



# wwPDB X-ray Structure Validation Summary Report

Jun 16, 2014 – 07:43 PM BST

PDB ID : 4V67  
Title : Crystal structure of a translation termination complex formed with release factor RF2.  
Authors : Korostelev, A.; Asahara, H.; Lancaster, L.; Laurberg, M.; Hirschi, A.; Noller, H.F.  
Deposited on : 2008-10-27  
Resolution : 3.00 Å(reported)

This is a wwPDB validation summary report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

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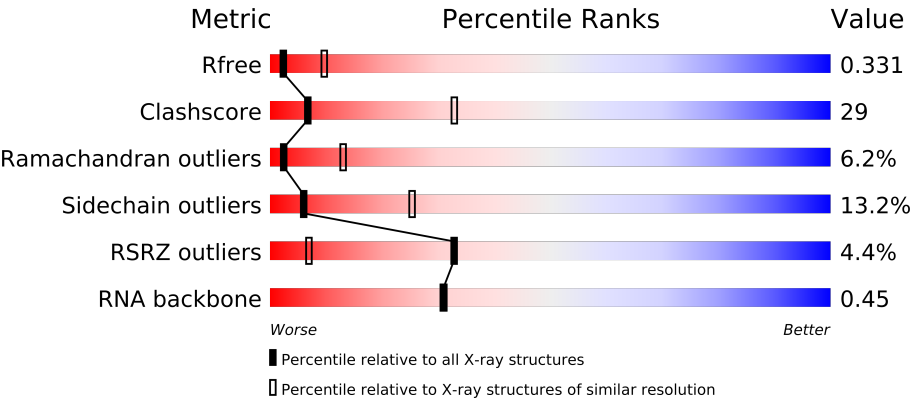
The following versions of software and data (see [references](#)) were used in the production of this report:

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 3.00 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R <sub>free</sub>	66092	1216 (3.00-3.00)
Clashscore	79885	1594 (3.00-3.00)
Ramachandran outliers	78287	1537 (3.00-3.00)
Sidechain outliers	78261	1540 (3.00-3.00)
RSRZ outliers	66119	1217 (3.00-3.00)
RNA backbone	1838	1070 (3.50-2.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	1525	
1	CA	1525	
2	AY	77	
2	AZ	77	
2	CY	77	
2	CZ	77	
3	AV	27	
3	CV	27	
4	AB	256	
4	CB	256	
5	AC	239	
5	CC	239	

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Mol	Chain	Length	Quality of chain
6	AD	209	
6	CD	209	
7	AE	162	
7	CE	162	
8	AF	101	
8	CF	101	
9	AG	156	
9	CG	156	
10	AH	138	
10	CH	138	
11	AI	128	
11	CI	128	
12	AJ	105	
12	CJ	105	
13	AK	129	
13	CK	129	
14	AL	134	
14	CL	134	
15	AM	126	
15	CM	126	
16	AN	61	
16	CN	61	
17	AO	89	
17	CO	89	
18	AP	88	
18	CP	88	
19	AQ	105	
19	CQ	105	
20	AR	88	
20	CR	88	
21	AS	93	
21	CS	93	
22	AT	106	
22	CT	106	
23	AU	27	
23	CU	27	
24	AX	378	
24	CX	378	
25	BA	2894	
25	DA	2894	
26	BB	124	
26	DB	124	

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Mol	Chain	Length	Quality of chain
27	BD	276	
27	DD	276	
28	BE	206	
28	DE	206	
29	BF	210	
29	DF	210	
30	BG	182	
30	DG	182	
31	BH	180	
31	DH	180	
32	BI	148	
32	DI	148	
33	BK	147	
33	DK	147	
34	BN	163	
34	DN	163	
35	BO	122	
35	DO	122	
36	BP	150	
36	DP	150	
37	BQ	141	
37	DQ	141	
38	BR	118	
38	DR	118	
39	BS	112	
39	DS	112	
40	BT	146	
40	DT	146	
41	BU	118	
41	DU	118	
42	BV	101	
42	DV	101	
43	BW	113	
43	DW	113	
44	BX	96	
44	DX	96	
45	BY	110	
45	DY	110	
46	BZ	206	
46	DZ	206	
47	B0	85	
47	D0	85	

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Mol	Chain	Length	Quality of chain
48	B1	98	
48	D1	98	
49	B2	72	
49	D2	72	
50	B3	60	
50	D3	60	
51	B4	97	
51	D4	97	
52	B5	60	
52	D5	60	
53	B6	54	
53	D6	54	
54	B7	49	
54	D7	49	
55	B8	65	
55	D8	65	

## 2 Entry composition

There are 57 unique types of molecules in this entry. The entry contains 301148 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.

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			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AA	466	G	C	CONFLICT	GB 155076
CA	466	G	C	CONFLICT	GB 155076

- Molecule 2 is a RNA chain called P AND E-SITE TRNA(FMET).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	AZ	77	Total	C	N	O	P	0	0	0
			1640	732	297	535	76			
2	AY	77	Total	C	N	O	P	0	0	0
			1640	732	297	535	76			
2	CZ	77	Total	C	N	O	P	0	0	0
			1640	732	297	535	76			
2	CY	77	Total	C	N	O	P	0	0	0
			1640	732	297	535	76			

- Molecule 3 is a RNA chain called MRNA.

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

- Molecule 4 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	AB	234	Total	C	N	O	S	0	0	0
			1900	1213	341	341	5			
4	CB	234	Total	C	N	O	S	0	0	0
			1900	1213	341	341	5			

- Molecule 5 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	AC	206	Total	C	N	O	S	0	0	0
			1612	1016	314	281	1			
5	CC	206	Total	C	N	O	S	0	0	0
			1612	1016	314	281	1			

- Molecule 6 is a protein called 30S ribosomal protein S4.

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

- Molecule 7 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	AE	151	Total	C	N	O	S	0	0	0
			1155	729	218	204	4			
7	CE	151	Total	C	N	O	S	0	0	0
			1155	729	218	204	4			

- Molecule 8 is a protein called 30S ribosomal protein S6.

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

- Molecule 9 is a protein called 30S ribosomal protein S7.

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

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

- Molecule 10 is a protein called 30S ribosomal protein S8.

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

- Molecule 11 is a protein called 30S ribosomal protein S9.

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

- Molecule 12 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	AJ	98	Total	C	N	O	S	0	0	0
			794	499	156	138	1			
12	CJ	98	Total	C	N	O	S	0	0	0
			794	499	156	138	1			

- Molecule 13 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	AK	114	Total	C	N	O	S	0	0	0
			842	522	159	158	3			
13	CK	114	Total	C	N	O	S	0	0	0
			842	522	159	158	3			

- Molecule 14 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	AL	122	Total	C	N	O	S	0	0	0
			956	603	193	159	1			
14	CL	122	Total	C	N	O	S	0	0	0
			956	603	193	159	1			



There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AL	2	ALA	-	INSERTION	UNP P61941
AL	3	LEU	-	INSERTION	UNP P61941
CL	2	ALA	-	INSERTION	UNP P61941
CL	3	LEU	-	INSERTION	UNP P61941

- Molecule 15 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	AM	117	Total	C	N	O	S	0	0	0
			933	577	192	162	2			
15	CM	117	Total	C	N	O	S	0	0	0
			933	577	192	162	2			

- Molecule 16 is a protein called 30S ribosomal protein S14.

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

- Molecule 17 is a protein called 30S ribosomal protein S15.

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

- Molecule 18 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
18	AP	83	Total	C	N	O	S	0	0	0
			700	443	139	117	1			
18	CP	83	Total	C	N	O	S	0	0	0
			700	443	139	117	1			

- Molecule 19 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	AQ	99	Total	C	N	O	S	0	0	0
			823	528	152	141	2			
19	CQ	99	Total	C	N	O	S	0	0	0
			823	528	152	141	2			

- Molecule 20 is a protein called 30S ribosomal protein S18.

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

- Molecule 21 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
21	AS	78	Total	C	N	O	S	0	0	0
			629	403	114	110	2			
21	CS	78	Total	C	N	O	S	0	0	0
			629	403	114	110	2			

- Molecule 22 is a protein called 30S ribosomal protein S20.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	AU	24	Total	C	N	O		0	0	0
			208	128	50	30				
23	CU	24	Total	C	N	O		0	0	0
			208	128	50	30				

- Molecule 24 is a protein called Bacterial peptide chain release factor 2 (RF-2).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	AX	362	Total	C	N	O	S	0	0	0
			2876	1794	518	556	8			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	CX	362	Total	C	N	O	S	0	0	0
			2876	1794	518	556	8			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
25	BA	2879	Total	C	N	O	P	0	0	0
			61997	27594	11582	19943	2878			
25	DA	2879	Total	C	N	O	P	0	0	0
			61997	27594	11582	19943	2878			

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

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
			2104	1329	416	356	3			
27	DD	271	Total	C	N	O	S	0	0	0
			2104	1329	416	356	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
			1563	988	299	270	6			
28	DE	204	Total	C	N	O	S	0	0	0
			1563	988	299	270	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
			1586	1011	297	275	3			
29	DF	202	Total	C	N	O	S	0	0	0
			1586	1011	297	275	3			

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
BF	1	MET	-	INSERTION	UNP Q72I05
BF	2	LYS	-	INSERTION	UNP Q72I05
BF	3	GLU	-	INSERTION	UNP Q72I05
BF	4	VAL	-	INSERTION	UNP Q72I05
BF	5	ALA	-	INSERTION	UNP Q72I05
DF	1	MET	-	INSERTION	UNP Q72I05
DF	2	LYS	-	INSERTION	UNP Q72I05
DF	3	GLU	-	INSERTION	UNP Q72I05
DF	4	VAL	-	INSERTION	UNP Q72I05
DF	5	ALA	-	INSERTION	UNP Q72I05

- 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
			1222	773	228	220	1			
31	DH	159	Total	C	N	O	S	0	0	0
			1222	773	228	220	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
			1132	724	200	207	1			
32	DI	145	Total	C	N	O	S	0	0	0
			1132	724	200	207	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			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
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
			1096	707	205	181	3			
34	DN	137	Total	C	N	O	S	0	0	0
			1096	707	205	181	3			

There are 48 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
BN	1	MET	-	INSERTION	UNP Q72IN1
BN	2	VAL	-	INSERTION	UNP Q72IN1
BN	3	LYS	-	INSERTION	UNP Q72IN1
BN	4	SER	-	INSERTION	UNP Q72IN1
BN	5	SER	-	INSERTION	UNP Q72IN1
BN	6	LEU	-	INSERTION	UNP Q72IN1
BN	7	ALA	-	INSERTION	UNP Q72IN1
BN	8	PHE	-	INSERTION	UNP Q72IN1
BN	9	LEU	-	INSERTION	UNP Q72IN1
BN	10	ARG	-	INSERTION	UNP Q72IN1
BN	11	GLY	-	INSERTION	UNP Q72IN1
BN	12	PRO	-	INSERTION	UNP Q72IN1
BN	13	PRO	-	INSERTION	UNP Q72IN1
BN	14	ILE	-	INSERTION	UNP Q72IN1
BN	15	PRO	-	INSERTION	UNP Q72IN1
BN	16	ARG	-	INSERTION	UNP Q72IN1
BN	17	GLN	-	INSERTION	UNP Q72IN1
BN	18	GLU	-	INSERTION	UNP Q72IN1
BN	19	GLN	-	INSERTION	UNP Q72IN1
BN	20	ARG	-	INSERTION	UNP Q72IN1
BN	21	ARG	-	INSERTION	UNP Q72IN1
BN	22	ALA	-	INSERTION	UNP Q72IN1
BN	23	LEU	-	INSERTION	UNP Q72IN1
BN	24	VAL	-	INSERTION	UNP Q72IN1
DN	1	MET	-	INSERTION	UNP Q72IN1
DN	2	VAL	-	INSERTION	UNP Q72IN1
DN	3	LYS	-	INSERTION	UNP Q72IN1
DN	4	SER	-	INSERTION	UNP Q72IN1

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Chain	Residue	Modelled	Actual	Comment	Reference
DN	5	SER	-	INSERTION	UNP Q72IN1
DN	6	LEU	-	INSERTION	UNP Q72IN1
DN	7	ALA	-	INSERTION	UNP Q72IN1
DN	8	PHE	-	INSERTION	UNP Q72IN1
DN	9	LEU	-	INSERTION	UNP Q72IN1
DN	10	ARG	-	INSERTION	UNP Q72IN1
DN	11	GLY	-	INSERTION	UNP Q72IN1
DN	12	PRO	-	INSERTION	UNP Q72IN1
DN	13	PRO	-	INSERTION	UNP Q72IN1
DN	14	ILE	-	INSERTION	UNP Q72IN1
DN	15	PRO	-	INSERTION	UNP Q72IN1
DN	16	ARG	-	INSERTION	UNP Q72IN1
DN	17	GLN	-	INSERTION	UNP Q72IN1
DN	18	GLU	-	INSERTION	UNP Q72IN1
DN	19	GLN	-	INSERTION	UNP Q72IN1
DN	20	ARG	-	INSERTION	UNP Q72IN1
DN	21	ARG	-	INSERTION	UNP Q72IN1
DN	22	ALA	-	INSERTION	UNP Q72IN1
DN	23	LEU	-	INSERTION	UNP Q72IN1
DN	24	VAL	-	INSERTION	UNP Q72IN1

- 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
			1064	680	201	178	5			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
37	DQ	134	Total	C	N	O	S	0	0	0
			1064	680	201	178	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
			770	486	154	130				
39	DS	98	Total	C	N	O		0	0	0
			770	486	154	130				

- 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
			1143	713	234	195	1			
40	DT	137	Total	C	N	O	S	0	0	0
			1143	713	234	195	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
			890	560	175	153	2			
43	DW	112	Total	C	N	O	S	0	0	0
			890	560	175	153	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
			725	471	131	123				
44	DX	92	Total	C	N	O		0	0	0
			725	471	131	123				

- 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
			775	500	148	123	4			
45	DY	100	Total	C	N	O	S	0	0	0
			775	500	148	123	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
			1482	945	264	271	2			
46	DZ	187	Total	C	N	O	S	0	0	0
			1482	945	264	271	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
			694	435	141	118			
48	D1	88	Total	C	N	O	0	0	0
			694	435	141	118			

- 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
			520	325	102	91	2			
49	D2	62	Total	C	N	O	S	0	0	0
			520	325	102	91	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
			467	298	90	78	1			
50	D3	59	Total	C	N	O	S	0	0	0
			467	298	90	78	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
			225	142	36	43	4			
51	D4	30	Total	C	N	O	S	0	0	0
			225	142	36	43	4			

There are 54 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B4	1	MET	-	INSERTION	UNP Q72JR0
B4	2	PRO	-	INSERTION	UNP Q72JR0
B4	3	LEU	-	INSERTION	UNP Q72JR0
B4	4	GLY	-	INSERTION	UNP Q72JR0
B4	5	VAL	-	INSERTION	UNP Q72JR0
B4	6	HIS	-	INSERTION	UNP Q72JR0
B4	7	PRO	-	INSERTION	UNP Q72JR0
B4	8	LEU	-	INSERTION	UNP Q72JR0
B4	9	TYR	-	INSERTION	UNP Q72JR0
B4	10	THR	-	INSERTION	UNP Q72JR0
B4	11	LYS	-	INSERTION	UNP Q72JR0

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Chain	Residue	Modelled	Actual	Comment	Reference
B4	12	ARG	-	INSERTION	UNP Q72JR0
B4	13	TRP	-	INSERTION	UNP Q72JR0
B4	14	LEU	-	INSERTION	UNP Q72JR0
B4	15	ALA	-	INSERTION	UNP Q72JR0
B4	16	HIS	-	INSERTION	UNP Q72JR0
B4	17	GLY	-	INSERTION	UNP Q72JR0
B4	18	GLN	-	INSERTION	UNP Q72JR0
B4	19	ASP	-	INSERTION	UNP Q72JR0
B4	20	ARG	-	INSERTION	UNP Q72JR0
B4	21	ALA	-	INSERTION	UNP Q72JR0
B4	22	LYS	-	INSERTION	UNP Q72JR0
B4	23	LYS	-	INSERTION	UNP Q72JR0
B4	24	GLU	-	INSERTION	UNP Q72JR0
B4	25	ALA	-	INSERTION	UNP Q72JR0
B4	26	ASN	-	INSERTION	UNP Q72JR0
B4	27	VAL	-	INSERTION	UNP Q72JR0
D4	1	MET	-	INSERTION	UNP Q72JR0
D4	2	PRO	-	INSERTION	UNP Q72JR0
D4	3	LEU	-	INSERTION	UNP Q72JR0
D4	4	GLY	-	INSERTION	UNP Q72JR0
D4	5	VAL	-	INSERTION	UNP Q72JR0
D4	6	HIS	-	INSERTION	UNP Q72JR0
D4	7	PRO	-	INSERTION	UNP Q72JR0
D4	8	LEU	-	INSERTION	UNP Q72JR0
D4	9	TYR	-	INSERTION	UNP Q72JR0
D4	10	THR	-	INSERTION	UNP Q72JR0
D4	11	LYS	-	INSERTION	UNP Q72JR0
D4	12	ARG	-	INSERTION	UNP Q72JR0
D4	13	TRP	-	INSERTION	UNP Q72JR0
D4	14	LEU	-	INSERTION	UNP Q72JR0
D4	15	ALA	-	INSERTION	UNP Q72JR0
D4	16	HIS	-	INSERTION	UNP Q72JR0
D4	17	GLY	-	INSERTION	UNP Q72JR0
D4	18	GLN	-	INSERTION	UNP Q72JR0
D4	19	ASP	-	INSERTION	UNP Q72JR0
D4	20	ARG	-	INSERTION	UNP Q72JR0
D4	21	ALA	-	INSERTION	UNP Q72JR0
D4	22	LYS	-	INSERTION	UNP Q72JR0
D4	23	LYS	-	INSERTION	UNP Q72JR0
D4	24	GLU	-	INSERTION	UNP Q72JR0
D4	25	ALA	-	INSERTION	UNP Q72JR0
D4	26	ASN	-	INSERTION	UNP Q72JR0

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Chain	Residue	Modelled	Actual	Comment	Reference
D4	27	VAL	-	INSERTION	UNP Q72JR0

- 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
			404	255	79	65	5			
52	D5	52	Total	C	N	O	S	0	0	0
			404	255	79	65	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
			380	235	77	64	4			
53	D6	44	Total	C	N	O	S	0	0	0
			380	235	77	64	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
			418	257	104	55	2			
54	D7	48	Total	C	N	O	S	0	0	0
			418	257	104	55	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
			507	326	101	78	2			
55	D8	63	Total	C	N	O	S	0	0	0
			507	326	101	78	2			

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	CZ	14	Total	Mg	0	0
			14	14		
56	B4	2	Total	Mg	0	0
			2	2		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	BA	923	Total 923	Mg 923	0	0
56	AK	7	Total 7	Mg 7	0	0
56	DQ	2	Total 2	Mg 2	0	0
56	AB	7	Total 7	Mg 7	0	0
56	DF	1	Total 1	Mg 1	0	0
56	B8	4	Total 4	Mg 4	0	0
56	BE	6	Total 6	Mg 6	0	0
56	DU	1	Total 1	Mg 1	0	0
56	D8	1	Total 1	Mg 1	0	0
56	B1	7	Total 7	Mg 7	0	0
56	DY	1	Total 1	Mg 1	0	0
56	AN	1	Total 1	Mg 1	0	0
56	BP	2	Total 2	Mg 2	0	0
56	AX	14	Total 14	Mg 14	0	0
56	DN	1	Total 1	Mg 1	0	0
56	BI	6	Total 6	Mg 6	0	0
56	CY	14	Total 14	Mg 14	0	0
56	CH	2	Total 2	Mg 2	0	0
56	CA	222	Total 222	Mg 222	0	0
56	B5	2	Total 2	Mg 2	0	0
56	BB	35	Total 35	Mg 35	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	AJ	1	Total 1	Mg 1	0	0
56	BT	1	Total 1	Mg 1	0	0
56	DO	2	Total 2	Mg 2	0	0
56	AE	8	Total 8	Mg 8	0	0
56	DG	2	Total 2	Mg 2	0	0
56	CF	5	Total 5	Mg 5	0	0
56	DT	1	Total 1	Mg 1	0	0
56	BF	6	Total 6	Mg 6	0	0
56	AV	3	Total 3	Mg 3	0	0
56	BX	2	Total 2	Mg 2	0	0
56	DA	491	Total 491	Mg 491	0	0
56	B2	3	Total 3	Mg 3	0	0
56	AA	428	Total 428	Mg 428	0	0
56	BQ	6	Total 6	Mg 6	0	0
56	CQ	1	Total 1	Mg 1	0	0
56	D6	1	Total 1	Mg 1	0	0
56	AR	1	Total 1	Mg 1	0	0
56	B6	2	Total 2	Mg 2	0	0
56	DI	1	Total 1	Mg 1	0	0
56	AM	3	Total 3	Mg 3	0	0
56	BU	1	Total 1	Mg 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	DR	1	Total 1	Mg 1	0	0
56	CC	1	Total 1	Mg 1	0	0
56	AD	3	Total 3	Mg 3	0	0
56	BN	4	Total 4	Mg 4	0	0
56	CT	1	Total 1	Mg 1	0	0
56	CG	2	Total 2	Mg 2	0	0
56	BG	2	Total 2	Mg 2	0	0
56	AI	1	Total 1	Mg 1	0	0
56	BY	3	Total 3	Mg 3	0	0
56	DE	1	Total 1	Mg 1	0	0
56	BR	2	Total 2	Mg 2	0	0
56	AZ	15	Total 15	Mg 15	0	0
56	BK	3	Total 3	Mg 3	0	0
56	DP	1	Total 1	Mg 1	0	0
56	DD	9	Total 9	Mg 9	0	0
56	AL	4	Total 4	Mg 4	0	0
56	BV	3	Total 3	Mg 3	0	0
56	AG	2	Total 2	Mg 2	0	0
56	BO	5	Total 5	Mg 5	0	0
56	AQ	1	Total 1	Mg 1	0	0
56	D1	2	Total 2	Mg 2	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	AH	2	Total 2	Mg 2	0	0
56	BZ	1	Total 1	Mg 1	0	0
56	CO	1	Total 1	Mg 1	0	0
56	AC	4	Total 4	Mg 4	0	0
56	BS	3	Total 3	Mg 3	0	0
56	DB	12	Total 12	Mg 12	0	0
56	CS	1	Total 1	Mg 1	0	0
56	CB	2	Total 2	Mg 2	0	0
56	BD	7	Total 7	Mg 7	0	0
56	AT	2	Total 2	Mg 2	0	0
56	CL	1	Total 1	Mg 1	0	0
56	B0	3	Total 3	Mg 3	0	0
56	AO	2	Total 2	Mg 2	0	0
56	BW	2	Total 2	Mg 2	0	0
56	AY	26	Total 26	Mg 26	0	0
56	CK	3	Total 3	Mg 3	0	0
56	AF	2	Total 2	Mg 2	0	0
56	BH	4	Total 4	Mg 4	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

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
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

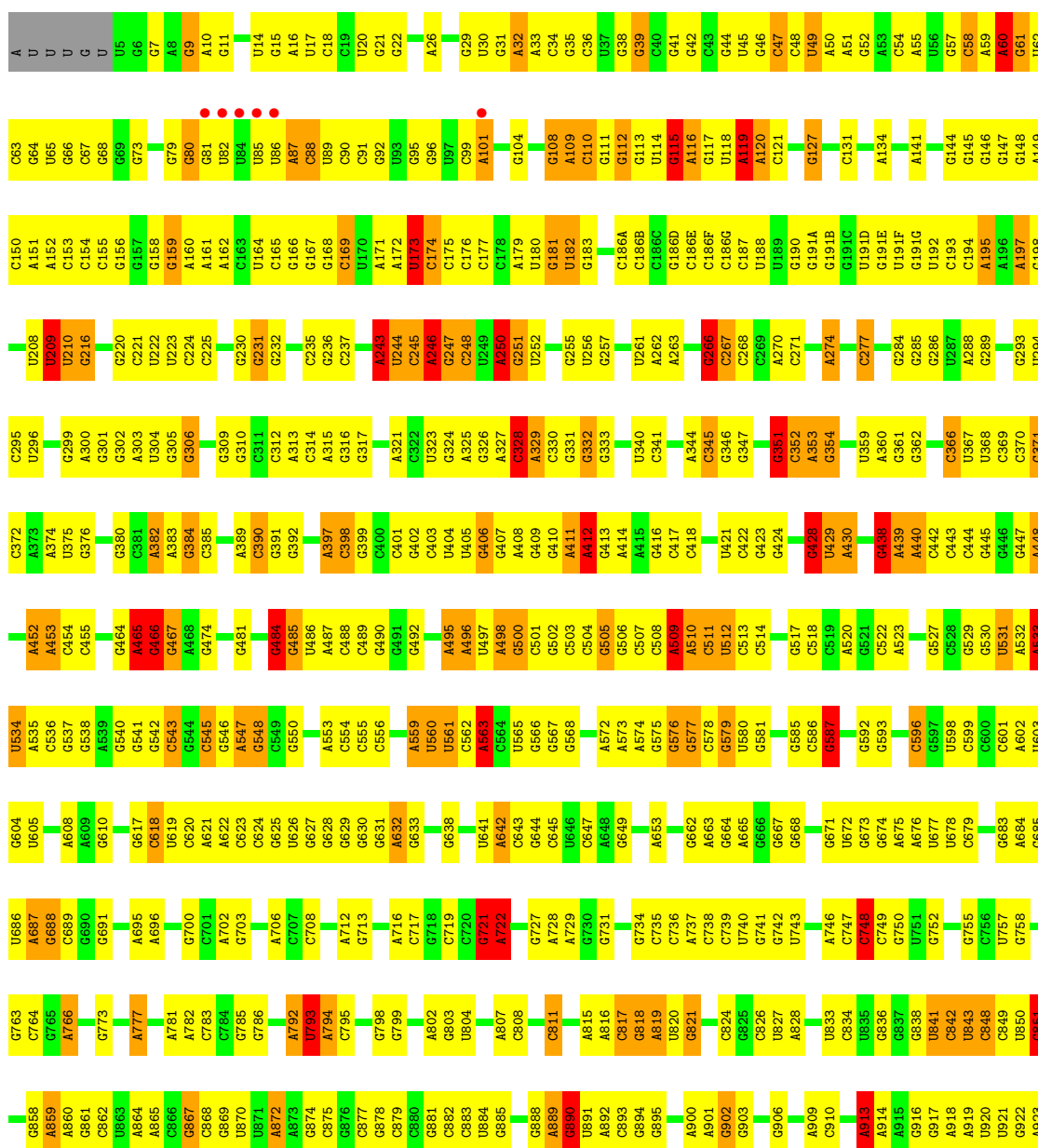


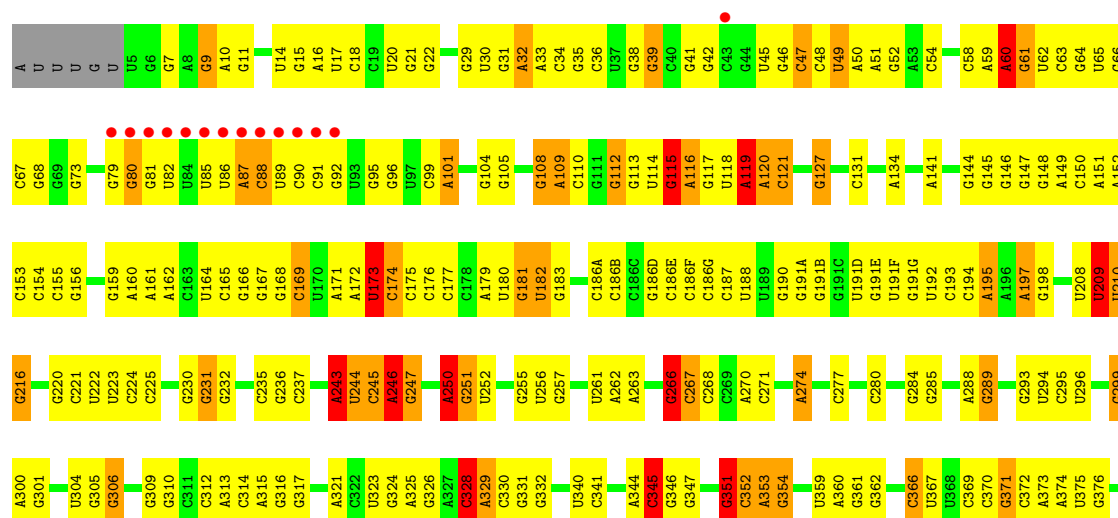
### 3 Residue-property plots

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

Chain AA: 





C1452	C1453	G1454	G1455	G1456	G1457	G1458	G1459	A1460	G1461	G1462	G1463	G1464	A1468	G1469	U1472	A1473	G1474	G1475	G1476	G1477	G1480	U1481	G1482	A1483	G1484	U1485	G1486	G1487	G1488	G1491	G1492	G1493	G1494	G1495	G1496	G1497	G1498	A1499	C1500	A1501	G1502	A1503	G1504	G1505	U1506	A1507	G1508	G1509	U1510	U1511	U1512	A1513	A1514	G1517	A1518	A1519	G1520	G1521	U1522	G1523
G1373	G1374	A1375	U1376	U1377	G1378	G1379	U1380	U1381	G1382	G1387	C1388	G1389	U1390	U1391	G1392	U1393	C1397	A1398	A1399	A1401	G1402	G1403	G1404	G1405	G1406	G1407	G1408	G1409	G1410	G1411	A1412	G1413	G1414	G1415	G1416	C417	C418	U421	C422	G423	G424	G428	U429	A430	G433	A439	A440	C443	C444	G445	G446	G447	U448	A452	A453	C454	C455	G537		
G1312	U1313	G1316	G1317	G1318	G1319	G1320	G1321	G1322	G1323	A1324	C1325	G1326	G1327	G1328	A1329	U1330	G1331	A1332	A1333	G1334	G1335	G1336	G1337	G1338	A1339	G1342	G1343	G1344	U1345	A1346	G1347	U1348	A1349	A1350	U1351	G1352	G1353	G1354	G1355	G1356	A1357	U1358	G1359	C1360	G1361	G1362	G1363	G1364	G1365	G1366	G1367	A1368	G1369	G1370	U1371	U1372				
A1245	G1182	A1183	G1184	G1185	G1186	G1187	A1188	G1189	G1190	G1193	U1196	G1197	G1198	U1199	A1200	G1201	G1202	C1203	A1204	U1205	G1206	G1207	G1208	G1209	U1210	U1211	U1212	A1213	G1214	G1215	G1216	G1217	G1218	U1219	G1220	G1221	G1222	C1223	G1224	A1225	G1226	A1227	G1228	C1229	G1230	G1231	U1232	G1233	G1234	U1235	A1236	G1237	G1238	A1239	U1240	G1241	C1244			
A1245	A1250	A1251	A1252	G1253	C1254	G1255	A1256	U1257	G1258	G1259	C1260	G1263	G1264	G1265	A1268	A1269	C1270	G1271	G1272	G1273	G1274	A1275	G1276	G1277	U1278	A1279	U1280	A1281	U1282	G1283	G1284	A1285	A1286	A1287	A1288	G1291	U1292	G1293	C1296	G1297	G1298	A1299	G1300	U1301	U1302	G1303	G1304	G1305	A1306	U1307	A1308	G1309	G1310	G1311						
G1312	U1313	G1316	G1317	G1318	G1319	G1320	G1321	G1322	G1323	A1324	C1325	G1326	G1327	G1328	A1329	U1330	G1331	A1332	A1333	G1334	G1335	G1336	G1337	G1338	A1339	G1342	G1343	G1344	U1345	A1346	G1347	U1348	A1349	A1350	U1351	G1352	G1353	G1354	G1355	G1356	A1357	U1358	G1359	C1360	G1361	G1362	G1363	G1364	G1365	G1366	G1367	A1368	G1369	G1370	U1371	U1372				
G1373	A1374	U1375	U1376	A1377	G1378	G1379	U1380	U1381	G1382	G1387	C1388	G1389	U1390	U1391	G1392	U1393	C1397	A1398	A1399	A1401	G1402	G1403	G1404	G1405	G1406	G1407	G1408	G1409	G1410	G1411	A1412	G1413	G1414	G1415	G1416	C417	C418	U421	C422	G423	G424	G428	U429	A430	G433	A439	A440	C443	C444	G445	G446	G447	U448	A452	A453	C454	C455	G537		
C1452	G1453	G1454	G1455	G1456	G1457	G1458	G1459	A1460	G1461	G1462	G1463	G1464	A1468	G1469	U1472	A1473	G1474	G1475	G1476	G1477	G1480	U1481	G1482	A1483	G1484	U1485	G1486	G1487	G1488	G1491	G1492	G1493	G1494	G1495	G1496	G1497	G1498	A1499	C1500	A1501	G1502	A1503	G1504	U1505	U1506	A1507	G1508	G1509	U1510	U1511	U1512	A1513	A1514	G1517	A1518	A1519	G1520	G1521	U1522	G1523

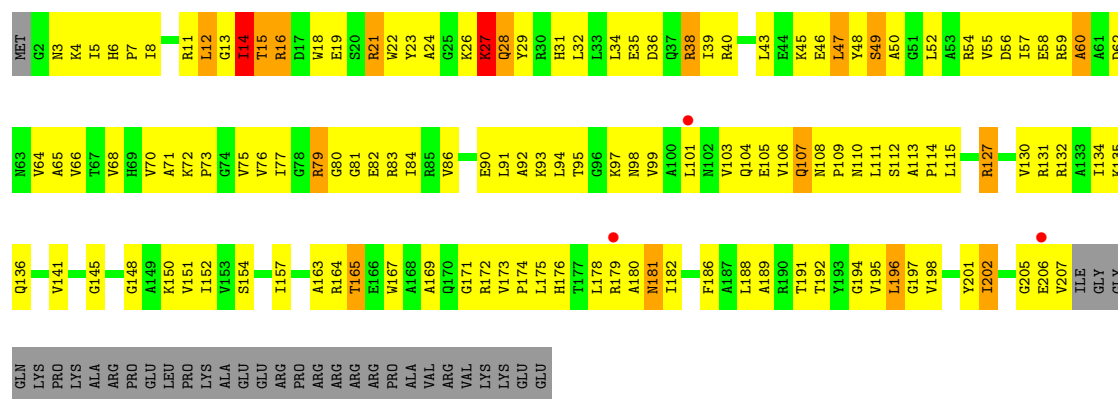


Chain AB:

Chain CB:

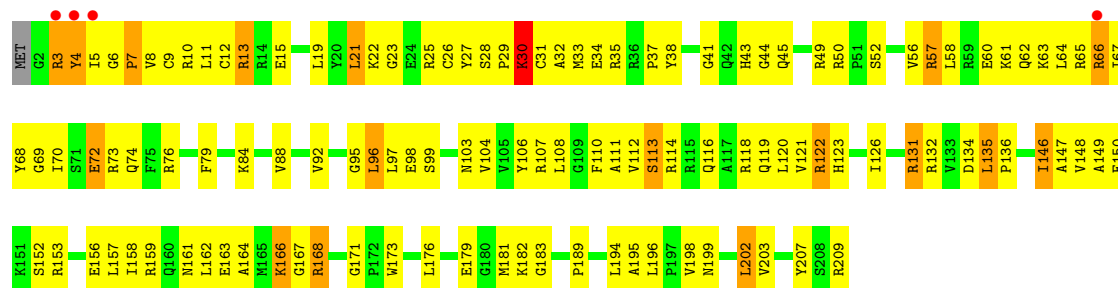
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Chain CC: 



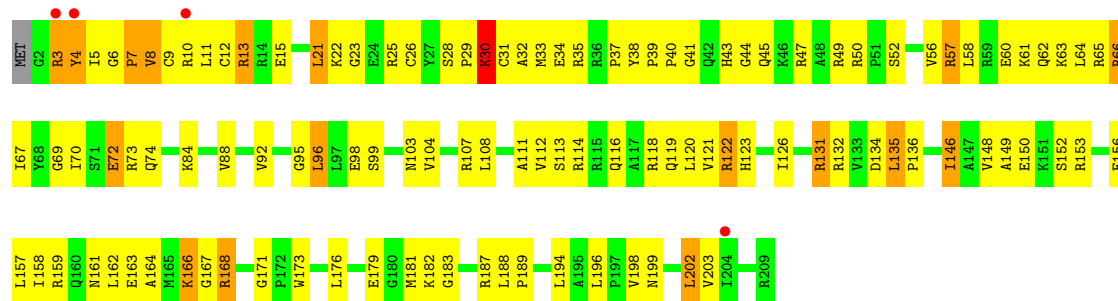
- Molecule 6: 30S ribosomal protein S4

Chain AD:



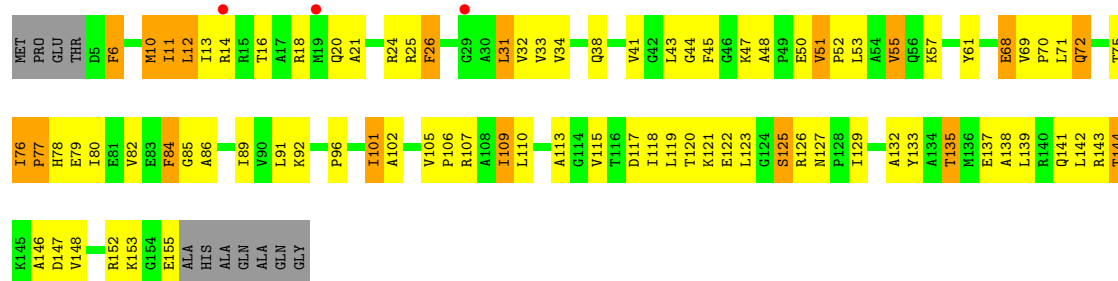
- Molecule 6: 30S ribosomal protein S4

Chain CD:



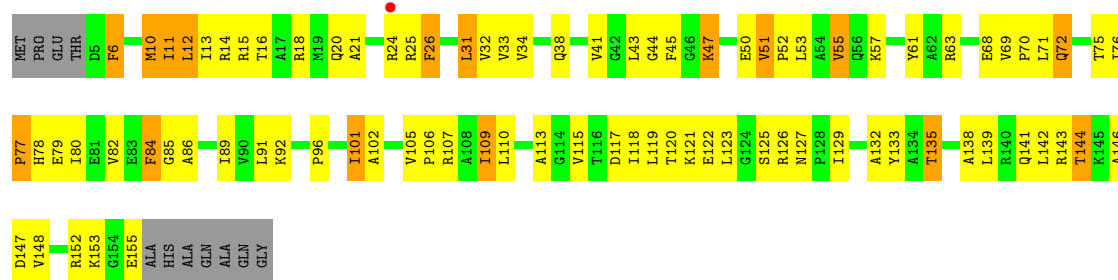
- Molecule 7: 30S ribosomal protein S5

Chain AE:



- Molecule 7: 30S ribosomal protein S5

Chain CE:



- Molecule 8: 30S ribosomal protein S6

Chain AF:



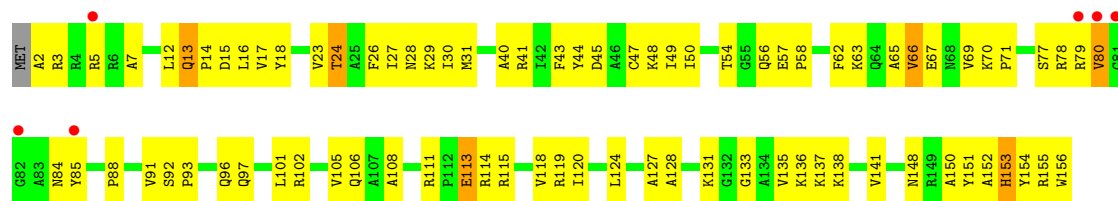
- Molecule 8: 30S ribosomal protein S6

Chain CF:



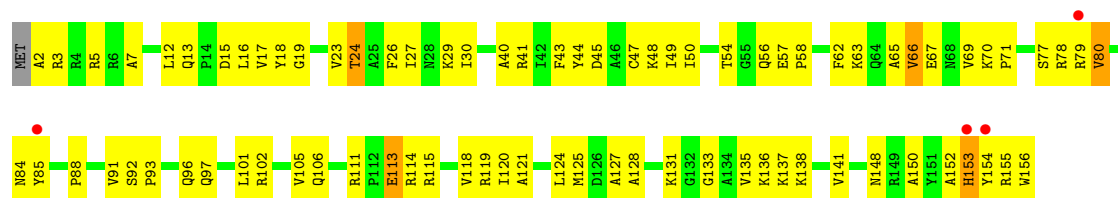
- Molecule 9: 30S ribosomal protein S7

Chain AG:



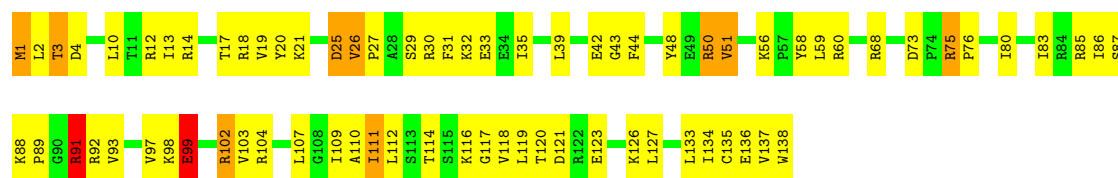
- Molecule 9: 30S ribosomal protein S7

Chain CG:



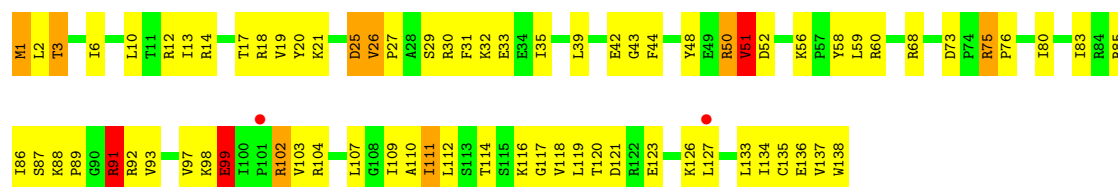
- Molecule 10: 30S ribosomal protein S8

Chain AH:



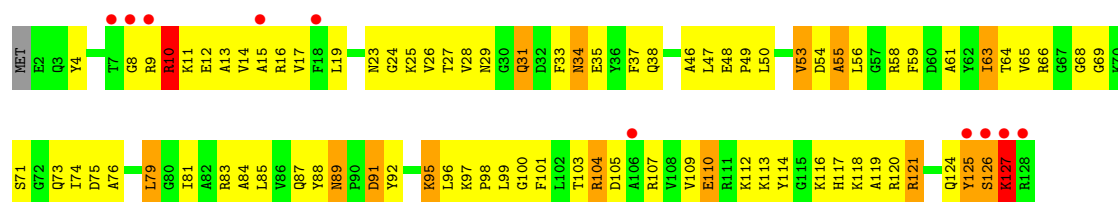
- Molecule 10: 30S ribosomal protein S8

Chain CH:



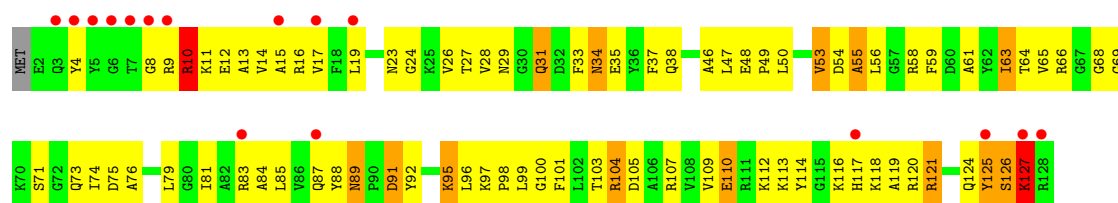
- Molecule 11: 30S ribosomal protein S9

Chain AI:



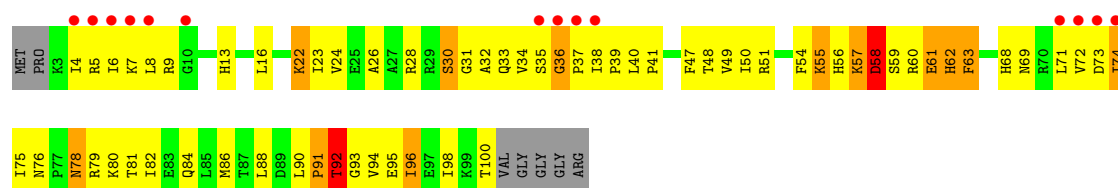
- Molecule 11: 30S ribosomal protein S9

Chain CI:



- Molecule 12: 30S ribosomal protein S10

Chain AJ:

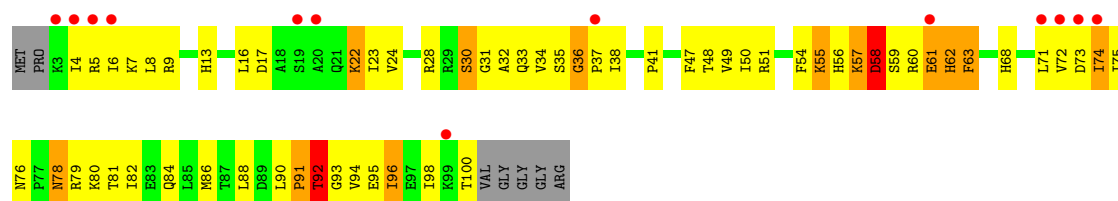


- Molecule 12: 30S ribosomal protein S10

Chain CJ:

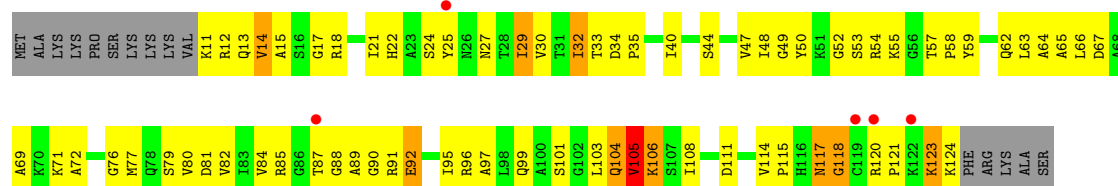






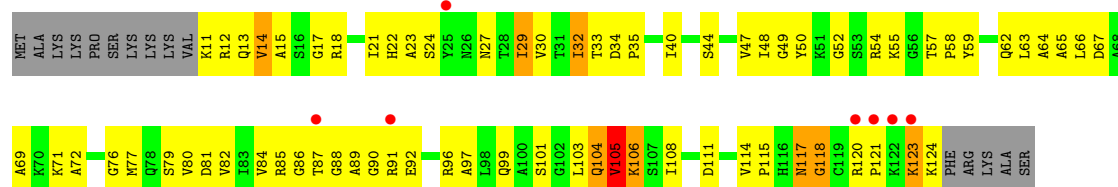
• Molecule 13: 30S ribosomal protein S11

Chain AK:



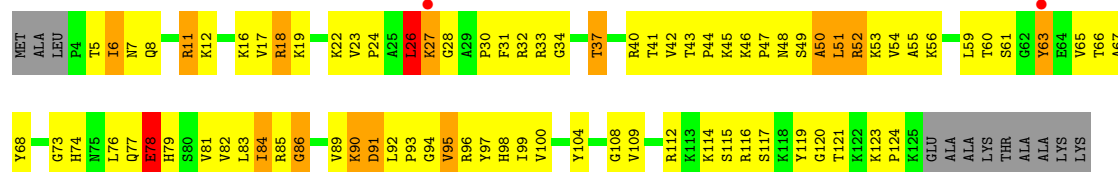
• Molecule 13: 30S ribosomal protein S11

Chain CK:



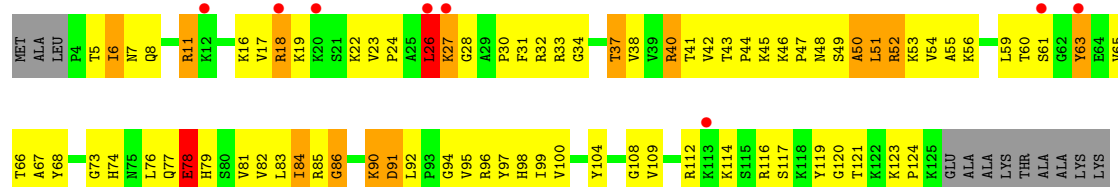
• Molecule 14: 30S ribosomal protein S12

Chain AL:



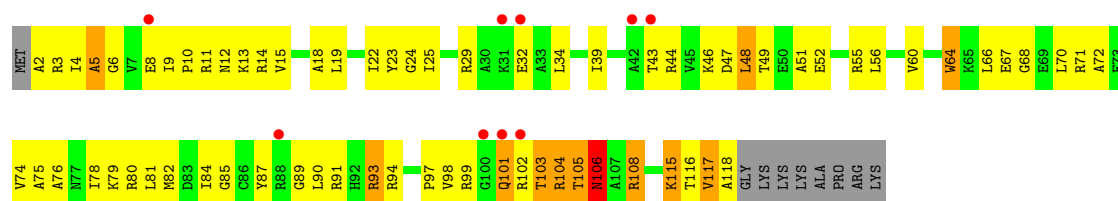
• Molecule 14: 30S ribosomal protein S12

Chain CL:



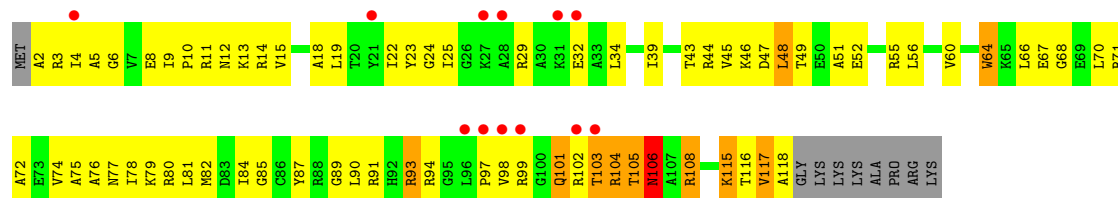
• Molecule 15: 30S ribosomal protein S13

Chain AM:



• Molecule 15: 30S ribosomal protein S13

Chain CM:



• Molecule 16: 30S ribosomal protein S14

Chain AN:



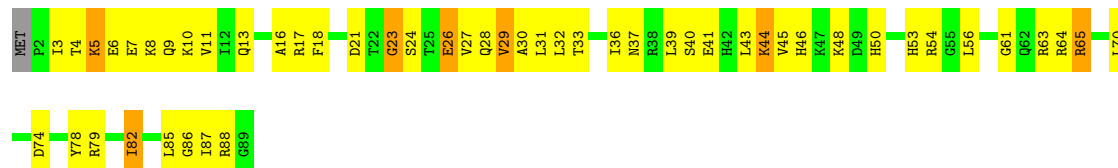
• Molecule 16: 30S ribosomal protein S14

Chain CN:



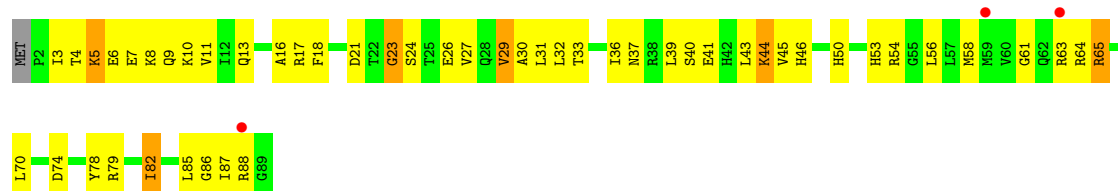
• Molecule 17: 30S ribosomal protein S15

Chain AO:



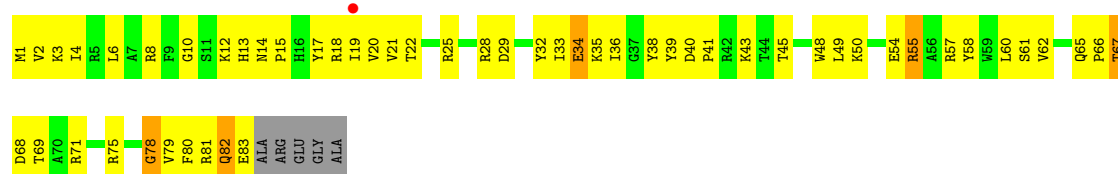
• Molecule 17: 30S ribosomal protein S15

Chain CO:



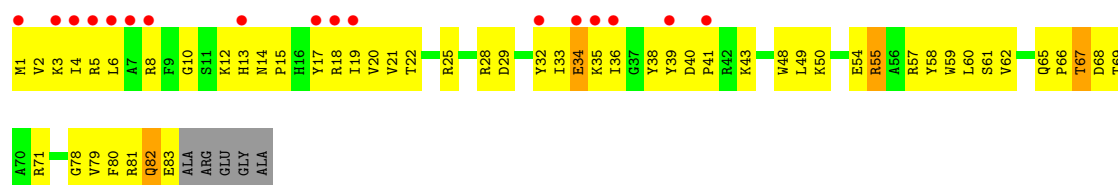
• Molecule 18: 30S ribosomal protein S16

Chain AP:



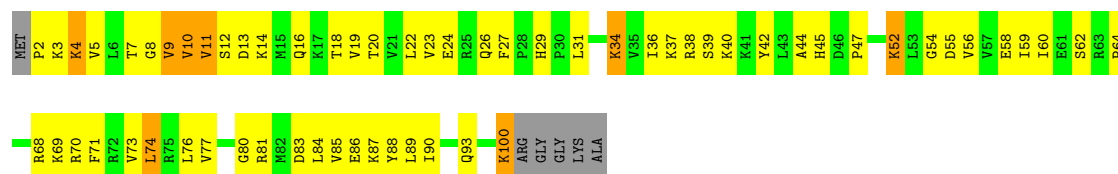
• Molecule 18: 30S ribosomal protein S16

Chain CP:



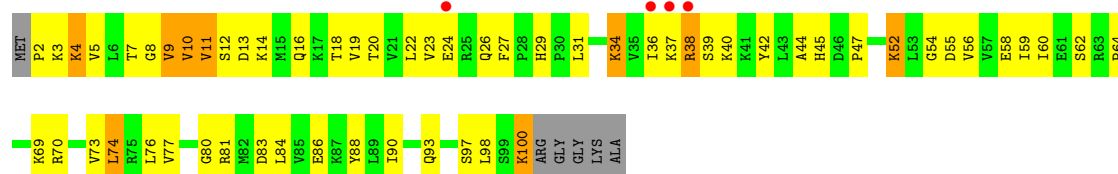
• Molecule 19: 30S ribosomal protein S17

Chain AQ:



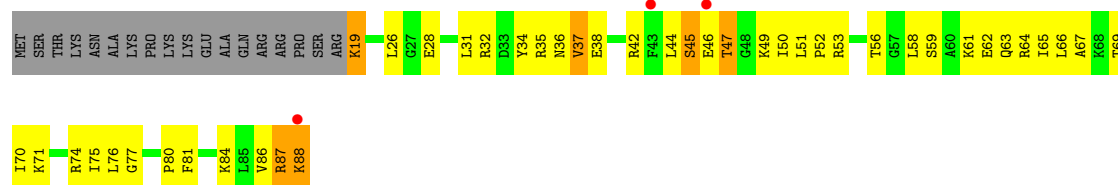
• Molecule 19: 30S ribosomal protein S17

Chain CQ:



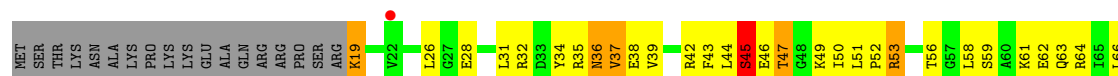
• Molecule 20: 30S ribosomal protein S18

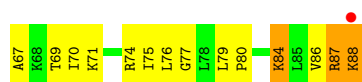
Chain AR:



• Molecule 20: 30S ribosomal protein S18

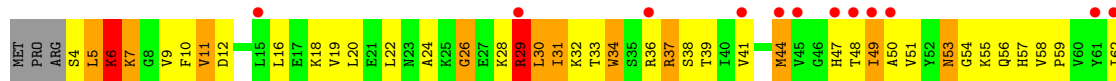
Chain CR:





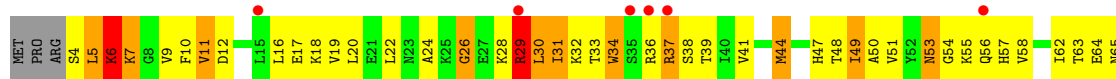
- Molecule 21: 30S ribosomal protein S19

Chain AS:



- Molecule 21: 30S ribosomal protein S19

Chain CS:



- Molecule 22: 30S ribosomal protein S20

Chain AT:



- Molecule 22: 30S ribosomal protein S20

Chain CT:



- Molecule 23: 30S ribosomal protein Thx

Chain AU:



- Molecule 23: 30S ribosomal protein Thx



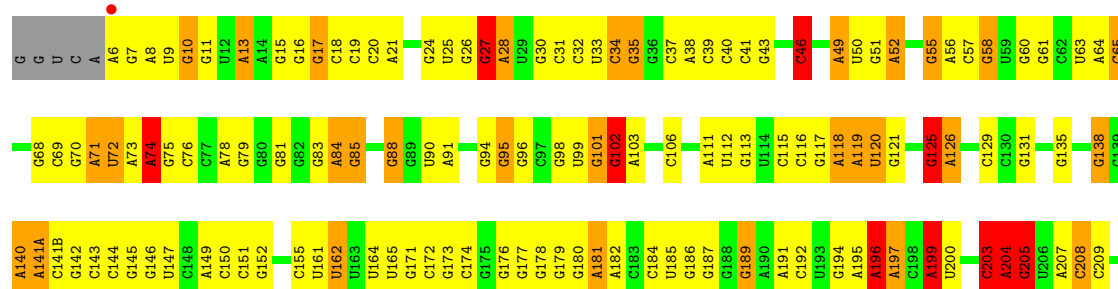
● Molecule 25: 23S RRNA

Chain BA:



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A64	C65	G68	C71B	G68	C69	G70	A71	U72	A73	C150	G75	C77	A78	U79	G80	G81	U164	U165	G83	A84	G85	A88	G89	U90	A91	G94	G95	G96	U99	G101	C102	A103	C106	A190	A191	C192	U193	G194	A195	C116	G117	A118	A119	U120	G121	G122	G125	A126	C130	G131	G135	G138	C139							
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G217	A218	G219	G220	A221	A222	A228	A229	U230	A230	C231	C232	A233	C234	U235	C236	U239	G240	A241	G242	G245	C246	G247	G248	C249	A250	A251	G252	A262	C263	C264	U185	A265	G266	U269	G307	G308	G309	C309	A310	A311	G312	G315	C316	C317	C318	C319	A320	G321	A322	C323	A324	G325	G326	G270U	G270V	G270W	G270X			
U271A	G271B	C271C	U271D	G271	C273G	G274	G275	A276	C277	G278	A278	C279	C280	U281	G282	G283	U284	C285	C286	C287	C288	A289	G290	C291	G295	C296	C297	C298	A299	C364	C365A	C366B	G372	U373	A374	G379	U380	G381	G382	U383	U384	C385	G386	U387	G388	G389	A390	G391	G392	C393	A394	U395	G396	G397	U398	A401				
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G617	G620	A621	G622	A627	G628	G629	G630	A631	A632	C633	G634	G635	G636	A637	G638	U639	G640	G641	G642	A643	A644	A645	A646	G647	G648	G649	A650	G651	G652	C653	G654	G655	G656	G657	G658	G659	G660	G661	G662	A663	G664	G665	G666	G667	G668	G669	A670	C671	G672	G673	G674	A675	A676	C679	A680	G681	G682	G683	A684	A685
G686	C687	U688	C692	G693	U694	G695	G696	C697	C698	A699	G700	G704	A705	U706	G707	G708	U709	G710	G711	G717	A718	G719	G720	C721	G722	A723	G726	A727	G728	G729	C730	G731	C732	G733	A734	G735	C736	G737	G738	G739	U740	G744	G745	A746	U747	A750	A751	A752	G753	C754	C755	G758								
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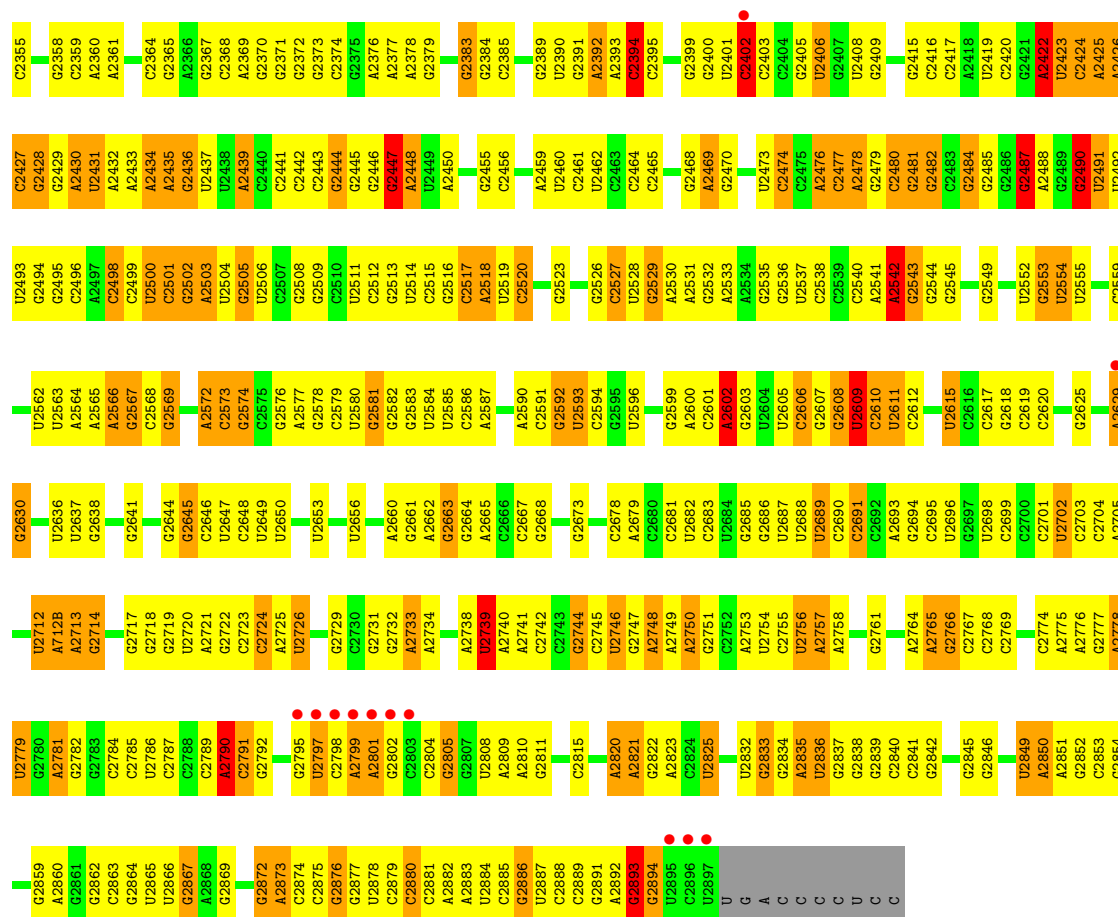






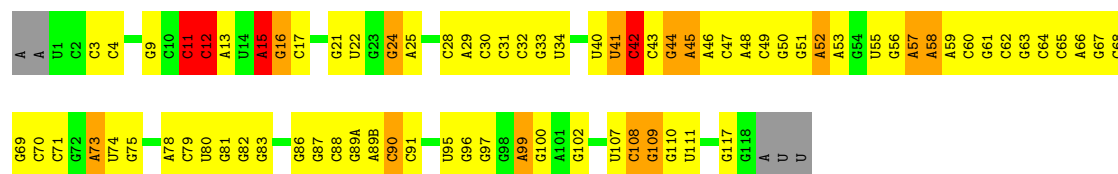


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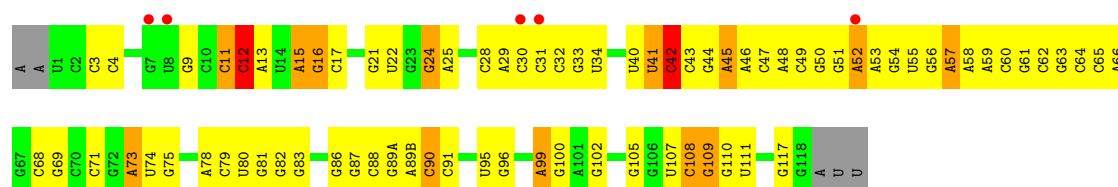
• Molecule 26: 5S rRNA

Chain BB:



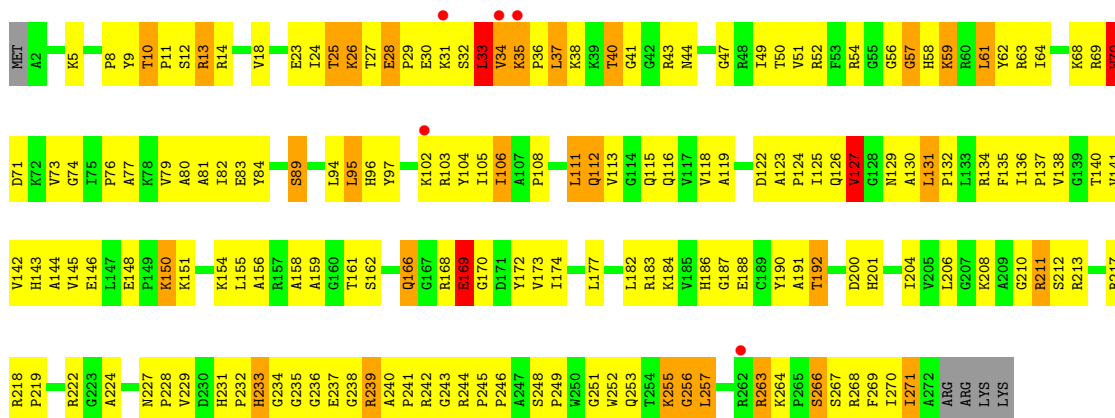
• Molecule 26: 5S rRNA

Chain DB:



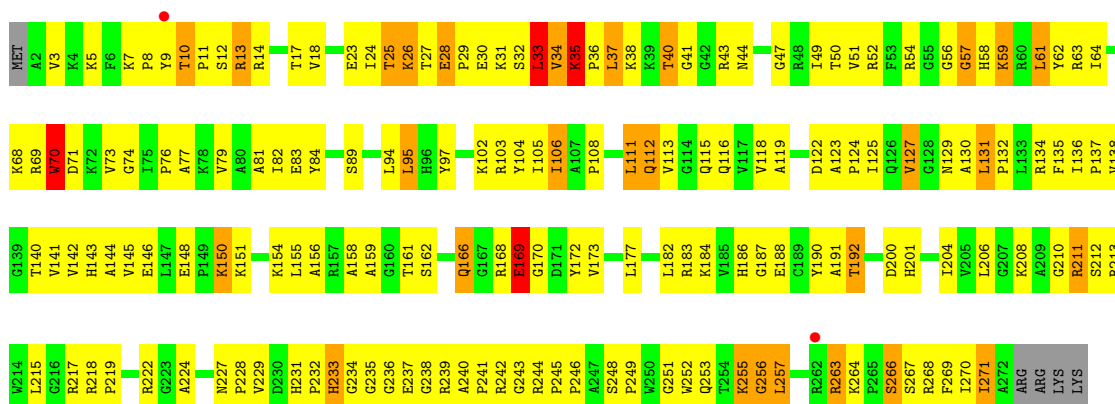
• Molecule 27: 50S ribosomal protein L2

Chain BD:



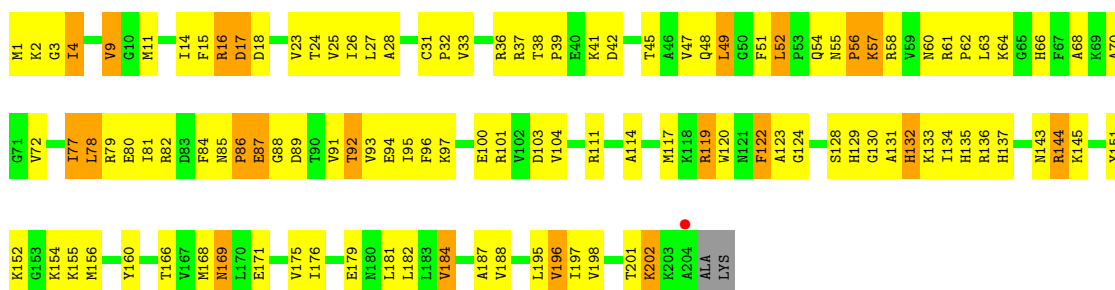
• Molecule 27: 50S ribosomal protein L2

Chain DD:



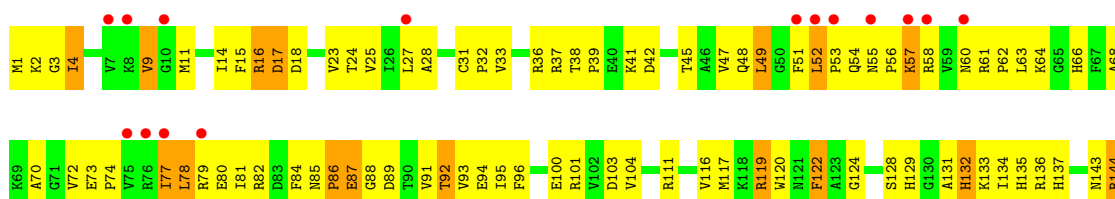
• Molecule 28: 50S ribosomal protein L3

Chain BE:



• Molecule 28: 50S ribosomal protein L3

Chain DE:

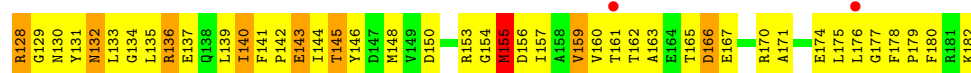




• Molecule 29: 50S ribosomal protein L4

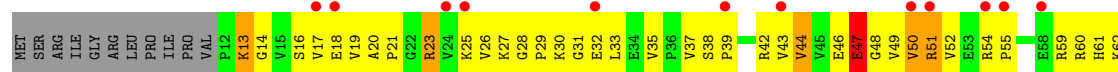
Chain BF:





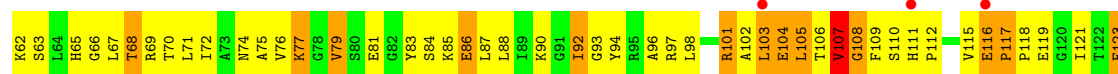
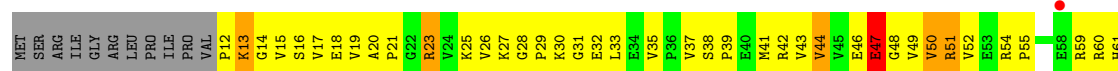
• Molecule 31: 50S ribosomal protein L6

Chain BH:



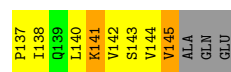
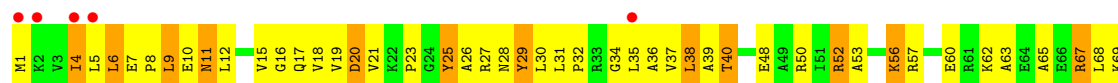
• Molecule 31: 50S ribosomal protein L6

Chain DH:



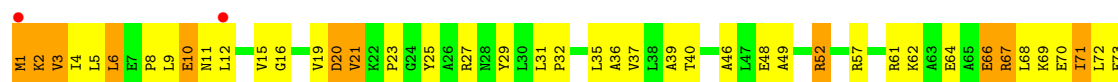
• Molecule 32: 50S ribosomal protein L9

Chain BI:



• Molecule 32: 50S ribosomal protein L9

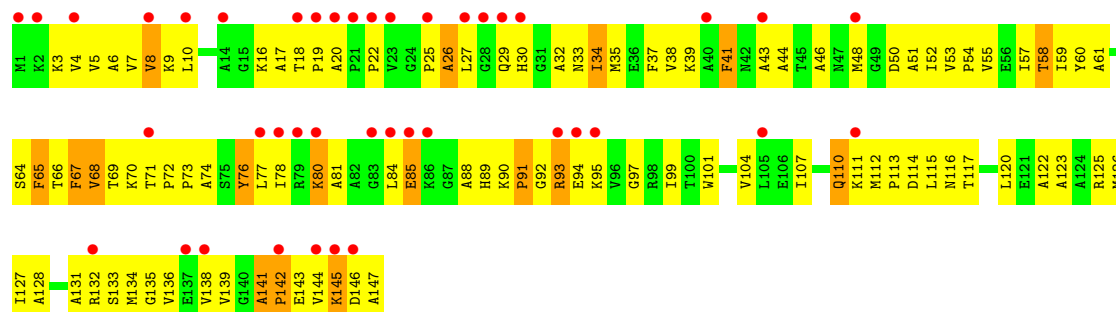
Chain DI:





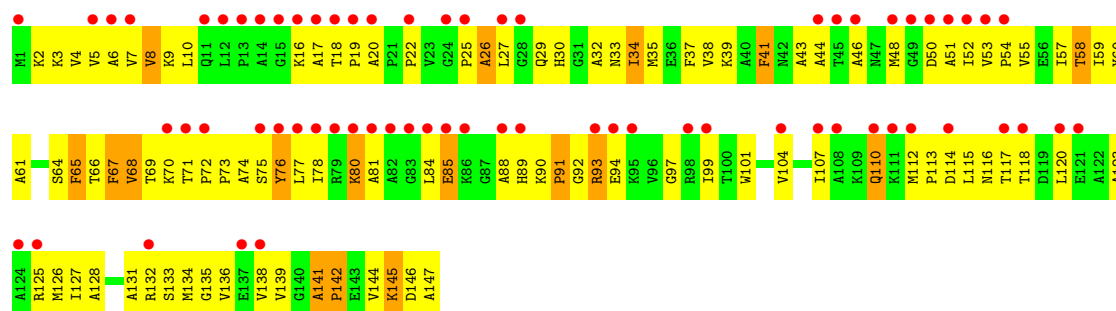
• Molecule 33: 50S ribosomal protein L11

Chain BK:



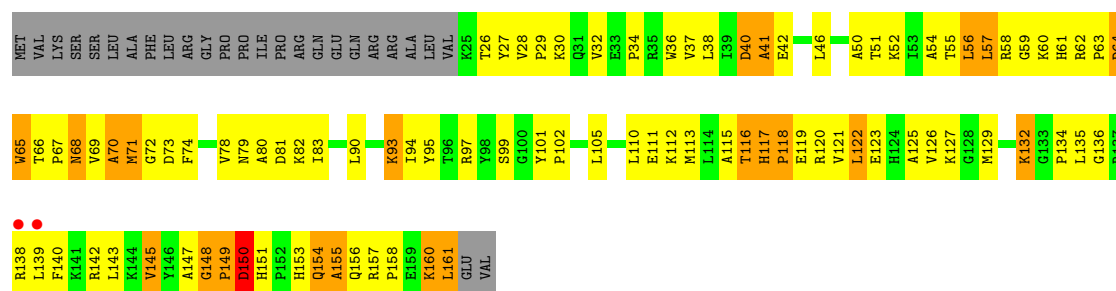
• Molecule 33: 50S ribosomal protein L11

Chain DK:



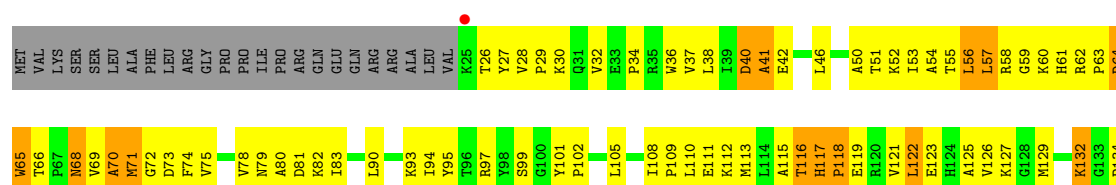
• Molecule 34: 50S ribosomal protein L13

Chain BN:



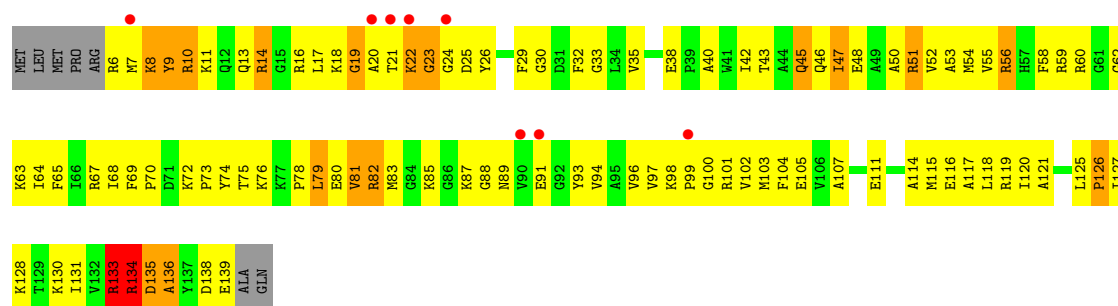
• Molecule 34: 50S ribosomal protein L13

Chain DN:



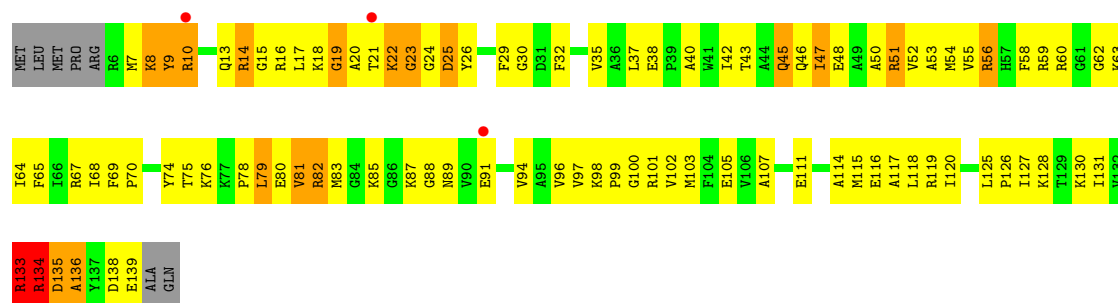






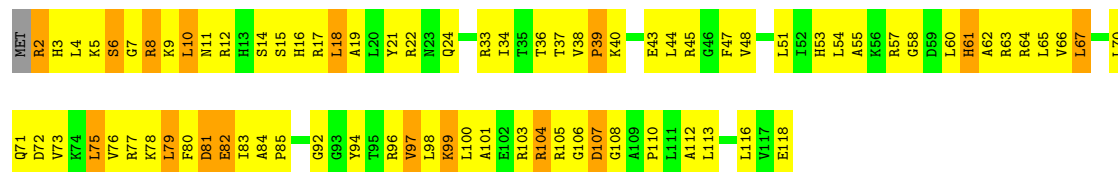
- Molecule 37: 50S ribosomal protein L16

Chain DQ:



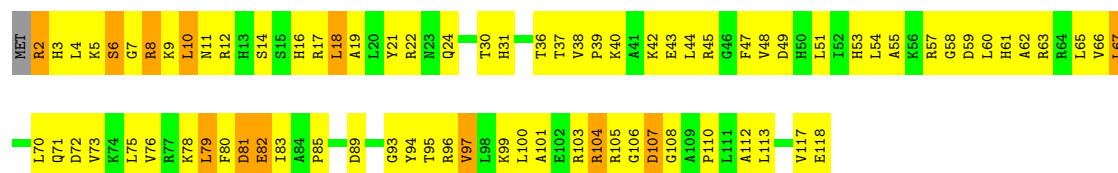
- Molecule 38: 50S ribosomal protein L17

Chain BR:



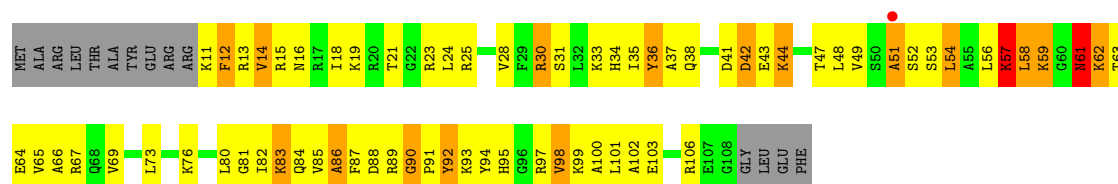
- Molecule 38: 50S ribosomal protein L17

Chain DR:



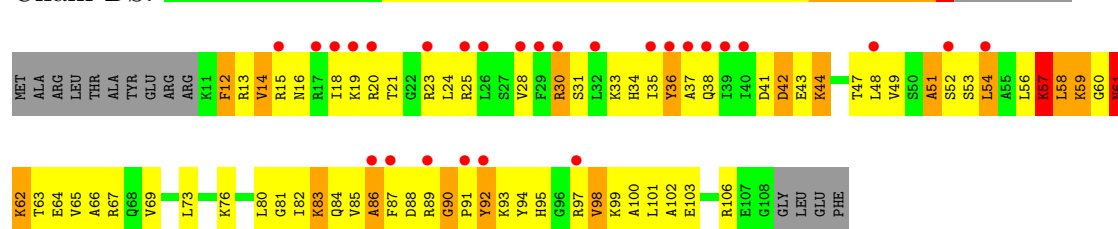
- Molecule 39: 50S ribosomal protein L18

Chain BS:



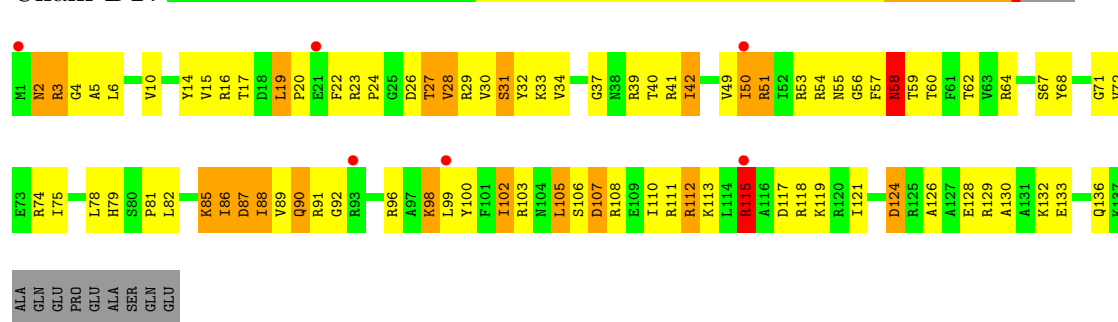
- Molecule 39: 50S ribosomal protein L18

Chain DS:



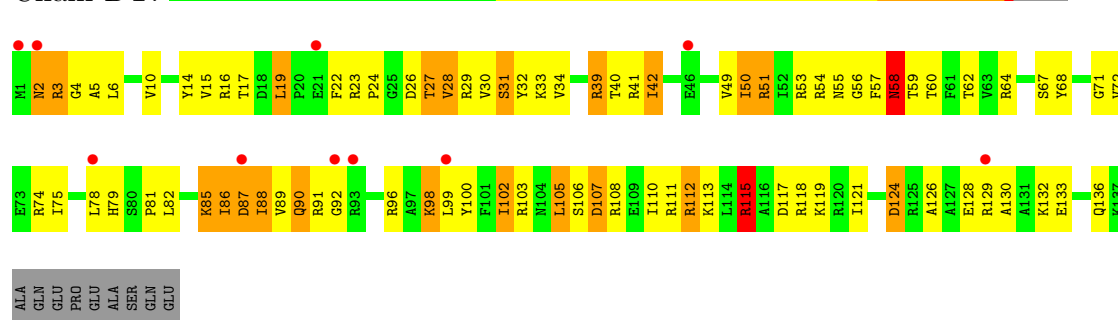
- Molecule 40: 50S ribosomal protein L19

Chain BT:



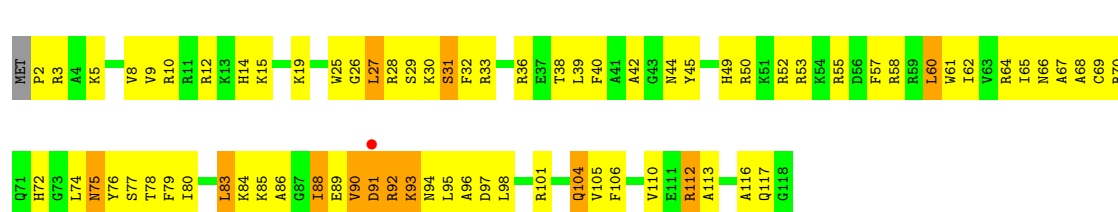
- Molecule 40: 50S ribosomal protein L19

Chain DT:



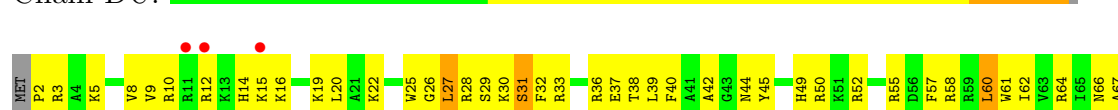
- Molecule 41: 50S ribosomal protein L20

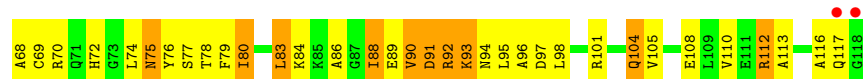
Chain BU:



- Molecule 41: 50S ribosomal protein L20

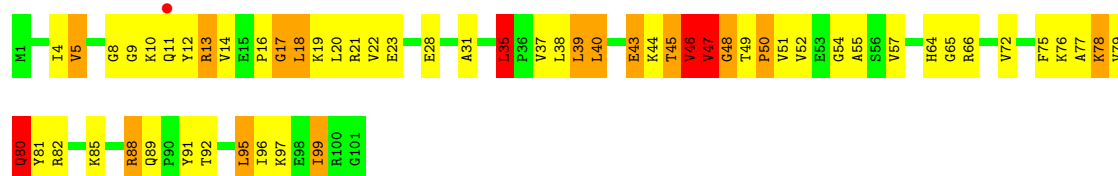
Chain DU:





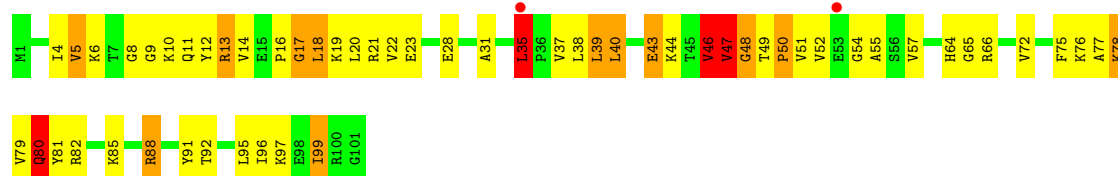
• Molecule 42: 50S ribosomal protein L21

Chain BV:



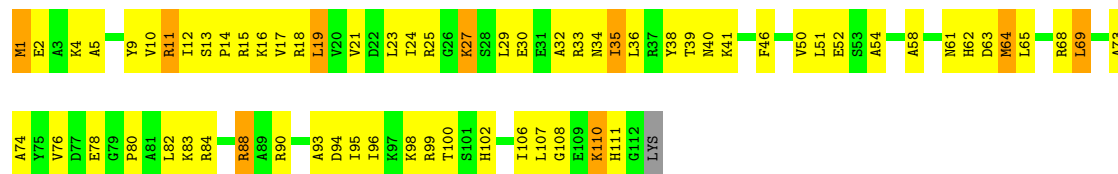
• Molecule 42: 50S ribosomal protein L21

Chain DV:



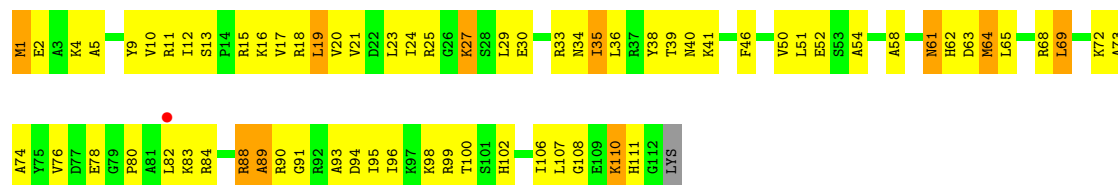
• Molecule 43: 50S ribosomal protein L22

Chain BW:



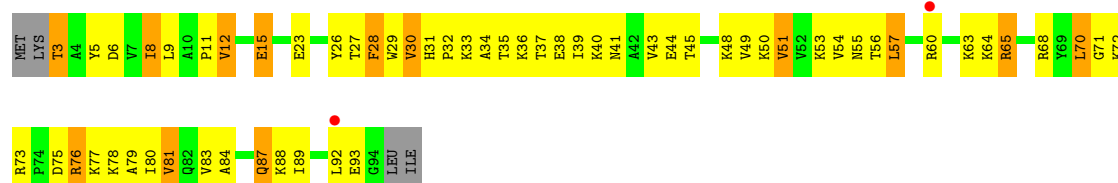
• Molecule 43: 50S ribosomal protein L22

Chain DW:



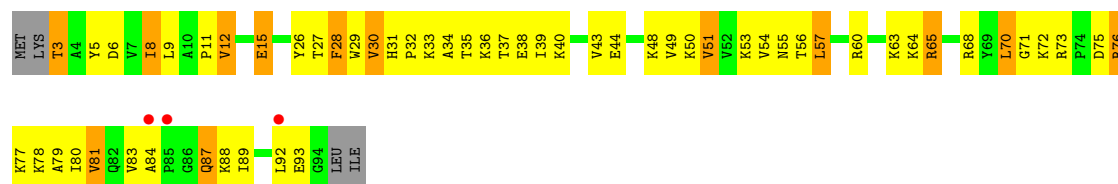
• Molecule 44: 50S ribosomal protein L23

Chain BX:



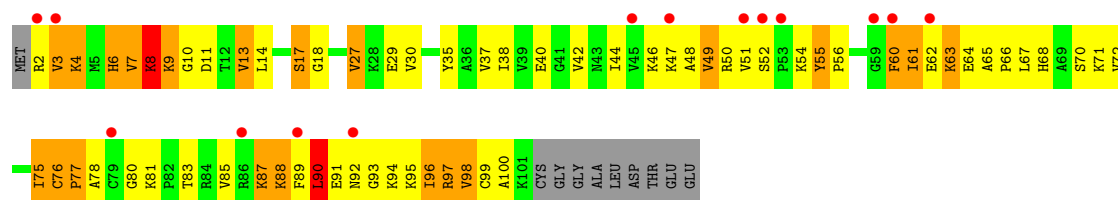
- Molecule 44: 50S ribosomal protein L23

Chain DX:



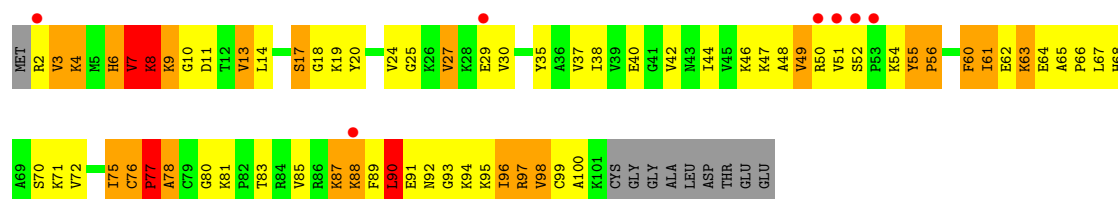
- Molecule 45: 50S ribosomal protein L24

Chain BY:



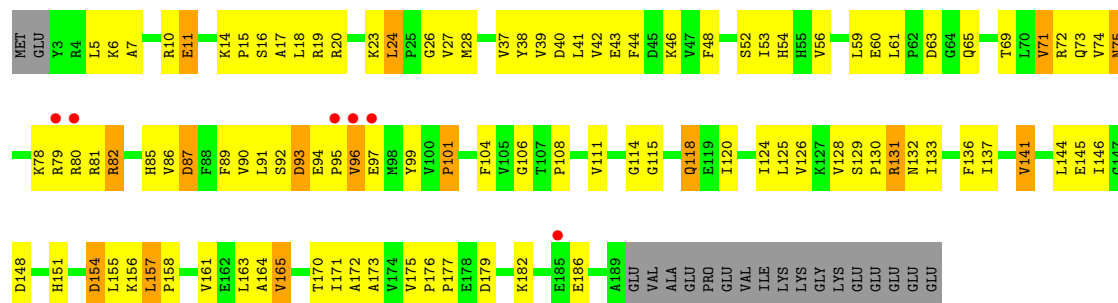
- Molecule 45: 50S ribosomal protein L24

Chain DY:



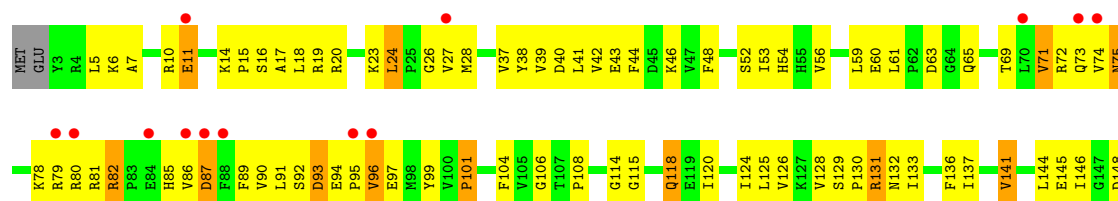
- Molecule 46: 50S ribosomal protein L25

Chain BZ:



- Molecule 46: 50S ribosomal protein L25

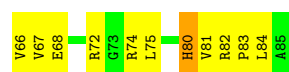
Chain DZ:





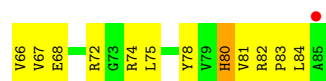
- Molecule 47: 50S ribosomal protein L27

Chain B0:



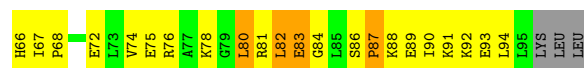
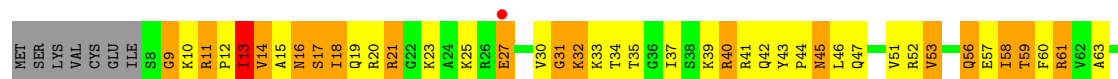
- Molecule 47: 50S ribosomal protein L27

Chain D0:



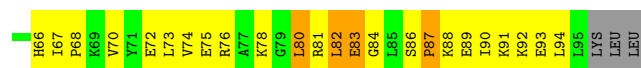
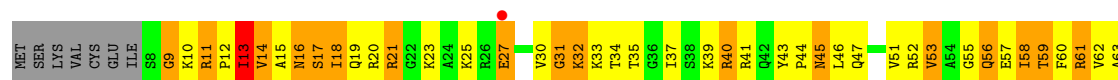
- Molecule 48: 50S ribosomal protein L28

Chain B1:



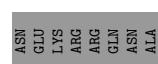
- Molecule 48: 50S ribosomal protein L28

Chain D1:



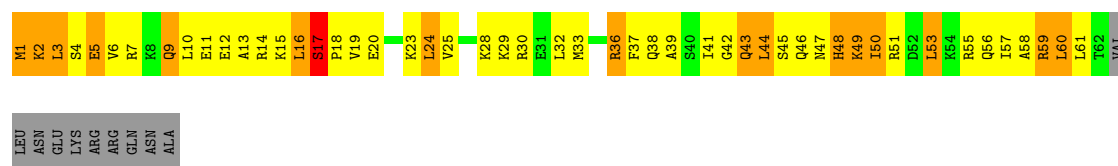
- Molecule 49: 50S ribosomal protein L29

Chain B2:



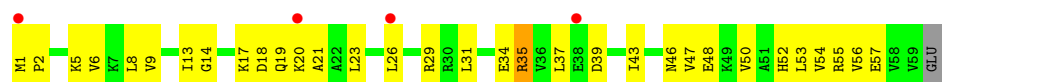
- Molecule 49: 50S ribosomal protein L29

Chain D2:



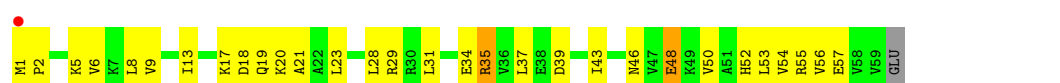
- Molecule 50: 50S ribosomal protein L30

Chain B3:



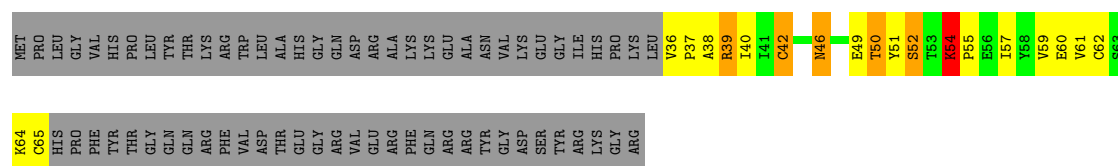
- Molecule 50: 50S ribosomal protein L30

Chain D3:



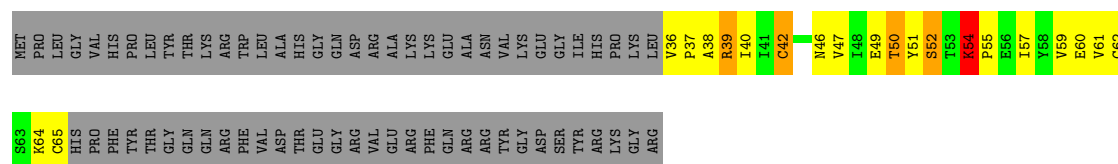
- Molecule 51: 50S ribosomal protein L31

Chain B4:



- Molecule 51: 50S ribosomal protein L31

Chain D4:



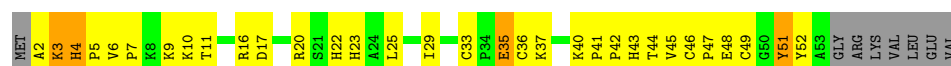
- Molecule 52: 50S ribosomal protein L32

Chain B5:



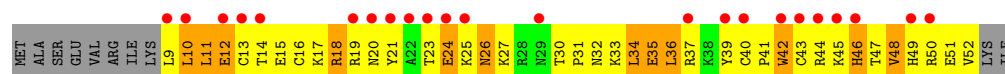
- Molecule 52: 50S ribosomal protein L32

Chain D5:



- Molecule 53: 50S ribosomal protein L33

Chain B6: 



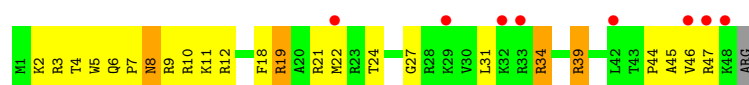
- Molecule 53: 50S ribosomal protein L33

Chain D6: 



- Molecule 54: 50S ribosomal protein L34

Chain B7: 



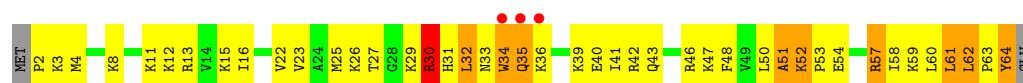
- Molecule 54: 50S ribosomal protein L34

Chain D7: 



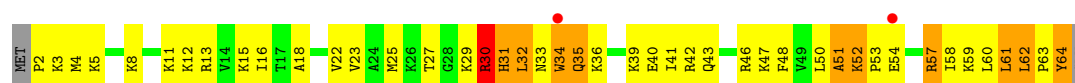
- Molecule 55: 50S ribosomal protein L35

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, $\alpha$ , $\beta$ , $\gamma$	211.24Å 456.78Å 618.71Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.95 – 3.00 50.99 – 2.99	Depositor EDS
% Data completeness (in resolution range)	97.3 (49.95-3.00) 97.2 (50.99-2.99)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.31 (at 3.01Å)	Xtriage
Refinement program	PHENIX (phenix.refine)	Depositor
R, $R_{free}$	0.280 , 0.316 0.299 , 0.331	Depositor DCC
$R_{free}$ test set	8188 reflections (0.71%)	DCC
Wilson B-factor (Å <sup>2</sup> )	56.2	Xtriage
Anisotropy	0.291	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.18 , 11.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.43$ , $\langle L^2 \rangle = 0.25$	Xtriage
Outliers	0 of 1158087 reflections	Xtriage
$F_o, F_c$ correlation	0.89	EDS
Total number of atoms	301148	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	95.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.24% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities 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	0.56	1/36194 (0.0%)	1.11	109/56493 (0.2%)
1	CA	0.55	1/36194 (0.0%)	1.10	110/56493 (0.2%)
2	AY	0.54	0/1832	1.03	2/2855 (0.1%)
2	AZ	0.46	0/1832	0.95	1/2855 (0.0%)
2	CY	0.54	0/1832	1.03	2/2855 (0.1%)
2	CZ	0.45	0/1832	0.94	1/2855 (0.0%)
3	AV	0.66	0/241	1.33	2/374 (0.5%)
3	CV	0.64	0/241	1.30	1/374 (0.3%)
4	AB	0.27	0/1935	0.46	0/2609
4	CB	0.27	0/1935	0.47	0/2609
5	AC	0.27	0/1636	0.46	0/2205
5	CC	0.28	0/1636	0.46	0/2205
6	AD	0.32	0/1733	0.50	0/2318
6	CD	0.30	0/1733	0.49	0/2318
7	AE	0.30	0/1171	0.50	0/1576
7	CE	0.29	0/1171	0.50	0/1576
8	AF	0.30	0/856	0.49	0/1154
8	CF	0.30	0/856	0.49	0/1154
9	AG	0.30	0/1276	0.47	0/1709
9	CG	0.28	0/1276	0.46	0/1709
10	AH	0.31	0/1136	0.52	0/1527
10	CH	0.29	0/1136	0.50	0/1527
11	AI	0.26	0/1029	0.45	0/1378
11	CI	0.26	0/1029	0.45	0/1378
12	AJ	0.29	0/807	0.49	0/1085
12	CJ	0.27	0/807	0.48	0/1085
13	AK	0.31	0/856	0.51	0/1157
13	CK	0.38	0/856	0.53	0/1157
14	AL	0.36	0/972	0.58	0/1301
14	CL	0.33	0/972	0.57	0/1301
15	AM	0.26	0/943	0.49	0/1265
15	CM	0.25	0/943	0.49	0/1265

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
16	AN	0.28	0/501	0.47	0/664
16	CN	0.30	0/501	0.47	0/664
17	AO	0.33	0/745	0.48	0/992
17	CO	0.32	0/745	0.48	0/992
18	AP	0.33	0/716	0.50	0/963
18	CP	0.27	0/716	0.47	0/963
19	AQ	0.32	0/836	0.50	0/1117
19	CQ	0.30	0/836	0.48	0/1117
20	AR	0.32	0/579	0.49	0/768
20	CR	0.32	0/579	0.50	0/768
21	AS	0.25	0/642	0.46	0/865
21	CS	0.25	0/642	0.46	0/865
22	AT	0.30	0/764	0.48	0/1006
22	CT	0.27	0/764	0.47	0/1006
23	AU	0.24	0/212	0.47	0/277
23	CU	0.25	0/212	0.45	0/277
24	AX	0.30	0/2926	0.49	0/3953
24	CX	0.27	0/2926	0.48	0/3953
25	BA	0.65	0/69437	1.22	337/108401 (0.3%)
25	DA	0.66	2/69437 (0.0%)	1.22	323/108401 (0.3%)
26	BB	0.53	0/2853	1.12	10/4451 (0.2%)
26	DB	0.52	0/2853	1.11	8/4451 (0.2%)
27	BD	0.46	0/2154	0.67	1/2905 (0.0%)
27	DD	0.47	0/2154	0.67	1/2905 (0.0%)
28	BE	0.35	0/1596	0.58	0/2153
28	DE	0.34	0/1596	0.57	0/2153
29	BF	0.37	0/1621	0.57	0/2194
29	DF	0.38	0/1621	0.57	0/2194
30	BG	0.28	0/1500	0.50	0/2017
30	DG	0.27	0/1500	0.49	0/2017
31	BH	0.26	0/1245	0.48	0/1682
31	DH	0.28	0/1245	0.49	0/1682
32	BI	0.31	0/1147	0.53	0/1552
32	DI	0.32	0/1147	0.55	0/1552
33	BK	0.24	0/1108	0.45	0/1500
33	DK	0.24	0/1108	0.45	0/1500
34	BN	0.32	0/1123	0.55	0/1515
34	DN	0.33	0/1123	0.55	0/1515
35	BO	0.38	0/942	0.56	0/1268
35	DO	0.35	0/942	0.55	0/1268
36	BP	0.38	0/1131	0.71	1/1504 (0.1%)
36	DP	0.40	0/1131	0.72	2/1504 (0.1%)
37	BQ	0.38	0/1084	0.60	0/1449

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
37	DQ	0.36	0/1084	0.59	0/1449
38	BR	0.38	0/974	0.59	0/1302
38	DR	0.36	0/974	0.57	0/1302
39	BS	0.28	0/778	0.50	0/1036
39	DS	0.26	0/778	0.48	0/1036
40	BT	0.37	0/1157	0.53	0/1544
40	DT	0.32	0/1157	0.51	0/1544
41	BU	0.37	0/982	0.53	0/1306
41	DU	0.42	0/982	0.54	0/1306
42	BV	0.35	0/790	0.57	0/1057
42	DV	0.37	0/790	0.59	0/1057
43	BW	0.36	0/901	0.56	0/1209
43	DW	0.37	0/901	0.56	0/1209
44	BX	0.40	0/739	0.55	0/993
44	DX	0.42	0/739	0.56	0/993
45	BY	0.33	0/788	0.57	0/1051
45	DY	0.39	0/788	0.59	0/1051
46	BZ	0.28	0/1514	0.50	0/2056
46	DZ	0.28	0/1514	0.49	0/2056
47	B0	0.34	0/613	0.54	0/816
47	D0	0.32	0/613	0.54	0/816
48	B1	0.44	0/701	0.71	1/932 (0.1%)
48	D1	0.42	0/701	0.70	1/932 (0.1%)
49	B2	0.37	0/522	0.62	0/690
49	D2	0.40	0/522	0.63	0/690
50	B3	0.30	0/472	0.48	0/634
50	D3	0.31	0/472	0.49	0/634
51	B4	0.28	0/228	0.52	0/309
51	D4	0.26	0/228	0.52	0/309
52	B5	0.32	0/418	0.55	0/567
52	D5	0.33	0/418	0.58	0/567
53	B6	0.30	0/387	0.51	0/518
53	D6	0.29	0/387	0.50	0/518
54	B7	0.41	0/426	0.58	0/561
54	D7	0.44	0/426	0.64	0/561
55	B8	0.46	0/515	0.66	0/679
55	D8	0.42	0/515	0.65	0/679
All	All	0.55	4/324432 (0.0%)	1.04	913/484634 (0.2%)

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
27	BD	0	1
27	DD	0	1
36	BP	0	3
36	DP	0	3
All	All	0	8

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	DA	74	A	C3'-O3'	5.67	1.50	1.42
25	DA	2447	G	C3'-O3'	5.48	1.49	1.42
1	AA	1064	G	C3'-O3'	5.40	1.49	1.42
1	CA	115	G	C3'-O3'	5.06	1.49	1.42

The worst 5 of 913 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	BA	1913	A	C1'-O4'-C4'	-12.89	99.59	109.90
25	DA	1559	G	C1'-O4'-C4'	-12.85	99.62	109.90
25	DA	945	A	C1'-O4'-C4'	-12.85	99.62	109.90
25	BA	1559	G	C1'-O4'-C4'	-12.81	99.65	109.90
25	DA	1786	A	C1'-O4'-C4'	-12.74	99.70	109.90

There are no chirality outliers.

5 of 8 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
27	BD	40	THR	Peptide
36	BP	51	PHE	Peptide
36	BP	52	GLU	Peptide
36	BP	9	ASN	Peptide
27	DD	40	THR	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	1066	0
1	CA	32332	0	16318	1109	0
2	AY	1640	0	837	39	0
2	AZ	1640	0	837	49	0
2	CY	1640	0	837	33	0
2	CZ	1640	0	837	48	0
3	AV	214	0	110	6	0
3	CV	214	0	110	4	0
4	AB	1900	0	1951	159	0
4	CB	1900	0	1951	160	0
5	AC	1612	0	1677	125	0
5	CC	1612	0	1677	129	0
6	AD	1703	0	1763	112	0
6	CD	1703	0	1763	105	0
7	AE	1155	0	1213	91	0
7	CE	1155	0	1213	84	0
8	AF	843	0	857	49	0
8	CF	843	0	857	48	0
9	AG	1257	0	1296	81	0
9	CG	1257	0	1296	79	0
10	AH	1116	0	1177	77	0
10	CH	1116	0	1177	80	0
11	AI	1011	0	1043	104	0
11	CI	1011	0	1043	106	0
12	AJ	794	0	840	102	0
12	CJ	794	0	840	97	0
13	AK	842	0	859	72	0
13	CK	842	0	859	74	0
14	AL	956	0	1046	112	0
14	CL	956	0	1046	109	0
15	AM	933	0	992	97	0
15	CM	933	0	992	108	0
16	AN	492	0	531	36	0
16	CN	492	0	532	41	0
17	AO	734	0	771	50	0
17	CO	734	0	771	51	0
18	AP	700	0	720	52	0
18	CP	700	0	720	59	0
19	AQ	823	0	893	54	0
19	CQ	823	0	893	52	0
20	AR	574	0	644	53	0
20	CR	574	0	644	51	0
21	AS	629	0	652	77	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
21	CS	629	0	652	76	0
22	AT	762	0	859	68	0
22	CT	762	0	859	64	0
23	AU	208	0	221	12	0
23	CU	208	0	221	12	0
24	AX	2876	0	2867	244	0
24	CX	2876	0	2867	242	0
25	BA	61997	0	31250	2146	0
25	DA	61997	0	31250	2152	1
26	BB	2551	0	1295	95	0
26	DB	2551	0	1295	93	1
27	BD	2104	0	2182	225	0
27	DD	2104	0	2182	228	0
28	BE	1563	0	1629	138	0
28	DE	1563	0	1629	129	0
29	BF	1586	0	1632	141	0
29	DF	1586	0	1632	144	0
30	BG	1475	0	1537	154	0
30	DG	1475	0	1537	151	0
31	BH	1222	0	1282	112	0
31	DH	1222	0	1282	114	0
32	BI	1132	0	1220	104	0
32	DI	1132	0	1220	91	0
33	BK	1088	0	1138	107	0
33	DK	1088	0	1138	107	0
34	BN	1096	0	1168	96	0
34	DN	1096	0	1168	93	0
35	BO	932	0	994	64	0
35	DO	932	0	994	61	0
36	BP	1114	0	1187	226	0
36	DP	1114	0	1187	229	0
37	BQ	1064	0	1114	141	0
37	DQ	1064	0	1114	129	0
38	BR	960	0	1021	106	0
38	DR	960	0	1021	101	0
39	BS	770	0	832	96	0
39	DS	770	0	832	98	0
40	BT	1143	0	1211	100	0
40	DT	1143	0	1211	98	0
41	BU	964	0	1022	92	0
41	DU	964	0	1022	102	0
42	BV	779	0	852	77	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
42	DV	779	0	852	78	0
43	BW	890	0	951	68	0
43	DW	890	0	951	70	0
44	BX	725	0	778	69	0
44	DX	725	0	778	71	0
45	BY	775	0	870	106	0
45	DY	775	0	870	110	0
46	BZ	1482	0	1507	106	0
46	DZ	1482	0	1507	106	0
47	B0	605	0	628	45	0
47	D0	605	0	628	49	0
48	B1	694	0	764	92	0
48	D1	694	0	764	91	0
49	B2	520	0	575	76	0
49	D2	520	0	575	77	0
50	B3	467	0	523	29	0
50	D3	467	0	523	29	0
51	B4	225	0	225	19	0
51	D4	225	0	225	22	0
52	B5	404	0	420	54	0
52	D5	404	0	420	53	0
53	B6	380	0	391	55	0
53	D6	380	0	391	56	0
54	B7	418	0	467	36	0
54	D7	418	0	467	38	0
55	B8	507	0	576	68	0
55	D8	507	0	576	79	0
56	AA	428	0	0	0	0
56	AB	7	0	0	0	0
56	AC	4	0	0	0	0
56	AD	3	0	0	0	0
56	AE	8	0	0	0	0
56	AF	2	0	0	0	0
56	AG	2	0	0	0	0
56	AH	2	0	0	0	0
56	AI	1	0	0	0	0
56	AJ	1	0	0	0	0
56	AK	7	0	0	0	0
56	AL	4	0	0	0	0
56	AM	3	0	0	0	0
56	AN	1	0	0	0	0
56	AO	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
56	AQ	1	0	0	0	0
56	AR	1	0	0	0	0
56	AT	2	0	0	0	0
56	AV	3	0	0	0	0
56	AX	14	0	0	0	0
56	AY	26	0	0	0	0
56	AZ	15	0	0	0	0
56	B0	3	0	0	0	0
56	B1	7	0	0	0	0
56	B2	3	0	0	0	0
56	B4	2	0	0	0	0
56	B5	2	0	0	0	0
56	B6	2	0	0	0	0
56	B8	4	0	0	0	0
56	BA	923	0	0	0	0
56	BB	35	0	0	0	0
56	BD	7	0	0	0	0
56	BE	6	0	0	0	0
56	BF	6	0	0	0	0
56	BG	2	0	0	0	0
56	BH	4	0	0	0	0
56	BI	6	0	0	0	0
56	BK	3	0	0	0	0
56	BN	4	0	0	0	0
56	BO	5	0	0	0	0
56	BP	2	0	0	0	0
56	BQ	6	0	0	0	0
56	BR	2	0	0	0	0
56	BS	3	0	0	0	0
56	BT	1	0	0	0	0
56	BU	1	0	0	0	0
56	BV	3	0	0	0	0
56	BW	2	0	0	0	0
56	BX	2	0	0	0	0
56	BY	3	0	0	0	0
56	BZ	1	0	0	0	0
56	CA	222	0	0	0	0
56	CB	2	0	0	0	0
56	CC	1	0	0	0	0
56	CF	5	0	0	0	0
56	CG	2	0	0	0	0
56	CH	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
56	CK	3	0	0	0	0
56	CL	1	0	0	0	0
56	CO	1	0	0	0	0
56	CQ	1	0	0	0	0
56	CS	1	0	0	0	0
56	CT	1	0	0	0	0
56	CY	14	0	0	0	0
56	CZ	14	0	0	0	0
56	D1	2	0	0	0	0
56	D6	1	0	0	0	0
56	D8	1	0	0	0	0
56	DA	491	0	0	0	0
56	DB	12	0	0	0	0
56	DD	9	0	0	0	0
56	DE	1	0	0	0	0
56	DF	1	0	0	0	0
56	DG	2	0	0	0	0
56	DI	1	0	0	0	0
56	DN	1	0	0	0	0
56	DO	2	0	0	0	0
56	DP	1	0	0	0	0
56	DQ	2	0	0	0	0
56	DR	1	0	0	0	0
56	DT	1	0	0	0	0
56	DU	1	0	0	0	0
56	DY	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	301148	0	204431	14693	1

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 29.

The worst 5 of 14693 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
55:B8:57:ARG:HB2	55:B8:57:ARG:HH11	1.11	1.16
48:B1:11:ARG:HB3	48:B1:12:PRO:HD2	1.14	1.13
48:D1:11:ARG:HB3	48:D1:12:PRO:HD2	1.18	1.12
36:BP:23:PRO:HD2	36:BP:33:ARG:NH2	1.67	1.09
25:BA:2630:G:H1'	25:BA:2894:G:H1'	1.35	1.09

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
25:DA:1411:C:O3'	26:DB:53:A:O2'[1.655]	2.14	0.06

## 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	AB	232/256 (91%)	175 (75%)	47 (20%)	10 (4%)	4	23
4	CB	232/256 (91%)	174 (75%)	48 (21%)	10 (4%)	4	23
5	AC	204/239 (85%)	138 (68%)	51 (25%)	15 (7%)	2	8
5	CC	204/239 (85%)	138 (68%)	52 (26%)	14 (7%)	2	9
6	AD	206/209 (99%)	166 (81%)	30 (15%)	10 (5%)	3	20
6	CD	206/209 (99%)	169 (82%)	26 (13%)	11 (5%)	3	18
7	AE	149/162 (92%)	117 (78%)	26 (17%)	6 (4%)	5	25
7	CE	149/162 (92%)	117 (78%)	26 (17%)	6 (4%)	5	25
8	AF	99/101 (98%)	87 (88%)	11 (11%)	1 (1%)	22	70
8	CF	99/101 (98%)	87 (88%)	11 (11%)	1 (1%)	22	70
9	AG	153/156 (98%)	124 (81%)	28 (18%)	1 (1%)	30	78
9	CG	153/156 (98%)	125 (82%)	27 (18%)	1 (1%)	30	78
10	AH	136/138 (99%)	112 (82%)	18 (13%)	6 (4%)	4	22
10	CH	136/138 (99%)	112 (82%)	18 (13%)	6 (4%)	4	22
11	AI	125/128 (98%)	93 (74%)	22 (18%)	10 (8%)	1	7
11	CI	125/128 (98%)	93 (74%)	23 (18%)	9 (7%)	2	8
12	AJ	96/105 (91%)	76 (79%)	14 (15%)	6 (6%)	2	12
12	CJ	96/105 (91%)	77 (80%)	13 (14%)	6 (6%)	2	12
13	AK	112/129 (87%)	94 (84%)	12 (11%)	6 (5%)	3	17
13	CK	112/129 (87%)	94 (84%)	12 (11%)	6 (5%)	3	17

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
14	AL	120/134 (90%)	87 (72%)	22 (18%)	11 (9%)	1	5
14	CL	120/134 (90%)	87 (72%)	22 (18%)	11 (9%)	1	5
15	AM	115/126 (91%)	91 (79%)	19 (16%)	5 (4%)	4	23
15	CM	115/126 (91%)	91 (79%)	20 (17%)	4 (4%)	6	30
16	AN	58/61 (95%)	46 (79%)	11 (19%)	1 (2%)	14	54
16	CN	58/61 (95%)	46 (79%)	11 (19%)	1 (2%)	14	54
17	AO	86/89 (97%)	70 (81%)	13 (15%)	3 (4%)	6	30
17	CO	86/89 (97%)	69 (80%)	14 (16%)	3 (4%)	6	30
18	AP	81/88 (92%)	59 (73%)	19 (24%)	3 (4%)	5	28
18	CP	81/88 (92%)	60 (74%)	18 (22%)	3 (4%)	5	28
19	AQ	97/105 (92%)	79 (81%)	16 (16%)	2 (2%)	11	47
19	CQ	97/105 (92%)	79 (81%)	16 (16%)	2 (2%)	11	47
20	AR	68/88 (77%)	45 (66%)	18 (26%)	5 (7%)	2	8
20	CR	68/88 (77%)	46 (68%)	17 (25%)	5 (7%)	2	8
21	AS	76/93 (82%)	50 (66%)	18 (24%)	8 (10%)	1	3
21	CS	76/93 (82%)	50 (66%)	18 (24%)	8 (10%)	1	3
22	AT	97/106 (92%)	72 (74%)	17 (18%)	8 (8%)	1	6
22	CT	97/106 (92%)	72 (74%)	18 (19%)	7 (7%)	2	8
23	AU	22/27 (82%)	12 (54%)	8 (36%)	2 (9%)	1	5
23	CU	22/27 (82%)	12 (54%)	8 (36%)	2 (9%)	1	5
24	AX	360/378 (95%)	288 (80%)	57 (16%)	15 (4%)	4	24
24	CX	360/378 (95%)	288 (80%)	58 (16%)	14 (4%)	5	26
27	BD	269/276 (98%)	208 (77%)	41 (15%)	20 (7%)	2	8
27	DD	269/276 (98%)	204 (76%)	46 (17%)	19 (7%)	2	9
28	BE	202/206 (98%)	157 (78%)	37 (18%)	8 (4%)	5	25
28	DE	202/206 (98%)	157 (78%)	37 (18%)	8 (4%)	5	25
29	BF	200/210 (95%)	162 (81%)	28 (14%)	10 (5%)	3	19
29	DF	200/210 (95%)	162 (81%)	26 (13%)	12 (6%)	2	14
30	BG	179/182 (98%)	128 (72%)	39 (22%)	12 (7%)	2	10
30	DG	179/182 (98%)	127 (71%)	39 (22%)	13 (7%)	2	8
31	BH	157/180 (87%)	120 (76%)	30 (19%)	7 (4%)	4	22

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
31	DH	157/180 (87%)	121 (77%)	28 (18%)	8 (5%)	3	18
32	BI	143/148 (97%)	107 (75%)	29 (20%)	7 (5%)	3	20
32	DI	143/148 (97%)	121 (85%)	19 (13%)	3 (2%)	11	47
33	BK	145/147 (99%)	101 (70%)	35 (24%)	9 (6%)	2	13
33	DK	145/147 (99%)	101 (70%)	35 (24%)	9 (6%)	2	13
34	BN	135/163 (83%)	103 (76%)	17 (13%)	15 (11%)	1	3
34	DN	135/163 (83%)	101 (75%)	19 (14%)	15 (11%)	1	3
35	BO	120/122 (98%)	102 (85%)	14 (12%)	4 (3%)	6	32
35	DO	120/122 (98%)	101 (84%)	15 (12%)	4 (3%)	6	32
36	BP	144/150 (96%)	86 (60%)	35 (24%)	23 (16%)	0	1
36	DP	144/150 (96%)	88 (61%)	34 (24%)	22 (15%)	0	1
37	BQ	132/141 (94%)	96 (73%)	22 (17%)	14 (11%)	1	3
37	DQ	132/141 (94%)	93 (70%)	24 (18%)	15 (11%)	1	3
38	BR	115/118 (98%)	89 (77%)	19 (16%)	7 (6%)	2	14
38	DR	115/118 (98%)	91 (79%)	19 (16%)	5 (4%)	4	23
39	BS	96/112 (86%)	56 (58%)	29 (30%)	11 (12%)	1	3
39	DS	96/112 (86%)	56 (58%)	29 (30%)	11 (12%)	1	3
40	BT	135/146 (92%)	91 (67%)	30 (22%)	14 (10%)	1	4
40	DT	135/146 (92%)	91 (67%)	31 (23%)	13 (10%)	1	4
41	BU	115/118 (98%)	92 (80%)	19 (16%)	4 (4%)	6	30
41	DU	115/118 (98%)	91 (79%)	19 (16%)	5 (4%)	4	23
42	BV	99/101 (98%)	74 (75%)	15 (15%)	10 (10%)	1	4
42	DV	99/101 (98%)	74 (75%)	15 (15%)	10 (10%)	1	4
43	BW	110/113 (97%)	88 (80%)	18 (16%)	4 (4%)	5	29
43	DW	110/113 (97%)	87 (79%)	18 (16%)	5 (4%)	4	22
44	BX	90/96 (94%)	73 (81%)	15 (17%)	2 (2%)	10	45
44	DX	90/96 (94%)	73 (81%)	15 (17%)	2 (2%)	10	45
45	BY	98/110 (89%)	64 (65%)	18 (18%)	16 (16%)	0	1
45	DY	98/110 (89%)	65 (66%)	17 (17%)	16 (16%)	0	1
46	BZ	185/206 (90%)	146 (79%)	31 (17%)	8 (4%)	4	23
46	DZ	185/206 (90%)	145 (78%)	32 (17%)	8 (4%)	4	23

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
47	B0	74/85 (87%)	61 (82%)	10 (14%)	3 (4%)	4	24
47	D0	74/85 (87%)	61 (82%)	10 (14%)	3 (4%)	4	24
48	B1	86/98 (88%)	59 (69%)	16 (19%)	11 (13%)	0	2
48	D1	86/98 (88%)	59 (69%)	16 (19%)	11 (13%)	0	2
49	B2	60/72 (83%)	43 (72%)	12 (20%)	5 (8%)	1	6
49	D2	60/72 (83%)	44 (73%)	11 (18%)	5 (8%)	1	6
50	B3	57/60 (95%)	50 (88%)	5 (9%)	2 (4%)	6	30
50	D3	57/60 (95%)	50 (88%)	5 (9%)	2 (4%)	6	30
51	B4	28/97 (29%)	18 (64%)	6 (21%)	4 (14%)	0	1
51	D4	28/97 (29%)	18 (64%)	6 (21%)	4 (14%)	0	1
52	B5	50/60 (83%)	40 (80%)	7 (14%)	3 (6%)	2	14
52	D5	50/60 (83%)	40 (80%)	7 (14%)	3 (6%)	2	14
53	B6	42/54 (78%)	27 (64%)	10 (24%)	5 (12%)	1	2
53	D6	42/54 (78%)	27 (64%)	10 (24%)	5 (12%)	1	2
54	B7	46/49 (94%)	43 (94%)	3 (6%)	0	100	100
54	D7	46/49 (94%)	42 (91%)	4 (9%)	0	100	100
55	B8	61/65 (94%)	42 (69%)	12 (20%)	7 (12%)	1	3
55	D8	61/65 (94%)	42 (69%)	12 (20%)	7 (12%)	1	3
All	All	12130/13206 (92%)	9225 (76%)	2153 (18%)	752 (6%)	2	13

5 of 752 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	AC	45	LYS
5	AC	47	LEU
6	AD	5	ILE
6	AD	44	GLY
7	AE	85	GLY

### 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	AB	202/220 (92%)	186 (92%)	16 (8%)	18	54
4	CB	202/220 (92%)	185 (92%)	17 (8%)	16	51
5	AC	160/188 (85%)	138 (86%)	22 (14%)	5	24
5	CC	160/188 (85%)	138 (86%)	22 (14%)	5	24
6	AD	180/181 (99%)	160 (89%)	20 (11%)	9	34
6	CD	180/181 (99%)	161 (89%)	19 (11%)	10	36
7	AE	116/123 (94%)	99 (85%)	17 (15%)	4	21
7	CE	116/123 (94%)	99 (85%)	17 (15%)	4	21
8	AF	90/90 (100%)	80 (89%)	10 (11%)	9	34
8	CF	90/90 (100%)	81 (90%)	9 (10%)	11	39
9	AG	126/127 (99%)	119 (94%)	7 (6%)	30	72
9	CG	126/127 (99%)	119 (94%)	7 (6%)	30	72
10	AH	119/119 (100%)	106 (89%)	13 (11%)	9	35
10	CH	119/119 (100%)	106 (89%)	13 (11%)	9	35
11	AI	98/99 (99%)	85 (87%)	13 (13%)	6	25
11	CI	98/99 (99%)	86 (88%)	12 (12%)	7	29
12	AJ	88/92 (96%)	75 (85%)	13 (15%)	4	21
12	CJ	88/92 (96%)	75 (85%)	13 (15%)	4	21
13	AK	86/99 (87%)	74 (86%)	12 (14%)	5	23
13	CK	86/99 (87%)	74 (86%)	12 (14%)	5	23
14	AL	103/110 (94%)	91 (88%)	12 (12%)	8	31
14	CL	103/110 (94%)	91 (88%)	12 (12%)	8	31
15	AM	94/101 (93%)	85 (90%)	9 (10%)	12	43
15	CM	94/101 (93%)	85 (90%)	9 (10%)	12	43
16	AN	49/50 (98%)	44 (90%)	5 (10%)	11	38
16	CN	49/50 (98%)	44 (90%)	5 (10%)	11	38
17	AO	79/80 (99%)	70 (89%)	9 (11%)	8	33
17	CO	79/80 (99%)	70 (89%)	9 (11%)	8	33
18	AP	72/74 (97%)	65 (90%)	7 (10%)	12	42
18	CP	72/74 (97%)	66 (92%)	6 (8%)	16	52
19	AQ	94/97 (97%)	86 (92%)	8 (8%)	15	51
19	CQ	94/97 (97%)	86 (92%)	8 (8%)	15	51

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
20	AR	61/77 (79%)	53 (87%)	8 (13%)	6	25
20	CR	61/77 (79%)	52 (85%)	9 (15%)	4	21
21	AS	69/80 (86%)	58 (84%)	11 (16%)	4	17
21	CS	69/80 (86%)	58 (84%)	11 (16%)	4	17
22	AT	76/82 (93%)	67 (88%)	9 (12%)	8	30
22	CT	76/82 (93%)	68 (90%)	8 (10%)	10	37
23	AU	19/22 (86%)	18 (95%)	1 (5%)	32	74
23	CU	19/22 (86%)	18 (95%)	1 (5%)	32	74
24	AX	305/319 (96%)	258 (85%)	47 (15%)	4	19
24	CX	305/319 (96%)	260 (85%)	45 (15%)	4	21
27	BD	213/218 (98%)	181 (85%)	32 (15%)	4	20
27	DD	213/218 (98%)	181 (85%)	32 (15%)	4	20
28	BE	165/166 (99%)	144 (87%)	21 (13%)	6	27
28	DE	165/166 (99%)	144 (87%)	21 (13%)	6	27
29	BF	161/166 (97%)	142 (88%)	19 (12%)	8	30
29	DF	161/166 (97%)	140 (87%)	21 (13%)	6	26
30	BG	155/156 (99%)	135 (87%)	20 (13%)	6	26
30	DG	155/156 (99%)	135 (87%)	20 (13%)	6	26
31	BH	132/148 (89%)	115 (87%)	17 (13%)	6	26
31	DH	132/148 (89%)	115 (87%)	17 (13%)	6	26
32	BI	122/124 (98%)	101 (83%)	21 (17%)	3	14
32	DI	122/124 (98%)	103 (84%)	19 (16%)	4	18
33	BK	111/111 (100%)	95 (86%)	16 (14%)	5	22
33	DK	111/111 (100%)	95 (86%)	16 (14%)	5	22
34	BN	116/139 (84%)	98 (84%)	18 (16%)	4	19
34	DN	116/139 (84%)	98 (84%)	18 (16%)	4	19
35	BO	100/100 (100%)	86 (86%)	14 (14%)	5	23
35	DO	100/100 (100%)	85 (85%)	15 (15%)	4	20
36	BP	112/116 (97%)	80 (71%)	32 (29%)	0	3
36	DP	112/116 (97%)	79 (70%)	33 (30%)	0	2
37	BQ	105/111 (95%)	91 (87%)	14 (13%)	6	25

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
37	DQ	105/111 (95%)	91 (87%)	14 (13%)	6	25
38	BR	100/101 (99%)	90 (90%)	10 (10%)	11	39
38	DR	100/101 (99%)	91 (91%)	9 (9%)	14	47
39	BS	77/88 (88%)	66 (86%)	11 (14%)	5	22
39	DS	77/88 (88%)	66 (86%)	11 (14%)	5	22
40	BT	121/128 (94%)	101 (84%)	20 (16%)	3	16
40	DT	121/128 (94%)	101 (84%)	20 (16%)	3	16
41	BU	93/94 (99%)	82 (88%)	11 (12%)	8	30
41	DU	93/94 (99%)	83 (89%)	10 (11%)	9	35
42	BV	82/82 (100%)	68 (83%)	14 (17%)	3	15
42	DV	82/82 (100%)	69 (84%)	13 (16%)	4	17
43	BW	91/92 (99%)	80 (88%)	11 (12%)	7	29
43	DW	91/92 (99%)	80 (88%)	11 (12%)	7	29
44	BX	74/78 (95%)	58 (78%)	16 (22%)	1	8
44	DX	74/78 (95%)	59 (80%)	15 (20%)	2	9
45	BY	84/91 (92%)	72 (86%)	12 (14%)	5	22
45	DY	84/91 (92%)	70 (83%)	14 (17%)	3	16
46	BZ	162/179 (90%)	151 (93%)	11 (7%)	22	63
46	DZ	162/179 (90%)	150 (93%)	12 (7%)	20	58
47	B0	61/67 (91%)	53 (87%)	8 (13%)	6	25
47	D0	61/67 (91%)	53 (87%)	8 (13%)	6	25
48	B1	73/83 (88%)	58 (80%)	15 (20%)	2	9
48	D1	73/83 (88%)	57 (78%)	16 (22%)	1	7
49	B2	58/67 (87%)	45 (78%)	13 (22%)	1	7
49	D2	58/67 (87%)	45 (78%)	13 (22%)	1	7
50	B3	51/52 (98%)	49 (96%)	2 (4%)	43	85
50	D3	51/52 (98%)	49 (96%)	2 (4%)	43	85
51	B4	27/84 (32%)	21 (78%)	6 (22%)	1	7
51	D4	27/84 (32%)	22 (82%)	5 (18%)	2	13
52	B5	45/52 (86%)	41 (91%)	4 (9%)	14	48
52	D5	45/52 (86%)	42 (93%)	3 (7%)	23	64

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
53	B6	43/52 (83%)	34 (79%)	9 (21%)	1	8
53	D6	43/52 (83%)	34 (79%)	9 (21%)	1	8
54	B7	41/42 (98%)	35 (85%)	6 (15%)	5	21
54	D7	41/42 (98%)	35 (85%)	6 (15%)	5	21
55	B8	53/55 (96%)	47 (89%)	6 (11%)	9	33
55	D8	53/55 (96%)	47 (89%)	6 (11%)	9	33
All	All	10228/10944 (94%)	8877 (87%)	1351 (13%)	6	25

5 of 1351 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
47	B0	21	LEU
8	CF	27	GLN
44	DX	30	VAL
48	B1	76	ARG
4	CB	102	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 287 such sidechains are listed below:

Mol	Chain	Res	Type
50	B3	19	GLN
8	CF	73	ASN
46	DZ	75	ASN
52	B5	22	HIS
4	CB	204	ASN

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	AA	1503/1525 (98%)	287 (19%)	107 (7%)
1	CA	1503/1525 (98%)	282 (18%)	106 (7%)
2	AY	76/77 (98%)	15 (19%)	6 (7%)
2	AZ	76/77 (98%)	15 (19%)	5 (6%)
2	CY	76/77 (98%)	14 (18%)	6 (7%)
2	CZ	76/77 (98%)	15 (19%)	5 (6%)
25	BA	2878/2894 (99%)	589 (20%)	178 (6%)
25	DA	2878/2894 (99%)	594 (20%)	173 (6%)
26	BB	118/124 (95%)	17 (14%)	6 (5%)

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
26	DB	118/124 (95%)	18 (15%)	6 (5%)
3	AV	10/27 (37%)	3 (30%)	3 (30%)
3	CV	10/27 (37%)	3 (30%)	3 (30%)
All	All	9322/9448 (98%)	1852 (19%)	604 (6%)

5 of 1852 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	AA	9	G
1	AA	22	G
1	AA	31	G
1	AA	32	A
1	AA	39	G

5 of 604 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
25	BA	2427	C
1	CA	466	G
25	DA	2145	C
25	BA	2573	C
1	CA	48	C

## 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 2392 ligands modelled in this entry, 2392 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	AA	1504/1525 (98%)	-0.43	18 (1%) 75 20	35, 78, 175, 261	0
1	CA	1504/1525 (98%)	-0.21	25 (1%) 67 15	34, 99, 199, 271	0
2	AY	77/77 (100%)	-0.60	0 100 100	60, 90, 124, 194	0
2	AZ	77/77 (100%)	0.99	17 (22%) 1 1	146, 211, 242, 260	0
2	CY	77/77 (100%)	-0.46	1 (1%) 74 19	59, 91, 127, 196	0
2	CZ	77/77 (100%)	1.46	21 (27%) 1 0	175, 231, 266, 276	0
3	AV	10/27 (37%)	0.20	1 (10%) 8 2	62, 77, 118, 184	0
3	CV	10/27 (37%)	0.53	1 (10%) 8 2	63, 104, 143, 196	0
4	AB	234/256 (91%)	0.18	8 (3%) 43 8	85, 126, 167, 194	0
4	CB	234/256 (91%)	0.26	9 (3%) 38 7	91, 127, 174, 204	0
5	AC	206/239 (86%)	0.02	2 (0%) 79 22	86, 121, 159, 183	0
5	CC	206/239 (86%)	0.11	3 (1%) 70 16	87, 126, 164, 178	0
6	AD	208/209 (99%)	0.09	4 (1%) 64 13	50, 79, 127, 164	0
6	CD	208/209 (99%)	0.34	4 (1%) 64 13	81, 115, 151, 184	0
7	AE	151/162 (93%)	0.03	3 (1%) 62 12	65, 90, 130, 192	0
7	CE	151/162 (93%)	0.06	1 (0%) 84 28	71, 100, 145, 173	0
8	AF	101/101 (100%)	-0.02	0 100 100	69, 98, 137, 176	0
8	CF	101/101 (100%)	-0.06	0 100 100	64, 94, 131, 149	0
9	AG	155/156 (99%)	0.05	6 (3%) 37 7	82, 113, 154, 172	0
9	CG	155/156 (99%)	0.14	4 (2%) 53 10	87, 125, 158, 181	0
10	AH	138/138 (100%)	0.03	0 100 100	64, 90, 135, 146	0
10	CH	138/138 (100%)	0.15	2 (1%) 72 18	80, 107, 145, 171	0
11	AI	127/128 (99%)	0.51	10 (7%) 13 3	90, 134, 168, 182	0
11	CI	127/128 (99%)	0.81	16 (12%) 4 1	105, 140, 173, 227	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
12	AJ	98/105 (93%)	0.70	14 (14%) 3 1	87, 125, 166, 184	0
12	CJ	98/105 (93%)	0.67	13 (13%) 4 1	106, 144, 175, 186	0
13	AK	114/129 (88%)	0.02	5 (4%) 33 7	59, 88, 123, 160	0
13	CK	114/129 (88%)	0.23	7 (6%) 21 5	64, 91, 135, 175	0
14	AL	122/134 (91%)	-0.03	2 (1%) 68 16	47, 67, 114, 144	0
14	CL	122/134 (91%)	0.26	8 (6%) 18 4	57, 89, 131, 185	0
15	AM	117/126 (92%)	0.32	9 (7%) 13 3	93, 122, 159, 171	0
15	CM	117/126 (92%)	0.56	12 (10%) 7 2	98, 143, 172, 188	0
16	AN	60/61 (98%)	0.43	5 (8%) 11 3	75, 109, 141, 193	0
16	CN	60/61 (98%)	0.50	5 (8%) 11 3	80, 113, 158, 175	0
17	AO	88/89 (98%)	0.05	0 100 100	57, 90, 123, 145	0
17	CO	88/89 (98%)	0.11	3 (3%) 43 8	60, 91, 130, 145	0
18	AP	83/88 (94%)	0.48	1 (1%) 75 20	58, 75, 119, 184	0
18	CP	83/88 (94%)	1.18	17 (20%) 1 1	90, 123, 155, 202	0
19	AQ	99/105 (94%)	-0.13	0 100 100	56, 79, 118, 142	0
19	CQ	99/105 (94%)	0.43	4 (4%) 36 7	76, 105, 140, 159	0
20	AR	70/88 (79%)	0.46	3 (4%) 34 7	68, 103, 147, 165	0
20	CR	70/88 (79%)	0.57	2 (2%) 49 9	64, 87, 139, 147	0
21	AS	78/93 (83%)	1.22	16 (20%) 1 1	98, 136, 170, 193	0
21	CS	78/93 (83%)	0.72	10 (12%) 4 1	114, 150, 184, 205	0
22	AT	99/106 (93%)	0.30	4 (4%) 36 7	51, 84, 138, 166	0
22	CT	99/106 (93%)	0.83	12 (12%) 5 1	87, 117, 160, 184	0
23	AU	24/27 (88%)	3.23	21 (87%) 0 0	93, 122, 162, 191	0
23	CU	24/27 (88%)	4.65	24 (100%) 0 0	100, 137, 178, 187	0
24	AX	362/378 (95%)	0.52	42 (11%) 5 2	61, 129, 207, 244	0
24	CX	362/378 (95%)	0.76	39 (10%) 6 2	94, 150, 244, 273	0
25	BA	2879/2894 (99%)	-0.43	51 (1%) 65 14	14, 64, 186, 278	0
25	DA	2879/2894 (99%)	-0.35	71 (2%) 54 11	10, 67, 204, 287	0
26	BB	119/124 (95%)	-0.34	0 100 100	69, 100, 144, 222	0
26	DB	119/124 (95%)	0.19	5 (4%) 35 7	87, 147, 205, 258	0
27	BD	271/276 (98%)	0.00	5 (1%) 65 14	27, 51, 99, 162	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
27	DD	271/276 (98%)	-0.02	2 (0%) 84 28	26, 51, 92, 146	0
28	BE	204/206 (99%)	-0.04	1 (0%) 88 36	36, 69, 126, 159	0
28	DE	204/206 (99%)	0.32	19 (9%) 9 2	45, 85, 137, 186	0
29	BF	202/210 (96%)	-0.09	3 (1%) 70 16	38, 71, 131, 153	0
29	DF	202/210 (96%)	0.06	1 (0%) 88 36	34, 66, 124, 190	0
30	BG	181/182 (99%)	0.39	12 (6%) 18 4	88, 121, 164, 179	0
30	DG	181/182 (99%)	0.48	11 (6%) 21 5	113, 153, 182, 206	0
31	BH	159/180 (88%)	0.50	15 (9%) 9 2	97, 139, 185, 202	0
31	DH	159/180 (88%)	0.19	8 (5%) 28 6	79, 111, 154, 174	0
32	BI	145/148 (97%)	0.25	6 (4%) 35 7	54, 106, 147, 198	0
32	DI	145/148 (97%)	0.02	2 (1%) 72 18	58, 94, 129, 147	0
33	BK	147/147 (100%)	1.51	41 (27%) 1 0	177, 205, 225, 240	0
33	DK	147/147 (100%)	2.49	67 (45%) 1 0	207, 236, 257, 274	0
34	BN	137/163 (84%)	0.25	2 (1%) 70 16	55, 87, 131, 153	0
34	DN	137/163 (84%)	0.05	3 (2%) 59 12	59, 80, 130, 164	0
35	BO	122/122 (100%)	-0.29	0 100 100	32, 61, 101, 118	0
35	DO	122/122 (100%)	-0.27	0 100 100	47, 72, 108, 129	0
36	BP	146/150 (97%)	0.35	6 (4%) 35 7	35, 89, 148, 203	0
36	DP	146/150 (97%)	0.24	5 (3%) 43 8	21, 93, 146, 183	0
37	BQ	134/141 (95%)	0.27	8 (5%) 21 5	44, 79, 136, 188	0
37	DQ	134/141 (95%)	0.18	3 (2%) 59 12	56, 91, 148, 192	0
38	BR	117/118 (99%)	-0.12	0 100 100	31, 63, 114, 165	0
38	DR	117/118 (99%)	0.08	0 100 100	48, 73, 130, 148	0
39	BS	98/112 (87%)	0.29	1 (1%) 79 22	66, 105, 140, 169	0
39	DS	98/112 (87%)	1.27	27 (27%) 1 0	106, 144, 177, 218	0
40	BT	137/146 (93%)	0.40	6 (4%) 33 7	41, 76, 136, 156	0
40	DT	137/146 (93%)	0.61	10 (7%) 15 3	66, 100, 155, 189	0
41	BU	117/118 (99%)	0.24	1 (0%) 81 24	45, 78, 124, 159	0
41	DU	117/118 (99%)	0.51	5 (4%) 34 7	39, 68, 120, 194	0
42	BV	101/101 (100%)	0.20	1 (0%) 79 22	63, 99, 144, 220	0
42	DV	101/101 (100%)	0.22	2 (1%) 62 12	46, 91, 143, 206	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
43	BW	112/113 (99%)	-0.11	0 100 100	39, 64, 111, 163	0
43	DW	112/113 (99%)	0.16	1 (0%) 81 24	31, 61, 119, 155	0
44	BX	92/96 (95%)	0.15	2 (2%) 59 12	50, 79, 122, 149	0
44	DX	92/96 (95%)	0.36	3 (3%) 44 8	38, 65, 114, 150	0
45	BY	100/110 (90%)	0.91	14 (14%) 3 1	75, 112, 179, 200	0
45	DY	100/110 (90%)	0.64	7 (7%) 16 4	53, 86, 160, 186	0
46	BZ	187/206 (90%)	0.24	6 (3%) 45 9	83, 119, 156, 196	0
46	DZ	187/206 (90%)	0.52	13 (6%) 16 4	107, 139, 176, 201	0
47	B0	76/85 (89%)	-0.06	0 100 100	56, 78, 115, 150	0
47	D0	76/85 (89%)	0.05	1 (1%) 74 19	73, 99, 139, 160	0
48	B1	88/98 (89%)	0.02	1 (1%) 77 21	31, 66, 119, 177	0
48	D1	88/98 (89%)	0.10	1 (1%) 77 21	34, 68, 143, 172	0
49	B2	62/72 (86%)	0.01	1 (1%) 68 16	55, 90, 131, 165	0
49	D2	62/72 (86%)	-0.07	0 100 100	37, 75, 147, 177	0
50	B3	59/60 (98%)	0.53	4 (6%) 17 4	65, 85, 145, 166	0
50	D3	59/60 (98%)	0.17	1 (1%) 67 15	57, 83, 129, 170	0
51	B4	30/97 (30%)	-0.10	0 100 100	101, 135, 178, 183	0
51	D4	30/97 (30%)	0.13	0 100 100	115, 149, 178, 183	0
52	B5	52/60 (86%)	0.18	2 (3%) 38 7	49, 79, 147, 166	0
52	D5	52/60 (86%)	-0.20	0 100 100	42, 80, 147, 167	0
53	B6	44/54 (81%)	2.51	23 (52%) 0 0	106, 136, 175, 224	0
53	D6	44/54 (81%)	2.54	27 (61%) 0 0	111, 140, 175, 192	0
54	B7	48/49 (97%)	0.96	8 (16%) 2 1	38, 57, 119, 143	0
54	D7	48/49 (97%)	0.73	6 (12%) 5 1	31, 44, 96, 161	0
55	B8	63/65 (96%)	0.30	3 (4%) 29 6	42, 59, 117, 156	0
55	D8	63/65 (96%)	0.39	2 (3%) 45 9	48, 72, 133, 168	0
All	All	21662/22654 (95%)	0.05	960 (4%) 33 7	10, 90, 190, 287	0

The worst 5 of 960 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	AA	84	U	14.8
2	CZ	56	C	12.6

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Mol	Chain	Res	Type	RSRZ
25	DA	2169	A	12.0
2	CZ	17(A)	U	11.8
2	AZ	17(A)	U	11.0

## 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
56	MG	AA	2027	1/1	0.11	-	27,27,27,27	0
56	MG	BA	3912	1/1	0.11	-	26,26,26,26	0
56	MG	BA	3169	1/1	0.16	-	67,67,67,67	0
56	MG	AB	307	1/1	0.07	-	45,45,45,45	0
56	MG	AA	1701	1/1	0.10	-	29,29,29,29	0
56	MG	DA	3318	1/1	0.39	-	45,45,45,45	0
56	MG	AA	1957	1/1	0.10	-	61,61,61,61	0
56	MG	AA	1797	1/1	0.37	-	21,21,21,21	0
56	MG	BA	3351	1/1	0.11	-	22,22,22,22	0
56	MG	DA	3149	1/1	0.25	-	3,3,3,3	0
56	MG	BA	3894	1/1	0.07	-	70,70,70,70	0
56	MG	DA	3331	1/1	0.17	-	23,23,23,23	0
56	MG	BA	3195	1/1	0.24	-	47,47,47,47	0
56	MG	BA	3867	1/1	0.30	-	50,50,50,50	0
56	MG	DA	3059	1/1	0.22	-	3,3,3,3	0
56	MG	AA	1691	1/1	0.16	-	37,37,37,37	0
56	MG	BA	3453	1/1	0.28	-	57,57,57,57	0
56	MG	BA	3356	1/1	0.24	-	54,54,54,54	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	BA	3211	1/1	0.11	-	80,80,80,80	0
56	MG	CA	1809	1/1	0.33	-	3,3,3,3	0
56	MG	AC	301	1/1	0.19	-	75,75,75,75	0
56	MG	AA	1649	1/1	0.17	-	37,37,37,37	0
56	MG	AA	1792	1/1	0.11	-	63,63,63,63	0
56	MG	DA	3110	1/1	0.06	-	48,48,48,48	0
56	MG	BA	3768	1/1	0.14	-	31,31,31,31	0
56	MG	BA	3574	1/1	0.37	-	74,74,74,74	0
56	MG	CA	1761	1/1	0.10	-	30,30,30,30	0
56	MG	AA	1718	1/1	0.13	-	79,79,79,79	0
56	MG	BA	3875	1/1	0.12	-	27,27,27,27	0
56	MG	AA	1866	1/1	0.10	-	26,26,26,26	0
56	MG	BA	3899	1/1	0.99	-	73,73,73,73	0
56	MG	B1	104	1/1	0.11	-	38,38,38,38	0
56	MG	BA	3576	1/1	0.19	-	43,43,43,43	0
56	MG	AY	116	1/1	0.26	-	40,40,40,40	0
56	MG	DA	3375	1/1	0.11	-	88,88,88,88	0
56	MG	DA	3021	1/1	0.17	-	4,4,4,4	0
56	MG	B5	102	1/1	0.10	-	49,49,49,49	0
56	MG	BA	3690	1/1	0.29	-	80,80,80,80	0
56	MG	BQ	203	1/1	0.17	-	46,46,46,46	0
56	MG	AA	1705	1/1	0.37	-	50,50,50,50	0
56	MG	CA	1815	1/1	0.25	-	63,63,63,63	0
56	MG	CA	1650	1/1	0.46	-	73,73,73,73	0
56	MG	AA	1735	1/1	0.11	-	44,44,44,44	0
56	MG	BA	3317	1/1	0.07	-	48,48,48,48	0
56	MG	DA	3437	1/1	0.54	-	3,3,3,3	0
56	MG	AA	1721	1/1	0.15	-	44,44,44,44	0
56	MG	BA	3003	1/1	0.10	-	36,36,36,36	0
56	MG	DA	3179	1/1	0.51	-	3,3,3,3	0
56	MG	BA	3799	1/1	0.12	-	29,29,29,29	0
56	MG	DB	212	1/1	0.22	-	3,3,3,3	0
56	MG	BA	3147	1/1	0.31	-	52,52,52,52	0
56	MG	DA	3477	1/1	0.21	-	3,3,3,3	0
56	MG	BA	3569	1/1	0.17	-	40,40,40,40	0
56	MG	BA	3257	1/1	0.16	-	28,28,28,28	0
56	MG	BA	3728	1/1	0.21	-	34,34,34,34	0
56	MG	CA	1678	1/1	0.21	-	49,49,49,49	0
56	MG	BA	3423	1/1	0.15	-	21,21,21,21	0
56	MG	DA	3259	1/1	0.22	-	4,4,4,4	0
56	MG	BA	3603	1/1	0.19	-	47,47,47,47	0
56	MG	BA	3161	1/1	0.42	-	103,103,103,103	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	BA	3425	1/1	0.26	-	48,48,48,48	0
56	MG	CA	1794	1/1	0.20	-	35,35,35,35	0
56	MG	BA	3725	1/1	0.12	-	23,23,23,23	0
56	MG	DA	3109	1/1	0.26	-	3,3,3,3	0
56	MG	DA	3470	1/1	0.21	-	4,4,4,4	0
56	MG	DA	3442	1/1	0.27	-	3,3,3,3	0
56	MG	DA	3399	1/1	0.29	-	58,58,58,58	0
56	MG	DA	3488	1/1	0.21	-	3,3,3,3	0
56	MG	AA	1761	1/1	0.15	-	39,39,39,39	0
56	MG	BA	3923	1/1	0.33	-	57,57,57,57	0
56	MG	BA	3463	1/1	0.12	-	38,38,38,38	0
56	MG	AA	1606	1/1	0.15	-	35,35,35,35	0
56	MG	BA	3836	1/1	0.26	-	20,20,20,20	0
56	MG	AA	1968	1/1	0.24	-	35,35,35,35	0
56	MG	BA	3052	1/1	0.17	-	71,71,71,71	0
56	MG	AA	1935	1/1	0.10	-	53,53,53,53	0
56	MG	BA	3319	1/1	0.07	-	44,44,44,44	0
56	MG	DA	3350	1/1	0.16	-	63,63,63,63	0
56	MG	BA	3645	1/1	0.16	-	30,30,30,30	0
56	MG	DA	3256	1/1	0.10	-	6,6,6,6	0
56	MG	BA	3464	1/1	0.17	-	75,75,75,75	0
56	MG	BA	3088	1/1	0.27	-	63,63,63,63	0
56	MG	DA	3142	1/1	0.42	-	3,3,3,3	0
56	MG	BA	3712	1/1	0.46	-	77,77,77,77	0
56	MG	AA	1777	1/1	0.23	-	53,53,53,53	0
56	MG	AA	1720	1/1	0.18	-	36,36,36,36	0
56	MG	BA	3021	1/1	0.40	-	37,37,37,37	0
56	MG	BA	3880	1/1	0.18	-	63,63,63,63	0
56	MG	BB	216	1/1	0.25	-	46,46,46,46	0
56	MG	BA	3379	1/1	0.29	-	115,115,115,115	0
56	MG	DA	3378	1/1	0.26	-	3,3,3,3	0
56	MG	BA	3013	1/1	1.09	-	103,103,103,103	0
56	MG	BA	3517	1/1	0.11	-	46,46,46,46	0
56	MG	CH	201	1/1	0.40	-	58,58,58,58	0
56	MG	BA	3391	1/1	0.11	-	51,51,51,51	0
56	MG	CA	1638	1/1	0.24	-	3,3,3,3	0
56	MG	DA	3261	1/1	0.27	-	3,3,3,3	0
56	MG	BA	3108	1/1	0.18	-	55,55,55,55	0
56	MG	BA	3660	1/1	0.25	-	12,12,12,12	0
56	MG	AA	1765	1/1	0.33	-	11,11,11,11	0
56	MG	BA	3911	1/1	0.05	-	22,22,22,22	0
56	MG	BA	3043	1/1	0.18	-	58,58,58,58	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	AA	1943	1/1	0.24	-	56,56,56,56	0
56	MG	CL	201	1/1	0.25	-	67,67,67,67	0
56	MG	AA	1834	1/1	0.11	-	43,43,43,43	0
56	MG	DA	3121	1/1	0.23	-	41,41,41,41	0
56	MG	BA	3580	1/1	0.18	-	54,54,54,54	0
56	MG	BA	3279	1/1	0.23	-	39,39,39,39	0
56	MG	BA	3483	1/1	0.35	-	47,47,47,47	0
56	MG	AA	1629	1/1	0.11	-	32,32,32,32	0
56	MG	DA	3327	1/1	0.27	-	4,4,4,4	0
56	MG	BA	3702	1/1	0.08	-	83,83,83,83	0
56	MG	BA	3429	1/1	0.19	-	51,51,51,51	0
56	MG	BA	3593	1/1	0.49	-	64,64,64,64	0
56	MG	AA	2000	1/1	0.14	-	46,46,46,46	0
56	MG	DA	3367	1/1	0.11	-	59,59,59,59	0
56	MG	BA	3264	1/1	0.24	-	60,60,60,60	0
56	MG	BA	3870	1/1	0.25	-	47,47,47,47	0
56	MG	AA	1913	1/1	0.09	-	54,54,54,54	0
56	MG	AL	204	1/1	0.07	-	43,43,43,43	0
56	MG	BA	3283	1/1	0.47	-	63,63,63,63	0
56	MG	DA	3062	1/1	0.29	-	4,4,4,4	0
56	MG	BA	3333	1/1	0.10	-	55,55,55,55	0
56	MG	BA	3535	1/1	0.24	-	62,62,62,62	0
56	MG	BA	3122	1/1	0.16	-	56,56,56,56	0
56	MG	BA	3862	1/1	0.10	-	85,85,85,85	0
56	MG	B1	106	1/1	0.20	-	56,56,56,56	0
56	MG	AA	1832	1/1	0.25	-	33,33,33,33	0
56	MG	BA	3184	1/1	0.12	-	45,45,45,45	0
56	MG	CA	1661	1/1	0.22	-	3,3,3,3	0
56	MG	DA	3146	1/1	0.29	-	3,3,3,3	0
56	MG	BA	3326	1/1	0.13	-	45,45,45,45	0
56	MG	AA	1927	1/1	0.24	-	29,29,29,29	0
56	MG	DA	3435	1/1	0.16	-	4,4,4,4	0
56	MG	AA	1995	1/1	0.14	-	44,44,44,44	0
56	MG	AB	302	1/1	0.12	-	50,50,50,50	0
56	MG	BA	3446	1/1	0.34	-	58,58,58,58	0
56	MG	AA	1754	1/1	0.16	-	70,70,70,70	0
56	MG	BA	3049	1/1	0.24	-	56,56,56,56	0
56	MG	BA	3514	1/1	0.33	-	53,53,53,53	0
56	MG	DA	3232	1/1	0.07	-	37,37,37,37	0
56	MG	AA	1851	1/1	0.42	-	69,69,69,69	0
56	MG	B0	101	1/1	0.43	-	63,63,63,63	0
56	MG	DA	3453	1/1	0.45	-	3,3,3,3	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	BA	3887	1/1	0.20	-	66,66,66,66	0
56	MG	BA	3732	1/1	0.56	-	68,68,68,68	0
56	MG	DA	3483	1/1	0.20	-	4,4,4,4	0
56	MG	CA	1780	1/1	0.09	-	51,51,51,51	0
56	MG	AA	1601	1/1	0.22	-	37,37,37,37	0
56	MG	DA	3090	1/1	0.27	-	3,3,3,3	0
56	MG	BA	3030	1/1	0.17	-	36,36,36,36	0
56	MG	AA	1915	1/1	0.13	-	109,109,109,109	0
56	MG	AA	1934	1/1	0.35	-	65,65,65,65	0
56	MG	DA	3050	1/1	0.37	-	3,3,3,3	0
56	MG	DN	201	1/1	0.57	-	3,3,3,3	0
56	MG	DA	3035	1/1	0.40	-	3,3,3,3	0
56	MG	AH	202	1/1	0.28	-	51,51,51,51	0
56	MG	BB	206	1/1	0.12	-	51,51,51,51	0
56	MG	AA	1811	1/1	0.25	-	37,37,37,37	0
56	MG	AA	1862	1/1	0.15	-	41,41,41,41	0
56	MG	AA	1624	1/1	0.13	-	43,43,43,43	0
56	MG	AY	126	1/1	0.34	-	68,68,68,68	0
56	MG	BA	3636	1/1	0.15	-	31,31,31,31	0
56	MG	CA	1677	1/1	0.17	-	103,103,103,103	0
56	MG	BA	3782	1/1	0.14	-	21,21,21,21	0
56	MG	AA	1871	1/1	0.27	-	68,68,68,68	0
56	MG	BA	3842	1/1	0.19	-	16,16,16,16	0
56	MG	BA	3865	1/1	0.56	-	37,37,37,37	0
56	MG	BA	3302	1/1	0.30	-	47,47,47,47	0
56	MG	AA	1677	1/1	0.12	-	74,74,74,74	0
56	MG	BA	3189	1/1	0.15	-	96,96,96,96	0
56	MG	DA	3273	1/1	0.28	-	3,3,3,3	0
56	MG	DA	3214	1/1	0.30	-	4,4,4,4	0
56	MG	CA	1730	1/1	0.28	-	4,4,4,4	0
56	MG	BA	3220	1/1	0.19	-	13,13,13,13	0
56	MG	BA	3917	1/1	0.11	-	51,51,51,51	0
56	MG	BA	3699	1/1	0.05	-	79,79,79,79	0
56	MG	AA	1666	1/1	0.12	-	61,61,61,61	0
56	MG	AA	1887	1/1	0.14	-	31,31,31,31	0
56	MG	DA	3393	1/1	0.05	-	47,47,47,47	0
56	MG	AA	1789	1/1	0.18	-	77,77,77,77	0
56	MG	BK	201	1/1	0.38	-	60,60,60,60	0
56	MG	BA	3048	1/1	0.55	-	58,58,58,58	0
56	MG	DA	3368	1/1	0.21	-	3,3,3,3	0
56	MG	AL	201	1/1	0.19	-	28,28,28,28	0
56	MG	DA	3027	1/1	0.15	-	6,6,6,6	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	BA	3407	1/1	0.42	-	56,56,56,56	0
56	MG	BA	3901	1/1	0.40	-	62,62,62,62	0
56	MG	DA	3423	1/1	0.47	-	28,28,28,28	0
56	MG	AA	1634	1/1	0.11	-	43,43,43,43	0
56	MG	CA	1790	1/1	0.23	-	57,57,57,57	0
56	MG	CA	1656	1/1	0.18	-	5,5,5,5	0
56	MG	DA	3407	1/1	0.26	-	3,3,3,3	0
56	MG	BA	3364	1/1	0.45	-	40,40,40,40	0
56	MG	BA	3753	1/1	0.45	-	65,65,65,65	0
56	MG	DA	3298	1/1	0.19	-	9,9,9,9	0
56	MG	BA	3539	1/1	0.18	-	12,12,12,12	0
56	MG	BA	3542	1/1	0.17	-	27,27,27,27	0
56	MG	AA	1739	1/1	0.34	-	55,55,55,55	0
56	MG	DA	3103	1/1	0.26	-	62,62,62,62	0
56	MG	BA	3618	1/1	0.10	-	19,19,19,19	0
56	MG	DA	3416	1/1	0.22	-	3,3,3,3	0
56	MG	CA	1754	1/1	0.20	-	3,3,3,3	0
56	MG	BB	213	1/1	0.20	-	53,53,53,53	0
56	MG	CA	1822	1/1	0.33	-	3,3,3,3	0
56	MG	BA	3309	1/1	0.22	-	17,17,17,17	0
56	MG	AX	413	1/1	0.35	-	32,32,32,32	0
56	MG	AA	1651	1/1	0.26	-	106,106,106,106	0
56	MG	CA	1674	1/1	0.39	-	57,57,57,57	0
56	MG	DA	3386	1/1	0.20	-	3,3,3,3	0
56	MG	CA	1784	1/1	0.26	-	3,3,3,3	0
56	MG	BA	3888	1/1	0.23	-	53,53,53,53	0
56	MG	AE	207	1/1	0.12	-	38,38,38,38	0
56	MG	BA	3525	1/1	0.12	-	77,77,77,77	0
56	MG	BE	301	1/1	0.08	-	55,55,55,55	0
56	MG	BA	3811	1/1	0.37	-	52,52,52,52	0
56	MG	BA	3864	1/1	0.32	-	78,78,78,78	0
56	MG	CA	1723	1/1	0.35	-	67,67,67,67	0
56	MG	BA	3530	1/1	0.15	-	60,60,60,60	0
56	MG	BA	3852	1/1	0.21	-	35,35,35,35	0
56	MG	BA	3729	1/1	0.23	-	38,38,38,38	0
56	MG	DA	3289	1/1	0.29	-	59,59,59,59	0
56	MG	BI	201	1/1	0.13	-	78,78,78,78	0
56	MG	BA	3222	1/1	0.36	-	39,39,39,39	0
56	MG	DA	3390	1/1	0.15	-	73,73,73,73	0
56	MG	AA	1948	1/1	0.13	-	56,56,56,56	0
56	MG	DA	3078	1/1	0.29	-	4,4,4,4	0
56	MG	AA	1687	1/1	0.10	-	47,47,47,47	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	DA	3200	1/1	0.41	-	3,3,3,3	0
56	MG	B2	102	1/1	0.30	-	62,62,62,62	0
56	MG	AA	1710	1/1	0.31	-	40,40,40,40	0
56	MG	BA	3694	1/1	0.13	-	77,77,77,77	0
56	MG	BA	3420	1/1	0.26	-	19,19,19,19	0
56	MG	CA	1719	1/1	0.22	-	60,60,60,60	0
56	MG	DA	3025	1/1	0.27	-	3,3,3,3	0
56	MG	BA	3345	1/1	0.15	-	42,42,42,42	0
56	MG	AA	1676	1/1	0.13	-	66,66,66,66	0
56	MG	BA	3620	1/1	0.19	-	53,53,53,53	0
56	MG	BA	3262	1/1	0.23	-	7,7,7,7	0
56	MG	BA	3209	1/1	0.30	-	54,54,54,54	0
56	MG	BA	3056	1/1	0.21	-	66,66,66,66	0
56	MG	BB	212	1/1	0.11	-	82,82,82,82	0
56	MG	DA	3267	1/1	0.16	-	3,3,3,3	0
56	MG	BA	3839	1/1	0.50	-	60,60,60,60	0
56	MG	DA	3034	1/1	0.11	-	6,6,6,6	0
56	MG	DA	3241	1/1	0.14	-	73,73,73,73	0
56	MG	DA	3408	1/1	0.25	-	4,4,4,4	0
56	MG	BA	3903	1/1	0.21	-	71,71,71,71	0
56	MG	AA	1697	1/1	0.21	-	48,48,48,48	0
56	MG	AA	1790	1/1	0.14	-	97,97,97,97	0
56	MG	BA	3545	1/1	0.16	-	23,23,23,23	0
56	MG	DA	3343	1/1	0.30	-	3,3,3,3	0
56	MG	DA	3148	1/1	0.19	-	4,4,4,4	0
56	MG	BA	3152	1/1	0.51	-	49,49,49,49	0
56	MG	BA	3914	1/1	0.14	-	47,47,47,47	0
56	MG	AA	1633	1/1	0.18	-	77,77,77,77	0
56	MG	AA	1708	1/1	0.31	-	33,33,33,33	0
56	MG	B6	102	1/1	0.10	-	57,57,57,57	0
56	MG	DA	3254	1/1	0.12	-	42,42,42,42	0
56	MG	AA	2002	1/1	0.17	-	47,47,47,47	0
56	MG	DA	3135	1/1	0.21	-	3,3,3,3	0
56	MG	DA	3160	1/1	0.34	-	3,3,3,3	0
56	MG	AA	1608	1/1	0.12	-	43,43,43,43	0
56	MG	AA	1846	1/1	0.38	-	68,68,68,68	0
56	MG	CS	101	1/1	0.25	-	3,3,3,3	0
56	MG	DA	3438	1/1	0.20	-	6,6,6,6	0
56	MG	BA	3451	1/1	0.17	-	13,13,13,13	0
56	MG	DA	3263	1/1	0.20	-	4,4,4,4	0
57	ZN	CD	5001	1/1	0.23	-	63,63,63,63	0
56	MG	CY	109	1/1	0.24	-	3,3,3,3	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	DA	3485	1/1	0.11	-	4,4,4,4	0
56	MG	AA	1920	1/1	0.23	-	26,26,26,26	0
56	MG	BA	3489	1/1	0.14	-	32,32,32,32	0
56	MG	DA	3197	1/1	0.18	-	3,3,3,3	0
56	MG	DA	3068	1/1	0.22	-	4,4,4,4	0
56	MG	BA	3469	1/1	0.22	-	46,46,46,46	0
56	MG	B0	103	1/1	0.14	-	30,30,30,30	0
56	MG	AA	1817	1/1	0.26	-	29,29,29,29	0
56	MG	CA	1604	1/1	0.27	-	3,3,3,3	0
56	MG	BA	3720	1/1	0.16	-	28,28,28,28	0
56	MG	DA	3244	1/1	0.07	-	5,5,5,5	0
56	MG	CF	201	1/1	0.15	-	40,40,40,40	0
56	MG	DA	3225	1/1	0.16	-	4,4,4,4	0
56	MG	DA	3037	1/1	0.25	-	4,4,4,4	0
56	MG	DA	3335	1/1	0.60	-	3,3,3,3	0
56	MG	AA	1766	1/1	0.39	-	33,33,33,33	0
56	MG	AY	101	1/1	0.28	-	68,68,68,68	0
56	MG	BA	3710	1/1	0.20	-	52,52,52,52	0
56	MG	DA	3246	1/1	0.22	-	3,3,3,3	0
56	MG	AA	1833	1/1	0.10	-	60,60,60,60	0
56	MG	DA	3356	1/1	0.07	-	56,56,56,56	0
56	MG	DA	3264	1/1	0.18	-	4,4,4,4	0
56	MG	B5	101	1/1	0.34	-	63,63,63,63	0
56	MG	DA	3326	1/1	0.15	-	4,4,4,4	0
56	MG	CA	1709	1/1	0.12	-	55,55,55,55	0
56	MG	AO	101	1/1	0.12	-	33,33,33,33	0
56	MG	BB	214	1/1	0.17	-	55,55,55,55	0
56	MG	DD	5002	1/1	0.14	-	33,33,33,33	0
56	MG	BA	3400	1/1	0.12	-	101,101,101,101	0
56	MG	BA	3528	1/1	0.36	-	60,60,60,60	0
56	MG	AA	2021	1/1	0.09	-	43,43,43,43	0
56	MG	BA	3116	1/1	0.23	-	44,44,44,44	0
56	MG	BA	3227	1/1	0.14	-	46,46,46,46	0
56	MG	BH	202	1/1	0.18	-	56,56,56,56	0
56	MG	AE	201	1/1	0.10	-	52,52,52,52	0
56	MG	DA	3340	1/1	0.13	-	5,5,5,5	0
56	MG	AX	410	1/1	0.09	-	73,73,73,73	0
56	MG	BA	3671	1/1	0.16	-	57,57,57,57	0
56	MG	CA	1760	1/1	0.14	-	18,18,18,18	0
56	MG	DA	3237	1/1	0.16	-	51,51,51,51	0
56	MG	BA	3245	1/1	0.15	-	39,39,39,39	0
56	MG	DA	3093	1/1	0.29	-	3,3,3,3	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	BA	3008	1/1	0.23	-	38,38,38,38	0
56	MG	DA	3253	1/1	0.22	-	3,3,3,3	0
56	MG	AE	206	1/1	0.07	-	57,57,57,57	0
56	MG	DA	3222	1/1	0.11	-	41,41,41,41	0
56	MG	BA	3381	1/1	0.22	-	48,48,48,48	0
56	MG	AA	1611	1/1	0.34	-	48,48,48,48	0
56	MG	DA	3143	1/1	0.23	-	3,3,3,3	0
56	MG	AA	1853	1/1	0.14	-	24,24,24,24	0
56	MG	DA	3063	1/1	0.25	-	3,3,3,3	0
56	MG	BA	3772	1/1	0.11	-	48,48,48,48	0
56	MG	DA	3220	1/1	0.31	-	21,21,21,21	0
56	MG	BA	3703	1/1	0.17	-	68,68,68,68	0
56	MG	DA	3141	1/1	0.10	-	4,4,4,4	0
56	MG	DA	3323	1/1	0.48	-	3,3,3,3	0
56	MG	DA	3336	1/1	0.16	-	25,25,25,25	0
56	MG	DA	3391	1/1	0.12	-	35,35,35,35	0
56	MG	BA	3774	1/1	0.27	-	42,42,42,42	0
56	MG	BA	3182	1/1	0.17	-	20,20,20,20	0
56	MG	AQ	201	1/1	0.09	-	52,52,52,52	0
56	MG	AY	110	1/1	0.14	-	31,31,31,31	0
56	MG	DA	3202	1/1	0.37	-	3,3,3,3	0
56	MG	BA	3509	1/1	0.22	-	34,34,34,34	0
56	MG	AA	1966	1/1	0.12	-	29,29,29,29	0
56	MG	DA	3051	1/1	0.28	-	3,3,3,3	0
56	MG	BA	3737	1/1	0.15	-	50,50,50,50	0
56	MG	AA	2022	1/1	0.11	-	35,35,35,35	0
56	MG	BA	3784	1/1	0.16	-	33,33,33,33	0
56	MG	AA	1796	1/1	0.14	-	60,60,60,60	0
56	MG	DA	3107	1/1	0.10	-	30,30,30,30	0
56	MG	CA	1734	1/1	0.12	-	29,29,29,29	0
56	MG	BA	3354	1/1	0.35	-	59,59,59,59	0
56	MG	AA	2013	1/1	0.33	-	40,40,40,40	0
56	MG	AA	1999	1/1	0.08	-	47,47,47,47	0
56	MG	DA	3250	1/1	0.22	-	3,3,3,3	0
56	MG	BA	3444	1/1	0.19	-	42,42,42,42	0
56	MG	BA	3718	1/1	0.23	-	51,51,51,51	0
56	MG	AA	1656	1/1	0.17	-	47,47,47,47	0
56	MG	DA	3047	1/1	0.20	-	3,3,3,3	0
56	MG	AA	1682	1/1	0.14	-	40,40,40,40	0
56	MG	AA	1827	1/1	0.25	-	44,44,44,44	0
56	MG	BA	3149	1/1	0.19	-	29,29,29,29	0
56	MG	BA	3005	1/1	0.27	-	51,51,51,51	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	BA	3304	1/1	0.30	-	25,25,25,25	0
56	MG	DA	3040	1/1	0.26	-	3,3,3,3	0
56	MG	BA	3878	1/1	0.22	-	44,44,44,44	0
56	MG	BA	3293	1/1	0.13	-	7,7,7,7	0
56	MG	DA	3440	1/1	0.12	-	4,4,4,4	0
56	MG	AK	205	1/1	0.40	-	61,61,61,61	0
56	MG	BA	3234	1/1	0.24	-	55,55,55,55	0
56	MG	BA	3286	1/1	0.24	-	17,17,17,17	0
56	MG	CA	1776	1/1	0.23	-	3,3,3,3	0
56	MG	AA	1703	1/1	0.10	-	48,48,48,48	0
56	MG	BA	3075	1/1	0.41	-	29,29,29,29	0
56	MG	DA	3321	1/1	0.28	-	4,4,4,4	0
56	MG	BG	201	1/1	0.23	-	64,64,64,64	0
56	MG	BA	3743	1/1	0.30	-	64,64,64,64	0
56	MG	CY	104	1/1	0.09	-	78,78,78,78	0
56	MG	BA	3808	1/1	0.20	-	18,18,18,18	0
56	MG	BA	3077	1/1	0.23	-	59,59,59,59	0
56	MG	BA	3616	1/1	0.09	-	12,12,12,12	0
56	MG	AA	1788	1/1	0.42	-	66,66,66,66	0
56	MG	CA	1689	1/1	0.37	-	81,81,81,81	0
56	MG	DA	3465	1/1	0.22	-	3,3,3,3	0
56	MG	BA	3759	1/1	0.23	-	47,47,47,47	0
56	MG	AA	1830	1/1	0.12	-	55,55,55,55	0
56	MG	CA	1669	1/1	0.52	-	79,79,79,79	0
56	MG	AA	1845	1/1	0.09	-	29,29,29,29	0
56	MG	BA	3573	1/1	0.18	-	62,62,62,62	0
56	MG	CA	1630	1/1	0.48	-	3,3,3,3	0
56	MG	BA	3450	1/1	0.18	-	24,24,24,24	0
56	MG	BA	3533	1/1	0.12	-	2,2,2,2	0
56	MG	DA	3168	1/1	0.20	-	4,4,4,4	0
56	MG	BA	3270	1/1	0.22	-	64,64,64,64	0
56	MG	BA	3508	1/1	0.17	-	33,33,33,33	0
56	MG	BA	3817	1/1	0.30	-	30,30,30,30	0
56	MG	DA	3086	1/1	0.29	-	3,3,3,3	0
56	MG	AA	1908	1/1	0.27	-	85,85,85,85	0
56	MG	CA	1785	1/1	0.27	-	83,83,83,83	0
56	MG	CA	1692	1/1	0.23	-	34,34,34,34	0
56	MG	AV	5502	1/1	0.55	-	89,89,89,89	0
56	MG	AA	1625	1/1	0.21	-	44,44,44,44	0
56	MG	DA	3461	1/1	0.16	-	4,4,4,4	0
56	MG	BA	3675	1/1	0.20	-	43,43,43,43	0
56	MG	DA	3042	1/1	0.04	-	69,69,69,69	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	BA	3552	1/1	0.07	-	15,15,15,15	0
56	MG	DA	3056	1/1	0.17	-	63,63,63,63	0
56	MG	AA	1764	1/1	0.45	-	72,72,72,72	0
56	MG	AY	104	1/1	0.08	-	64,64,64,64	0
56	MG	CA	1820	1/1	0.18	-	43,43,43,43	0
56	MG	DA	3462	1/1	0.25	-	3,3,3,3	0
56	MG	BA	3180	1/1	0.08	-	36,36,36,36	0
56	MG	DA	3424	1/1	0.36	-	14,14,14,14	0
56	MG	BB	226	1/1	0.24	-	72,72,72,72	0
56	MG	CA	1698	1/1	0.21	-	37,37,37,37	0
56	MG	DA	3441	1/1	0.22	-	4,4,4,4	0
56	MG	AZ	103	1/1	0.10	-	66,66,66,66	0
56	MG	DA	3019	1/1	0.24	-	3,3,3,3	0
56	MG	DA	3379	1/1	0.28	-	3,3,3,3	0
56	MG	BA	3401	1/1	0.29	-	86,86,86,86	0
56	MG	DA	3344	1/1	0.33	-	25,25,25,25	0
56	MG	BA	3874	1/1	0.74	-	103,103,103,103	0
56	MG	AA	1919	1/1	0.15	-	88,88,88,88	0
56	MG	BA	3773	1/1	0.15	-	25,25,25,25	0
56	MG	BA	3783	1/1	0.14	-	27,27,27,27	0
56	MG	BA	3607	1/1	0.20	-	40,40,40,40	0
56	MG	BA	3124	1/1	0.29	-	56,56,56,56	0
56	MG	AZ	113	1/1	0.08	-	60,60,60,60	0
56	MG	DA	3171	1/1	0.16	-	3,3,3,3	0
56	MG	DA	3097	1/1	0.15	-	4,4,4,4	0
56	MG	BA	3704	1/1	0.14	-	88,88,88,88	0
56	MG	AA	1970	1/1	0.15	-	52,52,52,52	0
56	MG	DA	3270	1/1	0.22	-	4,4,4,4	0
56	MG	CA	1612	1/1	0.15	-	3,3,3,3	0
56	MG	BA	3410	1/1	0.14	-	67,67,67,67	0
56	MG	BB	210	1/1	0.25	-	72,72,72,72	0
56	MG	DA	3333	1/1	0.30	-	4,4,4,4	0
56	MG	CZ	110	1/1	0.26	-	68,68,68,68	0
56	MG	AA	1652	1/1	0.29	-	63,63,63,63	0
56	MG	BA	3064	1/1	0.12	-	57,57,57,57	0
56	MG	BA	3538	1/1	0.41	-	30,30,30,30	0
56	MG	AE	204	1/1	0.09	-	51,51,51,51	0
56	MG	DA	3071	1/1	0.27	-	3,3,3,3	0
56	MG	BA	3416	1/1	0.35	-	55,55,55,55	0
56	MG	DA	3245	1/1	0.15	-	41,41,41,41	0
56	MG	BA	3419	1/1	0.22	-	50,50,50,50	0
56	MG	BA	3233	1/1	0.38	-	70,70,70,70	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	AA	1856	1/1	0.46	-	49,49,49,49	0
56	MG	AA	1690	1/1	0.10	-	19,19,19,19	0
56	MG	BA	3029	1/1	0.32	-	59,59,59,59	0
56	MG	CA	1633	1/1	0.28	-	3,3,3,3	0
56	MG	BB	202	1/1	0.06	-	50,50,50,50	0
56	MG	AA	1989	1/1	0.28	-	81,81,81,81	0
56	MG	BA	3691	1/1	0.13	-	73,73,73,73	0
56	MG	BA	3267	1/1	0.27	-	21,21,21,21	0
56	MG	BA	3624	1/1	0.16	-	89,89,89,89	0
56	MG	CA	1769	1/1	0.23	-	77,77,77,77	0
56	MG	CA	1736	1/1	0.32	-	3,3,3,3	0
56	MG	CZ	113	1/1	0.37	-	3,3,3,3	0
56	MG	BE	305	1/1	0.11	-	22,22,22,22	0
56	MG	BA	3781	1/1	0.25	-	85,85,85,85	0
56	MG	BA	3853	1/1	0.31	-	25,25,25,25	0
56	MG	BA	3430	1/1	0.11	-	45,45,45,45	0
56	MG	AA	1685	1/1	0.14	-	28,28,28,28	0
56	MG	BA	3516	1/1	0.18	-	43,43,43,43	0
56	MG	BA	3861	1/1	0.26	-	65,65,65,65	0
56	MG	AA	2014	1/1	0.19	-	21,21,21,21	0
56	MG	DA	3067	1/1	0.16	-	17,17,17,17	0
56	MG	DA	3328	1/1	0.19	-	23,23,23,23	0
56	MG	CA	1804	1/1	0.16	-	4,4,4,4	0
56	MG	BA	3863	1/1	0.22	-	62,62,62,62	0
56	MG	AA	1904	1/1	0.53	-	77,77,77,77	0
56	MG	B1	101	1/1	0.23	-	31,31,31,31	0
56	MG	AA	1932	1/1	0.10	-	64,64,64,64	0
56	MG	BA	3086	1/1	0.12	-	23,23,23,23	0
56	MG	BA	3421	1/1	0.27	-	45,45,45,45	0
56	MG	BA	3664	1/1	0.34	-	23,23,23,23	0
56	MG	BA	3382	1/1	0.09	-	75,75,75,75	0
56	MG	AA	1991	1/1	0.20	-	84,84,84,84	0
56	MG	BA	3389	1/1	0.81	-	75,75,75,75	0
56	MG	AB	304	1/1	0.13	-	73,73,73,73	0
56	MG	CA	1715	1/1	0.22	-	40,40,40,40	0
56	MG	BA	3910	1/1	0.24	-	40,40,40,40	0
56	MG	AA	1678	1/1	0.46	-	92,92,92,92	0
56	MG	BA	3908	1/1	0.22	-	26,26,26,26	0
56	MG	BA	3305	1/1	0.12	-	18,18,18,18	0
56	MG	CA	1788	1/1	0.28	-	94,94,94,94	0
56	MG	BA	3709	1/1	0.26	-	70,70,70,70	0
56	MG	AA	1770	1/1	0.35	-	52,52,52,52	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	BA	3591	1/1	0.14	-	29,29,29,29	0
56	MG	DA	3311	1/1	0.21	-	72,72,72,72	0
56	MG	CF	202	1/1	0.23	-	51,51,51,51	0
56	MG	DA	3045	1/1	0.28	-	3,3,3,3	0
56	MG	AA	1807	1/1	0.12	-	36,36,36,36	0
56	MG	CA	1710	1/1	0.22	-	46,46,46,46	0
56	MG	AA	1990	1/1	0.12	-	63,63,63,63	0
56	MG	DA	3456	1/1	0.19	-	5,5,5,5	0
56	MG	AA	1638	1/1	0.57	-	72,72,72,72	0
56	MG	BA	3099	1/1	0.30	-	29,29,29,29	0
56	MG	AA	1967	1/1	0.09	-	28,28,28,28	0
56	MG	BA	3438	1/1	0.21	-	67,67,67,67	0
56	MG	CT	201	1/1	0.29	-	3,3,3,3	0
56	MG	AA	1744	1/1	0.21	-	74,74,74,74	0
56	MG	DA	3426	1/1	0.18	-	5,5,5,5	0
56	MG	BB	228	1/1	0.41	-	63,63,63,63	0
56	MG	AA	1953	1/1	0.17	-	87,87,87,87	0
56	MG	DA	3188	1/1	0.22	-	3,3,3,3	0
56	MG	BA	3244	1/1	0.41	-	31,31,31,31	0
56	MG	CA	1748	1/1	0.25	-	3,3,3,3	0
56	MG	BA	3727	1/1	0.24	-	44,44,44,44	0
56	MG	BA	3479	1/1	0.20	-	30,30,30,30	0
56	MG	BA	3362	1/1	0.67	-	68,68,68,68	0
56	MG	BA	3541	1/1	0.15	-	30,30,30,30	0
56	MG	DA	3348	1/1	0.13	-	60,60,60,60	0
56	MG	CA	1814	1/1	0.15	-	66,66,66,66	0
56	MG	BA	3053	1/1	0.25	-	78,78,78,78	0
56	MG	BQ	201	1/1	0.35	-	45,45,45,45	0
56	MG	BA	3918	1/1	0.47	-	63,63,63,63	0
56	MG	DD	5001	1/1	0.12	-	33,33,33,33	0
56	MG	BA	3805	1/1	0.17	-	40,40,40,40	0
56	MG	BA	3682	1/1	0.12	-	20,20,20,20	0
56	MG	BA	3553	1/1	0.10	-	12,12,12,12	0
56	MG	AY	112	1/1	0.18	-	38,38,38,38	0
56	MG	AA	1931	1/1	0.19	-	31,31,31,31	0
56	MG	DA	3474	1/1	0.20	-	3,3,3,3	0
56	MG	BA	3522	1/1	0.05	-	36,36,36,36	0
56	MG	AC	304	1/1	0.20	-	72,72,72,72	0
56	MG	CY	113	1/1	0.18	-	27,27,27,27	0
56	MG	AY	125	1/1	0.49	-	36,36,36,36	0
56	MG	BA	3744	1/1	0.07	-	72,72,72,72	0
56	MG	BA	3387	1/1	0.11	-	56,56,56,56	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	DA	3249	1/1	0.12	-	6,6,6,6	0
56	MG	BA	3653	1/1	0.51	-	61,61,61,61	0
56	MG	CA	1697	1/1	0.23	-	52,52,52,52	0
56	MG	BA	3677	1/1	0.15	-	30,30,30,30	0
56	MG	B8	104	1/1	0.31	-	49,49,49,49	0
56	MG	DA	3341	1/1	0.36	-	3,3,3,3	0
56	MG	DA	3490	1/1	0.27	-	3,3,3,3	0
56	MG	BA	3770	1/1	0.14	-	30,30,30,30	0
56	MG	DA	3208	1/1	0.26	-	4,4,4,4	0
56	MG	AA	1945	1/1	0.12	-	34,34,34,34	0
56	MG	DA	3429	1/1	0.39	-	3,3,3,3	0
56	MG	BA	3373	1/1	0.23	-	50,50,50,50	0
56	MG	DA	3317	1/1	0.41	-	43,43,43,43	0
56	MG	BQ	202	1/1	0.12	-	18,18,18,18	0
56	MG	BA	3121	1/1	0.08	-	61,61,61,61	0
56	MG	CA	1724	1/1	0.15	-	36,36,36,36	0
56	MG	DA	3010	1/1	0.21	-	3,3,3,3	0
56	MG	CA	1796	1/1	0.18	-	77,77,77,77	0
56	MG	BA	3324	1/1	0.21	-	50,50,50,50	0
56	MG	BA	3726	1/1	0.07	-	25,25,25,25	0
56	MG	BA	3497	1/1	0.17	-	68,68,68,68	0
56	MG	CA	1676	1/1	0.70	-	42,42,42,42	0
56	MG	BA	3316	1/1	0.08	-	35,35,35,35	0
56	MG	BA	3166	1/1	0.33	-	63,63,63,63	0
56	MG	DY	201	1/1	0.12	-	3,3,3,3	0
56	MG	AA	2004	1/1	0.49	-	51,51,51,51	0
56	MG	CA	1646	1/1	0.26	-	3,3,3,3	0
56	MG	BA	3641	1/1	0.27	-	63,63,63,63	0
56	MG	BA	3396	1/1	0.29	-	42,42,42,42	0
56	MG	DA	3290	1/1	0.38	-	64,64,64,64	0
56	MG	CA	1695	1/1	0.19	-	59,59,59,59	0
56	MG	BN	201	1/1	0.16	-	70,70,70,70	0
56	MG	BA	3437	1/1	0.58	-	117,117,117,117	0
56	MG	BA	3656	1/1	0.26	-	16,16,16,16	0
56	MG	BA	3445	1/1	0.19	-	63,63,63,63	0
56	MG	AA	2017	1/1	0.25	-	47,47,47,47	0
56	MG	AA	1980	1/1	0.10	-	38,38,38,38	0
56	MG	AA	1973	1/1	0.17	-	56,56,56,56	0
56	MG	BA	3259	1/1	0.10	-	44,44,44,44	0
56	MG	DA	3398	1/1	0.49	-	55,55,55,55	0
56	MG	BA	3685	1/1	0.17	-	54,54,54,54	0
56	MG	BA	3798	1/1	0.23	-	54,54,54,54	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	CA	1645	1/1	0.14	-	6,6,6,6	0
56	MG	BF	305	1/1	0.13	-	63,63,63,63	0
56	MG	DG	201	1/1	0.18	-	3,3,3,3	0
56	MG	BA	3705	1/1	0.23	-	42,42,42,42	0
56	MG	BA	3650	1/1	0.10	-	5,5,5,5	0
56	MG	BA	3016	1/1	0.08	-	50,50,50,50	0
56	MG	BD	5005	1/1	0.20	-	10,10,10,10	0
56	MG	DA	3172	1/1	0.23	-	3,3,3,3	0
56	MG	DA	3276	1/1	0.22	-	4,4,4,4	0
56	MG	DO	201	1/1	0.29	-	3,3,3,3	0
56	MG	AA	1659	1/1	0.18	-	49,49,49,49	0
56	MG	BA	3776	1/1	0.22	-	43,43,43,43	0
56	MG	BA	3915	1/1	0.24	-	41,41,41,41	0
56	MG	BA	3107	1/1	0.10	-	49,49,49,49	0
56	MG	DA	3325	1/1	0.32	-	3,3,3,3	0
56	MG	AA	1746	1/1	0.24	-	39,39,39,39	0
56	MG	AA	2020	1/1	0.12	-	74,74,74,74	0
56	MG	BA	3435	1/1	0.13	-	32,32,32,32	0
56	MG	AA	1965	1/1	0.31	-	54,54,54,54	0
56	MG	BA	3260	1/1	0.26	-	75,75,75,75	0
56	MG	AA	1825	1/1	0.28	-	31,31,31,31	0
56	MG	D1	102	1/1	0.27	-	53,53,53,53	0
56	MG	AA	1660	1/1	0.08	-	77,77,77,77	0
56	MG	BA	3736	1/1	0.27	-	26,26,26,26	0
56	MG	DA	3454	1/1	0.14	-	45,45,45,45	0
56	MG	BA	3069	1/1	0.20	-	65,65,65,65	0
56	MG	CA	1798	1/1	0.38	-	3,3,3,3	0
56	MG	BA	3399	1/1	0.11	-	73,73,73,73	0
56	MG	CF	204	1/1	0.32	-	3,3,3,3	0
56	MG	AA	1801	1/1	0.08	-	55,55,55,55	0
56	MG	AA	1647	1/1	0.29	-	64,64,64,64	0
56	MG	CA	1759	1/1	0.25	-	48,48,48,48	0
56	MG	DD	5009	1/1	0.29	-	29,29,29,29	0
56	MG	AA	1679	1/1	0.41	-	51,51,51,51	0
56	MG	BA	3455	1/1	0.10	-	26,26,26,26	0
56	MG	CA	1664	1/1	0.15	-	3,3,3,3	0
56	MG	BA	3120	1/1	0.32	-	53,53,53,53	0
56	MG	BA	3132	1/1	0.17	-	40,40,40,40	0
56	MG	BA	3510	1/1	0.22	-	61,61,61,61	0
56	MG	BA	3713	1/1	0.21	-	33,33,33,33	0
56	MG	BA	3015	1/1	0.30	-	60,60,60,60	0
56	MG	BA	3619	1/1	0.18	-	42,42,42,42	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	BA	3742	1/1	0.13	-	70,70,70,70	0
56	MG	CY	105	1/1	0.15	-	52,52,52,52	0
56	MG	AA	1809	1/1	0.23	-	90,90,90,90	0
56	MG	BA	3328	1/1	0.08	-	38,38,38,38	0
56	MG	BA	3084	1/1	0.55	-	62,62,62,62	0
56	MG	BA	3081	1/1	0.29	-	31,31,31,31	0
56	MG	BA	3138	1/1	0.17	-	27,27,27,27	0
56	MG	AY	118	1/1	0.12	-	83,83,83,83	0
56	MG	BA	3274	1/1	0.14	-	21,21,21,21	0
56	MG	BA	3224	1/1	0.07	-	32,32,32,32	0
56	MG	BA	3544	1/1	0.36	-	72,72,72,72	0
56	MG	DA	3028	1/1	0.23	-	4,4,4,4	0
56	MG	DA	3361	1/1	0.55	-	78,78,78,78	0
56	MG	DA	3380	1/1	0.26	-	64,64,64,64	0
56	MG	AA	1978	1/1	0.19	-	35,35,35,35	0
56	MG	BA	3589	1/1	0.09	-	29,29,29,29	0
56	MG	DA	3475	1/1	0.13	-	3,3,3,3	0
56	MG	CA	1609	1/1	0.27	-	3,3,3,3	0
56	MG	BB	201	1/1	0.29	-	59,59,59,59	0
56	MG	BA	3551	1/1	0.23	-	19,19,19,19	0
56	MG	DA	3377	1/1	0.11	-	43,43,43,43	0
56	MG	BA	3427	1/1	0.16	-	34,34,34,34	0
56	MG	BA	3198	1/1	0.50	-	76,76,76,76	0
56	MG	CA	1752	1/1	0.30	-	3,3,3,3	0
56	MG	BA	3826	1/1	0.12	-	28,28,28,28	0
56	MG	AA	1895	1/1	0.12	-	52,52,52,52	0
56	MG	AA	1673	1/1	0.11	-	64,64,64,64	0
56	MG	BA	3070	1/1	0.25	-	37,37,37,37	0
56	MG	CA	1667	1/1	0.16	-	58,58,58,58	0
56	MG	CA	1706	1/1	0.28	-	62,62,62,62	0
56	MG	AA	1709	1/1	0.17	-	54,54,54,54	0
56	MG	BA	3820	1/1	0.24	-	59,59,59,59	0
56	MG	BA	3904	1/1	0.46	-	53,53,53,53	0
56	MG	BA	3599	1/1	0.51	-	50,50,50,50	0
56	MG	DA	3425	1/1	0.15	-	5,5,5,5	0
56	MG	CA	1683	1/1	0.16	-	61,61,61,61	0
56	MG	BA	3348	1/1	0.18	-	37,37,37,37	0
56	MG	DA	3359	1/1	0.10	-	42,42,42,42	0
56	MG	CA	1620	1/1	0.17	-	4,4,4,4	0
56	MG	BA	3882	1/1	0.20	-	42,42,42,42	0
56	MG	DA	3073	1/1	0.14	-	6,6,6,6	0
56	MG	AA	1918	1/1	0.05	-	58,58,58,58	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	AA	1602	1/1	0.47	-	74,74,74,74	0
56	MG	BA	3885	1/1	0.13	-	67,67,67,67	0
56	MG	BA	3488	1/1	0.24	-	52,52,52,52	0
56	MG	AT	202	1/1	0.08	-	58,58,58,58	0
56	MG	AA	2001	1/1	0.15	-	29,29,29,29	0
56	MG	AA	1829	1/1	0.23	-	43,43,43,43	0
56	MG	BA	3897	1/1	0.22	-	48,48,48,48	0
56	MG	AX	408	1/1	0.10	-	57,57,57,57	0
56	MG	BA	3604	1/1	0.48	-	50,50,50,50	0
56	MG	DA	3369	1/1	0.14	-	43,43,43,43	0
56	MG	CA	1688	1/1	0.30	-	54,54,54,54	0
56	MG	BA	3409	1/1	0.12	-	58,58,58,58	0
56	MG	BA	3560	1/1	0.32	-	52,52,52,52	0
56	MG	AA	1616	1/1	0.27	-	47,47,47,47	0
56	MG	DA	3221	1/1	0.38	-	52,52,52,52	0
56	MG	BA	3511	1/1	0.10	-	43,43,43,43	0
56	MG	AA	1778	1/1	0.22	-	37,37,37,37	0
56	MG	AA	1614	1/1	0.37	-	49,49,49,49	0
56	MG	AA	1655	1/1	0.13	-	61,61,61,61	0
56	MG	DA	3422	1/1	0.18	-	2,2,2,2	0
56	MG	DA	3402	1/1	0.15	-	32,32,32,32	0
56	MG	AA	1874	1/1	0.20	-	44,44,44,44	0
56	MG	DA	3268	1/1	0.11	-	4,4,4,4	0
56	MG	BA	3027	1/1	0.47	-	86,86,86,86	0
56	MG	CA	1631	1/1	0.21	-	3,3,3,3	0
56	MG	AA	1802	1/1	0.15	-	39,39,39,39	0
56	MG	AA	1897	1/1	0.36	-	62,62,62,62	0
56	MG	AA	1818	1/1	0.58	-	74,74,74,74	0
56	MG	DB	208	1/1	0.14	-	3,3,3,3	0
56	MG	BA	3701	1/1	0.10	-	58,58,58,58	0
56	MG	DA	3023	1/1	0.23	-	3,3,3,3	0
56	MG	DA	3159	1/1	0.29	-	3,3,3,3	0
56	MG	BA	3082	1/1	0.26	-	56,56,56,56	0
56	MG	BA	3502	1/1	0.13	-	61,61,61,61	0
56	MG	CA	1606	1/1	0.32	-	3,3,3,3	0
56	MG	BA	3349	1/1	0.17	-	46,46,46,46	0
56	MG	BA	3683	1/1	0.34	-	63,63,63,63	0
56	MG	DA	3466	1/1	0.23	-	3,3,3,3	0
56	MG	DA	3471	1/1	0.19	-	4,4,4,4	0
56	MG	DD	5003	1/1	0.22	-	65,65,65,65	0
56	MG	AA	1745	1/1	0.05	-	75,75,75,75	0
56	MG	CA	1684	1/1	0.18	-	74,74,74,74	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	AA	1627	1/1	0.12	-	29,29,29,29	0
56	MG	BA	3004	1/1	0.12	-	27,27,27,27	0
56	MG	BH	203	1/1	0.09	-	56,56,56,56	0
56	MG	AZ	101	1/1	0.12	-	63,63,63,63	0
56	MG	DA	3088	1/1	0.15	-	4,4,4,4	0
56	MG	BA	3403	1/1	0.41	-	98,98,98,98	0
56	MG	BA	3343	1/1	0.71	-	70,70,70,70	0
56	MG	CA	1771	1/1	0.33	-	80,80,80,80	0
56	MG	AA	1981	1/1	0.14	-	52,52,52,52	0
56	MG	DA	3436	1/1	0.20	-	4,4,4,4	0
56	MG	BA	3248	1/1	0.31	-	43,43,43,43	0
56	MG	BA	3639	1/1	0.22	-	42,42,42,42	0
56	MG	DA	3055	1/1	0.26	-	3,3,3,3	0
56	MG	DA	3032	1/1	0.07	-	6,6,6,6	0
56	MG	BA	3256	1/1	0.43	-	60,60,60,60	0
56	MG	BA	3232	1/1	0.10	-	58,58,58,58	0
56	MG	DA	3428	1/1	0.38	-	3,3,3,3	0
56	MG	DA	3396	1/1	0.19	-	66,66,66,66	0
56	MG	BB	205	1/1	0.51	-	100,100,100,100	0
56	MG	AA	1924	1/1	0.24	-	58,58,58,58	0
56	MG	BA	3023	1/1	0.22	-	44,44,44,44	0
56	MG	BR	201	1/1	0.12	-	34,34,34,34	0
56	MG	AX	412	1/1	0.17	-	56,56,56,56	0
56	MG	BA	3602	1/1	0.28	-	43,43,43,43	0
56	MG	BA	3765	1/1	0.44	-	60,60,60,60	0
56	MG	DA	3349	1/1	0.17	-	29,29,29,29	0
56	MG	DA	3299	1/1	0.18	-	50,50,50,50	0
56	MG	BA	3297	1/1	0.24	-	45,45,45,45	0
56	MG	AA	1688	1/1	0.08	-	68,68,68,68	0
56	MG	BA	3472	1/1	0.13	-	10,10,10,10	0
56	MG	AJ	201	1/1	0.10	-	49,49,49,49	0
56	MG	BA	3336	1/1	0.10	-	45,45,45,45	0
56	MG	BA	3357	1/1	0.16	-	31,31,31,31	0
56	MG	DA	3133	1/1	0.14	-	19,19,19,19	0
56	MG	DA	3016	1/1	0.15	-	3,3,3,3	0
56	MG	CA	1708	1/1	0.17	-	36,36,36,36	0
56	MG	DA	3193	1/1	0.16	-	7,7,7,7	0
56	MG	BB	223	1/1	0.10	-	27,27,27,27	0
56	MG	AA	1613	1/1	0.23	-	45,45,45,45	0
56	MG	DA	3227	1/1	0.32	-	3,3,3,3	0
56	MG	AA	1619	1/1	0.54	-	62,62,62,62	0
56	MG	BA	3298	1/1	0.28	-	30,30,30,30	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	DA	3491	1/1	0.32	-	3,3,3,3	0
56	MG	AA	1835	1/1	0.23	-	37,37,37,37	0
56	MG	AA	2006	1/1	0.16	-	53,53,53,53	0
56	MG	DA	3002	1/1	0.32	-	3,3,3,3	0
56	MG	AA	1632	1/1	0.12	-	35,35,35,35	0
56	MG	CA	1756	1/1	0.21	-	3,3,3,3	0
56	MG	BA	3193	1/1	0.49	-	83,83,83,83	0
56	MG	DA	3203	1/1	0.30	-	15,15,15,15	0
56	MG	BA	3659	1/1	0.19	-	43,43,43,43	0
56	MG	B8	103	1/1	0.17	-	61,61,61,61	0
56	MG	BA	3543	1/1	0.24	-	38,38,38,38	0
56	MG	BB	235	1/1	0.12	-	59,59,59,59	0
56	MG	CA	1764	1/1	0.27	-	3,3,3,3	0
56	MG	AX	407	1/1	0.65	-	60,60,60,60	0
56	MG	AA	1628	1/1	0.19	-	51,51,51,51	0
56	MG	AA	1670	1/1	0.21	-	67,67,67,67	0
56	MG	BA	3470	1/1	0.35	-	77,77,77,77	0
56	MG	BA	3167	1/1	0.40	-	22,22,22,22	0
56	MG	DA	3260	1/1	0.36	-	3,3,3,3	0
56	MG	BA	3572	1/1	0.16	-	34,34,34,34	0
56	MG	CA	1647	1/1	0.20	-	3,3,3,3	0
56	MG	BA	3284	1/1	0.18	-	15,15,15,15	0
56	MG	AA	1621	1/1	0.14	-	25,25,25,25	0
56	MG	DA	3224	1/1	0.13	-	5,5,5,5	0
56	MG	DA	3337	1/1	0.16	-	4,4,4,4	0
56	MG	BA	3457	1/1	0.28	-	11,11,11,11	0
56	MG	CA	1807	1/1	0.35	-	3,3,3,3	0
56	MG	BD	5007	1/1	0.23	-	55,55,55,55	0
56	MG	BA	3819	1/1	0.43	-	34,34,34,34	0
56	MG	AB	303	1/1	0.12	-	40,40,40,40	0
56	MG	AA	1992	1/1	0.18	-	77,77,77,77	0
56	MG	BQ	205	1/1	0.29	-	57,57,57,57	0
56	MG	BA	3350	1/1	0.24	-	31,31,31,31	0
56	MG	CA	1654	1/1	0.21	-	28,28,28,28	0
56	MG	CA	1601	1/1	0.26	-	3,3,3,3	0
56	MG	CA	1634	1/1	0.11	-	6,6,6,6	0
56	MG	BA	3059	1/1	0.10	-	74,74,74,74	0
56	MG	BA	3582	1/1	0.05	-	55,55,55,55	0
56	MG	DA	3482	1/1	0.20	-	4,4,4,4	0
56	MG	AA	1892	1/1	0.25	-	30,30,30,30	0
56	MG	AA	1642	1/1	0.15	-	57,57,57,57	0
56	MG	DA	3206	1/1	0.15	-	5,5,5,5	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	DA	3147	1/1	0.32	-	3,3,3,3	0
56	MG	BA	3155	1/1	0.37	-	46,46,46,46	0
56	MG	DA	3312	1/1	0.14	-	46,46,46,46	0
56	MG	BA	3635	1/1	0.07	-	37,37,37,37	0
56	MG	BA	3890	1/1	0.17	-	25,25,25,25	0
56	MG	CZ	106	1/1	0.21	-	82,82,82,82	0
56	MG	DA	3320	1/1	0.59	-	82,82,82,82	0
56	MG	BA	3322	1/1	0.18	-	40,40,40,40	0
56	MG	BA	3434	1/1	0.23	-	68,68,68,68	0
56	MG	CA	1743	1/1	0.09	-	52,52,52,52	0
56	MG	DA	3218	1/1	0.13	-	4,4,4,4	0
56	MG	CA	1789	1/1	0.34	-	43,43,43,43	0
56	MG	AX	404	1/1	0.45	-	92,92,92,92	0
56	MG	AZ	111	1/1	0.20	-	71,71,71,71	0
56	MG	CA	1773	1/1	0.13	-	66,66,66,66	0
56	MG	BU	201	1/1	0.33	-	83,83,83,83	0
56	MG	AA	1798	1/1	0.13	-	25,25,25,25	0
56	MG	CA	1626	1/1	0.50	-	3,3,3,3	0
56	MG	BA	3480	1/1	0.21	-	43,43,43,43	0
56	MG	DA	3211	1/1	0.23	-	4,4,4,4	0
56	MG	CY	101	1/1	0.25	-	3,3,3,3	0
56	MG	DA	3444	1/1	0.35	-	3,3,3,3	0
56	MG	DA	3266	1/1	0.25	-	3,3,3,3	0
56	MG	DA	3433	1/1	0.24	-	3,3,3,3	0
56	MG	BA	3824	1/1	0.15	-	17,17,17,17	0
56	MG	BA	3251	1/1	0.11	-	41,41,41,41	0
56	MG	BA	3441	1/1	0.55	-	70,70,70,70	0
56	MG	DA	3427	1/1	0.54	-	3,3,3,3	0
56	MG	AK	201	1/1	0.53	-	76,76,76,76	0
56	MG	DA	3286	1/1	0.22	-	33,33,33,33	0
56	MG	AA	1810	1/1	0.51	-	64,64,64,64	0
56	MG	BA	3253	1/1	0.35	-	71,71,71,71	0
56	MG	BA	3595	1/1	0.21	-	62,62,62,62	0
56	MG	BA	3339	1/1	0.36	-	66,66,66,66	0
56	MG	BA	3412	1/1	0.18	-	64,64,64,64	0
56	MG	DT	201	1/1	0.31	-	3,3,3,3	0
56	MG	AY	103	1/1	0.09	-	87,87,87,87	0
56	MG	AA	1933	1/1	0.14	-	75,75,75,75	0
56	MG	AD	5003	1/1	0.07	-	42,42,42,42	0
56	MG	BA	3563	1/1	0.13	-	57,57,57,57	0
56	MG	AA	1956	1/1	0.25	-	58,58,58,58	0
56	MG	BA	3201	1/1	0.23	-	67,67,67,67	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	BA	3178	1/1	0.20	-	51,51,51,51	0
56	MG	DA	3363	1/1	0.36	-	3,3,3,3	0
56	MG	CA	1741	1/1	0.27	-	50,50,50,50	0
56	MG	BA	3308	1/1	0.12	-	8,8,8,8	0
56	MG	AA	1645	1/1	0.21	-	42,42,42,42	0
56	MG	CA	1746	1/1	0.16	-	57,57,57,57	0
56	MG	AA	1724	1/1	0.09	-	35,35,35,35	0
56	MG	BA	3040	1/1	0.30	-	97,97,97,97	0
56	MG	BA	3140	1/1	0.22	-	33,33,33,33	0
56	MG	DA	3066	1/1	0.18	-	43,43,43,43	0
56	MG	DA	3014	1/1	0.33	-	3,3,3,3	0
56	MG	DA	3072	1/1	0.17	-	3,3,3,3	0
56	MG	AZ	107	1/1	0.08	-	78,78,78,78	0
56	MG	DA	3046	1/1	0.22	-	4,4,4,4	0
56	MG	DA	3196	1/1	0.26	-	4,4,4,4	0
56	MG	CY	106	1/1	0.30	-	66,66,66,66	0
56	MG	BA	3418	1/1	0.63	-	54,54,54,54	0
56	MG	AA	1942	1/1	0.16	-	34,34,34,34	0
56	MG	BA	3504	1/1	0.09	-	34,34,34,34	0
56	MG	B6	101	1/1	0.11	-	44,44,44,44	0
56	MG	BA	3816	1/1	0.18	-	38,38,38,38	0
56	MG	BA	3487	1/1	0.18	-	26,26,26,26	0
56	MG	AO	102	1/1	0.25	-	48,48,48,48	0
56	MG	BA	3700	1/1	0.14	-	72,72,72,72	0
56	MG	DA	3102	1/1	0.33	-	74,74,74,74	0
56	MG	CA	1727	1/1	0.11	-	53,53,53,53	0
56	MG	CA	1793	1/1	0.43	-	3,3,3,3	0
56	MG	AY	121	1/1	0.13	-	41,41,41,41	0
56	MG	CA	1675	1/1	0.30	-	65,65,65,65	0
56	MG	CA	1713	1/1	0.60	-	80,80,80,80	0
56	MG	CA	1610	1/1	0.18	-	4,4,4,4	0
56	MG	BA	3314	1/1	0.23	-	22,22,22,22	0
56	MG	CA	1619	1/1	0.24	-	4,4,4,4	0
56	MG	DA	3389	1/1	0.16	-	70,70,70,70	0
56	MG	BA	3035	1/1	0.32	-	51,51,51,51	0
56	MG	AA	1786	1/1	0.18	-	61,61,61,61	0
56	MG	BA	3162	1/1	0.29	-	58,58,58,58	0
56	MG	CY	114	1/1	0.34	-	39,39,39,39	0
56	MG	BA	3337	1/1	0.22	-	69,69,69,69	0
56	MG	BA	3500	1/1	0.10	-	21,21,21,21	0
56	MG	BA	3767	1/1	0.16	-	31,31,31,31	0
56	MG	AA	1643	1/1	0.34	-	50,50,50,50	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	BA	3719	1/1	0.23	-	37,37,37,37	0
56	MG	AB	305	1/1	0.18	-	56,56,56,56	0
56	MG	DA	3406	1/1	0.14	-	5,5,5,5	0
56	MG	DA	3265	1/1	0.19	-	3,3,3,3	0
56	MG	BA	3689	1/1	0.24	-	80,80,80,80	0
56	MG	CA	1628	1/1	0.19	-	4,4,4,4	0
56	MG	AA	1623	1/1	0.42	-	74,74,74,74	0
56	MG	DA	3163	1/1	0.22	-	3,3,3,3	0
56	MG	BA	3512	1/1	0.09	-	62,62,62,62	0
56	MG	BA	3252	1/1	0.11	-	80,80,80,80	0
56	MG	BA	3229	1/1	0.21	-	47,47,47,47	0
56	MG	BA	3892	1/1	0.17	-	46,46,46,46	0
56	MG	AA	1719	1/1	0.12	-	13,13,13,13	0
56	MG	AA	1750	1/1	0.14	-	97,97,97,97	0
56	MG	DA	3397	1/1	0.26	-	24,24,24,24	0
56	MG	DA	3004	1/1	0.40	-	3,3,3,3	0
56	MG	DA	3421	1/1	0.10	-	35,35,35,35	0
56	MG	BA	3507	1/1	0.20	-	82,82,82,82	0
56	MG	BF	304	1/1	0.31	-	65,65,65,65	0
56	MG	DD	5005	1/1	0.48	-	51,51,51,51	0
56	MG	AA	1890	1/1	0.17	-	21,21,21,21	0
56	MG	DA	3295	1/1	0.20	-	33,33,33,33	0
56	MG	BA	3039	1/1	0.46	-	67,67,67,67	0
56	MG	CA	1787	1/1	0.11	-	57,57,57,57	0
56	MG	BA	3128	1/1	0.24	-	60,60,60,60	0
56	MG	AA	1713	1/1	0.28	-	39,39,39,39	0
56	MG	AA	1658	1/1	0.15	-	29,29,29,29	0
56	MG	DA	3449	1/1	0.18	-	53,53,53,53	0
56	MG	BA	3678	1/1	0.41	-	37,37,37,37	0
56	MG	BA	3126	1/1	0.10	-	46,46,46,46	0
56	MG	DA	3414	1/1	0.12	-	5,5,5,5	0
56	MG	DA	3099	1/1	0.26	-	3,3,3,3	0
56	MG	CA	1704	1/1	0.35	-	63,63,63,63	0
56	MG	DA	3217	1/1	0.09	-	58,58,58,58	0
56	MG	CA	1652	1/1	0.62	-	44,44,44,44	0
56	MG	DA	3452	1/1	0.25	-	38,38,38,38	0
56	MG	AA	1639	1/1	0.23	-	59,59,59,59	0
56	MG	BA	3477	1/1	0.13	-	53,53,53,53	0
56	MG	CA	1802	1/1	0.27	-	3,3,3,3	0
56	MG	AA	1706	1/1	0.11	-	36,36,36,36	0
56	MG	CA	1806	1/1	0.29	-	3,3,3,3	0
56	MG	BA	3426	1/1	0.28	-	20,20,20,20	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	AA	1737	1/1	0.27	-	36,36,36,36	0
56	MG	BA	3311	1/1	0.25	-	44,44,44,44	0
56	MG	BA	3018	1/1	0.20	-	40,40,40,40	0
56	MG	CA	1725	1/1	0.05	-	54,54,54,54	0
56	MG	AA	1609	1/1	0.16	-	58,58,58,58	0
56	MG	DA	3210	1/1	0.34	-	3,3,3,3	0
56	MG	CY	112	1/1	0.25	-	3,3,3,3	0
56	MG	BA	3026	1/1	0.16	-	33,33,33,33	0
56	MG	DA	3353	1/1	0.06	-	61,61,61,61	0
56	MG	B1	107	1/1	0.12	-	56,56,56,56	0
56	MG	BA	3814	1/1	0.49	-	47,47,47,47	0
56	MG	AA	1663	1/1	0.12	-	33,33,33,33	0
56	MG	DA	3281	1/1	0.32	-	63,63,63,63	0
56	MG	CK	201	1/1	0.25	-	70,70,70,70	0
56	MG	AA	2012	1/1	0.30	-	55,55,55,55	0
56	MG	DD	5007	1/1	0.29	-	11,11,11,11	0
56	MG	BA	3643	1/1	0.37	-	68,68,68,68	0
56	MG	BA	3024	1/1	0.32	-	87,87,87,87	0
56	MG	CA	1672	1/1	0.34	-	3,3,3,3	0
56	MG	BA	3526	1/1	0.21	-	49,49,49,49	0
56	MG	DR	201	1/1	0.27	-	3,3,3,3	0
56	MG	AA	1824	1/1	0.55	-	34,34,34,34	0
56	MG	AA	1665	1/1	0.10	-	38,38,38,38	0
56	MG	AA	1618	1/1	0.15	-	50,50,50,50	0
56	MG	DA	3309	1/1	0.18	-	4,4,4,4	0
56	MG	BA	3830	1/1	0.13	-	12,12,12,12	0
56	MG	DA	3118	1/1	0.29	-	6,6,6,6	0
56	MG	BA	3666	1/1	0.13	-	46,46,46,46	0
56	MG	AA	1949	1/1	0.17	-	90,90,90,90	0
56	MG	DA	3345	1/1	0.59	-	3,3,3,3	0
56	MG	BA	3378	1/1	0.10	-	32,32,32,32	0
56	MG	BA	3447	1/1	0.26	-	31,31,31,31	0
57	ZN	AN	101	1/1	0.11	-	82,82,82,82	0
56	MG	BW	202	1/1	0.18	-	38,38,38,38	0
56	MG	DA	3385	1/1	0.20	-	51,51,51,51	0
56	MG	BA	3037	1/1	0.23	-	61,61,61,61	0
56	MG	AA	1972	1/1	0.14	-	43,43,43,43	0
56	MG	BA	3125	1/1	0.07	-	26,26,26,26	0
56	MG	BA	3657	1/1	0.53	-	56,56,56,56	0
56	MG	BA	3686	1/1	0.35	-	49,49,49,49	0
56	MG	DA	3092	1/1	0.24	-	4,4,4,4	0
56	MG	BA	3471	1/1	0.41	-	50,50,50,50	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	DA	3087	1/1	0.30	-	3,3,3,3	0
56	MG	AR	101	1/1	0.08	-	32,32,32,32	0
56	MG	AA	1987	1/1	0.08	-	40,40,40,40	0
56	MG	DA	3382	1/1	0.06	-	42,42,42,42	0
56	MG	BA	3621	1/1	0.15	-	50,50,50,50	0
56	MG	AA	1939	1/1	0.45	-	47,47,47,47	0
56	MG	BA	3263	1/1	0.57	-	47,47,47,47	0
56	MG	AA	1635	1/1	0.12	-	52,52,52,52	0
56	MG	BA	3687	1/1	0.22	-	59,59,59,59	0
56	MG	DA	3005	1/1	0.16	-	3,3,3,3	0
56	MG	BA	3714	1/1	0.30	-	60,60,60,60	0
56	MG	AA	1795	1/1	0.19	-	64,64,64,64	0
56	MG	BB	218	1/1	0.13	-	78,78,78,78	0
56	MG	BA	3762	1/1	0.17	-	28,28,28,28	0
56	MG	BA	3170	1/1	0.35	-	80,80,80,80	0
56	MG	AA	1738	1/1	0.21	-	47,47,47,47	0
56	MG	CA	1670	1/1	0.25	-	43,43,43,43	0
56	MG	CZ	108	1/1	0.18	-	69,69,69,69	0
56	MG	AA	1714	1/1	0.13	-	79,79,79,79	0
56	MG	AA	1727	1/1	0.36	-	59,59,59,59	0
56	MG	BA	3019	1/1	0.16	-	55,55,55,55	0
56	MG	DA	3293	1/1	0.34	-	61,61,61,61	0
56	MG	BA	3625	1/1	0.20	-	43,43,43,43	0
56	MG	DA	3394	1/1	0.25	-	53,53,53,53	0
56	MG	BA	3913	1/1	0.16	-	45,45,45,45	0
56	MG	DA	3124	1/1	0.13	-	14,14,14,14	0
56	MG	AA	1894	1/1	0.18	-	35,35,35,35	0
56	MG	AB	306	1/1	0.25	-	56,56,56,56	0
56	MG	CZ	105	1/1	0.05	-	74,74,74,74	0
56	MG	BA	3883	1/1	0.15	-	67,67,67,67	0
56	MG	BA	3282	1/1	0.13	-	34,34,34,34	0
56	MG	BA	3877	1/1	0.28	-	76,76,76,76	0
56	MG	AA	1781	1/1	0.24	-	28,28,28,28	0
56	MG	CA	1792	1/1	0.44	-	3,3,3,3	0
56	MG	DA	3430	1/1	0.15	-	6,6,6,6	0
56	MG	DA	3262	1/1	0.32	-	3,3,3,3	0
56	MG	DA	3478	1/1	0.36	-	3,3,3,3	0
56	MG	BX	101	1/1	0.13	-	67,67,67,67	0
56	MG	BA	3916	1/1	0.24	-	59,59,59,59	0
56	MG	DA	3292	1/1	0.25	-	74,74,74,74	0
56	MG	BA	3327	1/1	0.26	-	64,64,64,64	0
56	MG	BA	3587	1/1	0.13	-	40,40,40,40	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	CA	1644	1/1	0.28	-	3,3,3,3	0
56	MG	AA	1702	1/1	0.40	-	48,48,48,48	0
56	MG	CY	110	1/1	0.13	-	90,90,90,90	0
56	MG	AA	1782	1/1	0.33	-	24,24,24,24	0
56	MG	CA	1720	1/1	0.11	-	27,27,27,27	0
56	MG	DA	3162	1/1	0.22	-	3,3,3,3	0
56	MG	AA	1768	1/1	0.36	-	37,37,37,37	0
56	MG	AA	1865	1/1	0.13	-	73,73,73,73	0
56	MG	CC	301	1/1	0.33	-	3,3,3,3	0
56	MG	AA	1615	1/1	0.08	-	4,4,4,4	0
56	MG	AA	1929	1/1	0.20	-	71,71,71,71	0
56	MG	AA	1836	1/1	0.35	-	53,53,53,53	0
56	MG	AA	1867	1/1	0.20	-	51,51,51,51	0
56	MG	DB	206	1/1	0.13	-	4,4,4,4	0
56	MG	BA	3684	1/1	0.20	-	50,50,50,50	0
56	MG	DA	3176	1/1	0.27	-	4,4,4,4	0
56	MG	AA	1996	1/1	0.24	-	56,56,56,56	0
56	MG	BA	3637	1/1	0.40	-	61,61,61,61	0
56	MG	AA	1662	1/1	0.25	-	45,45,45,45	0
56	MG	BA	3640	1/1	0.12	-	24,24,24,24	0
56	MG	DA	3316	1/1	0.13	-	4,4,4,4	0
56	MG	BA	3672	1/1	0.06	-	18,18,18,18	0
56	MG	DA	3294	1/1	0.65	-	63,63,63,63	0
56	MG	DA	3330	1/1	0.22	-	5,5,5,5	0
56	MG	BA	3571	1/1	0.19	-	39,39,39,39	0
56	MG	BE	304	1/1	0.12	-	79,79,79,79	0
56	MG	BA	3879	1/1	0.35	-	46,46,46,46	0
56	MG	CA	1641	1/1	0.27	-	3,3,3,3	0
56	MG	DA	3347	1/1	0.10	-	35,35,35,35	0
56	MG	DA	3212	1/1	0.12	-	5,5,5,5	0
56	MG	BA	3374	1/1	0.37	-	85,85,85,85	0
56	MG	BA	3363	1/1	0.23	-	42,42,42,42	0
56	MG	CA	1621	1/1	0.29	-	3,3,3,3	0
56	MG	AA	1979	1/1	0.29	-	58,58,58,58	0
56	MG	BT	201	1/1	0.49	-	81,81,81,81	0
56	MG	AA	1812	1/1	0.23	-	65,65,65,65	0
56	MG	AA	1982	1/1	0.35	-	51,51,51,51	0
56	MG	BA	3841	1/1	0.15	-	31,31,31,31	0
56	MG	AA	1821	1/1	0.29	-	90,90,90,90	0
56	MG	BA	3089	1/1	0.34	-	69,69,69,69	0
56	MG	AA	1742	1/1	0.11	-	67,67,67,67	0
56	MG	AZ	102	1/1	0.13	-	71,71,71,71	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	CA	1690	1/1	0.17	-	54,54,54,54	0
56	MG	CA	1671	1/1	0.15	-	63,63,63,63	0
56	MG	BA	3758	1/1	0.54	-	94,94,94,94	0
56	MG	BA	3627	1/1	0.15	-	22,22,22,22	0
56	MG	DD	5006	1/1	0.19	-	47,47,47,47	0
56	MG	BA	3315	1/1	0.18	-	28,28,28,28	0
56	MG	AA	1784	1/1	0.33	-	25,25,25,25	0
56	MG	DA	3362	1/1	0.16	-	82,82,82,82	0
56	MG	CA	1699	1/1	0.16	-	8,8,8,8	0
56	MG	CA	1635	1/1	0.16	-	4,4,4,4	0
56	MG	BA	3051	1/1	0.09	-	44,44,44,44	0
56	MG	BA	3661	1/1	0.44	-	71,71,71,71	0
56	MG	DA	3365	1/1	0.20	-	3,3,3,3	0
56	MG	BA	3654	1/1	0.18	-	12,12,12,12	0
56	MG	BA	3134	1/1	0.18	-	23,23,23,23	0
56	MG	AA	1751	1/1	0.27	-	61,61,61,61	0
56	MG	AA	1843	1/1	0.10	-	41,41,41,41	0
56	MG	DA	3153	1/1	0.22	-	5,5,5,5	0
56	MG	AA	1872	1/1	0.18	-	59,59,59,59	0
56	MG	CA	1735	1/1	0.22	-	31,31,31,31	0
56	MG	BA	3537	1/1	0.13	-	38,38,38,38	0
56	MG	BA	3630	1/1	0.15	-	47,47,47,47	0
56	MG	BA	3748	1/1	0.20	-	35,35,35,35	0
56	MG	DA	3145	1/1	0.18	-	4,4,4,4	0
56	MG	BA	3034	1/1	0.14	-	43,43,43,43	0
56	MG	BA	3215	1/1	0.14	-	27,27,27,27	0
56	MG	BA	3823	1/1	0.20	-	14,14,14,14	0
56	MG	CA	1666	1/1	0.22	-	3,3,3,3	0
56	MG	BA	3190	1/1	0.41	-	77,77,77,77	0
56	MG	AE	205	1/1	0.13	-	65,65,65,65	0
56	MG	DA	3108	1/1	0.36	-	59,59,59,59	0
56	MG	BA	3292	1/1	0.87	-	36,36,36,36	0
56	MG	AA	1951	1/1	0.26	-	59,59,59,59	0
56	MG	BA	3221	1/1	0.50	-	33,33,33,33	0
56	MG	CA	1722	1/1	0.21	-	49,49,49,49	0
56	MG	BB	222	1/1	0.19	-	39,39,39,39	0
56	MG	AA	1696	1/1	0.26	-	59,59,59,59	0
56	MG	CA	1691	1/1	0.17	-	45,45,45,45	0
56	MG	AY	115	1/1	0.15	-	65,65,65,65	0
56	MG	BB	208	1/1	0.14	-	63,63,63,63	0
56	MG	DA	3026	1/1	0.30	-	3,3,3,3	0
56	MG	BV	202	1/1	0.70	-	38,38,38,38	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	AA	1819	1/1	0.17	-	76,76,76,76	0
56	MG	AF	202	1/1	0.11	-	41,41,41,41	0
56	MG	BA	3886	1/1	0.16	-	69,69,69,69	0
56	MG	BA	3181	1/1	0.24	-	23,23,23,23	0
56	MG	AA	1794	1/1	0.15	-	19,19,19,19	0
56	MG	DA	3271	1/1	0.23	-	3,3,3,3	0
56	MG	BA	3529	1/1	0.34	-	64,64,64,64	0
56	MG	AA	1823	1/1	0.25	-	47,47,47,47	0
56	MG	BA	3119	1/1	0.26	-	54,54,54,54	0
56	MG	DA	3226	1/1	0.11	-	4,4,4,4	0
56	MG	BB	215	1/1	0.10	-	103,103,103,103	0
56	MG	DF	301	1/1	0.40	-	3,3,3,3	0
56	MG	DA	3460	1/1	0.07	-	6,6,6,6	0
56	MG	BA	3681	1/1	0.78	-	59,59,59,59	0
56	MG	AA	1986	1/1	0.28	-	52,52,52,52	0
56	MG	BB	230	1/1	0.41	-	50,50,50,50	0
56	MG	AE	208	1/1	0.12	-	42,42,42,42	0
56	MG	DA	3443	1/1	0.27	-	3,3,3,3	0
56	MG	BA	3554	1/1	0.26	-	7,7,7,7	0
56	MG	BP	201	1/1	0.41	-	68,68,68,68	0
56	MG	AA	2003	1/1	0.16	-	54,54,54,54	0
56	MG	CA	1622	1/1	0.23	-	3,3,3,3	0
56	MG	DA	3077	1/1	0.11	-	5,5,5,5	0
56	MG	AB	301	1/1	0.12	-	62,62,62,62	0
56	MG	AA	1716	1/1	0.11	-	24,24,24,24	0
56	MG	CA	1623	1/1	0.37	-	4,4,4,4	0
56	MG	AA	1700	1/1	0.25	-	45,45,45,45	0
56	MG	DA	3463	1/1	0.12	-	4,4,4,4	0
56	MG	AA	1661	1/1	0.14	-	66,66,66,66	0
56	MG	DA	3029	1/1	0.18	-	4,4,4,4	0
56	MG	BA	3058	1/1	0.08	-	67,67,67,67	0
56	MG	BA	3596	1/1	0.15	-	13,13,13,13	0
56	MG	DA	3119	1/1	0.19	-	58,58,58,58	0
56	MG	BA	3153	1/1	0.32	-	41,41,41,41	0
56	MG	CA	1745	1/1	0.21	-	36,36,36,36	0
56	MG	BE	303	1/1	0.09	-	53,53,53,53	0
56	MG	DA	3310	1/1	0.21	-	57,57,57,57	0
56	MG	AX	406	1/1	0.21	-	48,48,48,48	0
56	MG	BA	3721	1/1	0.36	-	34,34,34,34	0
56	MG	BA	3527	1/1	0.15	-	38,38,38,38	0
56	MG	BA	3096	1/1	0.08	-	60,60,60,60	0
56	MG	BA	3218	1/1	0.39	-	25,25,25,25	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	DA	3183	1/1	0.21	-	3,3,3,3	0
56	MG	BA	3895	1/1	0.25	-	51,51,51,51	0
56	MG	DA	3319	1/1	0.18	-	43,43,43,43	0
56	MG	AA	1868	1/1	0.22	-	38,38,38,38	0
56	MG	BA	3585	1/1	0.17	-	35,35,35,35	0
56	MG	DA	3255	1/1	0.18	-	12,12,12,12	0
56	MG	BA	3276	1/1	0.33	-	52,52,52,52	0
56	MG	BI	206	1/1	0.18	-	67,67,67,67	0
56	MG	CF	205	1/1	0.15	-	57,57,57,57	0
56	MG	BA	3662	1/1	0.36	-	35,35,35,35	0
56	MG	BA	3505	1/1	0.14	-	92,92,92,92	0
56	MG	BA	3301	1/1	0.19	-	31,31,31,31	0
56	MG	AA	1983	1/1	0.48	-	67,67,67,67	0
56	MG	BA	3095	1/1	0.17	-	40,40,40,40	0
56	MG	BA	3546	1/1	0.18	-	40,40,40,40	0
56	MG	BA	3212	1/1	0.08	-	29,29,29,29	0
56	MG	CA	1642	1/1	0.50	-	3,3,3,3	0
56	MG	BA	3652	1/1	0.20	-	28,28,28,28	0
56	MG	DA	3243	1/1	0.18	-	4,4,4,4	0
56	MG	DA	3400	1/1	0.14	-	52,52,52,52	0
56	MG	BA	3577	1/1	0.15	-	60,60,60,60	0
56	MG	AA	1667	1/1	0.27	-	70,70,70,70	0
56	MG	BA	3310	1/1	0.65	-	73,73,73,73	0
56	MG	DA	3201	1/1	0.12	-	6,6,6,6	0
56	MG	DA	3075	1/1	0.12	-	4,4,4,4	0
56	MG	CA	1673	1/1	0.17	-	49,49,49,49	0
56	MG	AY	117	1/1	0.16	-	68,68,68,68	0
56	MG	BA	3289	1/1	0.15	-	31,31,31,31	0
56	MG	BA	3532	1/1	0.26	-	55,55,55,55	0
56	MG	AA	1930	1/1	0.05	-	59,59,59,59	0
56	MG	BA	3462	1/1	0.14	-	35,35,35,35	0
56	MG	BA	3306	1/1	0.46	-	52,52,52,52	0
56	MG	BA	3397	1/1	0.13	-	52,52,52,52	0
56	MG	BA	3741	1/1	0.11	-	52,52,52,52	0
56	MG	AZ	105	1/1	0.08	-	78,78,78,78	0
56	MG	AA	1808	1/1	0.14	-	46,46,46,46	0
56	MG	BA	3242	1/1	0.20	-	23,23,23,23	0
56	MG	DA	3126	1/1	0.65	-	66,66,66,66	0
56	MG	AA	1963	1/1	0.18	-	56,56,56,56	0
56	MG	AA	1799	1/1	0.10	-	31,31,31,31	0
56	MG	BA	3241	1/1	0.27	-	48,48,48,48	0
56	MG	AY	124	1/1	0.37	-	51,51,51,51	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	BA	3290	1/1	0.15	-	15,15,15,15	0
56	MG	BA	3605	1/1	0.26	-	12,12,12,12	0
56	MG	AA	1648	1/1	0.31	-	87,87,87,87	0
56	MG	BA	3405	1/1	0.21	-	44,44,44,44	0
56	MG	DA	3151	1/1	0.17	-	4,4,4,4	0
56	MG	BA	3833	1/1	0.22	-	9,9,9,9	0
56	MG	BA	3871	1/1	0.76	-	65,65,65,65	0
56	MG	AE	203	1/1	0.35	-	72,72,72,72	0
56	MG	BA	3847	1/1	0.40	-	62,62,62,62	0
56	MG	BA	3439	1/1	0.20	-	18,18,18,18	0
56	MG	BB	227	1/1	0.34	-	54,54,54,54	0
56	MG	BA	3171	1/1	0.38	-	77,77,77,77	0
56	MG	DA	3302	1/1	0.13	-	44,44,44,44	0
56	MG	BA	3708	1/1	0.17	-	28,28,28,28	0
56	MG	DA	3006	1/1	0.31	-	3,3,3,3	0
56	MG	AH	201	1/1	0.16	-	27,27,27,27	0
56	MG	BA	3258	1/1	0.20	-	50,50,50,50	0
56	MG	AA	1852	1/1	0.16	-	18,18,18,18	0
56	MG	AA	1610	1/1	0.19	-	65,65,65,65	0
56	MG	AZ	108	1/1	0.06	-	60,60,60,60	0
56	MG	AA	1889	1/1	0.56	-	30,30,30,30	0
56	MG	CA	1643	1/1	0.17	-	3,3,3,3	0
56	MG	BA	3104	1/1	0.12	-	67,67,67,67	0
56	MG	AD	5004	1/1	0.26	-	48,48,48,48	0
56	MG	CZ	107	1/1	0.21	-	57,57,57,57	0
56	MG	CA	1774	1/1	0.42	-	82,82,82,82	0
56	MG	BA	3715	1/1	0.17	-	28,28,28,28	0
56	MG	DA	3228	1/1	0.11	-	4,4,4,4	0
56	MG	DA	3284	1/1	0.07	-	8,8,8,8	0
56	MG	AA	1998	1/1	0.20	-	57,57,57,57	0
56	MG	BA	3567	1/1	0.20	-	23,23,23,23	0
56	MG	CA	1737	1/1	0.12	-	35,35,35,35	0
56	MG	CA	1732	1/1	0.30	-	63,63,63,63	0
56	MG	AA	1858	1/1	0.11	-	72,72,72,72	0
56	MG	BB	225	1/1	0.20	-	48,48,48,48	0
56	MG	CZ	112	1/1	0.17	-	63,63,63,63	0
56	MG	DA	3084	1/1	0.30	-	3,3,3,3	0
56	MG	AA	1909	1/1	0.16	-	55,55,55,55	0
56	MG	DA	3300	1/1	0.34	-	78,78,78,78	0
56	MG	BA	3002	1/1	0.28	-	47,47,47,47	0
56	MG	BA	3531	1/1	0.15	-	12,12,12,12	0
56	MG	BA	3164	1/1	0.72	-	35,35,35,35	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	AA	1780	1/1	0.16	-	24,24,24,24	0
56	MG	BA	3191	1/1	0.06	-	26,26,26,26	0
56	MG	DA	3352	1/1	0.30	-	3,3,3,3	0
56	MG	BA	3629	1/1	0.21	-	50,50,50,50	0
56	MG	BA	3730	1/1	0.52	-	86,86,86,86	0
56	MG	AA	1758	1/1	0.22	-	22,22,22,22	0
56	MG	AA	1975	1/1	0.32	-	66,66,66,66	0
56	MG	BA	3032	1/1	0.10	-	30,30,30,30	0
56	MG	BA	3465	1/1	0.27	-	59,59,59,59	0
56	MG	DA	3455	1/1	0.15	-	27,27,27,27	0
56	MG	AA	1722	1/1	0.08	-	34,34,34,34	0
56	MG	BA	3613	1/1	0.09	-	32,32,32,32	0
56	MG	BG	202	1/1	0.14	-	63,63,63,63	0
56	MG	BA	3481	1/1	0.72	-	65,65,65,65	0
56	MG	BA	3072	1/1	0.32	-	61,61,61,61	0
56	MG	BY	202	1/1	0.20	-	42,42,42,42	0
56	MG	BA	3432	1/1	0.12	-	52,52,52,52	0
56	MG	DA	3112	1/1	0.13	-	26,26,26,26	0
56	MG	DD	5004	1/1	0.14	-	42,42,42,42	0
56	MG	CA	1629	1/1	0.17	-	4,4,4,4	0
56	MG	AA	1922	1/1	0.43	-	46,46,46,46	0
56	MG	DA	3388	1/1	0.12	-	19,19,19,19	0
56	MG	BA	3688	1/1	0.12	-	74,74,74,74	0
56	MG	CA	1821	1/1	0.21	-	29,29,29,29	0
56	MG	AA	1816	1/1	0.32	-	55,55,55,55	0
56	MG	BA	3390	1/1	0.09	-	67,67,67,67	0
56	MG	BA	3787	1/1	0.16	-	47,47,47,47	0
56	MG	CB	302	1/1	0.16	-	3,3,3,3	0
56	MG	DA	3420	1/1	0.17	-	4,4,4,4	0
56	MG	AA	1672	1/1	0.32	-	69,69,69,69	0
56	MG	AA	1684	1/1	0.35	-	61,61,61,61	0
56	MG	DA	3122	1/1	0.25	-	4,4,4,4	0
56	MG	BA	3376	1/1	0.15	-	39,39,39,39	0
56	MG	BA	3168	1/1	0.46	-	52,52,52,52	0
56	MG	DA	3070	1/1	0.22	-	4,4,4,4	0
56	MG	BA	3194	1/1	0.10	-	36,36,36,36	0
56	MG	DU	201	1/1	0.34	-	3,3,3,3	0
56	MG	AA	1775	1/1	0.15	-	27,27,27,27	0
56	MG	BA	3240	1/1	0.48	-	40,40,40,40	0
56	MG	DA	3458	1/1	0.15	-	6,6,6,6	0
56	MG	BA	3558	1/1	0.20	-	10,10,10,10	0
56	MG	AK	202	1/1	0.14	-	95,95,95,95	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	BA	3801	1/1	0.18	-	51,51,51,51	0
56	MG	DA	3305	1/1	0.14	-	23,23,23,23	0
56	MG	AL	202	1/1	0.09	-	34,34,34,34	0
56	MG	DA	3012	1/1	0.27	-	3,3,3,3	0
56	MG	AA	1937	1/1	0.23	-	61,61,61,61	0
56	MG	DA	3297	1/1	1.12	-	89,89,89,89	0
56	MG	DA	3164	1/1	0.13	-	4,4,4,4	0
56	MG	AA	1888	1/1	0.35	-	39,39,39,39	0
56	MG	BA	3740	1/1	0.33	-	53,53,53,53	0
56	MG	BA	3615	1/1	0.16	-	56,56,56,56	0
56	MG	BA	3359	1/1	0.84	-	70,70,70,70	0
56	MG	DA	3048	1/1	0.23	-	4,4,4,4	0
56	MG	DA	3030	1/1	0.15	-	4,4,4,4	0
56	MG	AA	1842	1/1	0.58	-	75,75,75,75	0
56	MG	BA	3499	1/1	0.11	-	57,57,57,57	0
56	MG	BA	3127	1/1	0.09	-	22,22,22,22	0
56	MG	DA	3338	1/1	0.26	-	3,3,3,3	0
56	MG	DA	3123	1/1	0.12	-	5,5,5,5	0
56	MG	BA	3388	1/1	0.09	-	61,61,61,61	0
56	MG	DA	3280	1/1	0.31	-	34,34,34,34	0
56	MG	AG	201	1/1	0.14	-	72,72,72,72	0
56	MG	BA	3061	1/1	0.10	-	76,76,76,76	0
56	MG	BA	3398	1/1	0.09	-	56,56,56,56	0
56	MG	CA	1779	1/1	0.36	-	76,76,76,76	0
56	MG	BA	3146	1/1	0.17	-	33,33,33,33	0
56	MG	CA	1731	1/1	0.22	-	3,3,3,3	0
56	MG	BZ	301	1/1	0.16	-	81,81,81,81	0
56	MG	BA	3829	1/1	0.19	-	40,40,40,40	0
56	MG	BO	202	1/1	0.13	-	54,54,54,54	0
56	MG	BA	3411	1/1	0.17	-	51,51,51,51	0
56	MG	DA	3085	1/1	0.25	-	3,3,3,3	0
56	MG	AA	1641	1/1	0.13	-	27,27,27,27	0
56	MG	AA	1622	1/1	0.32	-	72,72,72,72	0
56	MG	BA	3103	1/1	0.35	-	78,78,78,78	0
56	MG	CA	1812	1/1	0.09	-	36,36,36,36	0
56	MG	DA	3439	1/1	0.23	-	4,4,4,4	0
56	MG	DA	3098	1/1	0.28	-	3,3,3,3	0
56	MG	AY	114	1/1	0.21	-	48,48,48,48	0
56	MG	DA	3074	1/1	0.39	-	3,3,3,3	0
56	MG	BA	3780	1/1	0.28	-	32,32,32,32	0
56	MG	AA	1884	1/1	0.17	-	26,26,26,26	0
56	MG	BA	3044	1/1	0.21	-	49,49,49,49	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	DA	3128	1/1	0.19	-	12,12,12,12	0
56	MG	AA	1605	1/1	0.32	-	88,88,88,88	0
56	MG	CA	1817	1/1	0.14	-	22,22,22,22	0
56	MG	AA	1848	1/1	0.32	-	56,56,56,56	0
56	MG	DA	3060	1/1	0.14	-	4,4,4,4	0
56	MG	DA	3373	1/1	0.27	-	92,92,92,92	0
56	MG	DA	3017	1/1	0.10	-	3,3,3,3	0
56	MG	BA	3268	1/1	0.27	-	45,45,45,45	0
56	MG	BB	224	1/1	0.20	-	65,65,65,65	0
56	MG	BA	3338	1/1	0.45	-	56,56,56,56	0
56	MG	CA	1712	1/1	0.25	-	39,39,39,39	0
56	MG	BA	3101	1/1	0.23	-	47,47,47,47	0
56	MG	BA	3494	1/1	0.14	-	44,44,44,44	0
56	MG	DA	3476	1/1	0.17	-	3,3,3,3	0
56	MG	BA	3778	1/1	0.19	-	63,63,63,63	0
56	MG	AA	1946	1/1	0.11	-	59,59,59,59	0
56	MG	BA	3845	1/1	0.45	-	68,68,68,68	0
56	MG	BB	232	1/1	0.15	-	58,58,58,58	0
56	MG	AX	411	1/1	0.61	-	75,75,75,75	0
56	MG	CZ	103	1/1	0.08	-	42,42,42,42	0
56	MG	CA	1668	1/1	0.39	-	3,3,3,3	0
56	MG	DA	3177	1/1	0.40	-	3,3,3,3	0
56	MG	BA	3320	1/1	0.46	-	84,84,84,84	0
56	MG	CA	1744	1/1	0.10	-	36,36,36,36	0
56	MG	CA	1701	1/1	0.16	-	13,13,13,13	0
56	MG	BA	3046	1/1	0.14	-	38,38,38,38	0
56	MG	BA	3810	1/1	0.25	-	12,12,12,12	0
56	MG	DA	3287	1/1	0.30	-	10,10,10,10	0
56	MG	DA	3024	1/1	0.15	-	3,3,3,3	0
56	MG	AA	1620	1/1	0.25	-	56,56,56,56	0
56	MG	BA	3588	1/1	0.09	-	24,24,24,24	0
56	MG	AA	1839	1/1	0.08	-	18,18,18,18	0
56	MG	DA	3190	1/1	0.20	-	4,4,4,4	0
56	MG	DA	3049	1/1	0.15	-	5,5,5,5	0
56	MG	CA	1810	1/1	0.64	-	59,59,59,59	0
56	MG	CA	1795	1/1	0.14	-	54,54,54,54	0
56	MG	AA	1878	1/1	0.29	-	67,67,67,67	0
56	MG	BA	3342	1/1	0.17	-	20,20,20,20	0
56	MG	BA	3617	1/1	0.21	-	66,66,66,66	0
56	MG	BA	3361	1/1	0.27	-	16,16,16,16	0
56	MG	BA	3634	1/1	0.50	-	33,33,33,33	0
56	MG	AA	1675	1/1	0.22	-	58,58,58,58	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	BA	3144	1/1	0.41	-	45,45,45,45	0
56	MG	BA	3436	1/1	0.35	-	47,47,47,47	0
56	MG	AA	1928	1/1	0.16	-	52,52,52,52	0
56	MG	BA	3851	1/1	0.21	-	17,17,17,17	0
56	MG	CA	1679	1/1	0.86	-	90,90,90,90	0
56	MG	BB	229	1/1	0.26	-	33,33,33,33	0
56	MG	CA	1819	1/1	0.12	-	36,36,36,36	0
56	MG	B4	102	1/1	0.21	-	31,31,31,31	0
56	MG	BA	3422	1/1	0.45	-	59,59,59,59	0
56	MG	BA	3791	1/1	0.37	-	63,63,63,63	0
56	MG	DA	3346	1/1	0.31	-	56,56,56,56	0
56	MG	BA	3859	1/1	0.23	-	80,80,80,80	0
56	MG	DA	3278	1/1	0.24	-	60,60,60,60	0
56	MG	BY	201	1/1	0.10	-	68,68,68,68	0
56	MG	DA	3219	1/1	0.34	-	3,3,3,3	0
56	MG	BA	3920	1/1	0.23	-	54,54,54,54	0
56	MG	BA	3503	1/1	0.07	-	41,41,41,41	0
56	MG	DA	3106	1/1	0.15	-	46,46,46,46	0
56	MG	AA	1800	1/1	0.13	-	54,54,54,54	0
56	MG	DA	3223	1/1	0.29	-	4,4,4,4	0
56	MG	DA	3307	1/1	0.15	-	39,39,39,39	0
56	MG	CA	1639	1/1	0.22	-	3,3,3,3	0
56	MG	BA	3097	1/1	0.16	-	54,54,54,54	0
56	MG	BA	3243	1/1	0.11	-	26,26,26,26	0
56	MG	AY	108	1/1	0.08	-	59,59,59,59	0
56	MG	BA	3747	1/1	0.39	-	64,64,64,64	0
56	MG	CA	1608	1/1	0.22	-	3,3,3,3	0
56	MG	BA	3549	1/1	0.31	-	27,27,27,27	0
56	MG	DB	204	1/1	0.23	-	3,3,3,3	0
56	MG	DA	3018	1/1	0.22	-	3,3,3,3	0
56	MG	BA	3321	1/1	0.16	-	40,40,40,40	0
56	MG	BI	203	1/1	0.14	-	53,53,53,53	0
56	MG	BA	3106	1/1	0.10	-	68,68,68,68	0
56	MG	BA	3033	1/1	0.22	-	38,38,38,38	0
56	MG	BA	3022	1/1	0.16	-	61,61,61,61	0
56	MG	DA	3129	1/1	0.34	-	57,57,57,57	0
56	MG	BA	3679	1/1	0.18	-	5,5,5,5	0
56	MG	AA	1906	1/1	0.12	-	57,57,57,57	0
56	MG	AA	1917	1/1	0.06	-	52,52,52,52	0
56	MG	AA	1630	1/1	0.30	-	65,65,65,65	0
56	MG	CA	1714	1/1	0.30	-	62,62,62,62	0
56	MG	BA	3583	1/1	0.11	-	71,71,71,71	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	AA	1776	1/1	0.15	-	30,30,30,30	0
56	MG	BA	3751	1/1	0.37	-	53,53,53,53	0
56	MG	BA	3815	1/1	0.28	-	28,28,28,28	0
56	MG	CA	1663	1/1	0.24	-	3,3,3,3	0
56	MG	BA	3080	1/1	0.18	-	29,29,29,29	0
56	MG	BA	3792	1/1	0.32	-	85,85,85,85	0
56	MG	BA	3670	1/1	0.27	-	37,37,37,37	0
56	MG	BA	3074	1/1	0.13	-	26,26,26,26	0
56	MG	AA	1755	1/1	0.22	-	47,47,47,47	0
56	MG	DA	3288	1/1	0.18	-	33,33,33,33	0
56	MG	AA	1752	1/1	0.16	-	66,66,66,66	0
56	MG	BA	3711	1/1	0.25	-	70,70,70,70	0
56	MG	AA	1962	1/1	0.55	-	48,48,48,48	0
56	MG	BA	3111	1/1	0.23	-	35,35,35,35	0
56	MG	BA	3647	1/1	0.16	-	48,48,48,48	0
56	MG	CY	111	1/1	0.26	-	60,60,60,60	0
56	MG	CA	1648	1/1	0.20	-	33,33,33,33	0
56	MG	AK	203	1/1	0.11	-	49,49,49,49	0
56	MG	AY	107	1/1	0.10	-	67,67,67,67	0
56	MG	BA	3889	1/1	0.17	-	44,44,44,44	0
56	MG	DA	3095	1/1	0.24	-	3,3,3,3	0
56	MG	BA	3214	1/1	0.32	-	19,19,19,19	0
56	MG	BH	201	1/1	0.05	-	54,54,54,54	0
56	MG	CA	1717	1/1	0.16	-	21,21,21,21	0
56	MG	BA	3261	1/1	0.18	-	14,14,14,14	0
56	MG	AA	1950	1/1	0.09	-	73,73,73,73	0
56	MG	AA	1974	1/1	0.23	-	48,48,48,48	0
56	MG	BA	3323	1/1	0.26	-	57,57,57,57	0
56	MG	DA	3450	1/1	0.22	-	12,12,12,12	0
56	MG	BA	3598	1/1	0.42	-	73,73,73,73	0
56	MG	CA	1747	1/1	0.48	-	3,3,3,3	0
56	MG	BA	3856	1/1	0.10	-	36,36,36,36	0
56	MG	DA	3374	1/1	0.25	-	3,3,3,3	0
56	MG	BA	3763	1/1	0.13	-	52,52,52,52	0
56	MG	BA	3633	1/1	0.15	-	36,36,36,36	0
56	MG	DA	3313	1/1	0.38	-	69,69,69,69	0
56	MG	BA	3628	1/1	0.15	-	71,71,71,71	0
56	MG	CA	1808	1/1	0.53	-	3,3,3,3	0
56	MG	DA	3234	1/1	0.18	-	3,3,3,3	0
56	MG	BA	3789	1/1	0.09	-	36,36,36,36	0
56	MG	BA	3157	1/1	0.46	-	55,55,55,55	0
56	MG	BA	3231	1/1	0.20	-	63,63,63,63	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	BA	3377	1/1	0.10	-	73,73,73,73	0
56	MG	AA	1787	1/1	0.29	-	54,54,54,54	0
56	MG	AA	1783	1/1	0.46	-	28,28,28,28	0
56	MG	DA	3154	1/1	0.23	-	3,3,3,3	0
56	MG	AA	2010	1/1	0.20	-	33,33,33,33	0
56	MG	DA	3489	1/1	0.19	-	4,4,4,4	0
56	MG	D1	101	1/1	0.33	-	3,3,3,3	0
56	MG	BA	3716	1/1	0.13	-	24,24,24,24	0
56	MG	BA	3137	1/1	0.12	-	19,19,19,19	0
56	MG	DA	3140	1/1	0.20	-	3,3,3,3	0
56	MG	AA	1740	1/1	0.23	-	30,30,30,30	0
56	MG	CA	1611	1/1	0.25	-	3,3,3,3	0
56	MG	CG	202	1/1	0.16	-	82,82,82,82	0
56	MG	AA	1607	1/1	0.17	-	62,62,62,62	0
56	MG	AA	1936	1/1	0.24	-	97,97,97,97	0
56	MG	AA	1748	1/1	0.08	-	41,41,41,41	0
56	MG	AA	1640	1/1	0.22	-	36,36,36,36	0
56	MG	BA	3347	1/1	0.09	-	43,43,43,43	0
56	MG	AX	405	1/1	0.08	-	74,74,74,74	0
56	MG	BA	3461	1/1	0.21	-	69,69,69,69	0
56	MG	CH	202	1/1	0.14	-	59,59,59,59	0
56	MG	BA	3565	1/1	0.28	-	50,50,50,50	0
56	MG	DA	3136	1/1	0.16	-	8,8,8,8	0
56	MG	DA	3308	1/1	0.19	-	46,46,46,46	0
56	MG	AA	1840	1/1	0.28	-	26,26,26,26	0
56	MG	CQ	201	1/1	0.37	-	3,3,3,3	0
56	MG	BA	3738	1/1	0.55	-	57,57,57,57	0
56	MG	BA	3825	1/1	0.23	-	45,45,45,45	0
56	MG	BA	3680	1/1	0.16	-	60,60,60,60	0
56	MG	DA	3252	1/1	0.38	-	23,23,23,23	0
56	MG	BA	3697	1/1	0.45	-	72,72,72,72	0
56	MG	BA	3518	1/1	0.26	-	58,58,58,58	0
56	MG	CK	202	1/1	0.20	-	91,91,91,91	0
56	MG	AF	201	1/1	0.18	-	87,87,87,87	0
56	MG	BA	3760	1/1	0.36	-	49,49,49,49	0
56	MG	BA	3614	1/1	0.23	-	56,56,56,56	0
56	MG	BA	3402	1/1	0.12	-	49,49,49,49	0
56	MG	BA	3506	1/1	0.21	-	59,59,59,59	0
56	MG	AA	1911	1/1	0.10	-	63,63,63,63	0
56	MG	BA	3287	1/1	0.22	-	27,27,27,27	0
56	MG	BA	3746	1/1	0.48	-	71,71,71,71	0
56	MG	AY	102	1/1	0.10	-	58,58,58,58	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	AD	5002	1/1	0.14	-	64,64,64,64	0
56	MG	BF	303	1/1	0.88	-	50,50,50,50	0
56	MG	BA	3367	1/1	0.26	-	53,53,53,53	0
56	MG	CA	1603	1/1	0.20	-	4,4,4,4	0
56	MG	BA	3547	1/1	0.18	-	16,16,16,16	0
56	MG	AA	2008	1/1	0.16	-	49,49,49,49	0
56	MG	BA	3898	1/1	0.31	-	38,38,38,38	0
56	MG	BA	3922	1/1	0.10	-	56,56,56,56	0
56	MG	CA	1775	1/1	0.41	-	91,91,91,91	0
56	MG	BA	3564	1/1	0.21	-	54,54,54,54	0
56	MG	AM	203	1/1	0.30	-	47,47,47,47	0
56	MG	BA	3281	1/1	0.16	-	61,61,61,61	0
56	MG	CA	1681	1/1	0.21	-	3,3,3,3	0
56	MG	BA	3142	1/1	0.16	-	24,24,24,24	0
56	MG	BA	3891	1/1	0.26	-	58,58,58,58	0
56	MG	AA	1903	1/1	0.49	-	54,54,54,54	0
56	MG	AA	1612	1/1	0.36	-	68,68,68,68	0
56	MG	CA	1659	1/1	0.20	-	3,3,3,3	0
56	MG	BA	3586	1/1	0.08	-	18,18,18,18	0
56	MG	BA	3296	1/1	0.39	-	68,68,68,68	0
56	MG	CA	1660	1/1	0.14	-	5,5,5,5	0
56	MG	DA	3387	1/1	0.14	-	77,77,77,77	0
56	MG	DA	3165	1/1	0.20	-	4,4,4,4	0
56	MG	BA	3163	1/1	0.30	-	91,91,91,91	0
56	MG	AA	1847	1/1	0.22	-	30,30,30,30	0
56	MG	AA	1964	1/1	0.45	-	79,79,79,79	0
56	MG	BA	3028	1/1	0.30	-	39,39,39,39	0
56	MG	BA	3524	1/1	0.09	-	44,44,44,44	0
56	MG	AA	1877	1/1	0.22	-	24,24,24,24	0
56	MG	BA	3649	1/1	0.27	-	30,30,30,30	0
56	MG	BA	3449	1/1	0.41	-	73,73,73,73	0
56	MG	BA	3876	1/1	0.37	-	88,88,88,88	0
56	MG	BA	3667	1/1	0.43	-	48,48,48,48	0
56	MG	BA	3139	1/1	0.40	-	59,59,59,59	0
56	MG	BA	3902	1/1	0.29	-	66,66,66,66	0
56	MG	DA	3447	1/1	0.31	-	15,15,15,15	0
56	MG	DA	3412	1/1	0.25	-	3,3,3,3	0
56	MG	BA	3485	1/1	0.19	-	71,71,71,71	0
56	MG	AA	1955	1/1	0.57	-	82,82,82,82	0
56	MG	BA	3466	1/1	0.27	-	67,67,67,67	0
56	MG	AA	1653	1/1	0.34	-	95,95,95,95	0
56	MG	BA	3696	1/1	0.24	-	69,69,69,69	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	CA	1693	1/1	0.22	-	58,58,58,58	0
56	MG	AA	2007	1/1	0.23	-	23,23,23,23	0
56	MG	AA	1896	1/1	0.18	-	26,26,26,26	0
56	MG	AA	1844	1/1	0.75	-	101,101,101,101	0
56	MG	DQ	202	1/1	0.23	-	3,3,3,3	0
56	MG	BA	3100	1/1	0.25	-	57,57,57,57	0
56	MG	BA	3493	1/1	0.07	-	50,50,50,50	0
56	MG	AA	1891	1/1	0.10	-	61,61,61,61	0
56	MG	AA	1769	1/1	0.47	-	87,87,87,87	0
56	MG	AA	1757	1/1	0.15	-	60,60,60,60	0
56	MG	BA	3271	1/1	0.16	-	57,57,57,57	0
56	MG	BA	3869	1/1	0.12	-	7,7,7,7	0
56	MG	AZ	112	1/1	0.09	-	46,46,46,46	0
56	MG	DA	3134	1/1	0.41	-	21,21,21,21	0
56	MG	DA	3209	1/1	0.35	-	3,3,3,3	0
56	MG	DA	3329	1/1	0.16	-	10,10,10,10	0
56	MG	DA	3357	1/1	0.25	-	3,3,3,3	0
56	MG	CZ	102	1/1	0.06	-	51,51,51,51	0
56	MG	BA	3288	1/1	0.18	-	43,43,43,43	0
56	MG	DA	3351	1/1	0.26	-	40,40,40,40	0
56	MG	DA	3279	1/1	0.37	-	30,30,30,30	0
57	ZN	AD	5001	1/1	0.23	-	41,41,41,41	0
56	MG	CA	1624	1/1	0.19	-	3,3,3,3	0
56	MG	AA	1985	1/1	0.19	-	52,52,52,52	0
56	MG	BY	203	1/1	0.19	-	58,58,58,58	0
56	MG	AZ	115	1/1	0.09	-	39,39,39,39	0
56	MG	BA	3145	1/1	0.16	-	22,22,22,22	0
56	MG	AZ	106	1/1	0.36	-	93,93,93,93	0
56	MG	AX	402	1/1	0.08	-	42,42,42,42	0
56	MG	DA	3113	1/1	0.17	-	85,85,85,85	0
56	MG	BA	3668	1/1	0.14	-	33,33,33,33	0
56	MG	AA	1882	1/1	0.35	-	53,53,53,53	0
56	MG	BA	3366	1/1	0.08	-	24,24,24,24	0
56	MG	DA	3417	1/1	0.21	-	4,4,4,4	0
56	MG	CA	1762	1/1	0.27	-	69,69,69,69	0
56	MG	DA	3274	1/1	0.36	-	3,3,3,3	0
56	MG	BA	3312	1/1	0.24	-	36,36,36,36	0
56	MG	BA	3255	1/1	0.17	-	72,72,72,72	0
56	MG	BA	3610	1/1	0.16	-	38,38,38,38	0
56	MG	BA	3779	1/1	0.09	-	22,22,22,22	0
56	MG	DA	3251	1/1	0.26	-	51,51,51,51	0
56	MG	CA	1739	1/1	0.34	-	3,3,3,3	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	BA	3519	1/1	0.14	-	82,82,82,82	0
56	MG	BA	3752	1/1	0.82	-	71,71,71,71	0
56	MG	BA	3501	1/1	0.12	-	58,58,58,58	0
56	MG	DA	3003	1/1	0.20	-	4,4,4,4	0
56	MG	AA	1826	1/1	0.12	-	46,46,46,46	0
56	MG	AA	2024	1/1	0.19	-	53,53,53,53	0
56	MG	BA	3467	1/1	0.40	-	21,21,21,21	0
56	MG	BA	3010	1/1	0.57	-	72,72,72,72	0
56	MG	AA	1910	1/1	0.12	-	88,88,88,88	0
56	MG	CA	1627	1/1	0.30	-	3,3,3,3	0
56	MG	BD	5006	1/1	0.13	-	11,11,11,11	0
56	MG	BA	3114	1/1	0.15	-	63,63,63,63	0
56	MG	BA	3185	1/1	0.15	-	8,8,8,8	0
56	MG	CA	1640	1/1	0.21	-	4,4,4,4	0
56	MG	BA	3094	1/1	0.09	-	76,76,76,76	0
56	MG	DA	3383	1/1	0.70	-	71,71,71,71	0
56	MG	BP	202	1/1	0.12	-	24,24,24,24	0
56	MG	DA	3101	1/1	0.69	-	64,64,64,64	0
56	MG	BA	3900	1/1	0.18	-	51,51,51,51	0
56	MG	AA	1944	1/1	0.10	-	48,48,48,48	0
56	MG	CA	1782	1/1	0.16	-	3,3,3,3	0
56	MG	BO	201	1/1	0.27	-	62,62,62,62	0
56	MG	DA	3459	1/1	0.34	-	4,4,4,4	0
56	MG	DA	3015	1/1	0.08	-	6,6,6,6	0
56	MG	BA	3331	1/1	0.09	-	74,74,74,74	0
56	MG	CA	1751	1/1	0.24	-	3,3,3,3	0
56	MG	BA	3386	1/1	0.24	-	79,79,79,79	0
56	MG	DA	3392	1/1	0.24	-	38,38,38,38	0
56	MG	CA	1753	1/1	0.18	-	3,3,3,3	0
56	MG	BA	3775	1/1	0.10	-	36,36,36,36	0
56	MG	CA	1625	1/1	0.29	-	3,3,3,3	0
56	MG	BA	3448	1/1	0.26	-	21,21,21,21	0
56	MG	BA	3250	1/1	0.22	-	81,81,81,81	0
56	MG	DA	3189	1/1	0.16	-	5,5,5,5	0
56	MG	B8	102	1/1	0.26	-	57,57,57,57	0
56	MG	BA	3148	1/1	0.33	-	35,35,35,35	0
56	MG	AN	102	1/1	0.16	-	57,57,57,57	0
56	MG	BA	3318	1/1	0.08	-	25,25,25,25	0
56	MG	DA	3487	1/1	0.28	-	3,3,3,3	0
56	MG	BA	3496	1/1	0.14	-	63,63,63,63	0
56	MG	DA	3364	1/1	0.22	-	3,3,3,3	0
56	MG	DA	3175	1/1	0.29	-	3,3,3,3	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	BA	3091	1/1	0.14	-	37,37,37,37	0
56	MG	BA	3490	1/1	0.17	-	75,75,75,75	0
56	MG	DA	3178	1/1	0.18	-	4,4,4,4	0
56	MG	AY	123	1/1	0.29	-	42,42,42,42	0
56	MG	AA	1692	1/1	0.20	-	79,79,79,79	0
56	MG	BA	3165	1/1	0.28	-	21,21,21,21	0
56	MG	BA	3031	1/1	0.40	-	74,74,74,74	0
56	MG	CA	1694	1/1	0.10	-	60,60,60,60	0
56	MG	BA	3724	1/1	0.14	-	29,29,29,29	0
56	MG	AA	1759	1/1	0.27	-	15,15,15,15	0
56	MG	BA	3380	1/1	0.09	-	43,43,43,43	0
56	MG	DA	3235	1/1	0.09	-	24,24,24,24	0
56	MG	BA	3828	1/1	0.34	-	46,46,46,46	0
56	MG	AY	113	1/1	0.78	-	89,89,89,89	0
56	MG	CA	1799	1/1	0.10	-	5,5,5,5	0
56	MG	BA	3213	1/1	0.23	-	43,43,43,43	0
56	MG	AA	1736	1/1	0.11	-	63,63,63,63	0
56	MG	BA	3247	1/1	0.35	-	42,42,42,42	0
56	MG	AX	401	1/1	0.12	-	74,74,74,74	0
56	MG	CA	1682	1/1	0.16	-	52,52,52,52	0
56	MG	BA	3187	1/1	0.33	-	54,54,54,54	0
56	MG	DA	3150	1/1	0.14	-	4,4,4,4	0
56	MG	DA	3115	1/1	0.12	-	62,62,62,62	0
56	MG	BA	3173	1/1	0.20	-	80,80,80,80	0
56	MG	BA	3001	1/1	0.18	-	38,38,38,38	0
56	MG	BA	3428	1/1	0.49	-	86,86,86,86	0
56	MG	BA	3237	1/1	0.11	-	28,28,28,28	0
56	MG	AA	1864	1/1	0.09	-	71,71,71,71	0
56	MG	DA	3082	1/1	0.38	-	3,3,3,3	0
56	MG	AA	1969	1/1	0.10	-	46,46,46,46	0
56	MG	BA	3850	1/1	0.34	-	54,54,54,54	0
56	MG	BA	3206	1/1	0.12	-	35,35,35,35	0
56	MG	BA	3006	1/1	0.16	-	11,11,11,11	0
56	MG	DA	3041	1/1	0.07	-	52,52,52,52	0
56	MG	BA	3893	1/1	0.04	-	62,62,62,62	0
56	MG	BA	3896	1/1	0.12	-	58,58,58,58	0
56	MG	AA	1854	1/1	0.11	-	39,39,39,39	0
56	MG	BA	3722	1/1	0.79	-	66,66,66,66	0
56	MG	BN	203	1/1	0.27	-	72,72,72,72	0
56	MG	BA	3118	1/1	0.16	-	23,23,23,23	0
56	MG	DA	3434	1/1	0.16	-	3,3,3,3	0
56	MG	DA	3054	1/1	0.13	-	5,5,5,5	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	BA	3788	1/1	0.18	-	69,69,69,69	0
56	MG	DA	3480	1/1	0.23	-	3,3,3,3	0
56	MG	CY	107	1/1	0.29	-	60,60,60,60	0
56	MG	DA	3451	1/1	0.49	-	23,23,23,23	0
56	MG	DA	3152	1/1	0.14	-	5,5,5,5	0
56	MG	AA	2016	1/1	0.30	-	43,43,43,43	0
56	MG	DA	3238	1/1	0.15	-	62,62,62,62	0
56	MG	BA	3020	1/1	0.42	-	73,73,73,73	0
56	MG	DA	3137	1/1	0.56	-	3,3,3,3	0
56	MG	BA	3609	1/1	0.32	-	39,39,39,39	0
56	MG	DA	3116	1/1	0.08	-	3,3,3,3	0
56	MG	AA	1923	1/1	0.30	-	79,79,79,79	0
56	MG	BA	3369	1/1	0.07	-	60,60,60,60	0
56	MG	BA	3745	1/1	0.76	-	70,70,70,70	0
56	MG	AA	1938	1/1	0.37	-	58,58,58,58	0
56	MG	DA	3213	1/1	0.12	-	4,4,4,4	0
56	MG	AT	201	1/1	0.19	-	57,57,57,57	0
56	MG	BA	3417	1/1	0.14	-	8,8,8,8	0
56	MG	BA	3590	1/1	0.22	-	32,32,32,32	0
56	MG	AA	1731	1/1	0.12	-	17,17,17,17	0
56	MG	DA	3303	1/1	0.10	-	10,10,10,10	0
56	MG	CA	1781	1/1	0.21	-	59,59,59,59	0
56	MG	BD	5001	1/1	0.22	-	61,61,61,61	0
56	MG	BA	3238	1/1	0.16	-	20,20,20,20	0
56	MG	AA	1733	1/1	0.21	-	38,38,38,38	0
56	MG	BA	3057	1/1	0.17	-	80,80,80,80	0
56	MG	BA	3313	1/1	0.07	-	33,33,33,33	0
56	MG	BA	3840	1/1	0.32	-	56,56,56,56	0
56	MG	BB	233	1/1	0.08	-	48,48,48,48	0
56	MG	BA	3199	1/1	0.26	-	65,65,65,65	0
56	MG	BA	3513	1/1	0.15	-	28,28,28,28	0
56	MG	AA	1626	1/1	0.28	-	20,20,20,20	0
56	MG	BA	3570	1/1	0.21	-	62,62,62,62	0
56	MG	DA	3448	1/1	0.20	-	21,21,21,21	0
56	MG	BA	3807	1/1	0.24	-	37,37,37,37	0
56	MG	BA	3655	1/1	0.16	-	38,38,38,38	0
56	MG	BA	3228	1/1	0.15	-	31,31,31,31	0
56	MG	DA	3185	1/1	0.22	-	4,4,4,4	0
56	MG	BA	3358	1/1	0.16	-	17,17,17,17	0
56	MG	BB	209	1/1	0.19	-	63,63,63,63	0
56	MG	AA	1831	1/1	0.13	-	68,68,68,68	0
56	MG	BA	3200	1/1	0.56	-	76,76,76,76	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	BA	3346	1/1	0.25	-	65,65,65,65	0
56	MG	BA	3592	1/1	0.18	-	47,47,47,47	0
56	MG	CA	1616	1/1	0.09	-	5,5,5,5	0
56	MG	BA	3757	1/1	0.63	-	76,76,76,76	0
56	MG	CZ	114	1/1	0.13	-	36,36,36,36	0
56	MG	AA	1644	1/1	0.19	-	54,54,54,54	0
56	MG	BA	3766	1/1	0.20	-	31,31,31,31	0
56	MG	AA	1617	1/1	0.12	-	48,48,48,48	0
56	MG	AY	122	1/1	0.16	-	58,58,58,58	0
56	MG	BA	3372	1/1	0.06	-	37,37,37,37	0
56	MG	CF	203	1/1	0.24	-	51,51,51,51	0
56	MG	DA	3376	1/1	0.10	-	75,75,75,75	0
56	MG	BA	3223	1/1	0.13	-	36,36,36,36	0
56	MG	BA	3482	1/1	0.33	-	63,63,63,63	0
56	MG	DA	3381	1/1	0.25	-	3,3,3,3	0
56	MG	BA	3123	1/1	0.08	-	55,55,55,55	0
56	MG	BB	207	1/1	0.28	-	84,84,84,84	0
56	MG	BA	3698	1/1	0.19	-	94,94,94,94	0
56	MG	DA	3096	1/1	0.33	-	3,3,3,3	0
56	MG	CA	1801	1/1	0.23	-	3,3,3,3	0
56	MG	AA	1773	1/1	0.15	-	46,46,46,46	0
56	MG	BA	3790	1/1	0.21	-	86,86,86,86	0
56	MG	DA	3199	1/1	0.22	-	59,59,59,59	0
56	MG	BA	3415	1/1	0.21	-	65,65,65,65	0
56	MG	CA	1653	1/1	0.21	-	62,62,62,62	0
56	MG	DA	3446	1/1	0.38	-	3,3,3,3	0
56	MG	BA	3837	1/1	0.82	-	71,71,71,71	0
56	MG	DA	3038	1/1	0.23	-	4,4,4,4	0
56	MG	BA	3299	1/1	0.13	-	9,9,9,9	0
56	MG	BB	231	1/1	0.27	-	54,54,54,54	0
56	MG	BA	3866	1/1	0.19	-	25,25,25,25	0
56	MG	DA	3354	1/1	0.07	-	43,43,43,43	0
56	MG	AA	1863	1/1	0.19	-	57,57,57,57	0
56	MG	AA	1729	1/1	0.33	-	60,60,60,60	0
56	MG	CA	1618	1/1	0.22	-	4,4,4,4	0
56	MG	BA	3265	1/1	0.23	-	42,42,42,42	0
56	MG	BA	3556	1/1	0.32	-	45,45,45,45	0
56	MG	DA	3013	1/1	0.24	-	3,3,3,3	0
56	MG	BA	3651	1/1	0.30	-	37,37,37,37	0
56	MG	BA	3092	1/1	0.41	-	73,73,73,73	0
56	MG	BA	3756	1/1	0.37	-	49,49,49,49	0
56	MG	BA	3921	1/1	0.26	-	53,53,53,53	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	BA	3047	1/1	0.20	-	54,54,54,54	0
56	MG	DA	3468	1/1	0.42	-	3,3,3,3	0
56	MG	AA	1693	1/1	0.27	-	79,79,79,79	0
56	MG	BA	3105	1/1	0.36	-	30,30,30,30	0
56	MG	DA	3304	1/1	0.36	-	76,76,76,76	0
56	MG	AA	2028	1/1	0.09	-	65,65,65,65	0
56	MG	BA	3038	1/1	0.16	-	41,41,41,41	0
56	MG	BR	202	1/1	0.27	-	89,89,89,89	0
56	MG	BA	3135	1/1	0.23	-	43,43,43,43	0
56	MG	BA	3370	1/1	0.05	-	46,46,46,46	0
56	MG	AX	403	1/1	0.09	-	68,68,68,68	0
56	MG	CA	1811	1/1	0.42	-	79,79,79,79	0
56	MG	AA	1861	1/1	0.04	-	47,47,47,47	0
56	MG	BV	201	1/1	0.10	-	53,53,53,53	0
56	MG	AA	1756	1/1	0.30	-	41,41,41,41	0
56	MG	DA	3431	1/1	0.20	-	3,3,3,3	0
56	MG	BS	203	1/1	0.14	-	52,52,52,52	0
56	MG	B2	101	1/1	0.23	-	76,76,76,76	0
56	MG	BI	202	1/1	0.07	-	53,53,53,53	0
56	MG	BA	3050	1/1	0.16	-	44,44,44,44	0
56	MG	BA	3273	1/1	0.35	-	74,74,74,74	0
56	MG	DA	3138	1/1	0.42	-	3,3,3,3	0
56	MG	CA	1651	1/1	0.21	-	28,28,28,28	0
56	MG	CA	1818	1/1	0.31	-	59,59,59,59	0
56	MG	B4	101	1/1	0.10	-	29,29,29,29	0
56	MG	AA	1886	1/1	0.18	-	50,50,50,50	0
56	MG	DB	202	1/1	0.24	-	3,3,3,3	0
56	MG	CA	1636	1/1	0.32	-	3,3,3,3	0
56	MG	DA	3167	1/1	0.12	-	6,6,6,6	0
56	MG	BA	3012	1/1	0.22	-	75,75,75,75	0
56	MG	AA	1650	1/1	0.14	-	45,45,45,45	0
56	MG	DA	3215	1/1	0.16	-	4,4,4,4	0
56	MG	DA	3334	1/1	0.42	-	3,3,3,3	0
56	MG	BA	3834	1/1	0.31	-	12,12,12,12	0
56	MG	BA	3623	1/1	0.18	-	103,103,103,103	0
56	MG	BA	3154	1/1	0.14	-	41,41,41,41	0
56	MG	BA	3809	1/1	0.12	-	13,13,13,13	0
56	MG	DA	3157	1/1	0.37	-	3,3,3,3	0
56	MG	BA	3846	1/1	0.17	-	55,55,55,55	0
56	MG	BA	3205	1/1	0.61	-	55,55,55,55	0
56	MG	BA	3600	1/1	0.46	-	47,47,47,47	0
56	MG	DA	3464	1/1	0.33	-	3,3,3,3	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	BA	3731	1/1	0.28	-	53,53,53,53	0
56	MG	BA	3130	1/1	0.20	-	32,32,32,32	0
56	MG	BA	3365	1/1	0.38	-	53,53,53,53	0
56	MG	AX	414	1/1	0.38	-	97,97,97,97	0
56	MG	AA	1907	1/1	0.28	-	76,76,76,76	0
56	MG	BA	3919	1/1	0.24	-	49,49,49,49	0
56	MG	AA	1717	1/1	0.25	-	75,75,75,75	0
56	MG	BA	3459	1/1	0.21	-	18,18,18,18	0
56	MG	BA	3498	1/1	0.25	-	45,45,45,45	0
56	MG	BA	3093	1/1	0.72	-	80,80,80,80	0
56	MG	CA	1777	1/1	0.28	-	4,4,4,4	0
56	MG	AA	1637	1/1	0.08	-	54,54,54,54	0
56	MG	BA	3750	1/1	0.17	-	45,45,45,45	0
56	MG	BA	3669	1/1	0.42	-	52,52,52,52	0
56	MG	BA	3041	1/1	0.39	-	98,98,98,98	0
56	MG	DP	201	1/1	0.34	-	3,3,3,3	0
56	MG	BA	3495	1/1	0.10	-	48,48,48,48	0
56	MG	DA	3139	1/1	0.39	-	3,3,3,3	0
56	MG	AA	1822	1/1	0.24	-	40,40,40,40	0
56	MG	CA	1721	1/1	0.30	-	49,49,49,49	0
56	MG	AA	1603	1/1	0.25	-	91,91,91,91	0
56	MG	BA	3676	1/1	0.17	-	44,44,44,44	0
56	MG	DA	3432	1/1	0.29	-	3,3,3,3	0
56	MG	BA	3385	1/1	0.12	-	63,63,63,63	0
56	MG	DA	3091	1/1	0.45	-	3,3,3,3	0
56	MG	DA	3182	1/1	0.28	-	3,3,3,3	0
56	MG	AA	1876	1/1	0.18	-	69,69,69,69	0
56	MG	AA	1883	1/1	0.23	-	42,42,42,42	0
56	MG	CA	1740	1/1	0.21	-	41,41,41,41	0
56	MG	DA	3131	1/1	0.36	-	31,31,31,31	0
56	MG	DA	3269	1/1	0.16	-	3,3,3,3	0
56	MG	DB	203	1/1	0.25	-	3,3,3,3	0
56	MG	BA	3291	1/1	0.15	-	9,9,9,9	0
56	MG	BA	3473	1/1	0.14	-	31,31,31,31	0
56	MG	DA	3275	1/1	0.27	-	4,4,4,4	0
56	MG	DA	3247	1/1	0.25	-	3,3,3,3	0
56	MG	DA	3105	1/1	0.22	-	55,55,55,55	0
56	MG	AA	1712	1/1	0.16	-	35,35,35,35	0
56	MG	DA	3277	1/1	0.30	-	3,3,3,3	0
56	MG	AA	1747	1/1	0.15	-	41,41,41,41	0
56	MG	BA	3179	1/1	0.13	-	32,32,32,32	0
56	MG	DA	3404	1/1	0.17	-	5,5,5,5	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	AA	1772	1/1	0.35	-	40,40,40,40	0
56	MG	BO	205	1/1	0.32	-	86,86,86,86	0
56	MG	DB	209	1/1	0.32	-	3,3,3,3	0
56	MG	BA	3838	1/1	0.12	-	29,29,29,29	0
56	MG	BA	3172	1/1	0.25	-	54,54,54,54	0
56	MG	AA	1686	1/1	0.21	-	43,43,43,43	0
56	MG	DA	3158	1/1	0.31	-	3,3,3,3	0
56	MG	BA	3764	1/1	0.19	-	45,45,45,45	0
56	MG	BB	234	1/1	0.09	-	23,23,23,23	0
56	MG	CA	1768	1/1	0.19	-	46,46,46,46	0
56	MG	DA	3230	1/1	0.21	-	58,58,58,58	0
56	MG	CA	1718	1/1	0.19	-	41,41,41,41	0
56	MG	DA	3052	1/1	0.24	-	3,3,3,3	0
56	MG	DA	3192	1/1	0.34	-	3,3,3,3	0
56	MG	BA	3534	1/1	0.29	-	61,61,61,61	0
56	MG	DA	3282	1/1	0.36	-	72,72,72,72	0
56	MG	AA	1898	1/1	0.13	-	27,27,27,27	0
56	MG	DA	3403	1/1	0.23	-	64,64,64,64	0
56	MG	DA	3360	1/1	0.33	-	56,56,56,56	0
56	MG	DA	3285	1/1	0.12	-	4,4,4,4	0
56	MG	BA	3375	1/1	0.14	-	76,76,76,76	0
56	MG	BA	3761	1/1	0.17	-	29,29,29,29	0
56	MG	DA	3418	1/1	0.26	-	3,3,3,3	0
56	MG	AY	120	1/1	0.08	-	40,40,40,40	0
56	MG	DA	3022	1/1	0.21	-	3,3,3,3	0
56	MG	BA	3045	1/1	0.40	-	56,56,56,56	0
56	MG	BA	3857	1/1	0.27	-	71,71,71,71	0
56	MG	AA	1762	1/1	0.17	-	43,43,43,43	0
56	MG	CA	1765	1/1	0.27	-	3,3,3,3	0
56	MG	BB	211	1/1	0.14	-	81,81,81,81	0
56	MG	AA	1959	1/1	0.11	-	54,54,54,54	0
56	MG	BH	204	1/1	0.12	-	77,77,77,77	0
56	MG	CA	1763	1/1	1.25	-	77,77,77,77	0
56	MG	BA	3383	1/1	0.17	-	53,53,53,53	0
56	MG	BA	3249	1/1	0.17	-	58,58,58,58	0
56	MG	BA	3303	1/1	0.22	-	12,12,12,12	0
56	MG	AA	2026	1/1	0.12	-	26,26,26,26	0
56	MG	BA	3278	1/1	0.27	-	67,67,67,67	0
56	MG	BA	3523	1/1	0.08	-	62,62,62,62	0
56	MG	DA	3195	1/1	0.41	-	3,3,3,3	0
56	MG	BA	3151	1/1	0.08	-	31,31,31,31	0
56	MG	BA	3458	1/1	0.34	-	50,50,50,50	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	BA	3521	1/1	0.33	-	45,45,45,45	0
56	MG	BN	202	1/1	0.20	-	46,46,46,46	0
56	MG	CA	1632	1/1	0.46	-	3,3,3,3	0
56	MG	CY	102	1/1	0.29	-	3,3,3,3	0
56	MG	DA	3191	1/1	0.25	-	4,4,4,4	0
56	MG	CA	1738	1/1	0.34	-	64,64,64,64	0
56	MG	DA	3144	1/1	0.21	-	4,4,4,4	0
56	MG	AI	201	1/1	0.33	-	59,59,59,59	0
56	MG	DA	3216	1/1	0.29	-	3,3,3,3	0
56	MG	DA	3166	1/1	0.25	-	3,3,3,3	0
56	MG	BA	3806	1/1	0.44	-	29,29,29,29	0
56	MG	BA	3174	1/1	0.16	-	83,83,83,83	0
56	MG	B1	105	1/1	0.32	-	87,87,87,87	0
56	MG	AK	207	1/1	0.07	-	65,65,65,65	0
56	MG	DA	3314	1/1	0.39	-	70,70,70,70	0
56	MG	DA	3342	1/1	0.16	-	7,7,7,7	0
56	MG	BX	102	1/1	0.19	-	25,25,25,25	0
56	MG	AM	201	1/1	0.21	-	86,86,86,86	0
56	MG	CG	201	1/1	0.14	-	70,70,70,70	0
56	MG	AA	2015	1/1	0.09	-	40,40,40,40	0
56	MG	BA	3226	1/1	0.16	-	43,43,43,43	0
56	MG	CA	1805	1/1	0.21	-	3,3,3,3	0
56	MG	AY	106	1/1	0.14	-	58,58,58,58	0
56	MG	AA	1997	1/1	0.30	-	56,56,56,56	0
56	MG	BA	3371	1/1	0.18	-	53,53,53,53	0
56	MG	DA	3411	1/1	0.18	-	3,3,3,3	0
56	MG	BD	5002	1/1	0.17	-	82,82,82,82	0
56	MG	BA	3454	1/1	0.32	-	63,63,63,63	0
56	MG	CA	1696	1/1	0.29	-	60,60,60,60	0
56	MG	BA	3076	1/1	0.45	-	51,51,51,51	0
56	MG	BA	3474	1/1	0.50	-	73,73,73,73	0
56	MG	CA	1726	1/1	0.06	-	37,37,37,37	0
56	MG	CA	1657	1/1	0.18	-	3,3,3,3	0
56	MG	AA	1838	1/1	0.28	-	18,18,18,18	0
56	MG	AA	1771	1/1	0.24	-	45,45,45,45	0
56	MG	BA	3341	1/1	0.35	-	70,70,70,70	0
56	MG	BA	3821	1/1	0.13	-	22,22,22,22	0
56	MG	BA	3208	1/1	0.08	-	86,86,86,86	0
56	MG	BA	3561	1/1	0.28	-	75,75,75,75	0
56	MG	DI	201	1/1	0.11	-	38,38,38,38	0
56	MG	DA	3187	1/1	0.33	-	3,3,3,3	0
56	MG	BA	3827	1/1	0.17	-	48,48,48,48	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	AA	1711	1/1	0.48	-	58,58,58,58	0
56	MG	BA	3559	1/1	0.14	-	31,31,31,31	0
56	MG	AA	1828	1/1	0.30	-	69,69,69,69	0
56	MG	AA	1669	1/1	0.15	-	58,58,58,58	0
56	MG	DA	3315	1/1	0.34	-	62,62,62,62	0
56	MG	DA	3229	1/1	0.20	-	3,3,3,3	0
56	MG	BA	3754	1/1	0.40	-	44,44,44,44	0
56	MG	CA	1662	1/1	0.14	-	4,4,4,4	0
56	MG	AA	1814	1/1	0.15	-	47,47,47,47	0
56	MG	BA	3536	1/1	0.29	-	70,70,70,70	0
56	MG	CO	101	1/1	0.18	-	33,33,33,33	0
56	MG	BW	201	1/1	0.40	-	80,80,80,80	0
56	MG	AV	5501	1/1	0.15	-	28,28,28,28	0
56	MG	BA	3131	1/1	0.46	-	72,72,72,72	0
56	MG	BA	3217	1/1	0.17	-	12,12,12,12	0
56	MG	BO	204	1/1	0.28	-	50,50,50,50	0
56	MG	BA	3246	1/1	0.30	-	60,60,60,60	0
56	MG	AA	1763	1/1	0.13	-	41,41,41,41	0
56	MG	DA	3242	1/1	0.31	-	3,3,3,3	0
56	MG	DA	3205	1/1	0.30	-	38,38,38,38	0
56	MG	CA	1700	1/1	0.08	-	12,12,12,12	0
56	MG	CA	1749	1/1	0.25	-	3,3,3,3	0
56	MG	BA	3141	1/1	0.13	-	68,68,68,68	0
56	MG	BA	3907	1/1	0.39	-	27,27,27,27	0
56	MG	BB	221	1/1	0.50	-	65,65,65,65	0
56	MG	BA	3597	1/1	0.57	-	48,48,48,48	0
56	MG	BA	3334	1/1	0.06	-	77,77,77,77	0
56	MG	AM	202	1/1	0.09	-	58,58,58,58	0
56	MG	BA	3408	1/1	0.23	-	50,50,50,50	0
56	MG	DA	3057	1/1	0.27	-	3,3,3,3	0
56	MG	DA	3061	1/1	0.25	-	4,4,4,4	0
56	MG	CZ	109	1/1	0.10	-	95,95,95,95	0
56	MG	DA	3169	1/1	0.28	-	3,3,3,3	0
56	MG	B8	101	1/1	0.27	-	30,30,30,30	0
56	MG	AX	409	1/1	0.18	-	47,47,47,47	0
56	MG	BV	203	1/1	0.05	-	52,52,52,52	0
56	MG	CA	1637	1/1	0.15	-	4,4,4,4	0
56	MG	DA	3240	1/1	0.19	-	3,3,3,3	0
56	MG	AA	1726	1/1	0.14	-	53,53,53,53	0
56	MG	CA	1686	1/1	0.32	-	48,48,48,48	0
56	MG	DA	3355	1/1	0.09	-	56,56,56,56	0
56	MG	BA	3579	1/1	0.12	-	69,69,69,69	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	DA	3180	1/1	0.39	-	3,3,3,3	0
56	MG	DA	3198	1/1	0.42	-	4,4,4,4	0
56	MG	AE	202	1/1	0.17	-	64,64,64,64	0
56	MG	BA	3083	1/1	0.29	-	71,71,71,71	0
56	MG	DA	3401	1/1	0.20	-	39,39,39,39	0
56	MG	AA	2019	1/1	0.17	-	70,70,70,70	0
56	MG	BA	3872	1/1	0.17	-	54,54,54,54	0
56	MG	BA	3777	1/1	0.15	-	32,32,32,32	0
56	MG	AA	1837	1/1	0.14	-	17,17,17,17	0
56	MG	CA	1800	1/1	0.39	-	3,3,3,3	0
56	MG	BA	3491	1/1	0.28	-	38,38,38,38	0
56	MG	BA	3160	1/1	0.20	-	54,54,54,54	0
56	MG	BA	3113	1/1	0.23	-	85,85,85,85	0
56	MG	DA	3069	1/1	0.37	-	3,3,3,3	0
56	MG	BA	3203	1/1	0.13	-	39,39,39,39	0
56	MG	AA	1695	1/1	0.13	-	52,52,52,52	0
56	MG	BA	3352	1/1	0.10	-	17,17,17,17	0
56	MG	BA	3638	1/1	0.25	-	48,48,48,48	0
56	MG	DA	3130	1/1	0.26	-	3,3,3,3	0
56	MG	DG	202	1/1	0.07	-	59,59,59,59	0
56	MG	DA	3079	1/1	0.36	-	3,3,3,3	0
56	MG	CA	1816	1/1	0.56	-	61,61,61,61	0
56	MG	DA	3007	1/1	0.08	-	25,25,25,25	0
56	MG	CZ	104	1/1	0.24	-	3,3,3,3	0
56	MG	BA	3143	1/1	0.66	-	64,64,64,64	0
56	MG	BA	3515	1/1	0.17	-	68,68,68,68	0
56	MG	BA	3183	1/1	0.15	-	57,57,57,57	0
56	MG	AA	1916	1/1	0.05	-	63,63,63,63	0
56	MG	BF	301	1/1	0.13	-	63,63,63,63	0
56	MG	DA	3114	1/1	0.23	-	83,83,83,83	0
56	MG	AA	1860	1/1	0.14	-	58,58,58,58	0
56	MG	BA	3803	1/1	0.11	-	32,32,32,32	0
56	MG	BA	3606	1/1	0.58	-	52,52,52,52	0
56	MG	DE	301	1/1	0.10	-	5,5,5,5	0
56	MG	BA	3906	1/1	0.21	-	67,67,67,67	0
56	MG	AA	1926	1/1	0.08	-	30,30,30,30	0
56	MG	BA	3832	1/1	0.23	-	28,28,28,28	0
56	MG	CA	1733	1/1	0.21	-	3,3,3,3	0
56	MG	AA	1707	1/1	0.13	-	37,37,37,37	0
56	MG	BA	3129	1/1	0.23	-	48,48,48,48	0
56	MG	BA	3844	1/1	0.14	-	36,36,36,36	0
56	MG	BA	3117	1/1	0.53	-	63,63,63,63	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	BA	3769	1/1	0.10	-	28,28,28,28	0
56	MG	AA	1680	1/1	0.46	-	51,51,51,51	0
56	MG	BA	3440	1/1	0.17	-	73,73,73,73	0
56	MG	AA	1805	1/1	0.08	-	22,22,22,22	0
56	MG	BA	3818	1/1	0.60	-	71,71,71,71	0
56	MG	BA	3475	1/1	0.10	-	22,22,22,22	0
56	MG	DA	3301	1/1	0.25	-	42,42,42,42	0
56	MG	BA	3601	1/1	0.16	-	30,30,30,30	0
56	MG	DA	3409	1/1	0.28	-	3,3,3,3	0
56	MG	BK	202	1/1	0.09	-	83,83,83,83	0
56	MG	AA	1671	1/1	0.22	-	59,59,59,59	0
56	MG	DA	3473	1/1	0.16	-	3,3,3,3	0
56	MG	DA	3181	1/1	0.36	-	3,3,3,3	0
56	MG	BA	3098	1/1	0.16	-	27,27,27,27	0
56	MG	BA	3066	1/1	0.10	-	67,67,67,67	0
56	MG	BA	3693	1/1	0.14	-	62,62,62,62	0
56	MG	AA	1732	1/1	0.15	-	21,21,21,21	0
56	MG	BA	3692	1/1	0.42	-	52,52,52,52	0
56	MG	DA	3174	1/1	0.18	-	3,3,3,3	0
56	MG	BB	204	1/1	0.09	-	51,51,51,51	0
56	MG	DA	3081	1/1	0.17	-	4,4,4,4	0
56	MG	CA	1742	1/1	0.22	-	54,54,54,54	0
56	MG	AZ	104	1/1	0.11	-	61,61,61,61	0
56	MG	BA	3196	1/1	0.40	-	50,50,50,50	0
56	MG	AA	1604	1/1	0.15	-	43,43,43,43	0
56	MG	BA	3285	1/1	0.15	-	48,48,48,48	0
56	MG	BA	3854	1/1	0.47	-	60,60,60,60	0
56	MG	BA	3158	1/1	0.11	-	42,42,42,42	0
56	MG	AA	1767	1/1	0.16	-	45,45,45,45	0
56	MG	BA	3294	1/1	0.28	-	4,4,4,4	0
56	MG	BA	3216	1/1	0.19	-	54,54,54,54	0
56	MG	AV	5500	1/1	0.20	-	71,71,71,71	0
56	MG	DA	3173	1/1	0.19	-	3,3,3,3	0
56	MG	BI	204	1/1	0.25	-	32,32,32,32	0
56	MG	AA	1694	1/1	0.15	-	52,52,52,52	0
56	MG	BA	3071	1/1	0.18	-	35,35,35,35	0
56	MG	AA	1977	1/1	0.36	-	64,64,64,64	0
56	MG	BA	3460	1/1	0.92	-	75,75,75,75	0
56	MG	DA	3127	1/1	0.30	-	3,3,3,3	0
56	MG	BA	3612	1/1	0.10	-	9,9,9,9	0
56	MG	BA	3329	1/1	0.09	-	79,79,79,79	0
56	MG	CA	1766	1/1	0.12	-	64,64,64,64	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	DA	3089	1/1	0.15	-	4,4,4,4	0
56	MG	DA	3258	1/1	0.10	-	6,6,6,6	0
56	MG	CZ	101	1/1	0.11	-	72,72,72,72	0
56	MG	AA	1899	1/1	0.36	-	59,59,59,59	0
56	MG	D8	101	1/1	0.31	-	3,3,3,3	0
56	MG	BA	3734	1/1	0.25	-	59,59,59,59	0
56	MG	BA	3017	1/1	0.15	-	52,52,52,52	0
56	MG	BA	3665	1/1	0.10	-	24,24,24,24	0
56	MG	AL	203	1/1	0.08	-	43,43,43,43	0
56	MG	AA	1901	1/1	0.21	-	88,88,88,88	0
56	MG	AA	1704	1/1	0.18	-	48,48,48,48	0
56	MG	BA	3802	1/1	0.12	-	47,47,47,47	0
56	MG	AA	1984	1/1	0.28	-	39,39,39,39	0
56	MG	AA	1857	1/1	0.25	-	43,43,43,43	0
56	MG	CA	1605	1/1	0.40	-	3,3,3,3	0
56	MG	BA	3025	1/1	0.16	-	58,58,58,58	0
56	MG	AY	111	1/1	0.19	-	60,60,60,60	0
56	MG	BA	3566	1/1	0.11	-	43,43,43,43	0
56	MG	BA	3822	1/1	0.33	-	34,34,34,34	0
56	MG	AA	1815	1/1	0.32	-	43,43,43,43	0
56	MG	BA	3239	1/1	0.46	-	69,69,69,69	0
56	MG	BA	3442	1/1	0.14	-	46,46,46,46	0
56	MG	CA	1711	1/1	0.88	-	57,57,57,57	0
56	MG	BA	3186	1/1	0.11	-	67,67,67,67	0
56	MG	AY	119	1/1	0.10	-	50,50,50,50	0
56	MG	AA	1715	1/1	0.27	-	50,50,50,50	0
56	MG	DA	3064	1/1	0.22	-	4,4,4,4	0
56	MG	BF	306	1/1	0.17	-	47,47,47,47	0
56	MG	BA	3060	1/1	0.06	-	83,83,83,83	0
56	MG	BA	3793	1/1	0.14	-	54,54,54,54	0
56	MG	BA	3394	1/1	0.21	-	41,41,41,41	0
56	MG	BA	3384	1/1	0.19	-	60,60,60,60	0
56	MG	BA	3188	1/1	0.07	-	53,53,53,53	0
56	MG	DA	3011	1/1	0.20	-	3,3,3,3	0
56	MG	CA	1703	1/1	0.10	-	29,29,29,29	0
56	MG	DA	3020	1/1	0.27	-	3,3,3,3	0
56	MG	AA	1954	1/1	0.42	-	74,74,74,74	0
56	MG	BA	3036	1/1	0.21	-	88,88,88,88	0
56	MG	AA	1753	1/1	0.17	-	62,62,62,62	0
56	MG	BA	3368	1/1	0.26	-	63,63,63,63	0
56	MG	BK	203	1/1	0.16	-	72,72,72,72	0
56	MG	DA	3231	1/1	0.17	-	72,72,72,72	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	BA	3009	1/1	0.61	-	59,59,59,59	0
56	MG	BB	220	1/1	0.42	-	84,84,84,84	0
56	MG	AA	1881	1/1	0.48	-	98,98,98,98	0
56	MG	BA	3843	1/1	0.19	-	60,60,60,60	0
56	MG	B1	103	1/1	0.08	-	37,37,37,37	0
56	MG	BA	3492	1/1	0.09	-	48,48,48,48	0
56	MG	CA	1665	1/1	0.26	-	3,3,3,3	0
56	MG	AA	1849	1/1	0.15	-	10,10,10,10	0
56	MG	DA	3484	1/1	0.31	-	3,3,3,3	0
56	MG	BA	3848	1/1	0.19	-	61,61,61,61	0
56	MG	BA	3608	1/1	0.21	-	40,40,40,40	0
56	MG	BA	3868	1/1	0.12	-	11,11,11,11	0
56	MG	DA	3236	1/1	0.09	-	53,53,53,53	0
56	MG	DA	3125	1/1	0.21	-	28,28,28,28	0
56	MG	AA	2018	1/1	0.21	-	23,23,23,23	0
56	MG	DA	3008	1/1	0.23	-	4,4,4,4	0
56	MG	BA	3540	1/1	0.29	-	65,65,65,65	0
56	MG	AA	1699	1/1	0.23	-	61,61,61,61	0
56	MG	BA	3646	1/1	0.17	-	47,47,47,47	0
56	MG	DA	3036	1/1	0.21	-	5,5,5,5	0
56	MG	AA	1734	1/1	0.20	-	27,27,27,27	0
56	MG	BA	3468	1/1	0.39	-	22,22,22,22	0
56	MG	AA	1813	1/1	0.27	-	67,67,67,67	0
56	MG	DA	3410	1/1	0.18	-	3,3,3,3	0
56	MG	BA	3804	1/1	0.16	-	44,44,44,44	0
56	MG	AA	1636	1/1	0.08	-	67,67,67,67	0
56	MG	BA	3219	1/1	0.14	-	17,17,17,17	0
56	MG	BA	3065	1/1	0.14	-	78,78,78,78	0
56	MG	AA	2023	1/1	0.11	-	33,33,33,33	0
56	MG	BA	3584	1/1	0.22	-	54,54,54,54	0
56	MG	BA	3102	1/1	0.32	-	89,89,89,89	0
56	MG	BA	3325	1/1	0.13	-	66,66,66,66	0
56	MG	BA	3785	1/1	0.20	-	25,25,25,25	0
56	MG	BA	3813	1/1	0.10	-	15,15,15,15	0
56	MG	AA	1912	1/1	0.18	-	62,62,62,62	0
56	MG	BA	3581	1/1	0.12	-	69,69,69,69	0
56	MG	AA	1803	1/1	0.18	-	55,55,55,55	0
56	MG	DA	3472	1/1	0.27	-	4,4,4,4	0
56	MG	CA	1614	1/1	0.23	-	3,3,3,3	0
56	MG	BA	3063	1/1	0.04	-	86,86,86,86	0
56	MG	AA	1730	1/1	0.24	-	72,72,72,72	0
56	MG	AA	1925	1/1	0.09	-	43,43,43,43	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	BB	203	1/1	0.06	-	51,51,51,51	0
56	MG	BA	3632	1/1	0.17	-	51,51,51,51	0
56	MG	AZ	110	1/1	0.12	-	69,69,69,69	0
56	MG	AA	1988	1/1	0.14	-	65,65,65,65	0
56	MG	BA	3393	1/1	0.25	-	61,61,61,61	0
56	MG	AA	1804	1/1	0.46	-	56,56,56,56	0
56	MG	DA	3445	1/1	0.22	-	4,4,4,4	0
56	MG	DA	3058	1/1	0.18	-	3,3,3,3	0
56	MG	BA	3133	1/1	0.31	-	53,53,53,53	0
56	MG	AA	1914	1/1	0.23	-	70,70,70,70	0
56	MG	BA	3340	1/1	0.49	-	73,73,73,73	0
56	MG	DB	201	1/1	0.28	-	3,3,3,3	0
56	MG	BA	3881	1/1	0.43	-	68,68,68,68	0
56	MG	AA	1859	1/1	0.14	-	76,76,76,76	0
56	MG	DA	3415	1/1	0.20	-	4,4,4,4	0
56	MG	AA	1961	1/1	0.26	-	61,61,61,61	0
56	MG	DA	3324	1/1	0.47	-	3,3,3,3	0
56	MG	BA	3159	1/1	0.17	-	61,61,61,61	0
56	MG	B0	102	1/1	0.20	-	37,37,37,37	0
56	MG	BA	3272	1/1	0.18	-	54,54,54,54	0
56	MG	BA	3204	1/1	0.09	-	34,34,34,34	0
56	MG	DB	207	1/1	0.16	-	4,4,4,4	0
56	MG	CA	1716	1/1	0.20	-	58,58,58,58	0
56	MG	AA	1741	1/1	0.15	-	60,60,60,60	0
56	MG	AA	2005	1/1	0.20	-	49,49,49,49	0
56	MG	CB	301	1/1	0.13	-	39,39,39,39	0
56	MG	BS	201	1/1	0.17	-	46,46,46,46	0
56	MG	DA	3296	1/1	0.56	-	46,46,46,46	0
56	MG	CA	1680	1/1	0.23	-	34,34,34,34	0
56	MG	BA	3707	1/1	0.54	-	77,77,77,77	0
56	MG	BA	3626	1/1	0.16	-	62,62,62,62	0
56	MG	BA	3087	1/1	0.27	-	24,24,24,24	0
56	MG	BN	204	1/1	0.10	-	43,43,43,43	0
56	MG	CY	108	1/1	0.09	-	60,60,60,60	0
56	MG	CK	203	1/1	0.08	-	85,85,85,85	0
56	MG	DQ	201	1/1	0.20	-	4,4,4,4	0
56	MG	BA	3835	1/1	0.14	-	8,8,8,8	0
56	MG	CA	1803	1/1	0.26	-	3,3,3,3	0
56	MG	BA	3849	1/1	0.34	-	52,52,52,52	0
56	MG	DA	3479	1/1	0.24	-	3,3,3,3	0
56	MG	BA	3673	1/1	0.24	-	19,19,19,19	0
56	MG	CA	1783	1/1	0.30	-	65,65,65,65	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	DA	3366	1/1	0.19	-	86,86,86,86	0
56	MG	CA	1702	1/1	0.12	-	24,24,24,24	0
56	MG	AA	1873	1/1	0.31	-	77,77,77,77	0
56	MG	BA	3755	1/1	0.23	-	58,58,58,58	0
56	MG	AA	1728	1/1	0.36	-	46,46,46,46	0
56	MG	AA	1779	1/1	0.59	-	34,34,34,34	0
56	MG	CZ	111	1/1	0.31	-	3,3,3,3	0
56	MG	DA	3457	1/1	0.24	-	4,4,4,4	0
56	MG	AA	1875	1/1	0.53	-	83,83,83,83	0
56	MG	BA	3578	1/1	0.09	-	48,48,48,48	0
56	MG	AA	1993	1/1	0.23	-	46,46,46,46	0
56	MG	BA	3674	1/1	0.19	-	12,12,12,12	0
56	MG	DA	3370	1/1	0.17	-	71,71,71,71	0
56	MG	DA	3044	1/1	0.17	-	3,3,3,3	0
56	MG	BA	3794	1/1	0.13	-	65,65,65,65	0
56	MG	BA	3452	1/1	0.12	-	44,44,44,44	0
56	MG	BA	3395	1/1	0.18	-	22,22,22,22	0
56	MG	DA	3372	1/1	0.30	-	3,3,3,3	0
56	MG	B2	103	1/1	0.35	-	36,36,36,36	0
56	MG	BA	3079	1/1	0.30	-	51,51,51,51	0
56	MG	AA	1631	1/1	0.18	-	39,39,39,39	0
56	MG	BA	3796	1/1	0.16	-	30,30,30,30	0
56	MG	AA	1947	1/1	0.13	-	45,45,45,45	0
56	MG	BA	3424	1/1	0.41	-	55,55,55,55	0
56	MG	BA	3658	1/1	0.10	-	36,36,36,36	0
56	MG	BA	3392	1/1	0.11	-	52,52,52,52	0
56	MG	BA	3575	1/1	0.12	-	53,53,53,53	0
56	MG	CA	1770	1/1	0.11	-	54,54,54,54	0
56	MG	DA	3083	1/1	0.20	-	3,3,3,3	0
56	MG	AA	1668	1/1	0.08	-	46,46,46,46	0
56	MG	DA	3272	1/1	0.31	-	3,3,3,3	0
56	MG	AA	1681	1/1	0.09	-	27,27,27,27	0
56	MG	AA	1880	1/1	0.08	-	40,40,40,40	0
56	MG	DA	3283	1/1	0.81	-	70,70,70,70	0
56	MG	CA	1772	1/1	0.21	-	3,3,3,3	0
56	MG	BA	3360	1/1	0.25	-	65,65,65,65	0
56	MG	BA	3909	1/1	0.16	-	39,39,39,39	0
56	MG	DD	5008	1/1	0.14	-	13,13,13,13	0
56	MG	AY	109	1/1	0.15	-	47,47,47,47	0
56	MG	BA	3192	1/1	0.20	-	50,50,50,50	0
56	MG	BA	3090	1/1	0.09	-	43,43,43,43	0
56	MG	AZ	114	1/1	0.11	-	60,60,60,60	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	BA	3443	1/1	0.16	-	71,71,71,71	0
56	MG	AC	302	1/1	0.50	-	88,88,88,88	0
56	MG	AA	1879	1/1	0.17	-	49,49,49,49	0
56	MG	CA	1602	1/1	0.09	-	5,5,5,5	0
56	MG	DA	3009	1/1	0.30	-	3,3,3,3	0
56	MG	AA	1785	1/1	0.40	-	70,70,70,70	0
56	MG	AA	1683	1/1	0.10	-	74,74,74,74	0
56	MG	BO	203	1/1	0.23	-	55,55,55,55	0
56	MG	AA	1646	1/1	0.17	-	38,38,38,38	0
56	MG	BA	3156	1/1	0.49	-	53,53,53,53	0
56	MG	B1	102	1/1	0.07	-	9,9,9,9	0
56	MG	BA	3431	1/1	0.15	-	63,63,63,63	0
56	MG	BA	3520	1/1	0.13	-	61,61,61,61	0
56	MG	AA	1952	1/1	0.14	-	83,83,83,83	0
56	MG	BA	3266	1/1	0.32	-	24,24,24,24	0
56	MG	BA	3175	1/1	0.19	-	69,69,69,69	0
56	MG	BA	3433	1/1	0.29	-	67,67,67,67	0
56	MG	AA	1664	1/1	0.21	-	73,73,73,73	0
56	MG	BA	3054	1/1	0.27	-	63,63,63,63	0
56	MG	BA	3067	1/1	0.06	-	48,48,48,48	0
56	MG	AA	1793	1/1	0.40	-	82,82,82,82	0
56	MG	CA	1797	1/1	0.35	-	28,28,28,28	0
56	MG	DA	3039	1/1	0.19	-	4,4,4,4	0
56	MG	CA	1687	1/1	0.32	-	46,46,46,46	0
56	MG	DA	3384	1/1	0.27	-	3,3,3,3	0
56	MG	AA	1791	1/1	0.09	-	81,81,81,81	0
56	MG	DA	3306	1/1	0.22	-	3,3,3,3	0
56	MG	CA	1615	1/1	0.25	-	3,3,3,3	0
56	MG	AZ	109	1/1	0.12	-	79,79,79,79	0
56	MG	CA	1813	1/1	0.13	-	64,64,64,64	0
56	MG	BA	3007	1/1	0.41	-	20,20,20,20	0
56	MG	BA	3478	1/1	0.17	-	52,52,52,52	0
56	MG	BA	3800	1/1	0.46	-	74,74,74,74	0
56	MG	DA	3339	1/1	0.25	-	6,6,6,6	0
56	MG	BA	3210	1/1	0.10	-	69,69,69,69	0
56	MG	BA	3831	1/1	0.25	-	34,34,34,34	0
56	MG	AA	1806	1/1	0.33	-	27,27,27,27	0
56	MG	DB	211	1/1	0.25	-	3,3,3,3	0
56	MG	BA	3735	1/1	0.11	-	29,29,29,29	0
56	MG	CA	1617	1/1	0.11	-	4,4,4,4	0
56	MG	CA	1705	1/1	0.61	-	60,60,60,60	0
56	MG	DA	3132	1/1	0.48	-	65,65,65,65	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	AY	105	1/1	0.08	-	39,39,39,39	0
56	MG	BA	3136	1/1	0.18	-	45,45,45,45	0
56	MG	AA	1869	1/1	0.18	-	47,47,47,47	0
56	MG	AA	1893	1/1	0.25	-	52,52,52,52	0
56	MG	BA	3277	1/1	0.19	-	57,57,57,57	0
56	MG	BA	3404	1/1	0.13	-	11,11,11,11	0
56	MG	DA	3043	1/1	0.19	-	3,3,3,3	0
56	MG	BA	3797	1/1	0.21	-	52,52,52,52	0
56	MG	BA	3611	1/1	0.21	-	8,8,8,8	0
56	MG	BA	3786	1/1	0.36	-	18,18,18,18	0
56	MG	BA	3085	1/1	0.19	-	29,29,29,29	0
56	MG	BA	3406	1/1	0.29	-	23,23,23,23	0
56	MG	BE	302	1/1	0.49	-	67,67,67,67	0
56	MG	AA	1976	1/1	0.15	-	70,70,70,70	0
56	MG	CA	1685	1/1	0.31	-	68,68,68,68	0
56	MG	CA	1750	1/1	0.15	-	4,4,4,4	0
56	MG	DA	3094	1/1	0.37	-	3,3,3,3	0
56	MG	DA	3184	1/1	0.23	-	3,3,3,3	0
56	MG	AA	1971	1/1	0.31	-	57,57,57,57	0
56	MG	BA	3344	1/1	0.40	-	47,47,47,47	0
56	MG	DA	3170	1/1	0.25	-	3,3,3,3	0
56	MG	DA	3120	1/1	0.37	-	28,28,28,28	0
56	MG	CA	1791	1/1	0.48	-	54,54,54,54	0
56	MG	DA	3467	1/1	0.15	-	3,3,3,3	0
56	MG	AA	1698	1/1	0.32	-	53,53,53,53	0
56	MG	DA	3257	1/1	0.28	-	3,3,3,3	0
56	MG	DA	3186	1/1	0.11	-	4,4,4,4	0
56	MG	BE	306	1/1	0.13	-	71,71,71,71	0
56	MG	CA	1767	1/1	0.11	-	64,64,64,64	0
56	MG	AA	2011	1/1	0.29	-	75,75,75,75	0
56	MG	BA	3236	1/1	0.15	-	35,35,35,35	0
56	MG	BA	3717	1/1	0.14	-	67,67,67,67	0
56	MG	BA	3295	1/1	0.22	-	22,22,22,22	0
56	MG	BA	3011	1/1	0.17	-	47,47,47,47	0
56	MG	BA	3663	1/1	0.43	-	50,50,50,50	0
56	MG	DA	3111	1/1	0.26	-	3,3,3,3	0
56	MG	AA	1674	1/1	0.10	-	52,52,52,52	0
56	MG	AA	2025	1/1	0.25	-	58,58,58,58	0
56	MG	BA	3112	1/1	0.16	-	40,40,40,40	0
56	MG	DA	3405	1/1	0.11	-	4,4,4,4	0
56	MG	DA	3161	1/1	0.34	-	3,3,3,3	0
56	MG	BA	3269	1/1	0.10	-	31,31,31,31	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	CA	1607	1/1	0.21	-	3,3,3,3	0
56	MG	BA	3197	1/1	0.28	-	85,85,85,85	0
56	MG	BA	3176	1/1	0.46	-	66,66,66,66	0
56	MG	DA	3033	1/1	0.15	-	4,4,4,4	0
56	MG	AK	204	1/1	0.10	-	82,82,82,82	0
56	MG	BA	3548	1/1	0.14	-	36,36,36,36	0
56	MG	CA	1649	1/1	0.09	-	35,35,35,35	0
56	MG	BA	3335	1/1	0.14	-	52,52,52,52	0
56	MG	CA	1758	1/1	0.17	-	78,78,78,78	0
56	MG	DA	3291	1/1	0.23	-	44,44,44,44	0
56	MG	AK	206	1/1	0.24	-	69,69,69,69	0
56	MG	AA	1921	1/1	0.12	-	60,60,60,60	0
56	MG	BA	3280	1/1	0.17	-	29,29,29,29	0
56	MG	BB	217	1/1	0.29	-	74,74,74,74	0
56	MG	BA	3275	1/1	0.26	-	46,46,46,46	0
56	MG	DA	3001	1/1	0.09	-	55,55,55,55	0
56	MG	BF	302	1/1	0.21	-	59,59,59,59	0
56	MG	AA	1994	1/1	0.30	-	52,52,52,52	0
56	MG	BA	3230	1/1	0.10	-	60,60,60,60	0
56	MG	BA	3860	1/1	0.08	-	62,62,62,62	0
56	MG	AA	1905	1/1	0.14	-	50,50,50,50	0
56	MG	BA	3723	1/1	0.15	-	7,7,7,7	0
56	MG	DA	3395	1/1	0.31	-	41,41,41,41	0
56	MG	AG	202	1/1	0.11	-	56,56,56,56	0
56	MG	BA	3414	1/1	0.18	-	23,23,23,23	0
56	MG	DA	3065	1/1	0.15	-	45,45,45,45	0
56	MG	BA	3207	1/1	0.14	-	73,73,73,73	0
56	MG	AC	303	1/1	0.09	-	56,56,56,56	0
56	MG	AA	1743	1/1	0.11	-	63,63,63,63	0
56	MG	BA	3307	1/1	0.14	-	34,34,34,34	0
56	MG	DA	3332	1/1	0.21	-	33,33,33,33	0
56	MG	DA	3239	1/1	0.08	-	78,78,78,78	0
56	MG	DA	3080	1/1	0.27	-	3,3,3,3	0
56	MG	DA	3486	1/1	0.38	-	3,3,3,3	0
56	MG	BA	3225	1/1	0.10	-	27,27,27,27	0
56	MG	DB	210	1/1	0.21	-	3,3,3,3	0
56	MG	BA	3068	1/1	0.23	-	50,50,50,50	0
56	MG	BA	3042	1/1	0.50	-	74,74,74,74	0
56	MG	DA	3031	1/1	0.42	-	3,3,3,3	0
56	MG	BA	3073	1/1	0.45	-	57,57,57,57	0
56	MG	CA	1658	1/1	0.26	-	3,3,3,3	0
56	MG	DA	3248	1/1	0.16	-	3,3,3,3	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	BA	3631	1/1	0.30	-	67,67,67,67	0
56	MG	BA	3062	1/1	0.12	-	56,56,56,56	0
56	MG	AA	1774	1/1	0.14	-	39,39,39,39	0
56	MG	BA	3300	1/1	0.46	-	61,61,61,61	0
56	MG	BA	3550	1/1	0.31	-	42,42,42,42	0
56	MG	DA	3076	1/1	0.18	-	3,3,3,3	0
56	MG	BA	3353	1/1	0.28	-	37,37,37,37	0
56	MG	AA	1689	1/1	0.13	-	55,55,55,55	0
56	MG	DA	3204	1/1	0.35	-	43,43,43,43	0
56	MG	BA	3706	1/1	0.17	-	45,45,45,45	0
56	MG	AA	2009	1/1	0.33	-	47,47,47,47	0
56	MG	BA	3110	1/1	0.09	-	65,65,65,65	0
56	MG	CA	1655	1/1	0.34	-	38,38,38,38	0
56	MG	BA	3202	1/1	0.39	-	57,57,57,57	0
56	MG	AA	1960	1/1	0.31	-	53,53,53,53	0
56	MG	AA	1654	1/1	0.12	-	75,75,75,75	0
56	MG	DA	3322	1/1	0.29	-	3,3,3,3	0
56	MG	DA	3104	1/1	0.35	-	21,21,21,21	0
56	MG	AA	1760	1/1	0.09	-	8,8,8,8	0
56	MG	AA	1841	1/1	0.24	-	8,8,8,8	0
56	MG	CA	1786	1/1	0.27	-	67,67,67,67	0
56	MG	BA	3733	1/1	0.28	-	38,38,38,38	0
56	MG	AA	1870	1/1	0.24	-	85,85,85,85	0
56	MG	AA	1820	1/1	0.15	-	46,46,46,46	0
56	MG	CA	1757	1/1	0.29	-	66,66,66,66	0
56	MG	DA	3469	1/1	0.36	-	3,3,3,3	0
56	MG	BA	3858	1/1	0.28	-	60,60,60,60	0
56	MG	BA	3749	1/1	0.55	-	53,53,53,53	0
56	MG	DA	3194	1/1	0.18	-	3,3,3,3	0
56	MG	DA	3233	1/1	0.15	-	43,43,43,43	0
56	MG	BA	3812	1/1	0.18	-	40,40,40,40	0
56	MG	BA	3150	1/1	0.16	-	41,41,41,41	0
56	MG	DA	3419	1/1	0.30	-	3,3,3,3	0
56	MG	BA	3622	1/1	0.09	-	60,60,60,60	0
56	MG	CA	1729	1/1	0.33	-	36,36,36,36	0
56	MG	BA	3235	1/1	0.14	-	47,47,47,47	0
56	MG	DA	3155	1/1	0.19	-	4,4,4,4	0
56	MG	BA	3484	1/1	0.17	-	47,47,47,47	0
56	MG	AA	1958	1/1	0.86	-	87,87,87,87	0
56	MG	BA	3905	1/1	0.31	-	65,65,65,65	0
56	MG	BA	3855	1/1	0.15	-	49,49,49,49	0
56	MG	DB	205	1/1	0.27	-	3,3,3,3	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	AA	1940	1/1	0.36	-	53,53,53,53	0
56	MG	AA	1855	1/1	0.19	-	21,21,21,21	0
56	MG	DA	3413	1/1	0.20	-	3,3,3,3	0
56	MG	BQ	204	1/1	0.13	-	80,80,80,80	0
56	MG	BA	3795	1/1	0.30	-	84,84,84,84	0
56	MG	BA	3644	1/1	0.23	-	26,26,26,26	0
56	MG	CA	1755	1/1	0.22	-	4,4,4,4	0
56	MG	AA	1902	1/1	0.51	-	61,61,61,61	0
56	MG	DA	3371	1/1	0.07	-	56,56,56,56	0
56	MG	BQ	206	1/1	0.07	-	13,13,13,13	0
56	MG	BA	3476	1/1	0.08	-	18,18,18,18	0
56	MG	CA	1778	1/1	0.17	-	3,3,3,3	0
56	MG	DO	202	1/1	0.10	-	4,4,4,4	0
56	MG	AA	1725	1/1	0.35	-	56,56,56,56	0
56	MG	BA	3562	1/1	0.09	-	28,28,28,28	0
56	MG	BA	3568	1/1	0.16	-	33,33,33,33	0
56	MG	BA	3456	1/1	0.16	-	24,24,24,24	0
56	MG	BA	3771	1/1	0.34	-	72,72,72,72	0
56	MG	AA	1723	1/1	0.27	-	76,76,76,76	0
56	MG	BI	205	1/1	0.12	-	45,45,45,45	0
56	MG	DA	3481	1/1	0.19	-	4,4,4,4	0
56	MG	AA	1657	1/1	0.09	-	45,45,45,45	0
56	MG	BB	219	1/1	0.24	-	41,41,41,41	0
56	MG	BA	3330	1/1	0.12	-	55,55,55,55	0
56	MG	BA	3014	1/1	0.44	-	65,65,65,65	0
56	MG	BA	3109	1/1	0.17	-	70,70,70,70	0
56	MG	BA	3078	1/1	0.16	-	51,51,51,51	0
56	MG	BA	3873	1/1	0.39	-	44,44,44,44	0
56	MG	CA	1707	1/1	0.12	-	36,36,36,36	0
56	MG	BD	5004	1/1	0.14	-	50,50,50,50	0
56	MG	AA	1850	1/1	0.11	-	38,38,38,38	0
56	MG	AA	1885	1/1	0.30	-	58,58,58,58	0
56	MG	DA	3117	1/1	0.14	-	28,28,28,28	0
56	MG	AA	1941	1/1	0.28	-	42,42,42,42	0
56	MG	BS	202	1/1	0.07	-	42,42,42,42	0
56	MG	BA	3557	1/1	0.27	-	29,29,29,29	0
56	MG	DA	3358	1/1	0.11	-	54,54,54,54	0
56	MG	BA	3648	1/1	0.20	-	48,48,48,48	0
57	ZN	CN	101	1/1	0.16	-	100,100,100,100	0
56	MG	CY	103	1/1	0.10	-	31,31,31,31	0
56	MG	BD	5003	1/1	0.14	-	57,57,57,57	0
56	MG	BA	3355	1/1	0.08	-	33,33,33,33	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	DA	3156	1/1	0.39	-	3,3,3,3	0
56	MG	DA	3207	1/1	0.62	-	50,50,50,50	0
56	MG	CA	1728	1/1	0.14	-	57,57,57,57	0
56	MG	AA	1900	1/1	0.34	-	39,39,39,39	0
56	MG	BA	3594	1/1	0.22	-	12,12,12,12	0
56	MG	BA	3055	1/1	0.21	-	73,73,73,73	0
56	MG	BA	3695	1/1	0.16	-	70,70,70,70	0
56	MG	DA	3100	1/1	0.17	-	4,4,4,4	0
56	MG	BA	3884	1/1	0.28	-	80,80,80,80	0
56	MG	BA	3555	1/1	0.20	-	7,7,7,7	0
56	MG	BA	3642	1/1	0.16	-	67,67,67,67	0
56	MG	BA	3486	1/1	0.16	-	36,36,36,36	0
56	MG	CA	1613	1/1	0.17	-	3,3,3,3	0
56	MG	BA	3332	1/1	0.10	-	90,90,90,90	0
56	MG	BA	3177	1/1	0.11	-	40,40,40,40	0
56	MG	BA	3413	1/1	0.07	-	43,43,43,43	0
56	MG	AA	1749	1/1	0.14	-	68,68,68,68	0
56	MG	DA	3053	1/1	0.16	-	4,4,4,4	0
56	MG	BA	3254	1/1	0.22	-	79,79,79,79	0
56	MG	BA	3739	1/1	0.23	-	23,23,23,23	0
56	MG	D6	101	1/1	0.15	-	43,43,43,43	0
56	MG	BA	3115	1/1	0.10	-	61,61,61,61	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.