



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 17, 2026 – 02:59 AM UTC

PDB ID : 4V5A / pdb_00004v5a
Title : Structure of the Ribosome Recycling Factor bound to the Thermus thermophilus 70S ribosome with mRNA, ASL-Phe and tRNA-fMet
Authors : Weixlbaumer, A.; Petry, S.; Dunham, C.M.; Selmer, M.; Kelley, A.C.; Ramakrishnan, V.
Deposited on : 2007-06-28
Resolution : 3.50 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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	FAILED
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.48.1

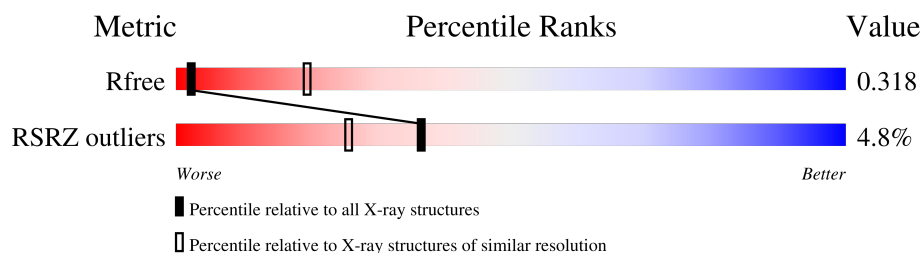
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.50 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	164625	1094 (3.56-3.44)
RSRZ outliers	164620	1093 (3.56-3.44)

MolProbity failed to run properly - the sequence quality summary graphics cannot be shown.

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
57	MG	AA	1653	-	-	-	X
57	MG	AA	1691	-	-	-	X
57	MG	AA	1720	-	-	-	X
57	MG	AA	1743	-	-	-	X
57	MG	AA	1789	-	-	-	X
57	MG	AA	1797	-	-	-	X
57	MG	AW	112	-	-	-	X
57	MG	BA	3014	-	-	-	X
57	MG	BA	3035	-	-	-	X
57	MG	BA	3103	-	-	-	X
57	MG	BA	3130	-	-	-	X
57	MG	BA	3206	-	-	-	X
57	MG	BA	3227	-	-	-	X
57	MG	BA	3379	-	-	-	X
57	MG	BA	3394	-	-	-	X
57	MG	BA	3423	-	-	-	X
57	MG	CA	1640	-	-	-	X
57	MG	CA	1651	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
57	MG	CA	1681	-	-	-	X
57	MG	CA	1736	-	-	-	X
57	MG	CA	1785	-	-	-	X
57	MG	CA	1796	-	-	-	X
57	MG	CW	110	-	-	-	X
57	MG	CW	116	-	-	-	X
57	MG	DA	3048	-	-	-	X
57	MG	DA	3049	-	-	-	X
57	MG	DA	3090	-	-	-	X
57	MG	DA	3141	-	-	-	X
57	MG	DA	3206	-	-	-	X
57	MG	DA	3214	-	-	-	X
57	MG	DA	3219	-	-	-	X
57	MG	DA	3273	-	-	-	X
57	MG	DA	3295	-	-	-	X
57	MG	DA	3358	-	-	-	X
57	MG	DA	3409	-	-	-	X

2 Entry composition

There are 58 unique types of molecules in this entry. The entry contains 290487 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 ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	AA	1504	Total	C	N	O	P	0	0	0
			32329	14390	5992	10444	1503			
1	CA	1504	Total	C	N	O	P	0	0	0
			32329	14390	5992	10444	1503			

- Molecule 2 is a protein called 30S RIBOSOMAL PROTEIN S2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	AB	235	Total	C	N	O	S	0	0	1
			1901	1213	342	341	5			
2	CB	235	Total	C	N	O	S	0	0	1
			1901	1213	342	341	5			

- Molecule 3 is a protein called 30S RIBOSOMAL PROTEIN S3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	AC	207	Total	C	N	O	S	0	0	1
			1613	1016	315	281	1			
3	CC	207	Total	C	N	O	S	0	0	1
			1613	1016	315	281	1			

- Molecule 4 is a protein called 30S RIBOSOMAL PROTEIN S4.

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

- Molecule 5 is a protein called 30S RIBOSOMAL PROTEIN S5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	AE	151	Total	C	N	O	S	0	0	1
			1147	724	218	201	4			
5	CE	151	Total	C	N	O	S	0	0	1
			1147	724	218	201	4			

- Molecule 6 is a protein called 30S RIBOSOMAL PROTEIN S6.

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

- Molecule 7 is a protein called 30S RIBOSOMAL PROTEIN S7.

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

- Molecule 8 is a protein called 30S RIBOSOMAL PROTEIN S8.

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

- Molecule 9 is a protein called 30S RIBOSOMAL PROTEIN S9.

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

- Molecule 10 is a protein called 30S RIBOSOMAL PROTEIN S10.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	AJ	99	Total	C	N	O	S	0	0	1
			795	499	157	138	1			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	CJ	99	Total	C	N	O	S	0	0	1
			795	499	157	138	1			

- Molecule 11 is a protein called 30S RIBOSOMAL PROTEIN S11.

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

- Molecule 12 is a protein called 30S RIBOSOMAL PROTEIN S12.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	AL	125	Total	C	N	O	S	0	0	1
			971	611	196	163	1			
12	CL	125	Total	C	N	O	S	0	0	1
			971	611	196	163	1			

- Molecule 13 is a protein called 30S RIBOSOMAL PROTEIN S13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	AM	125	Total	C	N	O	S	0	0	1
			988	611	206	169	2			
13	CM	125	Total	C	N	O	S	0	0	1
			988	611	206	169	2			

- Molecule 14 is a protein called 30S RIBOSOMAL PROTEIN S14.

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

- Molecule 15 is a protein called 30S RIBOSOMAL PROTEIN S15.

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

- Molecule 16 is a protein called 30S RIBOSOMAL PROTEIN S16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	AP	84	Total	C	N	O	S	0	0	1
			701	443	140	117	1			
16	CP	84	Total	C	N	O	S	0	0	1
			701	443	140	117	1			

- Molecule 17 is a protein called 30S RIBOSOMAL PROTEIN S17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	AQ	100	Total	C	N	O	S	0	0	1
			824	528	152	142	2			
17	CQ	100	Total	C	N	O	S	0	0	1
			824	528	152	142	2			

- Molecule 18 is a protein called 30S RIBOSOMAL PROTEIN S18.

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

- Molecule 19 is a protein called 30S RIBOSOMAL PROTEIN S19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	AS	79	Total	C	N	O	S	0	0	1
			630	403	115	110	2			
19	CS	79	Total	C	N	O	S	0	0	1
			630	403	115	110	2			

- Molecule 20 is a protein called 30S RIBOSOMAL PROTEIN S20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	AT	99	Total	C	N	O	S	0	0	0
			763	470	162	129	2			
20	CT	99	Total	C	N	O	S	0	0	0
			763	470	162	129	2			

- Molecule 21 is a protein called 30S RIBOSOMAL PROTEIN THX.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
21	AU	25	Total	C	N	O	0	0	1
			209	128	51	30			
21	CU	25	Total	C	N	O	0	0	1
			209	128	51	30			

- Molecule 22 is a RNA chain called P-SITE RNA ASL-PHE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	AV	17	Total	C	N	O	P	0	0	0
			362	163	68	115	16			
22	CV	17	Total	C	N	O	P	0	0	0
			362	163	68	115	16			

- Molecule 23 is a RNA chain called TRNA-FMET.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	AW	77	Total	C	N	O	P	0	0	0
			1641	733	297	535	76			
23	CW	77	Total	C	N	O	P	0	0	0
			1641	733	297	535	76			

- Molecule 24 is a RNA chain called MRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	AX	11	Total	C	N	O	P	0	0	0
			230	104	38	78	10			
24	CX	11	Total	C	N	O	P	0	0	0
			230	104	38	78	10			

- Molecule 25 is a protein called RIBOSOME RECYCLING FACTOR.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
25	AY	185	Total	C	N	O	S	0	0	0
			1478	924	270	282	2			
25	CY	185	Total	C	N	O	S	0	0	0
			1478	924	270	282	2			

- Molecule 26 is a protein called 50S RIBOSOMAL PROTEIN L27.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	B0	85	Total	C	N	O	S	0	0	0
			652	403	137	111	1			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	D0	85	Total	C	N	O	S	0	0	0
			652	403	137	111	1			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B0	6	ALA	GLY	conflict	UNP P60493
B0	8	ALA	GLY	conflict	UNP P60493
D0	6	ALA	GLY	conflict	UNP P60493
D0	8	ALA	GLY	conflict	UNP P60493

- Molecule 27 is a protein called 50S RIBOSOMAL PROTEIN L28.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
27	B1	89	Total	C	N	O		0	0	1
			693	435	140	118				
27	D1	89	Total	C	N	O		0	0	1
			693	435	140	118				

- Molecule 28 is a protein called 50S RIBOSOMAL PROTEIN L29.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
28	B2	51	Total	C	N	O	S	0	0	1
			421	263	85	72	1			
28	D2	51	Total	C	N	O	S	0	0	1
			421	263	85	72	1			

- Molecule 29 is a protein called 50S RIBOSOMAL PROTEIN L30.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
29	B3	60	Total	C	N	O	S	0	0	1
			468	298	91	78	1			
29	D3	60	Total	C	N	O	S	0	0	1
			468	298	91	78	1			

- Molecule 30 is a protein called 50S RIBOSOMAL PROTEIN L31.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
30	B4	50	Total	C	N	O		0	0	1
			242	143	50	49				
30	D4	50	Total	C	N	O		0	0	1
			242	143	50	49				

- Molecule 31 is a protein called 50S RIBOSOMAL PROTEIN L32.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
31	B5	59	Total	C	N	O	S	0	0	0
			459	288	90	76	5			
31	D5	59	Total	C	N	O	S	0	0	0
			459	288	90	76	5			

- Molecule 32 is a protein called 50S RIBOSOMAL PROTEIN L33.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
32	B6	45	Total	C	N	O	S	0	0	1
			381	235	78	64	4			
32	D6	45	Total	C	N	O	S	0	0	1
			381	235	78	64	4			

- Molecule 33 is a protein called 50S RIBOSOMAL PROTEIN L34.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
33	B7	49	Total	C	N	O	S	0	0	1
			419	257	105	55	2			
33	D7	49	Total	C	N	O	S	0	0	1
			419	257	105	55	2			

- Molecule 34 is a protein called 50S RIBOSOMAL PROTEIN L35.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
34	B8	64	Total	C	N	O	S	0	0	1
			508	326	102	78	2			
34	D8	64	Total	C	N	O	S	0	0	1
			508	326	102	78	2			

- Molecule 35 is a RNA chain called 23S ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
35	BA	2767	Total	C	N	O	P	0	0	0
			59601	26526	11153	19156	2766			
35	DA	2767	Total	C	N	O	P	0	0	0
			59601	26526	11153	19156	2766			

- Molecule 36 is a RNA chain called 5S ribosomal RNA.

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

- Molecule 37 is a protein called 50S RIBOSOMAL PROTEIN L1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
37	BC	191	Total	C	N	O		0	0	1
			1142	691	221	230				
37	DC	191	Total	C	N	O		0	0	1
			1143	692	221	230				

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
DC	106	ALA	GLY	conflict	UNP Q5SLP7
DC	132	ALA	GLY	conflict	UNP Q5SLP7

- Molecule 38 is a protein called 50S RIBOSOMAL PROTEIN L2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
38	BD	272	Total	C	N	O	S	0	0	1
			2105	1329	417	356	3			
38	DD	272	Total	C	N	O	S	0	0	1
			2105	1329	417	356	3			

- Molecule 39 is a protein called 50S RIBOSOMAL PROTEIN L3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
39	BE	205	Total	C	N	O	S	0	0	1
			1564	988	300	270	6			
39	DE	205	Total	C	N	O	S	0	0	1
			1564	988	300	270	6			

- Molecule 40 is a protein called 50S RIBOSOMAL PROTEIN L4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
40	BF	208	Total	C	N	O	S	0	0	1
			1624	1035	304	282	3			
40	DF	208	Total	C	N	O	S	0	0	1
			1624	1035	304	282	3			

- Molecule 41 is a protein called 50S RIBOSOMAL PROTEIN L5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
41	BG	181	Total	C	N	O	S	0	0	0
			1474	942	268	260	4			
41	DG	181	Total	C	N	O	S	0	0	0
			1474	942	268	260	4			

- Molecule 42 is a protein called 50S RIBOSOMAL PROTEIN L6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
42	BH	160	Total	C	N	O	S	0	0	1
			1223	773	229	220	1			
42	DH	160	Total	C	N	O	S	0	0	1
			1223	773	229	220	1			

- Molecule 43 is a protein called 50S RIBOSOMAL PROTEIN L9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
43	BI	146	Total	C	N	O	S	0	0	1
			1132	723	201	207	1			
43	DI	146	Total	C	N	O	S	0	0	1
			1132	723	201	207	1			

- Molecule 44 is a protein called 50S RIBOSOMAL PROTEIN L13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
44	BN	139	Total	C	N	O	S	0	0	1
			1105	712	207	182	4			
44	DN	139	Total	C	N	O	S	0	0	1
			1105	712	207	182	4			

- Molecule 45 is a protein called 50S RIBOSOMAL PROTEIN L14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
45	BO	122	Total	C	N	O	S	0	0	0
			933	588	171	170	4			
45	DO	122	Total	C	N	O	S	0	0	0
			933	588	171	170	4			

- Molecule 46 is a protein called 50S RIBOSOMAL PROTEIN L15.

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

- Molecule 47 is a protein called 50S RIBOSOMAL PROTEIN L16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
47	BQ	136	Total	C	N	O	S	0	0	0
			1080	688	204	183	5			
47	DQ	136	Total	C	N	O	S	0	0	0
			1080	688	204	183	5			

- Molecule 48 is a protein called 50S RIBOSOMAL PROTEIN L17.

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

- Molecule 49 is a protein called 50S RIBOSOMAL PROTEIN L18.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
49	BS	99	Total	C	N	O		0	0	1
			771	486	155	130				
49	DS	99	Total	C	N	O		0	0	1
			771	486	155	130				

- Molecule 50 is a protein called 50S RIBOSOMAL PROTEIN L19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
50	BT	138	Total	C	N	O	S	0	0	1
			1142	710	235	196	1			
50	DT	138	Total	C	N	O	S	0	0	1
			1142	710	235	196	1			

- Molecule 51 is a protein called 50S RIBOSOMAL PROTEIN L20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
51	BU	117	Total	C	N	O	S	0	0	0
			958	604	202	151	1			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
51	DU	117	Total	C	N	O	S	0	0	0
			958	604	202	151	1			

- Molecule 52 is a protein called 50S RIBOSOMAL PROTEIN L21.

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

- Molecule 53 is a protein called 50S RIBOSOMAL PROTEIN L22.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
53	BW	113	Total	C	N	O	S	0	0	0
			896	563	176	155	2			
53	DW	113	Total	C	N	O	S	0	0	0
			896	563	176	155	2			

- Molecule 54 is a protein called 50S RIBOSOMAL PROTEIN L23.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
54	BX	93	Total	C	N	O		0	0	1
			726	471	132	123				
54	DX	93	Total	C	N	O		0	0	1
			726	471	132	123				

- Molecule 55 is a protein called 50S RIBOSOMAL PROTEIN L24.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
55	BY	101	Total	C	N	O	S	0	0	1
			776	500	149	123	4			
55	DY	101	Total	C	N	O	S	0	0	1
			776	500	149	123	4			

- Molecule 56 is a protein called 50S RIBOSOMAL PROTEIN L25.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
56	BZ	177	Total	C	N	O	S	0	0	1
			1404	897	253	252	2			
56	DZ	177	Total	C	N	O	S	0	0	1
			1404	897	253	252	2			

- Molecule 57 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	AA	204	Total 204	Mg 204	0	0
57	AD	2	Total 2	Mg 2	0	0
57	AE	2	Total 2	Mg 2	0	0
57	AG	1	Total 1	Mg 1	0	0
57	AK	1	Total 1	Mg 1	0	0
57	AL	2	Total 2	Mg 2	0	0
57	AM	1	Total 1	Mg 1	0	0
57	AV	4	Total 4	Mg 4	0	0
57	AW	23	Total 23	Mg 23	0	0
57	AX	5	Total 5	Mg 5	0	0
57	B1	4	Total 4	Mg 4	0	0
57	B2	2	Total 2	Mg 2	0	0
57	B3	1	Total 1	Mg 1	0	0
57	B5	2	Total 2	Mg 2	0	0
57	B7	1	Total 1	Mg 1	0	0
57	BA	445	Total 445	Mg 445	0	0
57	BB	20	Total 20	Mg 20	0	0
57	BD	3	Total 3	Mg 3	0	0
57	BE	1	Total 1	Mg 1	0	0
57	BF	4	Total 4	Mg 4	0	0
57	BG	1	Total 1	Mg 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	BN	4	Total 4	Mg 4	0	0
57	BO	1	Total 1	Mg 1	0	0
57	BP	3	Total 3	Mg 3	0	0
57	BU	2	Total 2	Mg 2	0	0
57	BX	2	Total 2	Mg 2	0	0
57	CA	208	Total 208	Mg 208	0	0
57	CE	3	Total 3	Mg 3	0	0
57	CG	1	Total 1	Mg 1	0	0
57	CL	2	Total 2	Mg 2	0	0
57	CN	1	Total 1	Mg 1	0	0
57	CV	4	Total 4	Mg 4	0	0
57	CW	23	Total 23	Mg 23	0	0
57	CX	4	Total 4	Mg 4	0	0
57	D1	4	Total 4	Mg 4	0	0
57	D2	2	Total 2	Mg 2	0	0
57	D3	1	Total 1	Mg 1	0	0
57	D5	1	Total 1	Mg 1	0	0
57	D7	1	Total 1	Mg 1	0	0
57	DA	441	Total 441	Mg 441	0	0
57	DB	19	Total 19	Mg 19	0	0
57	DD	3	Total 3	Mg 3	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	DE	2	Total	Mg	0	0
			2	2		
57	DF	5	Total	Mg	0	0
			5	5		
57	DG	1	Total	Mg	0	0
			1	1		
57	DH	1	Total	Mg	0	0
			1	1		
57	DN	2	Total	Mg	0	0
			2	2		
57	DP	4	Total	Mg	0	0
			4	4		
57	DS	1	Total	Mg	0	0
			1	1		
57	DU	3	Total	Mg	0	0
			3	3		
57	DV	1	Total	Mg	0	0
			1	1		
57	DX	3	Total	Mg	0	0
			3	3		

- Molecule 58 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

MolProbity failed to run properly - this section is therefore empty.

3 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	212.41Å 450.11Å 630.54Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 3.50 20.00 – 3.50	Depositor EDS
% Data completeness (in resolution range)	98.9 (20.00-3.50) 98.4 (20.00-3.50)	Depositor EDS
R_{merge}	0.30	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.30 (at 3.48Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.265 , 0.326 0.259 , 0.318	Depositor DCC
R_{free} test set	34086 reflections (4.58%)	wwPDB-VP
Wilson B-factor (Å ²)	81.4	Xtriage
Anisotropy	0.101	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.18 , 62.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.33$, $\langle L^2 \rangle = 0.16$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.87	EDS
Total number of atoms	290487	wwPDB-VP
Average B, all atoms (Å ²)	88.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.69% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

4 Model quality [i](#)

4.1 Standard geometry [i](#)

MolProbity failed to run properly - this section is therefore empty.

4.2 Too-close contacts [i](#)

MolProbity failed to run properly - this section is therefore empty.

4.3 Torsion angles [i](#)

4.3.1 Protein backbone [i](#)

MolProbity failed to run properly - this section is therefore empty.

4.3.2 Protein sidechains [i](#)

MolProbity failed to run properly - this section is therefore empty.

4.3.3 RNA [i](#)

MolProbity failed to run properly - this section is therefore empty.

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

2 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
23	5MU	AW	55	23	19,22,23	0.26	0	27,32,35	0.35	0
23	5MU	CW	55	23	19,22,23	0.29	0	27,32,35	0.52	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral

centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	5MU	AW	55	23	-	0/7/25/26	0/2/2/2
23	5MU	CW	55	23	-	0/7/25/26	0/2/2/2

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.

4.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

4.6 Ligand geometry [i](#)

Of 1486 ligands modelled in this entry, 1486 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.

4.7 Other polymers [i](#)

There are no such residues in this entry.

4.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
13	CM	5
13	AM	5
9	CI	2
9	AI	2
32	B6	1
32	D6	1
41	DG	1
52	DV	1
52	BV	1
41	BG	1

The worst 5 of 20 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B6	46:HIS	C	47:THR	N	6.15
1	D6	46:HIS	C	47:THR	N	6.12
1	CI	53:VAL	C	54:ASP	N	5.30
1	AI	53:VAL	C	54:ASP	N	5.29
1	DG	112:PRO	C	113:ARG	N	4.36

5 Fit of model and data ⓘ

5.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	AA	1504/1522 (98%)	0.41	54 (3%) 46 31	15, 82, 177, 200	0
1	CA	1504/1522 (98%)	0.54	103 (6%) 25 19	20, 90, 190, 200	0
2	AB	235/256 (91%)	0.15	9 (3%) 44 30	19, 113, 188, 200	0
2	CB	235/256 (91%)	0.23	12 (5%) 34 25	26, 127, 188, 200	0
3	AC	207/239 (86%)	0.06	5 (2%) 59 41	11, 98, 175, 200	0
3	CC	207/239 (86%)	0.15	3 (1%) 73 53	38, 121, 183, 200	0
4	AD	208/209 (99%)	0.10	8 (3%) 44 30	13, 75, 145, 200	0
4	CD	208/209 (99%)	0.15	10 (4%) 36 26	25, 89, 155, 200	0
5	AE	151/162 (93%)	-0.02	4 (2%) 57 39	21, 73, 158, 190	0
5	CE	151/162 (93%)	0.06	7 (4%) 38 27	26, 89, 157, 200	0
6	AF	101/101 (100%)	-0.06	1 (0%) 79 61	19, 100, 151, 189	0
6	CF	101/101 (100%)	0.07	2 (1%) 64 45	16, 83, 141, 170	0
7	AG	155/156 (99%)	0.21	7 (4%) 39 27	34, 104, 175, 194	0
7	CG	155/156 (99%)	0.37	14 (9%) 17 13	53, 123, 185, 200	0
8	AH	138/138 (100%)	-0.07	4 (2%) 54 36	33, 81, 145, 190	0
8	CH	138/138 (100%)	-0.02	2 (1%) 73 53	30, 91, 147, 165	0
9	AI	127/128 (99%)	0.40	11 (8%) 17 13	27, 123, 180, 200	0
9	CI	127/128 (99%)	0.63	9 (7%) 23 18	43, 140, 195, 200	0
10	AJ	99/105 (94%)	0.34	4 (4%) 43 29	47, 120, 180, 200	0
10	CJ	99/105 (94%)	0.61	10 (10%) 14 11	65, 140, 189, 200	0
11	AK	119/129 (92%)	-0.04	4 (3%) 48 32	13, 78, 163, 187	0
11	CK	119/129 (92%)	0.03	4 (3%) 48 32	30, 86, 164, 200	0
12	AL	125/135 (92%)	0.04	5 (4%) 43 29	19, 71, 146, 200	0
12	CL	125/135 (92%)	0.01	5 (4%) 43 29	12, 75, 143, 200	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	AM	125/126 (99%)	0.24	9 (7%) 23 18	56, 124, 183, 200	0
13	CM	125/126 (99%)	0.42	11 (8%) 17 13	41, 140, 199, 200	0
14	AN	60/61 (98%)	0.30	4 (6%) 25 19	38, 94, 181, 200	0
14	CN	60/61 (98%)	0.42	2 (3%) 49 33	57, 117, 171, 189	0
15	AO	88/89 (98%)	-0.13	0 100 100	11, 84, 147, 172	0
15	CO	88/89 (98%)	-0.01	5 (5%) 30 23	18, 88, 146, 167	0
16	AP	84/88 (95%)	-0.04	2 (2%) 59 41	17, 64, 135, 200	0
16	CP	84/88 (95%)	0.05	2 (2%) 59 41	32, 90, 139, 199	0
17	AQ	100/105 (95%)	0.17	3 (3%) 52 35	15, 81, 143, 200	0
17	CQ	100/105 (95%)	0.01	2 (2%) 64 45	20, 84, 134, 200	0
18	AR	70/88 (79%)	-0.14	1 (1%) 73 53	33, 87, 156, 200	0
18	CR	70/88 (79%)	-0.03	3 (4%) 40 27	17, 79, 137, 170	0
19	AS	79/93 (84%)	0.20	2 (2%) 58 40	60, 134, 200, 200	0
19	CS	79/93 (84%)	0.34	4 (5%) 34 25	76, 140, 200, 200	0
20	AT	99/106 (93%)	0.08	4 (4%) 43 29	21, 91, 178, 200	0
20	CT	99/106 (93%)	0.03	1 (1%) 79 61	45, 102, 167, 197	0
21	AU	25/27 (92%)	0.31	0 100 100	59, 114, 161, 200	0
21	CU	25/27 (92%)	0.42	2 (8%) 20 15	58, 131, 182, 200	0
22	AV	17/76 (22%)	0.35	1 (5%) 29 22	55, 68, 122, 125	0
22	CV	17/76 (22%)	0.18	0 100 100	56, 73, 128, 131	0
23	AW	76/77 (98%)	1.04	12 (15%) 6 6	63, 179, 200, 200	0
23	CW	76/77 (98%)	1.31	17 (22%) 3 2	62, 191, 200, 200	0
24	AX	11/31 (35%)	-0.15	0 100 100	23, 72, 120, 172	0
24	CX	11/31 (35%)	-0.21	0 100 100	41, 63, 93, 196	0
25	AY	185/185 (100%)	-0.31	2 (1%) 77 59	27, 99, 167, 200	0
25	CY	185/185 (100%)	0.02	7 (3%) 44 30	9, 93, 166, 198	0
26	B0	85/85 (100%)	0.41	6 (7%) 23 18	21, 80, 184, 199	0
26	D0	85/85 (100%)	0.66	7 (8%) 19 15	39, 95, 174, 200	0
27	B1	89/98 (90%)	-0.03	4 (4%) 39 27	5, 64, 138, 193	0
27	D1	89/98 (90%)	-0.09	3 (3%) 48 32	5, 62, 133, 200	0
28	B2	51/72 (70%)	0.09	2 (3%) 44 30	44, 103, 157, 200	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
28	D2	51/72 (70%)	0.26	3 (5%) 29 22	24, 93, 168, 200	0
29	B3	60/60 (100%)	-0.20	1 (1%) 69 49	15, 81, 158, 200	0
29	D3	60/60 (100%)	0.14	2 (3%) 49 33	21, 85, 167, 200	0
30	B4	50/71 (70%)	-0.08	0 100 100	71, 144, 192, 200	0
30	D4	50/71 (70%)	0.21	3 (6%) 29 22	86, 167, 192, 200	0
31	B5	59/60 (98%)	0.39	8 (13%) 8 7	22, 84, 184, 200	0
31	D5	59/60 (98%)	0.01	1 (1%) 69 49	6, 74, 191, 200	0
32	B6	45/54 (83%)	0.78	5 (11%) 12 9	53, 122, 184, 200	0
32	D6	45/54 (83%)	0.56	5 (11%) 12 9	54, 147, 188, 200	0
33	B7	49/49 (100%)	0.11	2 (4%) 42 28	5, 47, 114, 200	0
33	D7	49/49 (100%)	-0.24	0 100 100	3, 44, 105, 176	0
34	B8	64/65 (98%)	0.11	3 (4%) 37 26	7, 53, 145, 200	0
34	D8	64/65 (98%)	0.38	6 (9%) 15 12	27, 73, 140, 185	0
35	BA	2767/2782 (99%)	0.33	109 (3%) 44 30	9, 65, 172, 200	0
35	DA	2767/2782 (99%)	0.35	122 (4%) 39 27	6, 62, 169, 200	0
36	BB	119/122 (97%)	0.59	6 (5%) 35 25	60, 102, 160, 189	0
36	DB	119/122 (97%)	0.87	16 (13%) 8 7	69, 140, 188, 200	0
37	BC	191/229 (83%)	0.49	14 (7%) 22 18	76, 175, 200, 200	0
37	DC	191/229 (83%)	0.62	18 (9%) 15 12	120, 180, 200, 200	0
38	BD	272/276 (98%)	-0.21	5 (1%) 67 48	8, 56, 122, 200	0
38	DD	272/276 (98%)	-0.12	8 (2%) 54 36	1, 47, 114, 200	0
39	BE	205/206 (99%)	0.20	8 (3%) 44 30	10, 75, 160, 200	0
39	DE	205/206 (99%)	0.13	4 (1%) 64 45	7, 64, 153, 199	0
40	BF	208/210 (99%)	0.16	13 (6%) 27 20	1, 69, 164, 200	0
40	DF	208/210 (99%)	0.09	6 (2%) 54 36	6, 75, 170, 200	0
41	BG	181/182 (99%)	0.02	7 (3%) 44 30	36, 107, 171, 200	0
41	DG	181/182 (99%)	0.29	16 (8%) 17 13	45, 135, 191, 200	0
42	BH	160/180 (88%)	0.32	9 (5%) 31 23	47, 145, 200, 200	0
42	DH	160/180 (88%)	0.23	9 (5%) 31 23	36, 110, 180, 200	0
43	BI	146/148 (98%)	0.32	10 (6%) 25 19	25, 112, 184, 200	0
43	DI	146/148 (98%)	1.19	29 (19%) 3 3	17, 134, 200, 200	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å ²)	Q<0.9
44	BN	139/140 (99%)	0.27	5 (3%)	46	31	37, 98, 160, 200	0
44	DN	139/140 (99%)	0.15	7 (5%)	35	25	19, 76, 152, 195	0
45	BO	122/122 (100%)	-0.05	2 (1%)	70	51	15, 63, 116, 133	0
45	DO	122/122 (100%)	-0.35	0	100	100	10, 49, 100, 128	0
46	BP	146/150 (97%)	0.16	5 (3%)	48	32	6, 84, 167, 200	0
46	DP	146/150 (97%)	0.21	7 (4%)	36	26	18, 93, 168, 199	0
47	BQ	136/141 (96%)	0.20	9 (6%)	26	19	26, 90, 187, 200	0
47	DQ	136/141 (96%)	-0.01	5 (3%)	45	30	16, 73, 158, 200	0
48	BR	117/118 (99%)	-0.01	4 (3%)	48	32	8, 66, 138, 198	0
48	DR	117/118 (99%)	0.12	3 (2%)	57	39	8, 64, 136, 180	0
49	BS	99/112 (88%)	0.25	5 (5%)	34	25	32, 105, 186, 200	0
49	DS	99/112 (88%)	0.52	7 (7%)	23	18	62, 133, 182, 200	0
50	BT	138/146 (94%)	0.19	5 (3%)	46	31	21, 96, 190, 200	0
50	DT	138/146 (94%)	0.12	7 (5%)	34	25	17, 84, 173, 200	0
51	BU	117/118 (99%)	0.18	5 (4%)	40	27	15, 79, 161, 182	0
51	DU	117/118 (99%)	0.09	3 (2%)	57	39	12, 65, 141, 194	0
52	BV	101/101 (100%)	0.45	11 (10%)	12	10	26, 106, 188, 200	0
52	DV	101/101 (100%)	0.48	9 (8%)	17	13	29, 100, 178, 200	0
53	BW	113/113 (100%)	-0.12	2 (1%)	67	48	8, 55, 134, 200	0
53	DW	113/113 (100%)	-0.15	2 (1%)	67	48	16, 66, 148, 200	0
54	BX	93/96 (96%)	0.14	5 (5%)	32	23	12, 83, 163, 200	0
54	DX	93/96 (96%)	0.11	5 (5%)	32	23	18, 79, 147, 185	0
55	BY	101/110 (91%)	0.38	12 (11%)	10	9	16, 94, 187, 200	0
55	DY	101/110 (91%)	0.70	12 (11%)	10	9	21, 108, 187, 200	0
56	BZ	177/206 (85%)	-0.01	1 (0%)	85	72	46, 113, 178, 200	0
56	DZ	177/206 (85%)	0.11	8 (4%)	39	27	11, 114, 180, 200	0
All	All	21176/22108 (95%)	0.26	1009 (4%)	36	26	1, 84, 184, 200	0

The worst 5 of 1009 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
43	DI	92	VAL	14.3
26	D0	6	ALA	13.3

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Mol	Chain	Res	Type	RSRZ
35	DA	897	C	12.3
43	DI	90	GLY	11.4
43	DI	119	PRO	8.7

5.2 Non-standard residues in protein, DNA, RNA chains [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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
23	5MU	CW	55	21/22	0.13	0.20	177,200,200,200	0
23	5MU	AW	55	21/22	0.67	0.11	130,173,200,200	0

5.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.4 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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
57	MG	AA	1617	1/1	-0.60	0.06	6,6,6,6	1
57	MG	AW	118	1/1	-0.05	0.13	69,69,69,69	1
57	MG	DA	3212	1/1	0.12	0.22	86,86,86,86	1
57	MG	AA	1789	1/1	0.18	0.43	111,111,111,111	0
57	MG	BA	3206	1/1	0.20	0.54	1,1,1,1	1
57	MG	DH	201	1/1	0.24	0.22	12,12,12,12	1
57	MG	CA	1681	1/1	0.30	0.60	96,96,96,96	1
57	MG	DA	3214	1/1	0.34	0.54	64,64,64,64	1
57	MG	BA	3153	1/1	0.34	0.13	35,35,35,35	1
57	MG	DB	202	1/1	0.38	0.14	33,33,33,33	1
57	MG	BB	204	1/1	0.43	0.22	76,76,76,76	1
57	MG	CW	116	1/1	0.43	0.53	107,107,107,107	0
57	MG	CV	101	1/1	0.46	0.08	41,41,41,41	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	BA	3423	1/1	0.47	0.55	54,54,54,54	1
57	MG	DA	3273	1/1	0.48	0.51	97,97,97,97	1
57	MG	CW	110	1/1	0.48	0.62	66,66,66,66	1
57	MG	CA	1651	1/1	0.48	0.40	50,50,50,50	1
57	MG	CW	101	1/1	0.49	0.20	83,83,83,83	1
57	MG	CA	1796	1/1	0.50	0.76	95,95,95,95	1
57	MG	BB	220	1/1	0.50	0.23	71,71,71,71	1
57	MG	AA	1716	1/1	0.52	0.20	60,60,60,60	0
57	MG	CW	111	1/1	0.52	0.08	136,136,136,136	1
57	MG	CA	1737	1/1	0.54	0.12	1,1,1,1	1
57	MG	AA	1650	1/1	0.54	0.29	20,20,20,20	1
57	MG	CA	1767	1/1	0.55	0.20	94,94,94,94	0
57	MG	AW	120	1/1	0.55	0.18	58,58,58,58	1
57	MG	BA	3002	1/1	0.55	0.33	16,16,16,16	1
57	MG	DA	3382	1/1	0.56	0.20	71,71,71,71	0
57	MG	DA	3150	1/1	0.56	0.24	39,39,39,39	1
57	MG	CA	1759	1/1	0.56	0.13	108,108,108,108	1
57	MG	CA	1686	1/1	0.57	0.32	49,49,49,49	0
57	MG	CA	1736	1/1	0.57	0.66	71,71,71,71	0
57	MG	AA	1702	1/1	0.57	0.13	57,57,57,57	0
57	MG	BA	3348	1/1	0.58	0.23	84,84,84,84	0
57	MG	CA	1748	1/1	0.59	0.25	97,97,97,97	1
57	MG	CA	1785	1/1	0.59	0.82	112,112,112,112	0
57	MG	BA	3227	1/1	0.59	0.64	71,71,71,71	1
57	MG	AW	102	1/1	0.60	0.10	82,82,82,82	1
57	MG	AA	1653	1/1	0.61	0.41	93,93,93,93	1
57	MG	DA	3224	1/1	0.61	0.11	65,65,65,65	1
57	MG	AA	1788	1/1	0.62	0.13	40,40,40,40	0
57	MG	DX	103	1/1	0.62	0.07	48,48,48,48	1
57	MG	CA	1709	1/1	0.63	0.33	46,46,46,46	0
57	MG	AV	103	1/1	0.63	0.13	70,70,70,70	0
57	MG	DA	3371	1/1	0.63	0.22	35,35,35,35	1
57	MG	DA	3202	1/1	0.63	0.34	7,7,7,7	1
57	MG	BA	3231	1/1	0.63	0.21	102,102,102,102	0
57	MG	BA	3130	1/1	0.63	0.56	1,1,1,1	1
57	MG	DA	3220	1/1	0.63	0.11	86,86,86,86	0
57	MG	BA	3392	1/1	0.64	0.27	70,70,70,70	0
57	MG	DA	3361	1/1	0.64	0.28	88,88,88,88	0
57	MG	DA	3400	1/1	0.64	0.37	61,61,61,61	1
57	MG	BA	3417	1/1	0.65	0.08	17,17,17,17	1
57	MG	CA	1746	1/1	0.65	0.17	74,74,74,74	0
57	MG	DA	3101	1/1	0.66	0.20	17,17,17,17	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	BA	3281	1/1	0.66	0.29	43,43,43,43	1
57	MG	DU	202	1/1	0.66	0.37	1,1,1,1	1
57	MG	CA	1675	1/1	0.66	0.25	47,47,47,47	1
57	MG	BA	3412	1/1	0.67	0.33	34,34,34,34	1
57	MG	DA	3295	1/1	0.67	0.64	79,79,79,79	0
57	MG	BA	3394	1/1	0.67	0.44	7,7,7,7	1
57	MG	CA	1783	1/1	0.67	0.17	33,33,33,33	1
57	MG	CW	113	1/1	0.67	0.11	68,68,68,68	1
57	MG	DA	3206	1/1	0.68	0.44	32,32,32,32	1
57	MG	DA	3422	1/1	0.68	0.25	62,62,62,62	0
57	MG	DA	3320	1/1	0.68	0.24	75,75,75,75	0
57	MG	BA	3327	1/1	0.68	0.20	46,46,46,46	1
57	MG	DA	3250	1/1	0.68	0.18	1,1,1,1	0
57	MG	BA	3418	1/1	0.68	0.20	41,41,41,41	1
57	MG	AA	1688	1/1	0.69	0.24	12,12,12,12	1
57	MG	DA	3329	1/1	0.69	0.21	62,62,62,62	1
57	MG	DA	3358	1/1	0.69	0.68	11,11,11,11	1
57	MG	DA	3100	1/1	0.70	0.35	63,63,63,63	1
57	MG	BA	3264	1/1	0.70	0.19	66,66,66,66	0
57	MG	CA	1640	1/1	0.70	1.25	65,65,65,65	1
57	MG	DA	3326	1/1	0.71	0.13	96,96,96,96	1
57	MG	CA	1718	1/1	0.71	0.22	59,59,59,59	0
57	MG	DA	3158	1/1	0.71	0.12	23,23,23,23	0
57	MG	CE	202	1/1	0.71	0.12	85,85,85,85	1
57	MG	CA	1704	1/1	0.72	0.07	62,62,62,62	0
57	MG	AA	1680	1/1	0.72	0.15	53,53,53,53	0
57	MG	DA	3439	1/1	0.72	0.25	85,85,85,85	1
57	MG	DA	3441	1/1	0.72	0.12	44,44,44,44	1
57	MG	BA	3014	1/1	0.72	0.40	51,51,51,51	0
57	MG	DA	3219	1/1	0.72	0.41	21,21,21,21	1
57	MG	CA	1797	1/1	0.72	0.19	82,82,82,82	1
57	MG	DA	3323	1/1	0.72	0.16	63,63,63,63	1
57	MG	AW	112	1/1	0.73	2.04	64,64,64,64	1
57	MG	DA	3141	1/1	0.73	0.45	1,1,1,1	1
57	MG	DB	218	1/1	0.73	0.16	30,30,30,30	1
57	MG	CA	1727	1/1	0.73	0.32	92,92,92,92	0
57	MG	BA	3397	1/1	0.73	0.23	44,44,44,44	0
57	MG	BA	3154	1/1	0.73	0.06	56,56,56,56	0
57	MG	DA	3152	1/1	0.74	0.14	62,62,62,62	1
57	MG	BA	3279	1/1	0.74	0.17	35,35,35,35	1
57	MG	CW	103	1/1	0.74	0.28	61,61,61,61	1
57	MG	CA	1607	1/1	0.74	0.23	54,54,54,54	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	BA	3120	1/1	0.74	0.20	38,38,38,38	0
57	MG	BA	3213	1/1	0.74	0.33	49,49,49,49	1
57	MG	CA	1788	1/1	0.74	0.07	1,1,1,1	1
57	MG	DA	3049	1/1	0.74	0.60	43,43,43,43	0
57	MG	DA	3420	1/1	0.74	0.08	14,14,14,14	1
57	MG	DA	3090	1/1	0.74	0.41	97,97,97,97	0
57	MG	DA	3241	1/1	0.74	0.18	50,50,50,50	0
57	MG	AE	202	1/1	0.74	0.13	37,37,37,37	0
57	MG	CA	1680	1/1	0.74	0.09	75,75,75,75	1
57	MG	BA	3018	1/1	0.74	0.21	35,35,35,35	0
57	MG	DA	3299	1/1	0.74	0.26	13,13,13,13	1
57	MG	BA	3035	1/1	0.74	0.47	67,67,67,67	1
57	MG	DA	3322	1/1	0.74	0.11	34,34,34,34	1
57	MG	AA	1797	1/1	0.75	0.85	9,9,9,9	1
57	MG	DA	3262	1/1	0.75	0.27	79,79,79,79	1
57	MG	CA	1684	1/1	0.75	0.16	59,59,59,59	0
57	MG	AA	1800	1/1	0.75	0.17	38,38,38,38	0
57	MG	DA	3176	1/1	0.75	0.22	77,77,77,77	0
57	MG	DA	3319	1/1	0.75	0.20	116,116,116,116	1
57	MG	AA	1743	1/1	0.75	0.49	74,74,74,74	1
57	MG	CA	1793	1/1	0.75	0.09	74,74,74,74	0
57	MG	DA	3402	1/1	0.75	0.16	45,45,45,45	1
57	MG	BA	3210	1/1	0.76	0.10	10,10,10,10	1
57	MG	CA	1733	1/1	0.76	0.18	59,59,59,59	0
57	MG	AA	1748	1/1	0.76	0.07	73,73,73,73	0
57	MG	CA	1602	1/1	0.76	0.17	72,72,72,72	0
57	MG	AA	1769	1/1	0.76	0.11	48,48,48,48	0
57	MG	BA	3334	1/1	0.76	0.09	51,51,51,51	1
57	MG	CE	201	1/1	0.76	0.27	78,78,78,78	0
57	MG	DA	3068	1/1	0.76	0.15	24,24,24,24	0
57	MG	AA	1780	1/1	0.76	0.17	95,95,95,95	1
57	MG	AA	1799	1/1	0.76	0.20	58,58,58,58	1
57	MG	DA	3270	1/1	0.77	0.21	47,47,47,47	1
57	MG	DA	3026	1/1	0.77	0.36	1,1,1,1	0
57	MG	AA	1728	1/1	0.77	0.17	34,34,34,34	0
57	MG	AA	1651	1/1	0.77	0.16	32,32,32,32	0
57	MG	BA	3292	1/1	0.77	0.31	27,27,27,27	1
57	MG	DB	216	1/1	0.77	0.24	54,54,54,54	0
57	MG	BA	3294	1/1	0.77	0.19	55,55,55,55	0
57	MG	BA	3164	1/1	0.77	0.29	56,56,56,56	0
57	MG	CV	102	1/1	0.77	0.10	57,57,57,57	0
57	MG	DA	3409	1/1	0.77	0.47	83,83,83,83	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	BA	3373	1/1	0.78	0.09	1,1,1,1	1
57	MG	BA	3379	1/1	0.78	0.48	50,50,50,50	1
57	MG	BB	209	1/1	0.78	0.11	108,108,108,108	0
57	MG	DA	3406	1/1	0.78	0.39	57,57,57,57	0
57	MG	BB	210	1/1	0.78	0.18	68,68,68,68	1
57	MG	AA	1720	1/1	0.78	0.48	91,91,91,91	0
57	MG	BA	3324	1/1	0.78	0.16	56,56,56,56	0
57	MG	CW	119	1/1	0.78	0.19	57,57,57,57	1
57	MG	BA	3103	1/1	0.78	0.47	33,33,33,33	1
57	MG	DA	3048	1/1	0.78	0.59	56,56,56,56	1
57	MG	CA	1616	1/1	0.78	0.14	64,64,64,64	0
57	MG	BA	3402	1/1	0.78	0.06	13,13,13,13	1
57	MG	AA	1691	1/1	0.78	0.42	69,69,69,69	0
57	MG	BA	3251	1/1	0.78	0.13	64,64,64,64	0
57	MG	BA	3369	1/1	0.78	0.13	50,50,50,50	0
57	MG	CA	1668	1/1	0.79	0.17	43,43,43,43	0
57	MG	BA	3122	1/1	0.79	0.35	1,1,1,1	1
57	MG	BA	3006	1/1	0.79	0.30	77,77,77,77	0
57	MG	BB	213	1/1	0.79	0.17	33,33,33,33	1
57	MG	BA	3346	1/1	0.79	0.15	43,43,43,43	0
57	MG	AA	1710	1/1	0.79	0.14	113,113,113,113	1
57	MG	DA	3127	1/1	0.79	0.24	57,57,57,57	0
57	MG	AA	1683	1/1	0.79	0.12	1,1,1,1	1
57	MG	CW	102	1/1	0.79	0.09	38,38,38,38	1
57	MG	CA	1774	1/1	0.79	0.13	74,74,74,74	0
57	MG	DA	3157	1/1	0.79	0.22	37,37,37,37	0
57	MG	CA	1778	1/1	0.79	0.10	1,1,1,1	1
57	MG	DB	208	1/1	0.79	0.11	53,53,53,53	1
57	MG	BA	3320	1/1	0.79	0.06	37,37,37,37	1
57	MG	CA	1713	1/1	0.79	0.10	40,40,40,40	1
57	MG	BA	3322	1/1	0.79	0.14	21,21,21,21	1
57	MG	CA	1792	1/1	0.79	0.14	16,16,16,16	1
57	MG	BA	3276	1/1	0.79	0.16	34,34,34,34	1
57	MG	DA	3252	1/1	0.80	0.23	89,89,89,89	0
57	MG	DA	3258	1/1	0.80	0.12	23,23,23,23	1
57	MG	BA	3341	1/1	0.80	0.30	4,4,4,4	1
57	MG	BB	219	1/1	0.80	0.11	73,73,73,73	1
57	MG	CA	1670	1/1	0.80	0.15	23,23,23,23	0
57	MG	DA	3415	1/1	0.80	0.28	3,3,3,3	1
57	MG	D1	104	1/1	0.80	0.16	74,74,74,74	1
57	MG	DA	3006	1/1	0.80	0.14	93,93,93,93	0
57	MG	BA	3401	1/1	0.80	0.11	42,42,42,42	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	CA	1731	1/1	0.80	0.24	54,54,54,54	0
57	MG	CV	103	1/1	0.80	0.06	44,44,44,44	0
57	MG	BA	3425	1/1	0.80	0.13	23,23,23,23	0
57	MG	AA	1794	1/1	0.80	0.26	40,40,40,40	0
57	MG	AA	1715	1/1	0.80	0.20	29,29,29,29	1
57	MG	CW	106	1/1	0.80	0.06	47,47,47,47	1
57	MG	DS	201	1/1	0.80	0.12	1,1,1,1	1
57	MG	AA	1615	1/1	0.80	0.24	47,47,47,47	0
57	MG	CA	1643	1/1	0.80	0.10	73,73,73,73	1
57	MG	BA	3434	1/1	0.81	0.21	60,60,60,60	0
57	MG	CA	1617	1/1	0.81	0.27	29,29,29,29	0
57	MG	DA	3296	1/1	0.81	0.90	33,33,33,33	1
57	MG	BA	3435	1/1	0.81	0.14	85,85,85,85	0
57	MG	BA	3439	1/1	0.81	0.10	25,25,25,25	0
57	MG	CA	1649	1/1	0.81	0.31	14,14,14,14	1
57	MG	AA	1686	1/1	0.81	0.14	61,61,61,61	0
57	MG	DA	3221	1/1	0.81	0.37	79,79,79,79	1
57	MG	AA	1749	1/1	0.81	0.33	1,1,1,1	1
57	MG	DB	205	1/1	0.81	0.16	5,5,5,5	1
57	MG	AA	1676	1/1	0.81	0.23	32,32,32,32	0
57	MG	DA	3355	1/1	0.81	0.11	42,42,42,42	1
57	MG	AA	1638	1/1	0.81	0.25	39,39,39,39	0
57	MG	DB	219	1/1	0.81	0.23	56,56,56,56	1
57	MG	AD	301	1/1	0.81	0.14	15,15,15,15	1
57	MG	BA	3421	1/1	0.81	0.28	39,39,39,39	1
57	MG	AA	1682	1/1	0.81	0.24	46,46,46,46	0
57	MG	AA	1666	1/1	0.81	0.29	47,47,47,47	0
57	MG	AV	102	1/1	0.82	0.38	73,73,73,73	0
57	MG	AW	121	1/1	0.82	0.04	63,63,63,63	0
57	MG	DA	3245	1/1	0.82	0.38	67,67,67,67	0
57	MG	DA	3424	1/1	0.82	0.09	31,31,31,31	1
57	MG	DA	3434	1/1	0.82	0.50	98,98,98,98	0
57	MG	AA	1706	1/1	0.82	0.32	58,58,58,58	1
57	MG	CA	1677	1/1	0.82	0.14	36,36,36,36	0
57	MG	BA	3127	1/1	0.82	0.32	3,3,3,3	1
57	MG	BA	3350	1/1	0.82	0.12	70,70,70,70	0
57	MG	AA	1724	1/1	0.82	0.12	34,34,34,34	1
57	MG	DA	3366	1/1	0.82	0.16	46,46,46,46	1
57	MG	AA	1645	1/1	0.82	0.17	14,14,14,14	1
57	MG	DA	3292	1/1	0.82	0.10	45,45,45,45	0
57	MG	AW	113	1/1	0.82	0.04	60,60,60,60	0
57	MG	AA	1798	1/1	0.82	0.23	52,52,52,52	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	CA	1808	1/1	0.82	0.27	43,43,43,43	1
57	MG	CA	1762	1/1	0.82	0.10	7,7,7,7	1
57	MG	BA	3169	1/1	0.83	0.32	33,33,33,33	0
57	MG	BA	3189	1/1	0.83	0.21	87,87,87,87	0
57	MG	DA	3165	1/1	0.83	0.13	47,47,47,47	0
57	MG	BA	3349	1/1	0.83	0.08	86,86,86,86	0
57	MG	AA	1736	1/1	0.83	0.10	20,20,20,20	0
57	MG	CA	1742	1/1	0.83	0.29	1,1,1,1	1
57	MG	AA	1741	1/1	0.83	0.14	48,48,48,48	0
57	MG	BA	3059	1/1	0.83	0.09	9,9,9,9	0
57	MG	CA	1756	1/1	0.83	0.04	56,56,56,56	0
57	MG	BA	3060	1/1	0.83	0.20	42,42,42,42	0
57	MG	DA	3063	1/1	0.83	0.35	1,1,1,1	0
57	MG	CA	1692	1/1	0.83	0.40	74,74,74,74	1
57	MG	BA	3094	1/1	0.83	0.11	25,25,25,25	1
57	MG	AW	101	1/1	0.83	0.09	51,51,51,51	1
57	MG	BA	3112	1/1	0.83	0.17	34,34,34,34	1
57	MG	CA	1782	1/1	0.83	0.10	28,28,28,28	0
57	MG	DN	202	1/1	0.83	0.10	31,31,31,31	1
57	MG	CW	104	1/1	0.83	0.05	35,35,35,35	1
57	MG	BA	3166	1/1	0.83	0.11	66,66,66,66	0
57	MG	BA	3345	1/1	0.83	0.44	1,1,1,1	1
57	MG	BA	3287	1/1	0.84	0.28	45,45,45,45	1
57	MG	CA	1697	1/1	0.84	0.22	59,59,59,59	1
57	MG	DA	3159	1/1	0.84	0.17	21,21,21,21	0
57	MG	CA	1798	1/1	0.84	0.23	43,43,43,43	1
57	MG	DA	3418	1/1	0.84	0.04	24,24,24,24	1
57	MG	AW	116	1/1	0.84	0.11	61,61,61,61	0
57	MG	AA	1609	1/1	0.84	0.10	7,7,7,7	1
57	MG	BA	3310	1/1	0.84	0.14	5,5,5,5	1
57	MG	DA	3426	1/1	0.84	0.25	44,44,44,44	0
57	MG	CG	201	1/1	0.84	0.20	10,10,10,10	1
57	MG	AW	110	1/1	0.84	0.48	30,30,30,30	1
57	MG	DA	3062	1/1	0.84	0.25	21,21,21,21	0
57	MG	BA	3415	1/1	0.84	0.11	18,18,18,18	1
57	MG	CA	1781	1/1	0.84	0.23	1,1,1,1	1
57	MG	DA	3345	1/1	0.84	0.16	2,2,2,2	1
57	MG	BA	3139	1/1	0.84	0.34	8,8,8,8	1
57	MG	BA	3366	1/1	0.84	0.52	38,38,38,38	1
57	MG	BA	3323	1/1	0.84	0.17	74,74,74,74	0
57	MG	AA	1777	1/1	0.84	0.04	6,6,6,6	0
57	MG	DA	3370	1/1	0.84	0.18	100,100,100,100	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	AA	1755	1/1	0.84	0.04	47,47,47,47	0
57	MG	BA	3162	1/1	0.84	0.17	54,54,54,54	1
57	MG	CA	1794	1/1	0.84	0.26	68,68,68,68	0
57	MG	DA	3215	1/1	0.85	0.28	17,17,17,17	1
57	MG	AA	1737	1/1	0.85	0.10	30,30,30,30	1
57	MG	CA	1663	1/1	0.85	0.22	15,15,15,15	1
57	MG	AA	1791	1/1	0.85	0.38	35,35,35,35	1
57	MG	BA	3207	1/1	0.85	0.11	1,1,1,1	1
57	MG	DA	3324	1/1	0.85	0.10	40,40,40,40	0
57	MG	DA	3325	1/1	0.85	0.06	72,72,72,72	0
57	MG	CA	1673	1/1	0.85	0.17	57,57,57,57	0
57	MG	CA	1674	1/1	0.85	0.18	44,44,44,44	1
57	MG	DA	3336	1/1	0.85	0.16	60,60,60,60	0
57	MG	BA	3429	1/1	0.85	0.30	32,32,32,32	0
57	MG	DA	3346	1/1	0.85	0.08	115,115,115,115	0
57	MG	BA	3102	1/1	0.85	0.07	21,21,21,21	1
57	MG	CA	1612	1/1	0.85	0.26	75,75,75,75	0
57	MG	BA	3306	1/1	0.85	0.22	50,50,50,50	0
57	MG	DB	217	1/1	0.85	0.18	53,53,53,53	1
57	MG	DA	3190	1/1	0.85	0.24	32,32,32,32	0
57	MG	DA	3367	1/1	0.85	0.20	95,95,95,95	1
57	MG	BA	3337	1/1	0.85	0.14	1,1,1,1	1
57	MG	DA	3285	1/1	0.85	0.17	13,13,13,13	1
57	MG	AW	111	1/1	0.85	0.06	76,76,76,76	1
57	MG	BA	3216	1/1	0.85	0.07	49,49,49,49	0
57	MG	BA	3389	1/1	0.85	0.36	31,31,31,31	0
57	MG	DA	3393	1/1	0.86	0.34	1,1,1,1	1
57	MG	CW	115	1/1	0.86	0.27	93,93,93,93	1
57	MG	DA	3401	1/1	0.86	0.13	49,49,49,49	1
57	MG	CA	1650	1/1	0.86	0.36	98,98,98,98	1
57	MG	BA	3238	1/1	0.86	0.14	38,38,38,38	1
57	MG	DA	3187	1/1	0.86	0.08	83,83,83,83	1
57	MG	CA	1806	1/1	0.86	0.12	35,35,35,35	0
57	MG	CA	1653	1/1	0.86	0.09	41,41,41,41	0
57	MG	BA	3249	1/1	0.86	0.23	58,58,58,58	0
57	MG	DA	3035	1/1	0.86	0.12	48,48,48,48	0
57	MG	BA	3107	1/1	0.86	0.23	23,23,23,23	0
57	MG	BA	3180	1/1	0.86	0.10	1,1,1,1	1
57	MG	DA	3428	1/1	0.86	0.22	17,17,17,17	0
57	MG	CN	101	1/1	0.86	0.16	65,65,65,65	0
57	MG	CA	1776	1/1	0.86	0.19	32,32,32,32	0
57	MG	DA	3440	1/1	0.86	0.16	80,80,80,80	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	DA	3332	1/1	0.86	0.10	41,41,41,41	1
57	MG	CA	1672	1/1	0.86	0.11	44,44,44,44	0
57	MG	CA	1726	1/1	0.86	0.23	36,36,36,36	0
57	MG	BA	3406	1/1	0.86	0.20	19,19,19,19	0
57	MG	DB	209	1/1	0.86	0.47	96,96,96,96	1
57	MG	DB	212	1/1	0.86	0.11	55,55,55,55	0
57	MG	DA	3354	1/1	0.86	0.21	6,6,6,6	1
57	MG	CA	1728	1/1	0.86	0.15	41,41,41,41	1
57	MG	BA	3372	1/1	0.86	0.11	20,20,20,20	1
57	MG	AA	1764	1/1	0.86	0.34	35,35,35,35	0
57	MG	DA	3144	1/1	0.86	0.16	1,1,1,1	0
57	MG	CA	1623	1/1	0.86	0.23	84,84,84,84	1
57	MG	AA	1731	1/1	0.86	0.14	79,79,79,79	1
57	MG	DU	201	1/1	0.86	0.59	77,77,77,77	1
57	MG	AA	1762	1/1	0.86	0.12	58,58,58,58	0
57	MG	BA	3286	1/1	0.86	0.14	32,32,32,32	1
57	MG	AA	1750	1/1	0.87	0.19	42,42,42,42	0
57	MG	DA	3227	1/1	0.87	0.08	73,73,73,73	0
57	MG	BA	3224	1/1	0.87	0.45	80,80,80,80	0
57	MG	BA	3367	1/1	0.87	0.17	37,37,37,37	0
57	MG	CA	1729	1/1	0.87	0.06	63,63,63,63	0
57	MG	DA	3065	1/1	0.87	0.48	1,1,1,1	1
57	MG	BA	3225	1/1	0.87	0.30	67,67,67,67	0
57	MG	AW	114	1/1	0.87	0.13	78,78,78,78	0
57	MG	CA	1664	1/1	0.87	0.10	54,54,54,54	1
57	MG	BA	3315	1/1	0.87	0.51	87,87,87,87	0
57	MG	BB	203	1/1	0.87	0.08	60,60,60,60	0
57	MG	CA	1743	1/1	0.87	0.07	64,64,64,64	0
57	MG	AA	1746	1/1	0.87	0.09	29,29,29,29	0
57	MG	BB	208	1/1	0.87	0.23	38,38,38,38	1
57	MG	DA	3298	1/1	0.87	0.14	22,22,22,22	0
57	MG	BA	3381	1/1	0.87	0.18	23,23,23,23	0
57	MG	BA	3032	1/1	0.87	0.18	1,1,1,1	0
57	MG	DA	3438	1/1	0.87	0.12	48,48,48,48	1
57	MG	BA	3248	1/1	0.87	0.25	10,10,10,10	0
57	MG	AW	108	1/1	0.87	0.18	24,24,24,24	1
57	MG	BA	3175	1/1	0.87	0.25	21,21,21,21	0
57	MG	BA	3331	1/1	0.87	0.14	11,11,11,11	1
57	MG	DB	204	1/1	0.87	0.28	89,89,89,89	1
57	MG	AA	1757	1/1	0.87	0.09	51,51,51,51	1
57	MG	DA	3189	1/1	0.87	0.38	59,59,59,59	0
57	MG	CA	1690	1/1	0.87	0.46	20,20,20,20	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	DA	3194	1/1	0.87	0.42	57,57,57,57	0
57	MG	AA	1667	1/1	0.87	0.28	17,17,17,17	0
57	MG	DA	3337	1/1	0.87	0.09	92,92,92,92	0
57	MG	BA	3137	1/1	0.87	0.26	7,7,7,7	0
57	MG	B5	102	1/1	0.87	0.13	48,48,48,48	0
57	MG	CA	1706	1/1	0.87	0.13	47,47,47,47	1
57	MG	DA	3004	1/1	0.87	0.36	64,64,64,64	0
57	MG	BA	3147	1/1	0.87	0.47	1,1,1,1	1
57	MG	AA	1719	1/1	0.87	0.27	1,1,1,1	1
57	MG	BA	3290	1/1	0.87	0.19	33,33,33,33	1
57	MG	DA	3223	1/1	0.87	0.26	12,12,12,12	1
57	MG	CA	1738	1/1	0.88	0.21	67,67,67,67	0
57	MG	CA	1658	1/1	0.88	0.24	24,24,24,24	1
57	MG	AA	1744	1/1	0.88	0.06	22,22,22,22	0
57	MG	BA	3297	1/1	0.88	0.11	12,12,12,12	0
57	MG	CW	107	1/1	0.88	0.04	84,84,84,84	0
57	MG	DA	3210	1/1	0.88	0.12	93,93,93,93	1
57	MG	BA	3303	1/1	0.88	0.89	8,8,8,8	1
57	MG	DA	3213	1/1	0.88	0.15	24,24,24,24	0
57	MG	B1	102	1/1	0.88	0.20	7,7,7,7	1
57	MG	DA	3379	1/1	0.88	0.12	47,47,47,47	0
57	MG	AA	1745	1/1	0.88	0.08	79,79,79,79	0
57	MG	CA	1760	1/1	0.88	0.08	40,40,40,40	0
57	MG	DA	3395	1/1	0.88	0.26	1,1,1,1	0
57	MG	AW	109	1/1	0.88	0.16	37,37,37,37	1
57	MG	CA	1765	1/1	0.88	0.48	85,85,85,85	0
57	MG	AA	1732	1/1	0.88	0.32	31,31,31,31	0
57	MG	BA	3239	1/1	0.88	0.33	14,14,14,14	1
57	MG	BA	3390	1/1	0.88	0.16	24,24,24,24	0
57	MG	BA	3121	1/1	0.88	0.20	30,30,30,30	0
57	MG	BA	3176	1/1	0.88	0.21	21,21,21,21	1
57	MG	DA	3419	1/1	0.88	0.16	58,58,58,58	0
57	MG	BE	301	1/1	0.88	0.21	1,1,1,1	1
57	MG	BF	302	1/1	0.88	0.17	15,15,15,15	1
57	MG	DA	3053	1/1	0.88	0.26	3,3,3,3	0
57	MG	BN	204	1/1	0.88	0.05	20,20,20,20	1
57	MG	BU	201	1/1	0.88	0.17	12,12,12,12	1
57	MG	AA	1656	1/1	0.88	0.12	31,31,31,31	0
57	MG	DA	3278	1/1	0.88	0.23	36,36,36,36	1
57	MG	CA	1702	1/1	0.88	0.23	47,47,47,47	0
57	MG	DA	3069	1/1	0.88	0.23	21,21,21,21	0
57	MG	BA	3263	1/1	0.88	0.12	29,29,29,29	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	AA	1774	1/1	0.88	0.05	23,23,23,23	0
57	MG	BA	3197	1/1	0.88	0.32	25,25,25,25	1
57	MG	DA	3124	1/1	0.88	0.22	24,24,24,24	0
57	MG	BA	3338	1/1	0.88	0.12	46,46,46,46	0
57	MG	BA	3340	1/1	0.88	0.14	22,22,22,22	1
57	MG	CA	1624	1/1	0.88	0.26	40,40,40,40	0
57	MG	CA	1639	1/1	0.88	0.23	34,34,34,34	0
57	MG	AA	1727	1/1	0.88	0.14	63,63,63,63	0
57	MG	AA	1655	1/1	0.88	0.12	31,31,31,31	0
57	MG	AA	1752	1/1	0.88	0.05	42,42,42,42	1
57	MG	AA	1754	1/1	0.88	0.13	49,49,49,49	1
57	MG	DA	3331	1/1	0.88	0.08	79,79,79,79	1
57	MG	DA	3161	1/1	0.88	0.67	112,112,112,112	0
57	MG	CA	1735	1/1	0.88	0.11	1,1,1,1	1
57	MG	AA	1687	1/1	0.88	0.16	61,61,61,61	0
57	MG	BA	3217	1/1	0.88	0.23	35,35,35,35	0
57	MG	DA	3275	1/1	0.89	0.16	2,2,2,2	1
57	MG	AA	1708	1/1	0.89	0.23	37,37,37,37	0
57	MG	BP	202	1/1	0.89	0.23	9,9,9,9	1
57	MG	DA	3290	1/1	0.89	0.22	21,21,21,21	0
57	MG	BA	3232	1/1	0.89	0.14	30,30,30,30	0
57	MG	CW	121	1/1	0.89	0.04	28,28,28,28	1
57	MG	AA	1625	1/1	0.89	0.20	31,31,31,31	0
57	MG	D2	2602	1/1	0.89	0.17	6,6,6,6	1
57	MG	BA	3374	1/1	0.89	0.24	28,28,28,28	1
57	MG	DA	3192	1/1	0.89	0.24	27,27,27,27	0
57	MG	AV	101	1/1	0.89	0.16	46,46,46,46	0
57	MG	CA	1613	1/1	0.89	0.18	10,10,10,10	1
57	MG	CA	1801	1/1	0.89	0.47	2,2,2,2	1
57	MG	CA	1615	1/1	0.89	0.07	42,42,42,42	0
57	MG	DA	3429	1/1	0.89	0.46	36,36,36,36	1
57	MG	DA	3432	1/1	0.89	0.28	50,50,50,50	0
57	MG	AA	1725	1/1	0.89	0.17	48,48,48,48	0
57	MG	BA	3385	1/1	0.89	0.08	7,7,7,7	0
57	MG	AA	1713	1/1	0.89	0.12	25,25,25,25	0
57	MG	AA	1703	1/1	0.89	0.20	22,22,22,22	0
57	MG	BA	3305	1/1	0.89	0.07	37,37,37,37	0
57	MG	BA	3009	1/1	0.89	0.46	1,1,1,1	0
57	MG	BA	3396	1/1	0.89	0.20	15,15,15,15	0
57	MG	CA	1645	1/1	0.89	0.34	46,46,46,46	0
57	MG	CA	1766	1/1	0.89	0.07	1,1,1,1	0
57	MG	BA	3309	1/1	0.89	0.20	47,47,47,47	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	DA	3237	1/1	0.89	0.07	22,22,22,22	0
57	MG	AA	1674	1/1	0.89	0.45	30,30,30,30	1
57	MG	DA	3359	1/1	0.89	0.20	40,40,40,40	0
57	MG	BA	3265	1/1	0.89	0.11	37,37,37,37	0
57	MG	BA	3182	1/1	0.89	0.21	13,13,13,13	0
57	MG	CA	1725	1/1	0.89	0.11	43,43,43,43	1
57	MG	CW	108	1/1	0.89	0.04	28,28,28,28	1
57	MG	BA	3409	1/1	0.89	0.15	5,5,5,5	0
57	MG	DA	3265	1/1	0.89	0.32	70,70,70,70	0
57	MG	AA	1707	1/1	0.89	0.46	53,53,53,53	0
57	MG	BA	3229	1/1	0.89	0.19	39,39,39,39	0
57	MG	DA	3226	1/1	0.90	0.07	48,48,48,48	0
57	MG	CE	203	1/1	0.90	0.11	38,38,38,38	1
57	MG	CA	1744	1/1	0.90	0.15	33,33,33,33	0
57	MG	BA	3168	1/1	0.90	0.12	29,29,29,29	0
57	MG	AA	1669	1/1	0.90	0.32	5,5,5,5	0
57	MG	BA	3437	1/1	0.90	0.33	64,64,64,64	0
57	MG	BA	3328	1/1	0.90	0.07	33,33,33,33	0
57	MG	DA	3392	1/1	0.90	0.17	46,46,46,46	0
57	MG	CA	1631	1/1	0.90	0.07	57,57,57,57	0
57	MG	CA	1696	1/1	0.90	0.28	52,52,52,52	0
57	MG	BA	3282	1/1	0.90	0.65	72,72,72,72	0
57	MG	AA	1672	1/1	0.90	0.17	24,24,24,24	0
57	MG	BA	3128	1/1	0.90	0.12	1,1,1,1	0
57	MG	CA	1772	1/1	0.90	0.10	60,60,60,60	0
57	MG	DA	3155	1/1	0.90	0.12	21,21,21,21	0
57	MG	DA	3280	1/1	0.90	0.08	24,24,24,24	1
57	MG	DA	3281	1/1	0.90	0.21	64,64,64,64	0
57	MG	DA	3156	1/1	0.90	0.08	21,21,21,21	0
57	MG	AA	1633	1/1	0.90	0.17	26,26,26,26	0
57	MG	BA	3075	1/1	0.90	0.21	6,6,6,6	1
57	MG	BA	3183	1/1	0.90	0.42	52,52,52,52	0
57	MG	AA	1658	1/1	0.90	0.27	1,1,1,1	0
57	MG	CA	1719	1/1	0.90	0.06	56,56,56,56	1
57	MG	CA	1724	1/1	0.90	0.08	51,51,51,51	0
57	MG	DA	3304	1/1	0.90	0.22	1,1,1,1	1
57	MG	CW	117	1/1	0.90	0.05	57,57,57,57	1
57	MG	BA	3191	1/1	0.90	0.14	23,23,23,23	0
57	MG	CA	1656	1/1	0.90	0.06	19,19,19,19	1
57	MG	D1	101	1/1	0.90	0.25	55,55,55,55	0
57	MG	DA	3193	1/1	0.90	0.15	1,1,1,1	1
57	MG	BA	3005	1/1	0.90	0.09	25,25,25,25	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	AA	1678	1/1	0.90	0.10	13,13,13,13	0
57	MG	AW	106	1/1	0.90	0.11	26,26,26,26	1
57	MG	BA	3362	1/1	0.90	0.25	38,38,38,38	0
57	MG	DA	3013	1/1	0.90	0.18	7,7,7,7	1
57	MG	DA	3016	1/1	0.90	0.30	57,57,57,57	0
57	MG	BA	3208	1/1	0.90	0.18	23,23,23,23	1
57	MG	DA	3340	1/1	0.90	0.14	59,59,59,59	0
57	MG	DA	3341	1/1	0.90	0.06	20,20,20,20	0
57	MG	AA	1679	1/1	0.90	0.10	12,12,12,12	1
57	MG	DE	302	1/1	0.90	0.20	50,50,50,50	0
57	MG	DG	201	1/1	0.90	0.07	38,38,38,38	0
57	MG	BA	3316	1/1	0.90	0.30	1,1,1,1	1
57	MG	DA	3352	1/1	0.90	0.26	123,123,123,123	1
57	MG	DP	202	1/1	0.90	0.07	1,1,1,1	1
57	MG	CA	1610	1/1	0.90	0.06	15,15,15,15	1
57	MG	AW	119	1/1	0.90	0.07	71,71,71,71	1
57	MG	BA	3268	1/1	0.90	0.05	30,30,30,30	0
57	MG	AK	201	1/1	0.90	0.16	33,33,33,33	1
57	MG	BA	3236	1/1	0.91	0.21	1,1,1,1	0
57	MG	BA	3084	1/1	0.91	0.15	1,1,1,1	1
57	MG	CA	1657	1/1	0.91	0.24	67,67,67,67	0
57	MG	DA	3301	1/1	0.91	0.14	55,55,55,55	1
57	MG	BA	3088	1/1	0.91	0.11	1,1,1,1	1
57	MG	DA	3305	1/1	0.91	0.20	1,1,1,1	0
57	MG	DA	3307	1/1	0.91	0.17	43,43,43,43	0
57	MG	DA	3309	1/1	0.91	0.25	44,44,44,44	0
57	MG	CA	1659	1/1	0.91	0.15	34,34,34,34	1
57	MG	DA	3066	1/1	0.91	0.28	1,1,1,1	0
57	MG	BA	3167	1/1	0.91	0.15	50,50,50,50	0
57	MG	AX	101	1/1	0.91	0.08	15,15,15,15	1
57	MG	DA	3083	1/1	0.91	0.21	22,22,22,22	0
57	MG	DA	3084	1/1	0.91	0.06	13,13,13,13	0
57	MG	AA	1660	1/1	0.91	0.18	17,17,17,17	0
57	MG	DA	3328	1/1	0.91	0.07	63,63,63,63	0
57	MG	BA	3432	1/1	0.91	0.16	47,47,47,47	0
57	MG	BA	3253	1/1	0.91	0.24	56,56,56,56	1
57	MG	BA	3255	1/1	0.91	0.12	25,25,25,25	0
57	MG	DA	3125	1/1	0.91	0.41	4,4,4,4	1
57	MG	BA	3257	1/1	0.91	0.08	42,42,42,42	0
57	MG	DA	3339	1/1	0.91	0.08	1,1,1,1	1
57	MG	AA	1613	1/1	0.91	0.20	11,11,11,11	1
57	MG	CA	1786	1/1	0.91	0.10	39,39,39,39	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	DA	3344	1/1	0.91	0.15	20,20,20,20	0
57	MG	DA	3148	1/1	0.91	0.18	26,26,26,26	0
57	MG	BA	3441	1/1	0.91	0.15	6,6,6,6	1
57	MG	DA	3151	1/1	0.91	0.14	1,1,1,1	1
57	MG	CA	1679	1/1	0.91	0.23	22,22,22,22	0
57	MG	BA	3444	1/1	0.91	0.06	15,15,15,15	1
57	MG	AA	1721	1/1	0.91	0.09	44,44,44,44	0
57	MG	BA	3179	1/1	0.91	0.07	30,30,30,30	0
57	MG	CA	1685	1/1	0.91	0.24	25,25,25,25	1
57	MG	BA	3110	1/1	0.91	0.39	32,32,32,32	1
57	MG	CA	1689	1/1	0.91	0.10	87,87,87,87	0
57	MG	DA	3163	1/1	0.91	0.09	17,17,17,17	1
57	MG	DA	3164	1/1	0.91	0.06	72,72,72,72	0
57	MG	BA	3269	1/1	0.91	0.09	22,22,22,22	0
57	MG	BA	3358	1/1	0.91	0.15	22,22,22,22	0
57	MG	DA	3179	1/1	0.91	0.19	52,52,52,52	1
57	MG	AA	1787	1/1	0.91	0.06	53,53,53,53	1
57	MG	BB	217	1/1	0.91	0.16	49,49,49,49	0
57	MG	BA	3364	1/1	0.91	0.06	12,12,12,12	0
57	MG	AA	1603	1/1	0.91	0.14	20,20,20,20	0
57	MG	CL	202	1/1	0.91	0.09	5,5,5,5	1
57	MG	AA	1602	1/1	0.91	0.07	64,64,64,64	0
57	MG	CA	1707	1/1	0.91	0.10	32,32,32,32	0
57	MG	DA	3413	1/1	0.91	0.13	10,10,10,10	1
57	MG	BA	3010	1/1	0.91	0.21	17,17,17,17	1
57	MG	DA	3209	1/1	0.91	0.11	1,1,1,1	1
57	MG	BF	303	1/1	0.91	0.09	36,36,36,36	0
57	MG	CA	1714	1/1	0.91	0.18	53,53,53,53	0
57	MG	BA	3194	1/1	0.91	0.17	19,19,19,19	0
57	MG	BA	3125	1/1	0.91	0.23	1,1,1,1	0
57	MG	CA	1720	1/1	0.91	0.18	4,4,4,4	1
57	MG	CA	1721	1/1	0.91	0.25	17,17,17,17	1
57	MG	BA	3288	1/1	0.91	0.06	44,44,44,44	1
57	MG	BA	3375	1/1	0.91	0.29	62,62,62,62	0
57	MG	AA	1790	1/1	0.91	0.11	35,35,35,35	0
57	MG	AW	115	1/1	0.91	0.09	19,19,19,19	1
57	MG	BA	3030	1/1	0.91	0.10	56,56,56,56	1
57	MG	BA	3133	1/1	0.91	0.26	1,1,1,1	0
57	MG	AA	1726	1/1	0.91	0.21	10,10,10,10	0
57	MG	AA	1695	1/1	0.91	0.21	42,42,42,42	0
57	MG	DA	3243	1/1	0.91	0.15	18,18,18,18	0
57	MG	CW	118	1/1	0.91	0.09	1,1,1,1	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	BA	3141	1/1	0.91	0.07	6,6,6,6	1
57	MG	BA	3308	1/1	0.91	0.14	30,30,30,30	1
57	MG	DA	3256	1/1	0.91	0.23	1,1,1,1	0
57	MG	CW	123	1/1	0.91	0.14	1,1,1,1	1
57	MG	BA	3219	1/1	0.91	0.18	1,1,1,1	1
57	MG	BA	3145	1/1	0.91	0.19	4,4,4,4	0
57	MG	AA	1618	1/1	0.91	0.21	1,1,1,1	0
57	MG	BA	3405	1/1	0.91	0.09	22,22,22,22	0
57	MG	DF	301	1/1	0.91	0.09	38,38,38,38	1
57	MG	BA	3152	1/1	0.91	0.35	62,62,62,62	0
57	MG	AW	105	1/1	0.91	0.09	82,82,82,82	0
57	MG	BA	3065	1/1	0.91	0.19	7,7,7,7	0
57	MG	DP	201	1/1	0.91	0.16	1,1,1,1	1
57	MG	DA	3024	1/1	0.91	0.15	32,32,32,32	0
57	MG	CA	1754	1/1	0.91	0.13	42,42,42,42	0
57	MG	BA	3413	1/1	0.91	0.07	21,21,21,21	1
57	MG	DA	3042	1/1	0.91	0.07	17,17,17,17	1
57	MG	DU	203	1/1	0.91	0.21	49,49,49,49	1
57	MG	AA	1623	1/1	0.91	0.04	16,16,16,16	0
57	MG	DA	3174	1/1	0.92	0.14	50,50,50,50	1
57	MG	BA	3117	1/1	0.92	0.15	8,8,8,8	0
57	MG	AA	1742	1/1	0.92	0.07	36,36,36,36	0
57	MG	DA	3335	1/1	0.92	0.09	7,7,7,7	1
57	MG	CA	1758	1/1	0.92	0.11	21,21,21,21	1
57	MG	BA	3321	1/1	0.92	0.07	51,51,51,51	0
57	MG	AA	1634	1/1	0.92	0.14	28,28,28,28	0
57	MG	BA	3267	1/1	0.92	0.22	34,34,34,34	0
57	MG	BA	3163	1/1	0.92	0.26	33,33,33,33	0
57	MG	BN	201	1/1	0.92	0.11	47,47,47,47	1
57	MG	DA	3201	1/1	0.92	0.28	15,15,15,15	0
57	MG	BA	3064	1/1	0.92	0.20	1,1,1,1	0
57	MG	DA	3349	1/1	0.92	0.09	10,10,10,10	1
57	MG	D2	2601	1/1	0.92	0.22	73,73,73,73	1
57	MG	CA	1768	1/1	0.92	0.09	5,5,5,5	1
57	MG	D3	101	1/1	0.92	0.09	42,42,42,42	0
57	MG	BA	3270	1/1	0.92	0.07	6,6,6,6	0
57	MG	DA	3005	1/1	0.92	0.08	22,22,22,22	0
57	MG	BA	3329	1/1	0.92	0.10	61,61,61,61	0
57	MG	CA	1687	1/1	0.92	0.34	42,42,42,42	0
57	MG	BA	3123	1/1	0.92	0.19	35,35,35,35	0
57	MG	AW	117	1/1	0.92	0.04	19,19,19,19	1
57	MG	BA	3280	1/1	0.92	0.06	72,72,72,72	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	DA	3372	1/1	0.92	0.22	35,35,35,35	1
57	MG	AA	1767	1/1	0.92	0.07	21,21,21,21	0
57	MG	AA	1696	1/1	0.92	0.17	45,45,45,45	1
57	MG	DA	3046	1/1	0.92	0.17	1,1,1,1	0
57	MG	BA	3171	1/1	0.92	0.09	1,1,1,1	1
57	MG	DA	3228	1/1	0.92	0.40	41,41,41,41	0
57	MG	DA	3231	1/1	0.92	0.11	14,14,14,14	0
57	MG	DA	3233	1/1	0.92	0.15	1,1,1,1	1
57	MG	DA	3235	1/1	0.92	0.18	7,7,7,7	1
57	MG	BA	3416	1/1	0.92	0.06	13,13,13,13	0
57	MG	BA	3343	1/1	0.92	0.18	33,33,33,33	0
57	MG	DA	3412	1/1	0.92	0.14	12,12,12,12	0
57	MG	DA	3242	1/1	0.92	0.28	100,100,100,100	1
57	MG	DA	3414	1/1	0.92	0.14	16,16,16,16	0
57	MG	AA	1646	1/1	0.92	0.28	29,29,29,29	0
57	MG	DA	3416	1/1	0.92	0.19	1,1,1,1	1
57	MG	BA	3230	1/1	0.92	0.27	22,22,22,22	0
57	MG	CA	1629	1/1	0.92	0.20	2,2,2,2	1
57	MG	AA	1632	1/1	0.92	0.20	4,4,4,4	0
57	MG	BA	3019	1/1	0.92	0.08	1,1,1,1	0
57	MG	BA	3427	1/1	0.92	0.14	99,99,99,99	1
57	MG	CA	1802	1/1	0.92	0.18	39,39,39,39	0
57	MG	CA	1641	1/1	0.92	0.08	17,17,17,17	0
57	MG	DA	3086	1/1	0.92	0.19	1,1,1,1	1
57	MG	CA	1642	1/1	0.92	0.16	2,2,2,2	0
57	MG	DA	3099	1/1	0.92	0.15	1,1,1,1	1
57	MG	BA	3293	1/1	0.92	0.17	19,19,19,19	0
57	MG	CA	1644	1/1	0.92	0.09	31,31,31,31	0
57	MG	DA	3108	1/1	0.92	0.17	13,13,13,13	0
57	MG	BA	3138	1/1	0.92	0.20	12,12,12,12	0
57	MG	DA	3288	1/1	0.92	0.15	7,7,7,7	1
57	MG	CA	1647	1/1	0.92	0.29	82,82,82,82	0
57	MG	BA	3296	1/1	0.92	0.18	11,11,11,11	0
57	MG	DB	207	1/1	0.92	0.07	16,16,16,16	1
57	MG	DA	3140	1/1	0.92	0.07	25,25,25,25	0
57	MG	BA	3181	1/1	0.92	0.24	17,17,17,17	0
57	MG	CA	1730	1/1	0.92	0.20	1,1,1,1	0
57	MG	DA	3145	1/1	0.92	0.20	56,56,56,56	1
57	MG	BA	3299	1/1	0.92	0.15	26,26,26,26	1
57	MG	AA	1779	1/1	0.92	0.17	1,1,1,1	1
57	MG	CV	104	1/1	0.92	0.19	45,45,45,45	1
57	MG	BA	3104	1/1	0.92	0.15	1,1,1,1	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	BA	3442	1/1	0.92	0.05	33,33,33,33	0
57	MG	DF	303	1/1	0.92	0.10	4,4,4,4	1
57	MG	DA	3317	1/1	0.92	0.14	78,78,78,78	1
57	MG	BA	3142	1/1	0.92	0.16	67,67,67,67	0
57	MG	BA	3143	1/1	0.92	0.19	1,1,1,1	1
57	MG	DA	3321	1/1	0.92	0.04	85,85,85,85	0
57	MG	AA	1704	1/1	0.92	0.17	11,11,11,11	0
57	MG	DP	203	1/1	0.92	0.17	1,1,1,1	1
57	MG	AA	1785	1/1	0.92	0.06	19,19,19,19	0
57	MG	BA	3377	1/1	0.92	0.34	95,95,95,95	0
57	MG	CA	1745	1/1	0.92	0.52	112,112,112,112	1
57	MG	BA	3312	1/1	0.92	0.14	1,1,1,1	0
57	MG	BA	3044	1/1	0.92	0.15	36,36,36,36	0
57	MG	AA	1773	1/1	0.93	0.17	16,16,16,16	1
57	MG	BA	3160	1/1	0.93	0.16	6,6,6,6	0
57	MG	BA	3215	1/1	0.93	0.12	38,38,38,38	1
57	MG	BN	202	1/1	0.93	0.15	3,3,3,3	1
57	MG	DA	3338	1/1	0.93	0.14	16,16,16,16	1
57	MG	DA	3195	1/1	0.93	0.07	15,15,15,15	0
57	MG	BN	203	1/1	0.93	0.06	56,56,56,56	1
57	MG	AA	1751	1/1	0.93	0.11	14,14,14,14	0
57	MG	CA	1769	1/1	0.93	0.15	28,28,28,28	0
57	MG	DA	3207	1/1	0.93	0.07	36,36,36,36	1
57	MG	BA	3330	1/1	0.93	0.04	35,35,35,35	0
57	MG	BA	3037	1/1	0.93	0.18	27,27,27,27	0
57	MG	CA	1775	1/1	0.93	0.07	1,1,1,1	1
57	MG	DA	3353	1/1	0.93	0.20	107,107,107,107	1
57	MG	BA	3041	1/1	0.93	0.07	46,46,46,46	1
57	MG	AA	1639	1/1	0.93	0.05	8,8,8,8	1
57	MG	CA	1688	1/1	0.93	0.17	21,21,21,21	0
57	MG	DA	3216	1/1	0.93	0.05	28,28,28,28	1
57	MG	BA	3284	1/1	0.93	0.06	12,12,12,12	1
57	MG	CA	1611	1/1	0.93	0.10	22,22,22,22	0
57	MG	BA	3285	1/1	0.93	0.34	40,40,40,40	0
57	MG	BA	3055	1/1	0.93	0.22	1,1,1,1	0
57	MG	AA	1614	1/1	0.93	0.30	11,11,11,11	0
57	MG	CA	1790	1/1	0.93	0.05	19,19,19,19	0
57	MG	DA	3373	1/1	0.93	0.06	74,74,74,74	0
57	MG	AA	1802	1/1	0.93	0.08	18,18,18,18	0
57	MG	AA	1671	1/1	0.93	0.30	47,47,47,47	0
57	MG	DA	3385	1/1	0.93	0.08	44,44,44,44	0
57	MG	CA	1618	1/1	0.93	0.12	22,22,22,22	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	BA	3422	1/1	0.93	0.17	30,30,30,30	0
57	MG	CA	1708	1/1	0.93	0.12	99,99,99,99	0
57	MG	DA	3236	1/1	0.93	0.08	14,14,14,14	0
57	MG	BA	3004	1/1	0.93	0.46	31,31,31,31	1
57	MG	CA	1710	1/1	0.93	0.12	16,16,16,16	0
57	MG	DA	3403	1/1	0.93	0.14	47,47,47,47	1
57	MG	DA	3405	1/1	0.93	0.22	30,30,30,30	1
57	MG	CA	1625	1/1	0.93	0.09	23,23,23,23	0
57	MG	BA	3074	1/1	0.93	0.24	1,1,1,1	1
57	MG	CA	1630	1/1	0.93	0.09	40,40,40,40	0
57	MG	AA	1723	1/1	0.93	0.09	55,55,55,55	0
57	MG	BA	3082	1/1	0.93	0.35	1,1,1,1	1
57	MG	DA	3253	1/1	0.93	0.09	25,25,25,25	0
57	MG	DA	3107	1/1	0.93	0.09	34,34,34,34	0
57	MG	BA	3431	1/1	0.93	0.18	12,12,12,12	0
57	MG	BA	3083	1/1	0.93	0.11	18,18,18,18	0
57	MG	BA	3241	1/1	0.93	0.08	27,27,27,27	0
57	MG	AG	201	1/1	0.93	0.12	5,5,5,5	1
57	MG	DA	3423	1/1	0.93	0.21	49,49,49,49	0
57	MG	DA	3136	1/1	0.93	0.21	9,9,9,9	1
57	MG	DA	3274	1/1	0.93	0.17	65,65,65,65	0
57	MG	DA	3138	1/1	0.93	0.15	17,17,17,17	0
57	MG	AA	1759	1/1	0.93	0.05	20,20,20,20	0
57	MG	DA	3279	1/1	0.93	0.34	75,75,75,75	0
57	MG	BA	3184	1/1	0.93	0.19	44,44,44,44	0
57	MG	CA	1646	1/1	0.93	0.29	56,56,56,56	0
57	MG	BA	3307	1/1	0.93	0.48	35,35,35,35	0
57	MG	AA	1628	1/1	0.93	0.12	1,1,1,1	1
57	MG	DA	3289	1/1	0.93	0.27	36,36,36,36	0
57	MG	BA	3101	1/1	0.93	0.12	1,1,1,1	1
57	MG	DB	203	1/1	0.93	0.13	60,60,60,60	0
57	MG	BA	3256	1/1	0.93	0.12	1,1,1,1	1
57	MG	AA	1763	1/1	0.93	0.07	40,40,40,40	1
57	MG	DA	3154	1/1	0.93	0.15	83,83,83,83	1
57	MG	DA	3297	1/1	0.93	0.26	11,11,11,11	1
57	MG	CA	1655	1/1	0.93	0.10	69,69,69,69	1
57	MG	DB	210	1/1	0.93	0.07	49,49,49,49	1
57	MG	BB	206	1/1	0.93	0.21	13,13,13,13	1
57	MG	DB	215	1/1	0.93	0.07	63,63,63,63	1
57	MG	DA	3300	1/1	0.93	0.27	38,38,38,38	0
57	MG	CA	1739	1/1	0.93	0.12	32,32,32,32	0
57	MG	CW	109	1/1	0.93	0.04	30,30,30,30	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	BA	3313	1/1	0.93	0.24	18,18,18,18	0
57	MG	DA	3160	1/1	0.93	0.05	1,1,1,1	1
57	MG	BA	3258	1/1	0.93	0.20	32,32,32,32	0
57	MG	AA	1690	1/1	0.93	0.09	40,40,40,40	0
57	MG	DF	304	1/1	0.93	0.06	66,66,66,66	0
57	MG	BA	3202	1/1	0.93	0.12	14,14,14,14	0
57	MG	BA	3150	1/1	0.93	0.06	22,22,22,22	0
57	MG	DA	3170	1/1	0.93	0.26	26,26,26,26	1
57	MG	CA	1666	1/1	0.93	0.16	1,1,1,1	0
57	MG	AA	1739	1/1	0.93	0.33	44,44,44,44	0
57	MG	DA	3177	1/1	0.93	0.09	22,22,22,22	0
57	MG	BA	3393	1/1	0.93	0.09	14,14,14,14	0
57	MG	DA	3180	1/1	0.93	0.10	47,47,47,47	0
57	MG	DA	3185	1/1	0.93	0.20	19,19,19,19	0
57	MG	BD	303	1/1	0.93	0.09	13,13,13,13	1
57	MG	AA	1648	1/1	0.93	0.26	3,3,3,3	1
57	MG	BA	3036	1/1	0.94	0.26	18,18,18,18	0
57	MG	BF	304	1/1	0.94	0.13	9,9,9,9	1
57	MG	BG	201	1/1	0.94	0.11	17,17,17,17	0
57	MG	BA	3289	1/1	0.94	0.57	60,60,60,60	1
57	MG	BA	3376	1/1	0.94	0.18	15,15,15,15	0
57	MG	AA	1644	1/1	0.94	0.12	1,1,1,1	0
57	MG	AA	1792	1/1	0.94	0.04	56,56,56,56	0
57	MG	CA	1705	1/1	0.94	0.11	5,5,5,5	0
57	MG	AA	1760	1/1	0.94	0.22	37,37,37,37	0
57	MG	BA	3054	1/1	0.94	0.13	20,20,20,20	0
57	MG	DA	3162	1/1	0.94	0.10	2,2,2,2	1
57	MG	AA	1796	1/1	0.94	0.23	9,9,9,9	0
57	MG	CA	1603	1/1	0.94	0.08	77,77,77,77	0
57	MG	AA	1673	1/1	0.94	0.10	12,12,12,12	1
57	MG	CA	1712	1/1	0.94	0.20	19,19,19,19	0
57	MG	DA	3173	1/1	0.94	0.11	52,52,52,52	1
57	MG	BA	3221	1/1	0.94	0.11	49,49,49,49	0
57	MG	AA	1612	1/1	0.94	0.17	36,36,36,36	0
57	MG	CA	1715	1/1	0.94	0.10	55,55,55,55	0
57	MG	CA	1716	1/1	0.94	0.08	75,75,75,75	0
57	MG	AA	1663	1/1	0.94	0.18	36,36,36,36	0
57	MG	AA	1765	1/1	0.94	0.17	41,41,41,41	0
57	MG	BA	3228	1/1	0.94	0.06	50,50,50,50	0
57	MG	BA	3068	1/1	0.94	0.15	1,1,1,1	0
57	MG	CW	112	1/1	0.94	0.06	24,24,24,24	1
57	MG	CA	1722	1/1	0.94	0.14	1,1,1,1	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	AA	1610	1/1	0.94	0.09	29,29,29,29	0
57	MG	AA	1803	1/1	0.94	0.17	9,9,9,9	0
57	MG	CA	1622	1/1	0.94	0.17	39,39,39,39	0
57	MG	AA	1712	1/1	0.94	0.12	50,50,50,50	0
57	MG	BA	3408	1/1	0.94	0.24	21,21,21,21	0
57	MG	BA	3235	1/1	0.94	0.21	22,22,22,22	0
57	MG	CW	122	1/1	0.94	0.05	70,70,70,70	0
57	MG	CA	1628	1/1	0.94	0.13	35,35,35,35	0
57	MG	BA	3411	1/1	0.94	0.17	99,99,99,99	1
57	MG	BA	3155	1/1	0.94	0.08	37,37,37,37	0
57	MG	DA	3375	1/1	0.94	0.21	74,74,74,74	1
57	MG	DA	3376	1/1	0.94	0.07	1,1,1,1	0
57	MG	DA	3377	1/1	0.94	0.47	62,62,62,62	1
57	MG	BA	3159	1/1	0.94	0.21	1,1,1,1	0
57	MG	DA	3380	1/1	0.94	0.07	16,16,16,16	1
57	MG	AW	122	1/1	0.94	0.07	47,47,47,47	0
57	MG	AD	302	1/1	0.94	0.09	28,28,28,28	0
57	MG	DA	3387	1/1	0.94	0.16	33,33,33,33	1
57	MG	DA	3390	1/1	0.94	0.09	34,34,34,34	0
57	MG	BA	3086	1/1	0.94	0.26	1,1,1,1	0
57	MG	AA	1770	1/1	0.94	0.12	16,16,16,16	1
57	MG	BA	3090	1/1	0.94	0.16	24,24,24,24	1
57	MG	DA	3012	1/1	0.94	0.23	1,1,1,1	0
57	MG	B5	101	1/1	0.94	0.14	1,1,1,1	0
57	MG	BA	3095	1/1	0.94	0.19	1,1,1,1	0
57	MG	DA	3225	1/1	0.94	0.07	35,35,35,35	0
57	MG	DA	3023	1/1	0.94	0.22	1,1,1,1	0
57	MG	AA	1747	1/1	0.94	0.18	5,5,5,5	0
57	MG	AA	1694	1/1	0.94	0.06	13,13,13,13	1
57	MG	DA	3411	1/1	0.94	0.06	19,19,19,19	0
57	MG	DA	3033	1/1	0.94	0.28	13,13,13,13	0
57	MG	DA	3034	1/1	0.94	0.18	33,33,33,33	0
57	MG	AL	202	1/1	0.94	0.06	1,1,1,1	0
57	MG	BA	3261	1/1	0.94	0.25	1,1,1,1	0
57	MG	DA	3044	1/1	0.94	0.14	60,60,60,60	0
57	MG	BA	3335	1/1	0.94	0.05	1,1,1,1	1
57	MG	AA	1729	1/1	0.94	0.08	19,19,19,19	0
57	MG	CA	1654	1/1	0.94	0.04	1,1,1,1	0
57	MG	AA	1654	1/1	0.94	0.05	65,65,65,65	0
57	MG	AA	1668	1/1	0.94	0.17	18,18,18,18	0
57	MG	BA	3266	1/1	0.94	0.27	65,65,65,65	0
57	MG	BA	3440	1/1	0.94	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
57	MG	AA	1781	1/1	0.94	0.14	7,7,7,7	1
57	MG	CA	1661	1/1	0.94	0.16	17,17,17,17	0
57	MG	DA	3260	1/1	0.94	0.08	8,8,8,8	1
57	MG	CA	1662	1/1	0.94	0.21	1,1,1,1	0
57	MG	DA	3436	1/1	0.94	0.14	41,41,41,41	0
57	MG	DA	3264	1/1	0.94	0.28	25,25,25,25	0
57	MG	DA	3073	1/1	0.94	0.23	1,1,1,1	1
57	MG	DA	3269	1/1	0.94	0.14	57,57,57,57	1
57	MG	BA	3113	1/1	0.94	0.16	1,1,1,1	0
57	MG	BA	3012	1/1	0.94	0.04	38,38,38,38	0
57	MG	BA	3445	1/1	0.94	0.05	25,25,25,25	1
57	MG	AA	1784	1/1	0.94	0.10	43,43,43,43	1
57	MG	BA	3275	1/1	0.94	0.10	37,37,37,37	0
57	MG	BB	205	1/1	0.94	0.10	6,6,6,6	1
57	MG	AA	1735	1/1	0.94	0.17	15,15,15,15	0
57	MG	DA	3102	1/1	0.94	0.18	3,3,3,3	0
57	MG	DA	3103	1/1	0.94	0.17	1,1,1,1	0
57	MG	DA	3287	1/1	0.94	0.10	28,28,28,28	0
57	MG	DB	214	1/1	0.94	0.29	25,25,25,25	1
57	MG	DA	3105	1/1	0.94	0.18	26,26,26,26	0
57	MG	BA	3351	1/1	0.94	0.30	68,68,68,68	1
57	MG	BA	3356	1/1	0.94	0.05	3,3,3,3	1
57	MG	DA	3291	1/1	0.94	0.13	1,1,1,1	1
57	MG	DA	3110	1/1	0.94	0.12	1,1,1,1	1
57	MG	DA	3294	1/1	0.94	0.09	73,73,73,73	1
57	MG	DA	3123	1/1	0.94	0.18	1,1,1,1	0
57	MG	CA	1676	1/1	0.94	0.08	43,43,43,43	1
57	MG	AA	1718	1/1	0.94	0.08	1,1,1,1	1
57	MG	DF	305	1/1	0.94	0.05	1,1,1,1	1
57	MG	BA	3028	1/1	0.94	0.25	1,1,1,1	0
57	MG	BB	214	1/1	0.94	0.09	34,34,34,34	0
57	MG	BA	3124	1/1	0.94	0.14	7,7,7,7	0
57	MG	CA	1682	1/1	0.94	0.11	9,9,9,9	0
57	MG	BA	3198	1/1	0.94	0.21	4,4,4,4	0
57	MG	BA	3199	1/1	0.94	0.04	5,5,5,5	1
57	MG	DA	3306	1/1	0.94	0.06	1,1,1,1	0
57	MG	AA	1642	1/1	0.94	0.10	26,26,26,26	0
57	MG	AA	1649	1/1	0.94	0.05	56,56,56,56	0
57	MG	DA	3310	1/1	0.94	0.19	7,7,7,7	1
57	MG	AA	1758	1/1	0.94	0.07	11,11,11,11	0
57	MG	BX	102	1/1	0.95	0.16	1,1,1,1	1
57	MG	AA	1621	1/1	0.95	0.05	3,3,3,3	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	DA	3087	1/1	0.95	0.17	17,17,17,17	1
57	MG	BA	3173	1/1	0.95	0.18	24,24,24,24	0
57	MG	DA	3094	1/1	0.95	0.18	1,1,1,1	1
57	MG	DA	3097	1/1	0.95	0.12	55,55,55,55	1
57	MG	BA	3426	1/1	0.95	0.16	27,27,27,27	0
57	MG	CA	1609	1/1	0.95	0.13	62,62,62,62	0
57	MG	AA	1611	1/1	0.95	0.14	24,24,24,24	0
57	MG	DA	3363	1/1	0.95	0.17	13,13,13,13	1
57	MG	DA	3365	1/1	0.95	0.15	24,24,24,24	1
57	MG	AA	1616	1/1	0.95	0.09	24,24,24,24	1
57	MG	BA	3274	1/1	0.95	0.24	55,55,55,55	0
57	MG	BA	3178	1/1	0.95	0.09	38,38,38,38	0
57	MG	CW	105	1/1	0.95	0.07	79,79,79,79	1
57	MG	BA	3140	1/1	0.95	0.09	24,24,24,24	1
57	MG	CA	1747	1/1	0.95	0.05	19,19,19,19	1
57	MG	DA	3112	1/1	0.95	0.22	1,1,1,1	0
57	MG	AA	1705	1/1	0.95	0.07	38,38,38,38	0
57	MG	DA	3248	1/1	0.95	0.16	5,5,5,5	1
57	MG	CA	1749	1/1	0.95	0.05	49,49,49,49	1
57	MG	DA	3251	1/1	0.95	0.07	10,10,10,10	1
57	MG	CA	1752	1/1	0.95	0.07	85,85,85,85	0
57	MG	BA	3058	1/1	0.95	0.11	3,3,3,3	1
57	MG	DA	3254	1/1	0.95	0.26	109,109,109,109	1
57	MG	DA	3128	1/1	0.95	0.13	1,1,1,1	1
57	MG	DA	3131	1/1	0.95	0.16	22,22,22,22	0
57	MG	AA	1753	1/1	0.95	0.12	48,48,48,48	0
57	MG	BA	3380	1/1	0.95	0.09	63,63,63,63	0
57	MG	DA	3396	1/1	0.95	0.07	14,14,14,14	0
57	MG	DA	3139	1/1	0.95	0.32	53,53,53,53	0
57	MG	AA	1714	1/1	0.95	0.09	23,23,23,23	0
57	MG	DA	3268	1/1	0.95	0.15	24,24,24,24	0
57	MG	BA	3383	1/1	0.95	0.18	39,39,39,39	1
57	MG	DA	3404	1/1	0.95	0.06	43,43,43,43	0
57	MG	CA	1761	1/1	0.95	0.27	1,1,1,1	1
57	MG	AW	104	1/1	0.95	0.04	14,14,14,14	1
57	MG	DA	3408	1/1	0.95	0.05	1,1,1,1	0
57	MG	CA	1764	1/1	0.95	0.06	49,49,49,49	0
57	MG	BA	3386	1/1	0.95	0.14	13,13,13,13	0
57	MG	DA	3276	1/1	0.95	0.07	47,47,47,47	0
57	MG	BB	202	1/1	0.95	0.03	9,9,9,9	1
57	MG	CA	1693	1/1	0.95	0.12	14,14,14,14	1
57	MG	AA	1733	1/1	0.95	0.10	5,5,5,5	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	BA	3114	1/1	0.95	0.14	1,1,1,1	0
57	MG	DA	3282	1/1	0.95	0.16	1,1,1,1	1
57	MG	DA	3284	1/1	0.95	0.23	18,18,18,18	0
57	MG	BA	3391	1/1	0.95	0.11	30,30,30,30	0
57	MG	AA	1756	1/1	0.95	0.05	58,58,58,58	0
57	MG	BA	3119	1/1	0.95	0.14	4,4,4,4	0
57	MG	D7	101	1/1	0.95	0.13	93,93,93,93	1
57	MG	BA	3246	1/1	0.95	0.11	23,23,23,23	1
57	MG	AA	1640	1/1	0.95	0.26	18,18,18,18	0
57	MG	CA	1779	1/1	0.95	0.07	34,34,34,34	0
57	MG	DA	3431	1/1	0.95	0.13	16,16,16,16	0
57	MG	BA	3158	1/1	0.95	0.12	32,32,32,32	0
57	MG	BA	3020	1/1	0.95	0.12	21,21,21,21	0
57	MG	DA	3435	1/1	0.95	0.08	48,48,48,48	0
57	MG	BA	3252	1/1	0.95	0.21	23,23,23,23	0
57	MG	DA	3168	1/1	0.95	0.12	36,36,36,36	1
57	MG	DA	3017	1/1	0.95	0.12	11,11,11,11	0
57	MG	BB	218	1/1	0.95	0.07	18,18,18,18	0
57	MG	CA	1648	1/1	0.95	0.15	14,14,14,14	1
57	MG	DA	3025	1/1	0.95	0.18	5,5,5,5	0
57	MG	DA	3302	1/1	0.95	0.26	80,80,80,80	1
57	MG	BA	3204	1/1	0.95	0.09	38,38,38,38	0
57	MG	DA	3178	1/1	0.95	0.12	1,1,1,1	1
57	MG	DA	3030	1/1	0.95	0.17	2,2,2,2	0
57	MG	AA	1657	1/1	0.95	0.12	8,8,8,8	1
57	MG	BA	3407	1/1	0.95	0.04	10,10,10,10	0
57	MG	BA	3347	1/1	0.95	0.13	1,1,1,1	0
57	MG	DA	3314	1/1	0.95	0.04	1,1,1,1	1
57	MG	AX	103	1/1	0.95	0.06	1,1,1,1	1
57	MG	B1	101	1/1	0.95	0.27	27,27,27,27	0
57	MG	BA	3033	1/1	0.95	0.13	20,20,20,20	0
57	MG	AA	1775	1/1	0.95	0.10	14,14,14,14	1
57	MG	BA	3353	1/1	0.95	0.23	41,41,41,41	1
57	MG	DA	3050	1/1	0.95	0.41	136,136,136,136	1
57	MG	DD	303	1/1	0.95	0.11	1,1,1,1	0
57	MG	BA	3214	1/1	0.95	0.06	106,106,106,106	1
57	MG	DA	3056	1/1	0.95	0.11	11,11,11,11	0
57	MG	DA	3203	1/1	0.95	0.06	1,1,1,1	1
57	MG	DA	3205	1/1	0.95	0.17	13,13,13,13	0
57	MG	CA	1804	1/1	0.95	0.20	45,45,45,45	0
57	MG	AA	1717	1/1	0.95	0.11	12,12,12,12	1
57	MG	DA	3064	1/1	0.95	0.09	18,18,18,18	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	DN	201	1/1	0.95	0.12	21,21,21,21	1
57	MG	BA	3359	1/1	0.95	0.03	21,21,21,21	1
57	MG	DA	3211	1/1	0.95	0.05	39,39,39,39	1
57	MG	BO	201	1/1	0.95	0.05	1,1,1,1	1
57	MG	BA	3091	1/1	0.95	0.14	1,1,1,1	0
57	MG	AL	201	1/1	0.95	0.05	1,1,1,1	1
57	MG	DA	3070	1/1	0.95	0.24	40,40,40,40	1
57	MG	CA	1667	1/1	0.95	0.19	8,8,8,8	0
57	MG	DA	3218	1/1	0.95	0.35	12,12,12,12	0
57	MG	BU	202	1/1	0.95	0.15	18,18,18,18	1
57	MG	CA	1660	1/1	0.96	0.23	8,8,8,8	0
57	MG	BA	3038	1/1	0.96	0.21	22,22,22,22	1
57	MG	DA	3067	1/1	0.96	0.18	1,1,1,1	0
57	MG	BA	3093	1/1	0.96	0.17	1,1,1,1	0
57	MG	CA	1732	1/1	0.96	0.14	10,10,10,10	0
57	MG	DA	3343	1/1	0.96	0.30	1,1,1,1	1
57	MG	BA	3186	1/1	0.96	0.07	5,5,5,5	1
57	MG	AA	1793	1/1	0.96	0.10	6,6,6,6	1
57	MG	DA	3081	1/1	0.96	0.12	11,11,11,11	0
57	MG	DA	3347	1/1	0.96	0.03	35,35,35,35	1
57	MG	DA	3082	1/1	0.96	0.10	20,20,20,20	0
57	MG	CA	1665	1/1	0.96	0.16	34,34,34,34	0
57	MG	AA	1772	1/1	0.96	0.30	52,52,52,52	0
57	MG	BA	3098	1/1	0.96	0.15	1,1,1,1	0
57	MG	BP	203	1/1	0.96	0.12	1,1,1,1	1
57	MG	DA	3356	1/1	0.96	0.14	57,57,57,57	0
57	MG	BA	3049	1/1	0.96	0.17	17,17,17,17	0
57	MG	BA	3146	1/1	0.96	0.16	1,1,1,1	0
57	MG	DA	3096	1/1	0.96	0.22	1,1,1,1	0
57	MG	DA	3362	1/1	0.96	0.18	15,15,15,15	0
57	MG	BA	3419	1/1	0.96	0.07	57,57,57,57	1
57	MG	DA	3364	1/1	0.96	0.04	42,42,42,42	0
57	MG	BA	3051	1/1	0.96	0.27	1,1,1,1	0
57	MG	BA	3360	1/1	0.96	0.18	10,10,10,10	0
57	MG	BA	3013	1/1	0.96	0.16	1,1,1,1	0
57	MG	BA	3363	1/1	0.96	0.12	90,90,90,90	0
57	MG	CA	1678	1/1	0.96	0.14	4,4,4,4	0
57	MG	DA	3232	1/1	0.96	0.34	1,1,1,1	0
57	MG	AA	1681	1/1	0.96	0.12	14,14,14,14	0
57	MG	CA	1753	1/1	0.96	0.07	7,7,7,7	1
57	MG	BA	3365	1/1	0.96	0.14	36,36,36,36	0
57	MG	BA	3205	1/1	0.96	0.15	23,23,23,23	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	DA	3378	1/1	0.96	0.10	18,18,18,18	1
57	MG	DA	3238	1/1	0.96	0.21	1,1,1,1	0
57	MG	BA	3106	1/1	0.96	0.06	19,19,19,19	1
57	MG	DA	3115	1/1	0.96	0.26	6,6,6,6	0
57	MG	AA	1624	1/1	0.96	0.15	9,9,9,9	0
57	MG	AA	1637	1/1	0.96	0.13	11,11,11,11	0
57	MG	DA	3247	1/1	0.96	0.19	13,13,13,13	0
57	MG	AA	1697	1/1	0.96	0.13	17,17,17,17	1
57	MG	BA	3062	1/1	0.96	0.20	1,1,1,1	0
57	MG	CA	1763	1/1	0.96	0.07	15,15,15,15	0
57	MG	DA	3129	1/1	0.96	0.11	1,1,1,1	0
57	MG	DA	3398	1/1	0.96	0.11	13,13,13,13	1
57	MG	DA	3130	1/1	0.96	0.16	33,33,33,33	0
57	MG	CA	1620	1/1	0.96	0.13	34,34,34,34	0
57	MG	DA	3134	1/1	0.96	0.16	8,8,8,8	0
57	MG	BA	3025	1/1	0.96	0.13	3,3,3,3	0
57	MG	CX	103	1/1	0.96	0.06	45,45,45,45	1
57	MG	BA	3026	1/1	0.96	0.06	8,8,8,8	0
57	MG	D1	102	1/1	0.96	0.23	51,51,51,51	0
57	MG	BA	3118	1/1	0.96	0.27	33,33,33,33	1
57	MG	DA	3142	1/1	0.96	0.25	21,21,21,21	0
57	MG	DA	3143	1/1	0.96	0.28	24,24,24,24	0
57	MG	BA	3378	1/1	0.96	0.08	31,31,31,31	0
57	MG	BA	3443	1/1	0.96	0.20	49,49,49,49	0
57	MG	DA	3146	1/1	0.96	0.12	3,3,3,3	0
57	MG	CA	1770	1/1	0.96	0.14	78,78,78,78	1
57	MG	D5	101	1/1	0.96	0.10	20,20,20,20	0
57	MG	BA	3067	1/1	0.96	0.38	1,1,1,1	1
57	MG	CA	1698	1/1	0.96	0.08	22,22,22,22	0
57	MG	DA	3153	1/1	0.96	0.12	1,1,1,1	0
57	MG	DA	3421	1/1	0.96	0.09	40,40,40,40	0
57	MG	BA	3271	1/1	0.96	0.14	9,9,9,9	0
57	MG	BA	3326	1/1	0.96	0.10	23,23,23,23	1
57	MG	DA	3008	1/1	0.96	0.51	1,1,1,1	0
57	MG	DA	3009	1/1	0.96	0.09	1,1,1,1	1
57	MG	DA	3286	1/1	0.96	0.18	12,12,12,12	0
57	MG	CA	1634	1/1	0.96	0.14	25,25,25,25	0
57	MG	BA	3027	1/1	0.96	0.09	1,1,1,1	1
57	MG	BA	3072	1/1	0.96	0.09	100,100,100,100	0
57	MG	BA	3001	1/1	0.96	0.14	8,8,8,8	0
57	MG	BA	3388	1/1	0.96	0.30	4,4,4,4	1
57	MG	AW	107	1/1	0.96	0.07	57,57,57,57	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	BA	3226	1/1	0.96	0.14	1,1,1,1	1
57	MG	BA	3332	1/1	0.96	0.07	64,64,64,64	0
57	MG	DA	3166	1/1	0.96	0.27	43,43,43,43	0
57	MG	DA	3167	1/1	0.96	0.14	12,12,12,12	0
57	MG	DB	201	1/1	0.96	0.08	22,22,22,22	1
57	MG	BA	3333	1/1	0.96	0.04	41,41,41,41	0
57	MG	DA	3169	1/1	0.96	0.17	1,1,1,1	1
57	MG	BA	3076	1/1	0.96	0.15	1,1,1,1	0
57	MG	BB	216	1/1	0.96	0.09	1,1,1,1	1
57	MG	DB	206	1/1	0.96	0.04	72,72,72,72	0
57	MG	BA	3079	1/1	0.96	0.18	1,1,1,1	0
57	MG	DA	3303	1/1	0.96	0.18	4,4,4,4	0
57	MG	DA	3041	1/1	0.96	0.08	24,24,24,24	0
57	MG	BA	3031	1/1	0.96	0.17	1,1,1,1	0
57	MG	BA	3003	1/1	0.96	0.12	68,68,68,68	1
57	MG	AA	1700	1/1	0.96	0.17	34,34,34,34	0
57	MG	BA	3132	1/1	0.96	0.06	24,24,24,24	1
57	MG	DA	3181	1/1	0.96	0.08	47,47,47,47	1
57	MG	DA	3313	1/1	0.96	0.09	5,5,5,5	0
57	MG	BA	3403	1/1	0.96	0.06	55,55,55,55	1
57	MG	DA	3316	1/1	0.96	0.05	14,14,14,14	1
57	MG	CA	1803	1/1	0.96	0.13	83,83,83,83	0
57	MG	DA	3318	1/1	0.96	0.11	7,7,7,7	1
57	MG	DA	3188	1/1	0.96	0.29	26,26,26,26	0
57	MG	DA	3051	1/1	0.96	0.24	1,1,1,1	0
57	MG	AM	201	1/1	0.96	0.11	28,28,28,28	0
57	MG	DA	3191	1/1	0.96	0.05	5,5,5,5	1
57	MG	BA	3344	1/1	0.96	0.07	1,1,1,1	1
57	MG	DA	3058	1/1	0.96	0.17	42,42,42,42	0
57	MG	DA	3059	1/1	0.96	0.12	1,1,1,1	0
57	MG	DA	3060	1/1	0.96	0.22	1,1,1,1	0
57	MG	DA	3197	1/1	0.96	0.18	3,3,3,3	0
57	MG	DA	3199	1/1	0.96	0.12	5,5,5,5	0
57	MG	DA	3200	1/1	0.96	0.13	2,2,2,2	0
57	MG	CA	1807	1/1	0.96	0.16	1,1,1,1	0
57	MG	DA	3333	1/1	0.96	0.06	15,15,15,15	0
57	MG	DA	3334	1/1	0.96	0.04	30,30,30,30	0
57	MG	AA	1643	1/1	0.96	0.09	43,43,43,43	0
57	MG	DX	101	1/1	0.96	0.06	52,52,52,52	1
57	MG	AA	1738	1/1	0.96	0.42	18,18,18,18	1
57	MG	BA	3250	1/1	0.97	0.22	24,24,24,24	0
57	MG	DA	3011	1/1	0.97	0.05	42,42,42,42	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	BA	3108	1/1	0.97	0.04	25,25,25,25	0
57	MG	CA	1751	1/1	0.97	0.10	10,10,10,10	0
57	MG	BA	3428	1/1	0.97	0.17	1,1,1,1	0
57	MG	DA	3330	1/1	0.97	0.07	73,73,73,73	0
57	MG	BA	3339	1/1	0.97	0.21	3,3,3,3	0
57	MG	DA	3018	1/1	0.97	0.24	12,12,12,12	0
57	MG	DA	3020	1/1	0.97	0.21	1,1,1,1	0
57	MG	DA	3184	1/1	0.97	0.13	1,1,1,1	0
57	MG	DA	3021	1/1	0.97	0.13	2,2,2,2	1
57	MG	DA	3186	1/1	0.97	0.23	24,24,24,24	0
57	MG	BA	3109	1/1	0.97	0.12	3,3,3,3	0
57	MG	CA	1755	1/1	0.97	0.05	1,1,1,1	0
57	MG	AA	1627	1/1	0.97	0.10	9,9,9,9	0
57	MG	AA	1801	1/1	0.97	0.31	1,1,1,1	0
57	MG	AA	1607	1/1	0.97	0.17	1,1,1,1	0
57	MG	BA	3436	1/1	0.97	0.09	6,6,6,6	1
57	MG	AA	1698	1/1	0.97	0.10	1,1,1,1	0
57	MG	BA	3177	1/1	0.97	0.07	36,36,36,36	1
57	MG	DA	3036	1/1	0.97	0.22	13,13,13,13	1
57	MG	DA	3039	1/1	0.97	0.13	2,2,2,2	0
57	MG	BA	3007	1/1	0.97	0.07	37,37,37,37	0
57	MG	BA	3262	1/1	0.97	0.07	32,32,32,32	1
57	MG	BA	3008	1/1	0.97	0.34	19,19,19,19	0
57	MG	BA	3061	1/1	0.97	0.19	3,3,3,3	0
57	MG	DA	3047	1/1	0.97	0.14	1,1,1,1	0
57	MG	AA	1804	1/1	0.97	0.16	20,20,20,20	0
57	MG	DA	3357	1/1	0.97	0.04	52,52,52,52	0
57	MG	BA	3352	1/1	0.97	0.25	44,44,44,44	1
57	MG	BA	3063	1/1	0.97	0.14	6,6,6,6	0
57	MG	AA	1635	1/1	0.97	0.16	2,2,2,2	0
57	MG	BA	3357	1/1	0.97	0.13	105,105,105,105	1
57	MG	CA	1773	1/1	0.97	0.14	9,9,9,9	0
57	MG	DA	3057	1/1	0.97	0.14	3,3,3,3	0
57	MG	CA	1669	1/1	0.97	0.20	32,32,32,32	0
57	MG	BA	3011	1/1	0.97	0.06	15,15,15,15	0
57	MG	CA	1671	1/1	0.97	0.07	21,21,21,21	0
57	MG	DA	3368	1/1	0.97	0.07	78,78,78,78	0
57	MG	DA	3369	1/1	0.97	0.16	142,142,142,142	1
57	MG	BA	3185	1/1	0.97	0.14	1,1,1,1	0
57	MG	DA	3217	1/1	0.97	0.16	31,31,31,31	0
57	MG	AA	1782	1/1	0.97	0.11	47,47,47,47	0
57	MG	BA	3361	1/1	0.97	0.31	1,1,1,1	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	AE	201	1/1	0.97	0.09	28,28,28,28	0
57	MG	BA	3126	1/1	0.97	0.20	1,1,1,1	0
57	MG	CA	1784	1/1	0.97	0.09	1,1,1,1	1
57	MG	BA	3193	1/1	0.97	0.09	1,1,1,1	0
57	MG	BB	215	1/1	0.97	0.04	49,49,49,49	1
57	MG	CA	1787	1/1	0.97	0.08	11,11,11,11	0
57	MG	DA	3071	1/1	0.97	0.31	1,1,1,1	0
57	MG	BA	3069	1/1	0.97	0.15	1,1,1,1	0
57	MG	DA	3076	1/1	0.97	0.17	1,1,1,1	0
57	MG	DA	3389	1/1	0.97	0.08	33,33,33,33	1
57	MG	DA	3078	1/1	0.97	0.22	58,58,58,58	1
57	MG	DA	3391	1/1	0.97	0.05	19,19,19,19	0
57	MG	BA	3196	1/1	0.97	0.04	19,19,19,19	0
57	MG	AA	1783	1/1	0.97	0.08	39,39,39,39	1
57	MG	DA	3394	1/1	0.97	0.05	30,30,30,30	1
57	MG	BA	3368	1/1	0.97	0.04	1,1,1,1	1
57	MG	BA	3129	1/1	0.97	0.07	8,8,8,8	1
57	MG	BD	302	1/1	0.97	0.16	1,1,1,1	0
57	MG	DA	3399	1/1	0.97	0.11	19,19,19,19	0
57	MG	DA	3240	1/1	0.97	0.09	72,72,72,72	0
57	MG	BA	3370	1/1	0.97	0.05	37,37,37,37	0
57	MG	BA	3073	1/1	0.97	0.26	1,1,1,1	0
57	MG	DA	3092	1/1	0.97	0.23	1,1,1,1	0
57	MG	CA	1800	1/1	0.97	0.10	9,9,9,9	0
57	MG	BA	3201	1/1	0.97	0.10	31,31,31,31	0
57	MG	AA	1761	1/1	0.97	0.05	13,13,13,13	0
57	MG	AA	1701	1/1	0.97	0.05	8,8,8,8	1
57	MG	BA	3136	1/1	0.97	0.16	1,1,1,1	0
57	MG	DA	3410	1/1	0.97	0.10	31,31,31,31	1
57	MG	CA	1805	1/1	0.97	0.24	1,1,1,1	0
57	MG	AA	1630	1/1	0.97	0.08	19,19,19,19	0
57	MG	CA	1695	1/1	0.97	0.08	1,1,1,1	1
57	MG	AA	1661	1/1	0.97	0.06	10,10,10,10	1
57	MG	DA	3257	1/1	0.97	0.05	54,54,54,54	0
57	MG	BA	3080	1/1	0.97	0.15	26,26,26,26	0
57	MG	BA	3209	1/1	0.97	0.15	18,18,18,18	0
57	MG	DA	3261	1/1	0.97	0.28	30,30,30,30	0
57	MG	CA	1699	1/1	0.97	0.11	6,6,6,6	1
57	MG	AA	1734	1/1	0.97	0.20	36,36,36,36	0
57	MG	CA	1703	1/1	0.97	0.03	12,12,12,12	0
57	MG	DA	3267	1/1	0.97	0.18	28,28,28,28	1
57	MG	DA	3116	1/1	0.97	0.25	1,1,1,1	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	DA	3425	1/1	0.97	0.30	19,19,19,19	0
57	MG	DA	3121	1/1	0.97	0.10	20,20,20,20	0
57	MG	DA	3122	1/1	0.97	0.07	8,8,8,8	0
57	MG	BA	3211	1/1	0.97	0.04	50,50,50,50	1
57	MG	AA	1766	1/1	0.97	0.06	1,1,1,1	1
57	MG	AW	123	1/1	0.97	0.06	1,1,1,1	1
57	MG	BA	3387	1/1	0.97	0.17	42,42,42,42	0
57	MG	AA	1631	1/1	0.97	0.07	1,1,1,1	1
57	MG	CA	1601	1/1	0.97	0.12	21,21,21,21	1
57	MG	BA	3302	1/1	0.97	0.04	19,19,19,19	1
57	MG	BA	3144	1/1	0.97	0.15	40,40,40,40	0
57	MG	AA	1675	1/1	0.97	0.08	41,41,41,41	1
57	MG	DA	3135	1/1	0.97	0.31	12,12,12,12	0
57	MG	BA	3089	1/1	0.97	0.25	6,6,6,6	1
57	MG	AX	105	1/1	0.97	0.06	35,35,35,35	0
57	MG	BA	3222	1/1	0.97	0.20	1,1,1,1	0
57	MG	BA	3223	1/1	0.97	0.11	9,9,9,9	1
57	MG	BA	3148	1/1	0.97	0.08	8,8,8,8	0
57	MG	BA	3400	1/1	0.97	0.16	1,1,1,1	0
57	MG	BA	3149	1/1	0.97	0.11	36,36,36,36	0
57	MG	AA	1665	1/1	0.97	0.27	21,21,21,21	0
57	MG	AA	1771	1/1	0.97	0.04	9,9,9,9	0
57	MG	BA	3404	1/1	0.97	0.16	108,108,108,108	0
57	MG	DB	211	1/1	0.97	0.06	1,1,1,1	1
57	MG	B1	104	1/1	0.97	0.12	62,62,62,62	0
57	MG	DB	213	1/1	0.97	0.04	28,28,28,28	1
57	MG	DA	3149	1/1	0.97	0.12	27,27,27,27	0
57	MG	AA	1677	1/1	0.97	0.14	42,42,42,42	0
57	MG	BA	3096	1/1	0.97	0.08	1,1,1,1	1
57	MG	BA	3156	1/1	0.97	0.09	12,12,12,12	1
57	MG	AA	1626	1/1	0.97	0.12	1,1,1,1	0
57	MG	BA	3410	1/1	0.97	0.06	6,6,6,6	1
57	MG	BA	3100	1/1	0.97	0.05	1,1,1,1	1
57	MG	CX	101	1/1	0.97	0.14	56,56,56,56	1
57	MG	B7	101	1/1	0.97	0.10	8,8,8,8	0
57	MG	CA	1734	1/1	0.97	0.09	46,46,46,46	1
57	MG	CA	1632	1/1	0.97	0.14	36,36,36,36	0
57	MG	DA	3308	1/1	0.97	0.15	3,3,3,3	0
57	MG	BA	3161	1/1	0.97	0.06	7,7,7,7	1
57	MG	BA	3042	1/1	0.97	0.17	1,1,1,1	0
57	MG	DA	3312	1/1	0.97	0.04	1,1,1,1	0
57	MG	BA	3240	1/1	0.97	0.23	8,8,8,8	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	BA	3043	1/1	0.97	0.05	26,26,26,26	0
57	MG	BA	3243	1/1	0.97	0.11	1,1,1,1	0
57	MG	AA	1740	1/1	0.97	0.10	35,35,35,35	0
57	MG	DP	204	1/1	0.97	0.06	15,15,15,15	1
57	MG	BA	3247	1/1	0.97	0.10	26,26,26,26	1
57	MG	AA	1647	1/1	0.97	0.07	17,17,17,17	1
57	MG	BA	3050	1/1	0.97	0.08	1,1,1,1	1
57	MG	DA	3007	1/1	0.97	0.19	14,14,14,14	0
57	MG	BA	3336	1/1	0.97	0.07	8,8,8,8	1
57	MG	DX	102	1/1	0.97	0.05	23,23,23,23	1
57	MG	DA	3171	1/1	0.97	0.07	33,33,33,33	0
57	MG	BA	3070	1/1	0.98	0.06	24,24,24,24	0
57	MG	DA	3106	1/1	0.98	0.11	1,1,1,1	0
57	MG	BA	3071	1/1	0.98	0.05	20,20,20,20	0
57	MG	CA	1750	1/1	0.98	0.12	14,14,14,14	0
57	MG	CW	120	1/1	0.98	0.03	20,20,20,20	1
57	MG	DA	3230	1/1	0.98	0.06	35,35,35,35	0
57	MG	AA	1620	1/1	0.98	0.09	3,3,3,3	0
57	MG	DA	3360	1/1	0.98	0.20	5,5,5,5	0
57	MG	BA	3355	1/1	0.98	0.03	37,37,37,37	0
57	MG	BP	201	1/1	0.98	0.05	11,11,11,11	1
57	MG	DA	3117	1/1	0.98	0.23	5,5,5,5	0
57	MG	DA	3119	1/1	0.98	0.11	1,1,1,1	0
57	MG	DA	3120	1/1	0.98	0.12	1,1,1,1	1
57	MG	BA	3300	1/1	0.98	0.06	1,1,1,1	1
57	MG	AA	1636	1/1	0.98	0.07	16,16,16,16	0
57	MG	BA	3116	1/1	0.98	0.06	13,13,13,13	0
57	MG	BA	3034	1/1	0.98	0.10	15,15,15,15	0
57	MG	AA	1659	1/1	0.98	0.22	27,27,27,27	0
57	MG	DA	3244	1/1	0.98	0.05	57,57,57,57	0
57	MG	AA	1606	1/1	0.98	0.14	1,1,1,1	0
57	MG	AA	1768	1/1	0.98	0.11	7,7,7,7	0
57	MG	DA	3374	1/1	0.98	0.04	28,28,28,28	0
57	MG	AA	1652	1/1	0.98	0.14	11,11,11,11	0
57	MG	CA	1604	1/1	0.98	0.04	41,41,41,41	0
57	MG	CA	1606	1/1	0.98	0.12	29,29,29,29	0
57	MG	DA	3132	1/1	0.98	0.13	34,34,34,34	0
57	MG	AA	1699	1/1	0.98	0.06	1,1,1,1	1
57	MG	BA	3311	1/1	0.98	0.11	1,1,1,1	0
57	MG	AA	1684	1/1	0.98	0.06	25,25,25,25	0
57	MG	DA	3137	1/1	0.98	0.08	5,5,5,5	1
57	MG	BA	3259	1/1	0.98	0.04	1,1,1,1	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	BA	3314	1/1	0.98	0.03	23,23,23,23	0
57	MG	BA	3430	1/1	0.98	0.10	1,1,1,1	1
57	MG	DA	3010	1/1	0.98	0.19	1,1,1,1	0
57	MG	DA	3263	1/1	0.98	0.04	16,16,16,16	0
57	MG	CA	1614	1/1	0.98	0.18	6,6,6,6	0
57	MG	AA	1685	1/1	0.98	0.04	12,12,12,12	0
57	MG	AA	1601	1/1	0.98	0.03	21,21,21,21	0
57	MG	DA	3014	1/1	0.98	0.13	14,14,14,14	0
57	MG	CA	1694	1/1	0.98	0.03	59,59,59,59	0
57	MG	BA	3433	1/1	0.98	0.10	33,33,33,33	0
57	MG	CA	1777	1/1	0.98	0.05	47,47,47,47	0
57	MG	BA	3371	1/1	0.98	0.11	53,53,53,53	1
57	MG	CA	1619	1/1	0.98	0.11	3,3,3,3	0
57	MG	CA	1780	1/1	0.98	0.12	31,31,31,31	1
57	MG	DA	3277	1/1	0.98	0.10	22,22,22,22	0
57	MG	BA	3317	1/1	0.98	0.06	60,60,60,60	0
57	MG	BA	3318	1/1	0.98	0.06	1,1,1,1	0
57	MG	DA	3407	1/1	0.98	0.05	9,9,9,9	0
57	MG	CA	1700	1/1	0.98	0.12	10,10,10,10	0
57	MG	DA	3027	1/1	0.98	0.24	55,55,55,55	1
57	MG	DA	3028	1/1	0.98	0.04	59,59,59,59	1
57	MG	DA	3283	1/1	0.98	0.03	7,7,7,7	1
57	MG	DA	3029	1/1	0.98	0.10	1,1,1,1	0
57	MG	CA	1701	1/1	0.98	0.13	3,3,3,3	0
57	MG	DA	3031	1/1	0.98	0.10	2,2,2,2	0
57	MG	BA	3087	1/1	0.98	0.05	18,18,18,18	0
57	MG	BA	3438	1/1	0.98	0.11	44,44,44,44	0
57	MG	BA	3048	1/1	0.98	0.18	1,1,1,1	0
57	MG	CA	1626	1/1	0.98	0.04	23,23,23,23	0
57	MG	CA	1789	1/1	0.98	0.12	73,73,73,73	0
57	MG	AA	1795	1/1	0.98	0.06	1,1,1,1	0
57	MG	AA	1664	1/1	0.98	0.03	4,4,4,4	0
57	MG	AA	1722	1/1	0.98	0.06	37,37,37,37	0
57	MG	BA	3325	1/1	0.98	0.03	30,30,30,30	0
57	MG	CA	1795	1/1	0.98	0.03	34,34,34,34	0
57	MG	BA	3131	1/1	0.98	0.15	1,1,1,1	0
57	MG	DA	3427	1/1	0.98	0.11	1,1,1,1	0
57	MG	CA	1711	1/1	0.98	0.22	37,37,37,37	1
57	MG	CA	1633	1/1	0.98	0.10	2,2,2,2	0
57	MG	DA	3430	1/1	0.98	0.10	13,13,13,13	0
57	MG	CA	1799	1/1	0.98	0.08	39,39,39,39	1
57	MG	AA	1619	1/1	0.98	0.11	25,25,25,25	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	DA	3433	1/1	0.98	0.04	28,28,28,28	1
57	MG	CA	1638	1/1	0.98	0.07	6,6,6,6	0
57	MG	BB	201	1/1	0.98	0.09	32,32,32,32	1
57	MG	AW	103	1/1	0.98	0.06	1,1,1,1	1
57	MG	BA	3384	1/1	0.98	0.06	1,1,1,1	1
57	MG	DA	3183	1/1	0.98	0.07	11,11,11,11	0
57	MG	BA	3135	1/1	0.98	0.17	38,38,38,38	0
57	MG	BA	3273	1/1	0.98	0.13	57,57,57,57	1
57	MG	BA	3056	1/1	0.98	0.05	1,1,1,1	0
57	MG	DA	3311	1/1	0.98	0.12	11,11,11,11	1
57	MG	AX	102	1/1	0.98	0.04	4,4,4,4	0
57	MG	CA	1723	1/1	0.98	0.05	10,10,10,10	1
57	MG	AA	1778	1/1	0.98	0.05	16,16,16,16	1
57	MG	AX	104	1/1	0.98	0.07	55,55,55,55	1
57	MG	BB	211	1/1	0.98	0.09	44,44,44,44	1
57	MG	BB	212	1/1	0.98	0.06	1,1,1,1	1
57	MG	AA	1689	1/1	0.98	0.10	6,6,6,6	0
57	MG	AA	1629	1/1	0.98	0.12	22,22,22,22	0
57	MG	CA	1652	1/1	0.98	0.13	1,1,1,1	1
57	MG	DA	3196	1/1	0.98	0.05	7,7,7,7	1
57	MG	AA	1641	1/1	0.98	0.09	26,26,26,26	0
57	MG	DA	3198	1/1	0.98	0.07	11,11,11,11	0
57	MG	DA	3077	1/1	0.98	0.14	1,1,1,1	0
57	MG	AA	1692	1/1	0.98	0.07	3,3,3,3	1
57	MG	BA	3105	1/1	0.98	0.12	1,1,1,1	0
57	MG	BA	3188	1/1	0.98	0.04	12,12,12,12	0
57	MG	B2	601	1/1	0.98	0.11	22,22,22,22	0
57	MG	DA	3204	1/1	0.98	0.17	51,51,51,51	1
57	MG	DE	301	1/1	0.98	0.11	1,1,1,1	1
57	MG	BA	3342	1/1	0.98	0.03	26,26,26,26	1
57	MG	BA	3190	1/1	0.98	0.15	17,17,17,17	0
57	MG	BA	3029	1/1	0.98	0.28	1,1,1,1	1
57	MG	DA	3088	1/1	0.98	0.05	1,1,1,1	1
57	MG	DA	3089	1/1	0.98	0.13	3,3,3,3	0
57	MG	BA	3192	1/1	0.98	0.05	15,15,15,15	0
57	MG	CA	1740	1/1	0.98	0.06	44,44,44,44	0
57	MG	CA	1741	1/1	0.98	0.05	1,1,1,1	1
57	MG	BF	301	1/1	0.98	0.10	14,14,14,14	0
57	MG	BA	3291	1/1	0.98	0.08	7,7,7,7	0
57	MG	DA	3342	1/1	0.98	0.03	1,1,1,1	1
57	MG	DA	3098	1/1	0.98	0.07	5,5,5,5	0
57	MG	B3	101	1/1	0.98	0.05	14,14,14,14	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	AA	1693	1/1	0.98	0.09	80,80,80,80	0
57	MG	CW	114	1/1	0.98	0.10	4,4,4,4	1
57	MG	BA	3244	1/1	0.98	0.10	1,1,1,1	0
57	MG	BA	3295	1/1	0.98	0.06	1,1,1,1	0
57	MG	DV	201	1/1	0.98	0.03	1,1,1,1	0
57	MG	DA	3350	1/1	0.98	0.06	73,73,73,73	1
57	MG	DA	3351	1/1	0.98	0.08	11,11,11,11	1
57	MG	DA	3104	1/1	0.98	0.05	9,9,9,9	1
57	MG	DA	3037	1/1	0.99	0.07	1,1,1,1	0
57	MG	DA	3038	1/1	0.99	0.07	3,3,3,3	1
57	MG	DA	3246	1/1	0.99	0.03	57,57,57,57	0
57	MG	AA	1662	1/1	0.99	0.06	41,41,41,41	1
57	MG	DA	3040	1/1	0.99	0.05	1,1,1,1	0
57	MG	DA	3249	1/1	0.99	0.04	1,1,1,1	0
57	MG	CA	1605	1/1	0.99	0.11	18,18,18,18	0
57	MG	BA	3218	1/1	0.99	0.04	50,50,50,50	0
57	MG	B2	602	1/1	0.99	0.11	1,1,1,1	1
57	MG	DA	3045	1/1	0.99	0.03	10,10,10,10	0
57	MG	BA	3220	1/1	0.99	0.04	16,16,16,16	1
57	MG	DA	3255	1/1	0.99	0.02	1,1,1,1	0
57	MG	DA	3147	1/1	0.99	0.04	22,22,22,22	0
57	MG	AA	1605	1/1	0.99	0.09	3,3,3,3	0
57	MG	BA	3078	1/1	0.99	0.12	1,1,1,1	0
57	MG	DA	3259	1/1	0.99	0.06	22,22,22,22	0
57	MG	BA	3052	1/1	0.99	0.03	51,51,51,51	0
57	MG	BA	3053	1/1	0.99	0.08	1,1,1,1	0
57	MG	AA	1776	1/1	0.99	0.20	33,33,33,33	1
57	MG	DA	3052	1/1	0.99	0.11	1,1,1,1	0
57	MG	DA	3381	1/1	0.99	0.07	65,65,65,65	0
57	MG	AA	1608	1/1	0.99	0.06	3,3,3,3	0
57	MG	DA	3383	1/1	0.99	0.08	42,42,42,42	1
57	MG	DA	3384	1/1	0.99	0.04	1,1,1,1	1
57	MG	DA	3054	1/1	0.99	0.06	1,1,1,1	0
57	MG	DA	3386	1/1	0.99	0.03	19,19,19,19	0
57	MG	CA	1683	1/1	0.99	0.18	19,19,19,19	0
57	MG	DA	3388	1/1	0.99	0.23	39,39,39,39	0
57	MG	BA	3115	1/1	0.99	0.04	3,3,3,3	0
57	MG	AA	1786	1/1	0.99	0.04	1,1,1,1	1
57	MG	BA	3278	1/1	0.99	0.03	8,8,8,8	0
57	MG	DA	3271	1/1	0.99	0.27	113,113,113,113	1
57	MG	DA	3272	1/1	0.99	0.09	5,5,5,5	0
57	MG	BA	3085	1/1	0.99	0.08	1,1,1,1	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	DA	3061	1/1	0.99	0.04	31,31,31,31	0
57	MG	CA	1757	1/1	0.99	0.20	35,35,35,35	0
57	MG	DA	3397	1/1	0.99	0.05	1,1,1,1	0
57	MG	BA	3057	1/1	0.99	0.08	7,7,7,7	0
57	MG	CA	1621	1/1	0.99	0.03	31,31,31,31	0
57	MG	AA	1709	1/1	0.99	0.06	3,3,3,3	0
57	MG	BA	3151	1/1	0.99	0.05	1,1,1,1	0
57	MG	BA	3283	1/1	0.99	0.10	2,2,2,2	0
57	MG	BA	3233	1/1	0.99	0.32	1,1,1,1	0
57	MG	BA	3234	1/1	0.99	0.04	12,12,12,12	0
57	MG	AA	1604	1/1	0.99	0.08	3,3,3,3	0
57	MG	BA	3015	1/1	0.99	0.08	6,6,6,6	0
57	MG	DA	3172	1/1	0.99	0.10	17,17,17,17	1
57	MG	DA	3072	1/1	0.99	0.07	1,1,1,1	1
57	MG	BA	3016	1/1	0.99	0.07	31,31,31,31	1
57	MG	DA	3175	1/1	0.99	0.06	43,43,43,43	1
57	MG	DA	3074	1/1	0.99	0.03	2,2,2,2	0
57	MG	DA	3075	1/1	0.99	0.10	1,1,1,1	0
57	MG	BB	207	1/1	0.99	0.03	11,11,11,11	0
57	MG	BA	3017	1/1	0.99	0.05	3,3,3,3	1
57	MG	DA	3293	1/1	0.99	0.16	1,1,1,1	1
57	MG	BA	3395	1/1	0.99	0.06	1,1,1,1	1
57	MG	DA	3417	1/1	0.99	0.10	71,71,71,71	0
57	MG	DA	3079	1/1	0.99	0.09	5,5,5,5	0
57	MG	DA	3182	1/1	0.99	0.04	1,1,1,1	1
57	MG	AA	1730	1/1	0.99	0.05	1,1,1,1	1
57	MG	CX	102	1/1	0.99	0.07	1,1,1,1	1
57	MG	CA	1635	1/1	0.99	0.09	6,6,6,6	0
57	MG	CX	104	1/1	0.99	0.06	39,39,39,39	0
57	MG	DA	3085	1/1	0.99	0.12	1,1,1,1	0
57	MG	CA	1636	1/1	0.99	0.11	1,1,1,1	0
57	MG	CA	1637	1/1	0.99	0.09	47,47,47,47	0
57	MG	BA	3157	1/1	0.99	0.04	28,28,28,28	0
57	MG	BA	3398	1/1	0.99	0.04	11,11,11,11	0
57	MG	BA	3399	1/1	0.99	0.14	56,56,56,56	1
57	MG	DA	3091	1/1	0.99	0.10	1,1,1,1	0
57	MG	BA	3242	1/1	0.99	0.04	1,1,1,1	0
57	MG	DA	3093	1/1	0.99	0.04	9,9,9,9	0
57	MG	AV	104	1/1	0.99	0.08	58,58,58,58	1
57	MG	DA	3095	1/1	0.99	0.09	1,1,1,1	0
57	MG	BA	3040	1/1	0.99	0.06	16,16,16,16	0
57	MG	DA	3001	1/1	0.99	0.09	49,49,49,49	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	DA	3437	1/1	0.99	0.06	59,59,59,59	1
57	MG	DA	3003	1/1	0.99	0.09	1,1,1,1	1
57	MG	DA	3315	1/1	0.99	0.10	6,6,6,6	0
57	MG	BA	3245	1/1	0.99	0.03	52,52,52,52	1
57	MG	BA	3066	1/1	0.99	0.06	20,20,20,20	0
57	MG	BA	3097	1/1	0.99	0.07	1,1,1,1	0
57	MG	BA	3298	1/1	0.99	0.10	1,1,1,1	1
57	MG	BD	301	1/1	0.99	0.16	1,1,1,1	0
57	MG	CA	1717	1/1	0.99	0.10	1,1,1,1	0
57	MG	B1	103	1/1	0.99	0.03	1,1,1,1	0
57	MG	DA	3208	1/1	0.99	0.08	14,14,14,14	0
57	MG	BA	3203	1/1	0.99	0.12	10,10,10,10	0
57	MG	BA	3301	1/1	0.99	0.05	24,24,24,24	0
57	MG	BA	3354	1/1	0.99	0.04	58,58,58,58	0
57	MG	DA	3327	1/1	0.99	0.04	2,2,2,2	1
57	MG	DA	3109	1/1	0.99	0.04	17,17,17,17	0
57	MG	BA	3099	1/1	0.99	0.09	45,45,45,45	1
57	MG	DA	3111	1/1	0.99	0.01	4,4,4,4	0
57	MG	DA	3015	1/1	0.99	0.04	1,1,1,1	1
57	MG	DA	3113	1/1	0.99	0.06	1,1,1,1	0
57	MG	BA	3021	1/1	0.99	0.05	2,2,2,2	0
57	MG	BA	3304	1/1	0.99	0.03	24,24,24,24	0
57	MG	BA	3414	1/1	0.99	0.03	20,20,20,20	0
57	MG	DA	3118	1/1	0.99	0.02	9,9,9,9	0
57	MG	DD	301	1/1	0.99	0.12	1,1,1,1	0
57	MG	DD	302	1/1	0.99	0.04	2,2,2,2	0
57	MG	BA	3165	1/1	0.99	0.04	4,4,4,4	1
57	MG	DA	3222	1/1	0.99	0.04	3,3,3,3	1
57	MG	BA	3022	1/1	0.99	0.23	1,1,1,1	0
57	MG	DA	3022	1/1	0.99	0.24	28,28,28,28	1
57	MG	DF	302	1/1	0.99	0.08	15,15,15,15	0
57	MG	BA	3254	1/1	0.99	0.03	5,5,5,5	0
57	MG	BA	3023	1/1	0.99	0.07	1,1,1,1	1
57	MG	BA	3134	1/1	0.99	0.08	1,1,1,1	0
57	MG	BA	3420	1/1	0.99	0.03	10,10,10,10	0
57	MG	DA	3229	1/1	0.99	0.13	1,1,1,1	0
57	MG	DA	3126	1/1	0.99	0.23	1,1,1,1	0
57	MG	BA	3046	1/1	0.99	0.03	15,15,15,15	0
57	MG	BA	3170	1/1	0.99	0.07	1,1,1,1	1
57	MG	BA	3047	1/1	0.99	0.12	1,1,1,1	0
57	MG	DA	3234	1/1	0.99	0.06	88,88,88,88	1
57	MG	BA	3424	1/1	0.99	0.07	37,37,37,37	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	BX	101	1/1	0.99	0.05	26,26,26,26	1
57	MG	DA	3032	1/1	0.99	0.03	23,23,23,23	0
57	MG	DA	3133	1/1	0.99	0.04	9,9,9,9	0
57	MG	DA	3239	1/1	0.99	0.05	4,4,4,4	0
57	MG	BA	3260	1/1	0.99	0.06	1,1,1,1	0
57	MG	BA	3172	1/1	0.99	0.23	100,100,100,100	1
57	MG	AA	1670	1/1	0.99	0.07	22,22,22,22	0
57	MG	BA	3174	1/1	0.99	0.05	1,1,1,1	1
58	ZN	AD	303	1/1	0.99	0.10	26,26,26,26	0
58	ZN	AN	101	1/1	0.99	0.07	143,143,143,143	0
58	ZN	CD	301	1/1	0.99	0.10	35,35,35,35	0
58	ZN	CN	102	1/1	0.99	0.03	114,114,114,114	0
57	MG	BA	3319	1/1	1.00	0.05	1,1,1,1	0
57	MG	D1	103	1/1	1.00	0.02	33,33,33,33	0
57	MG	AA	1622	1/1	1.00	0.05	1,1,1,1	1
57	MG	DA	3080	1/1	1.00	0.02	1,1,1,1	1
57	MG	DA	3266	1/1	1.00	0.03	17,17,17,17	1
57	MG	BA	3272	1/1	1.00	0.02	1,1,1,1	1
57	MG	BA	3039	1/1	1.00	0.01	1,1,1,1	0
57	MG	BA	3111	1/1	1.00	0.07	1,1,1,1	0
57	MG	DA	3114	1/1	1.00	0.07	1,1,1,1	0
57	MG	BA	3024	1/1	1.00	0.19	44,44,44,44	1
57	MG	DA	3055	1/1	1.00	0.02	1,1,1,1	0
57	MG	BA	3195	1/1	1.00	0.05	39,39,39,39	1
57	MG	BA	3277	1/1	1.00	0.02	28,28,28,28	1
57	MG	DA	3002	1/1	1.00	0.03	6,6,6,6	1
57	MG	BA	3081	1/1	1.00	0.03	1,1,1,1	0
57	MG	BA	3045	1/1	1.00	0.03	1,1,1,1	1
57	MG	BA	3187	1/1	1.00	0.08	1,1,1,1	0
57	MG	BA	3237	1/1	1.00	0.04	8,8,8,8	1
57	MG	BA	3382	1/1	1.00	0.02	38,38,38,38	0
57	MG	CL	201	1/1	1.00	0.04	1,1,1,1	0
57	MG	AA	1711	1/1	1.00	0.06	21,21,21,21	1
57	MG	CA	1791	1/1	1.00	0.01	1,1,1,1	1
57	MG	DA	3348	1/1	1.00	0.02	9,9,9,9	1
57	MG	BA	3212	1/1	1.00	0.01	2,2,2,2	0
57	MG	BA	3200	1/1	1.00	0.06	5,5,5,5	1
57	MG	CA	1771	1/1	1.00	0.07	1,1,1,1	1
57	MG	CA	1627	1/1	1.00	0.11	5,5,5,5	0
57	MG	CA	1608	1/1	1.00	0.11	17,17,17,17	0
57	MG	DA	3043	1/1	1.00	0.03	6,6,6,6	0
57	MG	BA	3077	1/1	1.00	0.06	1,1,1,1	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	BA	3092	1/1	1.00	0.02	5,5,5,5	0
57	MG	CA	1691	1/1	1.00	0.04	1,1,1,1	0
57	MG	DA	3019	1/1	1.00	0.01	23,23,23,23	0

5.5 Other polymers [i](#)

There are no such residues in this entry.