



# wwPDB X-ray Structure Validation Summary Report ⓘ

May 19, 2020 – 06:17 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 X-ray Structure 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

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

with specific help available everywhere you see the ⓘ symbol.

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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
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11



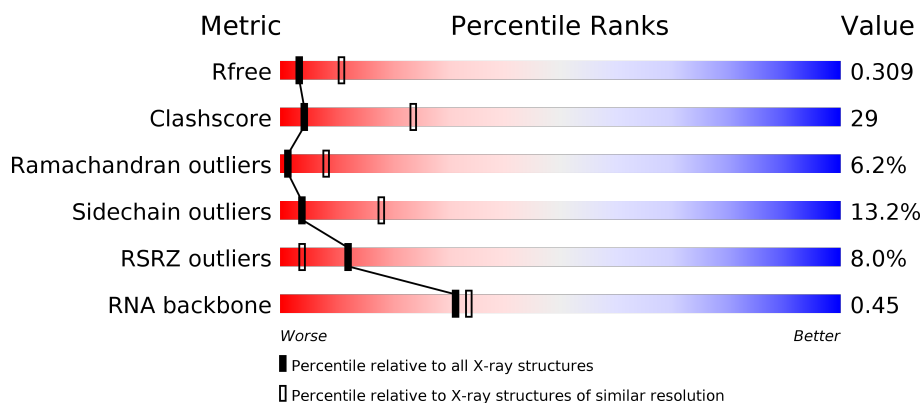
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 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))
$R_{free}$	130704	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (3.00-3.00)
RNA backbone	3102	1173 (3.30-2.70)

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 respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	AA	1525	<div> <div>33%</div> <div>49%</div> <div>14%</div> <div>••</div> </div>
1	CA	1525	<div> <div>31%</div> <div>51%</div> <div>13%</div> <div>••</div> </div>
2	AY	77	<div> <div>38%</div> <div>45%</div> <div>17%</div> </div>
2	AZ	77	<div> <div>25%</div> <div>36%</div> <div>47%</div> <div>16%</div> <div>•</div> </div>

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Mol	Chain	Length	Quality of chain
2	CY	77	
2	CZ	77	
3	AV	27	
3	CV	27	
4	AB	256	
4	CB	256	
5	AC	239	
5	CC	239	
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	

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Mol	Chain	Length	Quality of chain
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	

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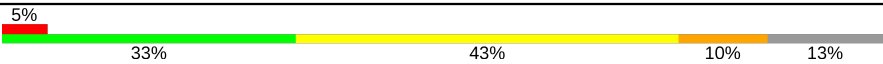



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Mol	Chain	Length	Quality of chain
39	DS	112	
40	BT	146	
40	DT	146	
41	BU	118	
41	DU	118	
42	BV	101	
42	DV	101	
43	BW	113	
43	DW	113	
44	BX	96	
44	DX	96	
45	BY	110	
45	DY	110	
46	BZ	206	
46	DZ	206	
47	B0	85	
47	D0	85	
48	B1	98	
48	D1	98	
49	B2	72	
49	D2	72	
50	B3	60	
50	D3	60	
51	B4	97	
51	D4	97	

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Mol	Chain	Length	Quality of chain
52	B5	60	
52	D5	60	
53	B6	54	
53	D6	54	
54	B7	49	
54	D7	49	
55	B8	65	
55	D8	65	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
56	MG	AA	1605	-	-	-	X
56	MG	AA	1619	-	-	-	X
56	MG	AA	1638	-	-	-	X
56	MG	AA	1653	-	-	-	X
56	MG	AA	1678	-	-	-	X
56	MG	AA	1684	-	-	-	X
56	MG	AA	1764	-	-	-	X
56	MG	AA	1769	-	-	-	X
56	MG	AA	1770	-	-	-	X
56	MG	AA	1875	-	-	-	X
56	MG	AA	1881	-	-	-	X
56	MG	AA	1902	-	-	-	X
56	MG	AA	1955	-	-	-	X
56	MG	AA	1958	-	-	-	X
56	MG	AA	1964	-	-	-	X
56	MG	AA	1989	-	-	-	X
56	MG	AV	5502	-	-	-	X
56	MG	AX	411	-	-	-	X
56	MG	AY	101	-	-	-	X
56	MG	AY	113	-	-	-	X
56	MG	AZ	106	-	-	-	X
56	MG	BA	3009	-	-	-	X
56	MG	BA	3013	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
56	MG	BA	3048	-	-	-	X
56	MG	BA	3093	-	-	-	X
56	MG	BA	3117	-	-	-	X
56	MG	BA	3147	-	-	-	X
56	MG	BA	3156	-	-	-	X
56	MG	BA	3171	-	-	-	X
56	MG	BA	3176	-	-	-	X
56	MG	BA	3193	-	-	-	X
56	MG	BA	3198	-	-	-	X
56	MG	BA	3233	-	-	-	X
56	MG	BA	3239	-	-	-	X
56	MG	BA	3263	-	-	-	X
56	MG	BA	3273	-	-	-	X
56	MG	BA	3296	-	-	-	X
56	MG	BA	3306	-	-	-	X
56	MG	BA	3340	-	-	-	X
56	MG	BA	3343	-	-	-	X
56	MG	BA	3362	-	-	-	X
56	MG	BA	3374	-	-	-	X
56	MG	BA	3389	-	-	-	X
56	MG	BA	3436	-	-	-	X
56	MG	BA	3437	-	-	-	X
56	MG	BA	3441	-	-	-	X
56	MG	BA	3449	-	-	-	X
56	MG	BA	3474	-	-	-	X
56	MG	BA	3593	-	-	-	X
56	MG	BA	3597	-	-	-	X
56	MG	BA	3598	-	-	-	X
56	MG	BA	3600	-	-	-	X
56	MG	BA	3653	-	-	-	X
56	MG	BA	3697	-	-	-	X
56	MG	BA	3712	-	-	-	X
56	MG	BA	3730	-	-	-	X
56	MG	BA	3738	-	-	-	X
56	MG	BA	3745	-	-	-	X
56	MG	BA	3746	-	-	-	X
56	MG	BA	3747	-	-	-	X
56	MG	BA	3757	-	-	-	X
56	MG	BA	3758	-	-	-	X
56	MG	BA	3847	-	-	-	X
56	MG	BA	3874	-	-	-	X
56	MG	BA	3876	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
56	MG	BA	3899	-	-	-	X
56	MG	BB	201	-	-	-	X
56	MG	BB	205	-	-	-	X
56	MG	BB	220	-	-	-	X
56	MG	BF	303	-	-	-	X
56	MG	BT	201	-	-	-	X
56	MG	BU	201	-	-	-	X
56	MG	BW	201	-	-	-	X
56	MG	CA	1669	-	-	-	X
56	MG	CA	1679	-	-	-	X
56	MG	CA	1685	-	-	-	X
56	MG	CA	1689	-	-	-	X
56	MG	CA	1705	-	-	-	X
56	MG	CA	1711	-	-	-	X
56	MG	CA	1713	-	-	-	X
56	MG	CA	1763	-	-	-	X
56	MG	CY	111	-	-	-	X
56	MG	DA	3101	-	-	-	X
56	MG	DA	3129	-	-	-	X
56	MG	DA	3297	-	-	-	X
56	MG	DA	3300	-	-	-	X
56	MG	DA	3320	-	-	-	X
56	MG	DD	5005	-	-	-	X



## 2 Entry composition [i](#)

There are 57 unique types of molecules in this entry. The entry contains 301148 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a RNA chain called 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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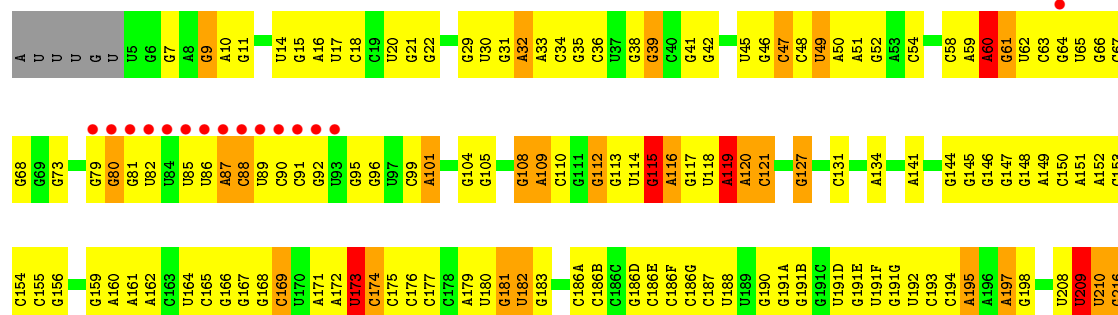
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
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57	CD	1	Total 1	Zn 1	0	0
57	AN	1	Total 1	Zn 1	0	0





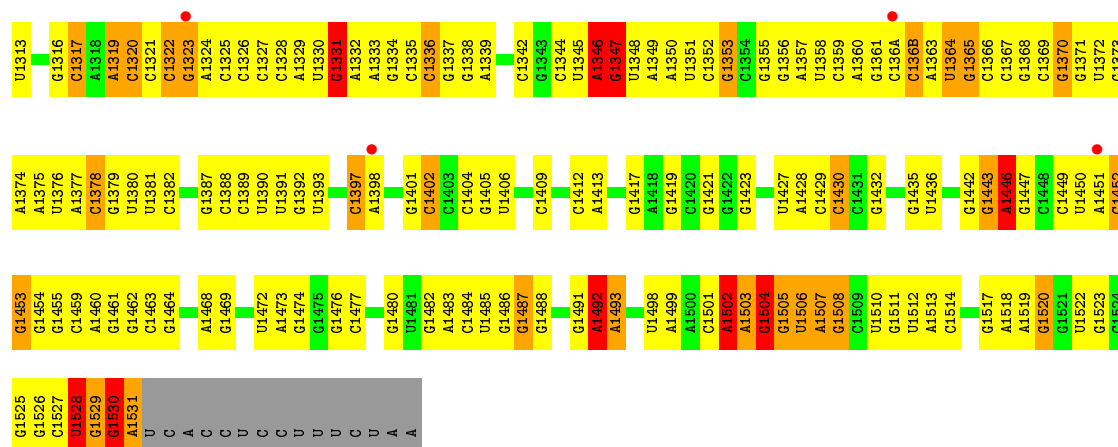




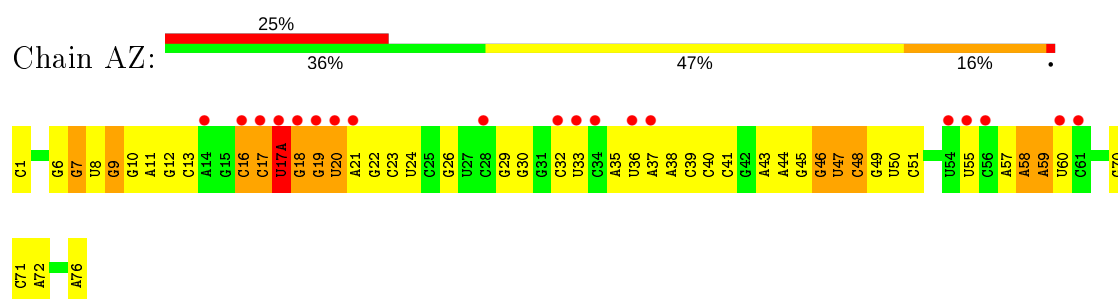


A1250	A1251	A1252	G1253	G1254	G1255	A1256	U1257	G1258	G1259	G1260	C1263	G1264	G1265	A1268	A1269	G1270	G1271	G1272	G1273	G1274	A1275	G1276	G1277	U1278	G1279	A1280	G1281	G1282	G1283	A1284	A1285	A1286	A1287	A1288	G1291	U1292	G1293	G1296	C1297	C1298	A1299	G1300	U1301	U1302	C1303	G1304	A1305	A1306	U1307	U1308	G1309	G1310	G1312																						
A1183	G1184	G1185	G1186	G1187	A1188	G1189	G1190	G1193	U1196	G1197	G1198	U1199	A1200	A1201	G1202	G1203	A1204	U1205	G1206	G1207	G1208	G1209	G1210	G1211	U1212	G1213	A1214	G1215	G1216	G1217	U1218	G1219	G1220	G1221	G1222	G1223	G1224	C1225	A1226	A1227	G1228	A1229	G1230	G1231	U1232	G1233	A1234	U1235	A1236	C1237	A1238	U1239	U1240	G1241	C1244	A1245																			
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G1116	G1117	C1118	U1121	U1122	A1123	G1124	U1125	U1126	G1127	G1128	G1129	A1130	G1131	C1132	G1133	G1134	U1135	U1136	C1137	G1138	G1139	G1140	C1141	G1142	G1143	G1144	G1145	A1146	C1147	U1148	U1149	A1150	A1151	A1152	C1153	G1154	G1155	G1156	A1157	C1158	U1159	G1160	C1161	C1162	C1163	A1169	A1170	G1171	U1172	A1173	G1174	A1175	G1176	G1177	U1178	A1179	C1180	C1181	G1182																
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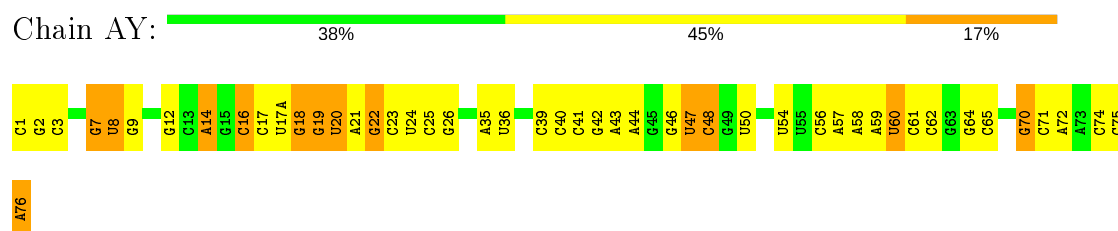




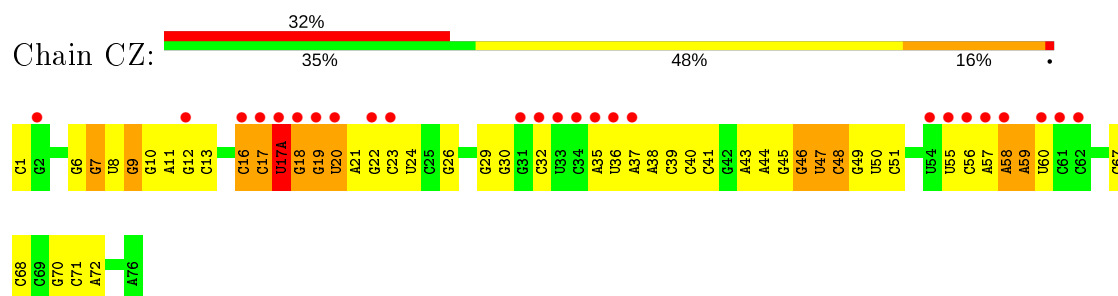
• Molecule 2: P AND E-SITE TRNA(FMET)



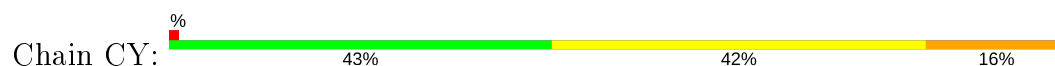
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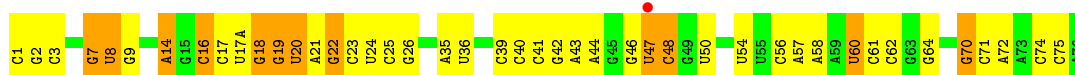
• Molecule 2: P AND E-SITE TRNA(FMET)



• Molecule 2: P AND E-SITE TRNA(FMET)







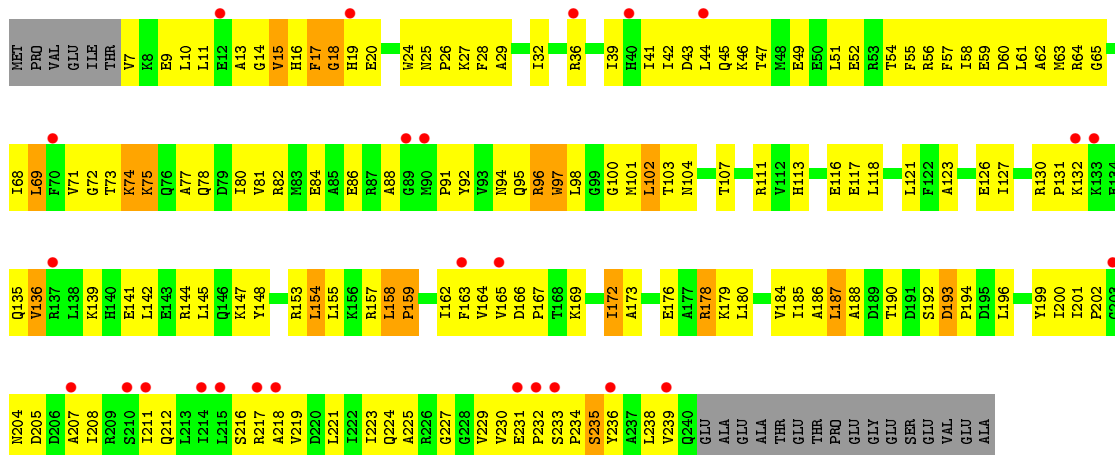
• Molecule 3: MRNA



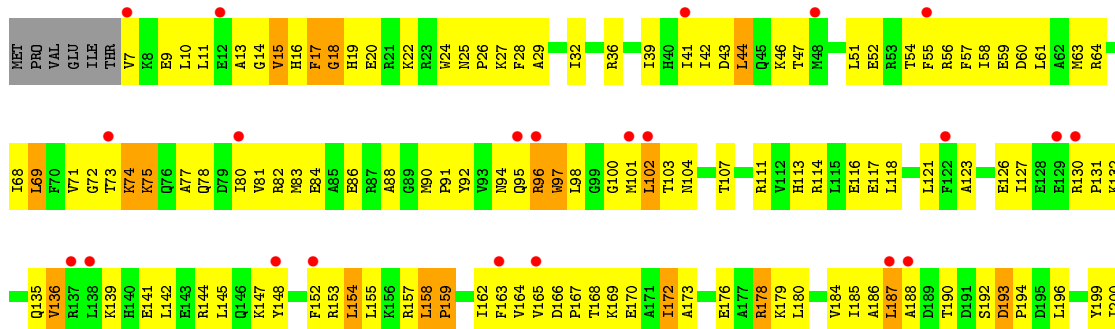
• Molecule 3: MRNA



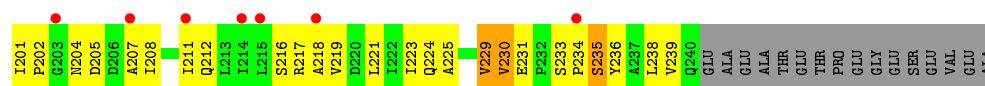
• Molecule 4: 30S ribosomal protein S2



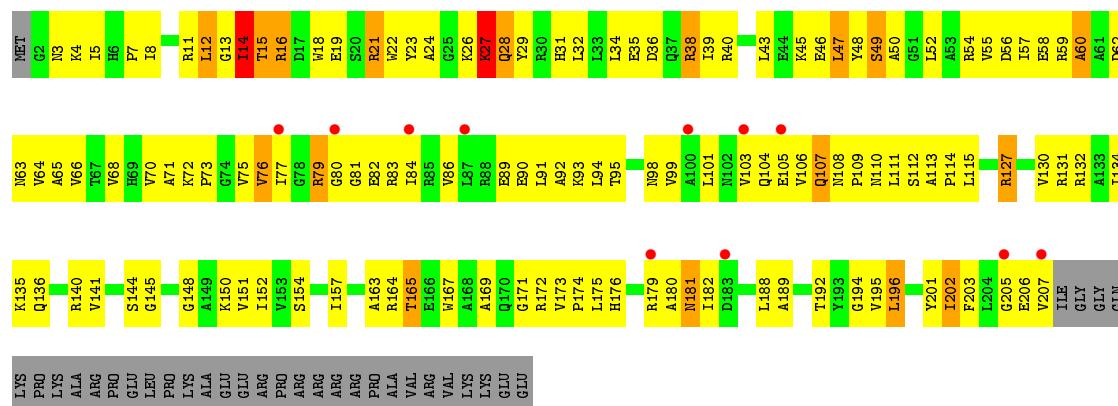
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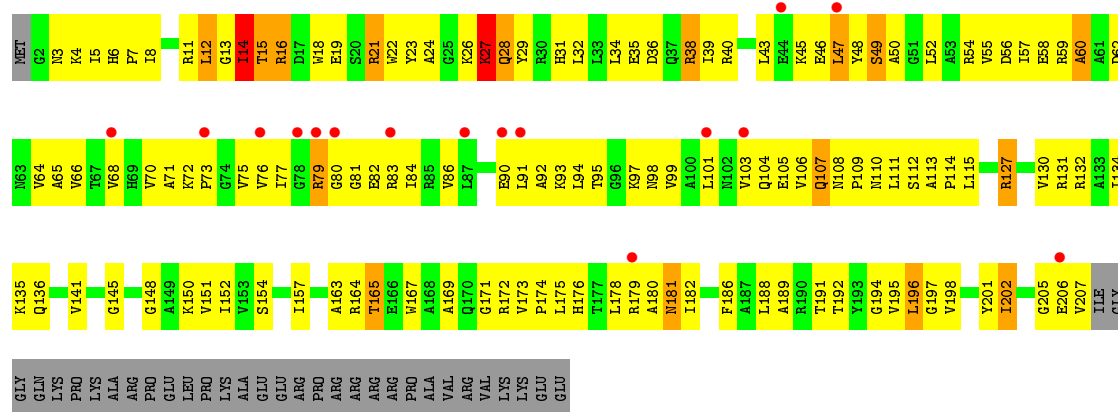




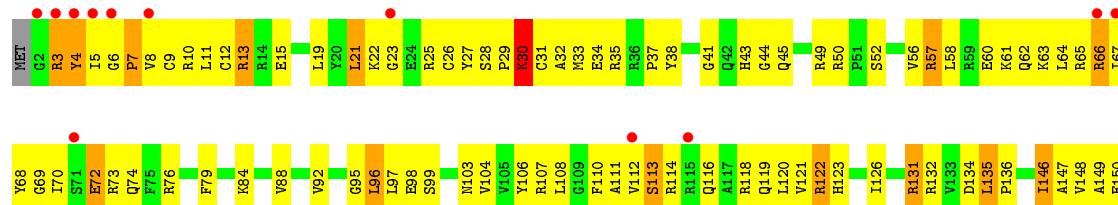
• Molecule 5: 30S ribosomal protein S3



• Molecule 5: 30S ribosomal protein S3



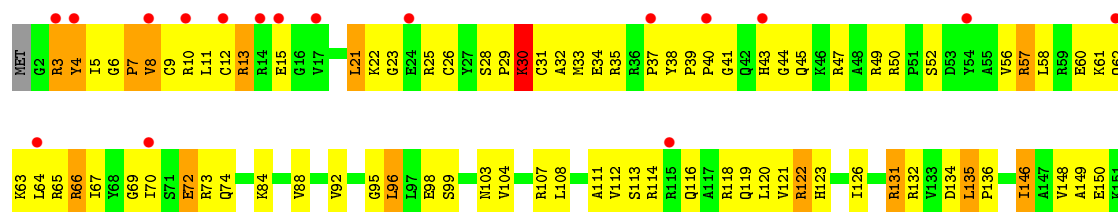
• Molecule 6: 30S ribosomal protein S4



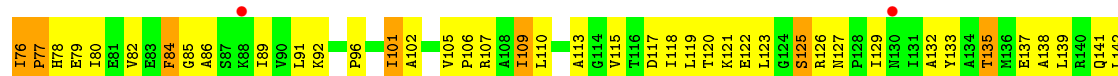
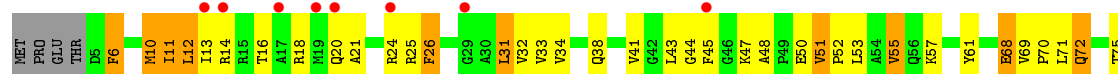
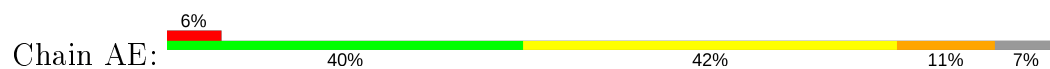




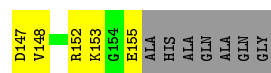
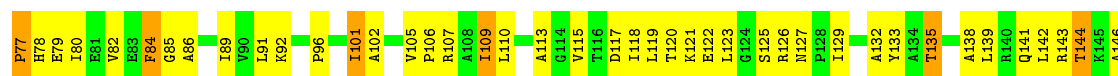
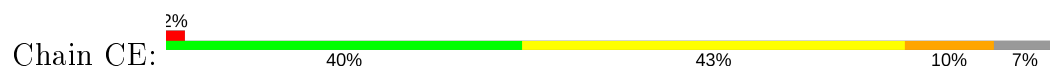
• Molecule 6: 30S ribosomal protein S4



• Molecule 7: 30S ribosomal protein S5



• Molecule 7: 30S ribosomal protein S5



• Molecule 8: 30S ribosomal protein S6

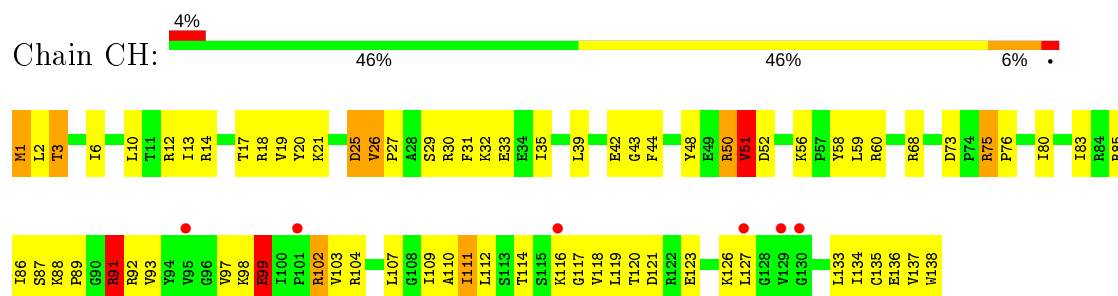




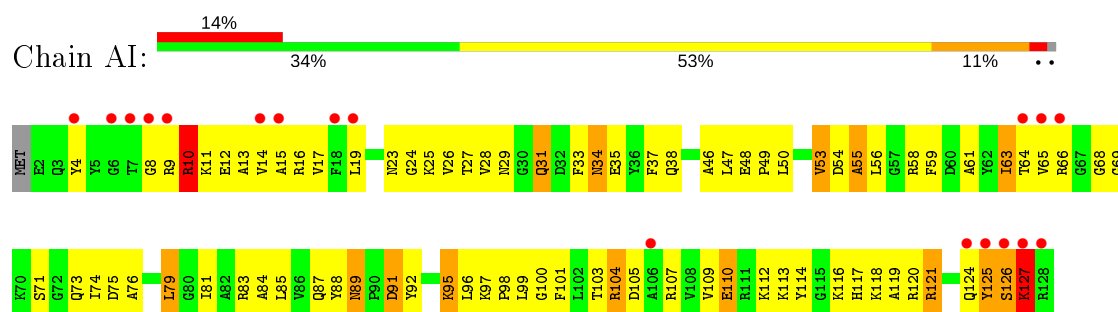




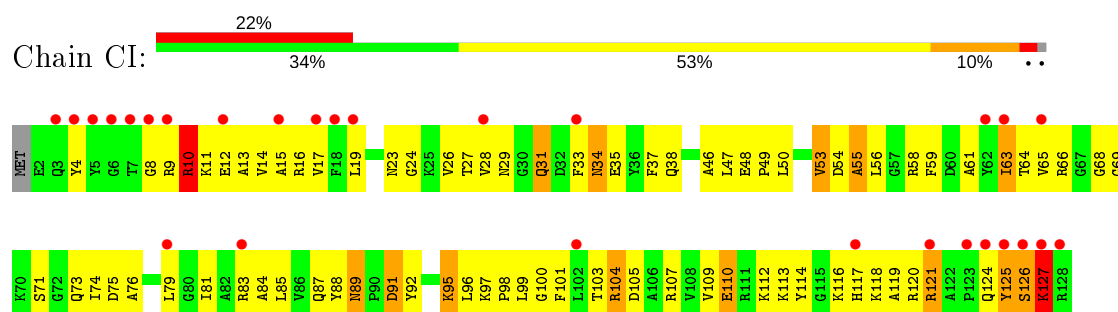
- Molecule 10: 30S ribosomal protein S8



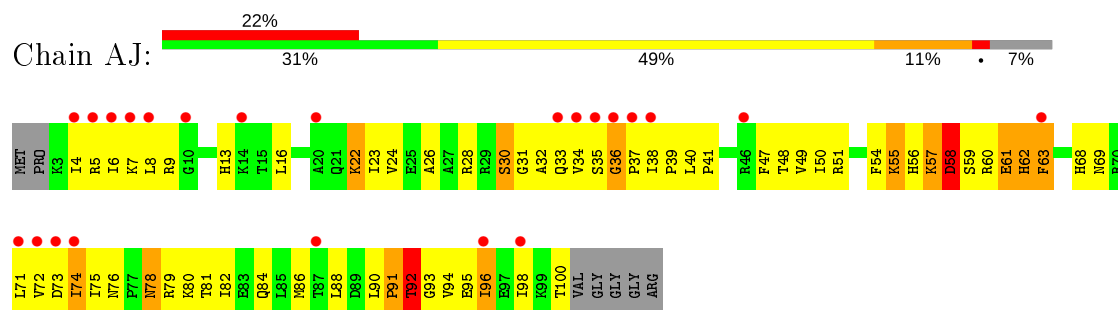
- Molecule 11: 30S ribosomal protein S9



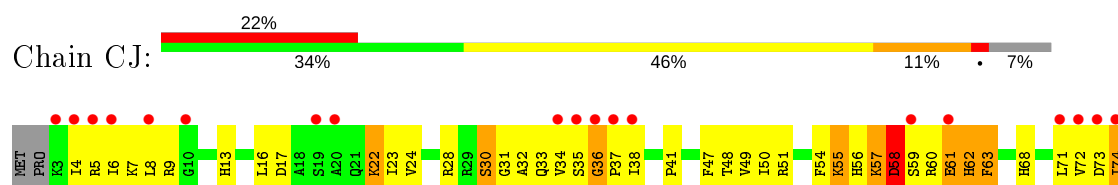
- Molecule 11: 30S ribosomal protein S9



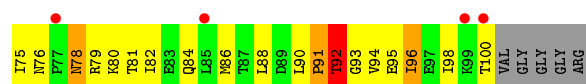
- Molecule 12: 30S ribosomal protein S10



- Molecule 12: 30S ribosomal protein S10







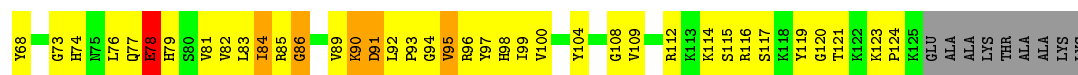
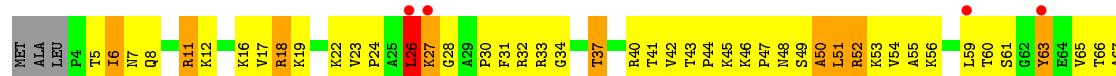
- Molecule 13: 30S ribosomal protein S11



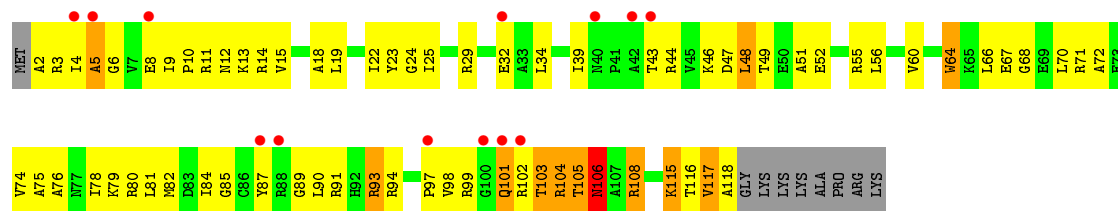
- Molecule 13: 30S ribosomal protein S11



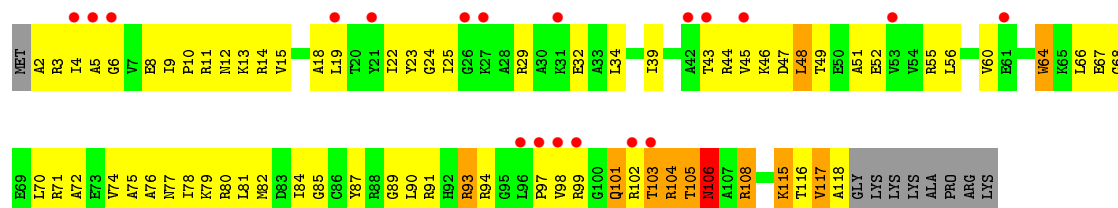
- Molecule 14: 30S ribosomal protein S12







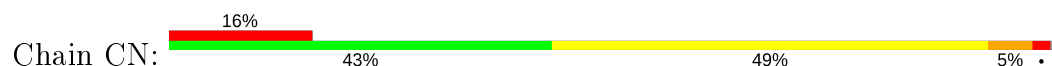
• Molecule 15: 30S ribosomal protein S13



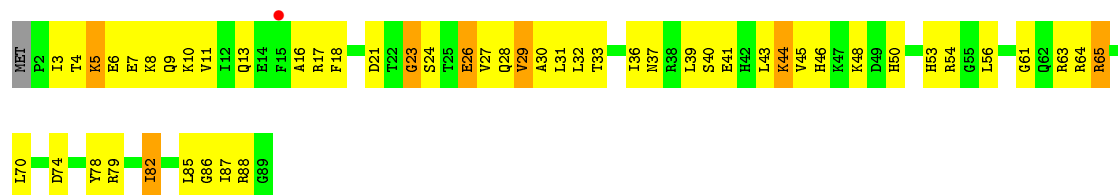
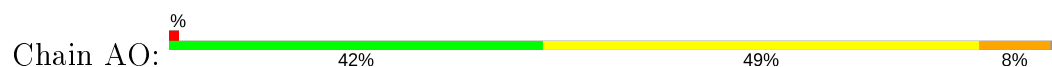
• Molecule 16: 30S ribosomal protein S14



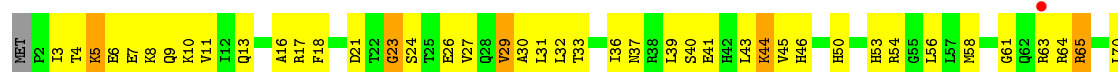
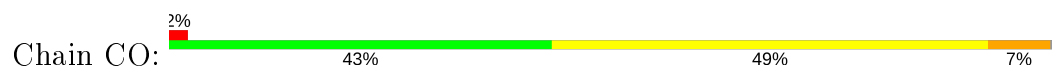
• Molecule 16: 30S ribosomal protein S14



• Molecule 17: 30S ribosomal protein S15



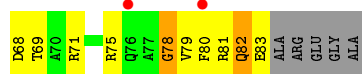
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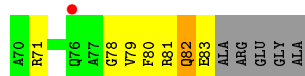
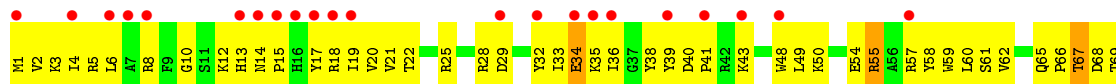




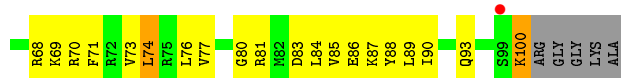
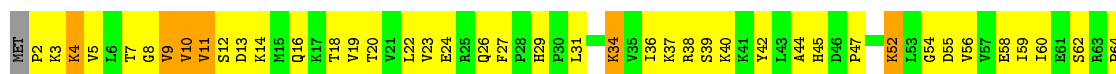
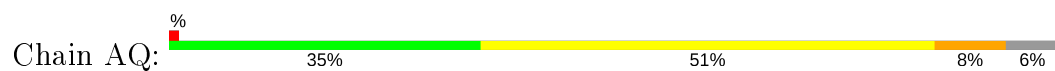
- Molecule 18: 30S ribosomal protein S16



- Molecule 18: 30S ribosomal protein S16



- Molecule 19: 30S ribosomal protein S17



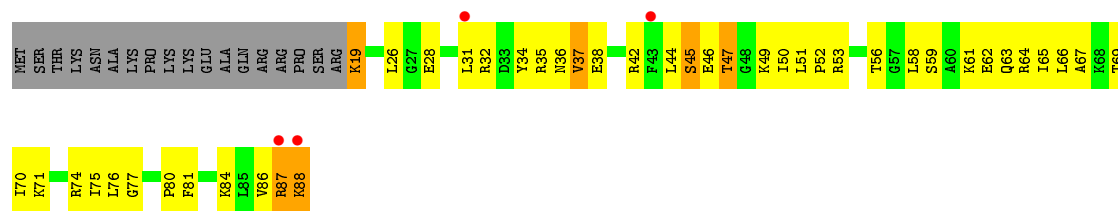
- Molecule 19: 30S ribosomal protein S17



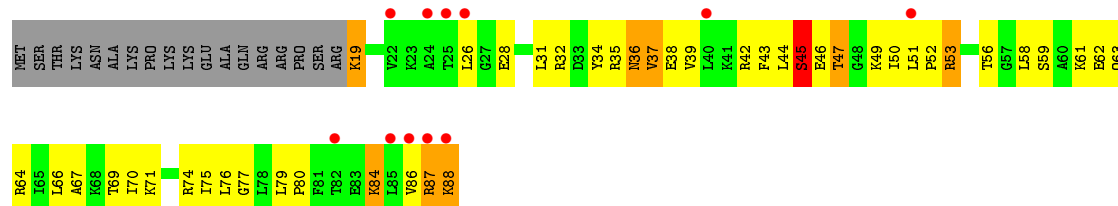
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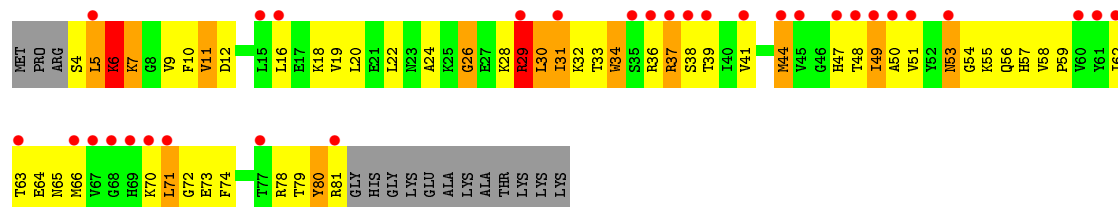




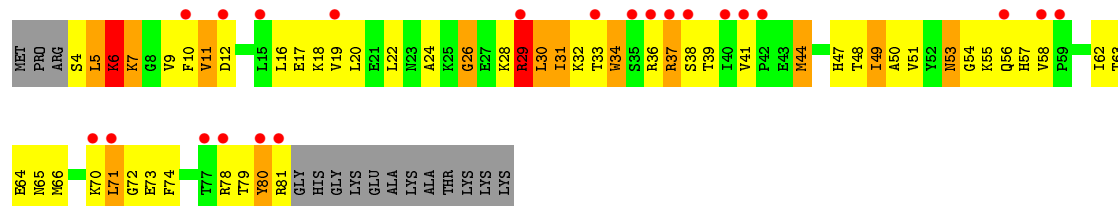
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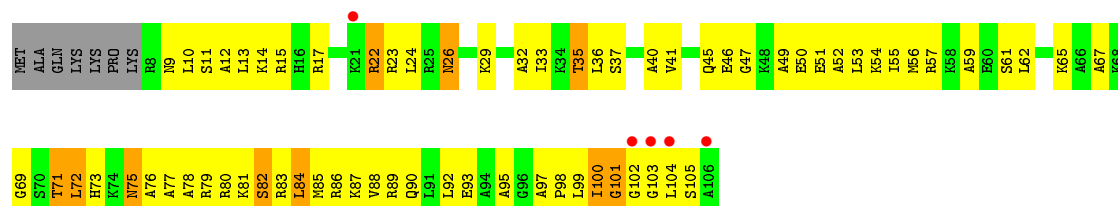
• Molecule 21: 30S ribosomal protein S19



• Molecule 21: 30S ribosomal protein S19



• Molecule 22: 30S ribosomal protein S20

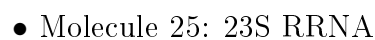




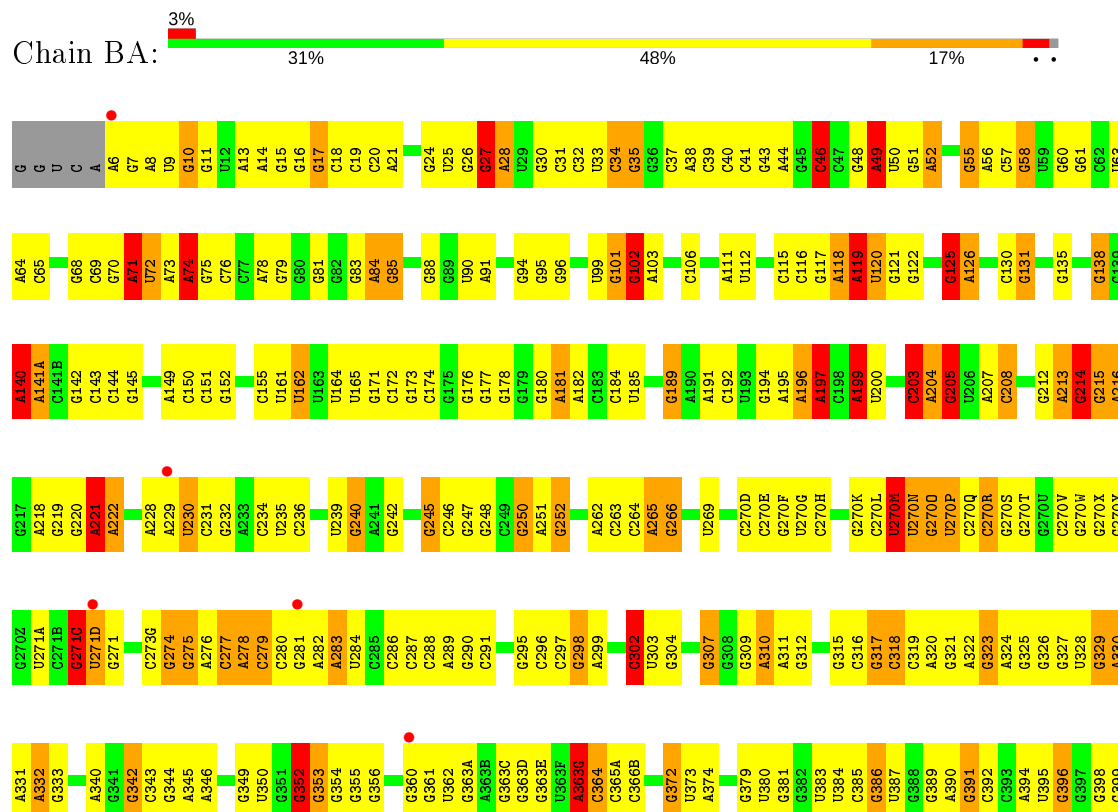




- Chain CX:



Chain BA:



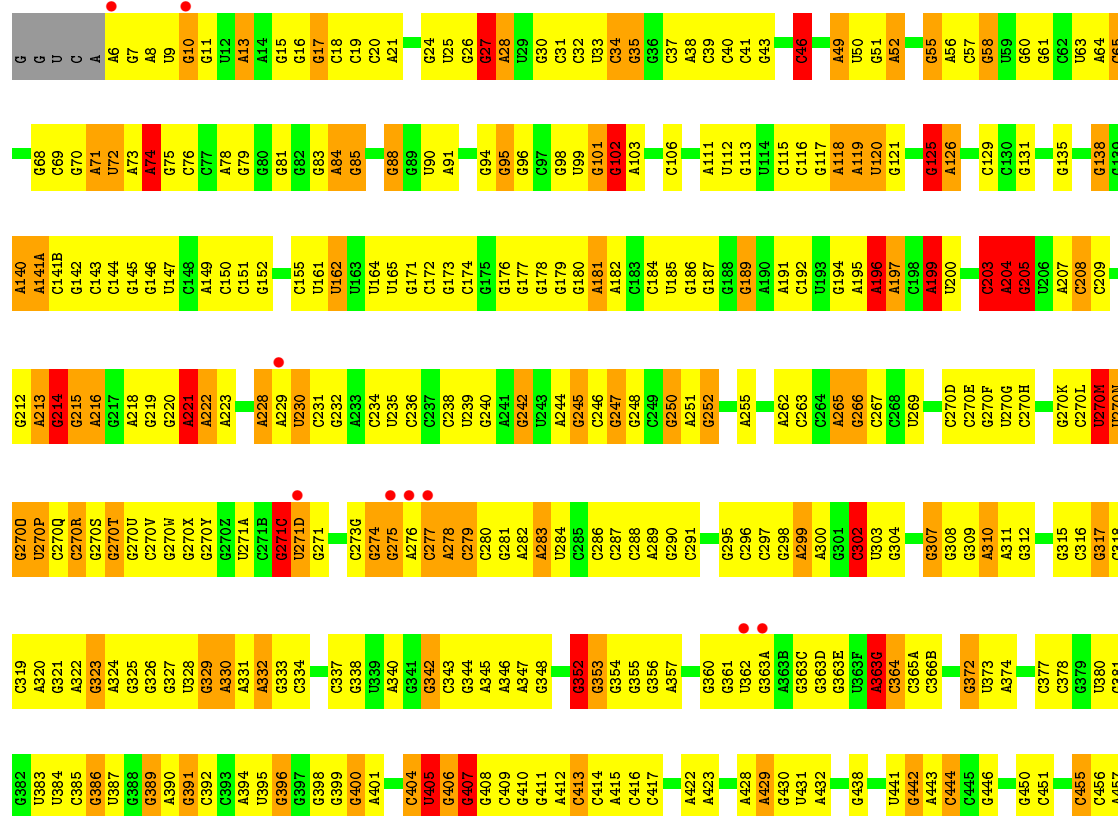


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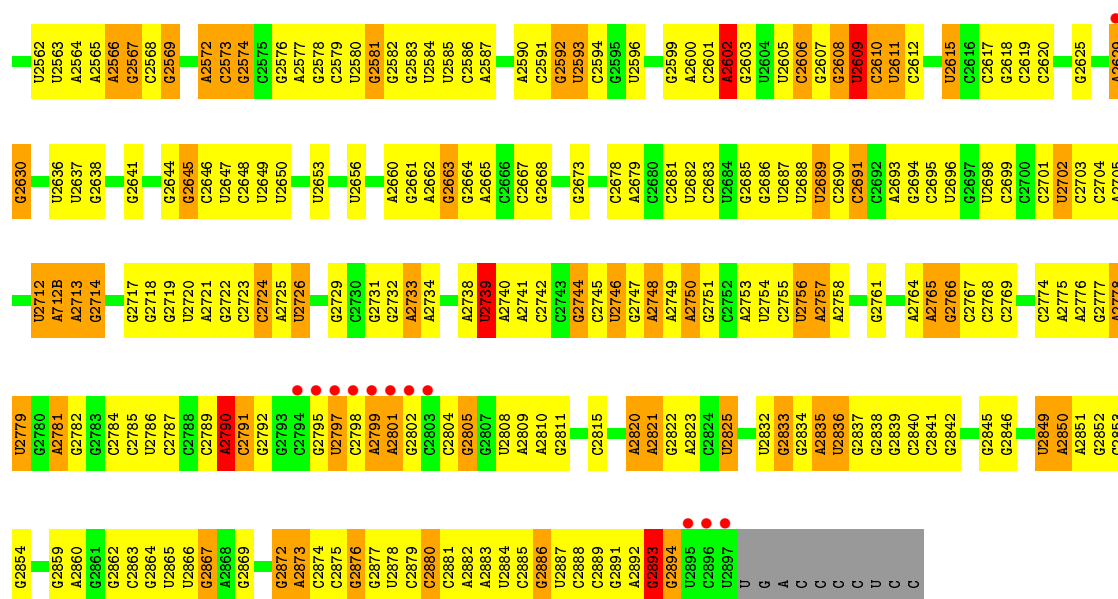


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A1510	U1438	C1293	A1221	A1077	U1009	C935	A866	G791	C720	G648	C580	A507
A1511	A1385	U1300	G1221	U1078	A1009	C936	C867	G792	C721	G649	C581	G508
G1512	U1372	A1301	G1227	C1080	A1010	U937	U868	G793	A722	C850	G582	C509
C1513	G1443	G1302	G1228	U1081	G1011	G938	G869	A793	G723	G851	G583	C510
U1514	G1444	C1303	U1229	U1082	U1012	G939	A870	G794	U724	U852	A586	A515
C1515	A1448	G1304	G1230	U1083	C1013	G940	U871	C795	A727	C653	C587	G512
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G1517	G1446	A1307	G1232	U1085	U1018	G942	C876	C797	G729	A655	C589	A514
C1518	G1447	U1308	C1233	A1086	U1019	U943	C876	G801	C730	G856	A590	A515
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G1521	G1380	C1311	U1236	U1089	G1022	G946	G882	A804	A735	C660	U594	U519
C1522	U1397	U1312	G1238	U1090	U1023	G947	G883	G805	A736	G661	G594	G520
G1523	G1451	U1313	G1239	G1091	G1024	C951	C884	C806	C736	G662	U594	G521
A1524	A1453	C1314	G1244	C1092	G1025	G952	C885	C807	C737	G663	C595	G522
G1525	U1454	U1315	U1244	U1093	A1026	G953	C886	U808	G738	C664	G598	G523
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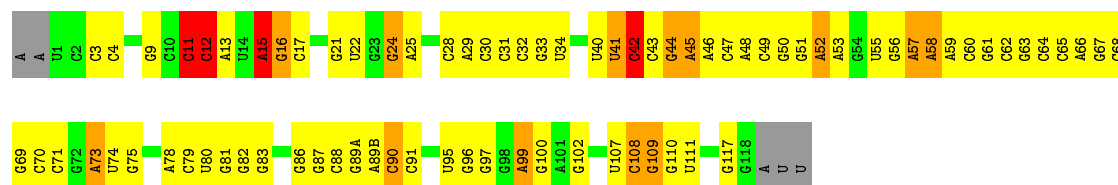
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	A2425	A2352	C2285	G2216	G2066	G2002		A1853		A1677	
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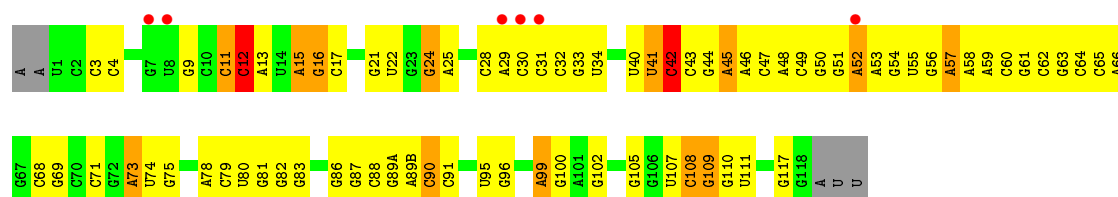
• Molecule 26: 5S rRNA

Chain BB: 32% 50% 10%



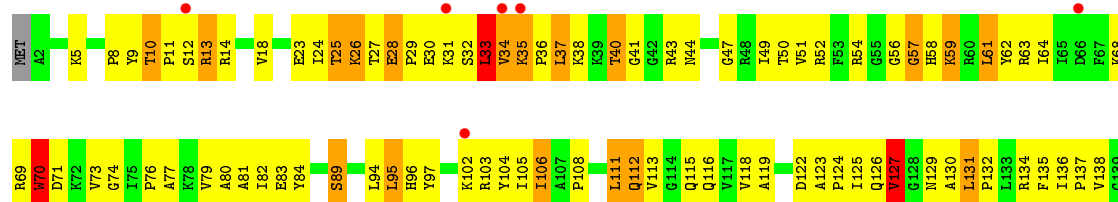
• Molecule 26: 5S rRNA

Chain DB: 33% 51% 10%

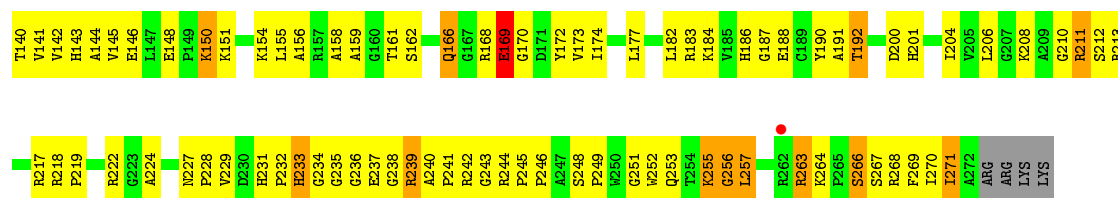


• Molecule 27: 50S ribosomal protein L2

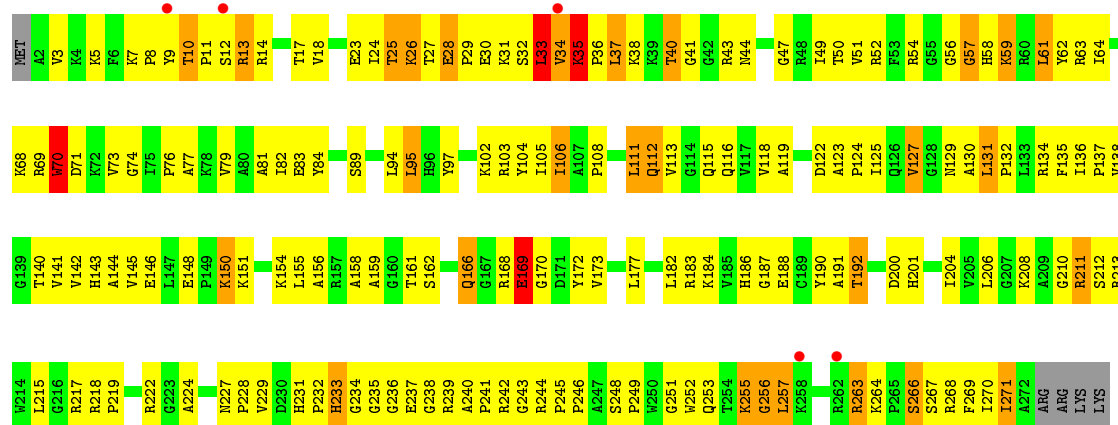
Chain BD: 3% 36% 50% 11%



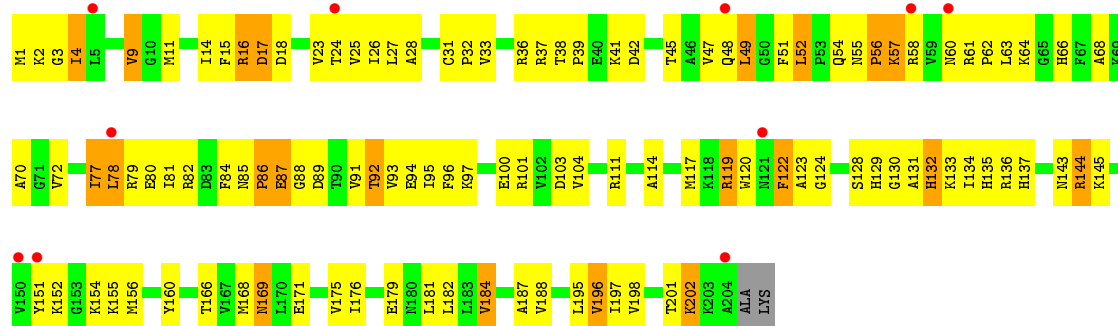




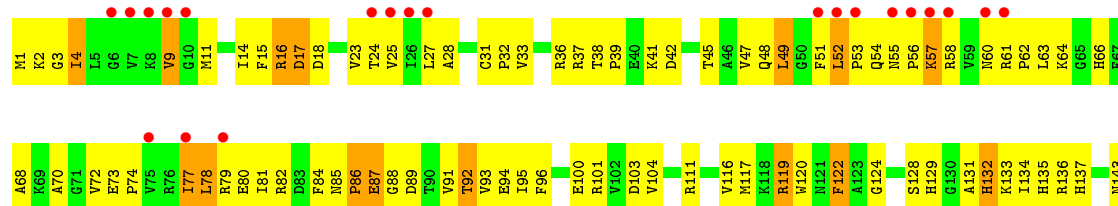
• Molecule 27: 50S ribosomal protein L2



• Molecule 28: 50S ribosomal protein L3



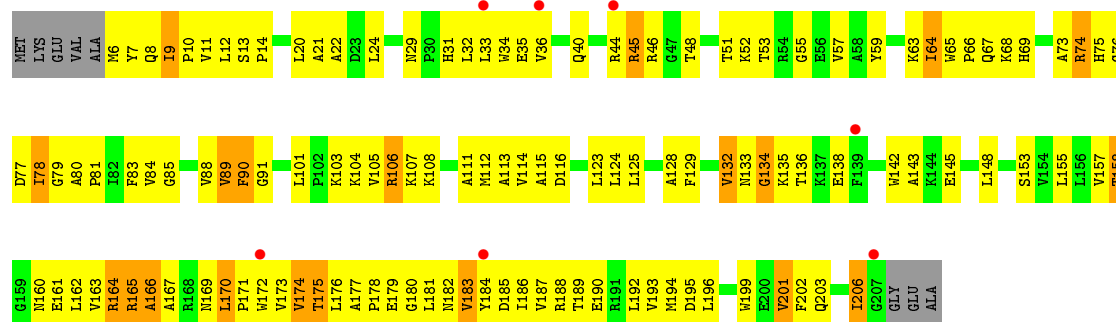
• Molecule 28: 50S ribosomal protein L3



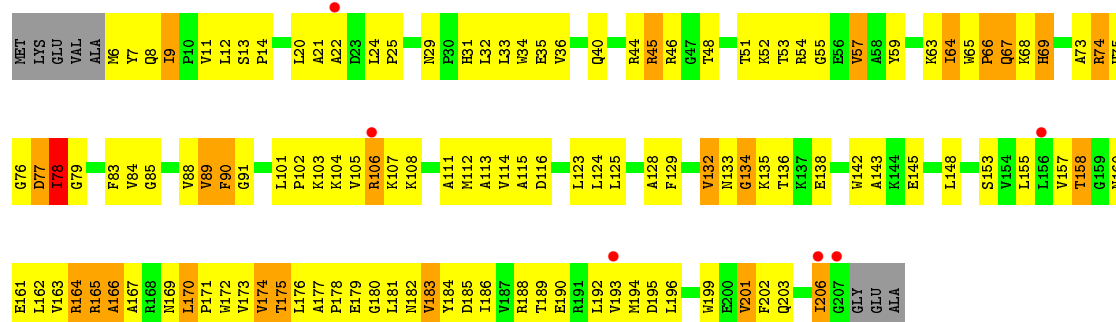




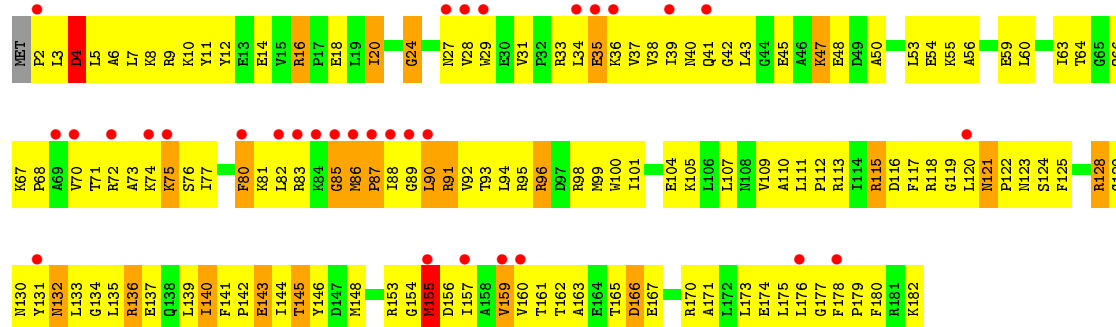
- Molecule 29: 50S ribosomal protein L4



- Molecule 29: 50S ribosomal protein L4



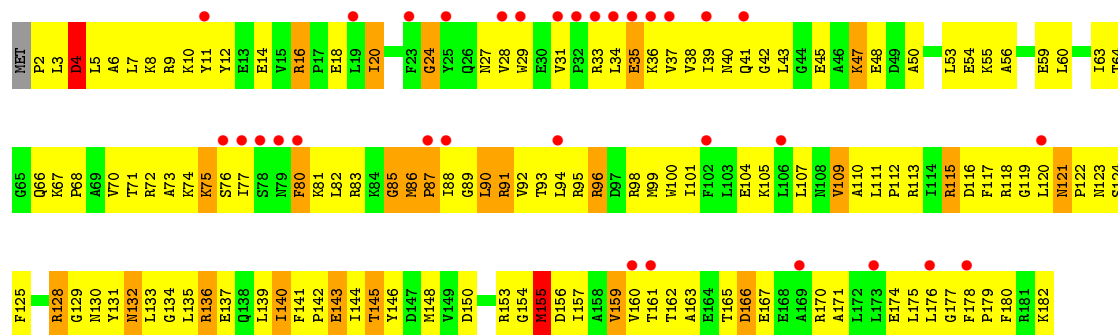
- Molecule 30: 50S ribosomal protein L5



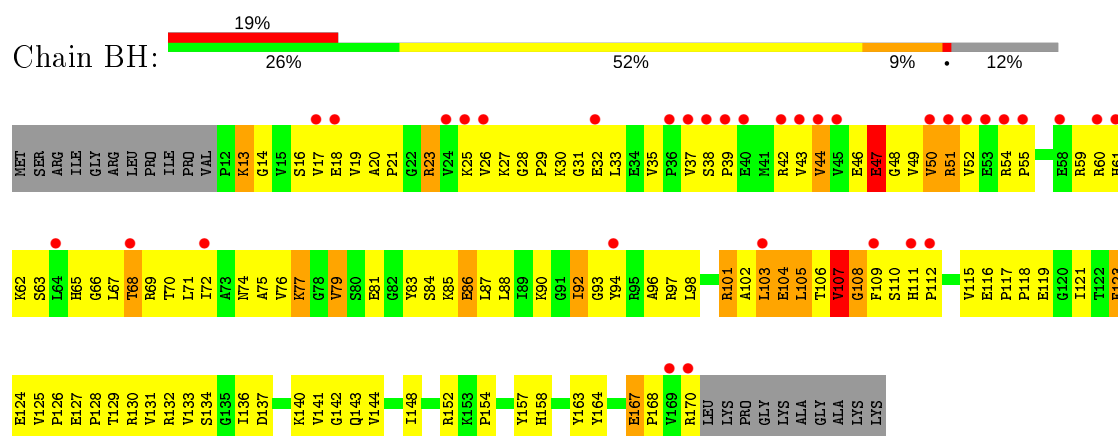
- Molecule 30: 50S ribosomal protein L5



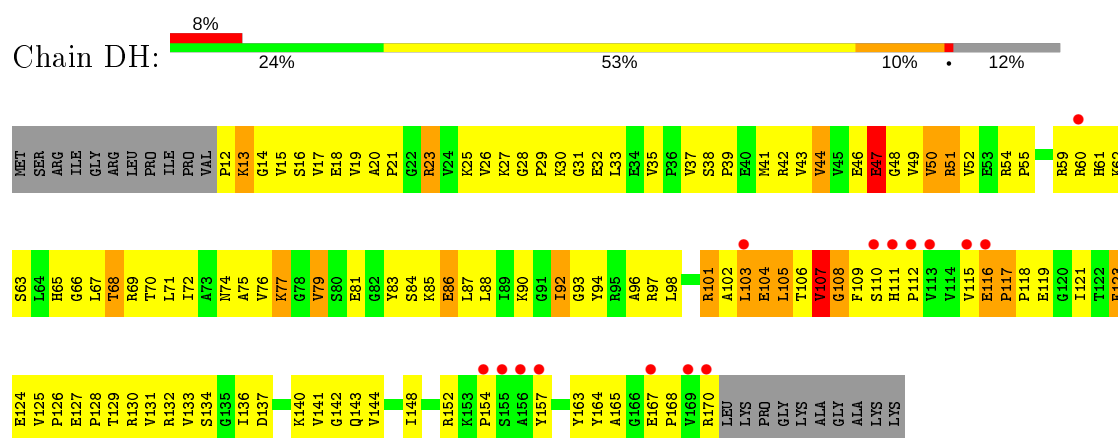




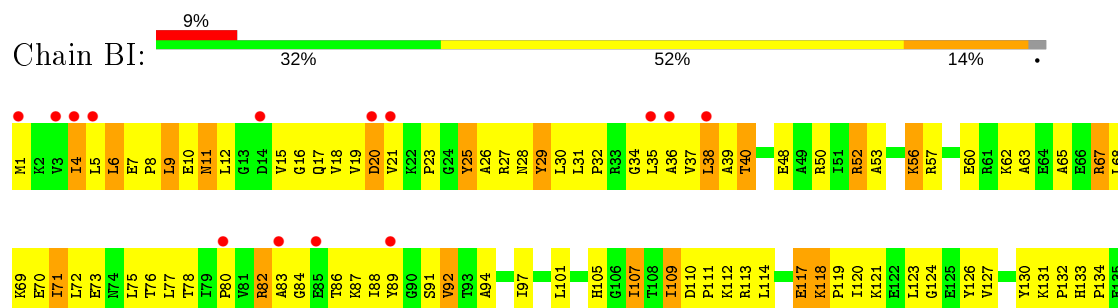
• Molecule 31: 50S ribosomal protein L6



• Molecule 31: 50S ribosomal protein L6



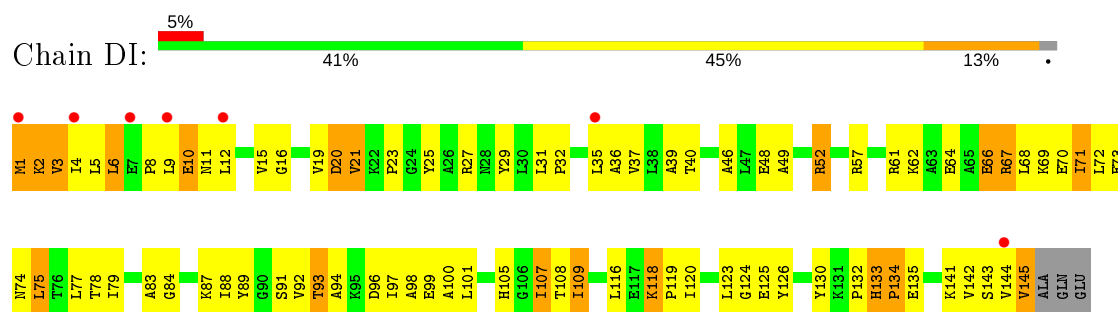
• Molecule 32: 50S ribosomal protein L9



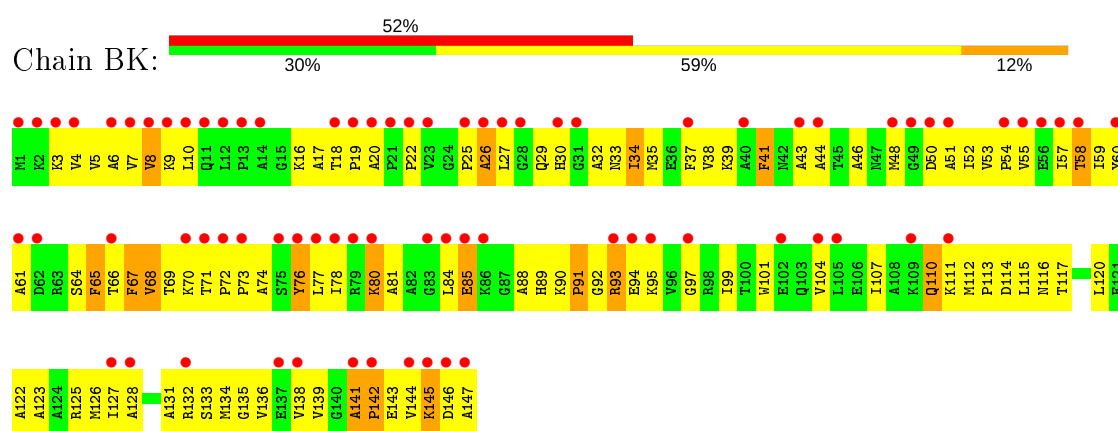




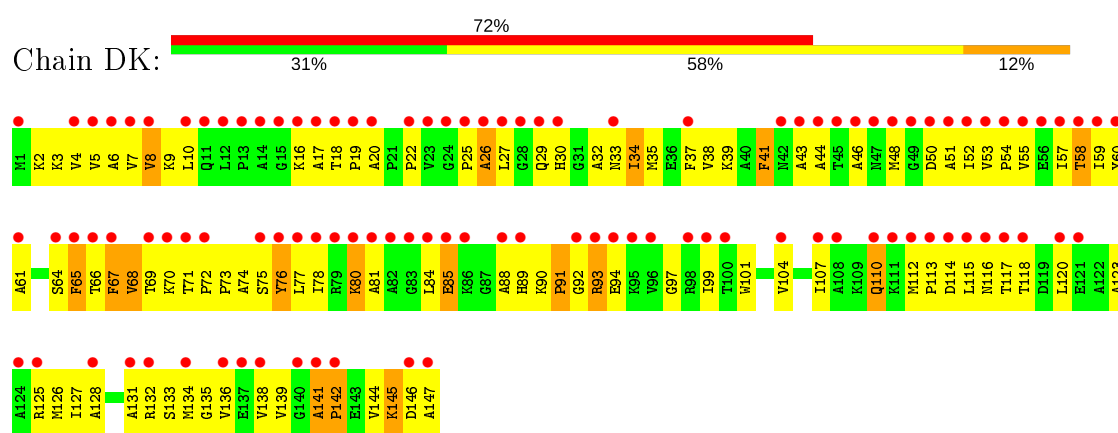
• Molecule 32: 50S ribosomal protein L9



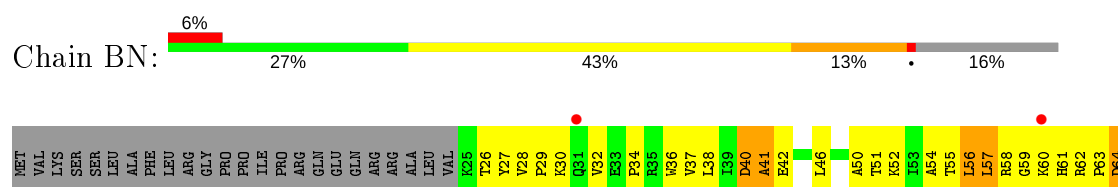
• Molecule 33: 50S ribosomal protein L11



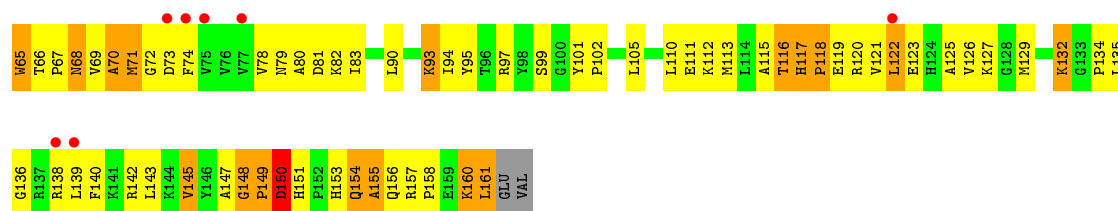
• Molecule 33: 50S ribosomal protein L11



• Molecule 34: 50S ribosomal protein L13



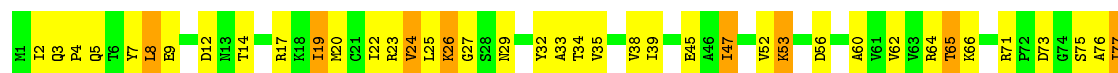




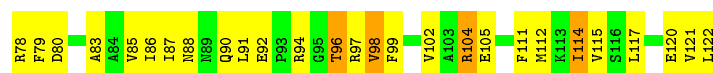
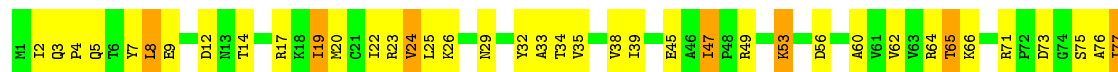
• Molecule 34: 50S ribosomal protein L13



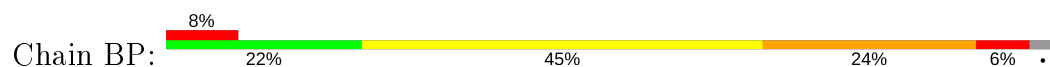
• Molecule 35: 50S ribosomal protein L14



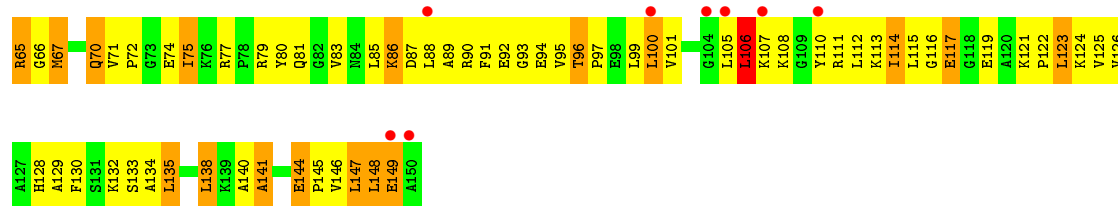
• Molecule 35: 50S ribosomal protein L14



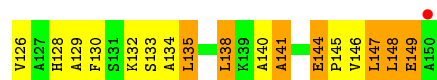
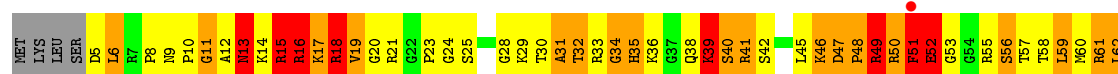
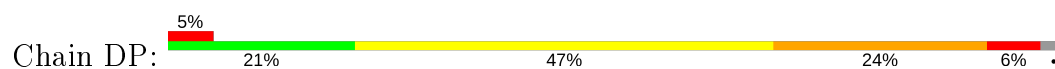
• Molecule 36: 50S ribosomal protein L15



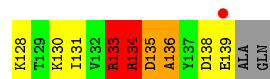
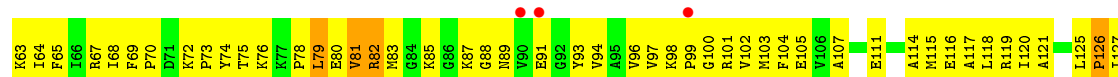




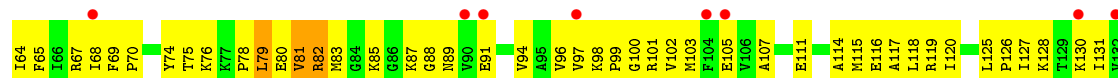
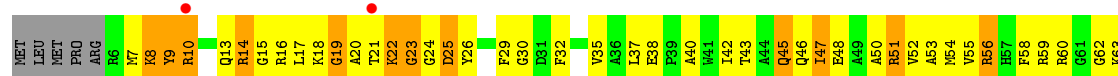
• Molecule 36: 50S ribosomal protein L15



• Molecule 37: 50S ribosomal protein L16

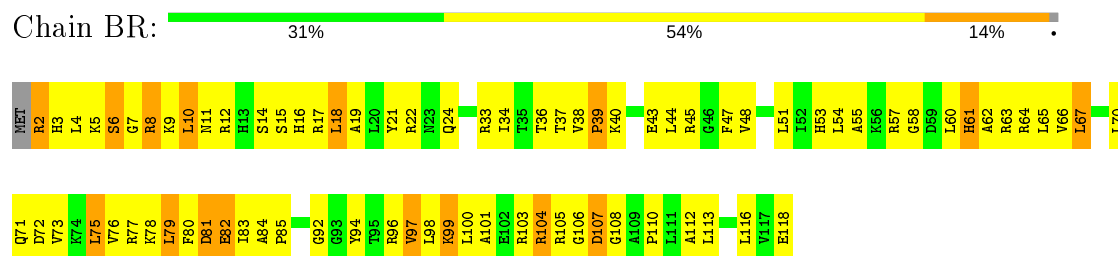


• Molecule 37: 50S ribosomal protein L16

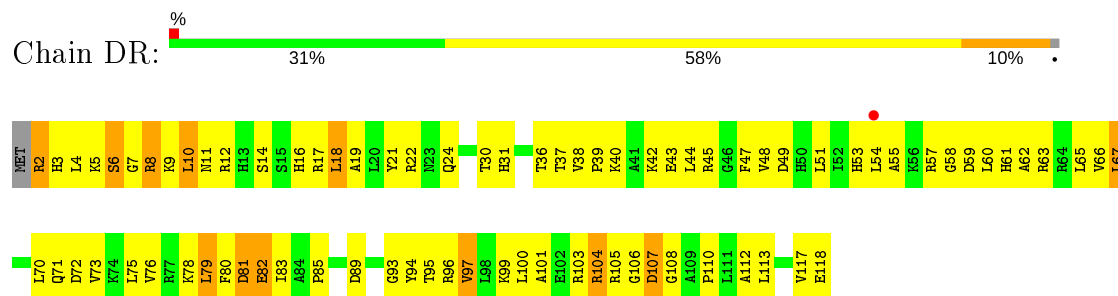




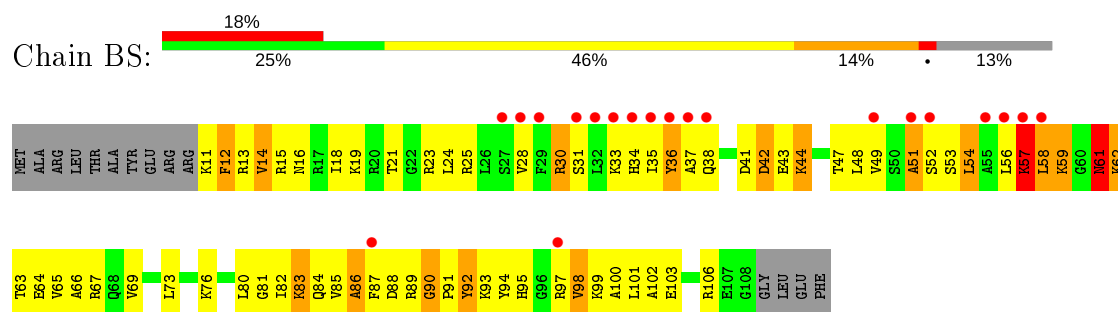
- Molecule 38: 50S ribosomal protein L17



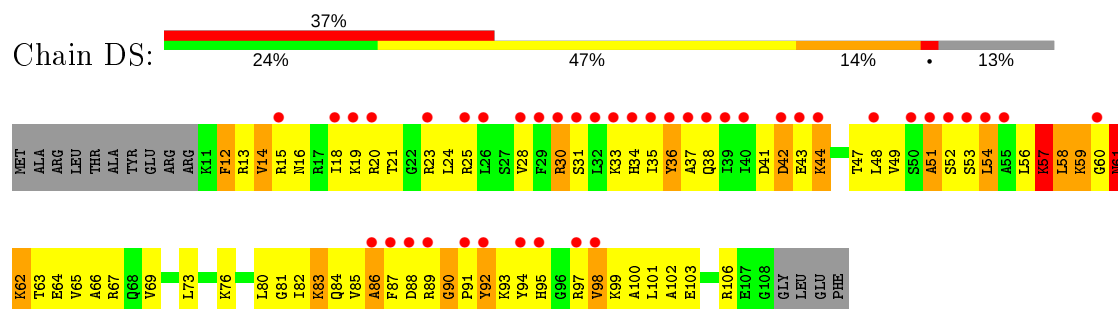
- Molecule 38: 50S ribosomal protein L17



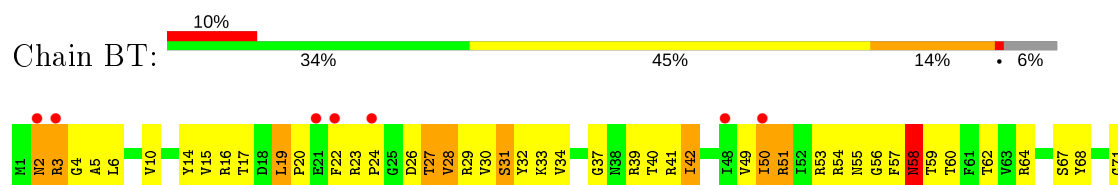
- Molecule 39: 50S ribosomal protein L18



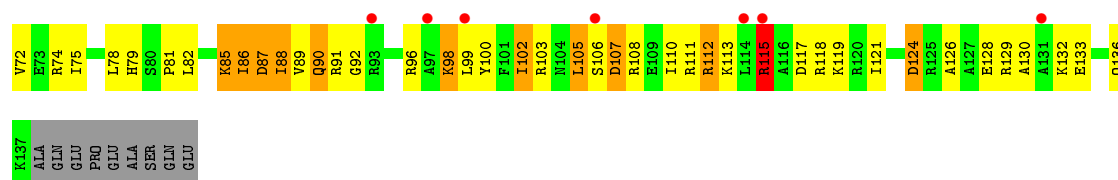
- Molecule 39: 50S ribosomal protein L18



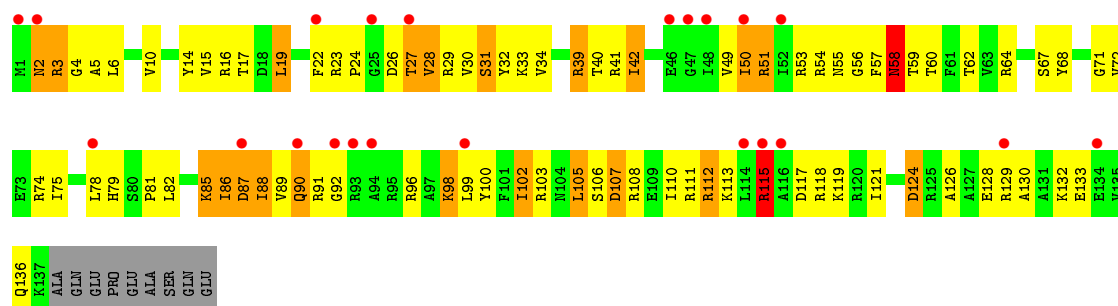
- Molecule 40: 50S ribosomal protein L19



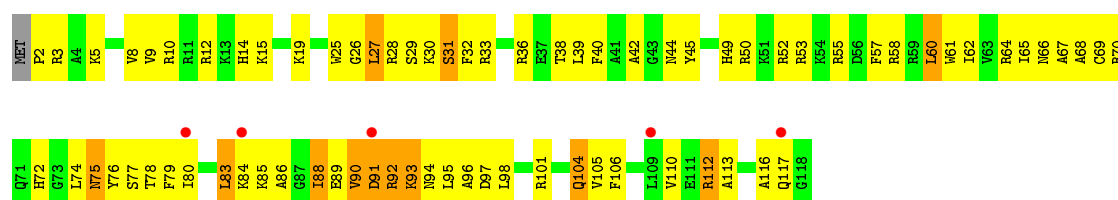




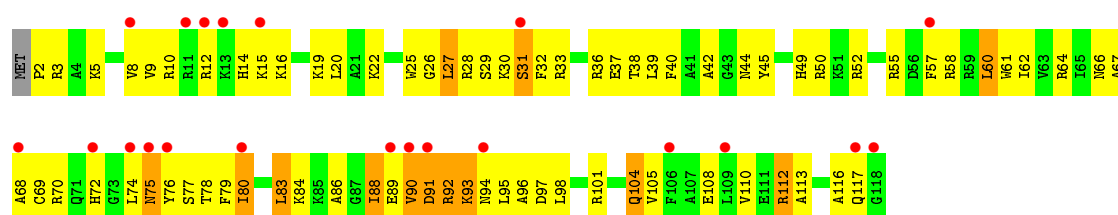
- Molecule 40: 50S ribosomal protein L19



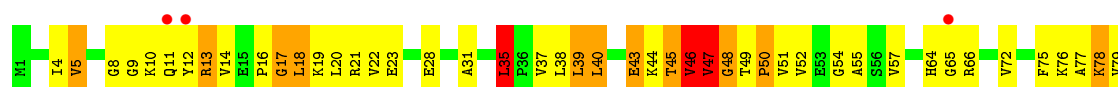
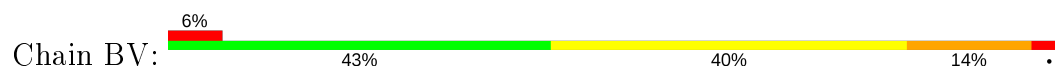
- Molecule 41: 50S ribosomal protein L20



- Molecule 41: 50S ribosomal protein L20



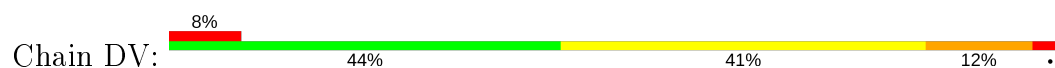
- Molecule 42: 50S ribosomal protein L21



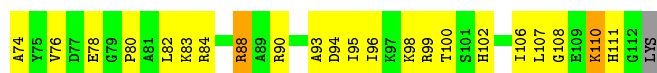
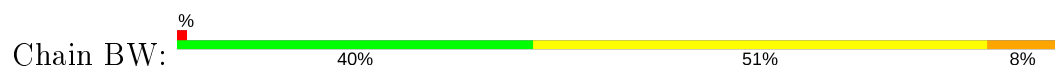




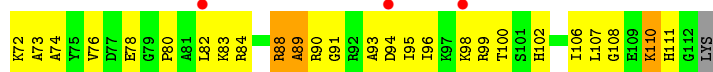
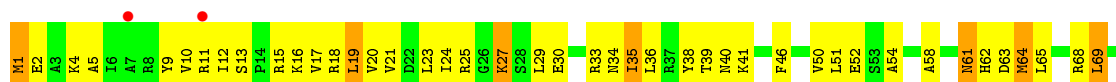
- Molecule 42: 50S ribosomal protein L21



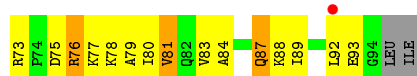
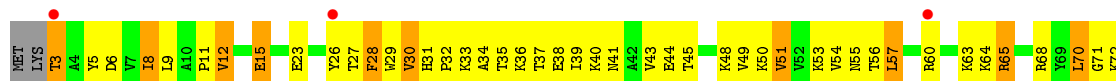
- Molecule 43: 50S ribosomal protein L22



- Molecule 43: 50S ribosomal protein L22



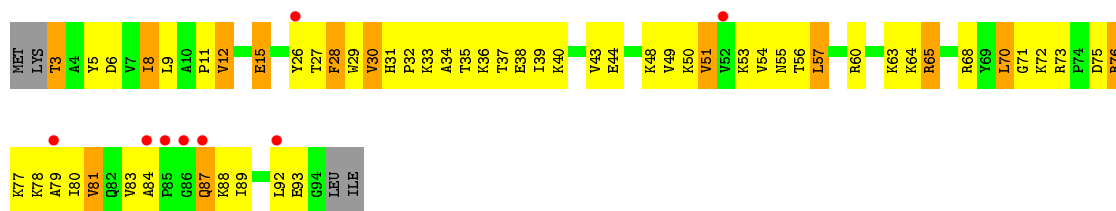
- Molecule 44: 50S ribosomal protein L23



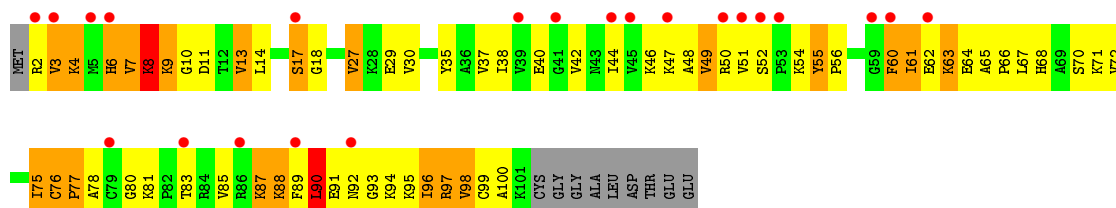
- Molecule 44: 50S ribosomal protein L23



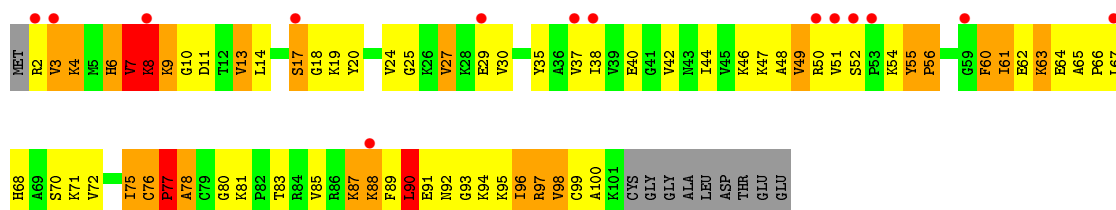




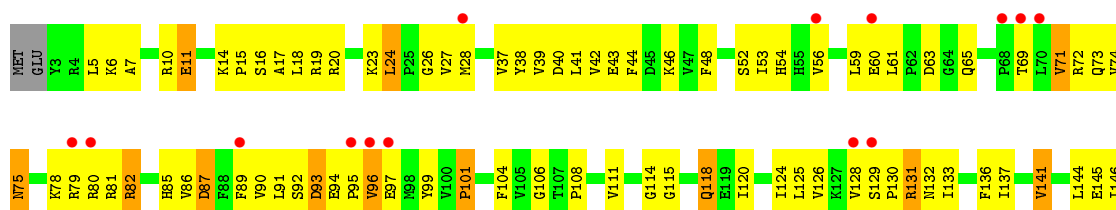
• Molecule 45: 50S ribosomal protein L24



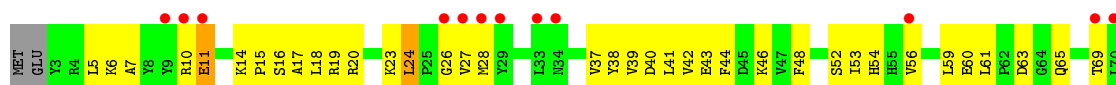
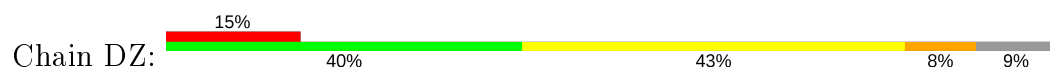
• Molecule 45: 50S ribosomal protein L24



• Molecule 46: 50S ribosomal protein L25



• Molecule 46: 50S ribosomal protein L25

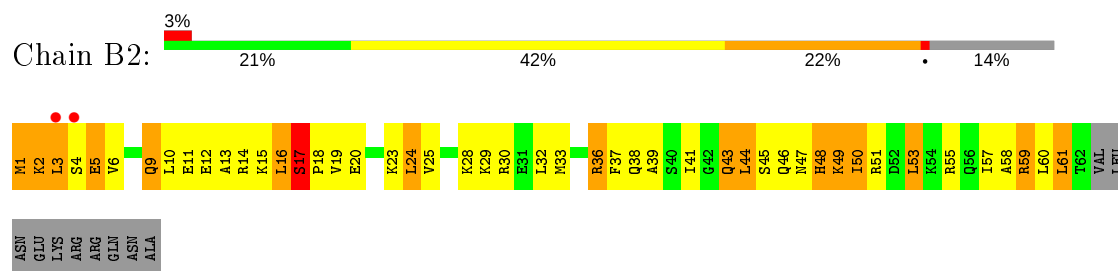




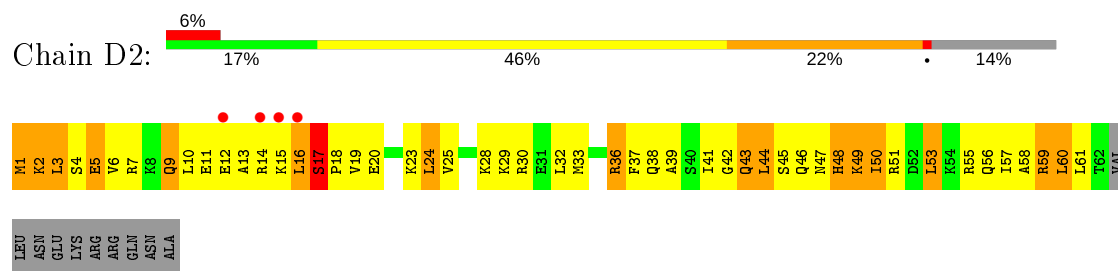




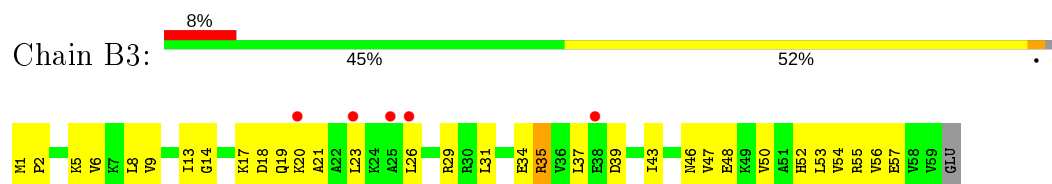
- Molecule 49: 50S ribosomal protein L29



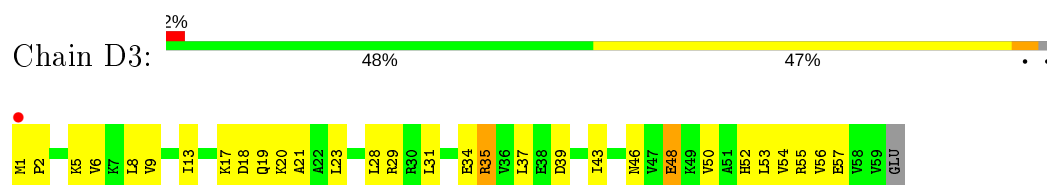
- Molecule 49: 50S ribosomal protein L29



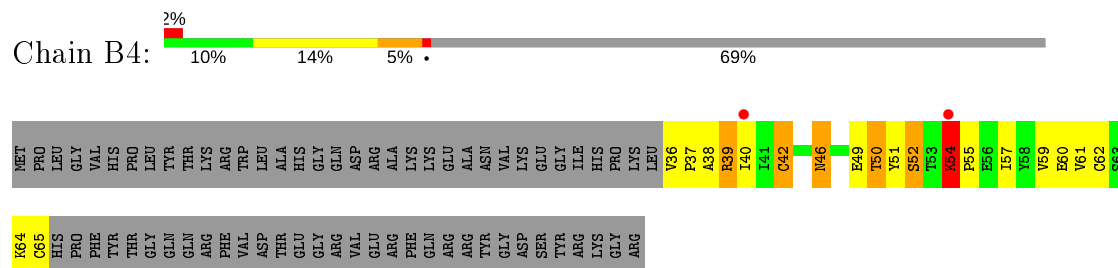
- Molecule 50: 50S ribosomal protein L30



- Molecule 50: 50S ribosomal protein L30



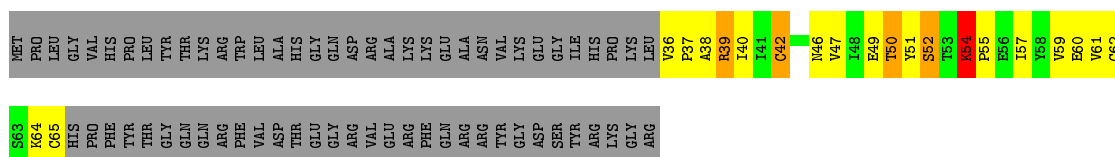
- Molecule 51: 50S ribosomal protein L31



- Molecule 51: 50S ribosomal protein L31







- Molecule 52: 50S ribosomal protein L32



- Molecule 52: 50S ribosomal protein L32



- Molecule 53: 50S ribosomal protein L33



- Molecule 53: 50S ribosomal protein L33



- Molecule 54: 50S ribosomal protein L34

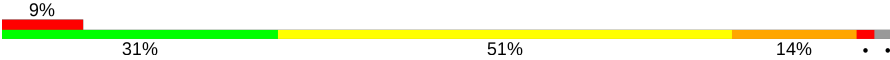


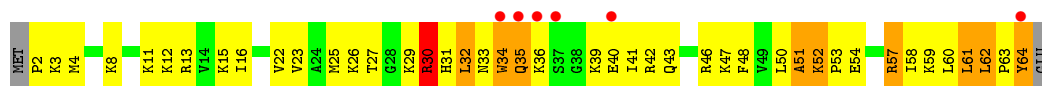
- Molecule 54: 50S ribosomal protein L34






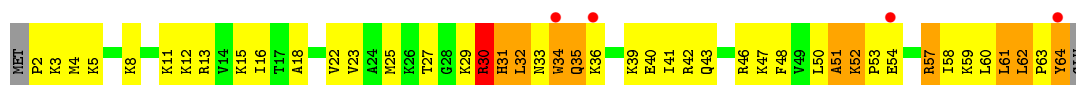
## ● Molecule 55: 50S ribosomal protein L35

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), CNS 1.2	Depositor
R, $R_{free}$	0.280 , 0.316 0.274 , 0.309	Depositor DCC
$R_{free}$ test set	10573 reflections (0.91%)	wwPDB-VP
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 , 49.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.43$ , $\langle L^2 \rangle = 0.25$	Xtriage
Estimated twinning fraction	No twinning to report.	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.

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



## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, MG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z  > 5$	RMSZ	# $ Z  > 5$
1	AA	0.56	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 Too-close contacts ⓘ

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

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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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
20	CR	574	0	644	51	0
21	AS	629	0	652	77	0
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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
41	DU	964	0	1022	102	0
42	BV	779	0	852	77	0
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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
56	AN	1	0	0	0	0
56	AO	2	0	0	0	0
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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
56	CG	2	0	0	0	0
56	CH	2	0	0	0	0
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

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 29.

The worst 5 of 14693 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
55:B8:57:ARG:HB2	55:B8:57:ARG:HH11	1.11	1.16

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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	Interatomic distance (Å)	Clash overlap (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%)	2	15
4	CB	232/256 (91%)	174 (75%)	48 (21%)	10 (4%)	2	15
5	AC	204/239 (85%)	138 (68%)	51 (25%)	15 (7%)	1	5
5	CC	204/239 (85%)	138 (68%)	52 (26%)	14 (7%)	1	6
6	AD	206/209 (99%)	166 (81%)	30 (15%)	10 (5%)	2	13
6	CD	206/209 (99%)	169 (82%)	26 (13%)	11 (5%)	2	11
7	AE	149/162 (92%)	117 (78%)	26 (17%)	6 (4%)	3	17
7	CE	149/162 (92%)	117 (78%)	26 (17%)	6 (4%)	3	17
8	AF	99/101 (98%)	87 (88%)	11 (11%)	1 (1%)	15	53
8	CF	99/101 (98%)	87 (88%)	11 (11%)	1 (1%)	15	53
9	AG	153/156 (98%)	124 (81%)	28 (18%)	1 (1%)	22	60
9	CG	153/156 (98%)	125 (82%)	27 (18%)	1 (1%)	22	60
10	AH	136/138 (99%)	112 (82%)	18 (13%)	6 (4%)	2	15

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
10	CH	136/138 (99%)	112 (82%)	18 (13%)	6 (4%)	2	15
11	AI	125/128 (98%)	93 (74%)	22 (18%)	10 (8%)	1	4
11	CI	125/128 (98%)	93 (74%)	23 (18%)	9 (7%)	1	5
12	AJ	96/105 (91%)	76 (79%)	14 (15%)	6 (6%)	1	7
12	CJ	96/105 (91%)	77 (80%)	13 (14%)	6 (6%)	1	7
13	AK	112/129 (87%)	94 (84%)	12 (11%)	6 (5%)	2	11
13	CK	112/129 (87%)	94 (84%)	12 (11%)	6 (5%)	2	11
14	AL	120/134 (90%)	87 (72%)	22 (18%)	11 (9%)	1	3
14	CL	120/134 (90%)	87 (72%)	22 (18%)	11 (9%)	1	3
15	AM	115/126 (91%)	91 (79%)	19 (16%)	5 (4%)	2	15
15	CM	115/126 (91%)	91 (79%)	20 (17%)	4 (4%)	3	20
16	AN	58/61 (95%)	46 (79%)	11 (19%)	1 (2%)	9	39
16	CN	58/61 (95%)	46 (79%)	11 (19%)	1 (2%)	9	39
17	AO	86/89 (97%)	70 (81%)	13 (15%)	3 (4%)	3	20
17	CO	86/89 (97%)	69 (80%)	14 (16%)	3 (4%)	3	20
18	AP	81/88 (92%)	59 (73%)	19 (24%)	3 (4%)	3	19
18	CP	81/88 (92%)	60 (74%)	18 (22%)	3 (4%)	3	19
19	AQ	97/105 (92%)	79 (81%)	16 (16%)	2 (2%)	7	33
19	CQ	97/105 (92%)	79 (81%)	16 (16%)	2 (2%)	7	33
20	AR	68/88 (77%)	45 (66%)	18 (26%)	5 (7%)	1	5
20	CR	68/88 (77%)	46 (68%)	17 (25%)	5 (7%)	1	5
21	AS	76/93 (82%)	50 (66%)	18 (24%)	8 (10%)	0	2
21	CS	76/93 (82%)	50 (66%)	18 (24%)	8 (10%)	0	2
22	AT	97/106 (92%)	72 (74%)	17 (18%)	8 (8%)	1	4
22	CT	97/106 (92%)	72 (74%)	18 (19%)	7 (7%)	1	5
23	AU	22/27 (82%)	12 (54%)	8 (36%)	2 (9%)	1	3
23	CU	22/27 (82%)	12 (54%)	8 (36%)	2 (9%)	1	3
24	AX	360/378 (95%)	288 (80%)	57 (16%)	15 (4%)	3	16
24	CX	360/378 (95%)	288 (80%)	58 (16%)	14 (4%)	3	17
27	BD	269/276 (98%)	208 (77%)	41 (15%)	20 (7%)	1	5
27	DD	269/276 (98%)	204 (76%)	46 (17%)	19 (7%)	1	5

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
28	BE	202/206 (98%)	157 (78%)	37 (18%)	8 (4%)	3	17
28	DE	202/206 (98%)	157 (78%)	37 (18%)	8 (4%)	3	17
29	BF	200/210 (95%)	162 (81%)	28 (14%)	10 (5%)	2	12
29	DF	200/210 (95%)	162 (81%)	26 (13%)	12 (6%)	1	9
30	BG	179/182 (98%)	128 (72%)	39 (22%)	12 (7%)	1	6
30	DG	179/182 (98%)	127 (71%)	39 (22%)	13 (7%)	1	5
31	BH	157/180 (87%)	120 (76%)	30 (19%)	7 (4%)	2	14
31	DH	157/180 (87%)	121 (77%)	28 (18%)	8 (5%)	2	12
32	BI	143/148 (97%)	107 (75%)	29 (20%)	7 (5%)	2	13
32	DI	143/148 (97%)	121 (85%)	19 (13%)	3 (2%)	7	33
33	BK	145/147 (99%)	101 (70%)	35 (24%)	9 (6%)	1	8
33	DK	145/147 (99%)	101 (70%)	35 (24%)	9 (6%)	1	8
34	BN	135/163 (83%)	103 (76%)	17 (13%)	15 (11%)	0	2
34	DN	135/163 (83%)	101 (75%)	19 (14%)	15 (11%)	0	2
35	BO	120/122 (98%)	102 (85%)	14 (12%)	4 (3%)	4	21
35	DO	120/122 (98%)	101 (84%)	15 (12%)	4 (3%)	4	21
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%)	0	2
37	DQ	132/141 (94%)	93 (70%)	24 (18%)	15 (11%)	0	2
38	BR	115/118 (98%)	89 (77%)	19 (16%)	7 (6%)	1	8
38	DR	115/118 (98%)	91 (79%)	19 (16%)	5 (4%)	2	15
39	BS	96/112 (86%)	56 (58%)	29 (30%)	11 (12%)	0	2
39	DS	96/112 (86%)	56 (58%)	29 (30%)	11 (12%)	0	2
40	BT	135/146 (92%)	91 (67%)	30 (22%)	14 (10%)	0	2
40	DT	135/146 (92%)	91 (67%)	31 (23%)	13 (10%)	0	3
41	BU	115/118 (98%)	92 (80%)	19 (16%)	4 (4%)	3	20
41	DU	115/118 (98%)	91 (79%)	19 (16%)	5 (4%)	2	15
42	BV	99/101 (98%)	74 (75%)	15 (15%)	10 (10%)	0	2
42	DV	99/101 (98%)	74 (75%)	15 (15%)	10 (10%)	0	2
43	BW	110/113 (97%)	88 (80%)	18 (16%)	4 (4%)	3	19

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
43	DW	110/113 (97%)	87 (79%)	18 (16%)	5 (4%)	2	14
44	BX	90/96 (94%)	73 (81%)	15 (17%)	2 (2%)	6	31
44	DX	90/96 (94%)	73 (81%)	15 (17%)	2 (2%)	6	31
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%)	2	15
46	DZ	185/206 (90%)	145 (78%)	32 (17%)	8 (4%)	2	15
47	B0	74/85 (87%)	61 (82%)	10 (14%)	3 (4%)	3	16
47	D0	74/85 (87%)	61 (82%)	10 (14%)	3 (4%)	3	16
48	B1	86/98 (88%)	59 (69%)	16 (19%)	11 (13%)	0	1
48	D1	86/98 (88%)	59 (69%)	16 (19%)	11 (13%)	0	1
49	B2	60/72 (83%)	43 (72%)	12 (20%)	5 (8%)	1	4
49	D2	60/72 (83%)	44 (73%)	11 (18%)	5 (8%)	1	4
50	B3	57/60 (95%)	50 (88%)	5 (9%)	2 (4%)	3	20
50	D3	57/60 (95%)	50 (88%)	5 (9%)	2 (4%)	3	20
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%)	1	9
52	D5	50/60 (83%)	40 (80%)	7 (14%)	3 (6%)	1	9
53	B6	42/54 (78%)	27 (64%)	10 (24%)	5 (12%)	0	1
53	D6	42/54 (78%)	27 (64%)	10 (24%)	5 (12%)	0	1
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%)	0	2
55	D8	61/65 (94%)	42 (69%)	12 (20%)	7 (12%)	0	2
All	All	12130/13206 (92%)	9225 (76%)	2153 (18%)	752 (6%)	1	8

5 of 752 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	AC	45	LYS
5	AC	47	LEU
6	AD	5	ILE

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Mol	Chain	Res	Type
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%)	12	41
4	CB	202/220 (92%)	185 (92%)	17 (8%)	11	38
5	AC	160/188 (85%)	138 (86%)	22 (14%)	3	17
5	CC	160/188 (85%)	138 (86%)	22 (14%)	3	17
6	AD	180/181 (99%)	160 (89%)	20 (11%)	6	25
6	CD	180/181 (99%)	161 (89%)	19 (11%)	6	26
7	AE	116/123 (94%)	99 (85%)	17 (15%)	3	15
7	CE	116/123 (94%)	99 (85%)	17 (15%)	3	15
8	AF	90/90 (100%)	80 (89%)	10 (11%)	6	25
8	CF	90/90 (100%)	81 (90%)	9 (10%)	7	29
9	AG	126/127 (99%)	119 (94%)	7 (6%)	21	56
9	CG	126/127 (99%)	119 (94%)	7 (6%)	21	56
10	AH	119/119 (100%)	106 (89%)	13 (11%)	6	25
10	CH	119/119 (100%)	106 (89%)	13 (11%)	6	25
11	AI	98/99 (99%)	85 (87%)	13 (13%)	4	17
11	CI	98/99 (99%)	86 (88%)	12 (12%)	5	21
12	AJ	88/92 (96%)	75 (85%)	13 (15%)	3	14
12	CJ	88/92 (96%)	75 (85%)	13 (15%)	3	14
13	AK	86/99 (87%)	74 (86%)	12 (14%)	3	16
13	CK	86/99 (87%)	74 (86%)	12 (14%)	3	16
14	AL	103/110 (94%)	91 (88%)	12 (12%)	5	22
14	CL	103/110 (94%)	91 (88%)	12 (12%)	5	22

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
15	AM	94/101 (93%)	85 (90%)	9 (10%)	8	32
15	CM	94/101 (93%)	85 (90%)	9 (10%)	8	32
16	AN	49/50 (98%)	44 (90%)	5 (10%)	7	28
16	CN	49/50 (98%)	44 (90%)	5 (10%)	7	28
17	AO	79/80 (99%)	70 (89%)	9 (11%)	5	24
17	CO	79/80 (99%)	70 (89%)	9 (11%)	5	24
18	AP	72/74 (97%)	65 (90%)	7 (10%)	8	31
18	CP	72/74 (97%)	66 (92%)	6 (8%)	11	39
19	AQ	94/97 (97%)	86 (92%)	8 (8%)	10	38
19	CQ	94/97 (97%)	86 (92%)	8 (8%)	10	38
20	AR	61/77 (79%)	53 (87%)	8 (13%)	4	18
20	CR	61/77 (79%)	52 (85%)	9 (15%)	3	14
21	AS	69/80 (86%)	58 (84%)	11 (16%)	2	12
21	CS	69/80 (86%)	58 (84%)	11 (16%)	2	12
22	AT	76/82 (93%)	67 (88%)	9 (12%)	5	22
22	CT	76/82 (93%)	68 (90%)	8 (10%)	7	27
23	AU	19/22 (86%)	18 (95%)	1 (5%)	22	58
23	CU	19/22 (86%)	18 (95%)	1 (5%)	22	58
24	AX	305/319 (96%)	258 (85%)	47 (15%)	2	13
24	CX	305/319 (96%)	260 (85%)	45 (15%)	3	14
27	BD	213/218 (98%)	181 (85%)	32 (15%)	3	14
27	DD	213/218 (98%)	181 (85%)	32 (15%)	3	14
28	BE	165/166 (99%)	144 (87%)	21 (13%)	4	19
28	DE	165/166 (99%)	144 (87%)	21 (13%)	4	19
29	BF	161/166 (97%)	142 (88%)	19 (12%)	5	22
29	DF	161/166 (97%)	140 (87%)	21 (13%)	4	19
30	BG	155/156 (99%)	135 (87%)	20 (13%)	4	19
30	DG	155/156 (99%)	135 (87%)	20 (13%)	4	19
31	BH	132/148 (89%)	115 (87%)	17 (13%)	4	19
31	DH	132/148 (89%)	115 (87%)	17 (13%)	4	19
32	BI	122/124 (98%)	101 (83%)	21 (17%)	2	10

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
32	DI	122/124 (98%)	103 (84%)	19 (16%)	2	13
33	BK	111/111 (100%)	95 (86%)	16 (14%)	3	15
33	DK	111/111 (100%)	95 (86%)	16 (14%)	3	15
34	BN	116/139 (84%)	98 (84%)	18 (16%)	2	13
34	DN	116/139 (84%)	98 (84%)	18 (16%)	2	13
35	BO	100/100 (100%)	86 (86%)	14 (14%)	3	16
35	DO	100/100 (100%)	85 (85%)	15 (15%)	3	14
36	BP	112/116 (97%)	80 (71%)	32 (29%)	0	2
36	DP	112/116 (97%)	79 (70%)	33 (30%)	0	1
37	BQ	105/111 (95%)	91 (87%)	14 (13%)	4	17
37	DQ	105/111 (95%)	91 (87%)	14 (13%)	4	17
38	BR	100/101 (99%)	90 (90%)	10 (10%)	7	29
38	DR	100/101 (99%)	91 (91%)	9 (9%)	9	35
39	BS	77/88 (88%)	66 (86%)	11 (14%)	3	15
39	DS	77/88 (88%)	66 (86%)	11 (14%)	3	15
40	BT	121/128 (94%)	101 (84%)	20 (16%)	2	11
40	DT	121/128 (94%)	101 (84%)	20 (16%)	2	11
41	BU	93/94 (99%)	82 (88%)	11 (12%)	5	22
41	DU	93/94 (99%)	83 (89%)	10 (11%)	6	26
42	BV	82/82 (100%)	68 (83%)	14 (17%)	2	10
42	DV	82/82 (100%)	69 (84%)	13 (16%)	2	12
43	BW	91/92 (99%)	80 (88%)	11 (12%)	5	21
43	DW	91/92 (99%)	80 (88%)	11 (12%)	5	21
44	BX	74/78 (95%)	58 (78%)	16 (22%)	1	5
44	DX	74/78 (95%)	59 (80%)	15 (20%)	1	6
45	BY	84/91 (92%)	72 (86%)	12 (14%)	3	15
45	DY	84/91 (92%)	70 (83%)	14 (17%)	2	11
46	BZ	162/179 (90%)	151 (93%)	11 (7%)	16	48
46	DZ	162/179 (90%)	150 (93%)	12 (7%)	13	44
47	B0	61/67 (91%)	53 (87%)	8 (13%)	4	18
47	D0	61/67 (91%)	53 (87%)	8 (13%)	4	18

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
48	B1	73/83 (88%)	58 (80%)	15 (20%)	1	6
48	D1	73/83 (88%)	57 (78%)	16 (22%)	1	5
49	B2	58/67 (87%)	45 (78%)	13 (22%)	1	4
49	D2	58/67 (87%)	45 (78%)	13 (22%)	1	4
50	B3	51/52 (98%)	49 (96%)	2 (4%)	32	69
50	D3	51/52 (98%)	49 (96%)	2 (4%)	32	69
51	B4	27/84 (32%)	21 (78%)	6 (22%)	1	4
51	D4	27/84 (32%)	22 (82%)	5 (18%)	1	8
52	B5	45/52 (86%)	41 (91%)	4 (9%)	9	35
52	D5	45/52 (86%)	42 (93%)	3 (7%)	16	49
53	B6	43/52 (83%)	34 (79%)	9 (21%)	1	5
53	D6	43/52 (83%)	34 (79%)	9 (21%)	1	5
54	B7	41/42 (98%)	35 (85%)	6 (15%)	3	15
54	D7	41/42 (98%)	35 (85%)	6 (15%)	3	15
55	B8	53/55 (96%)	47 (89%)	6 (11%)	6	24
55	D8	53/55 (96%)	47 (89%)	6 (11%)	6	24
All	All	10228/10944 (94%)	8877 (87%)	1351 (13%)	4	18

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%)
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.

No monomer is involved in short contacts.

## 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 [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

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%)	-0.34	19 (1%) 77 51	35, 78, 175, 261	0
1	CA	1504/1525 (98%)	-0.09	31 (2%) 63 34	34, 99, 199, 271	0
2	AY	77/77 (100%)	-0.48	0 100 100	60, 90, 124, 194	0
2	AZ	77/77 (100%)	1.27	19 (24%) 0 0	146, 211, 242, 260	0
2	CY	77/77 (100%)	-0.31	1 (1%) 77 51	59, 91, 127, 196	0
2	CZ	77/77 (100%)	1.88	25 (32%) 0 0	175, 231, 266, 276	0
3	AV	10/27 (37%)	0.18	0 100 100	62, 77, 118, 184	0
3	CV	10/27 (37%)	0.74	2 (20%) 1 0	63, 104, 143, 196	0
4	AB	234/256 (91%)	0.38	26 (11%) 5 1	85, 126, 167, 194	0
4	CB	234/256 (91%)	0.51	29 (12%) 4 1	91, 127, 174, 204	0
5	AC	206/239 (86%)	0.04	11 (5%) 26 10	86, 121, 159, 183	0
5	CC	206/239 (86%)	0.26	16 (7%) 13 4	87, 126, 164, 178	0
6	AD	208/209 (99%)	0.12	13 (6%) 20 6	50, 79, 127, 164	0
6	CD	208/209 (99%)	0.51	20 (9%) 8 2	81, 115, 151, 184	0
7	AE	151/162 (93%)	0.01	10 (6%) 18 5	65, 90, 130, 192	0
7	CE	151/162 (93%)	0.07	3 (1%) 65 36	71, 100, 145, 173	0
8	AF	101/101 (100%)	-0.02	2 (1%) 65 36	69, 98, 137, 176	0
8	CF	101/101 (100%)	-0.12	1 (0%) 82 59	64, 94, 131, 149	0
9	AG	155/156 (99%)	0.02	10 (6%) 18 5	82, 113, 154, 172	0
9	CG	155/156 (99%)	0.13	5 (3%) 47 20	87, 125, 158, 181	0
10	AH	138/138 (100%)	0.04	4 (2%) 51 23	64, 90, 135, 146	0
10	CH	138/138 (100%)	0.22	6 (4%) 35 13	80, 107, 145, 171	0
11	AI	127/128 (99%)	0.77	18 (14%) 2 1	90, 134, 168, 182	0
11	CI	127/128 (99%)	1.37	28 (22%) 0 0	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%)	1.18	23 (23%)	0 0	87, 125, 166, 184	0
12	CJ	98/105 (93%)	1.42	23 (23%)	0 0	106, 144, 175, 186	0
13	AK	114/129 (88%)	0.12	7 (6%)	21 7	59, 88, 123, 160	0
13	CK	114/129 (88%)	0.42	15 (13%)	3 1	64, 91, 135, 175	0
14	AL	122/134 (91%)	-0.05	4 (3%)	46 20	47, 67, 114, 144	0
14	CL	122/134 (91%)	0.23	10 (8%)	11 3	57, 89, 131, 185	0
15	AM	117/126 (92%)	0.43	13 (11%)	5 1	93, 122, 159, 171	0
15	CM	117/126 (92%)	0.86	19 (16%)	1 0	98, 143, 172, 188	0
16	AN	60/61 (98%)	0.69	8 (13%)	3 1	75, 109, 141, 193	0
16	CN	60/61 (98%)	0.93	10 (16%)	1 0	80, 113, 158, 175	0
17	AO	88/89 (98%)	0.13	1 (1%)	80 56	57, 90, 123, 145	0
17	CO	88/89 (98%)	0.07	2 (2%)	60 31	60, 91, 130, 145	0
18	AP	83/88 (94%)	0.52	7 (8%)	11 3	58, 75, 119, 184	0
18	CP	83/88 (94%)	1.34	23 (27%)	0 0	90, 123, 155, 202	0
19	AQ	99/105 (94%)	-0.07	1 (1%)	82 59	56, 79, 118, 142	0
19	CQ	99/105 (94%)	0.53	8 (8%)	12 3	76, 105, 140, 159	0
20	AR	70/88 (79%)	0.65	4 (5%)	23 8	68, 103, 147, 165	0
20	CR	70/88 (79%)	0.83	11 (15%)	2 1	64, 87, 139, 147	0
21	AS	78/93 (83%)	1.82	31 (39%)	0 0	98, 136, 170, 193	0
21	CS	78/93 (83%)	1.31	22 (28%)	0 0	114, 150, 184, 205	0
22	AT	99/106 (93%)	0.25	5 (5%)	28 10	51, 84, 138, 166	0
22	CT	99/106 (93%)	0.96	20 (20%)	1 0	87, 117, 160, 184	0
23	AU	24/27 (88%)	4.59	22 (91%)	0 0	93, 122, 162, 191	0
23	CU	24/27 (88%)	5.68	24 (100%)	0 0	100, 137, 178, 187	0
24	AX	362/378 (95%)	0.83	70 (19%)	1 0	61, 129, 207, 244	0
24	CX	362/378 (95%)	1.26	86 (23%)	0 0	94, 150, 244, 273	0
25	BA	2879/2894 (99%)	-0.33	74 (2%)	56 27	14, 64, 186, 278	0
25	DA	2879/2894 (99%)	-0.22	89 (3%)	49 21	10, 67, 204, 287	0
26	BB	119/124 (95%)	-0.27	0	100 100	69, 100, 144, 222	0
26	DB	119/124 (95%)	0.31	6 (5%)	28 10	87, 147, 205, 258	0
27	BD	271/276 (98%)	-0.07	7 (2%)	56 27	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%)	-0.10	5 (1%) 68 40	26, 51, 92, 146	0
28	BE	204/206 (99%)	0.04	10 (4%) 29 11	36, 69, 126, 159	0
28	DE	204/206 (99%)	0.46	29 (14%) 2 1	45, 85, 137, 186	0
29	BF	202/210 (96%)	-0.16	7 (3%) 44 18	38, 71, 131, 153	0
29	DF	202/210 (96%)	0.06	6 (2%) 50 22	34, 66, 124, 190	0
30	BG	181/182 (99%)	0.60	32 (17%) 1 0	88, 121, 164, 179	0
30	DG	181/182 (99%)	0.82	32 (17%) 1 0	113, 153, 182, 206	0
31	BH	159/180 (88%)	0.87	34 (21%) 0 0	97, 139, 185, 202	0
31	DH	159/180 (88%)	0.14	15 (9%) 8 3	79, 111, 154, 174	0
32	BI	145/148 (97%)	0.26	14 (9%) 7 2	54, 106, 147, 198	0
32	DI	145/148 (97%)	0.14	7 (4%) 30 11	58, 94, 129, 147	0
33	BK	147/147 (100%)	2.36	76 (51%) 0 0	177, 205, 225, 240	0
33	DK	147/147 (100%)	4.19	106 (72%) 0 0	207, 236, 257, 274	0
34	BN	137/163 (84%)	0.33	9 (6%) 18 5	55, 87, 131, 153	0
34	DN	137/163 (84%)	0.06	4 (2%) 51 23	59, 80, 130, 164	0
35	BO	122/122 (100%)	-0.41	0 100 100	32, 61, 101, 118	0
35	DO	122/122 (100%)	-0.41	0 100 100	47, 72, 108, 129	0
36	BP	146/150 (97%)	0.41	12 (8%) 11 3	35, 89, 148, 203	0
36	DP	146/150 (97%)	0.27	8 (5%) 25 9	21, 93, 146, 183	0
37	BQ	134/141 (95%)	0.24	8 (5%) 21 7	44, 79, 136, 188	0
37	DQ	134/141 (95%)	0.22	10 (7%) 14 4	56, 91, 148, 192	0
38	BR	117/118 (99%)	-0.17	0 100 100	31, 63, 114, 165	0
38	DR	117/118 (99%)	0.04	1 (0%) 84 63	48, 73, 130, 148	0
39	BS	98/112 (87%)	0.67	20 (20%) 1 0	66, 105, 140, 169	0
39	DS	98/112 (87%)	1.85	41 (41%) 0 0	106, 144, 177, 218	0
40	BT	137/146 (93%)	0.40	14 (10%) 6 2	41, 76, 136, 156	0
40	DT	137/146 (93%)	0.82	22 (16%) 1 0	66, 100, 155, 189	0
41	BU	117/118 (99%)	0.43	5 (4%) 35 13	45, 78, 124, 159	0
41	DU	117/118 (99%)	0.84	21 (17%) 1 0	39, 68, 120, 194	0
42	BV	101/101 (100%)	0.22	6 (5%) 22 7	63, 99, 144, 220	0
42	DV	101/101 (100%)	0.46	8 (7%) 12 4	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%)	-0.15	1 (0%) 84 63	39, 64, 111, 163	0
43	DW	112/113 (99%)	0.08	5 (4%) 33 12	31, 61, 119, 155	0
44	BX	92/96 (95%)	0.10	4 (4%) 35 13	50, 79, 122, 149	0
44	DX	92/96 (95%)	0.45	8 (8%) 10 3	38, 65, 114, 150	0
45	BY	100/110 (90%)	1.22	22 (22%) 0 0	75, 112, 179, 200	0
45	DY	100/110 (90%)	0.79	14 (14%) 2 1	53, 86, 160, 186	0
46	BZ	187/206 (90%)	0.32	16 (8%) 10 3	83, 119, 156, 196	0
46	DZ	187/206 (90%)	0.79	30 (16%) 1 1	107, 139, 176, 201	0
47	B0	76/85 (89%)	-0.13	0 100 100	56, 78, 115, 150	0
47	D0	76/85 (89%)	0.02	2 (2%) 56 27	73, 99, 139, 160	0
48	B1	88/98 (89%)	-0.02	2 (2%) 60 31	31, 66, 119, 177	0
48	D1	88/98 (89%)	0.14	3 (3%) 45 19	34, 68, 143, 172	0
49	B2	62/72 (86%)	0.13	2 (3%) 47 20	55, 90, 131, 165	0
49	D2	62/72 (86%)	0.03	4 (6%) 18 5	37, 75, 147, 177	0
50	B3	59/60 (98%)	0.38	5 (8%) 10 3	65, 85, 145, 166	0
50	D3	59/60 (98%)	0.14	1 (1%) 70 41	57, 83, 129, 170	0
51	B4	30/97 (30%)	0.30	2 (6%) 17 5	101, 135, 178, 183	0
51	D4	30/97 (30%)	0.05	0 100 100	115, 149, 178, 183	0
52	B5	52/60 (86%)	0.18	3 (5%) 23 7	49, 79, 147, 166	0
52	D5	52/60 (86%)	-0.29	2 (3%) 40 16	42, 80, 147, 167	0
53	B6	44/54 (81%)	4.64	32 (72%) 0 0	106, 136, 175, 224	0
53	D6	44/54 (81%)	5.17	36 (81%) 0 0	111, 140, 175, 192	0
54	B7	48/49 (97%)	1.28	11 (22%) 0 0	38, 57, 119, 143	0
54	D7	48/49 (97%)	0.70	6 (12%) 3 1	31, 44, 96, 161	0
55	B8	63/65 (96%)	0.37	6 (9%) 8 3	42, 59, 117, 156	0
55	D8	63/65 (96%)	0.36	4 (6%) 20 6	48, 72, 133, 168	0
All	All	21662/22654 (95%)	0.20	1727 (7%) 12 4	10, 90, 190, 287	0

The worst 5 of 1727 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
29	DF	207	GLY	20.4
53	B6	13	CYS	17.1

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Mol	Chain	Res	Type	RSRZ
11	CI	8	GLY	15.6
53	B6	23	THR	13.8
2	CZ	17(A)	U	13.1

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

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

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
56	MG	AA	1919	1/1	0.09	0.15	88,88,88,88	0
56	MG	CA	1679	1/1	0.22	0.94	90,90,90,90	0
56	MG	AA	1605	1/1	0.28	0.41	88,88,88,88	0
56	MG	AA	1915	1/1	0.31	0.20	109,109,109,109	0
56	MG	AA	1651	1/1	0.33	0.31	106,106,106,106	0
56	MG	BA	3623	1/1	0.34	0.21	103,103,103,103	0
56	MG	AA	1790	1/1	0.35	0.16	97,97,97,97	0
56	MG	BA	3437	1/1	0.36	0.41	117,117,117,117	0
56	MG	BA	3093	1/1	0.37	0.60	80,80,80,80	0
56	MG	BB	205	1/1	0.38	0.42	100,100,100,100	0
56	MG	DA	3320	1/1	0.38	0.71	82,82,82,82	0
56	MG	BA	3899	1/1	0.40	0.99	73,73,73,73	0
56	MG	BA	3874	1/1	0.41	0.66	103,103,103,103	0
56	MG	CZ	106	1/1	0.43	0.16	82,82,82,82	0
56	MG	AA	1684	1/1	0.43	0.47	61,61,61,61	0
56	MG	BA	3061	1/1	0.46	0.11	76,76,76,76	0
56	MG	CA	1738	1/1	0.46	0.32	64,64,64,64	0
56	MG	AA	1678	1/1	0.47	0.49	92,92,92,92	0
56	MG	CA	1769	1/1	0.47	0.20	77,77,77,77	0
56	MG	BA	3260	1/1	0.48	0.26	75,75,75,75	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	AA	1938	1/1	0.49	0.36	58,58,58,58	0
56	MG	BA	3445	1/1	0.49	0.28	63,63,63,63	0
56	MG	AA	1821	1/1	0.49	0.28	90,90,90,90	0
56	MG	AA	1653	1/1	0.49	0.43	95,95,95,95	0
56	MG	BA	3073	1/1	0.51	0.33	57,57,57,57	0
56	MG	BI	201	1/1	0.52	0.14	78,78,78,78	0
56	MG	BA	3643	1/1	0.53	0.38	68,68,68,68	0
56	MG	AA	1652	1/1	0.53	0.37	63,63,63,63	0
56	MG	BA	3117	1/1	0.53	0.53	63,63,63,63	0
56	MG	BA	3252	1/1	0.53	0.11	80,80,80,80	0
56	MG	AA	1949	1/1	0.54	0.31	90,90,90,90	0
56	MG	BA	3400	1/1	0.55	0.09	101,101,101,101	0
56	MG	BA	3048	1/1	0.56	0.88	58,58,58,58	0
56	MG	BA	3367	1/1	0.56	0.33	53,53,53,53	0
56	MG	BT	201	1/1	0.56	0.68	81,81,81,81	0
56	MG	BA	3454	1/1	0.56	0.32	63,63,63,63	0
56	MG	BB	235	1/1	0.56	0.13	59,59,59,59	0
56	MG	B2	101	1/1	0.56	0.35	76,76,76,76	0
56	MG	AZ	106	1/1	0.58	0.48	93,93,93,93	0
56	MG	BA	3758	1/1	0.58	0.53	94,94,94,94	0
56	MG	BA	3176	1/1	0.58	0.43	66,66,66,66	0
56	MG	BA	3505	1/1	0.58	0.16	92,92,92,92	0
56	MG	AA	1958	1/1	0.58	0.69	87,87,87,87	0
56	MG	BA	3884	1/1	0.58	0.24	80,80,80,80	0
56	MG	BA	3077	1/1	0.59	0.23	59,59,59,59	0
56	MG	BA	3653	1/1	0.59	0.51	61,61,61,61	0
56	MG	DA	3210	1/1	0.59	0.38	3,3,3,3	0
56	MG	BB	230	1/1	0.60	0.39	50,50,50,50	0
56	MG	BB	207	1/1	0.60	0.30	84,84,84,84	0
56	MG	BA	3624	1/1	0.60	0.17	89,89,89,89	0
56	MG	AA	1951	1/1	0.60	0.36	59,59,59,59	0
56	MG	BA	3332	1/1	0.60	0.15	90,90,90,90	0
56	MG	BA	3579	1/1	0.61	0.14	69,69,69,69	0
56	MG	AA	1875	1/1	0.62	0.55	83,83,83,83	0
56	MG	AV	5502	1/1	0.62	0.59	89,89,89,89	0
56	MG	BA	3306	1/1	0.62	0.43	52,52,52,52	0
56	MG	BW	201	1/1	0.63	0.42	80,80,80,80	0
56	MG	DA	3304	1/1	0.63	0.33	76,76,76,76	0
56	MG	BA	3704	1/1	0.63	0.17	88,88,88,88	0
56	MG	BA	3362	1/1	0.64	0.65	68,68,68,68	0
56	MG	CA	1713	1/1	0.64	0.58	80,80,80,80	0
56	MG	BA	3239	1/1	0.64	0.47	69,69,69,69	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	BA	3020	1/1	0.64	0.36	73,73,73,73	0
56	MG	BA	3431	1/1	0.64	0.17	63,63,63,63	0
56	MG	BA	3374	1/1	0.65	0.47	85,85,85,85	0
56	MG	DA	3373	1/1	0.65	0.28	92,92,92,92	0
56	MG	BA	3068	1/1	0.65	0.20	50,50,50,50	0
56	MG	BA	3329	1/1	0.65	0.17	79,79,79,79	0
56	MG	BB	212	1/1	0.65	0.17	82,82,82,82	0
56	MG	CA	1783	1/1	0.65	0.23	65,65,65,65	0
56	MG	BA	3661	1/1	0.65	0.38	71,71,71,71	0
56	MG	CA	1696	1/1	0.66	0.29	60,60,60,60	0
56	MG	BA	3193	1/1	0.66	0.55	83,83,83,83	0
56	MG	BA	3382	1/1	0.66	0.08	75,75,75,75	0
56	MG	AA	1969	1/1	0.66	0.09	46,46,46,46	0
56	MG	AA	1638	1/1	0.66	0.46	72,72,72,72	0
56	MG	AA	1950	1/1	0.66	0.15	73,73,73,73	0
56	MG	BB	220	1/1	0.66	0.58	84,84,84,84	0
56	MG	AA	1953	1/1	0.66	0.14	87,87,87,87	0
56	MG	AA	1964	1/1	0.67	0.41	79,79,79,79	0
56	MG	BA	3800	1/1	0.67	0.40	74,74,74,74	0
56	MG	BU	201	1/1	0.67	0.41	83,83,83,83	0
56	MG	BA	3600	1/1	0.67	0.43	47,47,47,47	0
56	MG	BA	3340	1/1	0.67	0.61	73,73,73,73	0
56	MG	AX	405	1/1	0.67	0.09	74,74,74,74	0
56	MG	BA	3795	1/1	0.67	0.35	84,84,84,84	0
56	MG	AA	1819	1/1	0.67	0.27	76,76,76,76	0
56	MG	AA	1947	1/1	0.67	0.12	45,45,45,45	0
56	MG	AA	1622	1/1	0.68	0.33	72,72,72,72	0
56	MG	CA	1781	1/1	0.68	0.21	59,59,59,59	0
56	MG	BD	5007	1/1	0.68	0.21	55,55,55,55	0
56	MG	AA	1885	1/1	0.68	0.32	58,58,58,58	0
56	MG	BA	3198	1/1	0.68	0.46	76,76,76,76	0
56	MG	BA	3470	1/1	0.68	0.35	77,77,77,77	0
56	MG	BA	3170	1/1	0.69	0.34	80,80,80,80	0
56	MG	BA	3598	1/1	0.69	0.48	73,73,73,73	0
56	MG	BA	3535	1/1	0.69	0.28	62,62,62,62	0
56	MG	BA	3506	1/1	0.69	0.25	59,59,59,59	0
56	MG	CA	1758	1/1	0.69	0.19	78,78,78,78	0
56	MG	BB	201	1/1	0.69	0.40	59,59,59,59	0
56	MG	BA	3296	1/1	0.69	0.43	68,68,68,68	0
56	MG	AA	1989	1/1	0.69	0.69	81,81,81,81	0
56	MG	AZ	102	1/1	0.69	0.13	71,71,71,71	0
56	MG	AA	1770	1/1	0.69	0.43	52,52,52,52	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	DA	3101	1/1	0.69	0.65	64,64,64,64	0
56	MG	BA	3496	1/1	0.69	0.25	63,63,63,63	0
56	MG	AA	1899	1/1	0.70	0.35	59,59,59,59	0
56	MG	BA	3171	1/1	0.70	0.68	77,77,77,77	0
56	MG	BA	3637	1/1	0.70	0.29	61,61,61,61	0
56	MG	BA	3751	1/1	0.70	0.34	53,53,53,53	0
56	MG	DA	3318	1/1	0.70	0.33	45,45,45,45	0
56	MG	AA	1619	1/1	0.70	0.44	62,62,62,62	0
56	MG	BA	3794	1/1	0.70	0.12	65,65,65,65	0
56	MG	BA	3343	1/1	0.70	0.64	70,70,70,70	0
56	MG	BA	3156	1/1	0.70	0.48	53,53,53,53	0
56	MG	BB	211	1/1	0.70	0.17	81,81,81,81	0
56	MG	CA	1762	1/1	0.71	0.29	69,69,69,69	0
56	MG	BZ	301	1/1	0.71	0.16	81,81,81,81	0
56	MG	BA	3057	1/1	0.71	0.16	80,80,80,80	0
56	MG	BA	3680	1/1	0.71	0.16	60,60,60,60	0
56	MG	BA	3698	1/1	0.71	0.20	94,94,94,94	0
56	MG	AA	2014	1/1	0.71	0.18	21,21,21,21	0
56	MG	CG	202	1/1	0.71	0.23	82,82,82,82	0
56	MG	AA	1664	1/1	0.71	0.19	73,73,73,73	0
56	MG	BA	3540	1/1	0.71	0.26	65,65,65,65	0
56	MG	AA	1769	1/1	0.72	0.69	87,87,87,87	0
56	MG	CA	1811	1/1	0.72	0.37	79,79,79,79	0
56	MG	BA	3412	1/1	0.72	0.19	64,64,64,64	0
56	MG	BA	3628	1/1	0.72	0.15	71,71,71,71	0
56	MG	BA	3864	1/1	0.72	0.29	78,78,78,78	0
56	MG	AX	411	1/1	0.72	0.46	75,75,75,75	0
56	MG	BO	205	1/1	0.72	0.33	86,86,86,86	0
56	MG	BA	3031	1/1	0.72	0.39	74,74,74,74	0
56	MG	AY	113	1/1	0.72	0.84	89,89,89,89	0
56	MG	DA	3314	1/1	0.72	0.36	70,70,70,70	0
56	MG	AA	1878	1/1	0.72	0.25	67,67,67,67	0
56	MG	BA	3013	1/1	0.72	0.63	103,103,103,103	0
56	MG	BA	3474	1/1	0.72	0.48	73,73,73,73	0
56	MG	BF	303	1/1	0.72	0.92	50,50,50,50	0
56	MG	BA	3422	1/1	0.72	0.36	59,59,59,59	0
56	MG	BA	3113	1/1	0.72	0.23	85,85,85,85	0
56	MG	BF	301	1/1	0.72	0.13	63,63,63,63	0
56	MG	DA	3114	1/1	0.72	0.33	83,83,83,83	0
56	MG	AA	1750	1/1	0.72	0.16	97,97,97,97	0
56	MG	AA	1752	1/1	0.72	0.23	66,66,66,66	0
56	MG	BA	3389	1/1	0.72	1.02	75,75,75,75	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	BA	3189	1/1	0.73	0.30	96,96,96,96	0
56	MG	DA	3313	1/1	0.73	0.39	69,69,69,69	0
56	MG	AE	204	1/1	0.73	0.09	51,51,51,51	0
56	MG	AA	1639	1/1	0.73	0.16	59,59,59,59	0
56	MG	BA	3233	1/1	0.73	0.41	70,70,70,70	0
56	MG	BA	3436	1/1	0.73	0.55	47,47,47,47	0
56	MG	AA	1793	1/1	0.73	0.31	82,82,82,82	0
56	MG	AA	1998	1/1	0.73	0.20	57,57,57,57	0
56	MG	BE	302	1/1	0.73	0.40	67,67,67,67	0
56	MG	CA	1685	1/1	0.73	0.50	68,68,68,68	0
56	MG	BA	3742	1/1	0.73	0.15	70,70,70,70	0
56	MG	BA	3923	1/1	0.73	0.29	57,57,57,57	0
56	MG	AY	103	1/1	0.73	0.10	87,87,87,87	0
56	MG	BA	3375	1/1	0.73	0.20	76,76,76,76	0
56	MG	BA	3745	1/1	0.73	0.75	70,70,70,70	0
56	MG	BA	3278	1/1	0.73	0.28	67,67,67,67	0
56	MG	AZ	103	1/1	0.73	0.09	66,66,66,66	0
56	MG	B1	105	1/1	0.73	0.34	87,87,87,87	0
56	MG	BA	3876	1/1	0.73	0.45	88,88,88,88	0
56	MG	BA	3709	1/1	0.74	0.29	70,70,70,70	0
56	MG	BA	3757	1/1	0.74	0.43	76,76,76,76	0
56	MG	BA	3801	1/1	0.74	0.19	51,51,51,51	0
56	MG	BA	3399	1/1	0.74	0.10	73,73,73,73	0
56	MG	DD	5005	1/1	0.74	0.64	51,51,51,51	0
56	MG	BA	3401	1/1	0.74	0.33	86,86,86,86	0
56	MG	BA	3630	1/1	0.74	0.18	47,47,47,47	0
56	MG	BA	3273	1/1	0.74	0.62	74,74,74,74	0
56	MG	BA	3350	1/1	0.74	0.26	31,31,31,31	0
56	MG	BA	3222	1/1	0.74	0.34	39,39,39,39	0
56	MG	AA	1935	1/1	0.74	0.11	53,53,53,53	0
56	MG	AK	206	1/1	0.74	0.30	69,69,69,69	0
56	MG	CA	1785	1/1	0.74	0.31	83,83,83,83	0
56	MG	BA	3839	1/1	0.74	0.38	60,60,60,60	0
56	MG	BA	3609	1/1	0.74	0.38	39,39,39,39	0
56	MG	CA	1763	1/1	0.74	1.37	77,77,77,77	0
56	MG	BB	226	1/1	0.74	0.32	72,72,72,72	0
56	MG	BD	5003	1/1	0.74	0.15	57,57,57,57	0
56	MG	BA	3525	1/1	0.74	0.10	77,77,77,77	0
56	MG	BA	3524	1/1	0.74	0.08	44,44,44,44	0
56	MG	BA	3747	1/1	0.75	0.43	64,64,64,64	0
56	MG	BA	3753	1/1	0.75	0.38	65,65,65,65	0
56	MG	BA	3792	1/1	0.75	0.31	85,85,85,85	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	BA	3250	1/1	0.75	0.23	81,81,81,81	0
56	MG	CA	1686	1/1	0.75	0.25	48,48,48,48	0
56	MG	BQ	205	1/1	0.75	0.25	57,57,57,57	0
56	MG	AA	1902	1/1	0.75	0.51	61,61,61,61	0
56	MG	CY	111	1/1	0.75	0.52	60,60,60,60	0
56	MG	BA	3471	1/1	0.75	0.36	50,50,50,50	0
56	MG	AA	1661	1/1	0.75	0.13	66,66,66,66	0
56	MG	DA	3370	1/1	0.75	0.21	71,71,71,71	0
56	MG	BA	3697	1/1	0.76	0.43	72,72,72,72	0
56	MG	CK	202	1/1	0.76	0.21	91,91,91,91	0
56	MG	BA	3265	1/1	0.76	0.24	42,42,42,42	0
56	MG	BA	3614	1/1	0.76	0.21	56,56,56,56	0
56	MG	AY	101	1/1	0.76	0.51	68,68,68,68	0
56	MG	AA	1929	1/1	0.76	0.21	71,71,71,71	0
56	MG	BA	3683	1/1	0.76	0.32	63,63,63,63	0
56	MG	BA	3891	1/1	0.76	0.32	58,58,58,58	0
56	MG	CY	107	1/1	0.76	0.27	60,60,60,60	0
56	MG	CA	1705	1/1	0.76	0.85	60,60,60,60	0
56	MG	AX	414	1/1	0.76	0.36	97,97,97,97	0
56	MG	AA	1667	1/1	0.76	0.26	70,70,70,70	0
56	MG	BA	3295	1/1	0.76	0.20	22,22,22,22	0
56	MG	BA	3011	1/1	0.76	0.22	47,47,47,47	0
56	MG	BA	3403	1/1	0.76	0.24	98,98,98,98	0
56	MG	AA	1923	1/1	0.76	0.33	79,79,79,79	0
56	MG	BA	3231	1/1	0.76	0.23	63,63,63,63	0
56	MG	CA	1711	1/1	0.76	0.84	57,57,57,57	0
56	MG	BA	3009	1/1	0.76	0.60	59,59,59,59	0
56	MG	BA	3550	1/1	0.76	0.32	42,42,42,42	0
56	MG	BA	3847	1/1	0.76	0.44	62,62,62,62	0
56	MG	AA	1881	1/1	0.76	0.48	98,98,98,98	0
56	MG	BA	3441	1/1	0.76	0.60	70,70,70,70	0
56	MG	BA	3109	1/1	0.76	0.18	70,70,70,70	0
56	MG	BA	3581	1/1	0.76	0.11	69,69,69,69	0
56	MG	BA	3133	1/1	0.76	0.34	53,53,53,53	0
56	MG	BA	3055	1/1	0.76	0.20	73,73,73,73	0
56	MG	BA	3738	1/1	0.76	1.02	57,57,57,57	0
56	MG	CA	1695	1/1	0.76	0.15	59,59,59,59	0
56	MG	BA	3914	1/1	0.77	0.16	47,47,47,47	0
56	MG	CA	1694	1/1	0.77	0.13	60,60,60,60	0
56	MG	BA	3790	1/1	0.77	0.23	86,86,86,86	0
56	MG	BA	3461	1/1	0.77	0.21	69,69,69,69	0
56	MG	AA	1764	1/1	0.77	0.43	72,72,72,72	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	CA	1669	1/1	0.77	0.56	79,79,79,79	0
56	MG	DA	3204	1/1	0.77	0.33	43,43,43,43	0
56	MG	BB	227	1/1	0.77	0.31	54,54,54,54	0
56	MG	CA	1743	1/1	0.77	0.10	52,52,52,52	0
56	MG	BA	3119	1/1	0.77	0.24	54,54,54,54	0
56	MG	AA	1723	1/1	0.77	0.32	76,76,76,76	0
56	MG	BA	3014	1/1	0.77	0.37	65,65,65,65	0
56	MG	CY	104	1/1	0.77	0.10	78,78,78,78	0
56	MG	BA	3114	1/1	0.77	0.15	63,63,63,63	0
56	MG	BA	3263	1/1	0.77	0.55	47,47,47,47	0
56	MG	BE	306	1/1	0.77	0.14	71,71,71,71	0
56	MG	AA	1897	1/1	0.77	0.36	62,62,62,62	0
56	MG	BA	3146	1/1	0.77	0.17	33,33,33,33	0
56	MG	BA	3300	1/1	0.78	0.39	61,61,61,61	0
56	MG	AA	1867	1/1	0.78	0.12	51,51,51,51	0
56	MG	BA	3210	1/1	0.78	0.14	69,69,69,69	0
56	MG	BA	3511	1/1	0.78	0.12	43,43,43,43	0
56	MG	BA	3397	1/1	0.78	0.09	52,52,52,52	0
56	MG	CH	202	1/1	0.78	0.15	59,59,59,59	0
56	MG	DA	3121	1/1	0.78	0.22	41,41,41,41	0
56	MG	BA	3593	1/1	0.78	0.47	64,64,64,64	0
56	MG	BA	3597	1/1	0.78	0.73	48,48,48,48	0
56	MG	BA	3334	1/1	0.78	0.13	77,77,77,77	0
56	MG	DA	3113	1/1	0.78	0.22	85,85,85,85	0
56	MG	AA	1864	1/1	0.78	0.12	71,71,71,71	0
56	MG	CA	1815	1/1	0.78	0.27	63,63,63,63	0
56	MG	AA	1636	1/1	0.78	0.12	67,67,67,67	0
56	MG	BA	3859	1/1	0.79	0.34	80,80,80,80	0
56	MG	CA	1796	1/1	0.79	0.20	77,77,77,77	0
56	MG	CA	1775	1/1	0.79	0.39	91,91,91,91	0
56	MG	DA	3129	1/1	0.79	0.59	57,57,57,57	0
56	MG	BA	3583	1/1	0.79	0.09	71,71,71,71	0
56	MG	AA	1853	1/1	0.79	0.15	24,24,24,24	0
56	MG	BA	3477	1/1	0.79	0.12	53,53,53,53	0
56	MG	DA	3300	1/1	0.79	0.42	78,78,78,78	0
56	MG	AA	1955	1/1	0.79	0.48	82,82,82,82	0
56	MG	BA	3688	1/1	0.79	0.14	74,74,74,74	0
56	MG	CA	1788	1/1	0.79	0.27	94,94,94,94	0
56	MG	BA	3691	1/1	0.79	0.15	73,73,73,73	0
56	MG	DA	3297	1/1	0.79	1.17	89,89,89,89	0
56	MG	BA	3024	1/1	0.79	0.33	87,87,87,87	0
56	MG	AA	1715	1/1	0.79	0.25	50,50,50,50	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	BA	3234	1/1	0.79	0.24	55,55,55,55	0
56	MG	AX	404	1/1	0.79	0.37	92,92,92,92	0
56	MG	BO	201	1/1	0.79	0.25	62,62,62,62	0
56	MG	DA	3396	1/1	0.79	0.19	66,66,66,66	0
56	MG	AA	1813	1/1	0.79	0.31	67,67,67,67	0
56	MG	BA	3712	1/1	0.79	0.41	77,77,77,77	0
56	MG	AY	123	1/1	0.79	0.28	42,42,42,42	0
56	MG	AA	1789	1/1	0.79	0.17	77,77,77,77	0
56	MG	CA	1712	1/1	0.79	0.27	39,39,39,39	0
56	MG	DA	3400	1/1	0.79	0.17	52,52,52,52	0
56	MG	AY	118	1/1	0.79	0.12	83,83,83,83	0
56	MG	CA	1689	1/1	0.79	0.46	81,81,81,81	0
56	MG	BA	3043	1/1	0.79	0.15	58,58,58,58	0
56	MG	BA	3409	1/1	0.79	0.11	58,58,58,58	0
56	MG	BA	3746	1/1	0.79	0.45	71,71,71,71	0
56	MG	BA	3100	1/1	0.80	0.18	57,57,57,57	0
56	MG	AA	1932	1/1	0.80	0.15	64,64,64,64	0
56	MG	BA	3199	1/1	0.80	0.25	65,65,65,65	0
56	MG	AA	1978	1/1	0.80	0.17	35,35,35,35	0
56	MG	DA	3376	1/1	0.80	0.10	75,75,75,75	0
56	MG	BA	3147	1/1	0.80	0.47	52,52,52,52	0
56	MG	BA	3730	1/1	0.80	0.52	86,86,86,86	0
56	MG	AA	1773	1/1	0.80	0.35	46,46,46,46	0
56	MG	DA	3251	1/1	0.80	0.27	51,51,51,51	0
56	MG	AA	1698	1/1	0.80	0.23	53,53,53,53	0
56	MG	BA	3072	1/1	0.80	0.31	61,61,61,61	0
56	MG	CA	1640	1/1	0.80	0.22	4,4,4,4	0
56	MG	BA	3543	1/1	0.80	0.27	38,38,38,38	0
56	MG	AA	1846	1/1	0.80	0.39	68,68,68,68	0
56	MG	DA	3290	1/1	0.80	0.37	64,64,64,64	0
56	MG	AB	306	1/1	0.80	0.29	56,56,56,56	0
56	MG	BA	3207	1/1	0.80	0.12	73,73,73,73	0
56	MG	BA	3036	1/1	0.80	0.35	88,88,88,88	0
56	MG	BX	101	1/1	0.80	0.27	67,67,67,67	0
56	MG	BA	3209	1/1	0.80	0.30	54,54,54,54	0
56	MG	BA	3095	1/1	0.80	0.13	40,40,40,40	0
56	MG	BA	3880	1/1	0.80	0.16	63,63,63,63	0
56	MG	AA	1699	1/1	0.80	0.41	61,61,61,61	0
56	MG	BA	3172	1/1	0.80	0.16	54,54,54,54	0
56	MG	BA	3690	1/1	0.80	0.32	80,80,80,80	0
56	MG	BA	3163	1/1	0.80	0.31	91,91,91,91	0
56	MG	BN	203	1/1	0.80	0.32	72,72,72,72	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	DA	3217	1/1	0.80	0.07	58,58,58,58	0
56	MG	BA	3509	1/1	0.80	0.17	34,34,34,34	0
56	MG	BA	3648	1/1	0.80	0.22	48,48,48,48	0
56	MG	BA	3449	1/1	0.80	0.84	73,73,73,73	0
56	MG	BA	3516	1/1	0.80	0.19	43,43,43,43	0
56	MG	AA	1936	1/1	0.80	0.20	97,97,97,97	0
56	MG	AA	1691	1/1	0.80	0.15	37,37,37,37	0
56	MG	DA	3383	1/1	0.81	1.05	71,71,71,71	0
56	MG	CK	201	1/1	0.81	0.34	70,70,70,70	0
56	MG	BA	3731	1/1	0.81	0.28	53,53,53,53	0
56	MG	BA	3565	1/1	0.81	0.20	50,50,50,50	0
56	MG	BA	3122	1/1	0.81	0.12	56,56,56,56	0
56	MG	BP	201	1/1	0.81	0.47	68,68,68,68	0
56	MG	CY	108	1/1	0.81	0.22	60,60,60,60	0
56	MG	DA	3398	1/1	0.81	0.41	55,55,55,55	0
56	MG	DA	3230	1/1	0.81	0.13	58,58,58,58	0
56	MG	BA	3534	1/1	0.81	0.31	61,61,61,61	0
56	MG	DA	3403	1/1	0.81	0.22	64,64,64,64	0
56	MG	BA	3518	1/1	0.81	0.29	58,58,58,58	0
56	MG	BA	3443	1/1	0.81	0.19	71,71,71,71	0
56	MG	CF	202	1/1	0.81	0.22	51,51,51,51	0
56	MG	AA	1833	1/1	0.81	0.13	60,60,60,60	0
56	MG	B0	101	1/1	0.81	0.62	63,63,63,63	0
56	MG	BN	202	1/1	0.81	0.20	46,46,46,46	0
56	MG	BA	3356	1/1	0.81	0.39	54,54,54,54	0
56	MG	BA	3850	1/1	0.81	0.30	54,54,54,54	0
56	MG	DA	3380	1/1	0.81	0.25	64,64,64,64	0
56	MG	AM	201	1/1	0.81	0.55	86,86,86,86	0
56	MG	AA	1956	1/1	0.81	0.21	58,58,58,58	0
56	MG	AY	124	1/1	0.81	0.44	51,51,51,51	0
56	MG	AA	1645	1/1	0.81	0.26	42,42,42,42	0
56	MG	CA	1767	1/1	0.81	0.10	64,64,64,64	0
56	MG	AA	1711	1/1	0.81	0.42	58,58,58,58	0
56	MG	DA	3315	1/1	0.81	0.34	62,62,62,62	0
56	MG	BA	3364	1/1	0.81	0.47	40,40,40,40	0
56	MG	AA	1906	1/1	0.81	0.16	57,57,57,57	0
56	MG	AA	1623	1/1	0.81	0.46	74,74,74,74	0
56	MG	CZ	109	1/1	0.81	0.10	95,95,95,95	0
56	MG	BE	304	1/1	0.81	0.19	79,79,79,79	0
56	MG	B8	104	1/1	0.81	0.28	49,49,49,49	0
56	MG	BA	3229	1/1	0.81	0.26	47,47,47,47	0
56	MG	DA	3107	1/1	0.81	0.09	30,30,30,30	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	DA	3388	1/1	0.81	0.11	19,19,19,19	0
56	MG	BA	3005	1/1	0.81	0.26	51,51,51,51	0
56	MG	BA	3196	1/1	0.81	0.37	50,50,50,50	0
56	MG	AA	1992	1/1	0.81	0.17	77,77,77,77	0
56	MG	CA	1677	1/1	0.81	0.26	103,103,103,103	0
56	MG	BA	3027	1/1	0.81	0.32	86,86,86,86	0
56	MG	DA	3199	1/1	0.81	0.26	59,59,59,59	0
56	MG	AA	1863	1/1	0.81	0.11	57,57,57,57	0
56	MG	AA	1882	1/1	0.81	0.32	53,53,53,53	0
56	MG	BA	3615	1/1	0.81	0.15	56,56,56,56	0
56	MG	AA	1609	1/1	0.81	0.13	58,58,58,58	0
56	MG	CA	1779	1/1	0.81	0.51	76,76,76,76	0
56	MG	B2	102	1/1	0.81	0.50	62,62,62,62	0
56	MG	BA	3510	1/1	0.82	0.26	61,61,61,61	0
56	MG	CZ	105	1/1	0.82	0.05	74,74,74,74	0
56	MG	DA	3311	1/1	0.82	0.19	72,72,72,72	0
56	MG	DA	3292	1/1	0.82	0.32	74,74,74,74	0
56	MG	BA	3116	1/1	0.82	0.34	44,44,44,44	0
56	MG	AI	201	1/1	0.82	0.28	59,59,59,59	0
56	MG	AA	1818	1/1	0.82	0.79	74,74,74,74	0
56	MG	AA	1670	1/1	0.82	0.33	67,67,67,67	0
56	MG	BA	3651	1/1	0.82	0.32	37,37,37,37	0
56	MG	BA	3049	1/1	0.82	0.24	56,56,56,56	0
56	MG	CA	1684	1/1	0.82	0.23	74,74,74,74	0
56	MG	BA	3076	1/1	0.82	0.46	51,51,51,51	0
56	MG	BB	217	1/1	0.82	0.42	74,74,74,74	0
56	MG	BA	3275	1/1	0.82	0.32	46,46,46,46	0
56	MG	DA	3281	1/1	0.82	0.27	63,63,63,63	0
56	MG	DB	210	1/1	0.82	0.20	3,3,3,3	0
56	MG	BA	3102	1/1	0.82	0.22	89,89,89,89	0
56	MG	BF	305	1/1	0.82	0.11	63,63,63,63	0
56	MG	BA	3776	1/1	0.82	0.23	43,43,43,43	0
56	MG	BA	3154	1/1	0.82	0.17	41,41,41,41	0
56	MG	AA	1786	1/1	0.82	0.18	61,61,61,61	0
56	MG	AA	1643	1/1	0.82	0.35	50,50,50,50	0
56	MG	DA	3428	1/1	0.82	0.39	3,3,3,3	0
56	MG	BA	3264	1/1	0.82	0.25	60,60,60,60	0
56	MG	BA	3771	1/1	0.82	0.52	72,72,72,72	0
56	MG	AA	1696	1/1	0.82	0.39	59,59,59,59	0
56	MG	BB	219	1/1	0.82	0.20	41,41,41,41	0
56	MG	BY	202	1/1	0.82	0.17	42,42,42,42	0
56	MG	DA	3283	1/1	0.82	0.82	70,70,70,70	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	AY	115	1/1	0.82	0.13	65,65,65,65	0
56	MG	BA	3861	1/1	0.82	0.19	65,65,65,65	0
56	MG	AA	1860	1/1	0.82	0.23	58,58,58,58	0
56	MG	CA	1670	1/1	0.82	0.23	43,43,43,43	0
56	MG	CA	1742	1/1	0.82	0.19	54,54,54,54	0
56	MG	BB	215	1/1	0.82	0.11	103,103,103,103	0
56	MG	BA	3149	1/1	0.83	0.18	29,29,29,29	0
56	MG	AA	1655	1/1	0.83	0.14	61,61,61,61	0
56	MG	AA	1823	1/1	0.83	0.23	47,47,47,47	0
56	MG	BA	3862	1/1	0.83	0.10	85,85,85,85	0
56	MG	BA	3692	1/1	0.83	0.41	52,52,52,52	0
56	MG	AA	1739	1/1	0.83	0.24	55,55,55,55	0
56	MG	CA	1718	1/1	0.83	0.21	41,41,41,41	0
56	MG	BA	3460	1/1	0.83	0.82	75,75,75,75	0
56	MG	AA	1754	1/1	0.83	0.30	70,70,70,70	0
56	MG	BA	3283	1/1	0.83	0.40	63,63,63,63	0
56	MG	CY	110	1/1	0.83	0.29	90,90,90,90	0
56	MG	AA	1647	1/1	0.83	0.28	64,64,64,64	0
56	MG	AA	1983	1/1	0.83	0.43	67,67,67,67	0
56	MG	BA	3384	1/1	0.83	0.18	60,60,60,60	0
56	MG	BA	3548	1/1	0.83	0.14	36,36,36,36	0
56	MG	BE	301	1/1	0.83	0.09	55,55,55,55	0
56	MG	DA	3231	1/1	0.83	0.18	72,72,72,72	0
56	MG	BA	3684	1/1	0.83	0.18	50,50,50,50	0
56	MG	BA	3410	1/1	0.83	0.15	67,67,67,67	0
56	MG	BA	3230	1/1	0.83	0.11	60,60,60,60	0
56	MG	BB	224	1/1	0.83	0.18	65,65,65,65	0
56	MG	BA	3010	1/1	0.83	0.96	72,72,72,72	0
56	MG	BA	3759	1/1	0.83	0.23	47,47,47,47	0
56	MG	BA	3480	1/1	0.83	0.18	43,43,43,43	0
56	MG	BA	3166	1/1	0.83	0.33	63,63,63,63	0
56	MG	BA	3065	1/1	0.83	0.13	78,78,78,78	0
56	MG	AE	203	1/1	0.83	0.29	72,72,72,72	0
56	MG	BA	3379	1/1	0.83	0.28	115,115,115,115	0
56	MG	AA	1730	1/1	0.83	0.25	72,72,72,72	0
56	MG	BA	3331	1/1	0.83	0.06	74,74,74,74	0
56	MG	AA	1771	1/1	0.83	0.26	45,45,45,45	0
56	MG	AA	2012	1/1	0.83	0.27	55,55,55,55	0
56	MG	BA	3483	1/1	0.83	0.43	47,47,47,47	0
56	MG	AA	1873	1/1	0.83	0.41	77,77,77,77	0
56	MG	AA	1633	1/1	0.83	0.19	77,77,77,77	0
56	MG	BA	3050	1/1	0.83	0.14	44,44,44,44	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	BA	3604	1/1	0.83	0.49	50,50,50,50	0
56	MG	AA	1827	1/1	0.83	0.26	44,44,44,44	0
56	MG	AA	1630	1/1	0.83	0.35	65,65,65,65	0
56	MG	CA	1722	1/1	0.83	0.20	49,49,49,49	0
56	MG	BA	3560	1/1	0.83	0.28	52,52,52,52	0
56	MG	BA	3481	1/1	0.84	0.82	65,65,65,65	0
56	MG	AZ	101	1/1	0.84	0.15	63,63,63,63	0
56	MG	BA	3840	1/1	0.84	0.42	56,56,56,56	0
56	MG	BA	3703	1/1	0.84	0.08	68,68,68,68	0
56	MG	BA	3058	1/1	0.84	0.08	67,67,67,67	0
56	MG	BH	204	1/1	0.84	0.13	77,77,77,77	0
56	MG	CF	203	1/1	0.84	0.27	51,51,51,51	0
56	MG	BB	218	1/1	0.84	0.10	78,78,78,78	0
56	MG	BA	3482	1/1	0.84	0.28	63,63,63,63	0
56	MG	AF	201	1/1	0.84	0.12	87,87,87,87	0
56	MG	BA	3039	1/1	0.84	0.43	67,67,67,67	0
56	MG	BA	3240	1/1	0.84	0.53	40,40,40,40	0
56	MG	AA	1957	1/1	0.84	0.07	61,61,61,61	0
56	MG	CY	105	1/1	0.84	0.18	52,52,52,52	0
56	MG	BA	3178	1/1	0.84	0.21	51,51,51,51	0
56	MG	AE	205	1/1	0.84	0.12	65,65,65,65	0
56	MG	CA	1741	1/1	0.84	0.28	50,50,50,50	0
56	MG	AA	1612	1/1	0.84	0.41	68,68,68,68	0
56	MG	AA	1743	1/1	0.84	0.11	63,63,63,63	0
56	MG	DA	3239	1/1	0.84	0.10	78,78,78,78	0
56	MG	CZ	110	1/1	0.84	0.18	68,68,68,68	0
56	MG	DI	201	1/1	0.84	0.11	38,38,38,38	0
56	MG	B5	101	1/1	0.84	0.28	63,63,63,63	0
56	MG	BA	3428	1/1	0.84	0.60	86,86,86,86	0
56	MG	BB	214	1/1	0.84	0.29	55,55,55,55	0
56	MG	CA	1680	1/1	0.84	0.19	34,34,34,34	0
56	MG	CA	1814	1/1	0.84	0.15	66,66,66,66	0
56	MG	BA	3918	1/1	0.84	0.56	63,63,63,63	0
56	MG	BA	3205	1/1	0.84	0.56	55,55,55,55	0
56	MG	AA	1610	1/1	0.84	0.23	65,65,65,65	0
56	MG	CA	1667	1/1	0.84	0.12	58,58,58,58	0
56	MG	BI	205	1/1	0.84	0.10	45,45,45,45	0
56	MG	DA	3294	1/1	0.84	0.63	63,63,63,63	0
56	MG	BA	3320	1/1	0.84	0.47	84,84,84,84	0
56	MG	DA	3131	1/1	0.84	0.30	31,31,31,31	0
56	MG	DA	3105	1/1	0.84	0.22	55,55,55,55	0
56	MG	AA	1646	1/1	0.84	0.20	38,38,38,38	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	BA	3906	1/1	0.84	0.24	67,67,67,67	0
56	MG	DA	3359	1/1	0.84	0.11	42,42,42,42	0
56	MG	BA	3617	1/1	0.84	0.24	66,66,66,66	0
56	MG	AA	1675	1/1	0.84	0.17	58,58,58,58	0
56	MG	BA	3254	1/1	0.84	0.23	79,79,79,79	0
56	MG	AK	201	1/1	0.85	0.56	76,76,76,76	0
56	MG	AA	2021	1/1	0.85	0.11	43,43,43,43	0
56	MG	BA	3519	1/1	0.85	0.15	82,82,82,82	0
56	MG	BA	3513	1/1	0.85	0.14	28,28,28,28	0
56	MG	DA	3282	1/1	0.85	0.52	72,72,72,72	0
56	MG	BA	3346	1/1	0.85	0.34	65,65,65,65	0
56	MG	BA	3612	1/1	0.85	0.10	9,9,9,9	0
56	MG	BA	3752	1/1	0.85	0.81	71,71,71,71	0
56	MG	AY	120	1/1	0.85	0.10	40,40,40,40	0
56	MG	DA	3440	1/1	0.85	0.12	4,4,4,4	0
56	MG	BI	203	1/1	0.85	0.14	53,53,53,53	0
56	MG	BA	3084	1/1	0.85	0.47	62,62,62,62	0
56	MG	DA	3390	1/1	0.85	0.13	73,73,73,73	0
56	MG	BA	3151	1/1	0.85	0.09	31,31,31,31	0
56	MG	AA	1948	1/1	0.85	0.12	56,56,56,56	0
56	MG	DA	3356	1/1	0.85	0.09	56,56,56,56	0
56	MG	BA	3725	1/1	0.85	0.12	23,23,23,23	0
56	MG	BA	3502	1/1	0.85	0.18	61,61,61,61	0
56	MG	BA	3349	1/1	0.85	0.17	46,46,46,46	0
56	MG	BA	3537	1/1	0.85	0.18	38,38,38,38	0
56	MG	CG	201	1/1	0.85	0.12	70,70,70,70	0
56	MG	AC	301	1/1	0.85	0.19	75,75,75,75	0
56	MG	BA	3124	1/1	0.85	0.25	56,56,56,56	0
56	MG	CA	1706	1/1	0.85	0.27	62,62,62,62	0
56	MG	AA	1847	1/1	0.85	0.18	30,30,30,30	0
56	MG	AA	1709	1/1	0.85	0.16	54,54,54,54	0
56	MG	BA	3157	1/1	0.85	0.39	55,55,55,55	0
56	MG	B4	101	1/1	0.85	0.10	29,29,29,29	0
56	MG	BA	3881	1/1	0.85	0.41	68,68,68,68	0
56	MG	CA	1757	1/1	0.85	0.34	66,66,66,66	0
56	MG	BF	304	1/1	0.85	0.36	65,65,65,65	0
56	MG	BA	3536	1/1	0.85	0.31	70,70,70,70	0
56	MG	BA	3377	1/1	0.85	0.14	73,73,73,73	0
56	MG	AA	1725	1/1	0.85	0.50	56,56,56,56	0
56	MG	CA	1678	1/1	0.85	0.18	49,49,49,49	0
56	MG	CA	1773	1/1	0.85	0.12	66,66,66,66	0
56	MG	BA	3181	1/1	0.85	0.20	23,23,23,23	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	BA	3529	1/1	0.85	0.41	64,64,64,64	0
56	MG	AA	1602	1/1	0.85	0.50	74,74,74,74	0
56	MG	BA	3676	1/1	0.85	0.14	44,44,44,44	0
56	MG	BA	3078	1/1	0.85	0.18	51,51,51,51	0
56	MG	BA	3360	1/1	0.85	0.26	65,65,65,65	0
56	MG	BA	3192	1/1	0.85	0.31	50,50,50,50	0
56	MG	AX	408	1/1	0.85	0.10	57,57,57,57	0
56	MG	AC	302	1/1	0.85	0.36	88,88,88,88	0
56	MG	AA	1785	1/1	0.85	0.26	70,70,70,70	0
56	MG	BA	3590	1/1	0.85	0.21	32,32,32,32	0
56	MG	BA	3528	1/1	0.85	0.27	60,60,60,60	0
56	MG	AF	202	1/1	0.86	0.09	41,41,41,41	0
56	MG	BA	3901	1/1	0.86	0.37	62,62,62,62	0
56	MG	CZ	108	1/1	0.86	0.15	69,69,69,69	0
56	MG	CA	1682	1/1	0.86	0.19	52,52,52,52	0
56	MG	DA	3308	1/1	0.86	0.13	46,46,46,46	0
56	MG	BA	3913	1/1	0.86	0.24	45,45,45,45	0
56	MG	BA	3045	1/1	0.86	0.59	56,56,56,56	0
56	MG	BA	3416	1/1	0.86	0.38	55,55,55,55	0
56	MG	BA	3425	1/1	0.86	0.29	48,48,48,48	0
56	MG	BA	3877	1/1	0.86	0.28	76,76,76,76	0
56	MG	DA	3456	1/1	0.86	0.19	5,5,5,5	0
56	MG	DA	3238	1/1	0.86	0.14	62,62,62,62	0
56	MG	BA	3458	1/1	0.86	0.33	50,50,50,50	0
56	MG	DA	3074	1/1	0.86	0.39	3,3,3,3	0
56	MG	AA	2003	1/1	0.86	0.15	54,54,54,54	0
56	MG	DA	3051	1/1	0.86	0.27	3,3,3,3	0
56	MG	AA	1744	1/1	0.86	0.32	74,74,74,74	0
56	MG	BE	303	1/1	0.86	0.09	53,53,53,53	0
56	MG	BA	3778	1/1	0.86	0.20	63,63,63,63	0
56	MG	BB	232	1/1	0.86	0.10	58,58,58,58	0
56	MG	AA	1868	1/1	0.86	0.25	38,38,38,38	0
56	MG	AA	1865	1/1	0.86	0.13	73,73,73,73	0
56	MG	BA	3152	1/1	0.86	0.40	49,49,49,49	0
56	MG	DA	3387	1/1	0.86	0.12	77,77,77,77	0
56	MG	DA	3424	1/1	0.86	0.39	14,14,14,14	0
56	MG	BA	3341	1/1	0.86	0.27	70,70,70,70	0
56	MG	DA	3295	1/1	0.86	0.16	33,33,33,33	0
56	MG	DA	3348	1/1	0.86	0.12	60,60,60,60	0
56	MG	AA	1828	1/1	0.86	0.28	69,69,69,69	0
56	MG	AA	1656	1/1	0.86	0.15	47,47,47,47	0
56	MG	BA	3603	1/1	0.86	0.25	47,47,47,47	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	BA	3123	1/1	0.86	0.07	55,55,55,55	0
56	MG	AA	1763	1/1	0.86	0.13	41,41,41,41	0
56	MG	BA	3345	1/1	0.86	0.17	42,42,42,42	0
56	MG	BA	3485	1/1	0.86	0.15	71,71,71,71	0
56	MG	BA	3871	1/1	0.86	0.78	65,65,65,65	0
56	MG	BA	3466	1/1	0.86	0.31	67,67,67,67	0
56	MG	AA	1708	1/1	0.86	0.33	33,33,33,33	0
56	MG	BA	3872	1/1	0.86	0.26	54,54,54,54	0
56	MG	BA	3837	1/1	0.86	0.48	71,71,71,71	0
56	MG	BA	3638	1/1	0.86	0.21	48,48,48,48	0
56	MG	BA	3022	1/1	0.86	0.19	61,61,61,61	0
56	MG	BA	3580	1/1	0.86	0.20	54,54,54,54	0
56	MG	BA	3556	1/1	0.86	0.30	45,45,45,45	0
56	MG	AA	1985	1/1	0.86	0.17	52,52,52,52	0
56	MG	BA	3092	1/1	0.86	0.40	73,73,73,73	0
56	MG	BA	3693	1/1	0.86	0.16	62,62,62,62	0
56	MG	AA	1693	1/1	0.86	0.20	79,79,79,79	0
56	MG	CA	1771	1/1	0.86	0.23	80,80,80,80	0
56	MG	BA	3497	1/1	0.86	0.10	68,68,68,68	0
56	MG	DD	5006	1/1	0.86	0.31	47,47,47,47	0
56	MG	BA	3202	1/1	0.86	0.54	57,57,57,57	0
56	MG	BA	3421	1/1	0.86	0.27	45,45,45,45	0
56	MG	BA	3749	1/1	0.86	0.53	53,53,53,53	0
56	MG	CA	1729	1/1	0.86	0.35	36,36,36,36	0
56	MG	BA	3255	1/1	0.86	0.16	72,72,72,72	0
56	MG	AA	1940	1/1	0.86	0.39	53,53,53,53	0
56	MG	AA	1766	1/1	0.86	0.36	33,33,33,33	0
56	MG	AY	111	1/1	0.86	0.18	60,60,60,60	0
56	MG	BA	3008	1/1	0.86	0.25	38,38,38,38	0
56	MG	BG	202	1/1	0.86	0.14	63,63,63,63	0
56	MG	BA	3501	1/1	0.86	0.13	58,58,58,58	0
56	MG	BF	306	1/1	0.86	0.15	47,47,47,47	0
56	MG	BA	3381	1/1	0.86	0.20	48,48,48,48	0
56	MG	BA	3037	1/1	0.86	0.41	61,61,61,61	0
56	MG	AA	1611	1/1	0.86	0.28	48,48,48,48	0
56	MG	BA	3432	1/1	0.86	0.10	52,52,52,52	0
56	MG	BA	3873	1/1	0.86	0.41	44,44,44,44	0
56	MG	BB	222	1/1	0.86	0.20	39,39,39,39	0
56	MG	BS	202	1/1	0.86	0.07	42,42,42,42	0
56	MG	AA	1876	1/1	0.86	0.21	69,69,69,69	0
56	MG	BA	3700	1/1	0.86	0.14	72,72,72,72	0
56	MG	AA	1672	1/1	0.86	0.35	69,69,69,69	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	BA	3407	1/1	0.86	0.43	56,56,56,56	0
56	MG	BA	3642	1/1	0.86	0.14	67,67,67,67	0
56	MG	DA	3389	1/1	0.86	0.17	70,70,70,70	0
56	MG	AK	202	1/1	0.86	0.17	95,95,95,95	0
56	MG	CA	1690	1/1	0.87	0.22	54,54,54,54	0
56	MG	DA	3449	1/1	0.87	0.12	53,53,53,53	0
56	MG	BN	201	1/1	0.87	0.14	70,70,70,70	0
56	MG	AA	2023	1/1	0.87	0.10	33,33,33,33	0
56	MG	CA	1652	1/1	0.87	0.62	44,44,44,44	0
56	MG	DA	3235	1/1	0.87	0.10	24,24,24,24	0
56	MG	BA	3828	1/1	0.87	0.23	46,46,46,46	0
56	MG	DA	3360	1/1	0.87	0.31	56,56,56,56	0
56	MG	AA	1607	1/1	0.87	0.21	62,62,62,62	0
56	MG	BA	3247	1/1	0.87	0.34	42,42,42,42	0
56	MG	DA	3153	1/1	0.87	0.22	5,5,5,5	0
56	MG	BA	3707	1/1	0.87	0.50	77,77,77,77	0
56	MG	AA	1748	1/1	0.87	0.09	41,41,41,41	0
56	MG	AA	1872	1/1	0.87	0.35	59,59,59,59	0
56	MG	BA	3819	1/1	0.87	0.48	34,34,34,34	0
56	MG	AA	1779	1/1	0.87	0.70	34,34,34,34	0
56	MG	BA	3390	1/1	0.87	0.10	67,67,67,67	0
56	MG	AA	1854	1/1	0.87	0.13	39,39,39,39	0
56	MG	BH	202	1/1	0.87	0.17	56,56,56,56	0
56	MG	AX	410	1/1	0.87	0.11	73,73,73,73	0
56	MG	BA	3168	1/1	0.87	0.42	52,52,52,52	0
56	MG	BA	3917	1/1	0.87	0.15	51,51,51,51	0
56	MG	CA	1723	1/1	0.87	0.42	67,67,67,67	0
56	MG	BA	3705	1/1	0.87	0.21	42,42,42,42	0
56	MG	AA	1937	1/1	0.87	0.27	61,61,61,61	0
56	MG	AA	1659	1/1	0.87	0.17	49,49,49,49	0
56	MG	AB	302	1/1	0.87	0.10	50,50,50,50	0
56	MG	AA	2020	1/1	0.87	0.13	74,74,74,74	0
56	MG	AA	1911	1/1	0.87	0.11	63,63,63,63	0
56	MG	BA	3666	1/1	0.87	0.14	46,46,46,46	0
56	MG	BB	202	1/1	0.87	0.07	50,50,50,50	0
56	MG	CA	1626	1/1	0.87	0.56	3,3,3,3	0
56	MG	BA	3807	1/1	0.87	0.23	37,37,37,37	0
56	MG	BA	3200	1/1	0.87	0.73	76,76,76,76	0
56	MG	DA	3132	1/1	0.87	0.53	65,65,65,65	0
56	MG	DB	208	1/1	0.87	0.20	3,3,3,3	0
56	MG	BA	3103	1/1	0.87	0.57	78,78,78,78	0
56	MG	CA	1791	1/1	0.87	0.41	54,54,54,54	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	BQ	203	1/1	0.87	0.19	46,46,46,46	0
56	MG	BA	3714	1/1	0.87	0.28	60,60,60,60	0
56	MG	BA	3088	1/1	0.87	0.35	63,63,63,63	0
56	MG	AA	1679	1/1	0.87	0.41	51,51,51,51	0
56	MG	DA	3391	1/1	0.87	0.11	35,35,35,35	0
56	MG	AA	1674	1/1	0.87	0.17	52,52,52,52	0
56	MG	BA	3101	1/1	0.87	0.26	47,47,47,47	0
56	MG	AK	204	1/1	0.87	0.12	82,82,82,82	0
56	MG	BH	203	1/1	0.87	0.10	56,56,56,56	0
56	MG	AA	1727	1/1	0.87	0.33	59,59,59,59	0
56	MG	BA	3768	1/1	0.87	0.15	31,31,31,31	0
56	MG	BA	3160	1/1	0.87	0.18	54,54,54,54	0
56	MG	BA	3781	1/1	0.87	0.21	85,85,85,85	0
56	MG	DA	3069	1/1	0.87	0.43	3,3,3,3	0
56	MG	BA	3195	1/1	0.87	0.22	47,47,47,47	0
56	MG	DG	202	1/1	0.87	0.14	59,59,59,59	0
56	MG	BA	3307	1/1	0.87	0.14	34,34,34,34	0
56	MG	DA	3332	1/1	0.87	0.27	33,33,33,33	0
56	MG	AA	1916	1/1	0.87	0.09	63,63,63,63	0
56	MG	AO	102	1/1	0.87	0.39	48,48,48,48	0
56	MG	AA	1934	1/1	0.87	0.39	65,65,65,65	0
56	MG	DA	3102	1/1	0.87	0.31	74,74,74,74	0
56	MG	BA	3248	1/1	0.87	0.28	43,43,43,43	0
56	MG	BA	3462	1/1	0.87	0.17	35,35,35,35	0
56	MG	BA	3818	1/1	0.87	0.56	71,71,71,71	0
56	MG	BK	202	1/1	0.87	0.18	83,83,83,83	0
56	MG	BA	3744	1/1	0.87	0.16	72,72,72,72	0
56	MG	BA	3038	1/1	0.87	0.14	41,41,41,41	0
56	MG	BA	3812	1/1	0.87	0.17	40,40,40,40	0
56	MG	BA	3135	1/1	0.87	0.24	43,43,43,43	0
56	MG	BA	3620	1/1	0.87	0.23	53,53,53,53	0
56	MG	BA	3905	1/1	0.87	0.25	65,65,65,65	0
56	MG	AA	1767	1/1	0.87	0.11	45,45,45,45	0
56	MG	AA	1836	1/1	0.87	0.29	53,53,53,53	0
56	MG	AA	1648	1/1	0.87	0.42	87,87,87,87	0
56	MG	DA	3050	1/1	0.87	0.36	3,3,3,3	0
56	MG	CA	1818	1/1	0.87	0.43	59,59,59,59	0
56	MG	BA	3802	1/1	0.87	0.18	47,47,47,47	0
56	MG	BA	3765	1/1	0.87	0.40	60,60,60,60	0
56	MG	DA	3481	1/1	0.87	0.20	4,4,4,4	0
56	MG	BB	213	1/1	0.87	0.20	53,53,53,53	0
56	MG	BA	3442	1/1	0.87	0.15	46,46,46,46	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	AH	202	1/1	0.87	0.27	51,51,51,51	0
56	MG	BA	3279	1/1	0.87	0.20	39,39,39,39	0
56	MG	AA	2024	1/1	0.87	0.23	53,53,53,53	0
56	MG	BA	3258	1/1	0.87	0.15	50,50,50,50	0
56	MG	AB	304	1/1	0.87	0.11	73,73,73,73	0
56	MG	AA	1889	1/1	0.87	0.42	30,30,30,30	0
56	MG	AX	407	1/1	0.87	0.47	60,60,60,60	0
56	MG	BA	3323	1/1	0.87	0.25	57,57,57,57	0
56	MG	CA	1737	1/1	0.87	0.16	35,35,35,35	0
56	MG	BA	3453	1/1	0.87	0.30	57,57,57,57	0
56	MG	BA	3486	1/1	0.87	0.12	36,36,36,36	0
56	MG	AA	1918	1/1	0.87	0.08	58,58,58,58	0
56	MG	BA	3646	1/1	0.87	0.15	47,47,47,47	0
56	MG	BA	3687	1/1	0.88	0.26	59,59,59,59	0
56	MG	BB	210	1/1	0.88	0.34	72,72,72,72	0
56	MG	BA	3756	1/1	0.88	0.39	49,49,49,49	0
56	MG	AA	1904	1/1	0.88	0.44	77,77,77,77	0
56	MG	B8	101	1/1	0.88	0.31	30,30,30,30	0
56	MG	AY	121	1/1	0.88	0.13	41,41,41,41	0
56	MG	AA	1628	1/1	0.88	0.18	51,51,51,51	0
56	MG	BA	3083	1/1	0.88	0.28	71,71,71,71	0
56	MG	BA	3870	1/1	0.88	0.29	47,47,47,47	0
56	MG	AA	1952	1/1	0.88	0.14	83,83,83,83	0
56	MG	AX	403	1/1	0.88	0.10	68,68,68,68	0
56	MG	DA	3154	1/1	0.88	0.17	3,3,3,3	0
56	MG	BA	3716	1/1	0.88	0.14	24,24,24,24	0
56	MG	CA	1794	1/1	0.88	0.17	35,35,35,35	0
56	MG	DA	3293	1/1	0.88	0.32	61,61,61,61	0
56	MG	BA	3625	1/1	0.88	0.21	43,43,43,43	0
56	MG	BA	3277	1/1	0.88	0.18	57,57,57,57	0
56	MG	BA	3404	1/1	0.88	0.15	11,11,11,11	0
56	MG	BA	3162	1/1	0.88	0.24	58,58,58,58	0
56	MG	BA	3490	1/1	0.88	0.28	75,75,75,75	0
56	MG	BA	3387	1/1	0.88	0.12	56,56,56,56	0
56	MG	DA	3237	1/1	0.88	0.20	51,51,51,51	0
56	MG	AA	1842	1/1	0.88	0.52	75,75,75,75	0
56	MG	BA	3542	1/1	0.88	0.17	27,27,27,27	0
56	MG	AA	2011	1/1	0.88	0.31	75,75,75,75	0
56	MG	BA	3398	1/1	0.88	0.09	56,56,56,56	0
56	MG	AA	1700	1/1	0.88	0.36	45,45,45,45	0
56	MG	AA	1732	1/1	0.88	0.17	21,21,21,21	0
56	MG	AA	2025	1/1	0.88	0.55	58,58,58,58	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	AA	1822	1/1	0.88	0.19	40,40,40,40	0
56	MG	AA	1603	1/1	0.88	0.31	91,91,91,91	0
56	MG	BA	3825	1/1	0.88	0.28	45,45,45,45	0
56	MG	BA	3770	1/1	0.88	0.15	30,30,30,30	0
56	MG	DA	3291	1/1	0.88	0.22	44,44,44,44	0
56	MG	BA	3173	1/1	0.88	0.43	80,80,80,80	0
56	MG	BA	3574	1/1	0.88	0.30	74,74,74,74	0
56	MG	AA	1856	1/1	0.88	0.48	49,49,49,49	0
56	MG	BA	3702	1/1	0.88	0.14	83,83,83,83	0
56	MG	BA	3434	1/1	0.88	0.24	68,68,68,68	0
56	MG	DD	5003	1/1	0.88	0.27	65,65,65,65	0
56	MG	BA	3878	1/1	0.88	0.17	44,44,44,44	0
56	MG	BA	3678	1/1	0.88	0.41	37,37,37,37	0
56	MG	AA	1996	1/1	0.88	0.28	56,56,56,56	0
56	MG	CA	1704	1/1	0.88	0.34	63,63,63,63	0
56	MG	BA	3003	1/1	0.88	0.10	36,36,36,36	0
56	MG	BA	3060	1/1	0.88	0.07	83,83,83,83	0
56	MG	BA	3922	1/1	0.88	0.11	56,56,56,56	0
56	MG	BA	3267	1/1	0.88	0.29	21,21,21,21	0
56	MG	AA	1689	1/1	0.88	0.12	55,55,55,55	0
56	MG	BA	3826	1/1	0.88	0.16	28,28,28,28	0
56	MG	CZ	103	1/1	0.88	0.10	42,42,42,42	0
56	MG	BA	3184	1/1	0.88	0.15	45,45,45,45	0
56	MG	DA	3323	1/1	0.88	0.51	3,3,3,3	0
56	MG	AA	1973	1/1	0.88	0.18	56,56,56,56	0
56	MG	CA	1683	1/1	0.88	0.30	61,61,61,61	0
56	MG	CA	1671	1/1	0.88	0.14	63,63,63,63	0
56	MG	CA	1736	1/1	0.88	0.36	3,3,3,3	0
56	MG	DA	3375	1/1	0.88	0.14	88,88,88,88	0
56	MG	AY	110	1/1	0.88	0.15	31,31,31,31	0
56	MG	AA	1751	1/1	0.88	0.17	61,61,61,61	0
56	MG	BA	3897	1/1	0.88	0.23	48,48,48,48	0
56	MG	BA	3727	1/1	0.88	0.28	44,44,44,44	0
56	MG	AA	2015	1/1	0.88	0.11	40,40,40,40	0
56	MG	AA	1858	1/1	0.88	0.10	72,72,72,72	0
56	MG	BB	225	1/1	0.88	0.16	48,48,48,48	0
56	MG	AZ	107	1/1	0.88	0.07	78,78,78,78	0
56	MG	AA	1859	1/1	0.88	0.12	76,76,76,76	0
56	MG	AA	2005	1/1	0.88	0.20	49,49,49,49	0
56	MG	CA	1714	1/1	0.88	0.35	62,62,62,62	0
56	MG	BA	3002	1/1	0.88	0.33	47,47,47,47	0
56	MG	CY	106	1/1	0.88	0.36	66,66,66,66	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	BA	3657	1/1	0.88	0.48	56,56,56,56	0
56	MG	DA	3108	1/1	0.88	0.35	59,59,59,59	0
56	MG	BA	3866	1/1	0.88	0.19	25,25,25,25	0
56	MG	AA	1942	1/1	0.88	0.20	34,34,34,34	0
56	MG	BA	3221	1/1	0.88	0.45	33,33,33,33	0
56	MG	CA	1790	1/1	0.88	0.32	57,57,57,57	0
56	MG	BO	204	1/1	0.88	0.32	50,50,50,50	0
56	MG	BA	3392	1/1	0.88	0.13	52,52,52,52	0
56	MG	AA	1668	1/1	0.88	0.08	46,46,46,46	0
56	MG	BA	3385	1/1	0.89	0.09	63,63,63,63	0
56	MG	AA	1944	1/1	0.89	0.07	48,48,48,48	0
56	MG	AY	107	1/1	0.89	0.08	67,67,67,67	0
56	MG	BA	3889	1/1	0.89	0.19	44,44,44,44	0
56	MG	CZ	112	1/1	0.89	0.14	63,63,63,63	0
56	MG	AA	1974	1/1	0.89	0.43	48,48,48,48	0
56	MG	BA	3423	1/1	0.89	0.16	21,21,21,21	0
56	MG	DA	3149	1/1	0.89	0.29	3,3,3,3	0
56	MG	AA	1692	1/1	0.89	0.50	79,79,79,79	0
56	MG	BA	3026	1/1	0.89	0.20	33,33,33,33	0
56	MG	BA	3465	1/1	0.89	0.44	59,59,59,59	0
56	MG	BA	3272	1/1	0.89	0.20	54,54,54,54	0
56	MG	AA	1741	1/1	0.89	0.17	60,60,60,60	0
56	MG	B1	107	1/1	0.89	0.14	56,56,56,56	0
56	MG	DA	3285	1/1	0.89	0.13	4,4,4,4	0
56	MG	BA	3161	1/1	0.89	0.42	103,103,103,103	0
56	MG	BA	3626	1/1	0.89	0.16	62,62,62,62	0
56	MG	BA	3761	1/1	0.89	0.15	29,29,29,29	0
56	MG	BA	3849	1/1	0.89	0.35	52,52,52,52	0
56	MG	BA	3190	1/1	0.89	0.25	77,77,77,77	0
56	MG	AZ	113	1/1	0.89	0.10	60,60,60,60	0
56	MG	AA	1762	1/1	0.89	0.12	43,43,43,43	0
56	MG	DA	3457	1/1	0.89	0.19	4,4,4,4	0
56	MG	DA	3286	1/1	0.89	0.24	33,33,33,33	0
56	MG	BA	3227	1/1	0.89	0.16	46,46,46,46	0
56	MG	BA	3373	1/1	0.89	0.19	50,50,50,50	0
56	MG	AA	2026	1/1	0.89	0.11	26,26,26,26	0
56	MG	AA	1933	1/1	0.89	0.14	75,75,75,75	0
56	MG	AD	5003	1/1	0.89	0.07	42,42,42,42	0
56	MG	BA	3304	1/1	0.89	0.33	25,25,25,25	0
56	MG	CA	1772	1/1	0.89	0.27	3,3,3,3	0
56	MG	BA	3896	1/1	0.89	0.19	58,58,58,58	0
56	MG	BA	3909	1/1	0.89	0.23	39,39,39,39	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	BA	3427	1/1	0.89	0.13	34,34,34,34	0
56	MG	BV	202	1/1	0.89	0.65	38,38,38,38	0
56	MG	BA	3788	1/1	0.89	0.19	69,69,69,69	0
56	MG	AA	1879	1/1	0.89	0.17	49,49,49,49	0
56	MG	BA	3894	1/1	0.89	0.10	70,70,70,70	0
56	MG	BA	3256	1/1	0.89	0.64	60,60,60,60	0
56	MG	BA	3140	1/1	0.89	0.20	33,33,33,33	0
56	MG	AA	1794	1/1	0.89	0.12	19,19,19,19	0
56	MG	BA	3520	1/1	0.89	0.19	61,61,61,61	0
56	MG	BA	3169	1/1	0.89	0.19	67,67,67,67	0
56	MG	BA	3175	1/1	0.89	0.30	69,69,69,69	0
56	MG	B6	102	1/1	0.89	0.09	57,57,57,57	0
56	MG	AA	2002	1/1	0.89	0.15	47,47,47,47	0
56	MG	CA	1687	1/1	0.89	0.29	46,46,46,46	0
56	MG	CA	1813	1/1	0.89	0.13	64,64,64,64	0
56	MG	AA	1738	1/1	0.89	0.20	47,47,47,47	0
56	MG	BA	3808	1/1	0.89	0.20	18,18,18,18	0
56	MG	AA	1688	1/1	0.89	0.08	68,68,68,68	0
56	MG	BA	3561	1/1	0.89	0.29	75,75,75,75	0
56	MG	BA	3357	1/1	0.89	0.16	31,31,31,31	0
56	MG	BB	233	1/1	0.89	0.09	48,48,48,48	0
56	MG	BA	3904	1/1	0.89	0.40	53,53,53,53	0
56	MG	BA	3599	1/1	0.89	0.55	50,50,50,50	0
56	MG	AA	1814	1/1	0.89	0.20	47,47,47,47	0
56	MG	BA	3570	1/1	0.89	0.20	62,62,62,62	0
56	MG	CO	101	1/1	0.89	0.21	33,33,33,33	0
56	MG	DA	3029	1/1	0.89	0.17	4,4,4,4	0
56	MG	BA	3228	1/1	0.89	0.18	31,31,31,31	0
56	MG	AY	126	1/1	0.89	0.42	68,68,68,68	0
56	MG	AA	1920	1/1	0.89	0.25	26,26,26,26	0
56	MG	BA	3268	1/1	0.89	0.20	45,45,45,45	0
56	MG	AA	1617	1/1	0.89	0.15	48,48,48,48	0
56	MG	AY	122	1/1	0.89	0.16	58,58,58,58	0
56	MG	AX	409	1/1	0.89	0.19	47,47,47,47	0
56	MG	BA	3029	1/1	0.89	0.30	59,59,59,59	0
56	MG	BA	3662	1/1	0.89	0.33	35,35,35,35	0
56	MG	CY	114	1/1	0.89	0.37	39,39,39,39	0
56	MG	BA	3337	1/1	0.89	0.24	69,69,69,69	0
56	MG	AA	1995	1/1	0.89	0.11	44,44,44,44	0
56	MG	AB	305	1/1	0.89	0.16	56,56,56,56	0
56	MG	BA	3685	1/1	0.89	0.17	54,54,54,54	0
56	MG	BA	3798	1/1	0.89	0.10	54,54,54,54	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	CA	1744	1/1	0.89	0.10	36,36,36,36	0
56	MG	BA	3143	1/1	0.89	0.55	64,64,64,64	0
56	MG	BA	3572	1/1	0.89	0.15	34,34,34,34	0
56	MG	DA	3447	1/1	0.89	0.32	15,15,15,15	0
56	MG	DA	3103	1/1	0.89	0.29	62,62,62,62	0
56	MG	AA	1729	1/1	0.89	0.32	60,60,60,60	0
56	MG	AZ	105	1/1	0.89	0.13	78,78,78,78	0
56	MG	BA	3507	1/1	0.89	0.16	82,82,82,82	0
56	MG	B5	102	1/1	0.89	0.10	49,49,49,49	0
56	MG	BA	3446	1/1	0.89	0.41	58,58,58,58	0
56	MG	BA	3791	1/1	0.89	0.70	63,63,63,63	0
56	MG	DA	3346	1/1	0.89	0.32	56,56,56,56	0
56	MG	AA	1616	1/1	0.89	0.30	47,47,47,47	0
56	MG	BB	204	1/1	0.89	0.11	51,51,51,51	0
56	MG	AX	402	1/1	0.89	0.08	42,42,42,42	0
56	MG	BA	3150	1/1	0.89	0.19	41,41,41,41	0
56	MG	AA	1800	1/1	0.89	0.15	54,54,54,54	0
56	MG	CA	1748	1/1	0.89	0.19	3,3,3,3	0
56	MG	AV	5500	1/1	0.89	0.32	71,71,71,71	0
56	MG	BA	3366	1/1	0.89	0.07	24,24,24,24	0
56	MG	BS	203	1/1	0.89	0.20	52,52,52,52	0
56	MG	BA	3108	1/1	0.89	0.14	55,55,55,55	0
56	MG	DA	3326	1/1	0.89	0.18	4,4,4,4	0
56	MG	BA	3610	1/1	0.89	0.17	38,38,38,38	0
56	MG	BA	3126	1/1	0.89	0.12	46,46,46,46	0
56	MG	AA	1852	1/1	0.89	0.16	18,18,18,18	0
56	MG	DA	3334	1/1	0.89	0.49	3,3,3,3	0
56	MG	AA	1966	1/1	0.89	0.14	29,29,29,29	0
56	MG	AB	307	1/1	0.89	0.08	45,45,45,45	0
56	MG	BA	3053	1/1	0.89	0.28	78,78,78,78	0
56	MG	BA	3567	1/1	0.89	0.34	23,23,23,23	0
56	MG	BA	3793	1/1	0.89	0.14	54,54,54,54	0
56	MG	AA	1910	1/1	0.89	0.08	88,88,88,88	0
56	MG	BD	5006	1/1	0.89	0.14	11,11,11,11	0
56	MG	AA	1717	1/1	0.89	0.24	75,75,75,75	0
56	MG	DA	3241	1/1	0.89	0.14	73,73,73,73	0
56	MG	AA	1637	1/1	0.89	0.08	54,54,54,54	0
56	MG	BA	3041	1/1	0.89	0.38	98,98,98,98	0
56	MG	BA	3843	1/1	0.89	0.20	60,60,60,60	0
56	MG	BA	3619	1/1	0.89	0.20	42,42,42,42	0
56	MG	BA	3426	1/1	0.89	0.28	20,20,20,20	0
56	MG	CA	1648	1/1	0.89	0.16	33,33,33,33	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	BA	3670	1/1	0.90	0.28	37,37,37,37	0
56	MG	DA	3366	1/1	0.90	0.15	86,86,86,86	0
56	MG	DA	3259	1/1	0.90	0.24	4,4,4,4	0
56	MG	BA	3415	1/1	0.90	0.18	65,65,65,65	0
56	MG	BA	3711	1/1	0.90	0.24	70,70,70,70	0
56	MG	BA	3419	1/1	0.90	0.24	50,50,50,50	0
56	MG	AB	301	1/1	0.90	0.12	62,62,62,62	0
56	MG	BA	3311	1/1	0.90	0.23	44,44,44,44	0
56	MG	BA	3395	1/1	0.90	0.13	22,22,22,22	0
56	MG	BK	201	1/1	0.90	0.30	60,60,60,60	0
56	MG	BA	3424	1/1	0.90	0.37	55,55,55,55	0
56	MG	BA	3640	1/1	0.90	0.14	24,24,24,24	0
56	MG	AA	1601	1/1	0.90	0.26	37,37,37,37	0
56	MG	DA	3119	1/1	0.90	0.22	58,58,58,58	0
56	MG	BB	221	1/1	0.90	0.43	65,65,65,65	0
56	MG	BA	3571	1/1	0.90	0.27	39,39,39,39	0
56	MG	BA	3856	1/1	0.90	0.09	36,36,36,36	0
56	MG	BA	3701	1/1	0.90	0.12	58,58,58,58	0
56	MG	AA	1888	1/1	0.90	0.44	39,39,39,39	0
56	MG	CH	201	1/1	0.90	0.41	58,58,58,58	0
56	MG	DA	3048	1/1	0.90	0.24	4,4,4,4	0
56	MG	BA	3743	1/1	0.90	0.27	64,64,64,64	0
56	MG	BV	201	1/1	0.90	0.14	53,53,53,53	0
56	MG	BA	3301	1/1	0.90	0.21	31,31,31,31	0
56	MG	DA	3367	1/1	0.90	0.10	59,59,59,59	0
56	MG	BA	3089	1/1	0.90	0.31	69,69,69,69	0
56	MG	DA	3189	1/1	0.90	0.16	5,5,5,5	0
56	MG	BA	3352	1/1	0.90	0.11	17,17,17,17	0
56	MG	BA	3433	1/1	0.90	0.23	67,67,67,67	0
56	MG	BA	3737	1/1	0.90	0.15	50,50,50,50	0
56	MG	DA	3130	1/1	0.90	0.32	3,3,3,3	0
56	MG	BA	3607	1/1	0.90	0.19	40,40,40,40	0
56	MG	DA	3007	1/1	0.90	0.10	25,25,25,25	0
56	MG	BA	3310	1/1	0.90	0.68	73,73,73,73	0
56	MG	BA	3532	1/1	0.90	0.28	55,55,55,55	0
56	MG	AY	114	1/1	0.90	0.23	48,48,48,48	0
56	MG	BA	3107	1/1	0.90	0.13	49,49,49,49	0
56	MG	BA	3724	1/1	0.90	0.20	29,29,29,29	0
56	MG	BA	3606	1/1	0.90	0.56	52,52,52,52	0
56	MG	BA	3044	1/1	0.90	0.23	49,49,49,49	0
56	MG	AA	1707	1/1	0.90	0.11	37,37,37,37	0
56	MG	BA	3365	1/1	0.90	0.38	53,53,53,53	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	DA	3467	1/1	0.90	0.19	3,3,3,3	0
56	MG	BA	3059	1/1	0.90	0.10	74,74,74,74	0
56	MG	AA	1907	1/1	0.90	0.26	76,76,76,76	0
56	MG	BA	3919	1/1	0.90	0.28	49,49,49,49	0
56	MG	AA	1848	1/1	0.90	0.29	56,56,56,56	0
56	MG	BA	3035	1/1	0.90	0.26	51,51,51,51	0
56	MG	BA	3741	1/1	0.90	0.12	52,52,52,52	0
56	MG	DA	3115	1/1	0.90	0.25	62,62,62,62	0
56	MG	AZ	104	1/1	0.90	0.11	61,61,61,61	0
56	MG	AA	2022	1/1	0.90	0.10	35,35,35,35	0
56	MG	CA	1721	1/1	0.90	0.32	49,49,49,49	0
56	MG	BA	3134	1/1	0.90	0.18	23,23,23,23	0
56	MG	BA	3125	1/1	0.90	0.07	26,26,26,26	0
56	MG	AA	1788	1/1	0.90	0.46	66,66,66,66	0
56	MG	DA	3182	1/1	0.90	0.27	3,3,3,3	0
56	MG	BA	3845	1/1	0.90	0.55	68,68,68,68	0
56	MG	DA	3041	1/1	0.90	0.07	52,52,52,52	0
56	MG	CA	1724	1/1	0.90	0.15	36,36,36,36	0
56	MG	BA	3723	1/1	0.90	0.12	7,7,7,7	0
56	MG	DA	3065	1/1	0.90	0.16	45,45,45,45	0
56	MG	CA	1735	1/1	0.90	0.20	31,31,31,31	0
56	MG	AA	1807	1/1	0.90	0.12	36,36,36,36	0
56	MG	AT	202	1/1	0.90	0.10	58,58,58,58	0
56	MG	AX	413	1/1	0.90	0.35	32,32,32,32	0
56	MG	BA	3588	1/1	0.90	0.09	24,24,24,24	0
56	MG	DA	3485	1/1	0.90	0.16	4,4,4,4	0
56	MG	BA	3281	1/1	0.90	0.18	61,61,61,61	0
56	MG	BA	3512	1/1	0.90	0.10	62,62,62,62	0
56	MG	AA	1774	1/1	0.90	0.14	39,39,39,39	0
56	MG	CA	1703	1/1	0.90	0.11	29,29,29,29	0
56	MG	BA	3369	1/1	0.90	0.07	60,60,60,60	0
56	MG	AA	1753	1/1	0.90	0.21	62,62,62,62	0
56	MG	AZ	108	1/1	0.90	0.09	60,60,60,60	0
56	MG	CA	1655	1/1	0.90	0.31	38,38,38,38	0
56	MG	AA	2004	1/1	0.90	0.14	51,51,51,51	0
56	MG	AA	1960	1/1	0.90	0.29	53,53,53,53	0
56	MG	DA	3104	1/1	0.90	0.40	21,21,21,21	0
56	MG	AA	1820	1/1	0.90	0.14	46,46,46,46	0
56	MG	DA	3369	1/1	0.90	0.21	43,43,43,43	0
56	MG	BA	3251	1/1	0.90	0.10	41,41,41,41	0
56	MG	DA	3421	1/1	0.90	0.12	35,35,35,35	0
56	MG	BA	3023	1/1	0.90	0.15	44,44,44,44	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	BR	201	1/1	0.90	0.14	34,34,34,34	0
56	MG	DA	3278	1/1	0.90	0.17	60,60,60,60	0
56	MG	BA	3920	1/1	0.90	0.22	54,54,54,54	0
56	MG	DA	3106	1/1	0.90	0.21	46,46,46,46	0
56	MG	DA	3413	1/1	0.90	0.17	3,3,3,3	0
56	MG	BA	3641	1/1	0.90	0.33	63,63,63,63	0
56	MG	BA	3655	1/1	0.90	0.18	38,38,38,38	0
56	MG	AA	1810	1/1	0.90	0.56	64,64,64,64	0
56	MG	BA	3785	1/1	0.90	0.20	25,25,25,25	0
56	MG	BA	3253	1/1	0.90	0.33	71,71,71,71	0
56	MG	BA	3063	1/1	0.90	0.05	86,86,86,86	0
56	MG	BA	3339	1/1	0.90	0.20	66,66,66,66	0
56	MG	BB	203	1/1	0.90	0.05	51,51,51,51	0
56	MG	AA	1988	1/1	0.90	0.10	65,65,65,65	0
56	MG	BA	3393	1/1	0.90	0.23	61,61,61,61	0
56	MG	AA	1844	1/1	0.90	0.64	101,101,101,101	0
56	MG	BA	3514	1/1	0.90	0.32	53,53,53,53	0
56	MG	BA	3472	1/1	0.90	0.14	10,10,10,10	0
56	MG	BA	3372	1/1	0.90	0.05	37,37,37,37	0
56	MG	BA	3270	1/1	0.90	0.42	64,64,64,64	0
56	MG	AZ	115	1/1	0.90	0.09	39,39,39,39	0
56	MG	BA	3469	1/1	0.90	0.20	46,46,46,46	0
56	MG	AA	1614	1/1	0.90	0.38	49,49,49,49	0
56	MG	BA	3681	1/1	0.90	0.88	59,59,59,59	0
56	MG	BA	3668	1/1	0.90	0.15	33,33,33,33	0
56	MG	AA	1666	1/1	0.90	0.13	61,61,61,61	0
56	MG	BA	3208	1/1	0.90	0.09	86,86,86,86	0
56	MG	DA	3437	1/1	0.91	0.54	3,3,3,3	0
56	MG	AA	1914	1/1	0.91	0.14	70,70,70,70	0
56	MG	BA	3523	1/1	0.91	0.08	62,62,62,62	0
56	MG	DA	3195	1/1	0.91	0.36	3,3,3,3	0
56	MG	DA	3423	1/1	0.91	0.56	28,28,28,28	0
56	MG	BA	3159	1/1	0.91	0.21	61,61,61,61	0
56	MG	AA	1660	1/1	0.91	0.11	77,77,77,77	0
56	MG	CA	1716	1/1	0.91	0.17	58,58,58,58	0
56	MG	CQ	201	1/1	0.91	0.35	3,3,3,3	0
56	MG	BB	216	1/1	0.91	0.25	46,46,46,46	0
56	MG	CY	113	1/1	0.91	0.19	27,27,27,27	0
56	MG	BA	3806	1/1	0.91	0.43	29,29,29,29	0
56	MG	BA	3576	1/1	0.91	0.15	43,43,43,43	0
56	MG	DA	3067	1/1	0.91	0.13	17,17,17,17	0
56	MG	DQ	201	1/1	0.91	0.24	4,4,4,4	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	AG	201	1/1	0.91	0.18	72,72,72,72	0
56	MG	DA	3062	1/1	0.91	0.32	4,4,4,4	0
56	MG	CA	1601	1/1	0.91	0.29	3,3,3,3	0
56	MG	AA	1997	1/1	0.91	0.22	56,56,56,56	0
56	MG	BA	3760	1/1	0.91	0.35	49,49,49,49	0
56	MG	BA	3719	1/1	0.91	0.17	37,37,37,37	0
56	MG	DA	3200	1/1	0.91	0.45	3,3,3,3	0
56	MG	DA	3394	1/1	0.91	0.17	53,53,53,53	0
56	MG	AA	1838	1/1	0.91	0.26	18,18,18,18	0
56	MG	AA	1641	1/1	0.91	0.13	27,27,27,27	0
56	MG	BA	3689	1/1	0.91	0.33	80,80,80,80	0
56	MG	DA	3482	1/1	0.91	0.20	4,4,4,4	0
56	MG	BA	3082	1/1	0.91	0.15	56,56,56,56	0
56	MG	AA	1970	1/1	0.91	0.14	52,52,52,52	0
56	MG	BG	201	1/1	0.91	0.34	64,64,64,64	0
56	MG	CA	1681	1/1	0.91	0.27	3,3,3,3	0
56	MG	DA	3310	1/1	0.91	0.17	57,57,57,57	0
56	MG	BA	3527	1/1	0.91	0.12	38,38,38,38	0
56	MG	AY	109	1/1	0.91	0.20	47,47,47,47	0
56	MG	AA	1719	1/1	0.91	0.13	13,13,13,13	0
56	MG	CA	1644	1/1	0.91	0.23	3,3,3,3	0
56	MG	BA	3138	1/1	0.91	0.21	27,27,27,27	0
56	MG	BA	3836	1/1	0.91	0.22	20,20,20,20	0
56	MG	BA	3246	1/1	0.91	0.32	60,60,60,60	0
56	MG	DA	3381	1/1	0.91	0.23	3,3,3,3	0
56	MG	AZ	111	1/1	0.91	0.15	71,71,71,71	0
56	MG	BA	3028	1/1	0.91	0.34	39,39,39,39	0
56	MG	BA	3544	1/1	0.91	0.41	72,72,72,72	0
56	MG	BA	3408	1/1	0.91	0.25	50,50,50,50	0
56	MG	BA	3546	1/1	0.91	0.28	40,40,40,40	0
56	MG	CA	1719	1/1	0.91	0.23	60,60,60,60	0
56	MG	BA	3577	1/1	0.91	0.16	60,60,60,60	0
56	MG	BA	3324	1/1	0.91	0.32	50,50,50,50	0
56	MG	DA	3039	1/1	0.91	0.21	4,4,4,4	0
56	MG	DA	3355	1/1	0.91	0.08	56,56,56,56	0
56	MG	AZ	109	1/1	0.91	0.16	79,79,79,79	0
56	MG	CA	1668	1/1	0.91	0.36	3,3,3,3	0
56	MG	CA	1715	1/1	0.91	0.28	40,40,40,40	0
56	MG	CA	1673	1/1	0.91	0.15	49,49,49,49	0
56	MG	CA	1787	1/1	0.91	0.11	57,57,57,57	0
56	MG	CA	1795	1/1	0.91	0.13	54,54,54,54	0
56	MG	AA	1662	1/1	0.91	0.48	45,45,45,45	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	AA	1695	1/1	0.91	0.20	52,52,52,52	0
56	MG	BA	3869	1/1	0.91	0.14	7,7,7,7	0
56	MG	AZ	112	1/1	0.91	0.10	46,46,46,46	0
56	MG	CZ	102	1/1	0.91	0.07	51,51,51,51	0
56	MG	BA	3128	1/1	0.91	0.26	60,60,60,60	0
56	MG	AA	1658	1/1	0.91	0.13	29,29,29,29	0
56	MG	DA	3211	1/1	0.91	0.28	4,4,4,4	0
56	MG	CA	1676	1/1	0.91	0.88	42,42,42,42	0
56	MG	CA	1819	1/1	0.91	0.11	36,36,36,36	0
56	MG	AA	1799	1/1	0.91	0.10	31,31,31,31	0
56	MG	DA	3110	1/1	0.91	0.06	48,48,48,48	0
56	MG	BA	3710	1/1	0.91	0.19	52,52,52,52	0
56	MG	BA	3405	1/1	0.91	0.20	44,44,44,44	0
56	MG	AA	1982	1/1	0.91	0.30	51,51,51,51	0
56	MG	DA	3033	1/1	0.91	0.17	4,4,4,4	0
56	MG	BY	201	1/1	0.91	0.14	68,68,68,68	0
56	MG	BA	3769	1/1	0.91	0.10	28,28,28,28	0
56	MG	DA	3138	1/1	0.91	0.41	3,3,3,3	0
56	MG	BA	3601	1/1	0.91	0.18	30,30,30,30	0
56	MG	AA	1851	1/1	0.91	0.36	69,69,69,69	0
56	MG	BA	3232	1/1	0.91	0.12	58,58,58,58	0
56	MG	AA	1742	1/1	0.91	0.10	67,67,67,67	0
56	MG	BF	302	1/1	0.91	0.24	59,59,59,59	0
56	MG	DA	3245	1/1	0.91	0.15	41,41,41,41	0
56	MG	BA	3595	1/1	0.91	0.21	62,62,62,62	0
56	MG	AA	1797	1/1	0.91	0.34	21,21,21,21	0
56	MG	BA	3309	1/1	0.91	0.23	17,17,17,17	0
56	MG	BA	3018	1/1	0.91	0.17	40,40,40,40	0
56	MG	CA	1635	1/1	0.91	0.17	4,4,4,4	0
56	MG	BA	3104	1/1	0.91	0.12	67,67,67,67	0
56	MG	BA	3071	1/1	0.91	0.23	35,35,35,35	0
56	MG	AA	1887	1/1	0.91	0.14	31,31,31,31	0
56	MG	CA	1709	1/1	0.91	0.13	55,55,55,55	0
56	MG	BA	3042	1/1	0.91	0.45	74,74,74,74	0
56	MG	BA	3887	1/1	0.91	0.20	66,66,66,66	0
56	MG	CA	1766	1/1	0.91	0.08	64,64,64,64	0
56	MG	CA	1732	1/1	0.91	0.35	63,63,63,63	0
56	MG	D8	101	1/1	0.91	0.36	3,3,3,3	0
56	MG	AA	1704	1/1	0.91	0.16	48,48,48,48	0
56	MG	DA	3353	1/1	0.91	0.06	61,61,61,61	0
56	MG	AA	1984	1/1	0.91	0.16	39,39,39,39	0
56	MG	BA	3025	1/1	0.91	0.23	58,58,58,58	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	BA	3297	1/1	0.91	0.17	45,45,45,45	0
56	MG	BA	3495	1/1	0.91	0.09	48,48,48,48	0
56	MG	BA	3201	1/1	0.91	0.24	67,67,67,67	0
56	MG	BA	3259	1/1	0.91	0.10	44,44,44,44	0
56	MG	BA	3091	1/1	0.91	0.17	37,37,37,37	0
56	MG	BA	3888	1/1	0.91	0.18	53,53,53,53	0
56	MG	DA	3432	1/1	0.91	0.31	3,3,3,3	0
56	MG	BB	228	1/1	0.91	0.30	63,63,63,63	0
56	MG	AA	1758	1/1	0.91	0.20	22,22,22,22	0
56	MG	BA	3032	1/1	0.91	0.09	30,30,30,30	0
56	MG	BA	3784	1/1	0.91	0.21	33,33,33,33	0
56	MG	AA	1665	1/1	0.91	0.11	38,38,38,38	0
56	MG	AA	1772	1/1	0.91	0.31	40,40,40,40	0
56	MG	AA	1632	1/1	0.91	0.11	35,35,35,35	0
56	MG	BA	3763	1/1	0.91	0.15	52,52,52,52	0
56	MG	BA	3732	1/1	0.91	0.58	68,68,68,68	0
56	MG	B1	106	1/1	0.91	0.24	56,56,56,56	0
56	MG	DA	3125	1/1	0.91	0.20	28,28,28,28	0
56	MG	AX	401	1/1	0.91	0.12	74,74,74,74	0
56	MG	AA	1657	1/1	0.91	0.11	45,45,45,45	0
56	MG	AA	1682	1/1	0.91	0.17	40,40,40,40	0
56	MG	BA	3187	1/1	0.91	0.27	54,54,54,54	0
56	MG	BA	3541	1/1	0.91	0.17	30,30,30,30	0
56	MG	CA	1691	1/1	0.91	0.16	45,45,45,45	0
56	MG	CA	1821	1/1	0.91	0.22	29,29,29,29	0
56	MG	BA	3686	1/1	0.91	0.58	49,49,49,49	0
56	MG	BB	208	1/1	0.91	0.20	63,63,63,63	0
56	MG	AA	1735	1/1	0.91	0.10	44,44,44,44	0
56	MG	BA	3376	1/1	0.91	0.18	39,39,39,39	0
56	MG	CA	1728	1/1	0.91	0.31	57,57,57,57	0
56	MG	AA	1987	1/1	0.91	0.07	40,40,40,40	0
56	MG	BA	3347	1/1	0.91	0.08	43,43,43,43	0
56	MG	AA	1939	1/1	0.91	0.37	47,47,47,47	0
56	MG	AZ	110	1/1	0.91	0.17	69,69,69,69	0
56	MG	BA	3383	1/1	0.91	0.12	53,53,53,53	0
56	MG	AA	1749	1/1	0.91	0.12	68,68,68,68	0
56	MG	BA	3886	1/1	0.91	0.17	69,69,69,69	0
56	MG	BA	3131	1/1	0.92	0.61	72,72,72,72	0
56	MG	BA	3879	1/1	0.92	0.31	46,46,46,46	0
56	MG	AA	1816	1/1	0.92	0.28	55,55,55,55	0
56	MG	AA	1834	1/1	0.92	0.14	43,43,43,43	0
56	MG	BA	3815	1/1	0.92	0.29	28,28,28,28	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	BA	3578	1/1	0.92	0.09	48,48,48,48	0
56	MG	BA	3787	1/1	0.92	0.22	47,47,47,47	0
56	MG	BA	3438	1/1	0.92	0.20	67,67,67,67	0
56	MG	DA	3468	1/1	0.92	0.46	3,3,3,3	0
56	MG	BA	3779	1/1	0.92	0.09	22,22,22,22	0
56	MG	DA	3169	1/1	0.92	0.34	3,3,3,3	0
56	MG	AB	303	1/1	0.92	0.13	40,40,40,40	0
56	MG	BA	3585	1/1	0.92	0.17	35,35,35,35	0
56	MG	BA	3276	1/1	0.92	0.26	52,52,52,52	0
56	MG	CF	205	1/1	0.92	0.15	57,57,57,57	0
56	MG	AA	1826	1/1	0.92	0.12	46,46,46,46	0
56	MG	BA	3841	1/1	0.92	0.15	31,31,31,31	0
56	MG	CA	1610	1/1	0.92	0.17	4,4,4,4	0
56	MG	AA	1761	1/1	0.92	0.16	39,39,39,39	0
56	MG	DA	3028	1/1	0.92	0.29	4,4,4,4	0
56	MG	DA	3361	1/1	0.92	0.62	78,78,78,78	0
56	MG	BA	3740	1/1	0.92	0.29	53,53,53,53	0
56	MG	BW	202	1/1	0.92	0.21	38,38,38,38	0
56	MG	BA	3359	1/1	0.92	0.78	70,70,70,70	0
56	MG	AA	1886	1/1	0.92	0.20	50,50,50,50	0
56	MG	BA	3212	1/1	0.92	0.07	29,29,29,29	0
56	MG	AA	1685	1/1	0.92	0.14	28,28,28,28	0
56	MG	CZ	104	1/1	0.92	0.24	3,3,3,3	0
56	MG	BA	3499	1/1	0.92	0.14	57,57,57,57	0
56	MG	BA	3386	1/1	0.92	0.13	79,79,79,79	0
56	MG	BA	3448	1/1	0.92	0.25	21,21,21,21	0
56	MG	DA	3466	1/1	0.92	0.28	3,3,3,3	0
56	MG	BA	3627	1/1	0.92	0.12	22,22,22,22	0
56	MG	AA	1710	1/1	0.92	0.24	40,40,40,40	0
56	MG	AA	1745	1/1	0.92	0.07	75,75,75,75	0
56	MG	AY	117	1/1	0.92	0.15	68,68,68,68	0
56	MG	DA	3246	1/1	0.92	0.25	3,3,3,3	0
56	MG	BA	3411	1/1	0.92	0.14	51,51,51,51	0
56	MG	AA	1680	1/1	0.92	0.47	51,51,51,51	0
56	MG	BA	3165	1/1	0.92	0.28	21,21,21,21	0
56	MG	DA	3087	1/1	0.92	0.23	3,3,3,3	0
56	MG	CA	1754	1/1	0.92	0.23	3,3,3,3	0
56	MG	BA	3085	1/1	0.92	0.24	29,29,29,29	0
56	MG	DA	3139	1/1	0.92	0.39	3,3,3,3	0
56	MG	BA	3479	1/1	0.92	0.15	30,30,30,30	0
56	MG	AA	1971	1/1	0.92	0.42	57,57,57,57	0
56	MG	CA	1812	1/1	0.92	0.11	36,36,36,36	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	CA	1789	1/1	0.92	0.31	43,43,43,43	0
56	MG	DA	3333	1/1	0.92	0.30	4,4,4,4	0
56	MG	CA	1799	1/1	0.92	0.13	5,5,5,5	0
56	MG	BA	3070	1/1	0.92	0.23	37,37,37,37	0
56	MG	BA	3245	1/1	0.92	0.24	39,39,39,39	0
56	MG	BA	3717	1/1	0.92	0.13	67,67,67,67	0
56	MG	BA	3762	1/1	0.92	0.22	28,28,28,28	0
56	MG	BA	3444	1/1	0.92	0.30	42,42,42,42	0
56	MG	BA	3663	1/1	0.92	0.32	50,50,50,50	0
56	MG	BA	3473	1/1	0.92	0.13	31,31,31,31	0
56	MG	AA	1798	1/1	0.92	0.11	25,25,25,25	0
56	MG	BA	3112	1/1	0.92	0.13	40,40,40,40	0
56	MG	BA	3269	1/1	0.92	0.11	31,31,31,31	0
56	MG	AA	1712	1/1	0.92	0.23	35,35,35,35	0
56	MG	BA	3292	1/1	0.92	0.78	36,36,36,36	0
56	MG	BA	3338	1/1	0.92	0.45	56,56,56,56	0
56	MG	AA	1634	1/1	0.92	0.13	43,43,43,43	0
56	MG	CA	1649	1/1	0.92	0.10	35,35,35,35	0
56	MG	BA	3734	1/1	0.92	0.28	59,59,59,59	0
56	MG	BA	3665	1/1	0.92	0.10	24,24,24,24	0
56	MG	CA	1768	1/1	0.92	0.22	46,46,46,46	0
56	MG	AA	1908	1/1	0.92	0.28	85,85,85,85	0
56	MG	BA	3494	1/1	0.92	0.10	44,44,44,44	0
56	MG	AA	1991	1/1	0.92	0.10	84,84,84,84	0
56	MG	AA	1994	1/1	0.92	0.30	52,52,52,52	0
56	MG	AH	201	1/1	0.92	0.20	27,27,27,27	0
56	MG	BA	3860	1/1	0.92	0.08	62,62,62,62	0
56	MG	AA	1815	1/1	0.92	0.24	43,43,43,43	0
56	MG	DA	3425	1/1	0.92	0.16	5,5,5,5	0
56	MG	BA	3287	1/1	0.92	0.22	27,27,27,27	0
56	MG	BA	3805	1/1	0.92	0.20	40,40,40,40	0
56	MG	AY	102	1/1	0.92	0.20	58,58,58,58	0
56	MG	AC	304	1/1	0.92	0.21	72,72,72,72	0
56	MG	DA	3172	1/1	0.92	0.27	3,3,3,3	0
56	MG	DA	3486	1/1	0.92	0.50	3,3,3,3	0
56	MG	DA	3047	1/1	0.92	0.29	3,3,3,3	0
56	MG	BA	3394	1/1	0.92	0.18	41,41,41,41	0
56	MG	AE	206	1/1	0.92	0.05	57,57,57,57	0
56	MG	AM	203	1/1	0.92	0.31	47,47,47,47	0
56	MG	BA	3062	1/1	0.92	0.12	56,56,56,56	0
56	MG	BA	3715	1/1	0.92	0.17	28,28,28,28	0
56	MG	AA	1676	1/1	0.92	0.09	66,66,66,66	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	AA	1871	1/1	0.92	0.29	68,68,68,68	0
56	MG	BA	3916	1/1	0.92	0.19	59,59,59,59	0
56	MG	AJ	201	1/1	0.92	0.10	49,49,49,49	0
56	MG	BA	3327	1/1	0.92	0.16	64,64,64,64	0
56	MG	BA	3677	1/1	0.92	0.14	30,30,30,30	0
56	MG	BA	3868	1/1	0.92	0.13	11,11,11,11	0
56	MG	BB	229	1/1	0.92	0.22	33,33,33,33	0
56	MG	AA	1760	1/1	0.92	0.10	8,8,8,8	0
56	MG	AA	1870	1/1	0.92	0.24	85,85,85,85	0
56	MG	AA	1792	1/1	0.92	0.23	63,63,63,63	0
56	MG	BA	3298	1/1	0.92	0.32	30,30,30,30	0
56	MG	BA	3858	1/1	0.92	0.24	60,60,60,60	0
56	MG	CY	102	1/1	0.92	0.33	3,3,3,3	0
56	MG	DA	3191	1/1	0.92	0.27	4,4,4,4	0
56	MG	AA	2006	1/1	0.92	0.21	53,53,53,53	0
56	MG	BA	3622	1/1	0.92	0.09	60,60,60,60	0
56	MG	DA	3350	1/1	0.92	0.14	63,63,63,63	0
56	MG	BA	3235	1/1	0.92	0.09	47,47,47,47	0
56	MG	AA	1986	1/1	0.92	0.27	52,52,52,52	0
56	MG	BA	3902	1/1	0.92	0.20	66,66,66,66	0
56	MG	AA	1975	1/1	0.92	0.30	66,66,66,66	0
56	MG	AA	1912	1/1	0.92	0.14	62,62,62,62	0
56	MG	BQ	204	1/1	0.92	0.18	80,80,80,80	0
56	MG	AA	1945	1/1	0.92	0.12	34,34,34,34	0
56	MG	BA	3659	1/1	0.92	0.26	43,43,43,43	0
56	MG	DO	202	1/1	0.92	0.10	4,4,4,4	0
56	MG	DD	5002	1/1	0.92	0.14	33,33,33,33	0
56	MG	BA	3120	1/1	0.92	0.37	53,53,53,53	0
56	MG	BA	3371	1/1	0.92	0.17	53,53,53,53	0
56	MG	DA	3307	1/1	0.92	0.14	39,39,39,39	0
56	MG	AY	108	1/1	0.92	0.11	59,59,59,59	0
56	MG	BA	3121	1/1	0.92	0.07	61,61,61,61	0
56	MG	AA	1757	1/1	0.92	0.12	60,60,60,60	0
56	MG	BA	3330	1/1	0.92	0.19	55,55,55,55	0
56	MG	CA	1726	1/1	0.92	0.09	37,37,37,37	0
56	MG	BA	3549	1/1	0.92	0.29	27,27,27,27	0
56	MG	BA	3321	1/1	0.92	0.15	40,40,40,40	0
56	MG	DA	3336	1/1	0.92	0.15	25,25,25,25	0
56	MG	CA	1801	1/1	0.92	0.24	3,3,3,3	0
56	MG	BA	3288	1/1	0.92	0.18	43,43,43,43	0
56	MG	DA	3279	1/1	0.92	0.40	30,30,30,30	0
56	MG	BA	3827	1/1	0.92	0.21	48,48,48,48	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	DA	3207	1/1	0.92	0.58	50,50,50,50	0
56	MG	CB	301	1/1	0.92	0.14	39,39,39,39	0
56	MG	BA	3106	1/1	0.92	0.08	68,68,68,68	0
56	MG	BA	3699	1/1	0.92	0.05	79,79,79,79	0
56	MG	CA	1653	1/1	0.92	0.28	62,62,62,62	0
56	MG	AA	1922	1/1	0.92	0.45	46,46,46,46	0
56	MG	AA	1687	1/1	0.92	0.12	47,47,47,47	0
56	MG	DA	3354	1/1	0.92	0.09	43,43,43,43	0
56	MG	BA	3720	1/1	0.92	0.16	28,28,28,28	0
56	MG	BA	3111	1/1	0.93	0.23	35,35,35,35	0
56	MG	AA	1728	1/1	0.93	0.40	46,46,46,46	0
56	MG	DA	3242	1/1	0.93	0.34	3,3,3,3	0
56	MG	BA	3647	1/1	0.93	0.17	48,48,48,48	0
56	MG	BA	3500	1/1	0.93	0.11	21,21,21,21	0
56	MG	DA	3222	1/1	0.93	0.21	41,41,41,41	0
56	MG	AM	202	1/1	0.93	0.07	58,58,58,58	0
56	MG	AK	203	1/1	0.93	0.13	49,49,49,49	0
56	MG	DA	3362	1/1	0.93	0.15	82,82,82,82	0
56	MG	BA	3908	1/1	0.93	0.18	26,26,26,26	0
56	MG	DA	3338	1/1	0.93	0.27	3,3,3,3	0
56	MG	BA	3545	1/1	0.93	0.12	23,23,23,23	0
56	MG	BA	3575	1/1	0.93	0.12	53,53,53,53	0
56	MG	CA	1770	1/1	0.93	0.12	54,54,54,54	0
56	MG	DA	3240	1/1	0.93	0.19	3,3,3,3	0
56	MG	CA	1697	1/1	0.93	0.28	52,52,52,52	0
56	MG	BA	3211	1/1	0.93	0.17	80,80,80,80	0
56	MG	AA	1825	1/1	0.93	0.17	31,31,31,31	0
56	MG	DA	3180	1/1	0.93	0.33	3,3,3,3	0
56	MG	DD	5008	1/1	0.93	0.13	13,13,13,13	0
56	MG	AE	202	1/1	0.93	0.15	64,64,64,64	0
56	MG	BA	3517	1/1	0.93	0.13	46,46,46,46	0
56	MG	DA	3401	1/1	0.93	0.21	39,39,39,39	0
56	MG	DA	3299	1/1	0.93	0.18	50,50,50,50	0
56	MG	BO	202	1/1	0.93	0.08	54,54,54,54	0
56	MG	BA	3900	1/1	0.93	0.17	51,51,51,51	0
56	MG	AA	1650	1/1	0.93	0.14	45,45,45,45	0
56	MG	CA	1808	1/1	0.93	0.48	3,3,3,3	0
56	MG	AA	1808	1/1	0.93	0.14	46,46,46,46	0
56	MG	AA	1963	1/1	0.93	0.22	56,56,56,56	0
56	MG	BA	3846	1/1	0.93	0.16	55,55,55,55	0
56	MG	AA	1777	1/1	0.93	0.29	53,53,53,53	0
56	MG	BA	3775	1/1	0.93	0.09	36,36,36,36	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	AA	1787	1/1	0.93	0.16	54,54,54,54	0
56	MG	DA	3019	1/1	0.93	0.23	3,3,3,3	0
56	MG	BA	3034	1/1	0.93	0.14	43,43,43,43	0
56	MG	AN	102	1/1	0.93	0.23	57,57,57,57	0
56	MG	CA	1615	1/1	0.93	0.25	3,3,3,3	0
56	MG	DA	3098	1/1	0.93	0.31	3,3,3,3	0
56	MG	DD	5009	1/1	0.93	0.38	29,29,29,29	0
56	MG	BA	3478	1/1	0.93	0.17	52,52,52,52	0
56	MG	BB	206	1/1	0.93	0.12	51,51,51,51	0
56	MG	BA	3780	1/1	0.93	0.27	32,32,32,32	0
56	MG	BA	3336	1/1	0.93	0.10	45,45,45,45	0
56	MG	AA	1990	1/1	0.93	0.12	63,63,63,63	0
56	MG	BA	3136	1/1	0.93	0.23	45,45,45,45	0
56	MG	BA	3019	1/1	0.93	0.18	55,55,55,55	0
56	MG	BA	3132	1/1	0.93	0.21	40,40,40,40	0
56	MG	AA	1624	1/1	0.93	0.14	43,43,43,43	0
56	MG	BA	3475	1/1	0.93	0.08	22,22,22,22	0
56	MG	AA	1976	1/1	0.93	0.16	70,70,70,70	0
56	MG	AK	205	1/1	0.93	0.41	61,61,61,61	0
56	MG	DA	3002	1/1	0.93	0.31	3,3,3,3	0
56	MG	BA	3066	1/1	0.93	0.11	67,67,67,67	0
56	MG	BA	3420	1/1	0.93	0.25	19,19,19,19	0
56	MG	AA	1720	1/1	0.93	0.18	36,36,36,36	0
56	MG	AA	1802	1/1	0.93	0.24	39,39,39,39	0
56	MG	BA	3636	1/1	0.93	0.14	31,31,31,31	0
56	MG	CA	1740	1/1	0.93	0.39	41,41,41,41	0
56	MG	AA	1946	1/1	0.93	0.12	59,59,59,59	0
56	MG	DB	203	1/1	0.93	0.26	3,3,3,3	0
56	MG	BA	3285	1/1	0.93	0.17	48,48,48,48	0
56	MG	BA	3563	1/1	0.93	0.14	57,57,57,57	0
56	MG	DA	3247	1/1	0.93	0.27	3,3,3,3	0
56	MG	AA	1694	1/1	0.93	0.15	52,52,52,52	0
56	MG	DA	3171	1/1	0.93	0.16	3,3,3,3	0
56	MG	DA	3405	1/1	0.93	0.11	4,4,4,4	0
56	MG	BA	3244	1/1	0.93	0.38	31,31,31,31	0
56	MG	BA	3179	1/1	0.93	0.12	32,32,32,32	0
56	MG	DA	3452	1/1	0.93	0.23	38,38,38,38	0
56	MG	AA	1649	1/1	0.93	0.15	37,37,37,37	0
56	MG	BA	3838	1/1	0.93	0.13	29,29,29,29	0
56	MG	AA	1782	1/1	0.93	0.33	24,24,24,24	0
56	MG	CL	201	1/1	0.93	0.30	67,67,67,67	0
56	MG	BA	3017	1/1	0.93	0.12	52,52,52,52	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	AA	1817	1/1	0.93	0.24	29,29,29,29	0
56	MG	BA	3280	1/1	0.93	0.18	29,29,29,29	0
56	MG	AL	203	1/1	0.93	0.08	43,43,43,43	0
56	MG	CA	1810	1/1	0.93	0.63	59,59,59,59	0
56	MG	DA	3052	1/1	0.93	0.32	3,3,3,3	0
56	MG	AD	5002	1/1	0.93	0.12	64,64,64,64	0
56	MG	CA	1746	1/1	0.93	0.18	57,57,57,57	0
56	MG	CA	1656	1/1	0.93	0.24	5,5,5,5	0
56	MG	BA	3898	1/1	0.93	0.36	38,38,38,38	0
56	MG	AG	202	1/1	0.93	0.11	56,56,56,56	0
56	MG	DB	206	1/1	0.93	0.13	4,4,4,4	0
56	MG	DA	3066	1/1	0.93	0.13	43,43,43,43	0
56	MG	BA	3564	1/1	0.93	0.18	54,54,54,54	0
56	MG	DA	3337	1/1	0.93	0.19	4,4,4,4	0
56	MG	DA	3022	1/1	0.93	0.21	3,3,3,3	0
56	MG	AA	1928	1/1	0.93	0.13	52,52,52,52	0
56	MG	CY	112	1/1	0.93	0.29	3,3,3,3	0
56	MG	CA	1765	1/1	0.93	0.35	3,3,3,3	0
56	MG	DA	3244	1/1	0.93	0.07	5,5,5,5	0
56	MG	AA	1722	1/1	0.93	0.08	34,34,34,34	0
56	MG	DA	3031	1/1	0.93	0.49	3,3,3,3	0
56	MG	BA	3464	1/1	0.93	0.35	75,75,75,75	0
56	MG	DA	3377	1/1	0.93	0.09	43,43,43,43	0
56	MG	BA	3664	1/1	0.93	0.38	23,23,23,23	0
56	MG	BA	3326	1/1	0.93	0.09	45,45,45,45	0
56	MG	BA	3718	1/1	0.93	0.39	51,51,51,51	0
56	MG	DD	5004	1/1	0.93	0.26	42,42,42,42	0
56	MG	DA	3219	1/1	0.93	0.45	3,3,3,3	0
56	MG	BA	3492	1/1	0.93	0.14	48,48,48,48	0
56	MG	BA	3848	1/1	0.93	0.17	61,61,61,61	0
56	MG	BA	3608	1/1	0.93	0.28	40,40,40,40	0
56	MG	DA	3347	1/1	0.93	0.10	35,35,35,35	0
56	MG	DA	3236	1/1	0.93	0.08	53,53,53,53	0
56	MG	BA	3733	1/1	0.93	0.30	38,38,38,38	0
56	MG	BA	3521	1/1	0.93	0.29	45,45,45,45	0
56	MG	CA	1675	1/1	0.93	0.31	65,65,65,65	0
56	MG	BA	3139	1/1	0.93	0.36	59,59,59,59	0
56	MG	BA	3363	1/1	0.93	0.21	42,42,42,42	0
56	MG	BA	3895	1/1	0.93	0.19	51,51,51,51	0
56	MG	BA	3592	1/1	0.93	0.20	47,47,47,47	0
56	MG	CA	1639	1/1	0.93	0.29	3,3,3,3	0
56	MG	BA	3097	1/1	0.93	0.14	54,54,54,54	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	DA	3319	1/1	0.93	0.17	43,43,43,43	0
56	MG	BA	3325	1/1	0.93	0.45	66,66,66,66	0
56	MG	CA	1621	1/1	0.93	0.27	3,3,3,3	0
56	MG	BA	3696	1/1	0.93	0.34	69,69,69,69	0
56	MG	AA	2007	1/1	0.93	0.24	23,23,23,23	0
56	MG	AA	1979	1/1	0.93	0.40	58,58,58,58	0
56	MG	DQ	202	1/1	0.93	0.30	3,3,3,3	0
56	MG	BD	5002	1/1	0.93	0.30	82,82,82,82	0
56	MG	CA	1654	1/1	0.93	0.18	28,28,28,28	0
56	MG	DA	3371	1/1	0.93	0.06	56,56,56,56	0
56	MG	AA	1812	1/1	0.93	0.20	65,65,65,65	0
56	MG	BA	3508	1/1	0.93	0.14	33,33,33,33	0
56	MG	BA	3568	1/1	0.93	0.16	33,33,33,33	0
56	MG	AA	1804	1/1	0.93	0.34	56,56,56,56	0
56	MG	BA	3033	1/1	0.93	0.18	38,38,38,38	0
56	MG	AA	1618	1/1	0.93	0.16	50,50,50,50	0
56	MG	BA	3194	1/1	0.93	0.12	36,36,36,36	0
56	MG	AY	112	1/1	0.93	0.21	38,38,38,38	0
56	MG	AA	1931	1/1	0.93	0.21	31,31,31,31	0
56	MG	AA	1892	1/1	0.93	0.22	30,30,30,30	0
56	MG	B0	102	1/1	0.93	0.15	37,37,37,37	0
56	MG	AL	202	1/1	0.93	0.10	34,34,34,34	0
56	MG	BB	231	1/1	0.93	0.24	54,54,54,54	0
56	MG	AA	1776	1/1	0.93	0.15	30,30,30,30	0
56	MG	BD	5004	1/1	0.93	0.17	50,50,50,50	0
56	MG	DA	3385	1/1	0.93	0.22	51,51,51,51	0
56	MG	AA	1968	1/1	0.93	0.27	35,35,35,35	0
56	MG	DA	3358	1/1	0.93	0.19	54,54,54,54	0
56	MG	BS	201	1/1	0.93	0.15	46,46,46,46	0
56	MG	DA	3164	1/1	0.93	0.16	4,4,4,4	0
56	MG	BA	3652	1/1	0.93	0.19	28,28,28,28	0
56	MG	BA	3650	1/1	0.93	0.12	5,5,5,5	0
56	MG	DA	3417	1/1	0.93	0.24	4,4,4,4	0
56	MG	CK	203	1/1	0.93	0.07	85,85,85,85	0
56	MG	AA	1913	1/1	0.93	0.09	54,54,54,54	0
56	MG	AA	1962	1/1	0.93	0.55	48,48,48,48	0
56	MG	BA	3673	1/1	0.93	0.28	19,19,19,19	0
56	MG	BA	3921	1/1	0.93	0.18	53,53,53,53	0
56	MG	BA	3047	1/1	0.93	0.21	54,54,54,54	0
56	MG	D1	102	1/1	0.94	0.24	53,53,53,53	0
56	MG	DA	3288	1/1	0.94	0.20	33,33,33,33	0
56	MG	CZ	111	1/1	0.94	0.33	3,3,3,3	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	DU	201	1/1	0.94	0.37	3,3,3,3	0
56	MG	AA	1721	1/1	0.94	0.11	44,44,44,44	0
56	MG	BA	3892	1/1	0.94	0.15	46,46,46,46	0
56	MG	AA	1726	1/1	0.94	0.23	53,53,53,53	0
56	MG	BA	3736	1/1	0.94	0.27	26,26,26,26	0
56	MG	BA	3452	1/1	0.94	0.14	44,44,44,44	0
56	MG	AA	1756	1/1	0.94	0.24	41,41,41,41	0
56	MG	B2	103	1/1	0.94	0.37	36,36,36,36	0
56	MG	BA	3079	1/1	0.94	0.28	51,51,51,51	0
56	MG	AA	1631	1/1	0.94	0.20	39,39,39,39	0
56	MG	DA	3305	1/1	0.94	0.13	23,23,23,23	0
56	MG	BA	3587	1/1	0.94	0.15	40,40,40,40	0
56	MG	DA	3003	1/1	0.94	0.22	4,4,4,4	0
56	MG	BA	3596	1/1	0.94	0.12	13,13,13,13	0
56	MG	DA	3454	1/1	0.94	0.14	45,45,45,45	0
56	MG	AA	2019	1/1	0.94	0.32	70,70,70,70	0
56	MG	AA	1880	1/1	0.94	0.11	40,40,40,40	0
56	MG	BA	3069	1/1	0.94	0.15	65,65,65,65	0
56	MG	AY	125	1/1	0.94	0.53	36,36,36,36	0
56	MG	AX	406	1/1	0.94	0.17	48,48,48,48	0
56	MG	CA	1720	1/1	0.94	0.11	27,27,27,27	0
56	MG	BA	3203	1/1	0.94	0.15	39,39,39,39	0
56	MG	DA	3215	1/1	0.94	0.16	4,4,4,4	0
56	MG	DA	3183	1/1	0.94	0.30	3,3,3,3	0
56	MG	AZ	114	1/1	0.94	0.10	60,60,60,60	0
56	MG	BA	3094	1/1	0.94	0.09	76,76,76,76	0
56	MG	BA	3875	1/1	0.94	0.10	27,27,27,27	0
56	MG	DA	3023	1/1	0.94	0.24	3,3,3,3	0
56	MG	CA	1602	1/1	0.94	0.10	5,5,5,5	0
56	MG	CA	1816	1/1	0.94	0.60	61,61,61,61	0
56	MG	AA	1683	1/1	0.94	0.16	74,74,74,74	0
56	MG	BO	203	1/1	0.94	0.21	55,55,55,55	0
56	MG	AA	1890	1/1	0.94	0.18	21,21,21,21	0
56	MG	BA	3127	1/1	0.94	0.11	22,22,22,22	0
56	MG	CA	1759	1/1	0.94	0.30	48,48,48,48	0
56	MG	BA	3515	1/1	0.94	0.11	68,68,68,68	0
56	MG	BA	3183	1/1	0.94	0.26	57,57,57,57	0
56	MG	AA	1866	1/1	0.94	0.10	26,26,26,26	0
56	MG	BA	3783	1/1	0.94	0.14	27,27,27,27	0
56	MG	DA	3392	1/1	0.94	0.18	38,38,38,38	0
56	MG	BA	3569	1/1	0.94	0.28	40,40,40,40	0
56	MG	CA	1797	1/1	0.94	0.53	28,28,28,28	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	AA	2027	1/1	0.94	0.11	27,27,27,27	0
56	MG	BA	3498	1/1	0.94	0.35	45,45,45,45	0
56	MG	DA	3384	1/1	0.94	0.34	3,3,3,3	0
56	MG	AE	201	1/1	0.94	0.08	52,52,52,52	0
56	MG	DA	3254	1/1	0.94	0.16	42,42,42,42	0
56	MG	BA	3669	1/1	0.94	0.35	52,52,52,52	0
56	MG	BA	3007	1/1	0.94	0.51	20,20,20,20	0
56	MG	B8	102	1/1	0.94	0.16	57,57,57,57	0
56	MG	DP	201	1/1	0.94	0.34	3,3,3,3	0
56	MG	DA	3339	1/1	0.94	0.25	6,6,6,6	0
56	MG	AA	2010	1/1	0.94	0.19	33,33,33,33	0
56	MG	DB	211	1/1	0.94	0.26	3,3,3,3	0
56	MG	DA	3298	1/1	0.94	0.18	9,9,9,9	0
56	MG	DA	3414	1/1	0.94	0.13	5,5,5,5	0
56	MG	DA	3181	1/1	0.94	0.28	3,3,3,3	0
56	MG	BA	3004	1/1	0.94	0.12	27,27,27,27	0
56	MG	BA	3021	1/1	0.94	0.41	37,37,37,37	0
56	MG	BA	3786	1/1	0.94	0.36	18,18,18,18	0
56	MG	AA	1809	1/1	0.94	0.23	90,90,90,90	0
56	MG	BA	3406	1/1	0.94	0.30	23,23,23,23	0
56	MG	AA	1640	1/1	0.94	0.18	36,36,36,36	0
56	MG	BA	3867	1/1	0.94	0.35	50,50,50,50	0
56	MG	CA	1809	1/1	0.94	0.32	3,3,3,3	0
56	MG	BA	3030	1/1	0.94	0.21	36,36,36,36	0
56	MG	BA	3344	1/1	0.94	0.38	47,47,47,47	0
56	MG	DA	3170	1/1	0.94	0.34	3,3,3,3	0
56	MG	BA	3224	1/1	0.94	0.07	32,32,32,32	0
56	MG	DA	3055	1/1	0.94	0.30	3,3,3,3	0
56	MG	AA	1884	1/1	0.94	0.16	26,26,26,26	0
56	MG	BA	3216	1/1	0.94	0.22	54,54,54,54	0
56	MG	B0	103	1/1	0.94	0.12	30,30,30,30	0
56	MG	BI	204	1/1	0.94	0.21	32,32,32,32	0
56	MG	BA	3213	1/1	0.94	0.27	43,43,43,43	0
56	MG	BA	3052	1/1	0.94	0.19	71,71,71,71	0
56	MG	AA	1977	1/1	0.94	0.27	64,64,64,64	0
56	MG	BA	3317	1/1	0.94	0.15	48,48,48,48	0
56	MG	DA	3071	1/1	0.94	0.26	3,3,3,3	0
56	MG	AA	2000	1/1	0.94	0.12	46,46,46,46	0
56	MG	AA	1924	1/1	0.94	0.25	58,58,58,58	0
56	MG	CZ	101	1/1	0.94	0.07	72,72,72,72	0
56	MG	CF	201	1/1	0.94	0.13	40,40,40,40	0
56	MG	BA	3396	1/1	0.94	0.24	42,42,42,42	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	AX	412	1/1	0.94	0.19	56,56,56,56	0
56	MG	DA	3082	1/1	0.94	0.37	3,3,3,3	0
56	MG	BA	3602	1/1	0.94	0.34	43,43,43,43	0
56	MG	BA	3402	1/1	0.94	0.09	49,49,49,49	0
56	MG	AA	1901	1/1	0.94	0.24	88,88,88,88	0
56	MG	DN	201	1/1	0.94	0.60	3,3,3,3	0
56	MG	BA	3262	1/1	0.94	0.25	7,7,7,7	0
56	MG	BA	3526	1/1	0.94	0.20	49,49,49,49	0
56	MG	BA	3722	1/1	0.94	0.76	66,66,66,66	0
56	MG	AA	1824	1/1	0.94	0.49	34,34,34,34	0
56	MG	BA	3566	1/1	0.94	0.14	43,43,43,43	0
56	MG	DA	3054	1/1	0.94	0.12	5,5,5,5	0
56	MG	BA	3051	1/1	0.94	0.09	44,44,44,44	0
56	MG	CA	1674	1/1	0.94	0.38	57,57,57,57	0
56	MG	AA	1905	1/1	0.94	0.23	50,50,50,50	0
56	MG	AA	2016	1/1	0.94	0.29	43,43,43,43	0
56	MG	BA	3186	1/1	0.94	0.11	67,67,67,67	0
56	MG	CA	1630	1/1	0.94	0.56	3,3,3,3	0
56	MG	DA	3006	1/1	0.94	0.46	3,3,3,3	0
56	MG	AA	2008	1/1	0.94	0.25	49,49,49,49	0
56	MG	DA	3118	1/1	0.94	0.33	6,6,6,6	0
56	MG	BA	3046	1/1	0.94	0.15	38,38,38,38	0
56	MG	BA	3056	1/1	0.94	0.21	66,66,66,66	0
56	MG	DA	3080	1/1	0.94	0.23	3,3,3,3	0
56	MG	BA	3188	1/1	0.94	0.10	53,53,53,53	0
56	MG	DA	3049	1/1	0.94	0.13	5,5,5,5	0
56	MG	AA	1954	1/1	0.94	0.27	74,74,74,74	0
56	MG	AT	201	1/1	0.94	0.19	57,57,57,57	0
56	MG	AA	2017	1/1	0.94	0.26	47,47,47,47	0
56	MG	BA	3447	1/1	0.94	0.47	31,31,31,31	0
56	MG	AA	1980	1/1	0.94	0.12	38,38,38,38	0
56	MG	DA	3072	1/1	0.94	0.19	3,3,3,3	0
56	MG	AA	1903	1/1	0.94	0.48	54,54,54,54	0
56	MG	BA	3634	1/1	0.94	0.77	33,33,33,33	0
56	MG	CA	1659	1/1	0.94	0.23	3,3,3,3	0
56	MG	BA	3748	1/1	0.94	0.23	35,35,35,35	0
56	MG	AA	2009	1/1	0.94	0.28	47,47,47,47	0
56	MG	BA	3110	1/1	0.94	0.08	65,65,65,65	0
56	MG	CZ	107	1/1	0.94	0.14	57,57,57,57	0
56	MG	DA	3165	1/1	0.94	0.23	4,4,4,4	0
56	MG	BA	3820	1/1	0.94	0.23	59,59,59,59	0
56	MG	AA	1654	1/1	0.94	0.14	75,75,75,75	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	DA	3216	1/1	0.94	0.32	3,3,3,3	0
56	MG	BB	209	1/1	0.94	0.14	63,63,63,63	0
56	MG	DA	3228	1/1	0.94	0.12	4,4,4,4	0
56	MG	CA	1666	1/1	0.94	0.22	3,3,3,3	0
56	MG	AA	1734	1/1	0.94	0.13	27,27,27,27	0
56	MG	BX	102	1/1	0.94	0.19	25,25,25,25	0
56	MG	BA	3804	1/1	0.94	0.15	44,44,44,44	0
56	MG	CA	1708	1/1	0.94	0.15	36,36,36,36	0
56	MG	BA	3418	1/1	0.94	0.47	54,54,54,54	0
56	MG	AL	201	1/1	0.94	0.14	28,28,28,28	0
56	MG	B6	101	1/1	0.94	0.10	44,44,44,44	0
56	MG	AE	207	1/1	0.94	0.09	38,38,38,38	0
56	MG	DA	3035	1/1	0.94	0.45	3,3,3,3	0
56	MG	BA	3621	1/1	0.94	0.17	50,50,50,50	0
56	MG	CA	1692	1/1	0.94	0.14	34,34,34,34	0
56	MG	AA	1803	1/1	0.94	0.17	55,55,55,55	0
56	MG	BA	3348	1/1	0.94	0.18	37,37,37,37	0
56	MG	BA	3903	1/1	0.94	0.16	71,71,71,71	0
56	MG	DA	3042	1/1	0.94	0.04	69,69,69,69	0
56	MG	B8	103	1/1	0.94	0.13	61,61,61,61	0
56	MG	DA	3026	1/1	0.94	0.42	3,3,3,3	0
56	MG	BE	305	1/1	0.94	0.11	22,22,22,22	0
56	MG	BA	3821	1/1	0.94	0.12	22,22,22,22	0
56	MG	DA	3445	1/1	0.94	0.22	4,4,4,4	0
56	MG	BA	3456	1/1	0.94	0.12	24,24,24,24	0
56	MG	AA	1697	1/1	0.94	0.11	48,48,48,48	0
56	MG	BA	3430	1/1	0.94	0.11	45,45,45,45	0
56	MG	BA	3493	1/1	0.94	0.07	50,50,50,50	0
56	MG	BQ	201	1/1	0.94	0.23	45,45,45,45	0
56	MG	CA	1820	1/1	0.94	0.23	43,43,43,43	0
56	MG	DA	3038	1/1	0.94	0.20	4,4,4,4	0
56	MG	AA	1669	1/1	0.94	0.16	58,58,58,58	0
56	MG	BA	3319	1/1	0.94	0.09	44,44,44,44	0
56	MG	BA	3204	1/1	0.94	0.09	34,34,34,34	0
56	MG	BA	3754	1/1	0.94	0.40	44,44,44,44	0
56	MG	DA	3260	1/1	0.94	0.30	3,3,3,3	0
56	MG	AA	2013	1/1	0.94	0.32	40,40,40,40	0
56	MG	BA	3435	1/1	0.94	0.12	32,32,32,32	0
56	MG	DA	3226	1/1	0.94	0.11	4,4,4,4	0
56	MG	BA	3557	1/1	0.94	0.20	29,29,29,29	0
56	MG	AV	5501	1/1	0.94	0.15	28,28,28,28	0
56	MG	CA	1618	1/1	0.94	0.25	4,4,4,4	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	AA	1965	1/1	0.94	0.33	54,54,54,54	0
56	MG	BA	3355	1/1	0.94	0.10	33,33,33,33	0
56	MG	DF	301	1/1	0.94	0.45	3,3,3,3	0
56	MG	DA	3021	1/1	0.94	0.19	4,4,4,4	0
56	MG	CA	1628	1/1	0.94	0.21	4,4,4,4	0
56	MG	BA	3695	1/1	0.94	0.15	70,70,70,70	0
56	MG	DA	3100	1/1	0.94	0.19	4,4,4,4	0
56	MG	BA	3835	1/1	0.94	0.17	8,8,8,8	0
56	MG	BA	3555	1/1	0.94	0.20	7,7,7,7	0
56	MG	AA	1778	1/1	0.94	0.34	37,37,37,37	0
56	MG	DA	3443	1/1	0.94	0.30	3,3,3,3	0
56	MG	DA	3148	1/1	0.94	0.21	4,4,4,4	0
56	MG	BA	3080	1/1	0.94	0.12	29,29,29,29	0
56	MG	DA	3262	1/1	0.94	0.35	3,3,3,3	0
56	MG	BA	3852	1/1	0.95	0.16	35,35,35,35	0
56	MG	BA	3299	1/1	0.95	0.13	9,9,9,9	0
56	MG	BA	3141	1/1	0.95	0.14	68,68,68,68	0
56	MG	AA	1891	1/1	0.95	0.13	61,61,61,61	0
56	MG	BA	3591	1/1	0.95	0.17	29,29,29,29	0
56	MG	BA	3308	1/1	0.95	0.13	8,8,8,8	0
56	MG	BA	3589	1/1	0.95	0.10	29,29,29,29	0
56	MG	DA	3044	1/1	0.95	0.19	3,3,3,3	0
56	MG	BA	3215	1/1	0.95	0.14	27,27,27,27	0
56	MG	DA	3061	1/1	0.95	0.24	4,4,4,4	0
56	MG	DA	3475	1/1	0.95	0.18	3,3,3,3	0
56	MG	BA	3772	1/1	0.95	0.10	48,48,48,48	0
56	MG	DA	3142	1/1	0.95	0.47	3,3,3,3	0
56	MG	CA	1624	1/1	0.95	0.24	3,3,3,3	0
56	MG	BV	203	1/1	0.95	0.04	52,52,52,52	0
56	MG	BA	3064	1/1	0.95	0.17	57,57,57,57	0
56	MG	BA	3658	1/1	0.95	0.12	36,36,36,36	0
56	MG	BY	203	1/1	0.95	0.18	58,58,58,58	0
56	MG	BA	3164	1/1	0.95	0.77	35,35,35,35	0
56	MG	BA	3145	1/1	0.95	0.18	22,22,22,22	0
56	MG	BA	3629	1/1	0.95	0.19	50,50,50,50	0
56	MG	AA	1681	1/1	0.95	0.10	27,27,27,27	0
56	MG	BA	3538	1/1	0.95	0.47	30,30,30,30	0
56	MG	DA	3198	1/1	0.95	0.36	4,4,4,4	0
56	MG	BA	3105	1/1	0.95	0.57	30,30,30,30	0
56	MG	DA	3196	1/1	0.95	0.22	4,4,4,4	0
56	MG	DA	3331	1/1	0.95	0.14	23,23,23,23	0
56	MG	AA	1673	1/1	0.95	0.18	64,64,64,64	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	BA	3257	1/1	0.95	0.08	28,28,28,28	0
56	MG	BA	3777	1/1	0.95	0.17	32,32,32,32	0
56	MG	CA	1800	1/1	0.95	0.42	3,3,3,3	0
56	MG	BA	3656	1/1	0.95	0.26	16,16,16,16	0
56	MG	BA	3613	1/1	0.95	0.11	32,32,32,32	0
56	MG	DA	3274	1/1	0.95	0.44	3,3,3,3	0
56	MG	BA	3312	1/1	0.95	0.17	36,36,36,36	0
56	MG	BA	3487	1/1	0.95	0.19	26,26,26,26	0
56	MG	BI	202	1/1	0.95	0.05	53,53,53,53	0
56	MG	AA	1967	1/1	0.95	0.09	28,28,28,28	0
56	MG	AL	204	1/1	0.95	0.07	43,43,43,43	0
56	MG	BA	3182	1/1	0.95	0.15	20,20,20,20	0
56	MG	CA	1651	1/1	0.95	0.21	28,28,28,28	0
56	MG	AA	1635	1/1	0.95	0.11	52,52,52,52	0
56	MG	CA	1727	1/1	0.95	0.11	53,53,53,53	0
56	MG	DA	3426	1/1	0.95	0.13	5,5,5,5	0
56	MG	AA	1795	1/1	0.95	0.16	64,64,64,64	0
56	MG	DA	3078	1/1	0.95	0.30	4,4,4,4	0
56	MG	BA	3728	1/1	0.95	0.17	34,34,34,34	0
56	MG	BA	3533	1/1	0.95	0.13	2,2,2,2	0
56	MG	CA	1619	1/1	0.95	0.27	4,4,4,4	0
56	MG	DA	3157	1/1	0.95	0.35	3,3,3,3	0
56	MG	DA	3168	1/1	0.95	0.20	4,4,4,4	0
56	MG	AA	1791	1/1	0.95	0.09	81,81,81,81	0
56	MG	DA	3306	1/1	0.95	0.25	3,3,3,3	0
56	MG	DE	301	1/1	0.95	0.09	5,5,5,5	0
56	MG	DA	3420	1/1	0.95	0.20	4,4,4,4	0
56	MG	BA	3832	1/1	0.95	0.26	28,28,28,28	0
56	MG	CA	1733	1/1	0.95	0.28	3,3,3,3	0
56	MG	DA	3203	1/1	0.95	0.26	15,15,15,15	0
56	MG	BA	3844	1/1	0.95	0.15	36,36,36,36	0
56	MG	CA	1645	1/1	0.95	0.12	6,6,6,6	0
56	MG	BA	3391	1/1	0.95	0.15	51,51,51,51	0
56	MG	BA	3831	1/1	0.95	0.22	34,34,34,34	0
56	MG	BP	202	1/1	0.95	0.12	24,24,24,24	0
56	MG	BA	3440	1/1	0.95	0.33	73,73,73,73	0
56	MG	CA	1822	1/1	0.95	0.38	3,3,3,3	0
56	MG	BA	3885	1/1	0.95	0.12	67,67,67,67	0
56	MG	AA	1869	1/1	0.95	0.16	47,47,47,47	0
56	MG	AA	1893	1/1	0.95	0.22	52,52,52,52	0
56	MG	BA	3488	1/1	0.95	0.16	52,52,52,52	0
56	MG	AA	1606	1/1	0.95	0.18	35,35,35,35	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	BA	3797	1/1	0.95	0.11	52,52,52,52	0
56	MG	AA	1671	1/1	0.95	0.17	59,59,59,59	0
56	MG	BA	3261	1/1	0.95	0.16	14,14,14,14	0
56	MG	CA	1751	1/1	0.95	0.28	3,3,3,3	0
56	MG	BA	3558	1/1	0.95	0.19	10,10,10,10	0
56	MG	AA	1894	1/1	0.95	0.30	35,35,35,35	0
56	MG	CA	1753	1/1	0.95	0.19	3,3,3,3	0
56	MG	DA	3184	1/1	0.95	0.25	3,3,3,3	0
56	MG	BA	3016	1/1	0.95	0.10	50,50,50,50	0
56	MG	DA	3232	1/1	0.95	0.05	37,37,37,37	0
56	MG	CA	1623	1/1	0.95	0.29	4,4,4,4	0
56	MG	DA	3012	1/1	0.95	0.25	3,3,3,3	0
56	MG	BA	3883	1/1	0.95	0.14	67,67,67,67	0
56	MG	BA	3429	1/1	0.95	0.24	51,51,51,51	0
56	MG	CA	1792	1/1	0.95	0.53	3,3,3,3	0
56	MG	DA	3234	1/1	0.95	0.19	3,3,3,3	0
56	MG	AA	1608	1/1	0.95	0.12	43,43,43,43	0
56	MG	DA	3178	1/1	0.95	0.20	4,4,4,4	0
56	MG	BA	3915	1/1	0.95	0.29	41,41,41,41	0
56	MG	BA	3675	1/1	0.95	0.24	43,43,43,43	0
56	MG	CA	1745	1/1	0.95	0.14	36,36,36,36	0
56	MG	DA	3127	1/1	0.95	0.35	3,3,3,3	0
56	MG	BA	3291	1/1	0.95	0.15	9,9,9,9	0
56	MG	BA	3354	1/1	0.95	0.33	59,59,59,59	0
56	MG	DA	3221	1/1	0.95	0.35	52,52,52,52	0
56	MG	D1	101	1/1	0.95	0.31	3,3,3,3	0
56	MG	BA	3197	1/1	0.95	0.32	85,85,85,85	0
56	MG	B1	104	1/1	0.95	0.12	38,38,38,38	0
56	MG	AY	104	1/1	0.95	0.09	64,64,64,64	0
56	MG	BA	3218	1/1	0.95	0.35	25,25,25,25	0
56	MG	BA	3388	1/1	0.95	0.09	61,61,61,61	0
56	MG	AA	1702	1/1	0.95	0.32	48,48,48,48	0
56	MG	BA	3335	1/1	0.95	0.15	52,52,52,52	0
56	MG	AA	1736	1/1	0.95	0.13	63,63,63,63	0
56	MG	AA	1686	1/1	0.95	0.18	43,43,43,43	0
56	MG	BB	234	1/1	0.95	0.11	23,23,23,23	0
56	MG	DA	3250	1/1	0.95	0.23	3,3,3,3	0
56	MG	DA	3397	1/1	0.95	0.22	24,24,24,24	0
56	MG	AA	1857	1/1	0.95	0.16	43,43,43,43	0
56	MG	BA	3180	1/1	0.95	0.07	36,36,36,36	0
56	MG	DA	3162	1/1	0.95	0.21	3,3,3,3	0
56	MG	DA	3192	1/1	0.95	0.39	3,3,3,3	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	DA	3150	1/1	0.95	0.15	4,4,4,4	0
56	MG	CA	1731	1/1	0.95	0.22	3,3,3,3	0
56	MG	AA	1898	1/1	0.95	0.10	27,27,27,27	0
56	MG	AA	1768	1/1	0.95	0.36	37,37,37,37	0
56	MG	BA	3829	1/1	0.95	0.15	40,40,40,40	0
56	MG	AY	119	1/1	0.95	0.09	50,50,50,50	0
56	MG	AC	303	1/1	0.95	0.07	56,56,56,56	0
56	MG	BA	3237	1/1	0.95	0.11	28,28,28,28	0
56	MG	AA	1874	1/1	0.95	0.22	44,44,44,44	0
56	MG	DA	3268	1/1	0.95	0.17	4,4,4,4	0
56	MG	DA	3474	1/1	0.95	0.22	3,3,3,3	0
56	MG	CY	109	1/1	0.95	0.24	3,3,3,3	0
56	MG	DA	3252	1/1	0.95	0.36	23,23,23,23	0
56	MG	BA	3225	1/1	0.95	0.13	27,27,27,27	0
56	MG	BA	3857	1/1	0.95	0.23	71,71,71,71	0
56	MG	BA	3893	1/1	0.95	0.05	62,62,62,62	0
56	MG	DA	3206	1/1	0.95	0.14	5,5,5,5	0
56	MG	DA	3386	1/1	0.95	0.21	3,3,3,3	0
56	MG	DA	3176	1/1	0.95	0.27	4,4,4,4	0
56	MG	DA	3248	1/1	0.95	0.13	3,3,3,3	0
56	MG	AA	1943	1/1	0.95	0.14	56,56,56,56	0
56	MG	BA	3322	1/1	0.95	0.20	40,40,40,40	0
56	MG	BA	3249	1/1	0.95	0.31	58,58,58,58	0
56	MG	AA	1713	1/1	0.95	0.24	39,39,39,39	0
56	MG	BA	3353	1/1	0.95	0.24	37,37,37,37	0
56	MG	DA	3328	1/1	0.95	0.17	23,23,23,23	0
56	MG	DA	3152	1/1	0.95	0.12	5,5,5,5	0
56	MG	BA	3489	1/1	0.95	0.09	32,32,32,32	0
56	MG	DA	3128	1/1	0.95	0.17	12,12,12,12	0
56	MG	DA	3330	1/1	0.95	0.22	5,5,5,5	0
56	MG	DA	3068	1/1	0.95	0.19	4,4,4,4	0
56	MG	BA	3912	1/1	0.95	0.10	26,26,26,26	0
56	MG	DA	3008	1/1	0.95	0.23	4,4,4,4	0
56	MG	DA	3322	1/1	0.95	0.30	3,3,3,3	0
56	MG	CA	1632	1/1	0.95	0.39	3,3,3,3	0
56	MG	CA	1780	1/1	0.95	0.08	51,51,51,51	0
56	MG	CA	1786	1/1	0.95	0.29	67,67,67,67	0
56	MG	DA	3099	1/1	0.95	0.26	3,3,3,3	0
56	MG	DA	3036	1/1	0.95	0.18	5,5,5,5	0
56	MG	BA	3842	1/1	0.95	0.19	16,16,16,16	0
56	MG	DA	3144	1/1	0.95	0.26	4,4,4,4	0
56	MG	BA	3455	1/1	0.95	0.11	26,26,26,26	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	DA	3253	1/1	0.95	0.23	3,3,3,3	0
56	MG	DA	3194	1/1	0.95	0.21	3,3,3,3	0
56	MG	BA	3219	1/1	0.95	0.16	17,17,17,17	0
56	MG	DA	3208	1/1	0.95	0.27	4,4,4,4	0
56	MG	DA	3419	1/1	0.95	0.33	3,3,3,3	0
56	MG	BA	3174	1/1	0.95	0.16	83,83,83,83	0
56	MG	BA	3584	1/1	0.95	0.27	54,54,54,54	0
56	MG	BA	3238	1/1	0.95	0.14	20,20,20,20	0
56	MG	DA	3155	1/1	0.95	0.18	4,4,4,4	0
56	MG	BA	3484	1/1	0.95	0.18	47,47,47,47	0
56	MG	DA	3040	1/1	0.95	0.24	3,3,3,3	0
56	MG	BA	3713	1/1	0.95	0.17	33,33,33,33	0
56	MG	BA	3855	1/1	0.95	0.14	49,49,49,49	0
56	MG	DB	205	1/1	0.95	0.29	3,3,3,3	0
56	MG	CA	1802	1/1	0.95	0.28	3,3,3,3	0
56	MG	AA	1855	1/1	0.95	0.24	21,21,21,21	0
56	MG	BA	3241	1/1	0.95	0.19	48,48,48,48	0
56	MG	AA	1706	1/1	0.95	0.12	36,36,36,36	0
56	MG	AY	106	1/1	0.95	0.11	58,58,58,58	0
56	MG	CA	1755	1/1	0.95	0.24	4,4,4,4	0
56	MG	BA	3290	1/1	0.95	0.16	15,15,15,15	0
56	MG	DA	3444	1/1	0.95	0.37	3,3,3,3	0
56	MG	BA	3015	1/1	0.95	0.20	60,60,60,60	0
56	MG	BA	3833	1/1	0.95	0.16	9,9,9,9	0
56	MG	BA	3562	1/1	0.95	0.12	28,28,28,28	0
56	MG	DA	3429	1/1	0.95	0.47	3,3,3,3	0
56	MG	BA	3810	1/1	0.95	0.27	12,12,12,12	0
56	MG	DA	3287	1/1	0.95	0.42	10,10,10,10	0
56	MG	AA	1620	1/1	0.95	0.18	56,56,56,56	0
56	MG	CA	1657	1/1	0.95	0.24	3,3,3,3	0
56	MG	AA	1677	1/1	0.95	0.10	74,74,74,74	0
56	MG	BA	3766	1/1	0.95	0.22	31,31,31,31	0
56	MG	DA	3190	1/1	0.95	0.24	4,4,4,4	0
56	MG	DA	3324	1/1	0.95	0.52	3,3,3,3	0
56	MG	CA	1661	1/1	0.95	0.25	3,3,3,3	0
56	MG	BA	3910	1/1	0.95	0.30	40,40,40,40	0
56	MG	BA	3328	1/1	0.95	0.14	38,38,38,38	0
56	MG	BA	3708	1/1	0.95	0.17	28,28,28,28	0
56	MG	CA	1707	1/1	0.95	0.14	36,36,36,36	0
56	MG	DA	3187	1/1	0.95	0.30	3,3,3,3	0
56	MG	AA	1850	1/1	0.95	0.11	38,38,38,38	0
56	MG	BA	3223	1/1	0.95	0.12	36,36,36,36	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	AA	1941	1/1	0.95	0.24	42,42,42,42	0
56	MG	AA	1981	1/1	0.95	0.16	52,52,52,52	0
56	MG	BA	3559	1/1	0.95	0.14	31,31,31,31	0
56	MG	DA	3010	1/1	0.95	0.18	3,3,3,3	0
56	MG	BA	3814	1/1	0.95	0.35	47,47,47,47	0
57	ZN	CN	101	1/1	0.95	0.16	100,100,100,100	0
56	MG	CY	103	1/1	0.95	0.17	31,31,31,31	0
56	MG	BA	3639	1/1	0.95	0.17	42,42,42,42	0
56	MG	DA	3229	1/1	0.95	0.22	3,3,3,3	0
56	MG	BA	3087	1/1	0.95	0.31	24,24,24,24	0
56	MG	BN	204	1/1	0.95	0.12	43,43,43,43	0
56	MG	BA	3530	1/1	0.95	0.16	60,60,60,60	0
56	MG	DA	3096	1/1	0.95	0.32	3,3,3,3	0
56	MG	DA	3225	1/1	0.95	0.18	4,4,4,4	0
56	MG	BA	3726	1/1	0.95	0.08	25,25,25,25	0
56	MG	AA	1703	1/1	0.95	0.12	48,48,48,48	0
56	MG	DA	3143	1/1	0.95	0.29	3,3,3,3	0
56	MG	CA	1774	1/1	0.95	0.50	82,82,82,82	0
56	MG	CA	1613	1/1	0.95	0.22	3,3,3,3	0
56	MG	DR	201	1/1	0.95	0.28	3,3,3,3	0
56	MG	BA	3177	1/1	0.95	0.10	40,40,40,40	0
56	MG	CA	1702	1/1	0.95	0.09	24,24,24,24	0
56	MG	DA	3053	1/1	0.95	0.21	4,4,4,4	0
56	MG	BA	3316	1/1	0.95	0.08	35,35,35,35	0
56	MG	D6	101	1/1	0.95	0.11	43,43,43,43	0
56	MG	DA	3408	1/1	0.96	0.29	4,4,4,4	0
56	MG	DA	3091	1/1	0.96	0.50	3,3,3,3	0
56	MG	BA	3380	1/1	0.96	0.07	43,43,43,43	0
56	MG	DA	3289	1/1	0.96	0.22	59,59,59,59	0
56	MG	AA	1883	1/1	0.96	0.20	42,42,42,42	0
56	MG	DA	3409	1/1	0.96	0.33	3,3,3,3	0
56	MG	DA	3477	1/1	0.96	0.25	3,3,3,3	0
56	MG	DA	3126	1/1	0.96	0.61	66,66,66,66	0
56	MG	DA	3473	1/1	0.96	0.18	3,3,3,3	0
56	MG	DA	3046	1/1	0.96	0.25	4,4,4,4	0
56	MG	CA	1688	1/1	0.96	0.31	54,54,54,54	0
56	MG	BA	3830	1/1	0.96	0.13	12,12,12,12	0
56	MG	BA	3315	1/1	0.96	0.12	28,28,28,28	0
56	MG	BA	3333	1/1	0.96	0.12	55,55,55,55	0
56	MG	CA	1817	1/1	0.96	0.15	22,22,22,22	0
56	MG	BA	3605	1/1	0.96	0.29	12,12,12,12	0
56	MG	DA	3060	1/1	0.96	0.16	4,4,4,4	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	DA	3037	1/1	0.96	0.27	4,4,4,4	0
56	MG	DB	209	1/1	0.96	0.35	3,3,3,3	0
56	MG	BA	3158	1/1	0.96	0.10	42,42,42,42	0
56	MG	DA	3017	1/1	0.96	0.09	3,3,3,3	0
56	MG	BA	3001	1/1	0.96	0.18	38,38,38,38	0
56	MG	AA	1801	1/1	0.96	0.07	55,55,55,55	0
56	MG	DA	3158	1/1	0.96	0.32	3,3,3,3	0
56	MG	BA	3773	1/1	0.96	0.15	25,25,25,25	0
56	MG	BA	3816	1/1	0.96	0.20	38,38,38,38	0
56	MG	BA	3618	1/1	0.96	0.09	19,19,19,19	0
56	MG	AA	1843	1/1	0.96	0.14	41,41,41,41	0
56	MG	BA	3439	1/1	0.96	0.17	18,18,18,18	0
56	MG	DA	3476	1/1	0.96	0.23	3,3,3,3	0
56	MG	BA	3911	1/1	0.96	0.08	22,22,22,22	0
56	MG	AA	1972	1/1	0.96	0.11	43,43,43,43	0
56	MG	DA	3089	1/1	0.96	0.14	4,4,4,4	0
56	MG	DA	3317	1/1	0.96	0.34	43,43,43,43	0
56	MG	CA	1764	1/1	0.96	0.29	3,3,3,3	0
56	MG	BQ	202	1/1	0.96	0.15	18,18,18,18	0
56	MG	DA	3434	1/1	0.96	0.18	3,3,3,3	0
56	MG	DA	3402	1/1	0.96	0.15	32,32,32,32	0
56	MG	DA	3145	1/1	0.96	0.24	4,4,4,4	0
56	MG	CA	1750	1/1	0.96	0.18	4,4,4,4	0
56	MG	DA	3094	1/1	0.96	0.37	3,3,3,3	0
56	MG	BA	3547	1/1	0.96	0.22	16,16,16,16	0
56	MG	BA	3351	1/1	0.96	0.16	22,22,22,22	0
56	MG	BA	3463	1/1	0.96	0.14	38,38,38,38	0
56	MG	DA	3382	1/1	0.96	0.07	42,42,42,42	0
56	MG	CA	1643	1/1	0.96	0.17	3,3,3,3	0
56	MG	DA	3220	1/1	0.96	0.27	21,21,21,21	0
56	MG	DA	3024	1/1	0.96	0.16	3,3,3,3	0
56	MG	DA	3186	1/1	0.96	0.11	4,4,4,4	0
56	MG	AA	1959	1/1	0.96	0.11	54,54,54,54	0
56	MG	AD	5004	1/1	0.96	0.19	48,48,48,48	0
56	MG	BA	3822	1/1	0.96	0.32	34,34,34,34	0
56	MG	BA	3236	1/1	0.96	0.17	35,35,35,35	0
56	MG	BA	3314	1/1	0.96	0.26	22,22,22,22	0
56	MG	AA	1839	1/1	0.96	0.08	18,18,18,18	0
56	MG	CA	1631	1/1	0.96	0.25	3,3,3,3	0
56	MG	DA	3224	1/1	0.96	0.14	5,5,5,5	0
56	MG	DA	3368	1/1	0.96	0.22	3,3,3,3	0
56	MG	BD	5001	1/1	0.96	0.35	61,61,61,61	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	BA	3586	1/1	0.96	0.11	18,18,18,18	0
56	MG	AA	1733	1/1	0.96	0.12	38,38,38,38	0
56	MG	AA	1705	1/1	0.96	0.39	50,50,50,50	0
56	MG	DA	3264	1/1	0.96	0.21	4,4,4,4	0
56	MG	DA	3027	1/1	0.96	0.15	6,6,6,6	0
56	MG	BA	3361	1/1	0.96	0.25	16,16,16,16	0
56	MG	BA	3774	1/1	0.96	0.23	42,42,42,42	0
56	MG	BA	3694	1/1	0.96	0.06	77,77,77,77	0
56	MG	DA	3448	1/1	0.96	0.12	21,21,21,21	0
56	MG	BA	3144	1/1	0.96	0.36	45,45,45,45	0
56	MG	DA	3045	1/1	0.96	0.35	3,3,3,3	0
56	MG	BA	3368	1/1	0.96	0.21	63,63,63,63	0
56	MG	BA	3649	1/1	0.96	0.33	30,30,30,30	0
56	MG	AA	1921	1/1	0.96	0.15	60,60,60,60	0
56	MG	DA	3166	1/1	0.96	0.27	3,3,3,3	0
56	MG	DA	3185	1/1	0.96	0.25	4,4,4,4	0
56	MG	DY	201	1/1	0.96	0.10	3,3,3,3	0
56	MG	DA	3001	1/1	0.96	0.16	55,55,55,55	0
56	MG	AA	1831	1/1	0.96	0.15	68,68,68,68	0
56	MG	AK	207	1/1	0.96	0.12	65,65,65,65	0
56	MG	DA	3084	1/1	0.96	0.34	3,3,3,3	0
56	MG	AQ	201	1/1	0.96	0.08	52,52,52,52	0
56	MG	AA	1714	1/1	0.96	0.19	79,79,79,79	0
56	MG	DA	3406	1/1	0.96	0.15	5,5,5,5	0
56	MG	DA	3395	1/1	0.96	0.23	41,41,41,41	0
56	MG	DA	3465	1/1	0.96	0.20	3,3,3,3	0
56	MG	BA	3226	1/1	0.96	0.18	43,43,43,43	0
56	MG	AA	1832	1/1	0.96	0.27	33,33,33,33	0
56	MG	DA	3471	1/1	0.96	0.16	4,4,4,4	0
56	MG	AA	1642	1/1	0.96	0.16	57,57,57,57	0
56	MG	DA	3411	1/1	0.96	0.22	3,3,3,3	0
56	MG	DA	3202	1/1	0.96	0.45	3,3,3,3	0
56	MG	DA	3124	1/1	0.96	0.15	14,14,14,14	0
56	MG	AA	1896	1/1	0.96	0.13	26,26,26,26	0
56	MG	DA	3455	1/1	0.96	0.20	27,27,27,27	0
56	MG	BA	3503	1/1	0.96	0.06	41,41,41,41	0
56	MG	DA	3147	1/1	0.96	0.37	3,3,3,3	0
56	MG	DA	3312	1/1	0.96	0.07	46,46,46,46	0
56	MG	AA	1845	1/1	0.96	0.09	29,29,29,29	0
56	MG	BA	3573	1/1	0.96	0.16	62,62,62,62	0
56	MG	DA	3135	1/1	0.96	0.18	3,3,3,3	0
56	MG	BA	3271	1/1	0.96	0.18	57,57,57,57	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	BA	3631	1/1	0.96	0.27	67,67,67,67	0
56	MG	DA	3453	1/1	0.96	0.46	3,3,3,3	0
56	MG	AY	116	1/1	0.96	0.31	40,40,40,40	0
56	MG	AE	208	1/1	0.96	0.11	42,42,42,42	0
56	MG	DA	3218	1/1	0.96	0.17	4,4,4,4	0
56	MG	DA	3076	1/1	0.96	0.17	3,3,3,3	0
56	MG	DA	3088	1/1	0.96	0.15	4,4,4,4	0
56	MG	AA	1925	1/1	0.96	0.10	43,43,43,43	0
57	ZN	AD	5001	1/1	0.96	0.24	41,41,41,41	0
56	MG	BA	3706	1/1	0.96	0.20	45,45,45,45	0
56	MG	DA	3263	1/1	0.96	0.27	4,4,4,4	0
56	MG	DA	3077	1/1	0.96	0.12	5,5,5,5	0
56	MG	AA	1690	1/1	0.96	0.10	19,19,19,19	0
56	MG	AA	1716	1/1	0.96	0.12	24,24,24,24	0
56	MG	BA	3679	1/1	0.96	0.24	5,5,5,5	0
56	MG	DA	3058	1/1	0.96	0.19	3,3,3,3	0
56	MG	DA	3109	1/1	0.96	0.27	3,3,3,3	0
56	MG	AA	1917	1/1	0.96	0.07	52,52,52,52	0
56	MG	BA	3817	1/1	0.96	0.24	30,30,30,30	0
56	MG	DB	201	1/1	0.96	0.28	3,3,3,3	0
56	MG	DA	3436	1/1	0.96	0.18	4,4,4,4	0
56	MG	DA	3086	1/1	0.96	0.26	3,3,3,3	0
56	MG	DA	3146	1/1	0.96	0.31	3,3,3,3	0
56	MG	AA	1895	1/1	0.96	0.08	52,52,52,52	0
56	MG	DA	3469	1/1	0.96	0.40	3,3,3,3	0
56	MG	CY	101	1/1	0.96	0.21	3,3,3,3	0
56	MG	BA	3153	1/1	0.96	0.29	41,41,41,41	0
56	MG	AA	1775	1/1	0.96	0.16	27,27,27,27	0
56	MG	DA	3470	1/1	0.96	0.24	4,4,4,4	0
56	MG	AA	1755	1/1	0.96	0.12	47,47,47,47	0
56	MG	BA	3824	1/1	0.96	0.14	17,17,17,17	0
56	MG	AA	2028	1/1	0.96	0.17	65,65,65,65	0
56	MG	CA	1734	1/1	0.96	0.10	29,29,29,29	0
56	MG	DA	3296	1/1	0.96	0.60	46,46,46,46	0
56	MG	BR	202	1/1	0.96	0.28	89,89,89,89	0
56	MG	CA	1739	1/1	0.96	0.35	3,3,3,3	0
56	MG	BA	3370	1/1	0.96	0.05	46,46,46,46	0
56	MG	BA	3811	1/1	0.96	0.25	52,52,52,52	0
56	MG	DA	3427	1/1	0.96	0.56	3,3,3,3	0
56	MG	AA	1861	1/1	0.96	0.05	47,47,47,47	0
56	MG	BA	3096	1/1	0.96	0.08	60,60,60,60	0
56	MG	DA	3461	1/1	0.96	0.19	4,4,4,4	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	CZ	113	1/1	0.96	0.45	3,3,3,3	0
56	MG	CA	1803	1/1	0.96	0.26	3,3,3,3	0
56	MG	DA	3435	1/1	0.96	0.16	4,4,4,4	0
56	MG	BA	3644	1/1	0.96	0.24	26,26,26,26	0
56	MG	DA	3479	1/1	0.96	0.23	3,3,3,3	0
56	MG	BD	5005	1/1	0.96	0.14	10,10,10,10	0
56	MG	DD	5001	1/1	0.96	0.15	33,33,33,33	0
56	MG	BQ	206	1/1	0.96	0.07	13,13,13,13	0
56	MG	AA	1999	1/1	0.96	0.11	47,47,47,47	0
56	MG	DA	3095	1/1	0.96	0.22	3,3,3,3	0
56	MG	BA	3214	1/1	0.96	0.36	19,19,19,19	0
56	MG	BA	3755	1/1	0.96	0.19	58,58,58,58	0
56	MG	BH	201	1/1	0.96	0.06	54,54,54,54	0
56	MG	DA	3056	1/1	0.96	0.31	63,63,63,63	0
56	MG	BA	3672	1/1	0.96	0.06	18,18,18,18	0
56	MG	DB	202	1/1	0.96	0.30	3,3,3,3	0
56	MG	DA	3167	1/1	0.96	0.11	6,6,6,6	0
56	MG	DA	3340	1/1	0.96	0.11	5,5,5,5	0
56	MG	BA	3674	1/1	0.96	0.15	12,12,12,12	0
56	MG	AA	1837	1/1	0.96	0.13	17,17,17,17	0
56	MG	BA	3220	1/1	0.96	0.23	13,13,13,13	0
56	MG	CA	1725	1/1	0.96	0.04	54,54,54,54	0
56	MG	DA	3073	1/1	0.96	0.11	6,6,6,6	0
56	MG	DA	3015	1/1	0.96	0.08	6,6,6,6	0
56	MG	DA	3374	1/1	0.96	0.29	3,3,3,3	0
56	MG	CA	1760	1/1	0.96	0.16	18,18,18,18	0
56	MG	CA	1641	1/1	0.96	0.33	3,3,3,3	0
56	MG	DA	3280	1/1	0.96	0.31	34,34,34,34	0
56	MG	DA	3117	1/1	0.96	0.11	28,28,28,28	0
56	MG	DA	3488	1/1	0.96	0.26	3,3,3,3	0
56	MG	CA	1638	1/1	0.96	0.30	3,3,3,3	0
56	MG	DA	3079	1/1	0.96	0.40	3,3,3,3	0
56	MG	CA	1625	1/1	0.96	0.34	3,3,3,3	0
56	MG	DA	3093	1/1	0.96	0.37	3,3,3,3	0
56	MG	DA	3083	1/1	0.96	0.21	3,3,3,3	0
56	MG	DA	3363	1/1	0.96	0.41	3,3,3,3	0
56	MG	BA	3863	1/1	0.96	0.16	62,62,62,62	0
56	MG	BA	3459	1/1	0.96	0.18	18,18,18,18	0
56	MG	DA	3156	1/1	0.96	0.40	3,3,3,3	0
56	MG	AA	1663	1/1	0.96	0.06	33,33,33,33	0
56	MG	BA	3148	1/1	0.96	0.35	35,35,35,35	0
56	MG	AA	1783	1/1	0.96	0.45	28,28,28,28	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	BA	3750	1/1	0.96	0.16	45,45,45,45	0
56	MG	DA	3016	1/1	0.96	0.17	3,3,3,3	0
56	MG	DA	3175	1/1	0.96	0.26	3,3,3,3	0
56	MG	CA	1698	1/1	0.96	0.19	37,37,37,37	0
56	MG	BA	3090	1/1	0.96	0.08	43,43,43,43	0
56	MG	DA	3193	1/1	0.96	0.14	7,7,7,7	0
56	MG	AA	1930	1/1	0.96	0.07	59,59,59,59	0
56	MG	BA	3137	1/1	0.96	0.11	19,19,19,19	0
56	MG	CA	1611	1/1	0.96	0.30	3,3,3,3	0
56	MG	BA	3129	1/1	0.96	0.17	48,48,48,48	0
56	MG	DD	5007	1/1	0.96	0.25	11,11,11,11	0
56	MG	BA	3040	1/1	0.96	0.32	97,97,97,97	0
56	MG	BA	3739	1/1	0.96	0.17	23,23,23,23	0
56	MG	BB	223	1/1	0.96	0.08	27,27,27,27	0
56	MG	BA	3115	1/1	0.96	0.08	61,61,61,61	0
56	MG	DA	3212	1/1	0.97	0.12	5,5,5,5	0
56	MG	DA	3011	1/1	0.97	0.21	3,3,3,3	0
56	MG	DA	3431	1/1	0.97	0.22	3,3,3,3	0
56	MG	DA	3112	1/1	0.97	0.10	26,26,26,26	0
56	MG	DA	3032	1/1	0.97	0.07	6,6,6,6	0
56	MG	DA	3214	1/1	0.97	0.30	4,4,4,4	0
56	MG	BA	3155	1/1	0.97	0.44	46,46,46,46	0
56	MG	BK	203	1/1	0.97	0.15	72,72,72,72	0
56	MG	CF	204	1/1	0.97	0.31	3,3,3,3	0
56	MG	B4	102	1/1	0.97	0.17	31,31,31,31	0
56	MG	DA	3345	1/1	0.97	0.61	3,3,3,3	0
56	MG	CA	1603	1/1	0.97	0.20	4,4,4,4	0
56	MG	AA	1759	1/1	0.97	0.26	15,15,15,15	0
56	MG	B1	103	1/1	0.97	0.09	37,37,37,37	0
56	MG	BA	3378	1/1	0.97	0.11	32,32,32,32	0
56	MG	CA	1665	1/1	0.97	0.29	3,3,3,3	0
56	MG	AA	1849	1/1	0.97	0.13	10,10,10,10	0
56	MG	CA	1662	1/1	0.97	0.19	4,4,4,4	0
56	MG	DA	3257	1/1	0.97	0.36	3,3,3,3	0
56	MG	BA	3635	1/1	0.97	0.13	37,37,37,37	0
57	ZN	AN	101	1/1	0.97	0.12	82,82,82,82	0
56	MG	BA	3012	1/1	0.97	0.34	75,75,75,75	0
56	MG	CB	302	1/1	0.97	0.14	3,3,3,3	0
56	MG	BI	206	1/1	0.97	0.27	67,67,67,67	0
56	MG	CA	1730	1/1	0.97	0.24	4,4,4,4	0
56	MG	BA	3217	1/1	0.97	0.17	12,12,12,12	0
56	MG	BA	3853	1/1	0.97	0.29	25,25,25,25	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	DA	3188	1/1	0.97	0.20	3,3,3,3	0
56	MG	DA	3111	1/1	0.97	0.26	3,3,3,3	0
56	MG	BA	3809	1/1	0.97	0.12	13,13,13,13	0
56	MG	BA	3468	1/1	0.97	0.41	22,22,22,22	0
56	MG	BA	3767	1/1	0.97	0.16	31,31,31,31	0
56	MG	DA	3410	1/1	0.97	0.18	3,3,3,3	0
56	MG	DA	3161	1/1	0.97	0.35	3,3,3,3	0
56	MG	CA	1700	1/1	0.97	0.09	12,12,12,12	0
56	MG	CA	1607	1/1	0.97	0.23	3,3,3,3	0
56	MG	CA	1749	1/1	0.97	0.34	3,3,3,3	0
56	MG	AA	2001	1/1	0.97	0.13	29,29,29,29	0
56	MG	BA	3907	1/1	0.97	0.34	27,27,27,27	0
56	MG	DA	3223	1/1	0.97	0.28	4,4,4,4	0
56	MG	AA	1829	1/1	0.97	0.31	43,43,43,43	0
56	MG	AA	1830	1/1	0.97	0.11	55,55,55,55	0
56	MG	BA	3130	1/1	0.97	0.17	32,32,32,32	0
56	MG	CA	1761	1/1	0.97	0.10	30,30,30,30	0
56	MG	BA	3813	1/1	0.97	0.10	15,15,15,15	0
56	MG	BA	3243	1/1	0.97	0.11	26,26,26,26	0
56	MG	AA	1718	1/1	0.97	0.17	79,79,79,79	0
56	MG	DA	3243	1/1	0.97	0.20	4,4,4,4	0
56	MG	AR	101	1/1	0.97	0.07	32,32,32,32	0
56	MG	DB	204	1/1	0.97	0.27	3,3,3,3	0
56	MG	BA	3539	1/1	0.97	0.17	12,12,12,12	0
56	MG	CA	1699	1/1	0.97	0.15	8,8,8,8	0
56	MG	BA	3632	1/1	0.97	0.23	51,51,51,51	0
56	MG	BA	3006	1/1	0.97	0.18	11,11,11,11	0
56	MG	DA	3438	1/1	0.97	0.21	6,6,6,6	0
56	MG	DA	3201	1/1	0.97	0.15	6,6,6,6	0
56	MG	DA	3075	1/1	0.97	0.12	4,4,4,4	0
56	MG	DA	3163	1/1	0.97	0.23	3,3,3,3	0
56	MG	BA	3667	1/1	0.97	0.32	48,48,48,48	0
56	MG	DA	3059	1/1	0.97	0.21	3,3,3,3	0
56	MG	BA	3289	1/1	0.97	0.17	31,31,31,31	0
56	MG	DA	3097	1/1	0.97	0.16	4,4,4,4	0
56	MG	DA	3063	1/1	0.97	0.31	3,3,3,3	0
56	MG	DA	3480	1/1	0.97	0.26	3,3,3,3	0
56	MG	CA	1650	1/1	0.97	0.59	73,73,73,73	0
56	MG	DA	3415	1/1	0.97	0.24	4,4,4,4	0
56	MG	AA	1961	1/1	0.97	0.38	61,61,61,61	0
56	MG	DA	3030	1/1	0.97	0.16	4,4,4,4	0
56	MG	AO	101	1/1	0.97	0.21	33,33,33,33	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	BA	3491	1/1	0.97	0.23	38,38,38,38	0
56	MG	DA	3267	1/1	0.97	0.16	3,3,3,3	0
56	MG	CA	1693	1/1	0.97	0.18	58,58,58,58	0
56	MG	DA	3137	1/1	0.97	0.65	3,3,3,3	0
56	MG	DA	3133	1/1	0.97	0.10	19,19,19,19	0
56	MG	CA	1658	1/1	0.97	0.28	3,3,3,3	0
56	MG	DA	3116	1/1	0.97	0.08	3,3,3,3	0
56	MG	DA	3269	1/1	0.97	0.20	3,3,3,3	0
56	MG	CA	1663	1/1	0.97	0.31	3,3,3,3	0
56	MG	DA	3004	1/1	0.97	0.40	3,3,3,3	0
56	MG	AA	1862	1/1	0.97	0.12	41,41,41,41	0
56	MG	BA	3242	1/1	0.97	0.19	23,23,23,23	0
56	MG	DA	3213	1/1	0.97	0.12	4,4,4,4	0
56	MG	DA	3483	1/1	0.97	0.20	4,4,4,4	0
56	MG	AA	1747	1/1	0.97	0.09	41,41,41,41	0
56	MG	DA	3422	1/1	0.97	0.23	2,2,2,2	0
56	MG	BA	3799	1/1	0.97	0.12	29,29,29,29	0
56	MG	AA	1613	1/1	0.97	0.24	45,45,45,45	0
56	MG	BA	3823	1/1	0.97	0.19	14,14,14,14	0
56	MG	DB	212	1/1	0.97	0.24	3,3,3,3	0
56	MG	DA	3090	1/1	0.97	0.28	3,3,3,3	0
56	MG	BA	3313	1/1	0.97	0.07	33,33,33,33	0
56	MG	BA	3803	1/1	0.97	0.14	32,32,32,32	0
56	MG	DA	3329	1/1	0.97	0.17	10,10,10,10	0
56	MG	BA	3764	1/1	0.97	0.15	45,45,45,45	0
56	MG	BA	3274	1/1	0.97	0.15	21,21,21,21	0
56	MG	AA	1841	1/1	0.97	0.23	8,8,8,8	0
56	MG	BA	3522	1/1	0.97	0.04	36,36,36,36	0
56	MG	DA	3351	1/1	0.97	0.25	40,40,40,40	0
56	MG	BA	3293	1/1	0.97	0.16	7,7,7,7	0
56	MG	DA	3085	1/1	0.97	0.23	3,3,3,3	0
56	MG	CA	1756	1/1	0.97	0.20	3,3,3,3	0
56	MG	BA	3782	1/1	0.97	0.15	21,21,21,21	0
56	MG	CA	1604	1/1	0.97	0.27	3,3,3,3	0
56	MG	DG	201	1/1	0.97	0.17	3,3,3,3	0
56	MG	AA	1993	1/1	0.97	0.22	46,46,46,46	0
56	MG	DA	3233	1/1	0.97	0.12	43,43,43,43	0
56	MG	CA	1717	1/1	0.97	0.16	21,21,21,21	0
56	MG	AA	1765	1/1	0.97	0.30	11,11,11,11	0
56	MG	BA	3305	1/1	0.97	0.09	18,18,18,18	0
56	MG	DA	3301	1/1	0.97	0.21	42,42,42,42	0
56	MG	BA	3282	1/1	0.97	0.12	34,34,34,34	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	DA	3159	1/1	0.97	0.40	3,3,3,3	0
56	MG	CA	1616	1/1	0.97	0.08	5,5,5,5	0
56	MG	DA	3249	1/1	0.97	0.11	6,6,6,6	0
56	MG	CZ	114	1/1	0.97	0.24	36,36,36,36	0
56	MG	BA	3796	1/1	0.97	0.14	30,30,30,30	0
56	MG	AA	1644	1/1	0.97	0.16	54,54,54,54	0
56	MG	BA	3098	1/1	0.97	0.09	27,27,27,27	0
56	MG	CA	1609	1/1	0.97	0.34	3,3,3,3	0
56	MG	BA	3286	1/1	0.97	0.24	17,17,17,17	0
56	MG	CA	1776	1/1	0.97	0.23	3,3,3,3	0
56	MG	BA	3633	1/1	0.97	0.23	36,36,36,36	0
56	MG	DA	3276	1/1	0.97	0.26	4,4,4,4	0
56	MG	DA	3081	1/1	0.97	0.16	4,4,4,4	0
56	MG	BA	3167	1/1	0.97	0.36	22,22,22,22	0
56	MG	AA	1724	1/1	0.97	0.08	35,35,35,35	0
56	MG	AA	1701	1/1	0.97	0.12	29,29,29,29	0
56	MG	AA	1604	1/1	0.97	0.21	43,43,43,43	0
56	MG	BA	3476	1/1	0.97	0.07	18,18,18,18	0
56	MG	BA	3789	1/1	0.97	0.09	36,36,36,36	0
56	MG	BA	3854	1/1	0.97	0.45	60,60,60,60	0
56	MG	AA	1737	1/1	0.97	0.26	36,36,36,36	0
56	MG	BA	3865	1/1	0.97	0.50	37,37,37,37	0
56	MG	CA	1647	1/1	0.97	0.24	3,3,3,3	0
56	MG	BA	3284	1/1	0.97	0.17	15,15,15,15	0
56	MG	AA	1621	1/1	0.97	0.14	25,25,25,25	0
56	MG	DA	3284	1/1	0.97	0.07	8,8,8,8	0
56	MG	DA	3460	1/1	0.97	0.07	6,6,6,6	0
56	MG	BA	3302	1/1	0.97	0.30	47,47,47,47	0
56	MG	CA	1633	1/1	0.97	0.27	3,3,3,3	0
56	MG	CA	1627	1/1	0.97	0.29	3,3,3,3	0
56	MG	DA	3446	1/1	0.97	0.34	3,3,3,3	0
56	MG	AA	1615	1/1	0.97	0.07	4,4,4,4	0
56	MG	AA	1740	1/1	0.97	0.24	30,30,30,30	0
56	MG	BA	3457	1/1	0.97	0.25	11,11,11,11	0
56	MG	B1	102	1/1	0.97	0.08	9,9,9,9	0
56	MG	CA	1807	1/1	0.97	0.32	3,3,3,3	0
56	MG	BA	3554	1/1	0.97	0.28	7,7,7,7	0
56	MG	DA	3325	1/1	0.97	0.30	3,3,3,3	0
56	MG	AA	1909	1/1	0.97	0.12	55,55,55,55	0
56	MG	DA	3177	1/1	0.97	0.41	3,3,3,3	0
56	MG	BA	3504	1/1	0.97	0.09	34,34,34,34	0
56	MG	BA	3054	1/1	0.97	0.28	63,63,63,63	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	BA	3067	1/1	0.97	0.07	48,48,48,48	0
56	MG	DA	3342	1/1	0.97	0.14	7,7,7,7	0
56	MG	CA	1784	1/1	0.97	0.30	3,3,3,3	0
56	MG	BA	3531	1/1	0.97	0.14	12,12,12,12	0
56	MG	DA	3335	1/1	0.97	0.63	3,3,3,3	0
56	MG	AA	1780	1/1	0.97	0.18	24,24,24,24	0
56	MG	CA	1710	1/1	0.97	0.33	46,46,46,46	0
56	MG	CA	1805	1/1	0.97	0.23	3,3,3,3	0
56	MG	DA	3441	1/1	0.97	0.24	4,4,4,4	0
56	MG	AA	1900	1/1	0.97	0.47	39,39,39,39	0
56	MG	AA	1629	1/1	0.97	0.13	32,32,32,32	0
56	MG	AA	1796	1/1	0.97	0.16	60,60,60,60	0
56	MG	DA	3316	1/1	0.97	0.13	4,4,4,4	0
56	MG	BA	3099	1/1	0.97	0.21	29,29,29,29	0
56	MG	CA	1672	1/1	0.97	0.33	3,3,3,3	0
56	MG	CA	1634	1/1	0.97	0.08	6,6,6,6	0
56	MG	DA	3379	1/1	0.97	0.34	3,3,3,3	0
56	MG	DA	3327	1/1	0.97	0.35	4,4,4,4	0
56	MG	DA	3344	1/1	0.97	0.36	25,25,25,25	0
56	MG	BA	3735	1/1	0.97	0.12	29,29,29,29	0
56	MG	CA	1617	1/1	0.97	0.11	4,4,4,4	0
56	MG	BA	3318	1/1	0.97	0.07	25,25,25,25	0
56	MG	DA	3487	1/1	0.97	0.32	3,3,3,3	0
56	MG	CA	1798	1/1	0.97	0.35	3,3,3,3	0
56	MG	DA	3364	1/1	0.97	0.20	3,3,3,3	0
56	MG	DA	3309	1/1	0.97	0.22	4,4,4,4	0
56	MG	DA	3092	1/1	0.98	0.30	4,4,4,4	0
56	MG	DA	3399	1/1	0.98	0.35	58,58,58,58	0
56	MG	DA	3484	1/1	0.98	0.39	3,3,3,3	0
56	MG	AA	1811	1/1	0.98	0.21	37,37,37,37	0
56	MG	AA	1625	1/1	0.98	0.21	44,44,44,44	0
56	MG	DA	3459	1/1	0.98	0.41	4,4,4,4	0
56	MG	DA	3255	1/1	0.98	0.23	12,12,12,12	0
56	MG	DA	3349	1/1	0.98	0.14	29,29,29,29	0
56	MG	AA	2018	1/1	0.98	0.23	23,23,23,23	0
56	MG	DA	3464	1/1	0.98	0.31	3,3,3,3	0
56	MG	AA	1626	1/1	0.98	0.27	20,20,20,20	0
56	MG	DA	3034	1/1	0.98	0.11	6,6,6,6	0
56	MG	DA	3009	1/1	0.98	0.26	3,3,3,3	0
56	MG	BA	3616	1/1	0.98	0.08	12,12,12,12	0
56	MG	AA	1926	1/1	0.98	0.07	30,30,30,30	0
56	MG	CA	1747	1/1	0.98	0.45	3,3,3,3	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	CA	1806	1/1	0.98	0.34	3,3,3,3	0
56	MG	DA	3378	1/1	0.98	0.27	3,3,3,3	0
56	MG	AA	1877	1/1	0.98	0.19	24,24,24,24	0
56	MG	BA	3358	1/1	0.98	0.18	17,17,17,17	0
56	MG	BA	3552	1/1	0.98	0.07	15,15,15,15	0
56	MG	BA	3882	1/1	0.98	0.25	42,42,42,42	0
56	MG	BA	3266	1/1	0.98	0.34	24,24,24,24	0
56	MG	CA	1777	1/1	0.98	0.23	4,4,4,4	0
56	MG	BA	3851	1/1	0.98	0.21	17,17,17,17	0
56	MG	AA	1805	1/1	0.98	0.05	22,22,22,22	0
56	MG	DA	3123	1/1	0.98	0.13	5,5,5,5	0
56	MG	DA	3005	1/1	0.98	0.17	3,3,3,3	0
56	MG	DA	3160	1/1	0.98	0.33	3,3,3,3	0
56	MG	DA	3270	1/1	0.98	0.22	4,4,4,4	0
56	MG	DA	3412	1/1	0.98	0.24	3,3,3,3	0
56	MG	CA	1642	1/1	0.98	0.43	3,3,3,3	0
56	MG	DT	201	1/1	0.98	0.37	3,3,3,3	0
56	MG	DA	3472	1/1	0.98	0.28	4,4,4,4	0
56	MG	CA	1614	1/1	0.98	0.25	3,3,3,3	0
56	MG	CA	1612	1/1	0.98	0.13	3,3,3,3	0
56	MG	BA	3729	1/1	0.98	0.28	38,38,38,38	0
56	MG	BA	3682	1/1	0.98	0.14	20,20,20,20	0
56	MG	BA	3553	1/1	0.98	0.14	12,12,12,12	0
56	MG	DA	3265	1/1	0.98	0.17	3,3,3,3	0
56	MG	DA	3489	1/1	0.98	0.20	4,4,4,4	0
56	MG	BA	3191	1/1	0.98	0.12	26,26,26,26	0
56	MG	DA	3174	1/1	0.98	0.20	3,3,3,3	0
56	MG	DA	3352	1/1	0.98	0.30	3,3,3,3	0
56	MG	AA	1806	1/1	0.98	0.31	27,27,27,27	0
56	MG	AA	1746	1/1	0.98	0.17	39,39,39,39	0
56	MG	DA	3140	1/1	0.98	0.18	3,3,3,3	0
56	MG	BA	3582	1/1	0.98	0.07	55,55,55,55	0
56	MG	AA	1627	1/1	0.98	0.12	29,29,29,29	0
56	MG	DA	3227	1/1	0.98	0.30	3,3,3,3	0
56	MG	AY	105	1/1	0.98	0.08	39,39,39,39	0
56	MG	DA	3442	1/1	0.98	0.36	3,3,3,3	0
56	MG	DA	3439	1/1	0.98	0.26	4,4,4,4	0
56	MG	CS	101	1/1	0.98	0.25	3,3,3,3	0
56	MG	DA	3134	1/1	0.98	0.42	21,21,21,21	0
56	MG	BA	3294	1/1	0.98	0.24	4,4,4,4	0
56	MG	DA	3043	1/1	0.98	0.20	3,3,3,3	0
56	MG	DA	3209	1/1	0.98	0.33	3,3,3,3	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	DA	3277	1/1	0.98	0.34	3,3,3,3	0
56	MG	DA	3173	1/1	0.98	0.21	3,3,3,3	0
56	MG	DA	3491	1/1	0.98	0.33	3,3,3,3	0
56	MG	DA	3357	1/1	0.98	0.23	3,3,3,3	0
56	MG	DA	3404	1/1	0.98	0.15	5,5,5,5	0
56	MG	AA	1835	1/1	0.98	0.20	37,37,37,37	0
56	MG	CA	1608	1/1	0.98	0.25	3,3,3,3	0
56	MG	DA	3462	1/1	0.98	0.24	3,3,3,3	0
56	MG	DA	3025	1/1	0.98	0.25	3,3,3,3	0
56	MG	DA	3018	1/1	0.98	0.23	3,3,3,3	0
56	MG	CA	1778	1/1	0.98	0.14	3,3,3,3	0
56	MG	DA	3205	1/1	0.98	0.22	38,38,38,38	0
56	MG	DA	3136	1/1	0.98	0.18	8,8,8,8	0
56	MG	DA	3120	1/1	0.98	0.39	28,28,28,28	0
56	MG	BA	3890	1/1	0.98	0.21	25,25,25,25	0
56	MG	AA	1927	1/1	0.98	0.16	29,29,29,29	0
56	MG	DA	3014	1/1	0.98	0.39	3,3,3,3	0
57	ZN	CD	5001	1/1	0.98	0.24	63,63,63,63	0
56	MG	AA	1781	1/1	0.98	0.20	28,28,28,28	0
56	MG	DA	3393	1/1	0.98	0.06	47,47,47,47	0
56	MG	BA	3206	1/1	0.98	0.12	35,35,35,35	0
56	MG	DA	3430	1/1	0.98	0.14	6,6,6,6	0
56	MG	BA	3450	1/1	0.98	0.14	24,24,24,24	0
56	MG	DA	3478	1/1	0.98	0.37	3,3,3,3	0
56	MG	DA	3416	1/1	0.98	0.20	3,3,3,3	0
56	MG	CT	201	1/1	0.98	0.29	3,3,3,3	0
56	MG	BA	3551	1/1	0.98	0.17	19,19,19,19	0
56	MG	DA	3463	1/1	0.98	0.12	4,4,4,4	0
56	MG	BA	3118	1/1	0.98	0.08	23,23,23,23	0
56	MG	DA	3151	1/1	0.98	0.19	4,4,4,4	0
56	MG	DA	3418	1/1	0.98	0.26	3,3,3,3	0
56	MG	DA	3261	1/1	0.98	0.30	3,3,3,3	0
56	MG	DA	3365	1/1	0.98	0.29	3,3,3,3	0
56	MG	BA	3654	1/1	0.98	0.20	12,12,12,12	0
56	MG	DA	3122	1/1	0.98	0.24	4,4,4,4	0
56	MG	DA	3451	1/1	0.98	0.48	23,23,23,23	0
56	MG	BA	3671	1/1	0.98	0.11	57,57,57,57	0
56	MG	DA	3064	1/1	0.98	0.32	4,4,4,4	0
56	MG	BA	3074	1/1	0.98	0.09	26,26,26,26	0
56	MG	DA	3273	1/1	0.98	0.25	3,3,3,3	0
56	MG	BA	3075	1/1	0.98	0.42	29,29,29,29	0
56	MG	DA	3341	1/1	0.98	0.36	3,3,3,3	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	DA	3302	1/1	0.98	0.11	44,44,44,44	0
56	MG	DA	3372	1/1	0.98	0.27	3,3,3,3	0
56	MG	DA	3490	1/1	0.98	0.29	3,3,3,3	0
56	MG	BA	3594	1/1	0.98	0.20	12,12,12,12	0
56	MG	BA	3303	1/1	0.98	0.26	12,12,12,12	0
56	MG	DA	3458	1/1	0.98	0.17	6,6,6,6	0
56	MG	DA	3321	1/1	0.98	0.31	4,4,4,4	0
56	MG	BA	3645	1/1	0.98	0.15	30,30,30,30	0
56	MG	BA	3721	1/1	0.98	0.27	34,34,34,34	0
56	MG	BA	3660	1/1	0.98	0.26	12,12,12,12	0
56	MG	BA	3185	1/1	0.98	0.14	8,8,8,8	0
56	MG	BA	3417	1/1	0.98	0.16	8,8,8,8	0
56	MG	CA	1636	1/1	0.98	0.37	3,3,3,3	0
56	MG	CA	1664	1/1	0.98	0.18	3,3,3,3	0
56	MG	BA	3413	1/1	0.98	0.08	43,43,43,43	0
56	MG	DA	3303	1/1	0.98	0.06	10,10,10,10	0
56	MG	DA	3272	1/1	0.98	0.28	3,3,3,3	0
56	MG	BA	3142	1/1	0.98	0.15	24,24,24,24	0
56	MG	BA	3414	1/1	0.98	0.11	23,23,23,23	0
56	MG	CC	301	1/1	0.98	0.25	3,3,3,3	0
56	MG	DA	3433	1/1	0.98	0.24	3,3,3,3	0
56	MG	BA	3342	1/1	0.99	0.16	20,20,20,20	0
56	MG	CA	1752	1/1	0.99	0.38	3,3,3,3	0
56	MG	CA	1620	1/1	0.99	0.17	4,4,4,4	0
56	MG	BA	3086	1/1	0.99	0.15	23,23,23,23	0
56	MG	DA	3258	1/1	0.99	0.11	6,6,6,6	0
56	MG	DA	3256	1/1	0.99	0.10	6,6,6,6	0
56	MG	DA	3141	1/1	0.99	0.15	4,4,4,4	0
56	MG	CA	1646	1/1	0.99	0.25	3,3,3,3	0
56	MG	DA	3070	1/1	0.99	0.27	4,4,4,4	0
56	MG	BA	3467	1/1	0.99	0.39	21,21,21,21	0
56	MG	CA	1793	1/1	0.99	0.42	3,3,3,3	0
56	MG	DA	3407	1/1	0.99	0.31	3,3,3,3	0
56	MG	BA	3451	1/1	0.99	0.14	13,13,13,13	0
56	MG	AA	1840	1/1	0.99	0.24	26,26,26,26	0
56	MG	DA	3013	1/1	0.99	0.30	3,3,3,3	0
56	MG	DA	3057	1/1	0.99	0.29	3,3,3,3	0
56	MG	DO	201	1/1	0.99	0.29	3,3,3,3	0
56	MG	CA	1605	1/1	0.99	0.33	3,3,3,3	0
56	MG	CA	1701	1/1	0.99	0.14	13,13,13,13	0
56	MG	AA	1731	1/1	0.99	0.08	17,17,17,17	0
56	MG	CA	1606	1/1	0.99	0.33	3,3,3,3	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	CA	1804	1/1	0.99	0.25	4,4,4,4	0
56	MG	BA	3834	1/1	0.99	0.34	12,12,12,12	0
56	MG	BA	3611	1/1	0.99	0.24	8,8,8,8	0
56	MG	CA	1637	1/1	0.99	0.15	4,4,4,4	0
56	MG	DA	3266	1/1	0.99	0.25	3,3,3,3	0
56	MG	CA	1629	1/1	0.99	0.21	4,4,4,4	0
56	MG	BA	3081	1/1	0.99	0.19	31,31,31,31	0
56	MG	DA	3179	1/1	0.99	0.47	3,3,3,3	0
56	MG	CA	1622	1/1	0.99	0.22	3,3,3,3	0
56	MG	CA	1782	1/1	0.99	0.17	3,3,3,3	0
56	MG	DB	207	1/1	0.99	0.18	4,4,4,4	0
56	MG	DA	3197	1/1	0.99	0.18	3,3,3,3	0
56	MG	CA	1660	1/1	0.99	0.13	5,5,5,5	0
56	MG	AA	1784	1/1	0.99	0.28	25,25,25,25	0
56	MG	DA	3275	1/1	0.99	0.29	4,4,4,4	0
56	MG	B1	101	1/1	0.99	0.26	31,31,31,31	0
56	MG	DA	3343	1/1	0.99	0.35	3,3,3,3	0
56	MG	DA	3271	1/1	0.99	0.21	3,3,3,3	0
56	MG	DA	3450	1/1	0.99	0.27	12,12,12,12	0
56	MG	DA	3020	1/1	0.99	0.31	3,3,3,3	0

## 6.5 Other polymers

There are no such residues in this entry.