	-	79,79,79,79	0
56	MG	AA	1725	1/1	0.53	-	121,121,121,121	0
56	MG	AA	1751	1/1	0.67	-	108,108,108,108	0
56	MG	BA	3636	1/1	0.47	-	28,28,28,28	0
56	MG	DA	3628	1/1	0.27	-	295,295,295,295	0
56	MG	DA	3581	1/1	0.34	-	69,69,69,69	0
56	MG	CA	1634	1/1	0.27	-	74,74,74,74	0
56	MG	AA	1651	1/1	0.37	-	84,84,84,84	0
56	MG	DA	3317	1/1	0.17	-	48,48,48,48	0
56	MG	DA	3463	1/1	0.36	-	60,60,60,60	0
56	MG	AA	1676	1/1	0.35	-	152,152,152,152	0
56	MG	DA	2920	1/1	0.20	-	83,83,83,83	0
56	MG	DA	3040	1/1	0.33	-	102,102,102,102	0
56	MG	DA	3131	1/1	0.54	-	40,40,40,40	0
56	MG	DA	3115	1/1	0.13	-	60,60,60,60	0
56	MG	AA	1619	1/1	0.70	-	69,69,69,69	0
56	MG	DA	3381	1/1	0.41	-	43,43,43,43	0
56	MG	DA	3346	1/1	0.28	-	90,90,90,90	0
56	MG	AA	1925	1/1	0.56	-	63,63,63,63	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	DA	3481	1/1	0.18	-	73,73,73,73	0
56	MG	DA	3173	1/1	0.63	-	46,46,46,46	0
56	MG	AA	1712	1/1	0.28	-	166,166,166,166	0
56	MG	CA	1701	1/1	0.24	-	88,88,88,88	0
56	MG	BA	2936	1/1	0.09	-	65,65,65,65	0
56	MG	BA	3712	1/1	0.55	-	52,52,52,52	0
56	MG	BA	3420	1/1	0.38	-	34,34,34,34	0
56	MG	AA	1746	1/1	0.36	-	93,93,93,93	0
56	MG	CA	1625	1/1	0.33	-	125,125,125,125	0
56	MG	BA	3504	1/1	0.16	-	39,39,39,39	0
56	MG	BA	3620	1/1	0.25	-	73,73,73,73	0
56	MG	CA	1860	1/1	0.26	-	133,133,133,133	0
56	MG	DA	3298	1/1	0.37	-	46,46,46,46	0
56	MG	BA	3396	1/1	0.38	-	43,43,43,43	0
56	MG	CA	1690	1/1	0.17	-	69,69,69,69	0
56	MG	CA	1760	1/1	0.18	-	67,67,67,67	0
56	MG	DA	3296	1/1	0.16	-	69,69,69,69	0
56	MG	AA	1823	1/1	0.23	-	96,96,96,96	0
56	MG	AA	1644	1/1	0.22	-	57,57,57,57	0
56	MG	BA	3691	1/1	0.25	-	45,45,45,45	0
56	MG	AA	1614	1/1	0.38	-	51,51,51,51	0
56	MG	BA	3135	1/1	0.47	-	55,55,55,55	0
56	MG	DA	3163	1/1	0.30	-	31,31,31,31	0
56	MG	BA	2913	1/1	0.28	-	77,77,77,77	0
56	MG	BA	3394	1/1	0.44	-	56,56,56,56	0
56	MG	CA	1750	1/1	0.24	-	222,222,222,222	0
56	MG	DA	3404	1/1	0.57	-	61,61,61,61	0
56	MG	DA	3433	1/1	0.18	-	27,27,27,27	0
56	MG	BA	3683	1/1	0.75	-	55,55,55,55	0
56	MG	DA	3148	1/1	0.55	-	34,34,34,34	0
56	MG	DB	212	1/1	0.12	-	84,84,84,84	0
56	MG	BA	3277	1/1	0.20	-	51,51,51,51	0
56	MG	DA	3215	1/1	0.48	-	46,46,46,46	0
56	MG	CA	1649	1/1	0.19	-	63,63,63,63	0
56	MG	DA	3516	1/1	0.49	-	70,70,70,70	0
56	MG	BA	3339	1/1	0.29	-	26,26,26,26	0
56	MG	BA	3435	1/1	1.39	-	112,112,112,112	0
56	MG	DA	3036	1/1	0.10	-	80,80,80,80	0
56	MG	BA	3443	1/1	0.36	-	18,18,18,18	0
56	MG	DA	3623	1/1	0.30	-	52,52,52,52	0
56	MG	BA	3036	1/1	0.26	-	131,131,131,131	0
56	MG	DA	3498	1/1	0.40	-	80,80,80,80	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	AA	1944	1/1	0.42	-	67,67,67,67	0
56	MG	DA	2983	1/1	0.33	-	77,77,77,77	0
56	MG	BA	2914	1/1	0.23	-	122,122,122,122	0
56	MG	BA	3202	1/1	0.19	-	205,205,205,205	0
56	MG	BA	3561	1/1	0.38	-	58,58,58,58	0
56	MG	BA	3558	1/1	0.29	-	71,71,71,71	0
56	MG	BA	3466	1/1	0.40	-	39,39,39,39	0
56	MG	DA	3183	1/1	0.33	-	16,16,16,16	0
56	MG	BA	3431	1/1	0.32	-	67,67,67,67	0
56	MG	BA	3671	1/1	0.28	-	84,84,84,84	0
56	MG	DA	3266	1/1	0.61	-	64,64,64,64	0
56	MG	BA	3056	1/1	0.25	-	117,117,117,117	0
56	MG	AA	1948	1/1	0.82	-	103,103,103,103	0
56	MG	AA	1730	1/1	0.19	-	78,78,78,78	0
56	MG	AA	1780	1/1	1.22	-	105,105,105,105	0
56	MG	BA	3232	1/1	0.18	-	65,65,65,65	0
56	MG	AA	1973	1/1	0.69	-	65,65,65,65	0
56	MG	BA	3402	1/1	0.34	-	37,37,37,37	0
56	MG	BA	3280	1/1	0.15	-	84,84,84,84	0
56	MG	CA	1804	1/1	0.36	-	78,78,78,78	0
56	MG	DA	2958	1/1	0.75	-	95,95,95,95	0
56	MG	DA	3010	1/1	0.77	-	54,54,54,54	0
56	MG	CA	1648	1/1	0.46	-	155,155,155,155	0
56	MG	BA	3385	1/1	0.36	-	50,50,50,50	0
56	MG	DA	3265	1/1	0.17	-	40,40,40,40	0
56	MG	CA	1786	1/1	0.30	-	84,84,84,84	0
56	MG	BA	3425	1/1	0.24	-	202,202,202,202	0
56	MG	AA	1657	1/1	0.27	-	112,112,112,112	0
56	MG	AA	1800	1/1	0.41	-	87,87,87,87	0
56	MG	BA	3328	1/1	0.57	-	35,35,35,35	0
56	MG	CA	1800	1/1	0.62	-	124,124,124,124	0
56	MG	CA	1899	1/1	0.41	-	41,41,41,41	0
56	MG	BA	3275	1/1	0.46	-	102,102,102,102	0
56	MG	CA	1827	1/1	0.09	-	45,45,45,45	0
56	MG	BA	2940	1/1	0.14	-	67,67,67,67	0
56	MG	AA	1989	1/1	0.24	-	70,70,70,70	0
56	MG	BA	3044	1/1	0.33	-	53,53,53,53	0

6.5 Other polymers ⓘ

There are no such residues in this entry.