



wwPDB X-ray Structure Validation Summary Report ⓘ

Apr 19, 2026 – 03:17 PM UTC

PDB ID : 4V9A / pdb_00004v9a
Title : Crystal Structure of the 70S ribosome with tetracycline.
Authors : Jenner, L.; Yusupov, M.; Yusupova, G.
Deposited on : 2012-07-18
Resolution : 3.30 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
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
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)	:	2.49

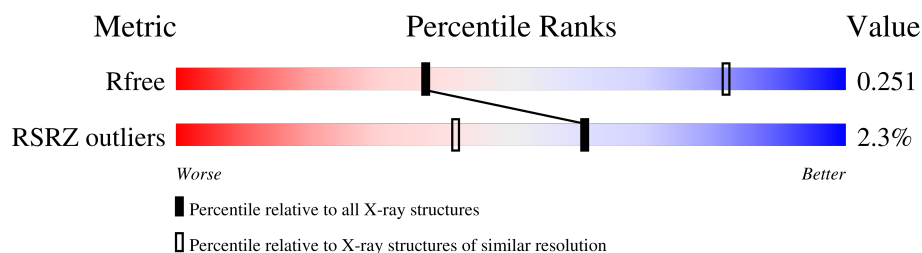
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.30 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}	180053	1169 (3.32-3.28)
RSRZ outliers	180081	1169 (3.32-3.28)

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
54	MG	AA	1674	-	-	-	X
54	MG	AC	108	-	-	-	X
54	MG	BA	3188	-	-	-	X
54	MG	BA	3507	-	-	-	X
54	MG	BA	3579	-	-	-	X
54	MG	BA	3592	-	-	-	X
54	MG	DA	3171	-	-	-	X
54	MG	DA	3248	-	-	-	X
54	MG	DA	3512	-	-	-	X
54	MG	DD	301	-	-	-	X

2 Entry composition

There are 56 unique types of molecules in this entry. The entry contains 292440 atoms, of which 1 is hydrogen 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	1506	Total	C	N	O	P	0	0	0
			32369	14408	5997	10459	1505			
1	CA	1506	Total	C	N	O	P	0	0	0
			32372	14408	5997	10461	1506			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	AE	237	Total	C	N	O	S	0	0	0
			1924	1228	344	347	5			
2	CE	237	Total	C	N	O	S	0	0	0
			1924	1228	344	347	5			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	AF	205	Total	C	N	O	S	0	0	0
			1605	1011	313	280	1			
3	CF	206	Total	C	N	O	S	0	0	0
			1612	1016	314	281	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	AG	208	Total	C	N	O	S	0	0	0
			1703	1066	339	291	7			
4	CG	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	AH	151	Total	C	N	O	S	0	0	0
			1155	729	218	204	4			
5	CH	151	Total	C	N	O	S	0	0	0
			1155	729	218	204	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	AI	101	Total	C	N	O	S	0	0	0
			843	531	155	154	3			
6	CI	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	AJ	155	Total	C	N	O	S	0	0	0
			1257	781	252	218	6			
7	CJ	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	AK	138	Total	C	N	O	S	0	0	0
			1116	705	215	193	3			
8	CK	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	AL	127	Total	C	N	O		0	0	0
			1010	639	197	174				
9	CL	127	Total	C	N	O		0	0	0
			1010	639	197	174				

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	AM	99	Total	C	N	O	S	0	0	0
			801	504	157	139	1			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	CM	99	Total	C	N	O	S	0	0	0
			801	504	157	139	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	AN	119	Total	C	N	O	S	0	0	0
			885	549	168	165	3			
11	CN	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	AO	125	Total	C	N	O	S	0	0	0
			975	614	196	164	1			
12	CO	125	Total	C	N	O	S	0	0	0
			975	614	196	164	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	AP	116	Total	C	N	O	S	0	0	0
			928	574	191	161	2			
13	CP	117	Total	C	N	O	S	0	0	0
			933	577	192	162	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	AQ	60	Total	C	N	O	S	0	0	0
			492	312	104	72	4			
14	CQ	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	AR	88	Total	C	N	O	S	0	0	0
			734	459	147	126	2			
15	CR	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	AS	84	Total	C	N	O	S	0	0	0
			705	446	140	118	1			
16	CS	84	Total	C	N	O	S	0	0	0
			705	446	140	118	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	AT	100	Total	C	N	O	S	0	0	0
			834	534	155	143	2			
17	CT	100	Total	C	N	O	S	0	0	0
			834	534	155	143	2			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
18	AU	72	Total	C	N	O	0	0	0
			591	376	117	98			
18	CU	72	Total	C	N	O	0	0	0
			591	376	117	98			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	AV	83	Total	C	N	O	S	0	0	0
			665	424	124	115	2			
19	CV	78	Total	C	N	O	S	0	0	0
			624	398	115	109	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	AW	99	Total	C	N	O	S	0	0	0
			763	470	162	129	2			
20	CW	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	AX	25	Total	C	N	O	0	0	0
			217	134	52	31			
21	CX	25	Total	C	N	O	0	0	0
			217	134	52	31			

- Molecule 22 is a RNA chain called TRNA-FMET.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	AC	77	Total	C	N	O	P	0	0	0
			1640	732	298	534	76			
22	CC	77	Total	C	N	O	P	0	0	0
			1640	732	298	534	76			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AC	17A	C	U	conflict	GB AP008226.1
AC	50	U	C	conflict	GB AP008226.1
AC	51	C	G	conflict	GB AP008226.1
AC	63	G	C	conflict	GB AP008226.1
CC	17A	C	U	conflict	GB AP008226.1
CC	50	U	C	conflict	GB AP008226.1
CC	51	C	G	conflict	GB AP008226.1
CC	63	G	C	conflict	GB AP008226.1

- Molecule 23 is a RNA chain called MRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	A1	4	Total	C	N	O	P	0	0	0
			85	38	14	29	4			
23	C1	4	Total	C	N	O	P	0	0	0
			85	38	14	29	4			

- Molecule 24 is a RNA chain called 23S ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	BA	2912	Total	C	N	O	P	0	0	0
			62707	27911	11722	20163	2911			
24	DA	2909	Total	C	N	O	P	0	0	0
			62647	27884	11716	20139	2908			

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
BA	161	U	-	insertion	GB AP008226.1
BA	654A	A	G	conflict	GB AP008226.1
BA	654E	C	G	conflict	GB AP008226.1
BA	654P	G	C	conflict	GB AP008226.1
BA	654T	A	C	conflict	GB AP008226.1
BA	1058	U	G	conflict	GB AP008226.1
BA	1080	A	C	conflict	GB AP008226.1
DA	158	U	-	insertion	GB AP008226.1
DA	654A	A	G	conflict	GB AP008226.1
DA	654E	C	G	conflict	GB AP008226.1
DA	654P	G	C	conflict	GB AP008226.1
DA	654T	A	C	conflict	GB AP008226.1
DA	1058	U	G	conflict	GB AP008226.1
DA	1080	A	C	conflict	GB AP008226.1

- Molecule 25 is a RNA chain called 5S RIBOSOMAL RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
25	BB	122	Total	C	N	O	P	0	0	0
			2617	1166	486	844	121			
25	DB	122	Total	C	N	O	P	0	0	0
			2617	1166	486	844	121			

- Molecule 26 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	BD	272	Total	C	N	O	S	0	0	0
			2115	1335	420	357	3			
26	DD	272	Total	C	N	O	S	0	0	0
			2115	1335	420	357	3			

- Molecule 27 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
27	BE	205	Total	C	N	O	S	0	0	0
			1568	991	300	271	6			
27	DE	205	Total	C	N	O	S	0	0	0
			1568	991	300	271	6			

- Molecule 28 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
28	BF	202	Total	C	N	O	S	0	0	0
			1585	1011	297	275	2			
28	DF	208	Total	C	N	O	S	0	0	0
			1627	1037	304	283	3			

- Molecule 29 is a protein called 50S ribosomal protein L5.

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

- Molecule 30 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
30	BH	170	Total	C	N	O	S	0	0	0
			1307	829	245	232	1			
30	DH	170	Total	C	N	O	S	0	0	0
			1307	829	245	232	1			

- Molecule 31 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
31	BK	146	Total	C	N	O	S	0	0	0
			1136	726	201	208	1			
31	DK	146	Total	C	N	O	S	0	0	0
			1136	726	201	208	1			

- Molecule 32 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
32	BM	138	Total	C	N	O	S	0	0	0
			1104	712	206	182	4			
32	DM	138	Total	C	N	O	S	0	0	0
			1104	712	206	182	4			

- Molecule 33 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
33	BN	122	Total	C	N	O	S	0	0	0
			933	588	171	170	4			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
33	DN	122	Total	C	N	O	S	0	0	0
			933	588	171	170	4			

- Molecule 34 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
34	BO	150	Total	C	N	O	S	0	0	0
			1145	712	232	198	3			
34	DO	150	Total	C	N	O	S	0	0	0
			1145	712	232	198	3			

- Molecule 35 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
35	BP	141	Total	C	N	O	S	0	0	0
			1122	715	212	188	7			
35	DP	141	Total	C	N	O	S	0	0	0
			1122	715	212	188	7			

- Molecule 36 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
36	B0	118	Total	C	N	O	S	0	0	0
			968	604	203	160	1			
36	D0	117	Total	C	N	O		0	0	0
			960	599	202	159				

- Molecule 37 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
37	BQ	111	Total	C	N	O	0	0	0
			882	556	176	150			
37	DQ	111	Total	C	N	O	0	0	0
			882	556	176	150			

- Molecule 38 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
38	BR	137	Total	C	N	O	S	0	0	0
			1141	710	234	196	1			
38	DR	137	Total	C	N	O	S	0	0	0
			1141	710	234	196	1			

- Molecule 39 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
39	B1	117	Total	C	N	O	S	0	0	0
			964	610	202	151	1			
39	D1	117	Total	C	N	O	S	0	0	0
			964	610	202	151	1			

- Molecule 40 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
40	B2	101	Total	C	N	O	S	0	0	0
			779	501	142	135	1			
40	D2	101	Total	C	N	O	S	0	0	0
			779	501	142	135	1			

- Molecule 41 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
41	BS	113	Total	C	N	O	S	0	0	0
			900	566	177	155	2			
41	DS	113	Total	C	N	O	S	0	0	0
			900	566	177	155	2			

- Molecule 42 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
42	BT	92	Total	C	N	O	0	0	0
			725	471	131	123			
42	DT	92	Total	C	N	O	0	0	0
			725	471	131	123			

- Molecule 43 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
43	BU	102	Total	C	N	O	S	0	0	0
			785	505	150	125	5			
43	DU	102	Total	C	N	O	S	0	0	0
			785	505	150	125	5			

- Molecule 44 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
44	BV	175	Total	C	N	O	S	0	0	0
			1397	892	251	251	3			
44	DV	179	Total	C	N	O	S	0	0	0
			1428	911	255	259	3			

- Molecule 45 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
45	B3	76	Total	C	N	O	S	0	0	0
			607	376	128	102	1			
45	D3	77	Total	C	N	O	S	0	0	0
			613	379	129	104	1			

- Molecule 46 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
46	BZ	97	Total	C	N	O	S	0	0	0
			763	481	150	131	1			
46	DZ	97	Total	C	N	O	S	0	0	0
			763	481	150	131	1			

- Molecule 47 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
47	BW	66	Total	C	N	O	S	0	0	0
			558	346	113	98	1			
47	DW	69	Total	C	N	O	S	0	0	0
			581	358	118	104	1			

- Molecule 48 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
48	BX	59	Total	C	N	O	0	0	0
			469	298	90	81			
48	DX	59	Total	C	N	O	0	0	0
			469	298	90	81			

- Molecule 49 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
49	B4	66	Total	C	N	O	S	0	0	0
			533	335	96	97	5			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
49	D4	63	Total	C	N	O	S	0	0	0
			515	326	93	91	5			

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

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

- Molecule 51 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
51	B6	45	Total	C	N	O	S	0	0	0
			389	241	79	65	4			
51	D6	45	Total	C	N	O	S	0	0	0
			389	241	79	65	4			

- Molecule 52 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
52	B7	49	Total	C	N	O	S	0	0	0
			430	263	108	57	2			
52	D7	49	Total	C	N	O	S	0	0	0
			430	263	108	57	2			

- Molecule 53 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
53	B8	61	Total	C	N	O	S	0	0	0
			488	312	99	75	2			
53	D8	61	Total	C	N	O	S	0	0	0
			488	312	99	75	2			

- Molecule 54 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
54	AA	232	Total	Mg	0	0
			232	232		
54	AG	2	Total	Mg	0	0
			2	2		

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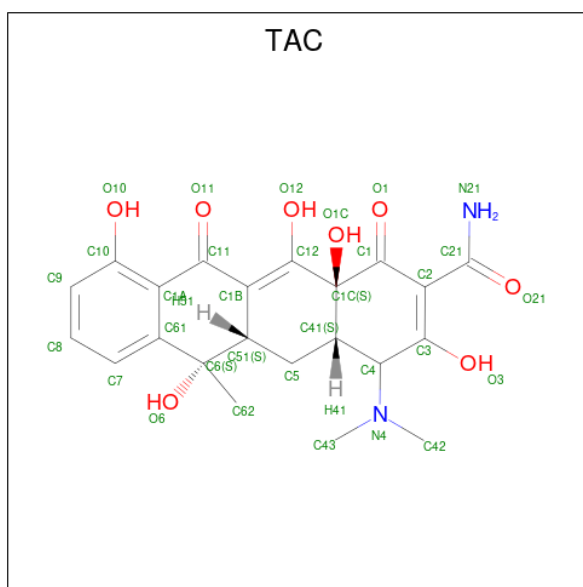
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
54	AH	2	Total 2	Mg 2	0	0
54	AJ	1	Total 1	Mg 1	0	0
54	AQ	2	Total 2	Mg 2	0	0
54	AR	1	Total 1	Mg 1	0	0
54	AS	1	Total 1	Mg 1	0	0
54	AC	9	Total 9	Mg 9	0	0
54	A1	1	Total 1	Mg 1	0	0
54	BA	627	Total 627	Mg 627	0	0
54	BB	17	Total 17	Mg 17	0	0
54	BE	5	Total 5	Mg 5	0	0
54	BF	2	Total 2	Mg 2	0	0
54	BO	3	Total 3	Mg 3	0	0
54	BP	1	Total 1	Mg 1	0	0
54	B1	2	Total 2	Mg 2	0	0
54	B2	1	Total 1	Mg 1	0	0
54	BU	2	Total 2	Mg 2	0	0
54	B3	2	Total 2	Mg 2	0	0
54	BZ	1	Total 1	Mg 1	0	0
54	B5	2	Total 2	Mg 2	0	0
54	B6	1	Total 1	Mg 1	0	0
54	B7	3	Total 3	Mg 3	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
54	B8	1	Total 1	Mg 1	0	0
54	CA	204	Total 204	Mg 204	0	0
54	CG	2	Total 2	Mg 2	0	0
54	CH	1	Total 1	Mg 1	0	0
54	CS	1	Total 1	Mg 1	0	0
54	CC	8	Total 8	Mg 8	0	0
54	DA	525	Total 525	Mg 525	0	0
54	DB	14	Total 14	Mg 14	0	0
54	DD	1	Total 1	Mg 1	0	0
54	DE	3	Total 3	Mg 3	0	0
54	DP	1	Total 1	Mg 1	0	0
54	DR	1	Total 1	Mg 1	0	0
54	D1	1	Total 1	Mg 1	0	0
54	DU	1	Total 1	Mg 1	0	0
54	DZ	2	Total 2	Mg 2	0	0
54	D5	1	Total 1	Mg 1	0	0

- Molecule 55 is TETRACYCLINE (CCD ID: TAC) (formula: $C_{22}H_{24}N_2O_8$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
55	AA	1	Total 33	C 22	H 1	N 2	O 8	0	0
55	CA	1	Total 32	C 22	N 2	O 8		0	0

- Molecule 56 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
56	AG	1	Total Zn 1 1	0	0
56	AQ	1	Total Zn 1 1	0	0
56	CG	1	Total Zn 1 1	0	0
56	CQ	1	Total Zn 1 1	0	0

MolProbit 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	209.27Å 448.54Å 615.75Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	173.07 – 3.30 173.07 – 3.30	Depositor EDS
% Data completeness (in resolution range)	100.0 (173.07-3.30) 93.5 (173.07-3.30)	Depositor EDS
R_{merge}	0.42	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.42 (at 3.33Å)	Xtriage
Refinement program	PHENIX dev_987	Depositor
R, R_{free}	0.202 , 0.254 0.198 , 0.251	Depositor DCC
R_{free} test set	2000 reflections (0.23%)	wwPDB-VP
Wilson B-factor (Å ²)	101.3	Xtriage
Anisotropy	0.267	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.25 , 56.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	292440	wwPDB-VP
Average B, all atoms (Å ²)	135.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.59% 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](#)

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

4.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

4.6 Ligand geometry [i](#)

Of 1693 ligands modelled in this entry, 1691 are monoatomic - leaving 2 for Mogul analysis.

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	$\# Z > 2$
55	TAC	AA	1833	54	34,35,35	1.52	5 (14%)	43,58,58	1.64	7 (16%)
55	TAC	CA	1805	54	34,35,35	1.46	5 (14%)	43,58,58	1.54	7 (16%)

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
55	TAC	AA	1833	54	-	4/8/74/74	0/4/4/4
55	TAC	CA	1805	54	-	8/8/74/74	0/4/4/4

The worst 5 of 10 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
55	AA	1833	TAC	C1A-C10	5.02	1.49	1.41
55	CA	1805	TAC	C1A-C10	4.69	1.48	1.41
55	AA	1833	TAC	C1A-C61	4.17	1.49	1.41
55	CA	1805	TAC	C1A-C61	3.92	1.48	1.41
55	AA	1833	TAC	C1C-C1	-3.39	1.50	1.55

The worst 5 of 14 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
55	AA	1833	TAC	C41-C1C-C1	-5.06	105.24	111.05
55	CA	1805	TAC	C41-C1C-C1	-4.84	105.49	111.05
55	AA	1833	TAC	O12-C12-C1C	4.60	120.03	113.37
55	CA	1805	TAC	O12-C12-C1C	4.22	119.48	113.37
55	AA	1833	TAC	C5-C41-C4	-3.94	108.04	113.73

There are no chirality outliers.

5 of 12 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
55	CA	1805	TAC	C1-C2-C21-O21
55	CA	1805	TAC	C1-C2-C21-N21
55	CA	1805	TAC	C3-C2-C21-O21

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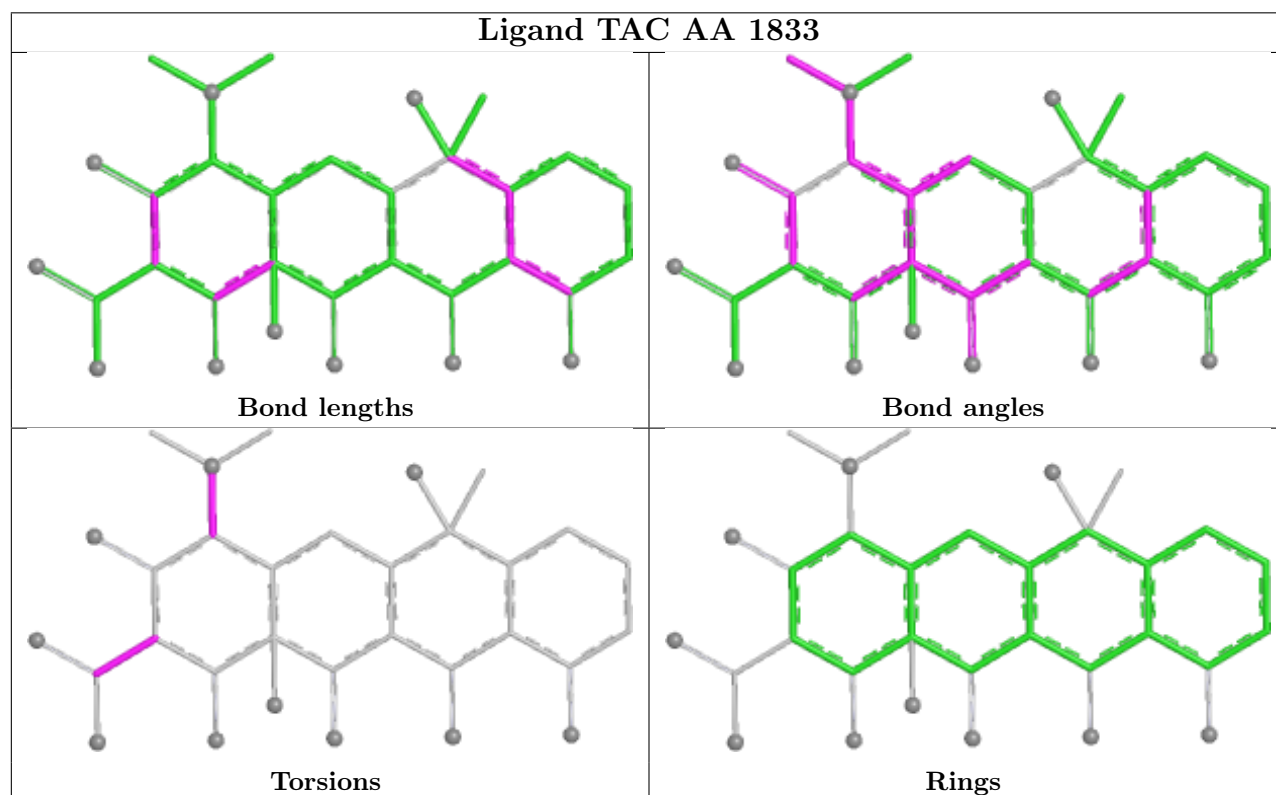
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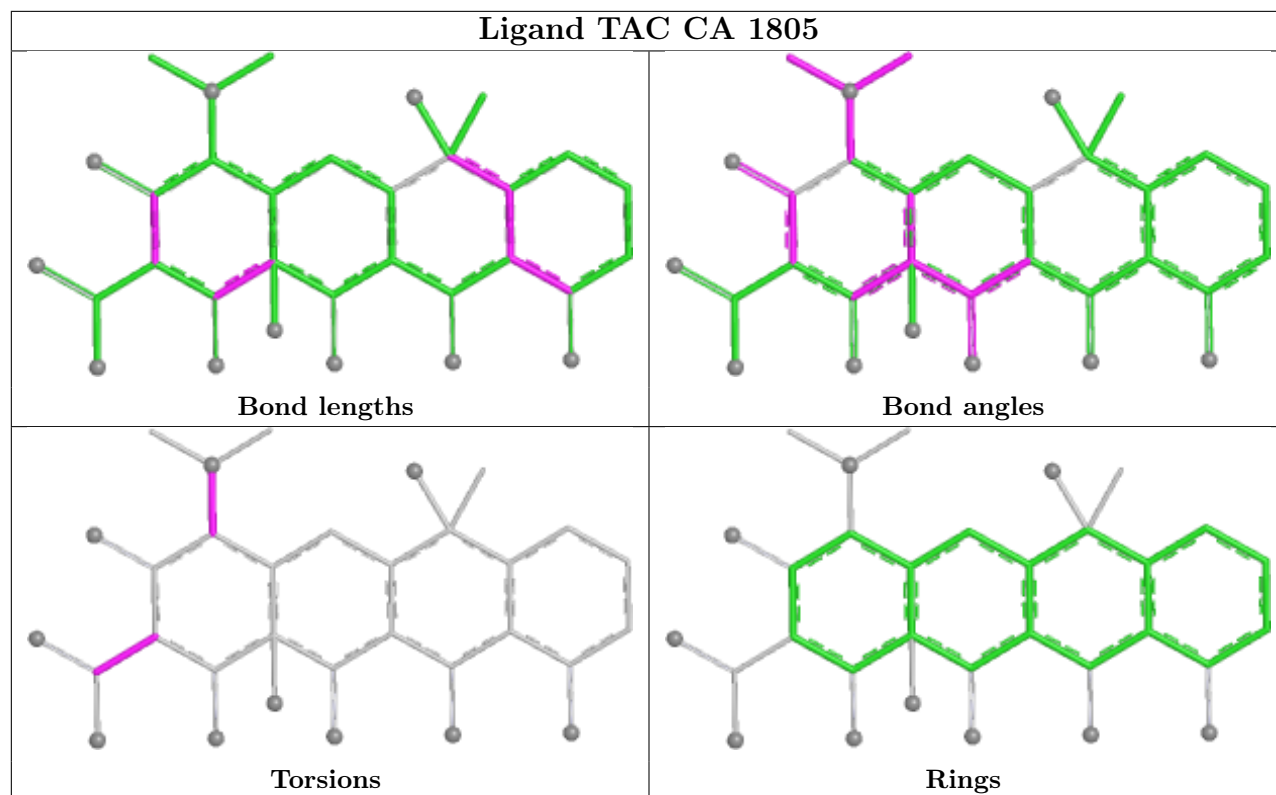
Mol	Chain	Res	Type	Atoms
55	CA	1805	TAC	C3-C2-C21-N21
55	CA	1805	TAC	C3-C4-N4-C42

There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





4.7 Other polymers [i](#)

There are no such residues in this entry.

4.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

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	1506/1506 (100%)	-0.68	23 (1%) 72 53	89, 141, 216, 277	0
1	CA	1506/1506 (100%)	-0.80	10 (0%) 84 70	103, 152, 218, 275	0
2	AE	237/256 (92%)	-0.29	4 (1%) 69 50	139, 172, 204, 216	0
2	CE	237/256 (92%)	-0.05	3 (1%) 75 56	160, 191, 219, 228	0
3	AF	205/239 (85%)	-0.09	7 (3%) 48 32	116, 151, 183, 201	0
3	CF	206/239 (86%)	0.38	9 (4%) 39 25	148, 179, 201, 211	0
4	AG	208/208 (100%)	0.03	1 (0%) 87 76	112, 149, 172, 183	0
4	CG	208/208 (100%)	-0.01	0 100 100	128, 153, 171, 180	0
5	AH	151/162 (93%)	-0.30	2 (1%) 75 56	111, 139, 161, 195	0
5	CH	151/162 (93%)	0.09	1 (0%) 84 70	129, 154, 177, 196	0
6	AI	101/101 (100%)	0.21	2 (1%) 65 46	116, 141, 162, 167	0
6	CI	101/101 (100%)	-0.36	1 (0%) 79 63	128, 149, 163, 178	0
7	AJ	155/156 (99%)	0.11	12 (7%) 19 14	129, 151, 187, 211	0
7	CJ	155/156 (99%)	-0.29	3 (1%) 66 48	146, 167, 195, 204	0
8	AK	138/138 (100%)	-0.48	0 100 100	118, 148, 162, 170	0
8	CK	138/138 (100%)	-0.16	1 (0%) 84 70	131, 159, 174, 180	0
9	AL	127/128 (99%)	-0.64	0 100 100	119, 168, 186, 192	0
9	CL	127/128 (99%)	-0.38	0 100 100	133, 185, 199, 208	0
10	AM	99/105 (94%)	-0.29	1 (1%) 79 63	119, 170, 197, 210	0
10	CM	99/105 (94%)	-0.14	1 (1%) 79 63	149, 191, 204, 209	0
11	AN	119/129 (92%)	0.56	9 (7%) 20 14	115, 137, 170, 198	0
11	CN	119/129 (92%)	-0.09	4 (3%) 48 32	124, 149, 178, 196	0
12	AO	125/128 (97%)	0.23	5 (4%) 42 28	106, 128, 150, 192	0
12	CO	125/128 (97%)	0.01	4 (3%) 50 34	111, 134, 159, 205	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	AP	116/126 (92%)	-0.53	0 100 100	103, 153, 174, 184	0
13	CP	117/126 (92%)	-0.28	1 (0%) 81 65	143, 179, 196, 205	0
14	AQ	60/61 (98%)	-0.15	1 (1%) 69 50	123, 143, 159, 161	0
14	CQ	60/61 (98%)	-0.02	1 (1%) 69 50	148, 176, 188, 191	0
15	AR	88/89 (98%)	-0.35	1 (1%) 78 60	109, 136, 155, 162	0
15	CR	88/89 (98%)	0.08	3 (3%) 48 32	121, 151, 168, 172	0
16	AS	84/88 (95%)	-0.08	1 (1%) 76 58	135, 156, 179, 198	0
16	CS	84/88 (95%)	-0.59	0 100 100	121, 143, 167, 203	0
17	AT	100/105 (95%)	-0.22	0 100 100	123, 147, 162, 173	0
17	CT	100/105 (95%)	0.06	4 (4%) 42 28	122, 145, 159, 182	0
18	AU	72/88 (81%)	0.79	10 (13%) 6 5	118, 142, 168, 195	0
18	CU	72/88 (81%)	-0.21	1 (1%) 73 55	134, 157, 181, 199	0
19	AV	83/93 (89%)	-0.41	0 100 100	133, 158, 180, 191	0
19	CV	78/93 (83%)	-0.35	1 (1%) 75 56	169, 195, 210, 221	0
20	AW	99/106 (93%)	-0.22	0 100 100	137, 159, 187, 196	0
20	CW	99/106 (93%)	-0.25	1 (1%) 79 63	112, 142, 177, 194	0
21	AX	25/27 (92%)	-0.80	0 100 100	120, 150, 170, 187	0
21	CX	25/27 (92%)	-0.32	0 100 100	144, 171, 192, 209	0
22	AC	77/77 (100%)	-0.58	1 (1%) 75 56	102, 125, 153, 175	0
22	CC	77/77 (100%)	-0.29	2 (2%) 57 38	106, 145, 175, 205	0
23	A1	4/4 (100%)	0.23	1 (25%) 2 1	106, 109, 114, 165	0
23	C1	4/4 (100%)	0.35	0 100 100	127, 131, 143, 184	0
24	BA	2912/2912 (100%)	-0.63	69 (2%) 59 40	68, 102, 240, 278	0
24	DA	2909/2912 (99%)	-0.62	40 (1%) 73 55	79, 114, 258, 279	0
25	BB	122/122 (100%)	-1.01	0 100 100	92, 122, 145, 211	0
25	DB	122/122 (100%)	-0.70	0 100 100	115, 152, 178, 226	0
26	BD	272/276 (98%)	0.31	15 (5%) 30 21	69, 96, 117, 140	0
26	DD	272/276 (98%)	0.10	9 (3%) 49 33	72, 106, 130, 155	0
27	BE	205/206 (99%)	0.30	10 (4%) 35 23	73, 117, 163, 177	0
27	DE	205/206 (99%)	0.08	2 (0%) 79 63	79, 122, 168, 196	0
28	BF	202/210 (96%)	-0.16	5 (2%) 58 39	74, 108, 149, 175	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
28	DF	208/210 (99%)	0.21	9 (4%) 40 25	82, 125, 187, 213	0
29	BG	181/182 (99%)	-0.51	1 (0%) 85 73	105, 127, 167, 186	0
29	DG	181/182 (99%)	0.09	1 (0%) 85 73	136, 166, 194, 204	0
30	BH	170/180 (94%)	-0.26	2 (1%) 76 58	103, 135, 159, 175	0
30	DH	170/180 (94%)	0.21	7 (4%) 41 27	154, 222, 249, 262	0
31	BK	146/148 (98%)	-0.25	1 (0%) 84 70	103, 151, 170, 178	0
31	DK	146/148 (98%)	-0.09	3 (2%) 63 44	111, 159, 178, 185	0
32	BM	138/140 (98%)	0.19	3 (2%) 62 43	90, 115, 153, 183	0
32	DM	138/140 (98%)	0.19	4 (2%) 53 35	93, 129, 168, 189	0
33	BN	122/122 (100%)	-0.07	2 (1%) 70 52	83, 111, 132, 139	0
33	DN	122/122 (100%)	0.22	3 (2%) 58 39	86, 116, 130, 140	0
34	BO	150/150 (100%)	0.62	16 (10%) 11 9	70, 113, 143, 207	0
34	DO	150/150 (100%)	0.20	11 (7%) 21 15	85, 129, 167, 206	0
35	BP	141/141 (100%)	0.04	1 (0%) 84 70	85, 107, 132, 163	0
35	DP	141/141 (100%)	-0.11	3 (2%) 63 44	95, 126, 152, 177	0
36	B0	118/118 (100%)	-0.09	1 (0%) 82 68	90, 110, 131, 148	0
36	D0	117/118 (99%)	-0.31	1 (0%) 81 65	88, 111, 135, 146	0
37	BQ	111/112 (99%)	-0.25	2 (1%) 67 49	90, 119, 148, 164	0
37	DQ	111/112 (99%)	-0.48	0 100 100	114, 146, 168, 190	0
38	BR	137/146 (93%)	0.17	4 (2%) 53 35	104, 125, 173, 202	0
38	DR	137/146 (93%)	0.11	4 (2%) 53 35	103, 121, 177, 212	0
39	B1	117/118 (99%)	0.02	2 (1%) 69 50	77, 106, 141, 168	0
39	D1	117/118 (99%)	-0.10	0 100 100	90, 122, 155, 178	0
40	B2	101/101 (100%)	0.18	2 (1%) 65 46	79, 122, 154, 181	0
40	D2	101/101 (100%)	0.46	8 (7%) 18 14	95, 149, 165, 181	0
41	BS	113/113 (100%)	0.22	5 (4%) 39 25	81, 102, 141, 191	0
41	DS	113/113 (100%)	0.02	4 (3%) 47 31	83, 107, 140, 194	0
42	BT	92/96 (95%)	-0.03	3 (3%) 49 33	81, 98, 126, 145	0
42	DT	92/96 (95%)	0.36	5 (5%) 31 21	96, 117, 140, 159	0
43	BU	102/110 (92%)	-0.02	2 (1%) 65 46	95, 123, 171, 190	0
43	DU	102/110 (92%)	0.83	12 (11%) 9 8	104, 142, 195, 212	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
44	BV	175/206 (84%)	0.32	5 (2%) 53 35	104, 142, 218, 229	0
44	DV	179/206 (86%)	-0.04	1 (0%) 85 73	132, 174, 237, 251	0
45	B3	76/85 (89%)	-0.51	2 (2%) 57 38	85, 101, 121, 163	0
45	D3	77/85 (90%)	-0.13	3 (3%) 43 29	98, 117, 141, 175	0
46	BZ	97/98 (98%)	0.20	4 (4%) 41 27	83, 106, 149, 195	0
46	DZ	97/98 (98%)	0.68	10 (10%) 12 10	87, 116, 159, 191	0
47	BW	66/72 (91%)	0.11	4 (6%) 27 18	80, 108, 133, 171	0
47	DW	69/72 (95%)	-0.09	2 (2%) 53 35	106, 138, 163, 196	0
48	BX	59/60 (98%)	0.02	2 (3%) 48 32	85, 106, 148, 160	0
48	DX	59/60 (98%)	0.34	3 (5%) 33 22	97, 126, 159, 194	0
49	B4	66/71 (92%)	-0.33	0 100 100	127, 176, 209, 219	0
49	D4	63/71 (88%)	0.36	1 (1%) 70 52	181, 212, 226, 235	0
50	B5	59/60 (98%)	0.46	4 (6%) 23 16	78, 115, 194, 210	0
50	D5	59/60 (98%)	0.20	4 (6%) 23 16	87, 114, 191, 218	0
51	B6	45/54 (83%)	0.32	1 (2%) 62 43	149, 184, 197, 201	0
51	D6	45/54 (83%)	0.72	7 (15%) 5 4	158, 195, 212, 215	0
52	B7	49/49 (100%)	0.17	4 (8%) 17 13	73, 83, 124, 154	0
52	D7	49/49 (100%)	0.22	3 (6%) 27 18	78, 91, 134, 156	0
53	B8	61/65 (93%)	0.15	3 (4%) 35 23	81, 96, 116, 145	0
53	D8	61/65 (93%)	0.46	4 (6%) 24 16	94, 109, 131, 161	0
All	All	20772/21286 (97%)	-0.29	471 (2%) 61 42	68, 133, 207, 279	0

The worst 5 of 471 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
7	AJ	81	GLY	8.7
50	B5	2	ALA	8.4
24	DA	2901	C	8.4
24	DA	2899	G	8.1
34	BO	94	GLU	8.1

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

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

5.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. 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($\text{\AA}^2$)	Q<0.9
54	MG	AA	1753	1/1	-0.15	0.24	143,143,143,143	0
54	MG	CA	1792	1/1	-0.06	0.18	160,160,160,160	0
54	MG	AA	1628	1/1	-0.05	0.24	142,142,142,142	0
54	MG	BA	3245	1/1	0.02	0.39	120,120,120,120	0
54	MG	AA	1772	1/1	0.05	0.27	155,155,155,155	0
54	MG	DA	3455	1/1	0.12	0.15	147,147,147,147	0
54	MG	DA	3339	1/1	0.14	0.23	152,152,152,152	0
54	MG	DA	3102	1/1	0.14	0.23	150,150,150,150	0
54	MG	AA	1765	1/1	0.16	0.17	137,137,137,137	0
54	MG	BA	3480	1/1	0.17	0.12	187,187,187,187	0
54	MG	DA	3164	1/1	0.19	0.21	136,136,136,136	0
54	MG	AA	1734	1/1	0.20	0.13	146,146,146,146	0
54	MG	CA	1757	1/1	0.21	0.17	149,149,149,149	0
54	MG	DB	206	1/1	0.24	0.15	142,142,142,142	0
54	MG	DA	3390	1/1	0.26	0.20	144,144,144,144	0
54	MG	CA	1780	1/1	0.30	0.17	137,137,137,137	0
54	MG	DA	3388	1/1	0.31	0.13	152,152,152,152	0
54	MG	BA	3373	1/1	0.33	0.15	131,131,131,131	0
54	MG	DA	3421	1/1	0.33	0.26	141,141,141,141	0
54	MG	BA	3535	1/1	0.35	0.27	116,116,116,116	0
54	MG	DA	3438	1/1	0.35	0.22	134,134,134,134	0
54	MG	BA	3429	1/1	0.35	0.19	129,129,129,129	0
54	MG	AA	1745	1/1	0.35	0.10	128,128,128,128	0
54	MG	DA	3041	1/1	0.37	0.19	142,142,142,142	0
54	MG	DA	3468	1/1	0.38	0.27	126,126,126,126	0
54	MG	CA	1799	1/1	0.38	0.17	150,150,150,150	0
54	MG	AA	1684	1/1	0.39	0.25	123,123,123,123	0
54	MG	BA	3132	1/1	0.40	0.29	127,127,127,127	0
54	MG	DA	3260	1/1	0.40	0.38	128,128,128,128	0
54	MG	BA	3617	1/1	0.40	0.12	134,134,134,134	0
54	MG	DA	3426	1/1	0.40	0.09	159,159,159,159	0
54	MG	BA	3191	1/1	0.41	0.32	111,111,111,111	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	BA	3443	1/1	0.42	0.30	124,124,124,124	0
54	MG	DA	3081	1/1	0.43	0.19	116,116,116,116	0
54	MG	AA	1671	1/1	0.43	0.31	110,110,110,110	0
54	MG	DA	3279	1/1	0.43	0.23	125,125,125,125	0
54	MG	AA	1689	1/1	0.44	0.11	153,153,153,153	0
54	MG	BA	3367	1/1	0.44	0.26	124,124,124,124	0
54	MG	BA	3116	1/1	0.44	0.14	137,137,137,137	0
54	MG	BA	3447	1/1	0.45	0.21	116,116,116,116	0
54	MG	DB	209	1/1	0.45	0.28	131,131,131,131	0
54	MG	AA	1674	1/1	0.46	0.67	119,119,119,119	0
54	MG	CA	1801	1/1	0.46	0.19	139,139,139,139	0
54	MG	BA	3446	1/1	0.46	0.12	127,127,127,127	0
54	MG	DA	3478	1/1	0.46	0.26	114,114,114,114	0
54	MG	AA	1696	1/1	0.46	0.21	104,104,104,104	0
54	MG	DA	3301	1/1	0.46	0.14	124,124,124,124	0
54	MG	CA	1750	1/1	0.47	0.25	122,122,122,122	0
54	MG	BA	3212	1/1	0.47	0.29	124,124,124,124	0
54	MG	CA	1644	1/1	0.48	0.27	133,133,133,133	0
54	MG	CC	101	1/1	0.48	0.11	130,130,130,130	0
54	MG	AA	1683	1/1	0.48	0.29	116,116,116,116	0
54	MG	CA	1793	1/1	0.48	0.22	115,115,115,115	0
54	MG	AQ	102	1/1	0.48	0.09	118,118,118,118	0
54	MG	DA	3098	1/1	0.49	0.06	139,139,139,139	0
54	MG	AA	1794	1/1	0.49	0.13	116,116,116,116	0
54	MG	DA	3485	1/1	0.49	0.19	104,104,104,104	0
54	MG	AA	1818	1/1	0.49	0.22	156,156,156,156	0
54	MG	DA	3405	1/1	0.49	0.22	121,121,121,121	0
54	MG	CA	1773	1/1	0.50	0.13	114,114,114,114	0
54	MG	CA	1631	1/1	0.51	0.17	134,134,134,134	0
54	MG	DA	3313	1/1	0.51	0.25	122,122,122,122	0
54	MG	BA	3188	1/1	0.51	0.49	120,120,120,120	0
54	MG	CA	1656	1/1	0.52	0.17	129,129,129,129	0
54	MG	CA	1695	1/1	0.52	0.27	111,111,111,111	0
54	MG	BA	3407	1/1	0.52	0.25	105,105,105,105	0
54	MG	CA	1769	1/1	0.53	0.13	136,136,136,136	0
54	MG	CA	1682	1/1	0.53	0.22	101,101,101,101	0
54	MG	BA	3395	1/1	0.53	0.27	105,105,105,105	0
54	MG	BA	3149	1/1	0.53	0.23	110,110,110,110	0
54	MG	BA	3472	1/1	0.53	0.13	114,114,114,114	0
54	MG	AG	301	1/1	0.54	0.24	114,114,114,114	0
54	MG	CC	103	1/1	0.54	0.17	150,150,150,150	0
54	MG	BA	3537	1/1	0.55	0.24	124,124,124,124	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	DA	3456	1/1	0.55	0.26	138,138,138,138	0
54	MG	BA	3517	1/1	0.55	0.12	121,121,121,121	0
54	MG	DA	3163	1/1	0.55	0.28	120,120,120,120	0
54	MG	CA	1776	1/1	0.55	0.18	125,125,125,125	0
54	MG	AA	1782	1/1	0.55	0.12	168,168,168,168	0
54	MG	DA	3450	1/1	0.55	0.28	130,130,130,130	0
54	MG	AA	1810	1/1	0.56	0.26	126,126,126,126	0
54	MG	AJ	201	1/1	0.56	0.18	108,108,108,108	0
54	MG	CA	1605	1/1	0.56	0.22	131,131,131,131	0
54	MG	BA	3319	1/1	0.56	0.26	129,129,129,129	0
54	MG	BA	3536	1/1	0.56	0.31	96,96,96,96	0
54	MG	AA	1676	1/1	0.57	0.26	132,132,132,132	0
54	MG	DA	3265	1/1	0.57	0.38	115,115,115,115	0
54	MG	DA	3096	1/1	0.57	0.24	125,125,125,125	0
54	MG	BA	3507	1/1	0.57	0.43	127,127,127,127	0
54	MG	DA	3248	1/1	0.58	0.49	112,112,112,112	0
54	MG	AA	1611	1/1	0.58	0.12	138,138,138,138	0
54	MG	AA	1778	1/1	0.58	0.13	136,136,136,136	0
54	MG	BA	3424	1/1	0.58	0.27	111,111,111,111	0
54	MG	AA	1699	1/1	0.58	0.17	122,122,122,122	0
54	MG	BA	3339	1/1	0.58	0.21	115,115,115,115	0
54	MG	DA	3329	1/1	0.58	0.14	110,110,110,110	0
54	MG	BA	3052	1/1	0.58	0.16	107,107,107,107	0
54	MG	BA	3060	1/1	0.58	0.19	105,105,105,105	0
54	MG	CA	1727	1/1	0.58	0.21	113,113,113,113	0
54	MG	BA	3562	1/1	0.58	0.29	97,97,97,97	0
54	MG	CA	1715	1/1	0.59	0.15	128,128,128,128	0
54	MG	DA	3203	1/1	0.59	0.28	90,90,90,90	0
54	MG	AA	1726	1/1	0.59	0.13	132,132,132,132	0
54	MG	CA	1745	1/1	0.59	0.18	132,132,132,132	0
54	MG	BB	207	1/1	0.59	0.21	131,131,131,131	0
54	MG	DA	3482	1/1	0.59	0.24	120,120,120,120	0
54	MG	BA	3539	1/1	0.59	0.36	99,99,99,99	0
54	MG	CA	1683	1/1	0.59	0.23	113,113,113,113	0
54	MG	DB	207	1/1	0.59	0.17	114,114,114,114	0
54	MG	AA	1717	1/1	0.59	0.12	137,137,137,137	0
54	MG	CA	1650	1/1	0.60	0.12	151,151,151,151	0
54	MG	AA	1716	1/1	0.60	0.32	107,107,107,107	0
54	MG	BA	3478	1/1	0.60	0.08	155,155,155,155	0
54	MG	AA	1673	1/1	0.60	0.15	133,133,133,133	0
54	MG	DA	3410	1/1	0.60	0.14	118,118,118,118	0
54	MG	DA	3032	1/1	0.60	0.33	127,127,127,127	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	DA	3348	1/1	0.61	0.32	108,108,108,108	0
54	MG	DA	3004	1/1	0.61	0.31	120,120,120,120	0
54	MG	AA	1709	1/1	0.61	0.09	155,155,155,155	0
54	MG	DA	3486	1/1	0.61	0.11	112,112,112,112	0
54	MG	DA	3333	1/1	0.61	0.08	128,128,128,128	0
54	MG	CA	1622	1/1	0.61	0.24	122,122,122,122	0
54	MG	DA	3347	1/1	0.61	0.24	116,116,116,116	0
54	MG	BA	3493	1/1	0.62	0.12	116,116,116,116	0
54	MG	CA	1652	1/1	0.62	0.25	120,120,120,120	0
54	MG	BA	3541	1/1	0.62	0.17	120,120,120,120	0
54	MG	BA	3419	1/1	0.62	0.21	129,129,129,129	0
54	MG	BA	3587	1/1	0.62	0.36	102,102,102,102	0
54	MG	CA	1684	1/1	0.62	0.34	115,115,115,115	0
54	MG	DA	3103	1/1	0.62	0.23	117,117,117,117	0
54	MG	DA	3152	1/1	0.62	0.28	112,112,112,112	0
54	MG	CA	1685	1/1	0.62	0.22	121,121,121,121	0
54	MG	BA	3432	1/1	0.62	0.16	126,126,126,126	0
54	MG	CA	1765	1/1	0.63	0.09	126,126,126,126	0
54	MG	DA	3428	1/1	0.63	0.08	89,89,89,89	0
54	MG	AA	1812	1/1	0.63	0.20	124,124,124,124	0
54	MG	DA	3158	1/1	0.63	0.12	113,113,113,113	0
54	MG	AA	1724	1/1	0.63	0.31	115,115,115,115	0
54	MG	CA	1740	1/1	0.63	0.15	109,109,109,109	0
54	MG	CA	1614	1/1	0.63	0.14	121,121,121,121	0
54	MG	BA	3558	1/1	0.63	0.24	118,118,118,118	0
54	MG	DA	3083	1/1	0.63	0.29	117,117,117,117	0
54	MG	CA	1751	1/1	0.63	0.28	118,118,118,118	0
54	MG	CA	1624	1/1	0.63	0.17	129,129,129,129	0
54	MG	CA	1762	1/1	0.63	0.27	116,116,116,116	0
54	MG	DA	3423	1/1	0.63	0.24	123,123,123,123	0
54	MG	DA	3424	1/1	0.63	0.21	115,115,115,115	0
54	MG	CH	201	1/1	0.64	0.29	114,114,114,114	0
54	MG	DA	3171	1/1	0.64	0.44	87,87,87,87	0
54	MG	CA	1790	1/1	0.64	0.35	118,118,118,118	0
54	MG	BA	3329	1/1	0.64	0.27	106,106,106,106	0
54	MG	DA	3375	1/1	0.64	0.15	127,127,127,127	0
54	MG	CA	1706	1/1	0.64	0.18	126,126,126,126	0
54	MG	CA	1667	1/1	0.64	0.14	139,139,139,139	0
54	MG	CA	1716	1/1	0.64	0.18	126,126,126,126	0
54	MG	DA	3292	1/1	0.64	0.18	129,129,129,129	0
54	MG	DA	3296	1/1	0.64	0.26	114,114,114,114	0
54	MG	DA	3153	1/1	0.64	0.15	145,145,145,145	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	DA	3074	1/1	0.64	0.18	109,109,109,109	0
54	MG	CA	1804	1/1	0.64	0.17	119,119,119,119	0
54	MG	BA	3292	1/1	0.65	0.13	113,113,113,113	0
54	MG	AA	1776	1/1	0.65	0.09	116,116,116,116	0
54	MG	BA	3056	1/1	0.65	0.25	101,101,101,101	0
54	MG	CA	1718	1/1	0.65	0.28	114,114,114,114	0
54	MG	CA	1626	1/1	0.65	0.18	117,117,117,117	0
54	MG	BA	3131	1/1	0.65	0.16	101,101,101,101	0
54	MG	CA	1803	1/1	0.65	0.28	123,123,123,123	0
54	MG	CA	1741	1/1	0.65	0.11	136,136,136,136	0
54	MG	CA	1705	1/1	0.65	0.30	114,114,114,114	0
54	MG	BA	3572	1/1	0.66	0.22	113,113,113,113	0
54	MG	AA	1646	1/1	0.66	0.08	150,150,150,150	0
54	MG	CA	1787	1/1	0.66	0.21	129,129,129,129	0
54	MG	AA	1725	1/1	0.66	0.07	111,111,111,111	0
54	MG	AA	1763	1/1	0.66	0.10	110,110,110,110	0
54	MG	BA	3124	1/1	0.66	0.22	110,110,110,110	0
54	MG	AC	102	1/1	0.66	0.15	123,123,123,123	0
54	MG	CA	1800	1/1	0.66	0.09	145,145,145,145	0
54	MG	BA	3398	1/1	0.66	0.29	105,105,105,105	0
54	MG	AA	1824	1/1	0.66	0.17	120,120,120,120	0
54	MG	BA	3317	1/1	0.66	0.25	99,99,99,99	0
54	MG	CA	1627	1/1	0.66	0.21	112,112,112,112	0
54	MG	BA	3137	1/1	0.66	0.12	105,105,105,105	0
54	MG	CA	1632	1/1	0.66	0.15	111,111,111,111	0
54	MG	CA	1639	1/1	0.66	0.21	129,129,129,129	0
54	MG	DA	3011	1/1	0.66	0.38	128,128,128,128	0
54	MG	DA	3028	1/1	0.66	0.22	122,122,122,122	0
54	MG	DA	3398	1/1	0.67	0.19	130,130,130,130	0
54	MG	DA	3113	1/1	0.67	0.18	105,105,105,105	0
54	MG	DA	3467	1/1	0.67	0.10	159,159,159,159	0
54	MG	AA	1714	1/1	0.67	0.10	115,115,115,115	0
54	MG	DA	3087	1/1	0.67	0.21	111,111,111,111	0
54	MG	AA	1821	1/1	0.67	0.24	110,110,110,110	0
54	MG	CC	108	1/1	0.67	0.16	129,129,129,129	0
54	MG	BA	3156	1/1	0.67	0.34	108,108,108,108	0
54	MG	BA	3456	1/1	0.67	0.06	108,108,108,108	0
54	MG	DA	3299	1/1	0.67	0.39	105,105,105,105	0
54	MG	DA	3183	1/1	0.67	0.30	92,92,92,92	0
54	MG	DA	3067	1/1	0.68	0.30	97,97,97,97	0
54	MG	CA	1676	1/1	0.68	0.30	102,102,102,102	0
54	MG	AA	1768	1/1	0.68	0.22	126,126,126,126	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	DA	3129	1/1	0.68	0.17	115,115,115,115	0
54	MG	DA	3256	1/1	0.68	0.10	103,103,103,103	0
54	MG	AA	1621	1/1	0.68	0.18	147,147,147,147	0
54	MG	BA	3285	1/1	0.68	0.15	114,114,114,114	0
54	MG	DA	3095	1/1	0.68	0.12	121,121,121,121	0
54	MG	CA	1663	1/1	0.68	0.20	105,105,105,105	0
54	MG	DA	3386	1/1	0.68	0.25	102,102,102,102	0
54	MG	BA	3109	1/1	0.68	0.32	94,94,94,94	0
54	MG	CA	1698	1/1	0.69	0.07	96,96,96,96	0
54	MG	DA	3342	1/1	0.69	0.28	114,114,114,114	0
54	MG	AA	1817	1/1	0.69	0.12	101,101,101,101	0
54	MG	BA	3242	1/1	0.69	0.29	115,115,115,115	0
54	MG	DA	3372	1/1	0.69	0.21	101,101,101,101	0
54	MG	AA	1718	1/1	0.69	0.17	124,124,124,124	0
54	MG	DA	3042	1/1	0.69	0.35	111,111,111,111	0
54	MG	DA	3138	1/1	0.69	0.30	79,79,79,79	0
54	MG	BA	3154	1/1	0.69	0.16	104,104,104,104	0
54	MG	AA	1820	1/1	0.69	0.17	130,130,130,130	0
54	MG	AA	1773	1/1	0.69	0.21	137,137,137,137	0
54	MG	BA	3096	1/1	0.69	0.28	129,129,129,129	0
54	MG	BA	3526	1/1	0.69	0.12	115,115,115,115	0
54	MG	BA	3451	1/1	0.69	0.19	102,102,102,102	0
54	MG	BA	3455	1/1	0.69	0.16	107,107,107,107	0
54	MG	BA	3465	1/1	0.70	0.40	107,107,107,107	0
54	MG	CA	1638	1/1	0.70	0.18	128,128,128,128	0
54	MG	BA	3469	1/1	0.70	0.31	125,125,125,125	0
54	MG	CA	1723	1/1	0.70	0.27	111,111,111,111	0
54	MG	DA	3441	1/1	0.70	0.37	116,116,116,116	0
54	MG	BA	3521	1/1	0.70	0.12	123,123,123,123	0
54	MG	CA	1738	1/1	0.70	0.21	114,114,114,114	0
54	MG	DA	3374	1/1	0.70	0.05	106,106,106,106	0
54	MG	BA	3095	1/1	0.70	0.10	92,92,92,92	0
54	MG	BA	3442	1/1	0.70	0.23	112,112,112,112	0
54	MG	BA	3579	1/1	0.70	0.55	85,85,85,85	0
54	MG	DA	3479	1/1	0.70	0.34	106,106,106,106	0
54	MG	DA	3037	1/1	0.70	0.16	117,117,117,117	0
54	MG	CA	1702	1/1	0.70	0.14	156,156,156,156	0
54	MG	BA	3241	1/1	0.70	0.18	91,91,91,91	0
54	MG	DA	3492	1/1	0.70	0.15	111,111,111,111	0
54	MG	BA	3196	1/1	0.70	0.14	109,109,109,109	0
54	MG	CA	1711	1/1	0.70	0.18	119,119,119,119	0
54	MG	DA	3080	1/1	0.70	0.21	114,114,114,114	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	CA	1726	1/1	0.71	0.17	111,111,111,111	0
54	MG	CA	1778	1/1	0.71	0.17	118,118,118,118	0
54	MG	CA	1713	1/1	0.71	0.15	137,137,137,137	0
54	MG	CA	1731	1/1	0.71	0.20	110,110,110,110	0
54	MG	DA	3334	1/1	0.71	0.18	136,136,136,136	0
54	MG	BA	3391	1/1	0.71	0.22	103,103,103,103	0
54	MG	AA	1701	1/1	0.71	0.29	115,115,115,115	0
54	MG	CC	107	1/1	0.71	0.11	120,120,120,120	0
54	MG	DA	3079	1/1	0.71	0.37	97,97,97,97	0
54	MG	AA	1758	1/1	0.71	0.30	111,111,111,111	0
54	MG	AA	1715	1/1	0.71	0.23	115,115,115,115	0
54	MG	CA	1774	1/1	0.71	0.10	110,110,110,110	0
54	MG	DA	3016	1/1	0.71	0.23	123,123,123,123	0
54	MG	DD	301	1/1	0.71	0.62	119,119,119,119	0
54	MG	DA	3407	1/1	0.72	0.23	114,114,114,114	0
54	MG	CA	1616	1/1	0.72	0.08	108,108,108,108	0
54	MG	DA	3104	1/1	0.72	0.18	107,107,107,107	0
54	MG	CA	1658	1/1	0.72	0.25	120,120,120,120	0
54	MG	CA	1794	1/1	0.72	0.19	109,109,109,109	0
54	MG	DA	3306	1/1	0.72	0.20	92,92,92,92	0
54	MG	BA	3439	1/1	0.72	0.16	109,109,109,109	0
54	MG	AA	1787	1/1	0.72	0.06	115,115,115,115	0
54	MG	BA	3093	1/1	0.72	0.17	154,154,154,154	0
54	MG	BA	3356	1/1	0.72	0.12	128,128,128,128	0
54	MG	DA	3162	1/1	0.72	0.22	108,108,108,108	0
54	MG	CA	1722	1/1	0.72	0.22	109,109,109,109	0
54	MG	CA	1772	1/1	0.72	0.18	109,109,109,109	0
54	MG	BA	3599	1/1	0.72	0.08	115,115,115,115	0
54	MG	DA	3367	1/1	0.72	0.15	125,125,125,125	0
54	MG	AA	1678	1/1	0.72	0.22	108,108,108,108	0
54	MG	DA	3085	1/1	0.72	0.12	113,113,113,113	0
54	MG	DA	3204	1/1	0.72	0.22	126,126,126,126	0
54	MG	DA	3377	1/1	0.72	0.23	102,102,102,102	0
54	MG	AA	1668	1/1	0.72	0.28	105,105,105,105	0
54	MG	BB	215	1/1	0.72	0.06	129,129,129,129	0
54	MG	BA	3374	1/1	0.72	0.18	104,104,104,104	0
54	MG	CA	1609	1/1	0.72	0.12	119,119,119,119	0
54	MG	BA	3097	1/1	0.72	0.36	83,83,83,83	0
54	MG	DA	3196	1/1	0.73	0.15	101,101,101,101	0
54	MG	AA	1830	1/1	0.73	0.23	135,135,135,135	0
54	MG	CA	1708	1/1	0.73	0.14	143,143,143,143	0
54	MG	DA	3058	1/1	0.73	0.14	109,109,109,109	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	BA	3396	1/1	0.73	0.21	101,101,101,101	0
54	MG	DA	3353	1/1	0.73	0.19	108,108,108,108	0
54	MG	DA	3362	1/1	0.73	0.20	120,120,120,120	0
54	MG	DA	3452	1/1	0.73	0.15	91,91,91,91	0
54	MG	AA	1691	1/1	0.73	0.29	105,105,105,105	0
54	MG	BA	3474	1/1	0.73	0.15	102,102,102,102	0
54	MG	DA	3465	1/1	0.73	0.09	111,111,111,111	0
54	MG	AG	302	1/1	0.73	0.07	162,162,162,162	0
54	MG	BA	3063	1/1	0.73	0.12	121,121,121,121	0
54	MG	BA	3486	1/1	0.73	0.26	108,108,108,108	0
54	MG	AA	1672	1/1	0.73	0.28	112,112,112,112	0
54	MG	CA	1797	1/1	0.73	0.18	127,127,127,127	0
54	MG	BA	3506	1/1	0.73	0.22	92,92,92,92	0
54	MG	DA	3310	1/1	0.73	0.10	111,111,111,111	0
54	MG	AA	1816	1/1	0.73	0.08	115,115,115,115	0
54	MG	DA	3315	1/1	0.73	0.08	125,125,125,125	0
54	MG	DA	3178	1/1	0.73	0.11	100,100,100,100	0
54	MG	DA	3419	1/1	0.73	0.11	100,100,100,100	0
54	MG	AA	1616	1/1	0.73	0.15	158,158,158,158	0
54	MG	AA	1710	1/1	0.74	0.09	116,116,116,116	0
54	MG	CA	1602	1/1	0.74	0.20	115,115,115,115	0
54	MG	BA	3320	1/1	0.74	0.29	104,104,104,104	0
54	MG	DA	3071	1/1	0.74	0.14	123,123,123,123	0
54	MG	DA	3366	1/1	0.74	0.27	103,103,103,103	0
54	MG	BA	3160	1/1	0.74	0.24	109,109,109,109	0
54	MG	DA	3105	1/1	0.74	0.14	110,110,110,110	0
54	MG	BA	3551	1/1	0.74	0.29	105,105,105,105	0
54	MG	CA	1642	1/1	0.74	0.14	105,105,105,105	0
54	MG	DA	3487	1/1	0.74	0.08	108,108,108,108	0
54	MG	BA	3614	1/1	0.74	0.33	109,109,109,109	0
54	MG	DA	3521	1/1	0.74	0.13	111,111,111,111	0
54	MG	AC	107	1/1	0.74	0.09	111,111,111,111	0
54	MG	BA	3071	1/1	0.74	0.15	103,103,103,103	0
54	MG	BB	214	1/1	0.74	0.14	108,108,108,108	0
54	MG	CA	1752	1/1	0.74	0.18	106,106,106,106	0
54	MG	BA	3112	1/1	0.75	0.22	97,97,97,97	0
54	MG	AA	1692	1/1	0.75	0.12	108,108,108,108	0
54	MG	DA	3149	1/1	0.75	0.19	112,112,112,112	0
54	MG	CA	1725	1/1	0.75	0.27	106,106,106,106	0
54	MG	AA	1741	1/1	0.75	0.14	130,130,130,130	0
54	MG	BA	3510	1/1	0.75	0.32	118,118,118,118	0
54	MG	BA	3354	1/1	0.75	0.20	113,113,113,113	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	CA	1732	1/1	0.75	0.11	144,144,144,144	0
54	MG	DA	3444	1/1	0.75	0.19	100,100,100,100	0
54	MG	AA	1613	1/1	0.75	0.12	144,144,144,144	0
54	MG	CA	1694	1/1	0.75	0.25	108,108,108,108	0
54	MG	BA	3364	1/1	0.75	0.14	137,137,137,137	0
54	MG	CA	1697	1/1	0.75	0.12	185,185,185,185	0
54	MG	BA	3280	1/1	0.75	0.21	106,106,106,106	0
54	MG	AA	1752	1/1	0.75	0.07	121,121,121,121	0
54	MG	BA	3477	1/1	0.75	0.27	93,93,93,93	0
54	MG	BA	3538	1/1	0.75	0.24	111,111,111,111	0
54	MG	DA	3253	1/1	0.75	0.20	103,103,103,103	0
54	MG	CS	101	1/1	0.75	0.17	115,115,115,115	0
54	MG	BE	303	1/1	0.75	0.32	72,72,72,72	0
54	MG	BP	201	1/1	0.75	0.29	115,115,115,115	0
54	MG	CA	1768	1/1	0.75	0.22	106,106,106,106	0
54	MG	BA	3085	1/1	0.75	0.38	95,95,95,95	0
54	MG	BA	3146	1/1	0.75	0.39	82,82,82,82	0
54	MG	DA	3402	1/1	0.75	0.25	105,105,105,105	0
54	MG	BA	3207	1/1	0.75	0.09	116,116,116,116	0
54	MG	CA	1612	1/1	0.75	0.14	122,122,122,122	0
54	MG	DA	3305	1/1	0.75	0.29	91,91,91,91	0
54	MG	AA	1769	1/1	0.76	0.08	124,124,124,124	0
54	MG	BA	3346	1/1	0.76	0.18	112,112,112,112	0
54	MG	CA	1796	1/1	0.76	0.17	115,115,115,115	0
54	MG	AA	1711	1/1	0.76	0.24	118,118,118,118	0
54	MG	B6	101	1/1	0.76	0.09	128,128,128,128	0
54	MG	AS	101	1/1	0.76	0.23	106,106,106,106	0
54	MG	CA	1709	1/1	0.76	0.20	110,110,110,110	0
54	MG	BA	3075	1/1	0.76	0.26	97,97,97,97	0
54	MG	DA	3449	1/1	0.76	0.21	106,106,106,106	0
54	MG	CA	1761	1/1	0.76	0.28	170,170,170,170	0
54	MG	BA	3282	1/1	0.76	0.24	107,107,107,107	0
54	MG	DA	3240	1/1	0.76	0.28	89,89,89,89	0
54	MG	BA	3117	1/1	0.76	0.25	102,102,102,102	0
54	MG	DA	3371	1/1	0.76	0.07	111,111,111,111	0
54	MG	BA	3291	1/1	0.76	0.30	99,99,99,99	0
54	MG	CA	1717	1/1	0.76	0.19	135,135,135,135	0
54	MG	DA	3472	1/1	0.76	0.08	102,102,102,102	0
54	MG	BA	3120	1/1	0.76	0.24	97,97,97,97	0
54	MG	AA	1813	1/1	0.76	0.16	131,131,131,131	0
54	MG	AA	1614	1/1	0.76	0.22	114,114,114,114	0
54	MG	AA	1790	1/1	0.76	0.27	115,115,115,115	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	BA	3399	1/1	0.76	0.09	90,90,90,90	0
54	MG	CA	1630	1/1	0.76	0.26	120,120,120,120	0
54	MG	DA	3399	1/1	0.76	0.06	126,126,126,126	0
54	MG	AA	1685	1/1	0.76	0.28	95,95,95,95	0
54	MG	CA	1789	1/1	0.76	0.07	121,121,121,121	0
54	MG	BA	3470	1/1	0.76	0.06	117,117,117,117	0
54	MG	CA	1637	1/1	0.76	0.15	121,121,121,121	0
54	MG	DA	3154	1/1	0.76	0.22	111,111,111,111	0
54	MG	DA	3425	1/1	0.77	0.24	122,122,122,122	0
54	MG	AA	1831	1/1	0.77	0.12	124,124,124,124	0
54	MG	DA	3343	1/1	0.77	0.23	95,95,95,95	0
54	MG	DA	3430	1/1	0.77	0.14	105,105,105,105	0
54	MG	BA	3264	1/1	0.77	0.39	75,75,75,75	0
54	MG	CA	1758	1/1	0.77	0.10	110,110,110,110	0
54	MG	BA	3623	1/1	0.77	0.26	86,86,86,86	0
54	MG	AA	1791	1/1	0.77	0.27	104,104,104,104	0
54	MG	CA	1764	1/1	0.77	0.14	110,110,110,110	0
54	MG	BB	212	1/1	0.77	0.14	103,103,103,103	0
54	MG	CA	1766	1/1	0.77	0.20	107,107,107,107	0
54	MG	BA	3389	1/1	0.77	0.20	102,102,102,102	0
54	MG	BA	3496	1/1	0.77	0.30	108,108,108,108	0
54	MG	AA	1728	1/1	0.77	0.08	85,85,85,85	0
54	MG	BA	3434	1/1	0.77	0.20	107,107,107,107	0
54	MG	BA	3225	1/1	0.77	0.27	92,92,92,92	0
54	MG	CA	1641	1/1	0.77	0.13	135,135,135,135	0
54	MG	BA	3515	1/1	0.77	0.18	112,112,112,112	0
54	MG	BA	3567	1/1	0.77	0.29	114,114,114,114	0
54	MG	CA	1781	1/1	0.77	0.11	126,126,126,126	0
54	MG	BA	3237	1/1	0.77	0.12	117,117,117,117	0
54	MG	AA	1707	1/1	0.77	0.10	94,94,94,94	0
54	MG	AA	1648	1/1	0.77	0.20	123,123,123,123	0
54	MG	DA	3512	1/1	0.77	0.44	81,81,81,81	0
54	MG	DA	3057	1/1	0.77	0.31	104,104,104,104	0
54	MG	CA	1747	1/1	0.77	0.16	122,122,122,122	0
54	MG	CA	1749	1/1	0.77	0.08	120,120,120,120	0
54	MG	DB	208	1/1	0.77	0.09	105,105,105,105	0
54	MG	BA	3530	1/1	0.77	0.11	110,110,110,110	0
54	MG	CA	1712	1/1	0.77	0.10	105,105,105,105	0
55	TAC	CA	1805	32/32	0.77	0.12	126,153,170,174	0
54	MG	DA	3110	1/1	0.78	0.24	75,75,75,75	0
54	MG	DA	3387	1/1	0.78	0.21	106,106,106,106	0
54	MG	DA	3075	1/1	0.78	0.27	105,105,105,105	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	AC	108	1/1	0.78	0.41	112,112,112,112	0
54	MG	BA	3592	1/1	0.78	0.47	112,112,112,112	0
54	MG	AA	1609	1/1	0.78	0.26	87,87,87,87	0
54	MG	B3	102	1/1	0.78	0.12	93,93,93,93	0
54	MG	DA	3258	1/1	0.78	0.27	98,98,98,98	0
54	MG	DA	3345	1/1	0.78	0.28	107,107,107,107	0
54	MG	CG	302	1/1	0.78	0.11	180,180,180,180	0
54	MG	DA	3412	1/1	0.78	0.21	110,110,110,110	0
54	MG	DA	3038	1/1	0.78	0.22	122,122,122,122	0
54	MG	DA	3156	1/1	0.78	0.10	113,113,113,113	0
54	MG	DA	3359	1/1	0.78	0.25	102,102,102,102	0
54	MG	DA	3093	1/1	0.78	0.11	106,106,106,106	0
54	MG	BA	3403	1/1	0.78	0.20	114,114,114,114	0
54	MG	BA	3378	1/1	0.78	0.06	129,129,129,129	0
54	MG	DA	3427	1/1	0.78	0.10	114,114,114,114	0
54	MG	DA	3522	1/1	0.78	0.37	113,113,113,113	0
54	MG	DA	3523	1/1	0.78	0.16	100,100,100,100	0
54	MG	DB	204	1/1	0.78	0.07	111,111,111,111	0
54	MG	BA	3318	1/1	0.78	0.25	88,88,88,88	0
54	MG	CA	1756	1/1	0.78	0.16	111,111,111,111	0
54	MG	DA	3431	1/1	0.78	0.06	101,101,101,101	0
54	MG	BA	3115	1/1	0.78	0.32	68,68,68,68	0
54	MG	AA	1747	1/1	0.78	0.09	159,159,159,159	0
54	MG	AA	1693	1/1	0.78	0.23	123,123,123,123	0
54	MG	AC	106	1/1	0.79	0.10	119,119,119,119	0
54	MG	BA	3167	1/1	0.79	0.19	95,95,95,95	0
54	MG	AA	1738	1/1	0.79	0.15	117,117,117,117	0
54	MG	DA	3435	1/1	0.79	0.11	99,99,99,99	0
54	MG	BA	3431	1/1	0.79	0.29	96,96,96,96	0
54	MG	CA	1655	1/1	0.79	0.17	125,125,125,125	0
54	MG	DA	3239	1/1	0.79	0.10	105,105,105,105	0
54	MG	BA	3122	1/1	0.79	0.21	114,114,114,114	0
54	MG	CA	1604	1/1	0.79	0.17	105,105,105,105	0
54	MG	CC	106	1/1	0.79	0.20	112,112,112,112	0
54	MG	AA	1675	1/1	0.79	0.14	93,93,93,93	0
54	MG	DA	3373	1/1	0.79	0.17	112,112,112,112	0
54	MG	BA	3489	1/1	0.79	0.36	104,104,104,104	0
54	MG	AA	1645	1/1	0.79	0.23	93,93,93,93	0
54	MG	DA	3007	1/1	0.79	0.11	116,116,116,116	0
54	MG	DA	3273	1/1	0.79	0.24	83,83,83,83	0
54	MG	AA	1732	1/1	0.79	0.24	112,112,112,112	0
54	MG	DA	3284	1/1	0.79	0.20	100,100,100,100	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	BA	3575	1/1	0.79	0.10	109,109,109,109	0
54	MG	CA	1619	1/1	0.79	0.23	111,111,111,111	0
54	MG	BA	3501	1/1	0.79	0.21	99,99,99,99	0
54	MG	CA	1687	1/1	0.79	0.16	106,106,106,106	0
54	MG	DA	3147	1/1	0.79	0.36	82,82,82,82	0
54	MG	DA	3406	1/1	0.79	0.21	103,103,103,103	0
54	MG	BA	3057	1/1	0.79	0.31	93,93,93,93	0
54	MG	BA	3232	1/1	0.79	0.24	93,93,93,93	0
54	MG	AA	1751	1/1	0.79	0.16	102,102,102,102	0
54	MG	BA	3449	1/1	0.79	0.23	118,118,118,118	0
54	MG	AA	1612	1/1	0.79	0.08	135,135,135,135	0
54	MG	AA	1815	1/1	0.79	0.15	88,88,88,88	0
54	MG	BA	3072	1/1	0.79	0.32	87,87,87,87	0
54	MG	BA	3251	1/1	0.79	0.15	109,109,109,109	0
54	MG	BA	3411	1/1	0.79	0.14	110,110,110,110	0
54	MG	DZ	102	1/1	0.79	0.16	88,88,88,88	0
54	MG	BA	3413	1/1	0.79	0.13	120,120,120,120	0
54	MG	AA	1619	1/1	0.80	0.18	96,96,96,96	0
54	MG	BA	3560	1/1	0.80	0.31	91,91,91,91	0
54	MG	BA	3054	1/1	0.80	0.28	91,91,91,91	0
54	MG	DA	3106	1/1	0.80	0.14	122,122,122,122	0
54	MG	BA	3340	1/1	0.80	0.27	95,95,95,95	0
54	MG	BA	3183	1/1	0.80	0.21	110,110,110,110	0
54	MG	BA	3350	1/1	0.80	0.18	115,115,115,115	0
54	MG	DA	3010	1/1	0.80	0.14	103,103,103,103	0
54	MG	AA	1694	1/1	0.80	0.14	105,105,105,105	0
54	MG	BA	3490	1/1	0.80	0.24	100,100,100,100	0
54	MG	DA	3023	1/1	0.80	0.25	86,86,86,86	0
54	MG	DA	3026	1/1	0.80	0.17	122,122,122,122	0
54	MG	DA	3436	1/1	0.80	0.17	120,120,120,120	0
54	MG	DA	3336	1/1	0.80	0.18	115,115,115,115	0
54	MG	BA	3127	1/1	0.80	0.32	109,109,109,109	0
54	MG	AA	1823	1/1	0.80	0.07	138,138,138,138	0
54	MG	BA	3498	1/1	0.80	0.30	107,107,107,107	0
54	MG	AA	1688	1/1	0.80	0.07	146,146,146,146	0
54	MG	BA	3502	1/1	0.80	0.26	90,90,90,90	0
54	MG	BA	3369	1/1	0.80	0.25	94,94,94,94	0
54	MG	BB	211	1/1	0.80	0.12	102,102,102,102	0
54	MG	DA	3172	1/1	0.80	0.27	110,110,110,110	0
54	MG	DA	3177	1/1	0.80	0.17	99,99,99,99	0
54	MG	BA	3370	1/1	0.80	0.20	111,111,111,111	0
54	MG	AA	1829	1/1	0.80	0.12	112,112,112,112	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	DA	3191	1/1	0.80	0.25	103,103,103,103	0
54	MG	AA	1632	1/1	0.80	0.12	116,116,116,116	0
54	MG	CA	1662	1/1	0.80	0.21	120,120,120,120	0
54	MG	BA	3307	1/1	0.80	0.22	90,90,90,90	0
54	MG	DA	3205	1/1	0.80	0.28	106,106,106,106	0
54	MG	BA	3388	1/1	0.80	0.37	100,100,100,100	0
54	MG	BA	3308	1/1	0.80	0.24	110,110,110,110	0
54	MG	BA	3452	1/1	0.80	0.22	131,131,131,131	0
54	MG	BA	3231	1/1	0.80	0.29	93,93,93,93	0
54	MG	DA	3255	1/1	0.80	0.27	87,87,87,87	0
54	MG	DA	3396	1/1	0.80	0.08	95,95,95,95	0
54	MG	AA	1634	1/1	0.80	0.10	97,97,97,97	0
54	MG	BA	3459	1/1	0.80	0.13	91,91,91,91	0
54	MG	DA	3400	1/1	0.80	0.30	105,105,105,105	0
54	MG	AA	1617	1/1	0.80	0.23	91,91,91,91	0
54	MG	BA	3077	1/1	0.80	0.19	77,77,77,77	0
54	MG	BA	3324	1/1	0.80	0.12	101,101,101,101	0
54	MG	BA	3325	1/1	0.80	0.24	89,89,89,89	0
54	MG	BA	3554	1/1	0.80	0.20	99,99,99,99	0
54	MG	DA	3351	1/1	0.81	0.32	90,90,90,90	0
54	MG	BA	3569	1/1	0.81	0.29	79,79,79,79	0
54	MG	DA	3254	1/1	0.81	0.31	74,74,74,74	0
54	MG	DA	3135	1/1	0.81	0.33	99,99,99,99	0
54	MG	AA	1623	1/1	0.81	0.22	81,81,81,81	0
54	MG	BA	3524	1/1	0.81	0.29	90,90,90,90	0
54	MG	BA	3214	1/1	0.81	0.09	93,93,93,93	0
54	MG	DA	3150	1/1	0.81	0.28	96,96,96,96	0
54	MG	BA	3372	1/1	0.81	0.32	99,99,99,99	0
54	MG	CA	1608	1/1	0.81	0.24	103,103,103,103	0
54	MG	BA	3588	1/1	0.81	0.38	109,109,109,109	0
54	MG	DA	3291	1/1	0.81	0.23	85,85,85,85	0
54	MG	AA	1704	1/1	0.81	0.18	112,112,112,112	0
54	MG	DA	3295	1/1	0.81	0.09	105,105,105,105	0
54	MG	CA	1746	1/1	0.81	0.15	92,92,92,92	0
54	MG	BA	3415	1/1	0.81	0.28	90,90,90,90	0
54	MG	DA	3475	1/1	0.81	0.23	121,121,121,121	0
54	MG	DA	3300	1/1	0.81	0.26	107,107,107,107	0
54	MG	AA	1686	1/1	0.81	0.15	120,120,120,120	0
54	MG	AA	1651	1/1	0.81	0.19	108,108,108,108	0
54	MG	DA	3090	1/1	0.81	0.21	90,90,90,90	0
54	MG	AA	1601	1/1	0.81	0.25	80,80,80,80	0
54	MG	AA	1796	1/1	0.81	0.30	109,109,109,109	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	DA	3022	1/1	0.81	0.28	86,86,86,86	0
54	MG	DA	3324	1/1	0.81	0.27	109,109,109,109	0
54	MG	DA	3519	1/1	0.81	0.14	94,94,94,94	0
54	MG	AA	1721	1/1	0.81	0.17	115,115,115,115	0
54	MG	DA	3188	1/1	0.81	0.36	69,69,69,69	0
54	MG	BA	3078	1/1	0.81	0.19	106,106,106,106	0
54	MG	DA	3420	1/1	0.81	0.12	108,108,108,108	0
54	MG	BA	3361	1/1	0.81	0.13	123,123,123,123	0
54	MG	CA	1760	1/1	0.81	0.09	135,135,135,135	0
54	MG	CA	1720	1/1	0.81	0.27	98,98,98,98	0
54	MG	BA	3205	1/1	0.81	0.10	88,88,88,88	0
54	MG	DB	214	1/1	0.81	0.06	118,118,118,118	0
54	MG	BA	3475	1/1	0.81	0.09	270,270,270,270	0
54	MG	AA	1622	1/1	0.81	0.20	96,96,96,96	0
54	MG	DA	3123	1/1	0.81	0.23	106,106,106,106	0
54	MG	DA	3190	1/1	0.82	0.42	80,80,80,80	0
54	MG	BA	3387	1/1	0.82	0.06	135,135,135,135	0
54	MG	DA	3341	1/1	0.82	0.18	107,107,107,107	0
54	MG	DA	3094	1/1	0.82	0.21	85,85,85,85	0
54	MG	DA	3005	1/1	0.82	0.33	86,86,86,86	0
54	MG	AA	1730	1/1	0.82	0.12	116,116,116,116	0
54	MG	CA	1737	1/1	0.82	0.32	97,97,97,97	0
54	MG	DA	3219	1/1	0.82	0.27	71,71,71,71	0
54	MG	B8	101	1/1	0.82	0.15	101,101,101,101	0
54	MG	BA	3228	1/1	0.82	0.22	85,85,85,85	0
54	MG	BA	3358	1/1	0.82	0.27	108,108,108,108	0
54	MG	CA	1704	1/1	0.82	0.17	95,95,95,95	0
54	MG	AA	1761	1/1	0.82	0.07	152,152,152,152	0
54	MG	BA	3323	1/1	0.82	0.38	116,116,116,116	0
54	MG	BA	3542	1/1	0.82	0.17	100,100,100,100	0
54	MG	DA	3461	1/1	0.82	0.06	102,102,102,102	0
54	MG	DA	3034	1/1	0.82	0.25	91,91,91,91	0
54	MG	DA	3466	1/1	0.82	0.14	94,94,94,94	0
54	MG	DA	3036	1/1	0.82	0.20	108,108,108,108	0
54	MG	BA	3150	1/1	0.82	0.14	90,90,90,90	0
54	MG	BA	3094	1/1	0.82	0.17	97,97,97,97	0
54	MG	DA	3139	1/1	0.82	0.33	67,67,67,67	0
54	MG	BA	3624	1/1	0.82	0.18	92,92,92,92	0
54	MG	CA	1755	1/1	0.82	0.10	97,97,97,97	0
54	MG	DA	3043	1/1	0.82	0.19	106,106,106,106	0
54	MG	CA	1618	1/1	0.82	0.11	123,123,123,123	0
54	MG	DA	3392	1/1	0.82	0.44	97,97,97,97	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	BA	3626	1/1	0.82	0.23	103,103,103,103	0
54	MG	DA	3066	1/1	0.82	0.22	79,79,79,79	0
54	MG	CA	1664	1/1	0.82	0.14	110,110,110,110	0
54	MG	CA	1666	1/1	0.82	0.13	120,120,120,120	0
54	MG	DA	3304	1/1	0.82	0.17	83,83,83,83	0
54	MG	AA	1742	1/1	0.82	0.22	108,108,108,108	0
54	MG	BA	3301	1/1	0.82	0.09	85,85,85,85	0
54	MG	AA	1750	1/1	0.82	0.10	110,110,110,110	0
54	MG	AA	1757	1/1	0.82	0.10	118,118,118,118	0
54	MG	BA	3177	1/1	0.82	0.56	101,101,101,101	0
54	MG	DA	3321	1/1	0.82	0.20	89,89,89,89	0
54	MG	CA	1767	1/1	0.82	0.24	90,90,90,90	0
54	MG	BA	3379	1/1	0.82	0.30	106,106,106,106	0
54	MG	DA	3332	1/1	0.82	0.32	120,120,120,120	0
54	MG	DU	201	1/1	0.82	0.23	103,103,103,103	0
54	MG	BA	3573	1/1	0.82	0.24	96,96,96,96	0
54	MG	CA	1729	1/1	0.82	0.36	115,115,115,115	0
54	MG	DA	3408	1/1	0.83	0.11	107,107,107,107	0
54	MG	DA	3409	1/1	0.83	0.10	132,132,132,132	0
54	MG	BA	3581	1/1	0.83	0.31	82,82,82,82	0
54	MG	BA	3584	1/1	0.83	0.38	100,100,100,100	0
54	MG	DA	3416	1/1	0.83	0.29	100,100,100,100	0
54	MG	BA	3038	1/1	0.83	0.25	67,67,67,67	0
54	MG	BA	3328	1/1	0.83	0.16	119,119,119,119	0
54	MG	BA	3258	1/1	0.83	0.29	74,74,74,74	0
54	MG	BA	3594	1/1	0.83	0.55	94,94,94,94	0
54	MG	DA	3025	1/1	0.83	0.32	88,88,88,88	0
54	MG	AA	1779	1/1	0.83	0.33	88,88,88,88	0
54	MG	CA	1633	1/1	0.83	0.18	107,107,107,107	0
54	MG	AA	1814	1/1	0.83	0.07	152,152,152,152	0
54	MG	DA	3318	1/1	0.83	0.18	91,91,91,91	0
54	MG	BA	3344	1/1	0.83	0.18	93,93,93,93	0
54	MG	BA	3392	1/1	0.83	0.19	110,110,110,110	0
54	MG	BA	3393	1/1	0.83	0.18	108,108,108,108	0
54	MG	AA	1667	1/1	0.83	0.33	88,88,88,88	0
54	MG	DA	3437	1/1	0.83	0.13	96,96,96,96	0
54	MG	BA	3532	1/1	0.83	0.20	100,100,100,100	0
54	MG	AA	1687	1/1	0.83	0.25	99,99,99,99	0
54	MG	AA	1736	1/1	0.83	0.10	122,122,122,122	0
54	MG	CA	1785	1/1	0.83	0.24	83,83,83,83	0
54	MG	CA	1654	1/1	0.83	0.08	128,128,128,128	0
54	MG	BA	3100	1/1	0.83	0.18	100,100,100,100	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	BA	3471	1/1	0.83	0.21	91,91,91,91	0
54	MG	CA	1728	1/1	0.83	0.10	144,144,144,144	0
54	MG	BA	3357	1/1	0.83	0.17	119,119,119,119	0
54	MG	AA	1705	1/1	0.83	0.16	98,98,98,98	0
54	MG	B1	202	1/1	0.83	0.17	100,100,100,100	0
54	MG	DA	3197	1/1	0.83	0.21	103,103,103,103	0
54	MG	DA	3357	1/1	0.83	0.21	105,105,105,105	0
54	MG	DA	3470	1/1	0.83	0.13	124,124,124,124	0
54	MG	BA	3110	1/1	0.83	0.13	92,92,92,92	0
54	MG	BA	3151	1/1	0.83	0.21	103,103,103,103	0
54	MG	BA	3366	1/1	0.83	0.19	95,95,95,95	0
54	MG	BA	3418	1/1	0.83	0.23	98,98,98,98	0
54	MG	DA	3226	1/1	0.83	0.26	81,81,81,81	0
54	MG	DA	3484	1/1	0.83	0.15	81,81,81,81	0
54	MG	DA	3227	1/1	0.83	0.30	83,83,83,83	0
54	MG	AA	1739	1/1	0.83	0.18	99,99,99,99	0
54	MG	AA	1602	1/1	0.83	0.20	95,95,95,95	0
54	MG	BA	3564	1/1	0.83	0.08	116,116,116,116	0
54	MG	AA	1801	1/1	0.83	0.19	97,97,97,97	0
54	MG	DA	3518	1/1	0.83	0.11	94,94,94,94	0
54	MG	BA	3164	1/1	0.83	0.26	80,80,80,80	0
54	MG	CA	1688	1/1	0.83	0.21	101,101,101,101	0
54	MG	CA	1689	1/1	0.83	0.11	122,122,122,122	0
54	MG	DA	3100	1/1	0.83	0.27	100,100,100,100	0
54	MG	CC	105	1/1	0.83	0.17	125,125,125,125	0
54	MG	DB	205	1/1	0.83	0.16	85,85,85,85	0
54	MG	DA	3394	1/1	0.83	0.11	106,106,106,106	0
54	MG	AA	1652	1/1	0.83	0.27	91,91,91,91	0
54	MG	AA	1661	1/1	0.83	0.41	94,94,94,94	0
54	MG	DA	3276	1/1	0.83	0.15	97,97,97,97	0
54	MG	BA	3376	1/1	0.83	0.27	96,96,96,96	0
54	MG	DA	3002	1/1	0.83	0.33	109,109,109,109	0
54	MG	DE	302	1/1	0.83	0.15	97,97,97,97	0
54	MG	DA	3107	1/1	0.83	0.32	100,100,100,100	0
54	MG	BA	3377	1/1	0.83	0.39	109,109,109,109	0
54	MG	CA	1759	1/1	0.83	0.06	157,157,157,157	0
54	MG	BA	3158	1/1	0.84	0.38	67,67,67,67	0
54	MG	BA	3255	1/1	0.84	0.19	110,110,110,110	0
54	MG	BA	3064	1/1	0.84	0.19	113,113,113,113	0
54	MG	AA	1811	1/1	0.84	0.06	154,154,154,154	0
54	MG	BA	3414	1/1	0.84	0.25	98,98,98,98	0
54	MG	BA	3482	1/1	0.84	0.17	88,88,88,88	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	DA	3326	1/1	0.84	0.27	82,82,82,82	0
54	MG	AC	104	1/1	0.84	0.48	107,107,107,107	0
54	MG	AA	1637	1/1	0.84	0.21	115,115,115,115	0
54	MG	DA	3434	1/1	0.84	0.31	110,110,110,110	0
54	MG	DA	3170	1/1	0.84	0.20	80,80,80,80	0
54	MG	CA	1623	1/1	0.84	0.07	180,180,180,180	0
54	MG	BA	3118	1/1	0.84	0.25	90,90,90,90	0
54	MG	DA	3338	1/1	0.84	0.34	95,95,95,95	0
54	MG	CA	1625	1/1	0.84	0.08	142,142,142,142	0
54	MG	AA	1664	1/1	0.84	0.36	96,96,96,96	0
54	MG	BA	3494	1/1	0.84	0.09	97,97,97,97	0
54	MG	BA	3121	1/1	0.84	0.20	87,87,87,87	0
54	MG	BA	3192	1/1	0.84	0.20	67,67,67,67	0
54	MG	BA	3499	1/1	0.84	0.10	103,103,103,103	0
54	MG	AA	1767	1/1	0.84	0.17	100,100,100,100	0
54	MG	DA	3460	1/1	0.84	0.22	96,96,96,96	0
54	MG	BA	3080	1/1	0.84	0.14	125,125,125,125	0
54	MG	BA	3314	1/1	0.84	0.16	104,104,104,104	0
54	MG	BA	3003	1/1	0.84	0.28	78,78,78,78	0
54	MG	BA	3612	1/1	0.84	0.12	99,99,99,99	0
54	MG	DA	3209	1/1	0.84	0.24	100,100,100,100	0
54	MG	BA	3128	1/1	0.84	0.27	99,99,99,99	0
54	MG	BA	3615	1/1	0.84	0.06	92,92,92,92	0
54	MG	AA	1680	1/1	0.84	0.17	104,104,104,104	0
54	MG	CA	1730	1/1	0.84	0.12	121,121,121,121	0
54	MG	BA	3217	1/1	0.84	0.21	92,92,92,92	0
54	MG	BA	3383	1/1	0.84	0.22	95,95,95,95	0
54	MG	BA	3522	1/1	0.84	0.05	106,106,106,106	0
54	MG	BA	3051	1/1	0.84	0.15	72,72,72,72	0
54	MG	CA	1739	1/1	0.84	0.20	112,112,112,112	0
54	MG	AA	1712	1/1	0.84	0.32	97,97,97,97	0
54	MG	DA	3101	1/1	0.84	0.30	94,94,94,94	0
54	MG	BA	3528	1/1	0.84	0.47	104,104,104,104	0
54	MG	DA	3513	1/1	0.84	0.12	95,95,95,95	0
54	MG	BA	3230	1/1	0.84	0.19	97,97,97,97	0
54	MG	AA	1719	1/1	0.84	0.10	110,110,110,110	0
54	MG	DA	3520	1/1	0.84	0.36	100,100,100,100	0
54	MG	CA	1665	1/1	0.84	0.15	103,103,103,103	0
54	MG	BB	216	1/1	0.84	0.22	111,111,111,111	0
54	MG	BB	217	1/1	0.84	0.09	132,132,132,132	0
54	MG	BA	3458	1/1	0.84	0.15	96,96,96,96	0
54	MG	AA	1650	1/1	0.84	0.22	85,85,85,85	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	BA	3464	1/1	0.84	0.38	80,80,80,80	0
54	MG	AQ	101	1/1	0.84	0.24	84,84,84,84	0
54	MG	BA	3240	1/1	0.84	0.22	93,93,93,93	0
54	MG	BA	3107	1/1	0.84	0.31	76,76,76,76	0
54	MG	AA	1760	1/1	0.84	0.09	122,122,122,122	0
54	MG	DA	3017	1/1	0.84	0.31	111,111,111,111	0
54	MG	BA	3545	1/1	0.84	0.07	108,108,108,108	0
54	MG	AA	1722	1/1	0.84	0.17	109,109,109,109	0
54	MG	DA	3307	1/1	0.84	0.28	102,102,102,102	0
54	MG	DA	3309	1/1	0.84	0.07	145,145,145,145	0
54	MG	BA	3604	1/1	0.85	0.19	97,97,97,97	0
54	MG	AH	202	1/1	0.85	0.18	108,108,108,108	0
54	MG	BA	3008	1/1	0.85	0.37	58,58,58,58	0
54	MG	DA	3021	1/1	0.85	0.20	77,77,77,77	0
54	MG	DA	3141	1/1	0.85	0.20	85,85,85,85	0
54	MG	BA	3305	1/1	0.85	0.22	80,80,80,80	0
54	MG	CA	1629	1/1	0.85	0.07	164,164,164,164	0
54	MG	DA	3422	1/1	0.85	0.24	93,93,93,93	0
54	MG	BA	3226	1/1	0.85	0.29	87,87,87,87	0
54	MG	DA	3151	1/1	0.85	0.14	113,113,113,113	0
54	MG	CA	1710	1/1	0.85	0.31	104,104,104,104	0
54	MG	DA	3311	1/1	0.85	0.19	92,92,92,92	0
54	MG	BA	3034	1/1	0.85	0.31	69,69,69,69	0
54	MG	AA	1743	1/1	0.85	0.10	136,136,136,136	0
54	MG	CA	1770	1/1	0.85	0.18	106,106,106,106	0
54	MG	AA	1754	1/1	0.85	0.12	85,85,85,85	0
54	MG	DA	3322	1/1	0.85	0.23	110,110,110,110	0
54	MG	CA	1714	1/1	0.85	0.07	94,94,94,94	0
54	MG	BB	201	1/1	0.85	0.10	99,99,99,99	0
54	MG	BB	204	1/1	0.85	0.18	86,86,86,86	0
54	MG	BA	3161	1/1	0.85	0.08	101,101,101,101	0
54	MG	DA	3439	1/1	0.85	0.10	84,84,84,84	0
54	MG	BB	208	1/1	0.85	0.25	90,90,90,90	0
54	MG	BB	209	1/1	0.85	0.09	116,116,116,116	0
54	MG	DA	3447	1/1	0.85	0.14	87,87,87,87	0
54	MG	DA	3176	1/1	0.85	0.09	112,112,112,112	0
54	MG	BA	3091	1/1	0.85	0.11	103,103,103,103	0
54	MG	BA	3484	1/1	0.85	0.14	116,116,116,116	0
54	MG	DA	3454	1/1	0.85	0.14	94,94,94,94	0
54	MG	AA	1690	1/1	0.85	0.16	128,128,128,128	0
54	MG	DA	3070	1/1	0.85	0.19	76,76,76,76	0
54	MG	DA	3458	1/1	0.85	0.08	115,115,115,115	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	BA	3321	1/1	0.85	0.18	71,71,71,71	0
54	MG	BA	3553	1/1	0.85	0.06	99,99,99,99	0
54	MG	AR	101	1/1	0.85	0.27	98,98,98,98	0
54	MG	BA	3126	1/1	0.85	0.15	89,89,89,89	0
54	MG	BA	3440	1/1	0.85	0.15	79,79,79,79	0
54	MG	AA	1654	1/1	0.85	0.15	113,113,113,113	0
54	MG	BA	3246	1/1	0.85	0.28	78,78,78,78	0
54	MG	CA	1735	1/1	0.85	0.11	103,103,103,103	0
54	MG	DA	3473	1/1	0.85	0.10	157,157,157,157	0
54	MG	BA	3190	1/1	0.85	0.26	93,93,93,93	0
54	MG	DA	3364	1/1	0.85	0.18	112,112,112,112	0
54	MG	DA	3089	1/1	0.85	0.23	117,117,117,117	0
54	MG	DA	3480	1/1	0.85	0.16	84,84,84,84	0
54	MG	BA	3334	1/1	0.85	0.20	115,115,115,115	0
54	MG	DA	3370	1/1	0.85	0.12	96,96,96,96	0
54	MG	BA	3570	1/1	0.85	0.16	82,82,82,82	0
54	MG	CG	301	1/1	0.85	0.19	115,115,115,115	0
54	MG	DA	3246	1/1	0.85	0.11	103,103,103,103	0
54	MG	DA	3488	1/1	0.85	0.21	105,105,105,105	0
54	MG	AA	1639	1/1	0.85	0.22	91,91,91,91	0
54	MG	DA	3510	1/1	0.85	0.31	77,77,77,77	0
54	MG	DA	3252	1/1	0.85	0.17	108,108,108,108	0
54	MG	CA	1680	1/1	0.85	0.29	94,94,94,94	0
54	MG	DA	3380	1/1	0.85	0.20	94,94,94,94	0
54	MG	DA	3381	1/1	0.85	0.08	97,97,97,97	0
54	MG	CA	1681	1/1	0.85	0.19	96,96,96,96	0
54	MG	AA	1733	1/1	0.85	0.11	120,120,120,120	0
54	MG	BA	3342	1/1	0.85	0.26	95,95,95,95	0
54	MG	AC	105	1/1	0.85	0.12	107,107,107,107	0
54	MG	BA	3271	1/1	0.85	0.23	96,96,96,96	0
54	MG	AA	1697	1/1	0.85	0.17	143,143,143,143	0
54	MG	DA	3272	1/1	0.85	0.36	92,92,92,92	0
54	MG	CA	1615	1/1	0.85	0.09	106,106,106,106	0
54	MG	DA	3275	1/1	0.85	0.20	93,93,93,93	0
54	MG	BA	3520	1/1	0.85	0.15	129,129,129,129	0
54	MG	DB	212	1/1	0.85	0.08	102,102,102,102	0
54	MG	DA	3401	1/1	0.85	0.10	103,103,103,103	0
54	MG	BA	3069	1/1	0.85	0.10	115,115,115,115	0
54	MG	AA	1764	1/1	0.85	0.07	118,118,118,118	0
54	MG	AA	1808	1/1	0.85	0.17	139,139,139,139	0
54	MG	DA	3117	1/1	0.85	0.33	72,72,72,72	0
54	MG	BA	3405	1/1	0.85	0.11	73,73,73,73	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	BA	3288	1/1	0.86	0.28	100,100,100,100	0
54	MG	BA	3152	1/1	0.86	0.06	90,90,90,90	0
54	MG	DA	3072	1/1	0.86	0.31	94,94,94,94	0
54	MG	BA	3513	1/1	0.86	0.13	112,112,112,112	0
54	MG	AA	1798	1/1	0.86	0.24	100,100,100,100	0
54	MG	AA	1749	1/1	0.86	0.08	112,112,112,112	0
54	MG	CA	1678	1/1	0.86	0.10	140,140,140,140	0
54	MG	CA	1679	1/1	0.86	0.16	94,94,94,94	0
54	MG	BA	3302	1/1	0.86	0.22	101,101,101,101	0
54	MG	CA	1802	1/1	0.86	0.12	136,136,136,136	0
54	MG	DA	3442	1/1	0.86	0.26	112,112,112,112	0
54	MG	DA	3443	1/1	0.86	0.08	103,103,103,103	0
54	MG	BA	3586	1/1	0.86	0.33	62,62,62,62	0
54	MG	DA	3350	1/1	0.86	0.30	82,82,82,82	0
54	MG	BA	3303	1/1	0.86	0.07	119,119,119,119	0
54	MG	BA	3359	1/1	0.86	0.16	92,92,92,92	0
54	MG	DA	3451	1/1	0.86	0.11	90,90,90,90	0
54	MG	DA	3354	1/1	0.86	0.17	105,105,105,105	0
54	MG	AA	1802	1/1	0.86	0.11	136,136,136,136	0
54	MG	BA	3525	1/1	0.86	0.15	96,96,96,96	0
54	MG	AH	201	1/1	0.86	0.16	118,118,118,118	0
54	MG	CA	1748	1/1	0.86	0.14	81,81,81,81	0
54	MG	BA	3365	1/1	0.86	0.14	104,104,104,104	0
54	MG	CC	104	1/1	0.86	0.28	95,95,95,95	0
54	MG	DA	3464	1/1	0.86	0.25	101,101,101,101	0
54	MG	BA	3607	1/1	0.86	0.24	94,94,94,94	0
54	MG	CA	1693	1/1	0.86	0.20	117,117,117,117	0
54	MG	AA	1679	1/1	0.86	0.15	105,105,105,105	0
54	MG	BA	3531	1/1	0.86	0.32	101,101,101,101	0
54	MG	DA	3469	1/1	0.86	0.23	107,107,107,107	0
54	MG	CA	1696	1/1	0.86	0.22	98,98,98,98	0
54	MG	BA	3123	1/1	0.86	0.21	73,73,73,73	0
54	MG	AA	1809	1/1	0.86	0.27	108,108,108,108	0
54	MG	DA	3474	1/1	0.86	0.23	107,107,107,107	0
54	MG	AA	1708	1/1	0.86	0.20	104,104,104,104	0
54	MG	DA	3476	1/1	0.86	0.29	99,99,99,99	0
54	MG	DA	3477	1/1	0.86	0.20	93,93,93,93	0
54	MG	BA	3022	1/1	0.86	0.30	65,65,65,65	0
54	MG	DA	3385	1/1	0.86	0.12	95,95,95,95	0
54	MG	BA	3104	1/1	0.86	0.27	70,70,70,70	0
54	MG	DA	3274	1/1	0.86	0.25	83,83,83,83	0
54	MG	BA	3481	1/1	0.86	0.22	99,99,99,99	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	DA	3124	1/1	0.86	0.16	69,69,69,69	0
54	MG	DA	3125	1/1	0.86	0.20	105,105,105,105	0
54	MG	BA	3025	1/1	0.86	0.36	65,65,65,65	0
54	MG	DA	3134	1/1	0.86	0.21	105,105,105,105	0
54	MG	DA	3491	1/1	0.86	0.25	65,65,65,65	0
54	MG	BB	206	1/1	0.86	0.12	97,97,97,97	0
54	MG	DA	3509	1/1	0.86	0.21	93,93,93,93	0
54	MG	BA	3108	1/1	0.86	0.34	82,82,82,82	0
54	MG	DA	3511	1/1	0.86	0.23	111,111,111,111	0
54	MG	BA	3544	1/1	0.86	0.20	77,77,77,77	0
54	MG	BA	3133	1/1	0.86	0.25	92,92,92,92	0
54	MG	DA	3517	1/1	0.86	0.28	106,106,106,106	0
54	MG	AA	1625	1/1	0.86	0.08	110,110,110,110	0
54	MG	BA	3262	1/1	0.86	0.31	63,63,63,63	0
54	MG	CA	1771	1/1	0.86	0.31	92,92,92,92	0
54	MG	DA	3033	1/1	0.86	0.21	89,89,89,89	0
54	MG	BA	3441	1/1	0.86	0.14	95,95,95,95	0
54	MG	CA	1645	1/1	0.86	0.12	103,103,103,103	0
54	MG	AA	1607	1/1	0.86	0.14	99,99,99,99	0
54	MG	BA	3147	1/1	0.86	0.27	64,64,64,64	0
54	MG	DA	3414	1/1	0.86	0.20	95,95,95,95	0
54	MG	AA	1641	1/1	0.86	0.11	90,90,90,90	0
54	MG	DA	3161	1/1	0.86	0.19	77,77,77,77	0
54	MG	BA	3079	1/1	0.86	0.30	99,99,99,99	0
54	MG	BE	304	1/1	0.86	0.23	112,112,112,112	0
54	MG	CA	1724	1/1	0.86	0.16	98,98,98,98	0
54	MG	DA	3166	1/1	0.86	0.27	65,65,65,65	0
54	MG	BA	3283	1/1	0.86	0.19	108,108,108,108	0
54	MG	D1	201	1/1	0.86	0.22	87,87,87,87	0
54	MG	BA	3450	1/1	0.86	0.20	99,99,99,99	0
54	MG	AA	1756	1/1	0.86	0.09	86,86,86,86	0
54	MG	DA	3068	1/1	0.86	0.13	122,122,122,122	0
54	MG	DA	3045	1/1	0.87	0.10	67,67,67,67	0
54	MG	DA	3335	1/1	0.87	0.17	78,78,78,78	0
54	MG	DA	3049	1/1	0.87	0.13	105,105,105,105	0
54	MG	DA	3052	1/1	0.87	0.14	120,120,120,120	0
54	MG	CA	1775	1/1	0.87	0.13	90,90,90,90	0
54	MG	DA	3340	1/1	0.87	0.19	89,89,89,89	0
54	MG	BA	3466	1/1	0.87	0.21	92,92,92,92	0
54	MG	CA	1777	1/1	0.87	0.08	133,133,133,133	0
54	MG	BA	3186	1/1	0.87	0.21	62,62,62,62	0
54	MG	AA	1658	1/1	0.87	0.15	79,79,79,79	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	DA	3189	1/1	0.87	0.28	65,65,65,65	0
54	MG	BA	3189	1/1	0.87	0.16	88,88,88,88	0
54	MG	CA	1782	1/1	0.87	0.17	98,98,98,98	0
54	MG	BA	3349	1/1	0.87	0.32	69,69,69,69	0
54	MG	AA	1660	1/1	0.87	0.14	126,126,126,126	0
54	MG	BA	3102	1/1	0.87	0.12	98,98,98,98	0
54	MG	BA	3410	1/1	0.87	0.18	120,120,120,120	0
54	MG	BA	3103	1/1	0.87	0.25	93,93,93,93	0
54	MG	BA	3193	1/1	0.87	0.28	76,76,76,76	0
54	MG	BA	3547	1/1	0.87	0.18	108,108,108,108	0
54	MG	BA	3011	1/1	0.87	0.27	72,72,72,72	0
54	MG	BA	3135	1/1	0.87	0.14	90,90,90,90	0
54	MG	DA	3234	1/1	0.87	0.16	92,92,92,92	0
54	MG	BA	3360	1/1	0.87	0.18	110,110,110,110	0
54	MG	BE	301	1/1	0.87	0.36	61,61,61,61	0
54	MG	BA	3070	1/1	0.87	0.21	119,119,119,119	0
54	MG	BA	3559	1/1	0.87	0.19	105,105,105,105	0
54	MG	BA	3488	1/1	0.87	0.22	109,109,109,109	0
54	MG	BA	3143	1/1	0.87	0.29	52,52,52,52	0
54	MG	CA	1672	1/1	0.87	0.23	101,101,101,101	0
54	MG	CA	1675	1/1	0.87	0.12	111,111,111,111	0
54	MG	BA	3426	1/1	0.87	0.14	77,77,77,77	0
54	MG	BA	3144	1/1	0.87	0.27	73,73,73,73	0
54	MG	BA	3568	1/1	0.87	0.17	105,105,105,105	0
54	MG	CA	1744	1/1	0.87	0.27	97,97,97,97	0
54	MG	DA	3483	1/1	0.87	0.19	88,88,88,88	0
54	MG	BA	3145	1/1	0.87	0.26	83,83,83,83	0
54	MG	AA	1638	1/1	0.87	0.20	104,104,104,104	0
54	MG	AA	1627	1/1	0.87	0.18	87,87,87,87	0
54	MG	DA	3109	1/1	0.87	0.32	63,63,63,63	0
54	MG	BA	3312	1/1	0.87	0.18	98,98,98,98	0
54	MG	BA	3030	1/1	0.87	0.21	66,66,66,66	0
54	MG	CA	1611	1/1	0.87	0.31	114,114,114,114	0
54	MG	DA	3495	1/1	0.87	0.30	78,78,78,78	0
54	MG	DA	3289	1/1	0.87	0.20	83,83,83,83	0
54	MG	AA	1826	1/1	0.87	0.08	94,94,94,94	0
54	MG	AA	1666	1/1	0.87	0.17	123,123,123,123	0
54	MG	CA	1754	1/1	0.87	0.20	97,97,97,97	0
54	MG	BA	3039	1/1	0.87	0.27	98,98,98,98	0
54	MG	CA	1691	1/1	0.87	0.18	95,95,95,95	0
54	MG	CA	1692	1/1	0.87	0.19	104,104,104,104	0
54	MG	BA	3153	1/1	0.87	0.13	89,89,89,89	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	AA	1762	1/1	0.87	0.09	124,124,124,124	0
54	MG	BA	3082	1/1	0.87	0.28	109,109,109,109	0
54	MG	CA	1621	1/1	0.87	0.21	84,84,84,84	0
54	MG	DA	3024	1/1	0.87	0.11	112,112,112,112	0
54	MG	BA	3119	1/1	0.87	0.22	78,78,78,78	0
54	MG	BA	3384	1/1	0.87	0.14	107,107,107,107	0
54	MG	CA	1700	1/1	0.87	0.15	92,92,92,92	0
54	MG	DA	3312	1/1	0.87	0.22	87,87,87,87	0
54	MG	AA	1800	1/1	0.87	0.29	92,92,92,92	0
54	MG	AA	1832	1/1	0.87	0.23	102,102,102,102	0
54	MG	AA	1784	1/1	0.87	0.12	91,91,91,91	0
54	MG	DA	3157	1/1	0.87	0.21	90,90,90,90	0
54	MG	BA	3457	1/1	0.87	0.05	112,112,112,112	0
54	MG	BA	3333	1/1	0.87	0.19	99,99,99,99	0
54	MG	DP	201	1/1	0.87	0.27	102,102,102,102	0
54	MG	AA	1785	1/1	0.87	0.08	131,131,131,131	0
54	MG	AA	1786	1/1	0.87	0.16	131,131,131,131	0
54	MG	BA	3618	1/1	0.87	0.10	107,107,107,107	0
54	MG	BA	3061	1/1	0.87	0.23	64,64,64,64	0
54	MG	BA	3468	1/1	0.88	0.09	84,84,84,84	0
54	MG	BA	3247	1/1	0.88	0.28	80,80,80,80	0
54	MG	DA	3232	1/1	0.88	0.20	78,78,78,78	0
54	MG	CA	1753	1/1	0.88	0.22	95,95,95,95	0
54	MG	BA	3609	1/1	0.88	0.21	102,102,102,102	0
54	MG	AA	1748	1/1	0.88	0.14	130,130,130,130	0
54	MG	DA	3355	1/1	0.88	0.24	89,89,89,89	0
54	MG	BA	3534	1/1	0.88	0.22	95,95,95,95	0
54	MG	BA	3253	1/1	0.88	0.12	89,89,89,89	0
54	MG	DA	3249	1/1	0.88	0.35	65,65,65,65	0
54	MG	DA	3457	1/1	0.88	0.27	102,102,102,102	0
54	MG	DA	3250	1/1	0.88	0.38	105,105,105,105	0
54	MG	DA	3459	1/1	0.88	0.08	108,108,108,108	0
54	MG	BA	3616	1/1	0.88	0.41	92,92,92,92	0
54	MG	BA	3201	1/1	0.88	0.30	122,122,122,122	0
54	MG	CA	1701	1/1	0.88	0.18	92,92,92,92	0
54	MG	BA	3368	1/1	0.88	0.22	93,93,93,93	0
54	MG	AA	1755	1/1	0.88	0.15	143,143,143,143	0
54	MG	CA	1763	1/1	0.88	0.17	94,94,94,94	0
54	MG	BA	3322	1/1	0.88	0.20	78,78,78,78	0
54	MG	BA	3625	1/1	0.88	0.20	99,99,99,99	0
54	MG	DA	3269	1/1	0.88	0.32	78,78,78,78	0
54	MG	DA	3471	1/1	0.88	0.11	102,102,102,102	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	CA	1707	1/1	0.88	0.12	109,109,109,109	0
54	MG	BA	3129	1/1	0.88	0.15	92,92,92,92	0
54	MG	BA	3427	1/1	0.88	0.29	91,91,91,91	0
54	MG	DA	3132	1/1	0.88	0.17	78,78,78,78	0
54	MG	BA	3210	1/1	0.88	0.26	78,78,78,78	0
54	MG	BA	3268	1/1	0.88	0.21	87,87,87,87	0
54	MG	BA	3326	1/1	0.88	0.21	89,89,89,89	0
54	MG	BA	3270	1/1	0.88	0.21	87,87,87,87	0
54	MG	BA	3435	1/1	0.88	0.10	109,109,109,109	0
54	MG	DA	3395	1/1	0.88	0.31	87,87,87,87	0
54	MG	BA	3436	1/1	0.88	0.15	118,118,118,118	0
54	MG	CA	1647	1/1	0.88	0.27	83,83,83,83	0
54	MG	BA	3555	1/1	0.88	0.08	67,67,67,67	0
54	MG	DA	3040	1/1	0.88	0.13	98,98,98,98	0
54	MG	AA	1806	1/1	0.88	0.23	100,100,100,100	0
54	MG	BA	3004	1/1	0.88	0.16	79,79,79,79	0
54	MG	BA	3216	1/1	0.88	0.23	95,95,95,95	0
54	MG	AA	1618	1/1	0.88	0.24	98,98,98,98	0
54	MG	BA	3385	1/1	0.88	0.23	72,72,72,72	0
54	MG	BE	302	1/1	0.88	0.51	104,104,104,104	0
54	MG	CA	1786	1/1	0.88	0.04	192,192,192,192	0
54	MG	BA	3163	1/1	0.88	0.17	104,104,104,104	0
54	MG	DA	3060	1/1	0.88	0.25	101,101,101,101	0
54	MG	BA	3089	1/1	0.88	0.32	77,77,77,77	0
54	MG	BF	301	1/1	0.88	0.08	100,100,100,100	0
54	MG	BA	3448	1/1	0.88	0.10	95,95,95,95	0
54	MG	AA	1727	1/1	0.88	0.14	110,110,110,110	0
54	MG	DA	3320	1/1	0.88	0.10	110,110,110,110	0
54	MG	BA	3571	1/1	0.88	0.24	85,85,85,85	0
54	MG	DA	3175	1/1	0.88	0.19	101,101,101,101	0
54	MG	BA	3345	1/1	0.88	0.07	95,95,95,95	0
54	MG	DA	3524	1/1	0.88	0.12	86,86,86,86	0
54	MG	BA	3020	1/1	0.88	0.41	109,109,109,109	0
54	MG	AA	1792	1/1	0.88	0.31	93,93,93,93	0
54	MG	DA	3078	1/1	0.88	0.16	97,97,97,97	0
54	MG	BA	3576	1/1	0.88	0.05	120,120,120,120	0
54	MG	DA	3429	1/1	0.88	0.22	97,97,97,97	0
54	MG	BA	3453	1/1	0.88	0.22	85,85,85,85	0
54	MG	BA	3066	1/1	0.88	0.14	97,97,97,97	0
54	MG	AA	1793	1/1	0.88	0.25	103,103,103,103	0
54	MG	BA	3304	1/1	0.88	0.18	90,90,90,90	0
54	MG	AA	1649	1/1	0.88	0.20	90,90,90,90	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	AA	1615	1/1	0.88	0.17	95,95,95,95	0
54	MG	AA	1647	1/1	0.88	0.20	96,96,96,96	0
54	MG	AA	1799	1/1	0.88	0.19	79,79,79,79	0
54	MG	CA	1617	1/1	0.88	0.17	140,140,140,140	0
54	MG	AA	1770	1/1	0.88	0.33	98,98,98,98	0
54	MG	BA	3546	1/1	0.89	0.18	97,97,97,97	0
54	MG	BA	3492	1/1	0.89	0.19	76,76,76,76	0
54	MG	BA	3548	1/1	0.89	0.15	96,96,96,96	0
54	MG	DA	3001	1/1	0.89	0.22	83,83,83,83	0
54	MG	DA	3346	1/1	0.89	0.26	93,93,93,93	0
54	MG	BA	3099	1/1	0.89	0.34	74,74,74,74	0
54	MG	CA	1635	1/1	0.89	0.14	78,78,78,78	0
54	MG	BA	3552	1/1	0.89	0.09	98,98,98,98	0
54	MG	AA	1797	1/1	0.89	0.41	82,82,82,82	0
54	MG	DA	3008	1/1	0.89	0.18	93,93,93,93	0
54	MG	BA	3495	1/1	0.89	0.18	73,73,73,73	0
54	MG	AA	1670	1/1	0.89	0.16	83,83,83,83	0
54	MG	BA	3125	1/1	0.89	0.21	88,88,88,88	0
54	MG	AA	1636	1/1	0.89	0.15	92,92,92,92	0
54	MG	BA	3024	1/1	0.89	0.09	81,81,81,81	0
54	MG	BA	3206	1/1	0.89	0.19	99,99,99,99	0
54	MG	DA	3462	1/1	0.89	0.17	102,102,102,102	0
54	MG	BA	3504	1/1	0.89	0.23	88,88,88,88	0
54	MG	BA	3058	1/1	0.89	0.10	103,103,103,103	0
54	MG	DA	3116	1/1	0.89	0.27	77,77,77,77	0
54	MG	CA	1653	1/1	0.89	0.15	122,122,122,122	0
54	MG	AA	1735	1/1	0.89	0.26	91,91,91,91	0
54	MG	BA	3265	1/1	0.89	0.26	96,96,96,96	0
54	MG	DA	3263	1/1	0.89	0.11	129,129,129,129	0
54	MG	DA	3264	1/1	0.89	0.21	80,80,80,80	0
54	MG	DA	3031	1/1	0.89	0.12	70,70,70,70	0
54	MG	BA	3511	1/1	0.89	0.14	80,80,80,80	0
54	MG	BA	3211	1/1	0.89	0.28	77,77,77,77	0
54	MG	BA	3462	1/1	0.89	0.07	113,113,113,113	0
54	MG	BA	3516	1/1	0.89	0.13	80,80,80,80	0
54	MG	CA	1779	1/1	0.89	0.14	112,112,112,112	0
54	MG	AA	1631	1/1	0.89	0.19	96,96,96,96	0
54	MG	DA	3140	1/1	0.89	0.19	74,74,74,74	0
54	MG	DA	3283	1/1	0.89	0.18	114,114,114,114	0
54	MG	DA	3481	1/1	0.89	0.32	101,101,101,101	0
54	MG	BA	3088	1/1	0.89	0.25	97,97,97,97	0
54	MG	DA	3287	1/1	0.89	0.19	67,67,67,67	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	BA	3421	1/1	0.89	0.10	106,106,106,106	0
54	MG	DA	3148	1/1	0.89	0.24	70,70,70,70	0
54	MG	BA	3279	1/1	0.89	0.30	74,74,74,74	0
54	MG	CA	1670	1/1	0.89	0.17	91,91,91,91	0
54	MG	DA	3044	1/1	0.89	0.10	96,96,96,96	0
54	MG	DA	3489	1/1	0.89	0.40	98,98,98,98	0
54	MG	BA	3162	1/1	0.89	0.14	72,72,72,72	0
54	MG	DA	3048	1/1	0.89	0.22	84,84,84,84	0
54	MG	CA	1603	1/1	0.89	0.22	93,93,93,93	0
54	MG	DA	3050	1/1	0.89	0.09	108,108,108,108	0
54	MG	BA	3331	1/1	0.89	0.22	74,74,74,74	0
54	MG	BA	3032	1/1	0.89	0.22	69,69,69,69	0
54	MG	AA	1657	1/1	0.89	0.27	63,63,63,63	0
54	MG	BA	3166	1/1	0.89	0.19	86,86,86,86	0
54	MG	BA	3092	1/1	0.89	0.10	111,111,111,111	0
54	MG	BA	3595	1/1	0.89	0.44	105,105,105,105	0
54	MG	DA	3417	1/1	0.89	0.20	110,110,110,110	0
54	MG	BA	3598	1/1	0.89	0.13	84,84,84,84	0
54	MG	BA	3229	1/1	0.89	0.18	89,89,89,89	0
54	MG	BA	3138	1/1	0.89	0.21	81,81,81,81	0
54	MG	AA	1603	1/1	0.89	0.13	109,109,109,109	0
54	MG	BA	3185	1/1	0.89	0.21	112,112,112,112	0
54	MG	DA	3525	1/1	0.89	0.15	103,103,103,103	0
54	MG	BA	3610	1/1	0.89	0.29	85,85,85,85	0
54	MG	DA	3077	1/1	0.89	0.13	96,96,96,96	0
54	MG	AA	1630	1/1	0.89	0.10	105,105,105,105	0
54	MG	DA	3180	1/1	0.89	0.19	82,82,82,82	0
54	MG	DA	3327	1/1	0.89	0.26	70,70,70,70	0
54	MG	BA	3483	1/1	0.89	0.14	89,89,89,89	0
54	MG	DB	211	1/1	0.89	0.17	107,107,107,107	0
54	MG	BA	3040	1/1	0.89	0.18	88,88,88,88	0
54	MG	BA	3540	1/1	0.89	0.31	122,122,122,122	0
54	MG	BA	3352	1/1	0.89	0.23	87,87,87,87	0
54	MG	DA	3084	1/1	0.89	0.18	98,98,98,98	0
54	MG	DE	303	1/1	0.89	0.26	70,70,70,70	0
54	MG	BA	3445	1/1	0.89	0.06	156,156,156,156	0
54	MG	DA	3337	1/1	0.89	0.20	88,88,88,88	0
54	MG	BA	3050	1/1	0.89	0.27	75,75,75,75	0
54	MG	DZ	101	1/1	0.89	0.19	113,113,113,113	0
54	MG	DA	3200	1/1	0.89	0.10	112,112,112,112	0
54	MG	AA	1723	1/1	0.89	0.22	92,92,92,92	0
54	MG	BA	3012	1/1	0.90	0.17	70,70,70,70	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	BA	3497	1/1	0.90	0.37	78,78,78,78	0
54	MG	AA	1819	1/1	0.90	0.09	81,81,81,81	0
54	MG	BB	210	1/1	0.90	0.23	78,78,78,78	0
54	MG	BA	3557	1/1	0.90	0.08	92,92,92,92	0
54	MG	BA	3021	1/1	0.90	0.35	72,72,72,72	0
54	MG	AA	1665	1/1	0.90	0.29	84,84,84,84	0
54	MG	BA	3155	1/1	0.90	0.07	113,113,113,113	0
54	MG	DA	3330	1/1	0.90	0.11	82,82,82,82	0
54	MG	CA	1651	1/1	0.90	0.16	116,116,116,116	0
54	MG	BA	3454	1/1	0.90	0.19	103,103,103,103	0
54	MG	DA	3185	1/1	0.90	0.31	66,66,66,66	0
54	MG	CA	1798	1/1	0.90	0.23	84,84,84,84	0
54	MG	BA	3505	1/1	0.90	0.40	108,108,108,108	0
54	MG	BA	3023	1/1	0.90	0.16	66,66,66,66	0
54	MG	BA	3248	1/1	0.90	0.41	74,74,74,74	0
54	MG	DA	3195	1/1	0.90	0.27	104,104,104,104	0
54	MG	BA	3408	1/1	0.90	0.07	109,109,109,109	0
54	MG	BA	3249	1/1	0.90	0.13	84,84,84,84	0
54	MG	CA	1661	1/1	0.90	0.13	98,98,98,98	0
54	MG	AA	1731	1/1	0.90	0.20	90,90,90,90	0
54	MG	BO	202	1/1	0.90	0.16	98,98,98,98	0
54	MG	BA	3514	1/1	0.90	0.36	90,90,90,90	0
54	MG	BA	3315	1/1	0.90	0.25	91,91,91,91	0
54	MG	DA	3217	1/1	0.90	0.18	89,89,89,89	0
54	MG	DA	3463	1/1	0.90	0.20	109,109,109,109	0
54	MG	DA	3091	1/1	0.90	0.24	87,87,87,87	0
54	MG	DA	3225	1/1	0.90	0.16	89,89,89,89	0
54	MG	DA	3352	1/1	0.90	0.19	81,81,81,81	0
54	MG	BU	201	1/1	0.90	0.11	105,105,105,105	0
54	MG	BA	3463	1/1	0.90	0.18	77,77,77,77	0
54	MG	DA	3229	1/1	0.90	0.31	94,94,94,94	0
54	MG	CA	1742	1/1	0.90	0.28	98,98,98,98	0
54	MG	BZ	101	1/1	0.90	0.09	69,69,69,69	0
54	MG	DA	3361	1/1	0.90	0.18	93,93,93,93	0
54	MG	DA	3097	1/1	0.90	0.29	74,74,74,74	0
54	MG	B5	102	1/1	0.90	0.14	92,92,92,92	0
54	MG	DA	3241	1/1	0.90	0.29	69,69,69,69	0
54	MG	CA	1673	1/1	0.90	0.18	89,89,89,89	0
54	MG	AA	1803	1/1	0.90	0.10	133,133,133,133	0
54	MG	B7	101	1/1	0.90	0.29	67,67,67,67	0
54	MG	BA	3084	1/1	0.90	0.25	110,110,110,110	0
54	MG	DA	3251	1/1	0.90	0.20	91,91,91,91	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	CA	1601	1/1	0.90	0.24	108,108,108,108	0
54	MG	BA	3027	1/1	0.90	0.29	69,69,69,69	0
54	MG	BA	3467	1/1	0.90	0.10	102,102,102,102	0
54	MG	BA	3261	1/1	0.90	0.18	90,90,90,90	0
54	MG	BA	3420	1/1	0.90	0.22	70,70,70,70	0
54	MG	DA	3382	1/1	0.90	0.27	80,80,80,80	0
54	MG	DA	3384	1/1	0.90	0.26	77,77,77,77	0
54	MG	CA	1607	1/1	0.90	0.27	83,83,83,83	0
54	MG	BA	3086	1/1	0.90	0.18	88,88,88,88	0
54	MG	DA	3114	1/1	0.90	0.24	82,82,82,82	0
54	MG	CA	1686	1/1	0.90	0.25	79,79,79,79	0
54	MG	DA	3019	1/1	0.90	0.31	84,84,84,84	0
54	MG	DA	3502	1/1	0.90	0.24	64,64,64,64	0
54	MG	DA	3506	1/1	0.90	0.42	61,61,61,61	0
54	MG	DA	3120	1/1	0.90	0.13	75,75,75,75	0
54	MG	BA	3527	1/1	0.90	0.09	109,109,109,109	0
54	MG	AA	1805	1/1	0.90	0.15	108,108,108,108	0
54	MG	BA	3529	1/1	0.90	0.23	89,89,89,89	0
54	MG	CA	1613	1/1	0.90	0.14	94,94,94,94	0
54	MG	BA	3114	1/1	0.90	0.28	83,83,83,83	0
54	MG	AA	1825	1/1	0.90	0.11	93,93,93,93	0
54	MG	DA	3280	1/1	0.90	0.05	94,94,94,94	0
54	MG	DA	3027	1/1	0.90	0.15	115,115,115,115	0
54	MG	BA	3428	1/1	0.90	0.23	80,80,80,80	0
54	MG	DA	3286	1/1	0.90	0.08	115,115,115,115	0
54	MG	BA	3269	1/1	0.90	0.11	85,85,85,85	0
54	MG	BA	3218	1/1	0.90	0.37	75,75,75,75	0
54	MG	BA	3223	1/1	0.90	0.25	84,84,84,84	0
54	MG	CA	1620	1/1	0.90	0.15	73,73,73,73	0
54	MG	BA	3278	1/1	0.90	0.22	101,101,101,101	0
54	MG	BA	3090	1/1	0.90	0.13	78,78,78,78	0
54	MG	DA	3415	1/1	0.90	0.18	84,84,84,84	0
54	MG	DA	3298	1/1	0.90	0.21	96,96,96,96	0
54	MG	BA	3178	1/1	0.90	0.32	78,78,78,78	0
54	MG	BA	3033	1/1	0.90	0.24	75,75,75,75	0
54	MG	BA	3485	1/1	0.90	0.10	90,90,90,90	0
54	MG	BA	3338	1/1	0.90	0.32	103,103,103,103	0
54	MG	BA	3619	1/1	0.90	0.06	88,88,88,88	0
54	MG	AA	1626	1/1	0.90	0.14	80,80,80,80	0
54	MG	BA	3067	1/1	0.90	0.35	108,108,108,108	0
54	MG	AA	1766	1/1	0.90	0.04	94,94,94,94	0
54	MG	DA	3160	1/1	0.90	0.35	84,84,84,84	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	BA	3343	1/1	0.90	0.18	86,86,86,86	0
54	MG	AA	1744	1/1	0.90	0.12	180,180,180,180	0
54	MG	AA	1775	1/1	0.90	0.18	80,80,80,80	0
54	MG	BA	3300	1/1	0.90	0.12	102,102,102,102	0
54	MG	DA	3173	1/1	0.91	0.15	92,92,92,92	0
54	MG	BA	3476	1/1	0.91	0.34	59,59,59,59	0
54	MG	DA	3314	1/1	0.91	0.25	83,83,83,83	0
54	MG	DA	3076	1/1	0.91	0.30	75,75,75,75	0
54	MG	DA	3316	1/1	0.91	0.14	124,124,124,124	0
54	MG	BA	3001	1/1	0.91	0.32	53,53,53,53	0
54	MG	BA	3433	1/1	0.91	0.22	107,107,107,107	0
54	MG	CA	1743	1/1	0.91	0.16	117,117,117,117	0
54	MG	AA	1643	1/1	0.91	0.09	112,112,112,112	0
54	MG	CA	1606	1/1	0.91	0.17	100,100,100,100	0
54	MG	AA	1662	1/1	0.91	0.24	111,111,111,111	0
54	MG	CC	102	1/1	0.91	0.21	83,83,83,83	0
54	MG	BA	3159	1/1	0.91	0.20	101,101,101,101	0
54	MG	BA	3533	1/1	0.91	0.25	106,106,106,106	0
54	MG	DA	3448	1/1	0.91	0.13	89,89,89,89	0
54	MG	DA	3194	1/1	0.91	0.25	91,91,91,91	0
54	MG	DA	3088	1/1	0.91	0.20	99,99,99,99	0
54	MG	AA	1605	1/1	0.91	0.16	108,108,108,108	0
54	MG	BA	3227	1/1	0.91	0.25	82,82,82,82	0
54	MG	DA	3198	1/1	0.91	0.23	95,95,95,95	0
54	MG	BA	3310	1/1	0.91	0.23	103,103,103,103	0
54	MG	DA	3202	1/1	0.91	0.28	88,88,88,88	0
54	MG	AA	1698	1/1	0.91	0.10	132,132,132,132	0
54	MG	BA	3351	1/1	0.91	0.24	84,84,84,84	0
54	MG	AA	1827	1/1	0.91	0.09	82,82,82,82	0
54	MG	DA	3207	1/1	0.91	0.27	86,86,86,86	0
54	MG	DA	3003	1/1	0.91	0.24	130,130,130,130	0
54	MG	DA	3213	1/1	0.91	0.23	67,67,67,67	0
54	MG	BA	3043	1/1	0.91	0.27	83,83,83,83	0
54	MG	BA	3316	1/1	0.91	0.26	82,82,82,82	0
54	MG	DA	3224	1/1	0.91	0.21	61,61,61,61	0
54	MG	DA	3006	1/1	0.91	0.33	69,69,69,69	0
54	MG	BA	3194	1/1	0.91	0.04	113,113,113,113	0
54	MG	BA	3543	1/1	0.91	0.13	90,90,90,90	0
54	MG	BA	3400	1/1	0.91	0.28	101,101,101,101	0
54	MG	BA	3401	1/1	0.91	0.21	91,91,91,91	0
54	MG	DA	3233	1/1	0.91	0.33	79,79,79,79	0
54	MG	BA	3044	1/1	0.91	0.08	58,58,58,58	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	DA	3235	1/1	0.91	0.19	89,89,89,89	0
54	MG	BA	3276	1/1	0.91	0.22	90,90,90,90	0
54	MG	BA	3046	1/1	0.91	0.26	86,86,86,86	0
54	MG	DA	3108	1/1	0.91	0.18	67,67,67,67	0
54	MG	DA	3244	1/1	0.91	0.17	84,84,84,84	0
54	MG	DA	3020	1/1	0.91	0.17	62,62,62,62	0
54	MG	DA	3247	1/1	0.91	0.24	89,89,89,89	0
54	MG	BA	3239	1/1	0.91	0.20	82,82,82,82	0
54	MG	BB	202	1/1	0.91	0.16	92,92,92,92	0
54	MG	BA	3362	1/1	0.91	0.37	70,70,70,70	0
54	MG	BB	205	1/1	0.91	0.23	93,93,93,93	0
54	MG	BA	3065	1/1	0.91	0.07	135,135,135,135	0
54	MG	DA	3119	1/1	0.91	0.21	65,65,65,65	0
54	MG	DA	3378	1/1	0.91	0.20	100,100,100,100	0
54	MG	BA	3412	1/1	0.91	0.22	94,94,94,94	0
54	MG	BA	3169	1/1	0.91	0.15	104,104,104,104	0
54	MG	CA	1634	1/1	0.91	0.12	110,110,110,110	0
54	MG	BA	3556	1/1	0.91	0.13	91,91,91,91	0
54	MG	DA	3128	1/1	0.91	0.27	65,65,65,65	0
54	MG	BA	3170	1/1	0.91	0.21	90,90,90,90	0
54	MG	BA	3460	1/1	0.91	0.22	90,90,90,90	0
54	MG	BA	3508	1/1	0.91	0.23	85,85,85,85	0
54	MG	DA	3389	1/1	0.91	0.20	94,94,94,94	0
54	MG	BA	3509	1/1	0.91	0.15	104,104,104,104	0
54	MG	DA	3137	1/1	0.91	0.18	74,74,74,74	0
54	MG	BA	3209	1/1	0.91	0.22	79,79,79,79	0
54	MG	BA	3417	1/1	0.91	0.16	78,78,78,78	0
54	MG	DA	3039	1/1	0.91	0.15	116,116,116,116	0
54	MG	BA	3565	1/1	0.91	0.11	86,86,86,86	0
54	MG	DA	3142	1/1	0.91	0.12	99,99,99,99	0
54	MG	BA	3566	1/1	0.91	0.16	100,100,100,100	0
54	MG	BA	3172	1/1	0.91	0.21	93,93,93,93	0
54	MG	BA	3173	1/1	0.91	0.23	62,62,62,62	0
54	MG	CA	1783	1/1	0.91	0.12	97,97,97,97	0
54	MG	BA	3049	1/1	0.91	0.18	88,88,88,88	0
54	MG	DA	3046	1/1	0.91	0.26	82,82,82,82	0
54	MG	DB	203	1/1	0.91	0.12	95,95,95,95	0
54	MG	DA	3290	1/1	0.91	0.17	107,107,107,107	0
54	MG	BE	305	1/1	0.91	0.12	111,111,111,111	0
54	MG	BA	3293	1/1	0.91	0.17	77,77,77,77	0
54	MG	DA	3155	1/1	0.91	0.12	80,80,80,80	0
54	MG	BO	201	1/1	0.91	0.13	90,90,90,90	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	BA	3422	1/1	0.91	0.19	120,120,120,120	0
54	MG	BA	3518	1/1	0.91	0.09	86,86,86,86	0
54	MG	BA	3294	1/1	0.91	0.25	79,79,79,79	0
54	MG	BA	3574	1/1	0.91	0.21	60,60,60,60	0
54	MG	DA	3302	1/1	0.91	0.21	79,79,79,79	0
54	MG	BA	3296	1/1	0.91	0.21	93,93,93,93	0
54	MG	BA	3336	1/1	0.91	0.32	109,109,109,109	0
54	MG	BA	3523	1/1	0.91	0.15	64,64,64,64	0
54	MG	BA	3580	1/1	0.91	0.48	64,64,64,64	0
54	MG	DA	3308	1/1	0.91	0.20	94,94,94,94	0
54	MG	BA	3337	1/1	0.91	0.07	75,75,75,75	0
54	MG	BA	3028	1/1	0.91	0.28	57,57,57,57	0
54	MG	AA	1655	1/1	0.91	0.18	106,106,106,106	0
54	MG	BA	3332	1/1	0.92	0.27	83,83,83,83	0
54	MG	DA	3145	1/1	0.92	0.14	110,110,110,110	0
54	MG	BA	3298	1/1	0.92	0.14	73,73,73,73	0
54	MG	DA	3063	1/1	0.92	0.24	76,76,76,76	0
54	MG	BA	3181	1/1	0.92	0.21	79,79,79,79	0
54	MG	BA	3335	1/1	0.92	0.13	96,96,96,96	0
54	MG	BA	3048	1/1	0.92	0.12	70,70,70,70	0
54	MG	BA	3503	1/1	0.92	0.17	105,105,105,105	0
54	MG	BA	3591	1/1	0.92	0.29	57,57,57,57	0
54	MG	DA	3453	1/1	0.92	0.25	104,104,104,104	0
54	MG	BA	3184	1/1	0.92	0.20	70,70,70,70	0
54	MG	DA	3356	1/1	0.92	0.28	64,64,64,64	0
54	MG	BA	3593	1/1	0.92	0.26	57,57,57,57	0
54	MG	DA	3358	1/1	0.92	0.25	73,73,73,73	0
54	MG	BA	3266	1/1	0.92	0.17	77,77,77,77	0
54	MG	DA	3360	1/1	0.92	0.19	85,85,85,85	0
54	MG	BA	3233	1/1	0.92	0.25	106,106,106,106	0
54	MG	BO	203	1/1	0.92	0.12	70,70,70,70	0
54	MG	BA	3596	1/1	0.92	0.12	88,88,88,88	0
54	MG	DA	3365	1/1	0.92	0.13	100,100,100,100	0
54	MG	BA	3236	1/1	0.92	0.18	97,97,97,97	0
54	MG	BA	3306	1/1	0.92	0.15	81,81,81,81	0
54	MG	DA	3369	1/1	0.92	0.34	76,76,76,76	0
54	MG	BA	3600	1/1	0.92	0.14	97,97,97,97	0
54	MG	BA	3603	1/1	0.92	0.47	113,113,113,113	0
54	MG	BA	3382	1/1	0.92	0.39	78,78,78,78	0
54	MG	DA	3277	1/1	0.92	0.35	77,77,77,77	0
54	MG	AA	1703	1/1	0.92	0.15	87,87,87,87	0
54	MG	DA	3009	1/1	0.92	0.29	74,74,74,74	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	BA	3165	1/1	0.92	0.10	119,119,119,119	0
54	MG	BA	3274	1/1	0.92	0.16	93,93,93,93	0
54	MG	DA	3013	1/1	0.92	0.18	69,69,69,69	0
54	MG	DA	3014	1/1	0.92	0.31	69,69,69,69	0
54	MG	BA	3275	1/1	0.92	0.27	111,111,111,111	0
54	MG	BA	3347	1/1	0.92	0.14	72,72,72,72	0
54	MG	DA	3018	1/1	0.92	0.07	83,83,83,83	0
54	MG	AA	1759	1/1	0.92	0.09	87,87,87,87	0
54	MG	BA	3062	1/1	0.92	0.24	70,70,70,70	0
54	MG	BA	3215	1/1	0.92	0.26	119,119,119,119	0
54	MG	BA	3437	1/1	0.92	0.14	81,81,81,81	0
54	MG	BA	3168	1/1	0.92	0.21	52,52,52,52	0
54	MG	BA	3621	1/1	0.92	0.24	66,66,66,66	0
54	MG	BA	3622	1/1	0.92	0.06	120,120,120,120	0
54	MG	CA	1671	1/1	0.92	0.31	75,75,75,75	0
54	MG	BA	3394	1/1	0.92	0.14	85,85,85,85	0
54	MG	DA	3397	1/1	0.92	0.30	96,96,96,96	0
54	MG	BA	3353	1/1	0.92	0.25	93,93,93,93	0
54	MG	CA	1674	1/1	0.92	0.40	117,117,117,117	0
54	MG	AC	109	1/1	0.92	0.06	105,105,105,105	0
54	MG	DA	3500	1/1	0.92	0.19	88,88,88,88	0
54	MG	BA	3355	1/1	0.92	0.29	90,90,90,90	0
54	MG	DA	3503	1/1	0.92	0.19	105,105,105,105	0
54	MG	CA	1733	1/1	0.92	0.10	124,124,124,124	0
54	MG	DA	3403	1/1	0.92	0.23	84,84,84,84	0
54	MG	DA	3112	1/1	0.92	0.25	71,71,71,71	0
54	MG	DA	3035	1/1	0.92	0.14	93,93,93,93	0
54	MG	CA	1788	1/1	0.92	0.27	87,87,87,87	0
54	MG	AA	1828	1/1	0.92	0.31	94,94,94,94	0
54	MG	DA	3515	1/1	0.92	0.25	94,94,94,94	0
54	MG	DA	3212	1/1	0.92	0.20	59,59,59,59	0
54	MG	CA	1736	1/1	0.92	0.26	85,85,85,85	0
54	MG	DA	3216	1/1	0.92	0.15	77,77,77,77	0
54	MG	DA	3317	1/1	0.92	0.11	131,131,131,131	0
54	MG	DA	3118	1/1	0.92	0.22	61,61,61,61	0
54	MG	DA	3319	1/1	0.92	0.19	77,77,77,77	0
54	MG	BA	3220	1/1	0.92	0.13	76,76,76,76	0
54	MG	DA	3222	1/1	0.92	0.20	62,62,62,62	0
54	MG	BB	203	1/1	0.92	0.20	73,73,73,73	0
54	MG	DA	3323	1/1	0.92	0.16	79,79,79,79	0
54	MG	BA	3286	1/1	0.92	0.19	98,98,98,98	0
54	MG	BA	3148	1/1	0.92	0.13	59,59,59,59	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	BA	3290	1/1	0.92	0.30	78,78,78,78	0
54	MG	DA	3126	1/1	0.92	0.12	58,58,58,58	0
54	MG	BA	3002	1/1	0.92	0.26	63,63,63,63	0
54	MG	AA	1644	1/1	0.92	0.19	72,72,72,72	0
54	MG	BA	3198	1/1	0.92	0.34	70,70,70,70	0
54	MG	AA	1702	1/1	0.92	0.32	77,77,77,77	0
54	MG	DA	3236	1/1	0.92	0.39	60,60,60,60	0
54	MG	DA	3238	1/1	0.92	0.20	117,117,117,117	0
54	MG	DA	3432	1/1	0.92	0.16	91,91,91,91	0
54	MG	BA	3179	1/1	0.92	0.12	108,108,108,108	0
54	MG	BA	3578	1/1	0.92	0.20	88,88,88,88	0
54	MG	DR	201	1/1	0.92	0.12	86,86,86,86	0
54	MG	DA	3051	1/1	0.92	0.32	81,81,81,81	0
54	MG	DA	3242	1/1	0.92	0.32	64,64,64,64	0
54	MG	BB	213	1/1	0.92	0.11	72,72,72,72	0
54	MG	DA	3055	1/1	0.92	0.26	59,59,59,59	0
55	TAC	AA	1833	32/32	0.92	0.11	99,129,142,143	0
54	MG	BA	3297	1/1	0.92	0.21	78,78,78,78	0
54	MG	DA	3245	1/1	0.93	0.10	83,83,83,83	0
54	MG	AA	1774	1/1	0.93	0.29	72,72,72,72	0
54	MG	BA	3272	1/1	0.93	0.23	52,52,52,52	0
54	MG	DA	3047	1/1	0.93	0.04	124,124,124,124	0
54	MG	BA	3029	1/1	0.93	0.23	74,74,74,74	0
54	MG	BA	3015	1/1	0.93	0.19	61,61,61,61	0
54	MG	BA	3363	1/1	0.93	0.14	73,73,73,73	0
54	MG	BA	3018	1/1	0.93	0.30	53,53,53,53	0
54	MG	BA	3219	1/1	0.93	0.24	123,123,123,123	0
54	MG	DA	3404	1/1	0.93	0.24	66,66,66,66	0
54	MG	DA	3054	1/1	0.93	0.28	88,88,88,88	0
54	MG	BA	3582	1/1	0.93	0.17	68,68,68,68	0
54	MG	BA	3583	1/1	0.93	0.22	59,59,59,59	0
54	MG	DA	3257	1/1	0.93	0.27	88,88,88,88	0
54	MG	BA	3134	1/1	0.93	0.15	130,130,130,130	0
54	MG	DA	3059	1/1	0.93	0.19	68,68,68,68	0
54	MG	DA	3411	1/1	0.93	0.12	68,68,68,68	0
54	MG	DA	3186	1/1	0.93	0.16	60,60,60,60	0
54	MG	DA	3413	1/1	0.93	0.08	115,115,115,115	0
54	MG	DA	3187	1/1	0.93	0.23	70,70,70,70	0
54	MG	BA	3309	1/1	0.93	0.17	84,84,84,84	0
54	MG	CA	1784	1/1	0.93	0.14	94,94,94,94	0
54	MG	DA	3065	1/1	0.93	0.09	103,103,103,103	0
54	MG	DA	3121	1/1	0.93	0.20	68,68,68,68	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	DA	3192	1/1	0.93	0.14	64,64,64,64	0
54	MG	DA	3012	1/1	0.93	0.08	129,129,129,129	0
54	MG	BA	3402	1/1	0.93	0.12	81,81,81,81	0
54	MG	DA	3349	1/1	0.93	0.22	88,88,88,88	0
54	MG	BA	3473	1/1	0.93	0.18	82,82,82,82	0
54	MG	DA	3278	1/1	0.93	0.15	80,80,80,80	0
54	MG	DA	3504	1/1	0.93	0.44	67,67,67,67	0
54	MG	DA	3015	1/1	0.93	0.20	98,98,98,98	0
54	MG	DA	3507	1/1	0.93	0.25	79,79,79,79	0
54	MG	DA	3508	1/1	0.93	0.25	68,68,68,68	0
54	MG	DA	3127	1/1	0.93	0.18	66,66,66,66	0
54	MG	DA	3199	1/1	0.93	0.14	77,77,77,77	0
54	MG	BA	3221	1/1	0.93	0.24	89,89,89,89	0
54	MG	DA	3201	1/1	0.93	0.25	73,73,73,73	0
54	MG	CA	1657	1/1	0.93	0.10	142,142,142,142	0
54	MG	DA	3288	1/1	0.93	0.18	95,95,95,95	0
54	MG	BA	3404	1/1	0.93	0.24	93,93,93,93	0
54	MG	DA	3133	1/1	0.93	0.16	74,74,74,74	0
54	MG	AA	1629	1/1	0.93	0.05	186,186,186,186	0
54	MG	BA	3195	1/1	0.93	0.13	82,82,82,82	0
54	MG	DA	3293	1/1	0.93	0.18	112,112,112,112	0
54	MG	BA	3444	1/1	0.93	0.03	186,186,186,186	0
54	MG	BA	3479	1/1	0.93	0.21	72,72,72,72	0
54	MG	BA	3371	1/1	0.93	0.19	81,81,81,81	0
54	MG	BA	3409	1/1	0.93	0.21	86,86,86,86	0
54	MG	BA	3284	1/1	0.93	0.11	121,121,121,121	0
54	MG	DA	3446	1/1	0.93	0.16	92,92,92,92	0
54	MG	CA	1668	1/1	0.93	0.15	145,145,145,145	0
54	MG	BA	3252	1/1	0.93	0.15	70,70,70,70	0
54	MG	AA	1669	1/1	0.93	0.30	79,79,79,79	0
54	MG	BA	3157	1/1	0.93	0.20	74,74,74,74	0
54	MG	BA	3256	1/1	0.93	0.20	68,68,68,68	0
54	MG	BA	3068	1/1	0.93	0.17	71,71,71,71	0
54	MG	BA	3036	1/1	0.93	0.19	63,63,63,63	0
54	MG	AA	1740	1/1	0.93	0.32	75,75,75,75	0
54	MG	DA	3092	1/1	0.93	0.25	80,80,80,80	0
54	MG	BA	3182	1/1	0.93	0.36	101,101,101,101	0
54	MG	AA	1746	1/1	0.93	0.15	92,92,92,92	0
54	MG	AA	1780	1/1	0.93	0.08	154,154,154,154	0
54	MG	DA	3237	1/1	0.93	0.17	63,63,63,63	0
54	MG	B2	201	1/1	0.93	0.08	90,90,90,90	0
54	MG	BA	3073	1/1	0.93	0.27	108,108,108,108	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	BA	3327	1/1	0.93	0.08	117,117,117,117	0
54	MG	AA	1604	1/1	0.93	0.08	135,135,135,135	0
54	MG	CA	1636	1/1	0.93	0.12	91,91,91,91	0
54	MG	AA	1633	1/1	0.93	0.20	80,80,80,80	0
56	ZN	AQ	103	1/1	0.93	0.14	186,186,186,186	0
54	MG	BA	3136	1/1	0.94	0.18	62,62,62,62	0
54	MG	DA	3056	1/1	0.94	0.17	86,86,86,86	0
54	MG	BA	3430	1/1	0.94	0.08	87,87,87,87	0
54	MG	AA	1656	1/1	0.94	0.16	71,71,71,71	0
54	MG	AA	1737	1/1	0.94	0.13	132,132,132,132	0
54	MG	DA	3376	1/1	0.94	0.12	87,87,87,87	0
54	MG	BA	3139	1/1	0.94	0.21	66,66,66,66	0
54	MG	DA	3061	1/1	0.94	0.26	64,64,64,64	0
54	MG	DA	3062	1/1	0.94	0.14	112,112,112,112	0
54	MG	BA	3348	1/1	0.94	0.23	90,90,90,90	0
54	MG	DA	3064	1/1	0.94	0.33	79,79,79,79	0
54	MG	DA	3383	1/1	0.94	0.25	84,84,84,84	0
54	MG	DA	3208	1/1	0.94	0.23	94,94,94,94	0
54	MG	DA	3130	1/1	0.94	0.16	92,92,92,92	0
54	MG	BA	3390	1/1	0.94	0.21	81,81,81,81	0
54	MG	DA	3303	1/1	0.94	0.07	140,140,140,140	0
54	MG	BA	3142	1/1	0.94	0.25	48,48,48,48	0
54	MG	DA	3215	1/1	0.94	0.14	80,80,80,80	0
54	MG	AA	1729	1/1	0.94	0.11	108,108,108,108	0
54	MG	BA	3311	1/1	0.94	0.23	100,100,100,100	0
54	MG	DA	3393	1/1	0.94	0.21	76,76,76,76	0
54	MG	DA	3069	1/1	0.94	0.08	101,101,101,101	0
54	MG	BA	3273	1/1	0.94	0.28	70,70,70,70	0
54	MG	DA	3223	1/1	0.94	0.16	54,54,54,54	0
54	MG	AA	1606	1/1	0.94	0.05	155,155,155,155	0
54	MG	BA	3234	1/1	0.94	0.40	84,84,84,84	0
54	MG	BA	3203	1/1	0.94	0.33	86,86,86,86	0
54	MG	AC	101	1/1	0.94	0.15	78,78,78,78	0
54	MG	DA	3228	1/1	0.94	0.09	80,80,80,80	0
54	MG	AA	1653	1/1	0.94	0.12	91,91,91,91	0
54	MG	DA	3230	1/1	0.94	0.40	65,65,65,65	0
54	MG	BA	3055	1/1	0.94	0.22	69,69,69,69	0
54	MG	BA	3281	1/1	0.94	0.32	106,106,106,106	0
54	MG	BA	3208	1/1	0.94	0.35	91,91,91,91	0
54	MG	DA	3490	1/1	0.94	0.16	120,120,120,120	0
54	MG	BA	3074	1/1	0.94	0.06	142,142,142,142	0
54	MG	CA	1734	1/1	0.94	0.17	93,93,93,93	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	BA	3243	1/1	0.94	0.06	122,122,122,122	0
54	MG	DA	3498	1/1	0.94	0.26	106,106,106,106	0
54	MG	BA	3014	1/1	0.94	0.28	68,68,68,68	0
54	MG	DA	3501	1/1	0.94	0.18	73,73,73,73	0
54	MG	DA	3325	1/1	0.94	0.33	74,74,74,74	0
54	MG	AA	1700	1/1	0.94	0.06	123,123,123,123	0
54	MG	DA	3086	1/1	0.94	0.15	84,84,84,84	0
54	MG	BA	3589	1/1	0.94	0.16	77,77,77,77	0
54	MG	BA	3287	1/1	0.94	0.17	95,95,95,95	0
54	MG	DA	3243	1/1	0.94	0.14	86,86,86,86	0
54	MG	BA	3017	1/1	0.94	0.17	67,67,67,67	0
54	MG	CA	1791	1/1	0.94	0.17	78,78,78,78	0
54	MG	BA	3180	1/1	0.94	0.46	73,73,73,73	0
54	MG	DA	3029	1/1	0.94	0.15	87,87,87,87	0
54	MG	BA	3101	1/1	0.94	0.25	58,58,58,58	0
54	MG	AA	1807	1/1	0.94	0.19	101,101,101,101	0
54	MG	DA	3516	1/1	0.94	0.13	92,92,92,92	0
54	MG	DA	3165	1/1	0.94	0.17	59,59,59,59	0
54	MG	CA	1795	1/1	0.94	0.12	112,112,112,112	0
54	MG	DA	3167	1/1	0.94	0.12	75,75,75,75	0
54	MG	DA	3168	1/1	0.94	0.24	95,95,95,95	0
54	MG	CA	1690	1/1	0.94	0.10	102,102,102,102	0
54	MG	AA	1659	1/1	0.94	0.12	71,71,71,71	0
54	MG	AA	1781	1/1	0.94	0.20	120,120,120,120	0
54	MG	DA	3099	1/1	0.94	0.12	74,74,74,74	0
54	MG	DA	3174	1/1	0.94	0.06	81,81,81,81	0
54	MG	DB	201	1/1	0.94	0.15	88,88,88,88	0
54	MG	BA	3295	1/1	0.94	0.21	70,70,70,70	0
54	MG	BA	3254	1/1	0.94	0.21	70,70,70,70	0
54	MG	BA	3106	1/1	0.94	0.11	52,52,52,52	0
54	MG	BA	3041	1/1	0.94	0.10	142,142,142,142	0
54	MG	DA	3179	1/1	0.94	0.07	85,85,85,85	0
54	MG	DA	3270	1/1	0.94	0.19	63,63,63,63	0
54	MG	DA	3440	1/1	0.94	0.22	83,83,83,83	0
54	MG	DB	210	1/1	0.94	0.18	73,73,73,73	0
54	MG	BA	3606	1/1	0.94	0.15	84,84,84,84	0
54	MG	AA	1608	1/1	0.94	0.07	111,111,111,111	0
54	MG	BA	3608	1/1	0.94	0.06	108,108,108,108	0
54	MG	BU	202	1/1	0.94	0.05	80,80,80,80	0
54	MG	DA	3445	1/1	0.94	0.22	89,89,89,89	0
54	MG	BA	3222	1/1	0.94	0.22	57,57,57,57	0
54	MG	CA	1649	1/1	0.94	0.12	113,113,113,113	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	BA	3423	1/1	0.94	0.25	89,89,89,89	0
54	MG	BA	3611	1/1	0.94	0.10	101,101,101,101	0
54	MG	BA	3512	1/1	0.94	0.12	97,97,97,97	0
54	MG	DA	3282	1/1	0.94	0.15	88,88,88,88	0
54	MG	AA	1771	1/1	0.94	0.07	117,117,117,117	0
54	MG	BA	3381	1/1	0.94	0.31	65,65,65,65	0
54	MG	BA	3087	1/1	0.94	0.06	142,142,142,142	0
54	MG	AA	1620	1/1	0.94	0.12	105,105,105,105	0
54	MG	CA	1677	1/1	0.95	0.08	114,114,114,114	0
54	MG	BA	3263	1/1	0.95	0.28	50,50,50,50	0
54	MG	DA	3231	1/1	0.95	0.23	74,74,74,74	0
54	MG	BA	3204	1/1	0.95	0.16	98,98,98,98	0
54	MG	DA	3169	1/1	0.95	0.22	76,76,76,76	0
54	MG	BA	3613	1/1	0.95	0.17	111,111,111,111	0
54	MG	BA	3416	1/1	0.95	0.08	70,70,70,70	0
54	MG	BA	3042	1/1	0.95	0.11	94,94,94,94	0
54	MG	BA	3313	1/1	0.95	0.20	61,61,61,61	0
54	MG	BA	3010	1/1	0.95	0.12	128,128,128,128	0
54	MG	BA	3577	1/1	0.95	0.25	61,61,61,61	0
54	MG	BA	3224	1/1	0.95	0.07	101,101,101,101	0
54	MG	DA	3433	1/1	0.95	0.19	66,66,66,66	0
54	MG	AA	1635	1/1	0.95	0.12	122,122,122,122	0
54	MG	BA	3081	1/1	0.95	0.13	88,88,88,88	0
54	MG	CA	1640	1/1	0.95	0.16	92,92,92,92	0
54	MG	BA	3045	1/1	0.95	0.28	66,66,66,66	0
54	MG	DA	3182	1/1	0.95	0.28	62,62,62,62	0
54	MG	BA	3026	1/1	0.95	0.19	66,66,66,66	0
54	MG	DA	3184	1/1	0.95	0.23	68,68,68,68	0
54	MG	BA	3397	1/1	0.95	0.17	92,92,92,92	0
54	MG	BA	3140	1/1	0.95	0.16	84,84,84,84	0
54	MG	CA	1646	1/1	0.95	0.14	101,101,101,101	0
54	MG	BA	3627	1/1	0.95	0.09	89,89,89,89	0
54	MG	BA	3111	1/1	0.95	0.12	68,68,68,68	0
54	MG	DA	3131	1/1	0.95	0.15	94,94,94,94	0
54	MG	BA	3519	1/1	0.95	0.26	75,75,75,75	0
54	MG	BA	3047	1/1	0.95	0.22	64,64,64,64	0
54	MG	CA	1699	1/1	0.95	0.07	81,81,81,81	0
54	MG	DA	3030	1/1	0.95	0.12	89,89,89,89	0
54	MG	BA	3299	1/1	0.95	0.41	78,78,78,78	0
54	MG	DA	3391	1/1	0.95	0.16	94,94,94,94	0
54	MG	BA	3590	1/1	0.95	0.51	116,116,116,116	0
54	MG	BA	3113	1/1	0.95	0.19	72,72,72,72	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	CA	1703	1/1	0.95	0.07	93,93,93,93	0
54	MG	BA	3491	1/1	0.95	0.16	84,84,84,84	0
54	MG	DA	3267	1/1	0.95	0.10	79,79,79,79	0
54	MG	BA	3461	1/1	0.95	0.07	79,79,79,79	0
54	MG	DB	202	1/1	0.95	0.09	113,113,113,113	0
54	MG	DA	3144	1/1	0.95	0.23	85,85,85,85	0
54	MG	BA	3277	1/1	0.95	0.09	97,97,97,97	0
54	MG	AA	1788	1/1	0.95	0.15	124,124,124,124	0
54	MG	CA	1659	1/1	0.95	0.09	158,158,158,158	0
54	MG	BA	3013	1/1	0.95	0.15	63,63,63,63	0
54	MG	BA	3597	1/1	0.95	0.20	69,69,69,69	0
54	MG	BA	3561	1/1	0.95	0.28	86,86,86,86	0
54	MG	BA	3406	1/1	0.95	0.25	86,86,86,86	0
54	MG	BA	3563	1/1	0.95	0.16	96,96,96,96	0
54	MG	AA	1795	1/1	0.95	0.10	102,102,102,102	0
54	MG	BA	3380	1/1	0.95	0.12	91,91,91,91	0
54	MG	BA	3605	1/1	0.95	0.10	82,82,82,82	0
54	MG	DA	3218	1/1	0.95	0.18	77,77,77,77	0
54	MG	CA	1669	1/1	0.95	0.13	130,130,130,130	0
54	MG	DA	3220	1/1	0.95	0.22	70,70,70,70	0
54	MG	BA	3257	1/1	0.95	0.24	70,70,70,70	0
54	MG	AA	1789	1/1	0.95	0.14	79,79,79,79	0
54	MG	BA	3260	1/1	0.95	0.10	126,126,126,126	0
54	MG	BA	3238	1/1	0.95	0.18	112,112,112,112	0
54	MG	BA	3031	1/1	0.95	0.31	63,63,63,63	0
54	MG	D5	101	1/1	0.95	0.09	63,63,63,63	0
54	MG	DA	3418	1/1	0.95	0.28	61,61,61,61	0
54	MG	BF	302	1/1	0.95	0.13	127,127,127,127	0
54	MG	CA	1628	1/1	0.95	0.06	149,149,149,149	0
54	MG	DA	3266	1/1	0.96	0.06	110,110,110,110	0
54	MG	BA	3175	1/1	0.96	0.08	80,80,80,80	0
54	MG	DA	3268	1/1	0.96	0.12	63,63,63,63	0
54	MG	DA	3493	1/1	0.96	0.15	64,64,64,64	0
54	MG	DA	3494	1/1	0.96	0.24	45,45,45,45	0
54	MG	BA	3105	1/1	0.96	0.13	68,68,68,68	0
54	MG	DA	3082	1/1	0.96	0.07	99,99,99,99	0
54	MG	DA	3271	1/1	0.96	0.29	62,62,62,62	0
54	MG	B5	101	1/1	0.96	0.14	61,61,61,61	0
54	MG	DA	3221	1/1	0.96	0.23	61,61,61,61	0
54	MG	BA	3197	1/1	0.96	0.11	66,66,66,66	0
54	MG	BA	3244	1/1	0.96	0.05	112,112,112,112	0
54	MG	DA	3505	1/1	0.96	0.14	72,72,72,72	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	BA	3438	1/1	0.96	0.21	62,62,62,62	0
54	MG	AA	1720	1/1	0.96	0.10	101,101,101,101	0
54	MG	BA	3199	1/1	0.96	0.09	78,78,78,78	0
54	MG	BA	3500	1/1	0.96	0.09	129,129,129,129	0
54	MG	BA	3076	1/1	0.96	0.07	74,74,74,74	0
54	MG	DA	3281	1/1	0.96	0.15	74,74,74,74	0
54	MG	BA	3202	1/1	0.96	0.22	65,65,65,65	0
54	MG	BA	3037	1/1	0.96	0.27	71,71,71,71	0
54	MG	DA	3181	1/1	0.96	0.13	74,74,74,74	0
54	MG	DA	3285	1/1	0.96	0.08	67,67,67,67	0
54	MG	DA	3136	1/1	0.96	0.25	64,64,64,64	0
54	MG	DA	3053	1/1	0.96	0.23	100,100,100,100	0
54	MG	BA	3602	1/1	0.96	0.33	66,66,66,66	0
54	MG	BA	3250	1/1	0.96	0.06	87,87,87,87	0
54	MG	AA	1682	1/1	0.96	0.04	113,113,113,113	0
54	MG	AA	1677	1/1	0.96	0.16	125,125,125,125	0
54	MG	AA	1610	1/1	0.96	0.22	71,71,71,71	0
54	MG	BA	3053	1/1	0.96	0.21	92,92,92,92	0
54	MG	DA	3294	1/1	0.96	0.32	64,64,64,64	0
54	MG	AC	103	1/1	0.96	0.28	75,75,75,75	0
54	MG	DA	3146	1/1	0.96	0.16	87,87,87,87	0
54	MG	DA	3297	1/1	0.96	0.09	71,71,71,71	0
54	MG	BA	3130	1/1	0.96	0.06	92,92,92,92	0
54	MG	BA	3098	1/1	0.96	0.28	75,75,75,75	0
54	MG	AA	1706	1/1	0.96	0.05	134,134,134,134	0
54	MG	BA	3019	1/1	0.96	0.17	49,49,49,49	0
54	MG	BA	3235	1/1	0.96	0.09	128,128,128,128	0
54	MG	BA	3341	1/1	0.96	0.20	71,71,71,71	0
54	MG	BA	3213	1/1	0.96	0.12	69,69,69,69	0
54	MG	BA	3289	1/1	0.96	0.11	83,83,83,83	0
54	MG	CA	1660	1/1	0.96	0.10	118,118,118,118	0
54	MG	DB	213	1/1	0.96	0.03	91,91,91,91	0
54	MG	BA	3550	1/1	0.96	0.05	99,99,99,99	0
54	MG	DA	3111	1/1	0.96	0.13	64,64,64,64	0
54	MG	DE	301	1/1	0.96	0.17	73,73,73,73	0
54	MG	BA	3487	1/1	0.96	0.09	116,116,116,116	0
54	MG	BA	3005	1/1	0.96	0.16	61,61,61,61	0
54	MG	DA	3073	1/1	0.96	0.14	102,102,102,102	0
54	MG	BA	3585	1/1	0.96	0.14	62,62,62,62	0
54	MG	AA	1804	1/1	0.96	0.08	130,130,130,130	0
54	MG	AA	1681	1/1	0.96	0.04	146,146,146,146	0
54	MG	DA	3259	1/1	0.96	0.29	76,76,76,76	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	AA	1713	1/1	0.96	0.09	107,107,107,107	0
54	MG	DA	3214	1/1	0.96	0.12	63,63,63,63	0
54	MG	BA	3375	1/1	0.96	0.31	80,80,80,80	0
54	MG	B3	101	1/1	0.96	0.17	77,77,77,77	0
54	MG	DA	3379	1/1	0.96	0.34	64,64,64,64	0
54	MG	DA	3261	1/1	0.97	0.17	78,78,78,78	0
54	MG	DA	3262	1/1	0.97	0.09	112,112,112,112	0
54	MG	AA	1783	1/1	0.97	0.07	125,125,125,125	0
54	MG	BA	3386	1/1	0.97	0.05	117,117,117,117	0
54	MG	DA	3206	1/1	0.97	0.34	58,58,58,58	0
54	MG	BA	3330	1/1	0.97	0.11	102,102,102,102	0
54	MG	AA	1642	1/1	0.97	0.09	103,103,103,103	0
54	MG	AA	1640	1/1	0.97	0.18	82,82,82,82	0
54	MG	DA	3211	1/1	0.97	0.12	71,71,71,71	0
54	MG	DA	3331	1/1	0.97	0.04	116,116,116,116	0
54	MG	BA	3171	1/1	0.97	0.09	87,87,87,87	0
54	MG	DA	3159	1/1	0.97	0.06	128,128,128,128	0
54	MG	DA	3496	1/1	0.97	0.10	72,72,72,72	0
54	MG	B7	102	1/1	0.97	0.18	75,75,75,75	0
54	MG	DA	3499	1/1	0.97	0.10	103,103,103,103	0
54	MG	B7	103	1/1	0.97	0.15	88,88,88,88	0
54	MG	CA	1719	1/1	0.97	0.04	116,116,116,116	0
54	MG	DA	3115	1/1	0.97	0.15	75,75,75,75	0
54	MG	A1	101	1/1	0.97	0.29	72,72,72,72	0
54	MG	BA	3620	1/1	0.97	0.10	72,72,72,72	0
54	MG	BA	3007	1/1	0.97	0.10	63,63,63,63	0
54	MG	BA	3174	1/1	0.97	0.10	61,61,61,61	0
54	MG	DA	3193	1/1	0.97	0.05	69,69,69,69	0
54	MG	DA	3143	1/1	0.97	0.05	117,117,117,117	0
54	MG	DA	3344	1/1	0.97	0.10	124,124,124,124	0
54	MG	BA	3141	1/1	0.97	0.09	63,63,63,63	0
54	MG	BA	3187	1/1	0.97	0.24	56,56,56,56	0
54	MG	DA	3122	1/1	0.97	0.15	67,67,67,67	0
54	MG	BA	3259	1/1	0.97	0.21	53,53,53,53	0
54	MG	AA	1624	1/1	0.97	0.09	98,98,98,98	0
54	MG	BA	3200	1/1	0.97	0.24	149,149,149,149	0
54	MG	CA	1648	1/1	0.97	0.07	96,96,96,96	0
54	MG	BA	3035	1/1	0.97	0.24	70,70,70,70	0
54	MG	CA	1610	1/1	0.97	0.05	147,147,147,147	0
56	ZN	CQ	101	1/1	0.97	0.10	188,188,188,188	0
54	MG	BA	3006	1/1	0.98	0.09	50,50,50,50	0
54	MG	DA	3514	1/1	0.98	0.06	71,71,71,71	0

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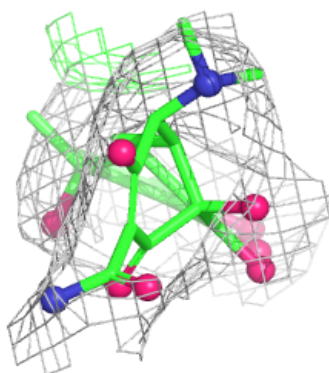
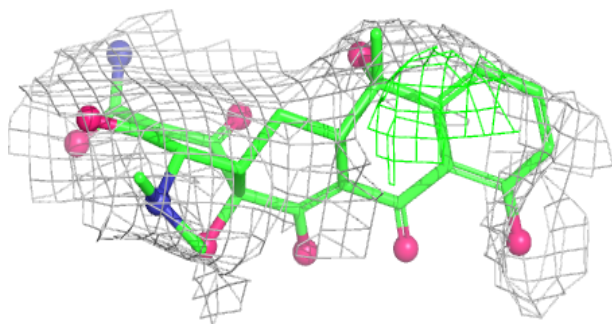
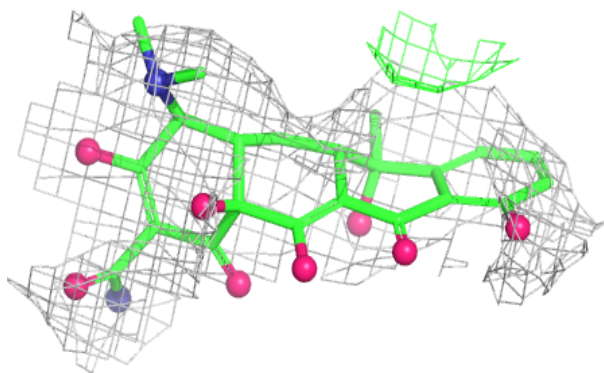
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	DA	3368	1/1	0.98	0.09	95,95,95,95	0
54	MG	AA	1695	1/1	0.98	0.05	152,152,152,152	0
54	MG	BA	3016	1/1	0.98	0.07	143,143,143,143	0
54	MG	BA	3083	1/1	0.98	0.06	108,108,108,108	0
54	MG	AA	1777	1/1	0.98	0.04	141,141,141,141	0
54	MG	CA	1721	1/1	0.98	0.04	128,128,128,128	0
54	MG	BA	3009	1/1	0.98	0.12	53,53,53,53	0
54	MG	BA	3267	1/1	0.98	0.03	126,126,126,126	0
54	MG	B1	201	1/1	0.98	0.18	61,61,61,61	0
54	MG	DA	3497	1/1	0.98	0.21	50,50,50,50	0
54	MG	CA	1643	1/1	0.98	0.04	148,148,148,148	0
56	ZN	CG	303	1/1	0.98	0.06	161,161,161,161	0
54	MG	DA	3210	1/1	0.98	0.16	63,63,63,63	0
54	MG	AA	1663	1/1	0.99	0.06	76,76,76,76	0
54	MG	BA	3549	1/1	0.99	0.02	140,140,140,140	0
54	MG	DA	3328	1/1	0.99	0.04	138,138,138,138	0
54	MG	BA	3176	1/1	0.99	0.04	89,89,89,89	0
54	MG	BA	3425	1/1	0.99	0.04	137,137,137,137	0
54	MG	DA	3363	1/1	0.99	0.04	125,125,125,125	0
56	ZN	AG	303	1/1	0.99	0.11	153,153,153,153	0
54	MG	BA	3059	1/1	0.99	0.03	144,144,144,144	0
54	MG	BA	3601	1/1	0.99	0.37	52,52,52,52	0
54	MG	AA	1822	1/1	0.99	0.02	144,144,144,144	0

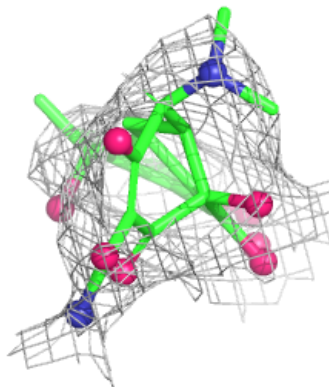
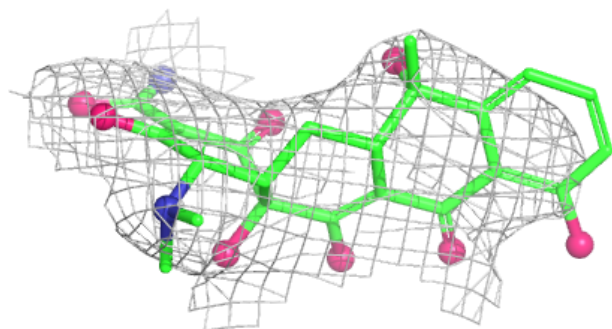
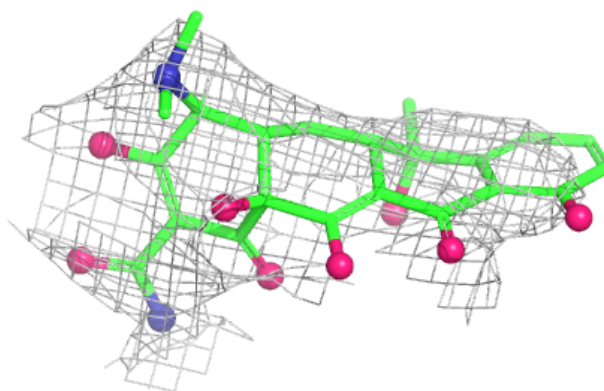
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around TAC CA 1805:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

**Electron density around TAC AA 1833:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



5.5 Other polymers [i](#)

There are no such residues in this entry.