



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 29, 2026 – 08:26 AM UTC

PDB ID : 4W2G / pdb_00004w2g
Title : Crystal structure of the *Thermus thermophilus* 70S ribosome in complex with pactamycin (soaked), mRNA and three deacylated tRNAs in the A, P and E sites
Authors : Polikanov, Y.S.; Osterman, I.A.; Szal, T.; Tashlitsky, V.N.; Serebryakova, M.V.; Kusochev, P.; Bulkley, D.; Malanicheva, I.A.; Efimenko, T.A.; Efremenkova, O.V.; Konevega, A.L.; Shaw, K.J.; Bogdanov, A.A.; Rodnina, M.V.; Dontsova, O.A.; Mankin, A.S.; Steitz, T.A.; Sergiev, P.V.
Deposited on : 2014-09-12
Resolution : 2.55 Å(reported)

This is a Full wwPDB X-ray Structure Validation 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

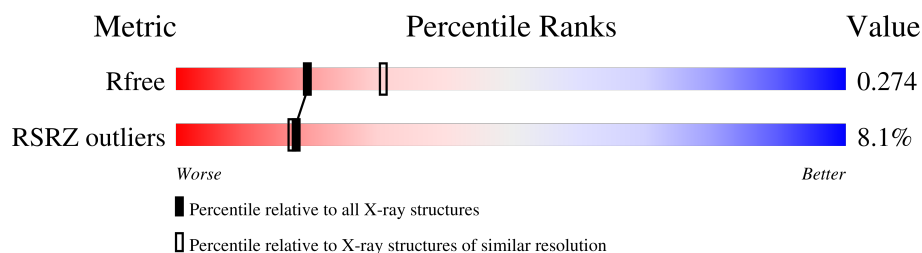
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.55 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	1091 (2.54-2.54)
RSRZ outliers	180081	1091 (2.54-2.54)

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

Ideal geometry (proteins) : Engh & Huber (2001)
 Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
 Validation Pipeline (wwPDB-VP) : 2.49

2 Entry composition

There are 61 unique types of molecules in this entry. The entry contains 297273 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a RNA chain called 16S Ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	AA	1498	Total	C	N	O	P	0	0	0
			32205	14333	5970	10404	1498			
1	CA	1503	Total	C	N	O	P	0	0	0
			32312	14381	5990	10438	1503			

- Molecule 2 is a protein called 30S Ribosomal Protein S2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	AB	231	Total	C	N	O	S	0	0	0
			1846	1179	331	331	5			
2	CB	231	Total	C	N	O	S	0	0	0
			1825	1167	326	327	5			

- Molecule 3 is a protein called 30S Ribosomal Protein S3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	AC	206	Total	C	N	O	S	0	0	0
			1552	976	302	273	1			
3	CC	206	Total	C	N	O	S	0	0	0
			1542	968	300	273	1			

- Molecule 4 is a protein called 30S Ribosomal Protein S4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	AD	208	Total	C	N	O	S	0	0	0
			1659	1040	326	286	7			
4	CD	208	Total	C	N	O	S	0	0	0
			1674	1050	333	284	7			

- Molecule 5 is a protein called 30S Ribosomal Protein S5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	AE	148	Total	C	N	O	S	0	0	0
			1129	714	213	198	4			
5	CE	148	Total	C	N	O	S	0	0	0
			1133	716	214	199	4			

- Molecule 6 is a protein called 30S Ribosomal Protein S6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	AF	100	Total	C	N	O	S	0	0	0
			806	511	143	149	3			
6	CF	100	Total	C	N	O	S	0	0	0
			816	516	146	151	3			

- Molecule 7 is a protein called 30S Ribosomal Protein S7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	AG	155	Total	C	N	O	S	0	0	0
			1231	766	243	216	6			
7	CG	155	Total	C	N	O	S	0	0	0
			1235	769	244	216	6			

- Molecule 8 is a protein called 30S Ribosomal Protein S8.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	AH	137	Total	C	N	O	S	0	0	0
			1088	689	206	191	2			
8	CH	137	Total	C	N	O	S	0	0	0
			1088	689	206	191	2			

- Molecule 9 is a protein called 30S Ribosomal Protein S9.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
9	AI	127	Total	C	N	O	0	0	0
			983	623	193	167			
9	CI	127	Total	C	N	O	0	0	0
			978	619	190	169			

- Molecule 10 is a protein called 30S Ribosomal Protein S10.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
10	AJ	97	Total	C	N	O	0	0	0
			709	440	138	131			

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
10	CJ	96	Total	C	N	O			
			714	445	138	131	0	0	0

- Molecule 11 is a protein called 30S Ribosomal Protein S11.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
11	AK	114	Total	C	N	O	S		
			829	516	155	155	3	0	0
11	CK	114	Total	C	N	O	S		
			833	519	156	155	3	0	0

- Molecule 12 is a protein called 30S Ribosomal Protein S12.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
12	AL	122	Total	C	N	O	S		
			930	585	185	159	1	0	0
12	CL	122	Total	C	N	O	S		
			930	585	185	159	1	0	0

- Molecule 13 is a protein called 30S Ribosomal Protein S13.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
13	AM	123	Total	C	N	O	S		
			958	592	198	166	2	0	0
13	CM	122	Total	C	N	O	S		
			950	586	197	165	2	0	0

- Molecule 14 is a protein called 30S Ribosomal Protein S14.

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

- Molecule 15 is a protein called 30S Ribosomal Protein S15.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
15	AO	88	Total	C	N	O	S		
			728	456	144	126	2	0	0
15	CO	88	Total	C	N	O	S		
			728	456	144	126	2	0	0

- Molecule 16 is a protein called 30S Ribosomal Protein S16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	AP	82	Total	C	N	O	S	0	0	0
			681	433	134	113	1			
16	CP	82	Total	C	N	O	S	0	0	0
			677	430	133	113	1			

- Molecule 17 is a protein called 30S Ribosomal Protein S17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	AQ	99	Total	C	N	O	S	0	0	0
			823	528	151	142	2			
17	CQ	99	Total	C	N	O	S	0	0	0
			823	528	151	142	2			

- Molecule 18 is a protein called 30S Ribosomal Protein S18.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
18	AR	68	Total	C	N	O	0	0	0
			555	355	108	92			
18	CR	68	Total	C	N	O	0	0	0
			555	355	108	92			

- Molecule 19 is a protein called 30S Ribosomal Protein S19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	AS	83	Total	C	N	O	S	0	0	0
			652	417	120	113	2			
19	CS	83	Total	C	N	O	S	0	0	0
			646	412	119	113	2			

- Molecule 20 is a protein called 30S Ribosomal Protein S20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	AT	96	Total	C	N	O	S	0	0	0
			728	446	156	124	2			
20	CT	96	Total	C	N	O	S	0	0	0
			727	446	155	124	2			

- Molecule 21 is a protein called 30S Ribosomal Protein THX.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
21	AU	23	Total	C	N	O	0	0	0
			199	122	48	29			
21	CU	23	Total	C	N	O	0	0	0
			199	122	48	29			

- Molecule 22 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	AV	13	Total	C	N	O	P	0	0	0
			277	125	51	88	13			
22	CV	13	Total	C	N	O	P	0	0	0
			277	125	51	88	13			

- Molecule 23 is a RNA chain called A/P-site tRNA.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
23	AW	74	Total	C	N	O	P	S	0	0	0
			1588	713	285	515	73	2			
23	AY	74	Total	C	N	O	P	S	0	0	0
			1581	707	285	515	73	1			
23	CW	72	Total	C	N	O	P	S	0	0	0
			1541	688	278	502	72	1			
23	CY	73	Total	C	N	O	P	S	0	0	0
			1561	698	283	507	72	1			

- Molecule 24 is a RNA chain called E-site tRNA.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
24	AX	76	Total	C	N	O	P	S	0	0	0
			1625	725	294	529	76	1			
24	CX	76	Total	C	N	O	P	S	0	0	0
			1625	725	294	529	76	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
25	BA	2819	Total	C	N	O	P	0	0	0
			60729	27026	11370	19515	2818			
25	DA	2800	Total	C	N	O	P	0	0	0
			60311	26840	11284	19388	2799			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	BB	120	Total	C	N	O	P	0	0	0
			2573	1146	476	832	119			
26	DB	120	Total	C	N	O	P	0	0	0
			2573	1146	476	832	119			

- Molecule 27 is a protein called 50S Ribosomal Protein L2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
27	BD	275	Total	C	N	O	S	0	0	0
			2136	1349	423	361	3			
27	DD	275	Total	C	N	O	S	0	0	0
			2136	1349	423	361	3			

- Molecule 28 is a protein called 50S Ribosomal Protein L3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
28	BE	204	Total	C	N	O	S	0	0	0
			1559	985	298	270	6			
28	DE	204	Total	C	N	O	S	0	0	0
			1559	985	298	270	6			

- Molecule 29 is a protein called 50S Ribosomal Protein L4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
29	BF	203	Total	C	N	O	S	0	0	1
			1584	1009	298	275	2			
29	DF	203	Total	C	N	O	S	0	0	1
			1580	1007	297	274	2			

- Molecule 30 is a protein called 50S Ribosomal Protein L5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
30	BG	181	Total	C	N	O	S	0	0	0
			1425	914	256	251	4			
30	DG	181	Total	C	N	O	S	0	0	0
			1424	911	258	251	4			

- Molecule 31 is a protein called 50S Ribosomal Protein L6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
31	BH	174	Total	C	N	O	S	0	0	0
			1330	845	248	236	1			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
31	DH	174	Total	C	N	O	S	0	0	0
			1330	845	248	236	1			

- Molecule 32 is a protein called 50S Ribosomal Protein L9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
32	BI	146	Total	C	N	O	S	0	0	0
			1085	693	189	202	1			
32	DI	146	Total	C	N	O	S	0	0	0
			1061	680	186	194	1			

- Molecule 33 is a protein called 50S Ribosomal Protein L13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
33	BN	140	Total	C	N	O	S	0	0	0
			1117	719	207	187	4			
33	DN	140	Total	C	N	O	S	0	0	0
			1117	719	207	187	4			

- Molecule 34 is a protein called 50S Ribosomal Protein L14.

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

- Molecule 35 is a protein called 50S Ribosomal Protein L15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
35	BP	149	Total	C	N	O	S	0	0	0
			1135	706	230	196	3			
35	DP	149	Total	C	N	O	S	0	0	0
			1135	706	230	196	3			

- Molecule 36 is a protein called 50S Ribosomal Protein L16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
36	BQ	141	Total	C	N	O	S	0	0	0
			1122	715	212	188	7			
36	DQ	141	Total	C	N	O	S	0	0	0
			1122	715	212	188	7			

- Molecule 37 is a protein called 50S Ribosomal Protein L17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
37	BR	118	Total	C	N	O	S	0	0	0
			968	604	203	160	1			
37	DR	118	Total	C	N	O	S	0	0	0
			968	604	203	160	1			

- Molecule 38 is a protein called 50S Ribosomal Protein L18.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
38	BS	110	Total	C	N	O		0	0	0
			877	553	175	149				
38	DS	110	Total	C	N	O		0	0	0
			870	549	173	148				

- Molecule 39 is a protein called 50S Ribosomal Protein L19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
39	BT	131	Total	C	N	O	S	0	0	0
			1091	680	225	185	1			
39	DT	131	Total	C	N	O	S	0	0	0
			1083	675	224	183	1			

- Molecule 40 is a protein called 50S Ribosomal Protein L20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
40	BU	116	Total	C	N	O	S	0	0	0
			959	608	201	149	1			
40	DU	116	Total	C	N	O	S	0	0	0
			959	608	201	149	1			

- Molecule 41 is a protein called 50S Ribosomal Protein L21.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
41	BV	101	Total	C	N	O	S	0	0	0
			771	495	140	135	1			
41	DV	101	Total	C	N	O	S	0	0	0
			771	495	140	135	1			

- Molecule 42 is a protein called 50S Ribosomal Protein L22.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
42	BW	112	Total	C	N	O	S	0	0	0
			886	557	174	153	2			
42	DW	112	Total	C	N	O	S	0	0	0
			886	557	174	153	2			

- Molecule 43 is a protein called 50S Ribosomal Protein L23.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
43	BX	95	Total	C	N	O	S	0	0	0
			750	488	135	126	1			
43	DX	95	Total	C	N	O	S	0	0	0
			750	488	135	126	1			

- Molecule 44 is a protein called 50S Ribosomal Protein L24.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
44	BY	107	Total	C	N	O	S	0	0	0
			806	517	152	131	6			
44	DY	107	Total	C	N	O	S	0	0	0
			806	517	152	131	6			

- Molecule 45 is a protein called 50S Ribosomal Protein L25.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
45	BZ	171	Total	C	N	O	S	0	0	0
			1349	862	243	242	2			
45	DZ	174	Total	C	N	O	S	0	0	0
			1360	870	243	245	2			

- Molecule 46 is a protein called 50S Ribosomal Protein L27.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
46	B0	83	Total	C	N	O	S	0	0	0
			653	404	139	109	1			
46	D0	83	Total	C	N	O	S	0	0	0
			653	404	139	109	1			

- Molecule 47 is a protein called 50S Ribosomal Protein L28.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
47	B1	97	Total	C	N	O	S	0	0	0
			755	475	148	131	1			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
47	D1	97	Total	C	N	O	S	0	0	0
			755	475	148	131	1			

- Molecule 48 is a protein called 50S Ribosomal Protein L29.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
48	B2	70	Total	C	N	O	S	0	0	0
			588	365	118	103	2			
48	D2	70	Total	C	N	O	S	0	0	0
			588	365	118	103	2			

- Molecule 49 is a protein called 50S Ribosomal Protein L30.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
49	B3	59	Total	C	N	O	0	0	0
			469	298	90	81			
49	D3	59	Total	C	N	O	0	0	0
			464	296	90	78			

- Molecule 50 is a protein called 50S Ribosomal Protein L31.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
50	B4	69	Total	C	N	O	S	0	0	0
			558	352	102	99	5			
50	D4	69	Total	C	N	O	S	0	0	0
			532	339	97	91	5			

- Molecule 51 is a protein called 50S Ribosomal Protein L32.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
51	B5	59	Total	C	N	O	S	0	0	0
			455	285	89	76	5			
51	D5	59	Total	C	N	O	S	0	0	0
			455	285	89	76	5			

- Molecule 52 is a protein called 50S Ribosomal Protein L33.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
52	B6	53	Total	C	N	O	S	0	0	0
			453	281	91	77	4			
52	D6	53	Total	C	N	O	S	0	0	0
			449	279	91	75	4			

- Molecule 53 is a protein called 50S Ribosomal Protein L34.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
53	B7	48	Total	C	N	O	S	0	0	0
			418	257	104	55	2			
53	D7	48	Total	C	N	O	S	0	0	0
			418	257	104	55	2			

- Molecule 54 is a protein called 50S Ribosomal Protein L35.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
54	B8	64	Total	C	N	O	S	0	0	0
			511	328	99	82	2			
54	D8	64	Total	C	N	O	S	0	0	0
			517	331	102	82	2			

- Molecule 55 is a protein called 50S Ribosomal Protein L36.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
55	B9	37	Total	C	N	O	S	0	0	0
			307	188	68	47	4			
55	D9	37	Total	C	N	O	S	0	0	0
			307	188	68	47	4			

- Molecule 56 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	AA	230	Total	Mg	0	0
			230	230		
56	AD	1	Total	Mg	0	0
			1	1		
56	AE	1	Total	Mg	0	0
			1	1		
56	AF	1	Total	Mg	0	0
			1	1		
56	AK	2	Total	Mg	0	0
			2	2		
56	AM	1	Total	Mg	0	0
			1	1		
56	AN	1	Total	Mg	0	0
			1	1		
56	AV	1	Total	Mg	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	AW	7	Total 7	Mg 7	0	0
56	AX	12	Total 12	Mg 12	0	0
56	AY	3	Total 3	Mg 3	0	0
56	BA	839	Total 839	Mg 839	0	0
56	BB	23	Total 23	Mg 23	0	0
56	BD	11	Total 11	Mg 11	0	0
56	BE	8	Total 8	Mg 8	0	0
56	BF	12	Total 12	Mg 12	0	0
56	BG	3	Total 3	Mg 3	0	0
56	BN	5	Total 5	Mg 5	0	0
56	BO	1	Total 1	Mg 1	0	0
56	BP	3	Total 3	Mg 3	0	0
56	BQ	5	Total 5	Mg 5	0	0
56	BR	5	Total 5	Mg 5	0	0
56	BU	9	Total 9	Mg 9	0	0
56	BV	5	Total 5	Mg 5	0	0
56	BW	3	Total 3	Mg 3	0	0
56	BX	2	Total 2	Mg 2	0	0
56	BY	1	Total 1	Mg 1	0	0
56	BZ	1	Total 1	Mg 1	0	0
56	B0	3	Total 3	Mg 3	0	0

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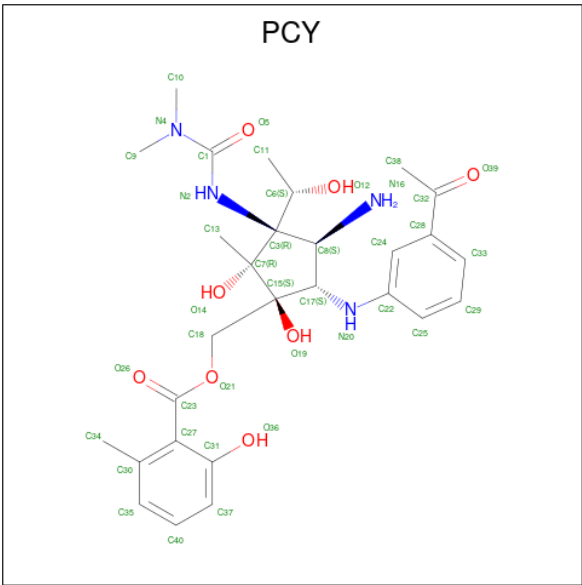
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	B1	2	Total 2	Mg 2	0	0
56	B2	1	Total 1	Mg 1	0	0
56	B3	3	Total 3	Mg 3	0	0
56	B4	1	Total 1	Mg 1	0	0
56	B5	4	Total 4	Mg 4	0	0
56	B6	2	Total 2	Mg 2	0	0
56	B7	2	Total 2	Mg 2	0	0
56	B8	3	Total 3	Mg 3	0	0
56	B9	1	Total 1	Mg 1	0	0
56	CA	177	Total 177	Mg 177	0	0
56	CE	2	Total 2	Mg 2	0	0
56	CF	1	Total 1	Mg 1	0	0
56	CJ	1	Total 1	Mg 1	0	0
56	CT	1	Total 1	Mg 1	0	0
56	CV	1	Total 1	Mg 1	0	0
56	CW	2	Total 2	Mg 2	0	0
56	CX	5	Total 5	Mg 5	0	0
56	CY	1	Total 1	Mg 1	0	0
56	DA	675	Total 675	Mg 675	0	0
56	DB	11	Total 11	Mg 11	0	0
56	DD	7	Total 7	Mg 7	0	0

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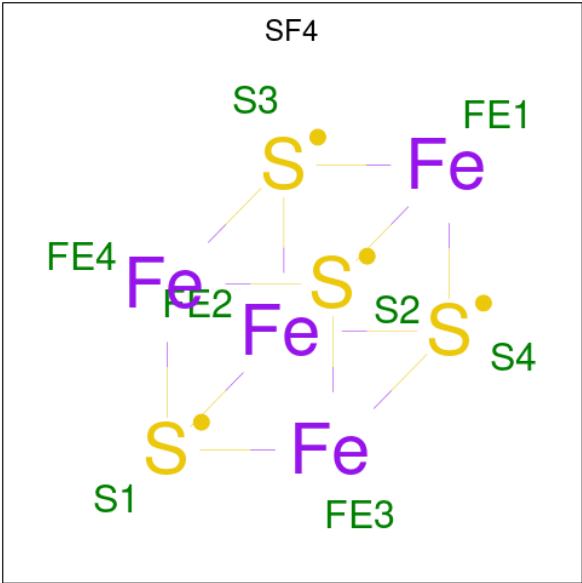
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	DE	4	Total 4	Mg 4	0	0
56	DF	5	Total 5	Mg 5	0	0
56	DG	1	Total 1	Mg 1	0	0
56	DN	1	Total 1	Mg 1	0	0
56	DO	1	Total 1	Mg 1	0	0
56	DQ	4	Total 4	Mg 4	0	0
56	DR	1	Total 1	Mg 1	0	0
56	DU	2	Total 2	Mg 2	0	0
56	DV	3	Total 3	Mg 3	0	0
56	DW	3	Total 3	Mg 3	0	0
56	DY	1	Total 1	Mg 1	0	0
56	D0	2	Total 2	Mg 2	0	0
56	D3	1	Total 1	Mg 1	0	0
56	D7	2	Total 2	Mg 2	0	0
56	D8	1	Total 1	Mg 1	0	0

- Molecule 57 is Pactamycin (CCD ID: PCY) (formula: $C_{28}H_{38}N_4O_8$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
57	AA	1	Total	C	N	O	0	0
			40	28	4	8		
57	CA	1	Total	C	N	O	0	0
			40	28	4	8		

- Molecule 58 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe₄S₄).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
58	AD	1	Total	Fe	S	0	0
			8	4	4		
58	CD	1	Total	Fe	S	0	0
			8	4	4		

- Molecule 59 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
59	AN	1	Total 1	Zn 1	0	0
59	BY	1	Total 1	Zn 1	0	0
59	B4	1	Total 1	Zn 1	0	0
59	B5	1	Total 1	Zn 1	0	0
59	B6	1	Total 1	Zn 1	0	0
59	B9	1	Total 1	Zn 1	0	0
59	CN	1	Total 1	Zn 1	0	0
59	DY	1	Total 1	Zn 1	0	0
59	D4	1	Total 1	Zn 1	0	0
59	D5	1	Total 1	Zn 1	0	0
59	D6	1	Total 1	Zn 1	0	0
59	D9	1	Total 1	Zn 1	0	0

- Molecule 60 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
60	AX	1	Total 1	K 1	0	0
60	CX	1	Total 1	K 1	0	0

- Molecule 61 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
61	AA	226	Total 226	O 226	0	0
61	AE	3	Total 3	O 3	0	0
61	AJ	1	Total 1	O 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
61	AL	4	Total 4	O 4	0	0
61	AM	1	Total 1	O 1	0	0
61	AV	4	Total 4	O 4	0	0
61	AW	6	Total 6	O 6	0	0
61	AX	8	Total 8	O 8	0	0
61	AY	3	Total 3	O 3	0	0
61	BA	1411	Total 1411	O 1411	0	0
61	BB	36	Total 36	O 36	0	0
61	BD	16	Total 16	O 16	0	0
61	BE	13	Total 13	O 13	0	0
61	BF	7	Total 7	O 7	0	0
61	BG	3	Total 3	O 3	0	0
61	BI	1	Total 1	O 1	0	0
61	BN	2	Total 2	O 2	0	0
61	BO	3	Total 3	O 3	0	0
61	BP	17	Total 17	O 17	0	0
61	BQ	2	Total 2	O 2	0	0
61	BR	2	Total 2	O 2	0	0
61	BT	1	Total 1	O 1	0	0
61	BU	6	Total 6	O 6	0	0
61	BV	2	Total 2	O 2	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
61	BW	4	Total 4	O 4	0	0
61	BX	1	Total 1	O 1	0	0
61	B0	4	Total 4	O 4	0	0
61	B1	2	Total 2	O 2	0	0
61	B3	2	Total 2	O 2	0	0
61	B5	5	Total 5	O 5	0	0
61	B6	1	Total 1	O 1	0	0
61	B7	3	Total 3	O 3	0	0
61	B8	11	Total 11	O 11	0	0
61	CA	173	Total 173	O 173	0	0
61	CJ	2	Total 2	O 2	0	0
61	CL	1	Total 1	O 1	0	0
61	CV	2	Total 2	O 2	0	0
61	CW	1	Total 1	O 1	0	0
61	CX	4	Total 4	O 4	0	0
61	DA	1002	Total 1002	O 1002	0	0
61	DB	10	Total 10	O 10	0	0
61	DD	17	Total 17	O 17	0	0
61	DE	11	Total 11	O 11	0	0
61	DF	5	Total 5	O 5	0	0
61	DN	2	Total 2	O 2	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
61	DO	2	Total	O	0	0
			2	2		
61	DP	8	Total	O	0	0
			8	8		
61	DQ	1	Total	O	0	0
			1	1		
61	DR	1	Total	O	0	0
			1	1		
61	DU	2	Total	O	0	0
			2	2		
61	DW	1	Total	O	0	0
			1	1		
61	DY	1	Total	O	0	0
			1	1		
61	D0	5	Total	O	0	0
			5	5		
61	D3	1	Total	O	0	0
			1	1		
61	D7	3	Total	O	0	0
			3	3		
61	D8	4	Total	O	0	0
			4	4		

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

3 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	209.35Å 449.01Å 621.98Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	145.52 – 2.55 145.52 – 2.55	Depositor EDS
% Data completeness (in resolution range)	99.0 (145.52-2.55) 99.0 (145.52-2.55)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.28 (at 2.55Å)	Xtriage
Refinement program	PHENIX 1.8.2_1309	Depositor
R, R_{free}	0.225 , 0.273 0.229 , 0.274	Depositor DCC
R_{free} test set	93275 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å ²)	48.2	Xtriage
Anisotropy	0.182	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 59.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.40$, $\langle L^2 \rangle = 0.23$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	297273	wwPDB-VP
Average B, all atoms (Å ²)	58.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.48% 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](#)

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
23	4SU	CW	8	23,56	18,21,22	1.69	5 (27%)	25,30,33	2.01	4 (16%)
24	4SU	AX	8	24	18,21,22	2.28	6 (33%)	25,30,33	1.74	7 (28%)
23	4SU	AW	8	23	18,21,22	1.81	6 (33%)	25,30,33	1.84	6 (24%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
23	PSU	AY	55	23	18,21,22	1.29	2 (11%)	21,30,33	2.06	6 (28%)
23	7MG	CY	46	23	23,26,27	1.39	4 (17%)	27,39,42	2.63	7 (25%)
23	PSU	CW	39	23	18,21,22	1.41	2 (11%)	21,30,33	1.64	3 (14%)
23	7MG	CW	46	23	23,26,27	1.33	4 (17%)	27,39,42	2.66	6 (22%)
23	5MU	AW	54	23	19,22,23	1.46	5 (26%)	27,32,35	1.71	5 (18%)
23	PSU	CY	32	23	18,21,22	1.37	2 (11%)	21,30,33	1.91	3 (14%)
23	MIA	CY	37	23	21,24,32	1.64	3 (14%)	30,35,47	2.03	8 (26%)
23	PSU	AW	39	23	18,21,22	1.37	2 (11%)	21,30,33	2.02	4 (19%)
23	MIA	AW	37	23	28,31,32	2.35	6 (21%)	38,44,47	2.67	13 (34%)
24	5MU	AX	54	56,24	19,22,23	1.44	6 (31%)	27,32,35	2.05	6 (22%)
23	7MG	AY	46	23	23,26,27	1.39	4 (17%)	27,39,42	2.61	6 (22%)
23	PSU	CY	55	23	18,21,22	1.40	2 (11%)	21,30,33	2.11	3 (14%)
23	PSU	AW	55	23	18,21,22	1.41	2 (11%)	21,30,33	2.03	3 (14%)
23	PSU	CW	32	23	18,21,22	1.37	4 (22%)	21,30,33	1.99	4 (19%)
23	PSU	CW	55	23	18,21,22	1.41	2 (11%)	21,30,33	2.10	3 (14%)
24	5MC	AX	32	24	19,22,23	1.68	3 (15%)	26,32,35	1.24	2 (7%)
23	7MG	AW	46	23	23,26,27	1.34	3 (13%)	27,39,42	2.64	7 (25%)
23	4SU	CY	8	23	18,21,22	1.76	4 (22%)	25,30,33	2.27	4 (16%)
23	PSU	AY	32	23	18,21,22	1.35	2 (11%)	21,30,33	2.06	4 (19%)
23	MIA	AY	37	23	21,24,32	1.64	4 (19%)	30,35,47	1.94	7 (23%)
23	5MU	CY	54	23	19,22,23	1.50	5 (26%)	27,32,35	1.95	9 (33%)
23	PSU	CY	39	23	18,21,22	1.46	3 (16%)	21,30,33	1.96	3 (14%)
23	5MU	AY	54	23	19,22,23	1.47	5 (26%)	27,32,35	1.63	6 (22%)
24	5MU	CX	54	24	19,22,23	1.38	6 (31%)	27,32,35	2.11	8 (29%)
23	MIA	CW	37	23	21,24,32	1.55	4 (19%)	30,35,47	2.15	8 (26%)
23	PSU	AW	32	23,56	18,21,22	1.39	3 (16%)	21,30,33	1.83	4 (19%)
24	PSU	CX	55	24	18,21,22	1.36	2 (11%)	21,30,33	1.99	6 (28%)
24	5MC	CX	32	24	19,22,23	1.63	3 (15%)	26,32,35	1.30	3 (11%)
23	5MU	CW	54	23	19,22,23	1.33	5 (26%)	27,32,35	1.98	7 (25%)
24	PSU	AX	55	24	18,21,22	1.35	2 (11%)	21,30,33	1.98	4 (19%)
23	4SU	AY	8	23	18,21,22	1.80	7 (38%)	25,30,33	1.57	5 (20%)
23	PSU	AY	39	23	18,21,22	1.50	3 (16%)	21,30,33	1.68	4 (19%)
24	4SU	CX	8	24	18,21,22	1.97	4 (22%)	25,30,33	1.34	4 (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
23	4SU	CW	8	23,56	-	0/7/25/26	0/2/2/2
24	4SU	AX	8	24	-	0/7/25/26	0/2/2/2
23	4SU	AW	8	23	-	0/7/25/26	0/2/2/2
23	PSU	AY	55	23	-	1/7/25/26	0/2/2/2
23	7MG	CY	46	23	-	2/7/37/38	0/3/3/3
23	PSU	CW	39	23	-	0/7/25/26	0/2/2/2
23	7MG	CW	46	23	-	2/7/37/38	0/3/3/3
23	5MU	AW	54	23	-	0/7/25/26	0/2/2/2
23	PSU	CY	32	23	-	1/7/25/26	0/2/2/2
23	MIA	CY	37	23	-	3/7/25/34	0/3/3/3
23	PSU	AW	39	23	-	0/7/25/26	0/2/2/2
23	MIA	AW	37	23	-	1/15/33/34	0/3/3/3
24	5MU	AX	54	56,24	-	0/7/25/26	0/2/2/2
23	7MG	AY	46	23	-	3/7/37/38	0/3/3/3
23	PSU	CY	55	23	-	3/7/25/26	0/2/2/2
23	PSU	AW	55	23	-	0/7/25/26	0/2/2/2
23	PSU	CW	32	23	-	4/7/25/26	0/2/2/2
23	PSU	CW	55	23	-	0/7/25/26	0/2/2/2
24	5MC	AX	32	24	-	0/7/25/26	0/2/2/2
23	7MG	AW	46	23	-	3/7/37/38	0/3/3/3
23	4SU	CY	8	23	-	2/7/25/26	0/2/2/2
23	PSU	AY	32	23	-	0/7/25/26	0/2/2/2
23	MIA	AY	37	23	-	1/7/25/34	0/3/3/3
23	5MU	CY	54	23	-	1/7/25/26	0/2/2/2
23	PSU	CY	39	23	-	2/7/25/26	0/2/2/2
23	5MU	AY	54	23	-	0/7/25/26	0/2/2/2
24	5MU	CX	54	24	-	0/7/25/26	0/2/2/2
23	MIA	CW	37	23	-	0/7/25/34	0/3/3/3
23	PSU	AW	32	23,56	-	0/7/25/26	0/2/2/2
24	PSU	CX	55	24	-	0/7/25/26	0/2/2/2
24	5MC	CX	32	24	-	0/7/25/26	0/2/2/2
23	5MU	CW	54	23	-	0/7/25/26	0/2/2/2
24	PSU	AX	55	24	-	0/7/25/26	0/2/2/2
23	4SU	AY	8	23	-	1/7/25/26	0/2/2/2
23	PSU	AY	39	23	-	2/7/25/26	0/2/2/2
24	4SU	CX	8	24	-	0/7/25/26	0/2/2/2

All (135) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	AW	37	MIA	C2-S10	-7.49	1.69	1.75
23	AW	37	MIA	C13-C14	6.84	1.52	1.32
24	AX	32	5MC	C5-C4	5.98	1.48	1.44
24	AX	8	4SU	C4-N3	-5.87	1.31	1.37
24	CX	32	5MC	C5-C4	5.67	1.48	1.44
23	CY	37	MIA	C5-C4	5.25	1.48	1.39
23	AY	37	MIA	C5-C4	5.23	1.48	1.39
23	CY	8	4SU	C4-S4	-4.93	1.60	1.68
23	CW	37	MIA	C5-C4	4.75	1.47	1.39
23	AW	8	4SU	C4-S4	-4.67	1.60	1.68
23	AW	37	MIA	C5-C4	4.61	1.47	1.39
24	AX	8	4SU	C4-S4	-4.48	1.60	1.68
23	CW	8	4SU	C4-S4	-4.48	1.60	1.68
24	CX	8	4SU	C4-N3	-4.44	1.33	1.37
23	AY	8	4SU	C4-S4	-4.39	1.60	1.68
24	CX	8	4SU	C4-S4	-4.31	1.61	1.68
23	CW	55	PSU	C6-C5	4.16	1.39	1.35
24	AX	8	4SU	C2-N3	-4.10	1.30	1.38
23	AW	55	PSU	C6-C5	4.05	1.39	1.35
23	AY	39	PSU	C6-C5	4.03	1.39	1.35
23	CY	32	PSU	C6-C5	4.01	1.39	1.35
24	CX	55	PSU	C6-C5	3.73	1.39	1.35
23	CW	39	PSU	C6-C5	3.72	1.39	1.35
23	CY	39	PSU	C6-C5	3.72	1.39	1.35
23	AY	46	7MG	C5-C4	3.70	1.49	1.37
23	AY	32	PSU	C6-C5	3.70	1.39	1.35
23	AY	55	PSU	C6-C5	3.69	1.39	1.35
23	CY	55	PSU	C6-C5	3.54	1.39	1.35
23	AW	39	PSU	C6-C5	3.53	1.39	1.35
23	CY	46	7MG	C5-C4	3.44	1.48	1.37
23	AW	46	7MG	C5-C4	3.40	1.48	1.37
23	AY	8	4SU	C4-N3	-3.39	1.34	1.37
23	AW	32	PSU	C6-C5	3.39	1.39	1.35
23	CW	46	7MG	C5-C4	3.35	1.47	1.37
24	CX	8	4SU	C5-C4	-3.34	1.38	1.42
23	CY	46	7MG	C4-N9	-3.23	1.33	1.37
23	CW	32	PSU	C6-C5	3.21	1.38	1.35
24	CX	32	5MC	C6-C5	3.16	1.39	1.34
23	AW	8	4SU	C4-N3	-3.10	1.34	1.37
24	AX	55	PSU	C6-C5	3.09	1.38	1.35
24	AX	8	4SU	C5-C4	-3.07	1.38	1.42
24	CX	8	4SU	C2-N3	-2.97	1.32	1.38
23	CY	54	5MU	C6-C5	2.93	1.39	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	CY	37	MIA	C5-C6	2.91	1.49	1.41
23	AY	37	MIA	C5-C6	2.91	1.49	1.41
23	CY	54	5MU	C2-N1	2.89	1.43	1.38
23	CY	8	4SU	C5-C4	-2.89	1.39	1.42
23	AW	8	4SU	C5-C4	-2.88	1.39	1.42
23	CW	8	4SU	C4-N3	-2.87	1.34	1.37
23	AW	54	5MU	C4-N3	-2.82	1.33	1.38
23	AW	54	5MU	C6-C5	2.80	1.39	1.34
23	AY	54	5MU	C6-C5	2.80	1.39	1.34
24	AX	54	5MU	C4-N3	-2.77	1.33	1.38
23	AW	46	7MG	C4-N9	-2.76	1.34	1.37
23	AW	32	PSU	C4-N3	-2.75	1.33	1.38
23	AY	54	5MU	C4-N3	-2.73	1.33	1.38
24	AX	32	5MC	C6-C5	2.72	1.39	1.34
24	AX	32	5MC	C6-N1	-2.70	1.33	1.38
24	AX	54	5MU	C6-C5	2.69	1.39	1.34
23	CW	37	MIA	C5-C6	2.68	1.48	1.41
24	CX	54	5MU	C6-C5	2.68	1.39	1.34
23	CW	39	PSU	C4-N3	-2.67	1.33	1.38
24	CX	54	5MU	C4-C5	2.65	1.49	1.44
23	CY	54	5MU	C4-C5	2.65	1.49	1.44
23	CW	54	5MU	C6-C5	2.65	1.38	1.34
23	CW	46	7MG	C4-N9	-2.64	1.34	1.37
23	AY	8	4SU	C5-C4	-2.60	1.39	1.42
24	CX	55	PSU	C4-N3	-2.59	1.34	1.38
23	CY	55	PSU	C4-N3	-2.56	1.34	1.38
23	AW	37	MIA	C5-N7	-2.54	1.34	1.39
23	CW	32	PSU	C4-N3	-2.53	1.34	1.38
24	AX	55	PSU	C4-N3	-2.53	1.34	1.38
23	AY	39	PSU	C4-N3	-2.53	1.34	1.38
23	CW	55	PSU	C4-N3	-2.49	1.34	1.38
23	CW	8	4SU	C2-N1	2.49	1.42	1.38
23	CY	54	5MU	C4-N3	-2.49	1.34	1.38
23	AY	46	7MG	C8-N9	2.48	1.47	1.45
23	AW	39	PSU	C4-N3	-2.48	1.34	1.38
23	CY	39	PSU	C4-N3	-2.48	1.34	1.38
23	AY	54	5MU	C4-C5	2.48	1.48	1.44
23	AW	55	PSU	C4-N3	-2.48	1.34	1.38
23	CW	54	5MU	C4-C5	2.47	1.48	1.44
24	CX	54	5MU	C4-N3	-2.45	1.34	1.38
23	CW	37	MIA	C5-N7	-2.44	1.34	1.39
23	CY	8	4SU	C2-N1	2.44	1.42	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	AY	37	MIA	C8-N7	2.43	1.36	1.31
23	CY	37	MIA	C8-N7	2.42	1.36	1.31
23	CY	8	4SU	C4-N3	-2.42	1.35	1.37
23	AY	32	PSU	C4-N3	-2.41	1.34	1.38
23	CY	46	7MG	C6-N1	-2.40	1.34	1.38
23	AW	54	5MU	C2-N1	2.38	1.42	1.38
23	AY	46	7MG	C4-N9	-2.38	1.34	1.37
24	AX	54	5MU	C4-C5	2.38	1.48	1.44
23	AW	37	MIA	C5-C6	2.36	1.47	1.41
23	AW	54	5MU	C4-C5	2.36	1.48	1.44
23	AY	54	5MU	C2-N1	2.36	1.42	1.38
23	AY	55	PSU	C4-N3	-2.35	1.34	1.38
23	CY	32	PSU	C4-N3	-2.33	1.34	1.38
23	AY	39	PSU	O4'-C1'	-2.33	1.40	1.43
23	AW	8	4SU	C2-N1	2.33	1.42	1.38
23	AY	46	7MG	C6-N1	-2.32	1.34	1.38
23	AW	54	5MU	C2-N3	-2.32	1.33	1.38
23	CW	37	MIA	C8-N7	2.31	1.36	1.31
24	AX	54	5MU	C2-N3	-2.30	1.34	1.38
23	AY	8	4SU	C2-N1	2.30	1.42	1.38
23	AW	46	7MG	C6-N1	-2.25	1.34	1.38
24	AX	8	4SU	O2-C2	2.24	1.27	1.23
23	AW	37	MIA	C8-N7	2.24	1.36	1.31
23	CW	54	5MU	C2-N1	2.24	1.42	1.38
23	CW	46	7MG	C6-N1	-2.23	1.34	1.38
23	CW	32	PSU	C4-C5	2.20	1.50	1.44
23	CW	46	7MG	C8-N9	2.18	1.47	1.45
24	CX	32	5MC	C6-N1	-2.16	1.34	1.38
23	AY	8	4SU	C2-N3	-2.12	1.34	1.38
23	CY	39	PSU	O4'-C1'	-2.12	1.40	1.43
23	AW	8	4SU	C2-N3	-2.11	1.34	1.38
23	CY	54	5MU	C2-N3	-2.10	1.34	1.38
24	AX	54	5MU	C2-N1	2.08	1.41	1.38
23	AW	32	PSU	C2-N3	-2.07	1.34	1.37
23	AY	8	4SU	O2-C2	2.07	1.26	1.23
23	CW	54	5MU	C4-N3	-2.07	1.35	1.38
24	AX	54	5MU	C6-N1	-2.06	1.34	1.38
24	AX	8	4SU	C6-C5	2.05	1.39	1.35
23	CW	8	4SU	C5-C4	-2.05	1.40	1.42
24	CX	54	5MU	C2-N1	2.05	1.41	1.38
24	CX	54	5MU	C2-N3	-2.05	1.34	1.38
23	AY	37	MIA	C5-N7	-2.03	1.35	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	CW	8	4SU	C6-C5	2.03	1.39	1.35
24	CX	54	5MU	C6-N1	-2.03	1.34	1.38
23	AY	54	5MU	C2-N3	-2.03	1.34	1.38
23	AY	8	4SU	C6-C5	2.01	1.39	1.35
23	CY	46	7MG	C8-N9	2.01	1.47	1.45
23	CW	32	PSU	C2-N3	-2.01	1.34	1.37
23	AW	8	4SU	O2-C2	2.00	1.26	1.23
23	CW	54	5MU	C6-N1	-2.00	1.34	1.38

All (192) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	AY	46	7MG	N9-C4-N3	9.30	139.09	125.46
23	AW	46	7MG	N9-C4-N3	9.21	138.96	125.46
23	CW	46	7MG	N9-C4-N3	9.01	138.66	125.46
23	CY	46	7MG	N9-C4-N3	8.82	138.38	125.46
23	AW	37	MIA	C12-C13-C14	-8.27	112.17	127.01
23	AW	37	MIA	C5-C4-N3	-7.69	119.08	127.18
23	CW	55	PSU	N1-C2-N3	6.62	122.15	115.17
23	AY	32	PSU	N1-C2-N3	6.44	121.96	115.17
23	CY	55	PSU	N1-C2-N3	6.44	121.96	115.17
23	CW	37	MIA	C5-C4-N3	-6.29	118.06	126.72
23	AW	55	PSU	N1-C2-N3	6.24	121.75	115.17
23	AW	37	MIA	N3-C4-N9	6.24	134.91	126.99
23	CY	39	PSU	N1-C2-N3	6.17	121.68	115.17
24	AX	55	PSU	N1-C2-N3	6.14	121.65	115.17
23	AW	39	PSU	N1-C2-N3	6.14	121.64	115.17
23	AY	55	PSU	N1-C2-N3	6.05	121.55	115.17
23	CY	8	4SU	C5-C4-N3	5.97	120.30	114.75
23	CW	8	4SU	C4-N3-C2	-5.96	121.60	127.31
23	CY	32	PSU	N1-C2-N3	5.93	121.42	115.17
23	CY	8	4SU	C4-N3-C2	-5.90	121.66	127.31
23	CW	46	7MG	C5-C4-N3	-5.83	117.19	128.13
23	AW	32	PSU	N1-C2-N3	5.83	121.31	115.17
24	CX	55	PSU	N1-C2-N3	5.76	121.24	115.17
23	CW	32	PSU	N1-C2-N3	5.73	121.21	115.17
23	AY	37	MIA	C5-C4-N3	-5.54	119.08	126.72
23	CY	37	MIA	C5-C4-N3	-5.52	119.11	126.72
23	AW	46	7MG	C5-C4-N3	-5.39	118.01	128.13
23	AY	46	7MG	C5-C4-N3	-5.37	118.04	128.13
23	CY	8	4SU	C5-C4-S4	-5.30	118.26	124.31
23	AW	8	4SU	C5-C4-N3	5.27	119.65	114.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	AW	46	7MG	N9-C8-N7	-5.27	95.92	103.37
23	CY	46	7MG	N9-C8-N7	-5.23	95.96	103.37
23	AY	39	PSU	N1-C2-N3	5.16	120.61	115.17
23	CY	46	7MG	C5-C4-N3	-5.12	118.53	128.13
24	CX	54	5MU	N3-C2-N1	5.08	121.51	114.89
23	CW	39	PSU	N1-C2-N3	5.05	120.50	115.17
24	CX	54	5MU	C4-N3-C2	-5.02	120.76	127.34
23	CW	37	MIA	N3-C4-N9	4.92	135.53	127.17
24	AX	54	5MU	C4-N3-C2	-4.92	120.89	127.34
23	CW	8	4SU	C5-C4-N3	4.90	119.31	114.75
23	CW	46	7MG	N9-C8-N7	-4.89	96.45	103.37
23	CY	37	MIA	N3-C4-N9	4.82	135.37	127.17
23	CW	46	7MG	C2-N3-C4	4.76	120.50	112.30
24	AX	54	5MU	C5-C4-N3	4.75	119.46	115.32
23	AY	46	7MG	N9-C8-N7	-4.71	96.71	103.37
24	AX	54	5MU	N3-C2-N1	4.60	120.88	114.89
23	CY	55	PSU	O2-C2-N1	-4.54	118.10	122.79
23	CW	54	5MU	C4-N3-C2	-4.48	121.46	127.34
23	AY	37	MIA	N3-C4-N9	4.48	134.78	127.17
23	CY	46	7MG	C2-N3-C4	4.40	119.87	112.30
23	CW	54	5MU	O4-C4-C5	-4.39	119.89	124.92
24	CX	55	PSU	C4-N3-C2	-4.37	120.35	126.37
23	AW	46	7MG	C2-N3-C4	4.36	119.80	112.30
24	CX	54	5MU	C5-C4-N3	4.34	119.09	115.32
23	CY	54	5MU	C5-C4-N3	4.30	119.06	115.32
23	AW	8	4SU	C4-N3-C2	-4.28	123.21	127.31
23	CY	39	PSU	O2-C2-N1	-4.26	118.40	122.79
23	AW	54	5MU	N3-C2-N1	4.24	120.41	114.89
23	AY	32	PSU	C4-N3-C2	-4.24	120.53	126.37
23	CY	54	5MU	C4-N3-C2	-4.23	121.79	127.34
23	CW	54	5MU	C5-C4-N3	4.23	119.00	115.32
23	AY	46	7MG	C2-N3-C4	4.23	119.58	112.30
23	CY	54	5MU	N3-C2-N1	4.22	120.38	114.89
23	AY	55	PSU	C4-N3-C2	-4.22	120.56	126.37
23	CW	54	5MU	N3-C2-N1	4.16	120.31	114.89
23	AY	8	4SU	C5-C4-N3	4.14	118.60	114.75
23	AW	39	PSU	C4-N3-C2	-4.13	120.68	126.37
23	AW	37	MIA	C15-C14-C13	-4.07	110.44	122.66
23	CY	55	PSU	C4-N3-C2	-4.06	120.78	126.37
23	CW	55	PSU	C4-N3-C2	-4.04	120.81	126.37
24	AX	8	4SU	C6-C5-C4	-4.03	116.46	119.95
23	AW	55	PSU	C4-N3-C2	-4.03	120.82	126.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	CW	37	MIA	C2-N3-C4	4.01	121.62	111.83
23	CW	8	4SU	N3-C2-N1	4.01	120.11	114.89
23	CW	37	MIA	N3-C2-N1	-3.98	122.55	128.58
24	AX	32	5MC	C5-C6-N1	-3.97	119.00	123.31
23	AW	37	MIA	C16-C14-C13	-3.95	110.80	122.66
24	AX	55	PSU	C4-N3-C2	-3.95	120.93	126.37
24	AX	8	4SU	O2-C2-N1	3.90	127.87	122.80
23	AW	54	5MU	C4-N3-C2	-3.80	122.36	127.34
24	AX	54	5MU	C5-C6-N1	-3.79	119.20	123.31
23	CW	32	PSU	C4-N3-C2	-3.77	121.17	126.37
24	CX	54	5MU	O4-C4-C5	-3.77	120.61	124.92
24	AX	54	5MU	O4-C4-C5	-3.74	120.64	124.92
23	CY	32	PSU	C4-N3-C2	-3.74	121.22	126.37
23	AW	54	5MU	C5-C4-N3	3.71	118.55	115.32
23	CW	55	PSU	O2-C2-N1	-3.65	119.02	122.79
24	AX	55	PSU	O2-C2-N1	-3.64	119.03	122.79
23	CW	37	MIA	C4-C5-N7	-3.61	106.45	110.58
23	AY	37	MIA	C2-N3-C4	3.60	120.63	111.83
23	AY	32	PSU	O2-C2-N1	-3.60	119.08	122.79
23	AW	8	4SU	C5-C4-S4	-3.58	120.21	124.31
23	AW	32	PSU	C4-N3-C2	-3.57	121.46	126.37
23	AY	54	5MU	C5-C4-N3	3.56	118.42	115.32
23	CY	37	MIA	C2-N3-C4	3.56	120.52	111.83
23	AY	54	5MU	N3-C2-N1	3.53	119.49	114.89
23	AY	8	4SU	C4-N3-C2	-3.52	123.94	127.31
23	CY	54	5MU	O4-C4-C5	-3.52	120.89	124.92
23	AW	39	PSU	O2-C2-N1	-3.51	119.17	122.79
23	AY	37	MIA	N3-C2-N1	-3.49	123.30	128.58
23	CY	37	MIA	N3-C2-N1	-3.48	123.32	128.58
23	CY	39	PSU	C4-N3-C2	-3.47	121.60	126.37
24	CX	32	5MC	C5-C6-N1	-3.45	119.57	123.31
23	CW	32	PSU	C6-C5-C4	-3.40	115.88	118.17
24	AX	8	4SU	S4-C4-N3	-3.40	116.65	120.20
24	CX	8	4SU	C6-C5-C4	-3.38	117.02	119.95
23	AY	55	PSU	O2-C2-N1	-3.36	119.32	122.79
23	AY	54	5MU	C4-N3-C2	-3.36	122.94	127.34
23	CY	8	4SU	N3-C2-N1	3.30	119.19	114.89
23	AW	37	MIA	N6-C6-N1	3.30	122.75	118.33
24	CX	32	5MC	C5-C4-N3	-3.25	118.42	121.75
23	AY	37	MIA	C4-C5-N7	-3.23	106.89	110.58
23	AW	37	MIA	C2-N3-C4	3.22	120.73	112.29
23	CY	32	PSU	O2-C2-N1	-3.21	119.48	122.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	CW	8	4SU	C5-C4-S4	-3.17	120.68	124.31
23	CY	37	MIA	C4-N9-C8	3.17	109.06	105.74
23	CY	37	MIA	C4-C5-N7	-3.13	107.00	110.58
24	CX	8	4SU	C1'-N1-C2	3.08	123.12	117.59
23	AW	54	5MU	O4-C4-C5	-3.06	121.41	124.92
23	AW	55	PSU	O2-C2-N1	-3.02	119.68	122.79
24	CX	54	5MU	C5-C6-N1	-3.00	120.05	123.31
23	AY	8	4SU	C1'-N1-C2	3.00	122.98	117.59
23	AW	37	MIA	C4-C5-N7	-2.98	107.17	110.58
23	CW	46	7MG	C5-C6-N1	2.97	116.17	110.94
23	CW	39	PSU	C4-N3-C2	-2.97	122.28	126.37
24	CX	32	5MC	O2-C2-N3	-2.91	117.73	122.33
23	AY	54	5MU	O4-C4-C5	-2.88	121.62	124.92
23	CY	54	5MU	C5-C6-N1	-2.88	120.19	123.31
24	AX	32	5MC	C5-C4-N3	-2.85	118.83	121.75
24	CX	54	5MU	O2-C2-N1	-2.84	119.10	122.80
23	CW	32	PSU	O2-C2-N1	-2.82	119.88	122.79
24	CX	54	5MU	C5M-C5-C4	2.82	121.79	118.78
24	AX	8	4SU	C5-C4-N3	2.79	117.35	114.75
23	CW	37	MIA	C5-N7-C8	2.78	107.82	103.45
23	AY	39	PSU	C6-C5-C4	-2.78	116.30	118.17
23	AW	54	5MU	C5-C6-N1	-2.74	120.34	123.31
23	AY	8	4SU	N3-C2-N1	2.73	118.45	114.89
23	AW	8	4SU	C1'-N1-C2	2.73	122.50	117.59
23	AY	46	7MG	C5-C4-N9	-2.71	102.86	106.33
23	CW	54	5MU	C5M-C5-C4	2.63	121.59	118.78
23	AY	39	PSU	C4-N3-C2	-2.62	122.76	126.37
24	CX	8	4SU	C5-C4-N3	2.59	117.16	114.75
23	AY	54	5MU	C5-C6-N1	-2.59	120.51	123.31
23	AW	46	7MG	C5-C4-N9	-2.58	103.03	106.33
23	AW	8	4SU	N3-C2-N1	2.57	118.24	114.89
23	AW	37	MIA	C6-C5-N7	2.56	135.22	132.43
23	CY	46	7MG	C5-C4-N9	-2.56	103.06	106.33
23	CY	54	5MU	C1'-N1-C2	2.53	122.14	117.59
24	AX	54	5MU	O2-C2-N1	-2.53	119.50	122.80
23	CW	54	5MU	C5-C6-N1	-2.52	120.58	123.31
23	AW	37	MIA	C2-N1-C6	2.52	122.32	117.54
23	AW	46	7MG	C5-C6-N1	2.51	115.35	110.94
23	CY	46	7MG	O4'-C1'-N9	-2.47	105.93	109.30
23	AW	37	MIA	C4-N9-C8	2.44	108.30	105.74
23	CY	37	MIA	C5-N7-C8	2.43	107.27	103.45
23	CY	54	5MU	C1'-N1-C6	-2.42	117.16	121.15

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	AX	8	4SU	O2-C2-N3	-2.42	117.03	121.49
23	CW	39	PSU	O2-C2-N1	-2.40	120.32	122.79
23	CY	54	5MU	C5M-C5-C4	2.40	121.34	118.78
24	AX	8	4SU	C1'-N1-C2	2.39	121.88	117.59
23	AY	54	5MU	C5M-C5-C4	2.38	121.33	118.78
23	AY	37	MIA	C4-N9-C8	2.37	108.23	105.74
23	AY	39	PSU	O2-C2-N1	-2.33	120.39	122.79
23	AY	55	PSU	C5-C6-N1	-2.31	118.94	122.14
24	CX	55	PSU	C5-C6-N1	-2.29	118.96	122.14
23	AW	37	MIA	C5-N7-C8	2.29	107.05	103.45
23	AY	37	MIA	C5-N7-C8	2.29	107.05	103.45
23	CW	54	5MU	O2-C2-N1	-2.27	119.84	122.80
23	CY	46	7MG	C5-C6-N1	2.27	114.93	110.94
23	AW	37	MIA	N3-C2-N1	-2.26	122.87	127.00
24	CX	55	PSU	C6-C5-C4	-2.26	116.65	118.17
23	CW	46	7MG	O6-C6-C5	-2.24	122.12	127.62
23	AY	8	4SU	C5-C4-S4	-2.20	121.79	124.31
23	AY	55	PSU	O4-C4-C5	-2.19	118.57	124.01
23	CW	37	MIA	C4-N9-C8	2.18	108.03	105.74
23	CY	54	5MU	O2-C2-N3	-2.17	117.49	121.49
23	AW	32	PSU	O2-C2-N1	-2.16	120.56	122.79
23	AY	46	7MG	C5-C6-N1	2.15	114.72	110.94
24	CX	55	PSU	O2-C2-N3	-2.11	118.12	121.86
24	CX	8	4SU	C6-N1-C2	-2.10	118.44	121.00
23	AW	32	PSU	O2-C2-N3	-2.10	118.12	121.86
23	AW	8	4SU	C6-C5-C4	-2.10	118.13	119.95
23	AY	32	PSU	C5-C6-N1	-2.10	119.22	122.14
23	AY	55	PSU	O4'-C1'-C2'	2.08	108.03	105.15
24	CX	55	PSU	O2-C2-N1	-2.08	120.64	122.79
24	AX	55	PSU	C5-C6-N1	-2.07	119.26	122.14
23	CW	37	MIA	C2-N1-C6	2.07	122.13	118.73
24	CX	54	5MU	C5M-C5-C6	-2.06	120.06	122.85
23	AW	46	7MG	O6-C6-C5	-2.06	122.57	127.62
24	AX	8	4SU	C4-N3-C2	2.05	129.28	127.31
23	CY	37	MIA	C2-N1-C6	2.04	122.08	118.73
23	AW	39	PSU	C5-C6-N1	-2.01	119.36	122.14

There are no chirality outliers.

All (32) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
23	AW	37	MIA	C12-C13-C14-C16

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Mol	Chain	Res	Type	Atoms
23	AY	46	7MG	C4'-C5'-O5'-P
23	CW	32	PSU	C2'-C1'-C5-C4
23	CW	32	PSU	C2'-C1'-C5-C6
23	CY	55	PSU	C2'-C1'-C5-C4
23	AY	39	PSU	C3'-C4'-C5'-O5'
23	CY	37	MIA	C3'-C4'-C5'-O5'
23	CY	39	PSU	C3'-C4'-C5'-O5'
23	CY	46	7MG	O4'-C4'-C5'-O5'
23	AY	39	PSU	O4'-C4'-C5'-O5'
23	CY	39	PSU	O4'-C4'-C5'-O5'
23	CY	8	4SU	O4'-C4'-C5'-O5'
23	CY	37	MIA	O4'-C4'-C5'-O5'
23	CY	46	7MG	C3'-C4'-C5'-O5'
23	CW	46	7MG	C2'-C1'-N9-C8
23	AY	46	7MG	C2'-C1'-N9-C8
23	AW	46	7MG	C3'-C4'-C5'-O5'
23	CY	55	PSU	C3'-C4'-C5'-O5'
23	AW	46	7MG	O4'-C4'-C5'-O5'
23	AY	37	MIA	C4'-C5'-O5'-P
23	AY	55	PSU	O4'-C1'-C5-C4
23	CW	32	PSU	O4'-C1'-C5-C4
23	CY	55	PSU	O4'-C1'-C5-C4
23	CY	37	MIA	C4'-C5'-O5'-P
23	CY	32	PSU	O4'-C4'-C5'-O5'
23	CY	8	4SU	C3'-C4'-C5'-O5'
23	CW	32	PSU	O4'-C1'-C5-C6
23	AY	46	7MG	O4'-C1'-N9-C8
23	CW	46	7MG	O4'-C1'-N9-C8
23	CY	54	5MU	C2'-C1'-N1-C2
23	AW	46	7MG	C4'-C5'-O5'-P
23	AY	8	4SU	C2'-C1'-N1-C2

There are no ring outliers.

No monomer is involved in short contacts.

4.5 Carbohydrates

There are no oligosaccharides in this entry.

4.6 Ligand geometry

Of 2152 ligands modelled in this entry, 2148 are monoatomic - leaving 4 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
58	SF4	AD	501	4	0,12,12	-	-	-		
57	PCY	AA	3231	-	34,42,42	1.73	5 (14%)	41,65,65	1.44	7 (17%)
58	SF4	CD	501	4	0,12,12	-	-	-		
57	PCY	CA	3178	-	34,42,42	1.70	4 (11%)	41,65,65	1.17	4 (9%)

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
58	SF4	AD	501	4	-	-	0/6/5/5
57	PCY	AA	3231	-	-	5/33/67/67	0/3/3/3
58	SF4	CD	501	4	-	-	0/6/5/5
57	PCY	CA	3178	-	-	8/33/67/67	0/3/3/3

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
57	AA	3231	PCY	C34-C30	-5.60	1.40	1.51
57	CA	3178	PCY	C34-C30	-5.56	1.40	1.51
57	CA	3178	PCY	C28-C32	-5.50	1.39	1.49
57	AA	3231	PCY	C28-C32	-5.35	1.39	1.49
57	AA	3231	PCY	C27-C23	-4.14	1.40	1.50
57	CA	3178	PCY	C27-C23	-3.71	1.41	1.50
57	CA	3178	PCY	C22-N20	-3.14	1.33	1.39
57	AA	3231	PCY	C22-N20	-2.86	1.34	1.39
57	AA	3231	PCY	C17-N20	2.32	1.48	1.45

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
57	AA	3231	PCY	C18-O21-C23	-4.84	107.00	116.55
57	CA	3178	PCY	C18-O21-C23	-3.69	109.27	116.55
57	AA	3231	PCY	O21-C23-C27	3.04	119.12	112.35
57	AA	3231	PCY	O21-C18-C15	2.78	112.92	107.79
57	AA	3231	PCY	O36-C31-C27	-2.29	116.91	121.14
57	CA	3178	PCY	C38-C32-C28	-2.19	115.07	119.21
57	AA	3231	PCY	C34-C30-C35	-2.18	116.08	120.28
57	AA	3231	PCY	C34-C30-C27	2.17	124.53	121.67
57	AA	3231	PCY	C30-C27-C23	2.17	126.64	120.47
57	CA	3178	PCY	C34-C30-C35	-2.05	116.32	120.28
57	CA	3178	PCY	C10-N4-C9	2.03	122.35	115.87

There are no chirality outliers.

All (13) torsion outliers are listed below:

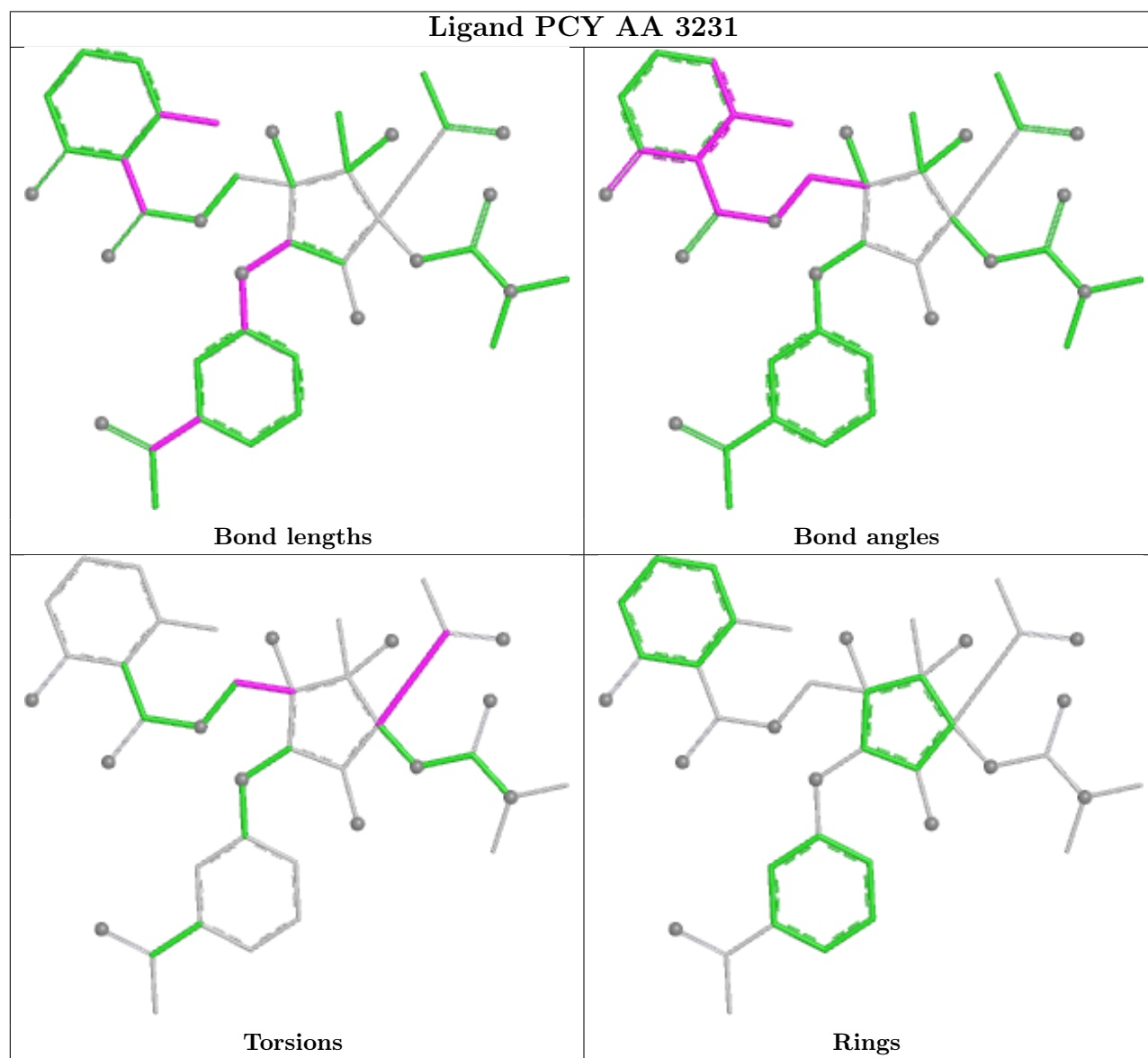
Mol	Chain	Res	Type	Atoms
57	AA	3231	PCY	N2-C3-C6-C11
57	AA	3231	PCY	C7-C3-C6-C11
57	AA	3231	PCY	C7-C15-C18-O21
57	AA	3231	PCY	C17-C15-C18-O21
57	AA	3231	PCY	O19-C15-C18-O21
57	CA	3178	PCY	N2-C3-C6-C11
57	CA	3178	PCY	N2-C3-C6-O12
57	CA	3178	PCY	C7-C3-C6-C11
57	CA	3178	PCY	C7-C3-C6-O12
57	CA	3178	PCY	O26-C23-C27-C30
57	CA	3178	PCY	O21-C23-C27-C30
57	CA	3178	PCY	O26-C23-C27-C31
57	CA	3178	PCY	O21-C23-C27-C31

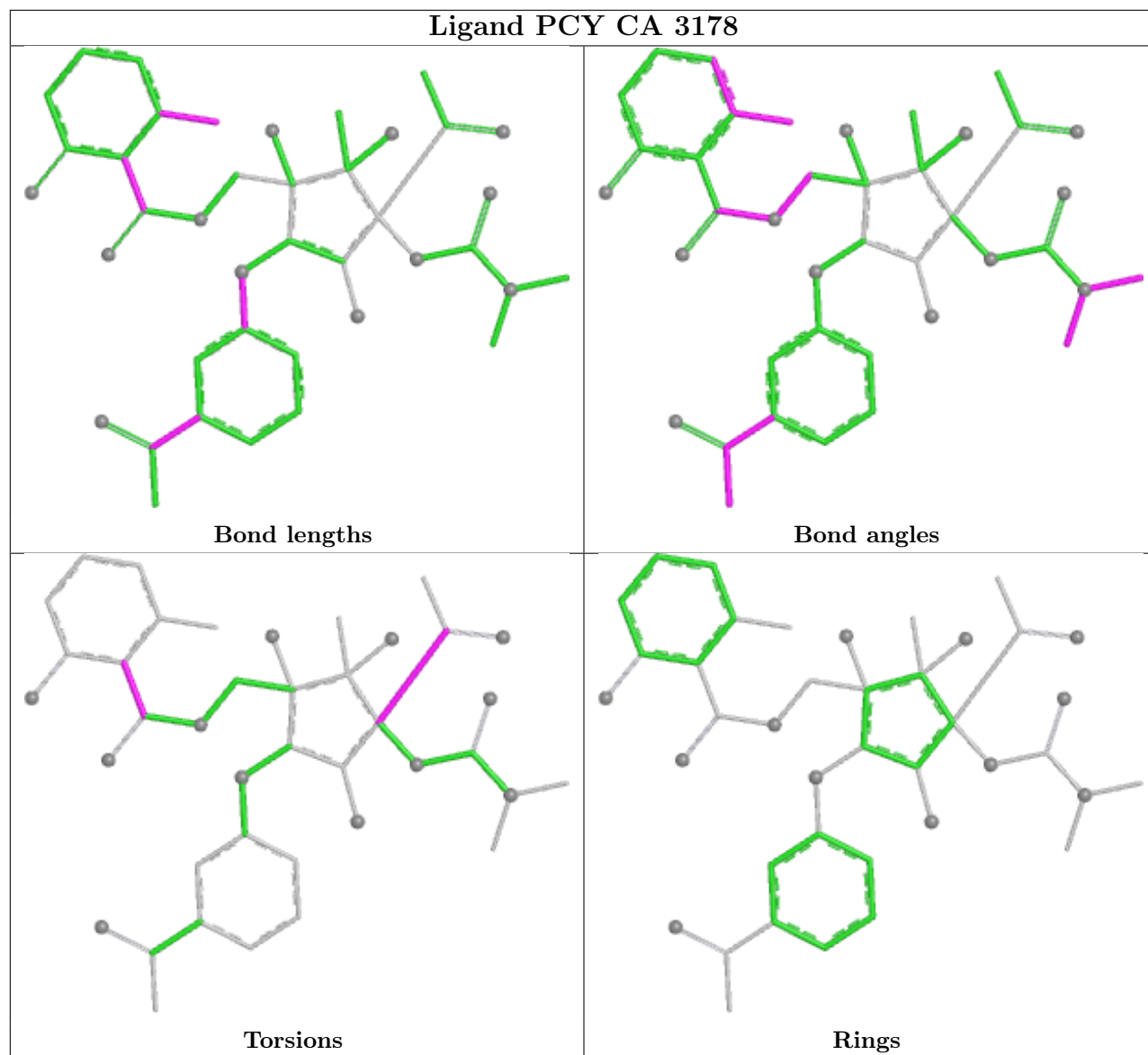
There are no ring outliers.

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	1498/1521 (98%)	0.43	45 (3%)	52	54	40, 67, 92, 106	0
1	CA	1503/1521 (98%)	0.51	62 (4%)	41	42	43, 69, 92, 106	0
2	AB	231/256 (90%)	1.32	43 (18%)	3	2	63, 80, 90, 94	0
2	CB	231/256 (90%)	1.72	71 (30%)	1	0	64, 82, 89, 96	0
3	AC	206/239 (86%)	1.20	24 (11%)	9	8	61, 74, 84, 92	0
3	CC	206/239 (86%)	1.55	52 (25%)	1	1	64, 76, 86, 92	0
4	AD	208/209 (99%)	1.40	43 (20%)	2	2	56, 68, 79, 87	0
4	CD	208/209 (99%)	1.06	22 (10%)	11	11	57, 68, 78, 87	0
5	AE	148/162 (91%)	1.11	9 (6%)	27	26	56, 67, 77, 91	0
5	CE	148/162 (91%)	1.08	18 (12%)	8	7	57, 69, 79, 92	0
6	AF	100/101 (99%)	1.00	7 (7%)	22	21	53, 66, 76, 82	0
6	CF	100/101 (99%)	0.80	1 (1%)	79	80	54, 66, 76, 82	0
7	AG	155/156 (99%)	1.17	14 (9%)	15	14	61, 71, 83, 93	0
7	CG	155/156 (99%)	1.48	33 (21%)	2	2	62, 73, 84, 96	0
8	AH	137/138 (99%)	1.27	19 (13%)	6	5	57, 69, 75, 83	0
8	CH	137/138 (99%)	1.00	7 (5%)	33	33	58, 71, 77, 84	0
9	AI	127/128 (99%)	1.51	31 (24%)	2	1	56, 78, 85, 90	0
9	CI	127/128 (99%)	2.16	67 (52%)	0	0	62, 79, 86, 89	0
10	AJ	97/105 (92%)	1.60	27 (27%)	1	1	57, 78, 90, 91	0
10	CJ	96/105 (91%)	2.31	53 (55%)	0	0	60, 80, 91, 93	0
11	AK	114/129 (88%)	1.08	12 (10%)	11	11	47, 66, 80, 83	0
11	CK	114/129 (88%)	1.12	15 (13%)	7	6	47, 67, 79, 83	0
12	AL	122/132 (92%)	0.80	8 (6%)	24	24	42, 56, 69, 75	0
12	CL	122/132 (92%)	0.78	6 (4%)	35	34	45, 58, 71, 75	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	AM	123/126 (97%)	0.98	14 (11%) 10 9	42, 63, 75, 80	0
13	CM	122/126 (96%)	1.88	48 (39%) 1 0	66, 79, 86, 90	0
14	AN	60/61 (98%)	1.42	10 (16%) 4 3	60, 70, 77, 81	0
14	CN	60/61 (98%)	2.37	33 (55%) 0 0	64, 73, 80, 83	0
15	AO	88/89 (98%)	1.26	10 (11%) 10 9	50, 66, 76, 82	0
15	CO	88/89 (98%)	0.90	6 (6%) 23 22	53, 68, 77, 82	0
16	AP	82/88 (93%)	1.64	26 (31%) 1 0	52, 68, 76, 80	0
16	CP	82/88 (93%)	1.15	8 (9%) 13 12	51, 68, 76, 79	0
17	AQ	99/105 (94%)	1.19	5 (5%) 33 33	55, 68, 77, 79	0
17	CQ	99/105 (94%)	1.09	8 (8%) 18 17	57, 69, 77, 80	0
18	AR	68/88 (77%)	0.97	3 (4%) 39 39	58, 66, 76, 80	0
18	CR	68/88 (77%)	0.85	3 (4%) 39 39	59, 68, 77, 80	0
19	AS	83/93 (89%)	1.28	12 (14%) 6 5	63, 73, 81, 91	0
19	CS	83/93 (89%)	1.78	28 (33%) 1 0	66, 76, 84, 92	0
20	AT	96/106 (90%)	1.06	9 (9%) 14 13	57, 68, 80, 86	0
20	CT	96/106 (90%)	1.31	16 (16%) 4 3	58, 68, 82, 87	0
21	AU	23/27 (85%)	1.23	5 (21%) 2 2	63, 66, 72, 75	0
21	CU	23/27 (85%)	1.74	7 (30%) 1 0	65, 68, 74, 77	0
22	AV	13/24 (54%)	0.98	2 (15%) 5 4	52, 64, 82, 98	0
22	CV	13/24 (54%)	1.07	3 (23%) 2 1	56, 67, 85, 99	0
23	AW	67/76 (88%)	0.81	7 (10%) 11 11	47, 84, 97, 104	0
23	AY	67/76 (88%)	1.65	18 (26%) 1 1	38, 97, 101, 104	0
23	CW	65/76 (85%)	1.23	11 (16%) 4 3	68, 91, 102, 104	0
23	CY	66/76 (86%)	1.82	23 (34%) 1 0	43, 97, 101, 104	0
24	AX	72/77 (93%)	0.69	5 (6%) 23 22	39, 68, 85, 93	0
24	CX	72/77 (93%)	0.52	2 (2%) 55 56	43, 71, 86, 94	0
25	BA	2819/2915 (96%)	-0.20	112 (3%) 42 43	23, 42, 88, 104	0
25	DA	2800/2915 (96%)	-0.10	81 (2%) 53 55	27, 47, 89, 108	0
26	BB	120/121 (99%)	0.08	0 100 100	35, 56, 70, 86	0
26	DB	120/121 (99%)	0.51	3 (2%) 58 59	42, 62, 73, 87	0
27	BD	275/276 (99%)	0.22	7 (2%) 58 59	23, 40, 55, 79	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
27	DD	275/276 (99%)	0.31	11 (4%) 42 43	26, 42, 56, 77	0
28	BE	204/206 (99%)	0.40	4 (1%) 65 65	22, 47, 66, 76	0
28	DE	204/206 (99%)	0.50	8 (3%) 43 44	28, 50, 67, 77	0
29	BF	203/210 (96%)	0.50	7 (3%) 48 49	23, 49, 73, 88	0
29	DF	203/210 (96%)	0.61	8 (3%) 43 44	27, 55, 75, 88	0
30	BG	181/182 (99%)	1.19	27 (14%) 5 5	44, 64, 78, 90	0
30	DG	181/182 (99%)	1.19	24 (13%) 7 6	50, 67, 80, 90	0
31	BH	174/180 (96%)	1.33	30 (17%) 4 3	51, 65, 76, 85	0
31	DH	174/180 (96%)	1.38	27 (15%) 5 4	57, 70, 80, 86	0
32	BI	146/148 (98%)	1.18	12 (8%) 17 17	50, 71, 82, 86	0
32	DI	146/148 (98%)	1.08	13 (8%) 15 14	53, 71, 82, 85	0
33	BN	140/140 (100%)	0.64	4 (2%) 53 55	32, 47, 68, 75	0
33	DN	140/140 (100%)	0.72	3 (2%) 63 64	36, 52, 70, 76	0
34	BO	122/122 (100%)	0.01	2 (1%) 70 71	25, 38, 59, 65	0
34	DO	122/122 (100%)	0.71	3 (2%) 58 59	47, 59, 74, 79	0
35	BP	149/150 (99%)	0.62	8 (5%) 31 31	24, 55, 74, 81	0
35	DP	149/150 (99%)	0.74	7 (4%) 36 36	29, 59, 76, 82	0
36	BQ	141/141 (100%)	0.52	0 100 100	31, 50, 66, 77	0
36	DQ	141/141 (100%)	0.92	8 (5%) 29 29	38, 54, 69, 80	0
37	BR	118/118 (100%)	-0.13	0 100 100	21, 32, 50, 58	0
37	DR	118/118 (100%)	0.49	2 (1%) 69 69	38, 53, 64, 74	0
38	BS	110/112 (98%)	0.17	0 100 100	32, 48, 64, 67	0
38	DS	110/112 (98%)	1.13	9 (8%) 17 17	58, 69, 80, 85	0
39	BT	131/146 (89%)	0.11	6 (4%) 37 38	31, 42, 68, 89	0
39	DT	131/146 (89%)	0.99	10 (7%) 20 19	51, 64, 78, 84	0
40	BU	116/118 (98%)	-0.45	1 (0%) 81 83	17, 28, 47, 65	0
40	DU	116/118 (98%)	0.76	4 (3%) 48 49	40, 62, 76, 82	0
41	BV	101/101 (100%)	-0.20	0 100 100	15, 35, 54, 67	0
41	DV	101/101 (100%)	1.21	9 (8%) 15 14	39, 74, 81, 88	0
42	BW	112/113 (99%)	-0.40	2 (1%) 67 68	17, 28, 53, 79	0
42	DW	112/113 (99%)	0.43	1 (0%) 81 83	38, 51, 68, 86	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
43	BX	95/96 (98%)	-0.05	1 (1%) 78 79	21, 35, 60, 75	0
43	DX	95/96 (98%)	1.01	12 (12%) 8 7	38, 56, 76, 85	0
44	BY	107/110 (97%)	0.13	3 (2%) 55 56	30, 46, 65, 83	0
44	DY	107/110 (97%)	1.46	24 (22%) 2 2	57, 71, 83, 86	0
45	BZ	171/206 (83%)	1.29	38 (22%) 2 2	35, 67, 94, 105	0
45	DZ	174/206 (84%)	1.97	66 (37%) 1 0	65, 83, 97, 103	0
46	B0	83/85 (97%)	-0.04	5 (6%) 27 27	20, 36, 57, 76	0
46	D0	83/85 (97%)	1.37	13 (15%) 5 4	44, 64, 74, 79	0
47	B1	97/98 (98%)	0.29	2 (2%) 63 64	24, 45, 70, 73	0
47	D1	97/98 (98%)	0.74	8 (8%) 17 17	37, 56, 75, 86	0
48	B2	70/72 (97%)	0.19	1 (1%) 73 74	30, 45, 58, 78	0
48	D2	70/72 (97%)	1.09	6 (8%) 16 15	53, 66, 78, 82	0
49	B3	59/60 (98%)	-0.17	2 (3%) 48 49	19, 31, 58, 75	0
49	D3	59/60 (98%)	1.16	6 (10%) 12 11	54, 66, 78, 88	0
50	B4	69/71 (97%)	1.17	11 (15%) 5 4	51, 70, 89, 99	0
50	D4	69/71 (97%)	1.63	17 (24%) 2 1	72, 82, 92, 93	0
51	B5	59/60 (98%)	-0.42	1 (1%) 69 69	17, 27, 43, 54	0
51	D5	59/60 (98%)	0.41	1 (1%) 69 69	35, 50, 66, 74	0
52	B6	53/54 (98%)	-0.02	1 (1%) 66 66	28, 39, 56, 67	0
52	D6	53/54 (98%)	0.78	3 (5%) 29 29	48, 59, 71, 76	0
53	B7	48/49 (97%)	-0.20	2 (4%) 40 41	18, 26, 62, 72	0
53	D7	48/49 (97%)	0.31	3 (6%) 26 25	30, 41, 61, 78	0
54	B8	64/65 (98%)	-0.36	0 100 100	19, 31, 40, 63	0
54	D8	64/65 (98%)	0.83	4 (6%) 26 25	44, 54, 65, 71	0
55	B9	37/37 (100%)	0.50	1 (2%) 56 57	26, 47, 63, 70	0
55	D9	37/37 (100%)	1.12	4 (10%) 11 10	45, 57, 68, 75	0
All	All	20900/21748 (96%)	0.56	1699 (8%) 18 17	15, 61, 87, 108	0

All (1699) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
7	CG	82	GLY	7.9
1	AA	1532	U	7.2

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Mol	Chain	Res	Type	RSRZ
13	CM	123	ALA	7.1
14	AN	2	ALA	6.7
7	AG	82	GLY	6.6
31	BH	2	SER	6.6
45	DZ	111	VAL	6.6
45	DZ	116	VAL	6.6
45	DZ	115	GLY	6.5
2	CB	237	ALA	6.4
13	AM	123	ALA	6.4
45	BZ	108	PRO	6.3
45	BZ	115	GLY	6.0
45	DZ	114	GLY	6.0
45	DZ	113	ALA	5.9
45	BZ	144	LEU	5.9
47	B1	2	SER	5.8
25	BA	2806	G	5.4
7	AG	79	ARG	5.4
25	BA	1221	G	5.4
19	CS	13	ASP	5.3
7	AG	80	VAL	5.3
14	CN	2	ALA	5.3
45	BZ	109	ALA	5.3
50	D4	49	PHE	5.2
7	CG	16	LEU	5.2
14	CN	39	LEU	5.1
11	CK	14	VAL	5.1
45	DZ	112	ARG	5.1
15	AO	87	ILE	5.1
10	AJ	4	ILE	5.0
2	CB	123	ALA	4.9
25	BA	932	C	4.9
9	CI	102	LEU	4.9
19	CS	9	VAL	4.9
32	BI	106	GLY	4.8
45	BZ	143	GLY	4.8
7	CG	81	GLY	4.8
46	D0	2	ALA	4.7
13	AM	124	PRO	4.7
45	DZ	144	LEU	4.7
11	AK	14	VAL	4.7
45	BZ	116	VAL	4.7
10	CJ	100	THR	4.7

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Mol	Chain	Res	Type	RSRZ
25	DA	883	G	4.7
7	CG	85	TYR	4.7
27	BD	276	LYS	4.7
9	CI	9	ARG	4.7
23	AW	1	G	4.7
44	DY	1	MET	4.6
28	DE	204	ALA	4.6
13	CM	6	GLY	4.6
27	DD	262	ARG	4.6
25	BA	942	A	4.6
43	DX	95	LEU	4.6
25	BA	931	C	4.5
23	CY	15	G	4.5
10	CJ	63	PHE	4.5
45	BZ	111	VAL	4.5
13	CM	124	PRO	4.5
23	CW	72	C	4.5
50	B4	49	PHE	4.4
2	CB	165	VAL	4.4
1	CA	1149	C	4.4
25	BA	2803	A	4.4
2	CB	236	TYR	4.4
50	D4	56	VAL	4.4
10	CJ	78	ASN	4.4
14	CN	18	VAL	4.3
25	BA	2180	A	4.3
43	DX	92	LEU	4.3
19	AS	13	ASP	4.3
13	CM	121	LYS	4.3
7	CG	84	ASN	4.3
23	CY	18	G	4.3
35	BP	15	ARG	4.3
1	CA	1030(B)	C	4.3
4	AD	194	LEU	4.3
46	D0	7	LEU	4.3
25	BA	934	A	4.2
9	CI	11	LYS	4.2
10	CJ	10	GLY	4.2
23	CY	34	G	4.2
33	BN	9	VAL	4.2
10	CJ	40	LEU	4.2
17	AQ	98	LEU	4.2

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Mol	Chain	Res	Type	RSRZ
30	BG	80	PHE	4.2
14	CN	34	TYR	4.2
22	CV	12	A	4.2
2	AB	237	ALA	4.2
7	AG	83	ALA	4.2
45	DZ	149	SER	4.1
9	AI	2	GLU	4.1
14	CN	38	GLY	4.1
45	BZ	114	GLY	4.1
45	DZ	168	GLU	4.1
13	CM	64	TRP	4.1
25	BA	271	U	4.1
39	BT	130	ALA	4.1
23	AW	71	G	4.1
9	CI	28	VAL	4.1
25	BA	2814	C	4.1
7	AG	85	TYR	4.1
2	CB	161	ALA	4.0
9	CI	44	VAL	4.0
25	BA	2816	G	4.0
1	AA	1503	A	4.0
45	BZ	1	MET	4.0
23	CY	36	A	4.0
50	B4	54	GLY	4.0
50	D4	66	SER	4.0
2	AB	50	GLU	4.0
10	CJ	55	LYS	4.0
45	DZ	170	THR	4.0
4	AD	201	GLN	4.0
45	BZ	113	ALA	3.9
44	DY	107	ASP	3.9
45	DZ	117	LEU	3.9
45	BZ	136	PHE	3.9
10	CJ	88	LEU	3.9
23	CW	71	G	3.9
43	DX	94	GLY	3.9
10	CJ	74	ILE	3.9
47	D1	2	SER	3.9
1	CA	1002	G	3.9
15	CO	60	VAL	3.9
25	DA	2116	G	3.9
25	BA	2815	C	3.9

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Mol	Chain	Res	Type	RSRZ
30	BG	146	TYR	3.9
43	DX	91	ALA	3.9
7	AG	84	ASN	3.9
45	BZ	117	LEU	3.9
45	DZ	109	ALA	3.8
45	DZ	147	GLY	3.8
13	CM	102	ARG	3.8
14	CN	44	LEU	3.8
10	CJ	41	PRO	3.8
23	AY	36	A	3.8
6	AF	46	ARG	3.8
25	BA	2168	C	3.8
17	AQ	36	ILE	3.8
2	AB	7	VAL	3.8
7	CG	83	ALA	3.8
39	DT	131	ALA	3.8
39	BT	38	ASN	3.8
25	BA	944	C	3.8
10	CJ	90	LEU	3.8
30	BG	48	GLU	3.8
10	AJ	33	GLN	3.8
9	CI	126	SER	3.8
7	CG	156	TRP	3.8
2	AB	12	GLU	3.8
44	DY	5	MET	3.8
2	CB	11	LEU	3.7
16	AP	68	ASP	3.7
38	DS	3	ARG	3.7
45	DZ	166	SER	3.7
11	CK	13	GLN	3.7
13	CM	4	ILE	3.7
3	CC	48	TYR	3.7
1	CA	1030(D)	A	3.7
10	CJ	87	THR	3.7
50	B4	50	VAL	3.7
13	AM	2	ALA	3.7
5	CE	23	GLY	3.7
10	CJ	23	ILE	3.7
10	CJ	86	MET	3.7
9	CI	4	TYR	3.7
45	DZ	164	ALA	3.6
9	CI	8	GLY	3.6

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Mol	Chain	Res	Type	RSRZ
12	CL	95	GLY	3.6
30	BG	42	GLY	3.6
45	BZ	110	GLY	3.6
8	AH	2	LEU	3.6
3	CC	182	ILE	3.6
26	DB	1	U	3.6
2	CB	97	TRP	3.6
14	CN	13	THR	3.6
45	BZ	157	LEU	3.6
11	CK	117	ASN	3.6
23	AY	34	G	3.6
50	D4	67	TYR	3.6
1	AA	1030(A)	G	3.6
14	CN	25	VAL	3.6
25	BA	2181	G	3.6
11	CK	89	ALA	3.6
16	CP	82	GLN	3.6
25	DA	896	A	3.6
45	BZ	118	GLN	3.6
30	DG	53	LEU	3.6
2	CB	41	ILE	3.6
25	BA	943	C	3.5
25	DA	884	C	3.5
25	BA	2154	U	3.5
2	CB	31	TYR	3.5
2	CB	33	TYR	3.5
1	AA	630	G	3.5
10	CJ	65	LEU	3.5
18	CR	66	LEU	3.5
25	DA	882	G	3.5
27	DD	2	ALA	3.5
45	DZ	57	ILE	3.5
10	CJ	76	ASN	3.5
30	BG	49	ASP	3.5
13	CM	120	LYS	3.5
13	CM	15	VAL	3.5
45	DZ	174	VAL	3.5
11	CK	25	TYR	3.5
9	AI	47	LEU	3.5
16	CP	48	TRP	3.5
20	CT	47	GLY	3.5
20	CT	97	ALA	3.5

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Mol	Chain	Res	Type	RSRZ
1	AA	1003	G	3.5
2	CB	17	PHE	3.5
23	CW	3	C	3.5
13	CM	101	GLN	3.5
19	CS	80	TYR	3.5
45	DZ	99	TYR	3.5
2	CB	154	LEU	3.5
46	D0	84	LEU	3.5
44	DY	80	GLY	3.5
46	B0	6	GLY	3.5
23	CW	70	G	3.5
25	DA	2159	G	3.5
45	DZ	157	LEU	3.5
9	CI	106	ALA	3.5
10	CJ	47	PHE	3.5
20	CT	74	LYS	3.5
1	AA	1447	A	3.4
1	CA	1001	A	3.4
25	BA	2153	G	3.4
25	BA	2163	G	3.4
3	CC	76	VAL	3.4
9	CI	7	THR	3.4
45	DZ	107	THR	3.4
20	CT	103	GLY	3.4
45	DZ	108	PRO	3.4
2	AB	127	ILE	3.4
9	CI	125	TYR	3.4
50	D4	59	PHE	3.4
11	CK	126	ARG	3.4
30	BG	26	GLN	3.4
4	AD	188	LEU	3.4
19	CS	2	PRO	3.4
19	AS	40	ILE	3.4
1	AA	1027	C	3.4
25	BA	2167	C	3.4
10	CJ	77	PRO	3.4
9	CI	69	GLY	3.4
39	DT	130	ALA	3.4
14	CN	35	ARG	3.4
50	B4	59	PHE	3.4
23	AW	72	C	3.4
25	BA	2183	C	3.4

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Mol	Chain	Res	Type	RSRZ
3	AC	18	TRP	3.4
14	CN	61	TRP	3.4
29	BF	89	VAL	3.4
30	BG	82	LEU	3.4
10	CJ	35	SER	3.4
4	AD	110	PHE	3.3
1	AA	163	C	3.3
25	DA	2139	C	3.3
4	AD	88	VAL	3.3
9	CI	17	VAL	3.3
19	AS	71	LEU	3.3
31	BH	44	VAL	3.3
9	CI	42	ARG	3.3
19	AS	84	GLY	3.3
23	AW	73	A	3.3
9	CI	61	ALA	3.3
16	AP	19	ILE	3.3
45	DZ	136	PHE	3.3
23	CY	19	G	3.3
2	CB	155	LEU	3.3
19	AS	9	VAL	3.3
14	CN	55	GLY	3.3
46	B0	3	HIS	3.3
30	BG	35	GLU	3.3
3	AC	65	ALA	3.3
5	CE	17	ALA	3.3
11	AK	75	TYR	3.3
10	CJ	33	GLN	3.3
23	CY	22	G	3.3
7	CG	80	VAL	3.3
10	CJ	56	HIS	3.3
12	CL	18	VAL	3.3
31	BH	17	VAL	3.3
3	AC	39	ILE	3.3
10	AJ	86	MET	3.3
30	BG	52	ILE	3.3
2	AB	236	TYR	3.3
16	AP	49	LEU	3.3
25	BA	930	G	3.3
49	D3	60	GLU	3.3
16	AP	69	THR	3.3
25	BA	2807	C	3.3

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Mol	Chain	Res	Type	RSRZ
4	AD	173	TRP	3.3
23	AY	35	A	3.2
23	CW	76	A	3.2
23	CY	21	A	3.2
1	AA	204	U	3.2
10	CJ	34	VAL	3.2
9	CI	64	THR	3.2
1	CA	1030	C	3.2
25	BA	34	C	3.2
25	BA	935	C	3.2
25	DA	2117	A	3.2
50	D4	65	ASP	3.2
2	CB	10	LEU	3.2
9	CI	2	GLU	3.2
1	AA	841	U	3.2
9	CI	14	VAL	3.2
1	AA	1030(B)	C	3.2
1	AA	1031	G	3.2
25	BA	929	G	3.2
25	DA	2155	G	3.2
2	CB	158	LEU	3.2
10	CJ	85	LEU	3.2
31	DH	173	PRO	3.2
32	BI	117	GLU	3.2
46	D0	3	HIS	3.2
12	AL	18	VAL	3.2
19	AS	48	THR	3.2
14	CN	3	ARG	3.2
25	DA	885	C	3.2
23	AY	15	G	3.2
2	AB	232	PRO	3.2
10	CJ	71	LEU	3.2
3	AC	184	TYR	3.2
3	CC	198	VAL	3.2
39	BT	37	GLY	3.2
41	DV	63	GLY	3.2
1	AA	1446	U	3.2
9	CI	103	THR	3.2
31	BH	3	ARG	3.1
17	CQ	100	LYS	3.1
45	DZ	16	SER	3.1
25	BA	936	C	3.1

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Mol	Chain	Res	Type	RSRZ
49	B3	2	PRO	3.1
50	D4	57	GLU	3.1
9	CI	56	LEU	3.1
9	CI	79	LEU	3.1
9	CI	80	GLY	3.1
14	CN	33	VAL	3.1
45	BZ	106	GLY	3.1
18	AR	25	THR	3.1
45	DZ	171	ILE	3.1
13	AM	122	LYS	3.1
2	CB	131	PRO	3.1
25	BA	2160	C	3.1
25	DA	2145	C	3.1
15	AO	86	GLY	3.1
19	CS	68	GLY	3.1
23	AY	18	G	3.1
25	BA	2805	G	3.1
7	CG	78	ARG	3.1
25	BA	945	A	3.1
25	BA	2195	A	3.1
25	DA	2158	A	3.1
30	BG	50	ALA	3.1
45	DZ	172	ALA	3.1
16	AP	50	LYS	3.1
53	B7	48	LYS	3.1
2	AB	125	PRO	3.1
11	CK	125	PHE	3.1
14	CN	37	PHE	3.1
3	CC	207	VAL	3.1
10	CJ	38	ILE	3.1
9	CI	5	TYR	3.1
13	CM	59	TYR	3.1
50	D4	63	TYR	3.1
45	DZ	118	GLN	3.1
1	AA	1023	G	3.1
13	CM	27	LYS	3.1
13	CM	30	ALA	3.1
25	BA	2146	G	3.1
25	BA	2155	G	3.1
23	AY	47	U	3.1
10	AJ	77	PRO	3.1
30	DG	17	PRO	3.1

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Mol	Chain	Res	Type	RSRZ
31	DH	168	PRO	3.1
45	DZ	92	SER	3.1
42	BW	112	GLY	3.1
25	BA	1555	C	3.1
16	AP	82	GLN	3.0
7	CG	7	ALA	3.0
39	DT	109	GLU	3.0
1	CA	1257	U	3.0
25	BA	273	G	3.0
25	DA	2115	G	3.0
3	CC	178	LEU	3.0
30	BG	53	LEU	3.0
32	BI	75	LEU	3.0
45	DZ	52	SER	3.0
4	AD	87	GLY	3.0
10	AJ	36	GLY	3.0
16	AP	59	TRP	3.0
45	DZ	143	GLY	3.0
31	DH	92	ILE	3.0
53	D7	46	VAL	3.0
45	BZ	107	THR	3.0
1	CA	1038	C	3.0
9	CI	15	ALA	3.0
23	CW	2	C	3.0
25	DA	888	C	3.0
11	CK	75	TYR	3.0
24	AX	47	U	3.0
3	AC	204	LEU	3.0
13	CM	90	LEU	3.0
32	DI	68	LEU	3.0
2	AB	195	ASP	3.0
1	CA	1003	G	3.0
25	BA	926	G	3.0
25	DA	2160	G	3.0
45	BZ	149	SER	3.0
5	CE	22	GLY	3.0
31	DH	174	GLY	3.0
2	AB	229	VAL	3.0
11	AK	13	GLN	3.0
11	AK	42	TRP	3.0
33	BN	131	GLN	3.0
3	AC	100	ALA	3.0

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Mol	Chain	Res	Type	RSRZ
5	AE	10	MET	3.0
14	CN	5	ALA	3.0
39	DT	1	MET	3.0
2	CB	92	TYR	3.0
9	CI	114	TYR	3.0
44	DY	55	TYR	3.0
45	DZ	167	PRO	3.0
15	AO	88	ARG	3.0
14	CN	16	PHE	3.0
13	CM	122	LYS	3.0
1	AA	1033	G	3.0
1	AA	1034	G	3.0
25	BA	2902	G	3.0
9	AI	30	GLY	3.0
29	BF	208	GLY	3.0
31	BH	66	GLY	3.0
9	CI	27	THR	3.0
13	AM	5	ALA	3.0
25	BA	2164	C	3.0
25	BA	2905	C	3.0
45	BZ	150	LEU	3.0
1	AA	1025	U	3.0
1	AA	1531	A	3.0
25	DA	229	A	3.0
10	CJ	36	GLY	3.0
2	AB	15	VAL	2.9
25	DA	1171	G	2.9
47	D1	83	GLU	2.9
3	CC	65	ALA	2.9
13	CM	33	ALA	2.9
44	DY	65	ALA	2.9
20	CT	98	PRO	2.9
30	DG	12	TYR	2.9
41	DV	85	LYS	2.9
46	D0	4	LYS	2.9
50	B4	63	TYR	2.9
1	CA	1043	C	2.9
25	BA	270	C	2.9
9	AI	126	SER	2.9
23	CW	73	A	2.9
3	CC	2	GLY	2.9
13	CM	119	GLY	2.9

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Mol	Chain	Res	Type	RSRZ
2	CB	39	ILE	2.9
10	CJ	75	ILE	2.9
4	AD	170	VAL	2.9
5	CE	51	VAL	2.9
31	DH	169	VAL	2.9
10	AJ	32	ALA	2.9
14	CN	10	ALA	2.9
25	BA	2147	G	2.9
25	DA	171	G	2.9
25	DA	2125	G	2.9
9	CI	19	LEU	2.9
7	CG	154	TYR	2.9
43	DX	69	TYR	2.9
11	AK	117	ASN	2.9
46	B0	8	GLY	2.9
2	CB	143	GLU	2.9
31	BH	18	GLU	2.9
28	BE	77	ILE	2.9
2	AB	230	VAL	2.9
31	BH	35	VAL	2.9
7	AG	2	ALA	2.9
10	CJ	37	PRO	2.9
19	CS	24	ALA	2.9
27	BD	275	LYS	2.9
31	BH	13	LYS	2.9
45	DZ	150	LEU	2.9
52	D6	11	LEU	2.9
1	AA	1032	G	2.9
1	AA	1036	G	2.9
1	CA	1034	G	2.9
25	BA	2813	G	2.9
9	AI	125	TYR	2.9
3	AC	205	GLY	2.9
4	CD	167	GLY	2.9
2	CB	208	ILE	2.9
9	CI	74	ILE	2.9
25	BA	2186	C	2.9
10	CJ	68	HIS	2.9
23	CY	14	A	2.9
25	BA	1219	A	2.9
25	BA	2157	A	2.9
25	BA	2901	A	2.9

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Mol	Chain	Res	Type	RSRZ
30	BG	83	ARG	2.9
9	AI	64	THR	2.9
10	CJ	42	THR	2.9
9	CI	36	TYR	2.9
14	CN	21	TYR	2.9
25	DA	2166	G	2.9
4	AD	179	GLU	2.9
2	CB	66	GLY	2.9
30	DG	42	GLY	2.9
7	CG	5	ARG	2.8
27	DD	275	LYS	2.8
30	BG	182	LYS	2.8
46	D0	5	LYS	2.8
33	BN	5	VAL	2.8
50	B4	56	VAL	2.8
25	DA	1536	C	2.8
25	DA	2136	C	2.8
10	AJ	87	THR	2.8
2	CB	34	ALA	2.8
23	CY	35	A	2.8
39	BT	131	ALA	2.8
45	DZ	173	ALA	2.8
32	DI	38	LEU	2.8
2	AB	97	TRP	2.8
10	AJ	73	ASP	2.8
7	CG	26	PHE	2.8
13	CM	50	GLU	2.8
19	CS	10	PHE	2.8
27	BD	28	GLU	2.8
32	DI	135	GLU	2.8
21	AU	18	TYR	2.8
9	CI	10	ARG	2.8
27	BD	38	LYS	2.8
27	DD	38	LYS	2.8
41	DV	86	GLY	2.8
25	DA	2133	G	2.8
45	BZ	142	SER	2.8
3	CC	195	VAL	2.8
16	AP	2	VAL	2.8
19	CS	41	VAL	2.8
33	DN	9	VAL	2.8
9	CI	91	ASP	2.8

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Mol	Chain	Res	Type	RSRZ
4	AD	49	ARG	2.8
3	CC	185	GLY	2.8
9	CI	62	TYR	2.8
9	CI	92	TYR	2.8
14	CN	51	GLY	2.8
45	DZ	121	HIS	2.8
30	BG	88	ILE	2.8
45	DZ	142	SER	2.8
13	CM	60	VAL	2.8
28	DE	59	VAL	2.8
29	DF	6	VAL	2.8
1	CA	1030(A)	G	2.8
25	BA	2182	G	2.8
25	DA	2802	G	2.8
1	CA	1020	U	2.8
2	CB	67	THR	2.8
25	BA	2135	U	2.8
20	AT	10	LEU	2.8
25	BA	933	C	2.8
26	DB	88	C	2.8
25	BA	2139	A	2.8
26	DB	120	A	2.8
3	CC	190	ARG	2.8
9	CI	105	ASP	2.8
9	AI	8	GLY	2.8
13	CM	100	GLY	2.8
19	CS	8	GLY	2.8
50	B4	4	GLY	2.8
50	B4	45	GLY	2.8
3	CC	193	TYR	2.8
6	AF	19	LEU	2.8
7	CG	12	LEU	2.8
10	AJ	100	THR	2.8
15	AO	57	LEU	2.8
20	AT	43	LEU	2.8
30	DG	161	THR	2.8
25	BA	924	U	2.8
25	BA	2906	U	2.8
25	DA	2144	U	2.8
25	DA	2150	U	2.8
24	AX	46	G	2.8
25	DA	2154	G	2.8

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Mol	Chain	Res	Type	RSRZ
1	AA	48	C	2.8
7	CG	4	ARG	2.8
54	D8	29	LYS	2.8
1	CA	1035	A	2.8
25	BA	2191	A	2.8
25	DA	2119	A	2.8
9	AI	105	ASP	2.8
2	AB	19	HIS	2.8
12	CL	63	GLY	2.7
2	CB	223	ILE	2.7
30	DG	52	ILE	2.7
21	CU	14	TRP	2.7
4	AD	189	PRO	2.7
8	AH	137	VAL	2.7
9	CI	109	VAL	2.7
10	CJ	49	VAL	2.7
7	AG	16	LEU	2.7
9	CI	52	ALA	2.7
16	CP	69	THR	2.7
45	DZ	125	LEU	2.7
30	DG	50	ALA	2.7
25	DA	2130	U	2.7
46	D0	24	LYS	2.7
48	D2	11	GLU	2.7
25	BA	2184	G	2.7
25	BA	2817	G	2.7
1	CA	1116	C	2.7
11	CK	36	ASP	2.7
16	AP	78	GLY	2.7
2	CB	32	ILE	2.7
2	CB	127	ILE	2.7
2	CB	222	ILE	2.7
3	CC	39	ILE	2.7
8	AH	80	ILE	2.7
14	CN	14	PRO	2.7
2	CB	81	VAL	2.7
13	CM	7	VAL	2.7
45	BZ	99	TYR	2.7
50	D4	50	VAL	2.7
4	AD	155	LEU	2.7
30	DG	139	LEU	2.7
13	CM	104	ARG	2.7

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Mol	Chain	Res	Type	RSRZ
25	BA	1985	U	2.7
19	CS	14	HIS	2.7
19	CS	84	GLY	2.7
25	DA	2156	G	2.7
2	CB	55	PHE	2.7
2	CB	57	PHE	2.7
25	DA	652(B)	A	2.7
25	DA	2134	A	2.7
3	CC	77	ILE	2.7
9	CI	81	ILE	2.7
45	DZ	146	ILE	2.7
10	AJ	72	VAL	2.7
45	DZ	42	VAL	2.7
2	AB	11	LEU	2.7
2	CB	121	LEU	2.7
6	AF	63	TYR	2.7
19	CS	5	LEU	2.7
7	CG	65	ALA	2.7
9	CI	66	ARG	2.7
14	CN	12	ARG	2.7
29	BF	17	ARG	2.7
5	AE	20	GLN	2.7
1	AA	1257	U	2.7
3	CC	194	GLY	2.7
20	AT	69	GLY	2.7
31	DH	14	GLY	2.7
41	DV	30	GLY	2.7
46	D0	76	GLY	2.7
45	DZ	159	PRO	2.7
55	B9	17	ILE	2.7
1	CA	1001(A)	G	2.7
1	CA	1054	C	2.7
1	CA	1286	A	2.7
23	AY	19	G	2.7
23	CW	19	G	2.7
23	CY	1	G	2.7
23	AY	13	C	2.7
23	CW	4	C	2.7
25	DA	1847	A	2.7
2	CB	215	LEU	2.7
3	AC	66	VAL	2.7
20	AT	13	LEU	2.7

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Mol	Chain	Res	Type	RSRZ
20	AT	62	LEU	2.7
30	BG	76	SER	2.7
19	AS	80	TYR	2.7
52	B6	4	GLU	2.7
10	AJ	10	GLY	2.6
28	DE	71	GLY	2.6
13	AM	39	ILE	2.6
21	CU	23	PRO	2.6
30	DG	20	ILE	2.6
31	DH	175	LYS	2.6
32	BI	109	ILE	2.6
45	BZ	104	PHE	2.6
53	D7	48	LYS	2.6
4	CD	132	ARG	2.6
13	CM	29	ARG	2.6
30	BG	51	ARG	2.6
45	BZ	112	ARG	2.6
7	CG	38	LEU	2.6
9	CI	99	LEU	2.6
19	CS	11	VAL	2.6
19	CS	16	LEU	2.6
25	BA	2162	C	2.6
25	BA	2179	G	2.6
25	DA	897	C	2.6
25	DA	2138	C	2.6
25	DA	2146	C	2.6
45	DZ	169	GLU	2.6
8	AH	28	ALA	2.6
10	CJ	32	ALA	2.6
44	DY	57	GLN	2.6
3	AC	2	GLY	2.6
5	AE	23	GLY	2.6
20	AT	103	GLY	2.6
31	DH	91	GLY	2.6
2	CB	234	PRO	2.6
45	BZ	146	ILE	2.6
55	D9	17	ILE	2.6
5	CE	18	ARG	2.6
31	BH	6	ARG	2.6
38	DS	61	ASN	2.6
3	CC	75	VAL	2.6
32	DI	41	GLU	2.6

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Mol	Chain	Res	Type	RSRZ
25	BA	2141	A	2.6
45	BZ	166	SER	2.6
9	AI	13	ALA	2.6
16	AP	45	THR	2.6
37	DR	101	ALA	2.6
45	BZ	170	THR	2.6
1	AA	1030(C)	G	2.6
4	CD	20	TYR	2.6
25	DA	892	G	2.6
42	BW	111	HIS	2.6
2	AB	18	GLY	2.6
9	CI	100	GLY	2.6
4	AD	73	ARG	2.6
8	AH	84	ARG	2.6
9	CI	49	PRO	2.6
10	CJ	79	ARG	2.6
13	AM	102	ARG	2.6
14	CN	7	ILE	2.6
14	CN	42	ILE	2.6
16	AP	4	ILE	2.6
31	DH	151	ILE	2.6
38	DS	20	ARG	2.6
43	DX	68	ARG	2.6
2	CB	69	LEU	2.6
9	AI	56	LEU	2.6
46	B0	7	LEU	2.6
32	BI	107	VAL	2.6
11	AK	89	ALA	2.6
44	DY	78	ALA	2.6
1	CA	1503	A	2.6
23	CY	23	A	2.6
25	DA	2135	A	2.6
1	AA	1397	C	2.6
1	CA	630	G	2.6
1	CA	998	G	2.6
23	AY	1	G	2.6
25	DA	2151	G	2.6
11	CK	49	GLY	2.6
2	CB	185	ILE	2.6
1	CA	1532	U	2.6
9	CI	18	PHE	2.6
17	AQ	27	PHE	2.6

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Mol	Chain	Res	Type	RSRZ
2	AB	187	LEU	2.6
4	CD	188	LEU	2.6
10	AJ	88	LEU	2.6
45	BZ	2	GLU	2.6
7	CG	37	ASN	2.6
6	AF	16	GLN	2.6
7	CG	66	VAL	2.6
13	CM	18	ALA	2.6
29	BF	15	SER	2.6
1	AA	1030(D)	A	2.6
20	CT	8	ARG	2.5
25	BA	2159	C	2.5
5	CE	74	GLY	2.5
31	BH	21	PRO	2.5
31	BH	174	GLY	2.5
39	BT	107	ASP	2.5
45	DZ	98	MET	2.5
48	D2	1	MET	2.5
1	CA	1190	G	2.5
10	AJ	75	ILE	2.5
23	CY	24	G	2.5
25	DA	2157	G	2.5
25	DA	2319	G	2.5
6	AF	60	PHE	2.5
9	AI	59	PHE	2.5
2	CB	61	LEU	2.5
8	AH	112	LEU	2.5
32	BI	140	LEU	2.5
2	CB	94	ASN	2.5
2	CB	164	VAL	2.5
2	AB	16	HIS	2.5
10	CJ	62	HIS	2.5
12	AL	126	LYS	2.5
13	CM	76	ALA	2.5
14	CN	20	ALA	2.5
35	BP	12	ALA	2.5
41	DV	92	THR	2.5
15	AO	68	ARG	2.5
1	CA	1004	A	2.5
1	CA	1005	A	2.5
16	AP	38	TYR	2.5
25	BA	302	A	2.5

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Mol	Chain	Res	Type	RSRZ
25	BA	572	A	2.5
25	DA	2114	A	2.5
44	BY	1	MET	2.5
1	AA	1028	C	2.5
2	AB	228	GLY	2.5
5	AE	85	GLY	2.5
10	CJ	58	ASP	2.5
25	BA	2165	C	2.5
40	DU	73	GLY	2.5
45	DZ	148	ASP	2.5
2	AB	200	ILE	2.5
13	CM	39	ILE	2.5
15	AO	3	ILE	2.5
2	AB	9	GLU	2.5
8	CH	2	LEU	2.5
10	CJ	54	PHE	2.5
1	CA	1031	G	2.5
13	AM	90	LEU	2.5
14	CN	6	LEU	2.5
25	BA	927	G	2.5
25	DA	1533	G	2.5
25	DA	2206	G	2.5
45	DZ	155	LEU	2.5
9	CI	86	VAL	2.5
11	AK	106	LYS	2.5
19	CS	19	VAL	2.5
30	DG	182	LYS	2.5
46	B0	5	LYS	2.5
2	AB	13	ALA	2.5
32	BI	146	ALA	2.5
43	DX	35	THR	2.5
2	AB	53	ARG	2.5
14	CN	29	ARG	2.5
21	CU	9	ARG	2.5
31	BH	42	ARG	2.5
54	D8	4	MET	2.5
1	CA	977	A	2.5
1	CA	983	A	2.5
19	AS	8	GLY	2.5
47	D1	28	GLY	2.5
3	CC	157	ILE	2.5
10	CJ	6	ILE	2.5

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Mol	Chain	Res	Type	RSRZ
25	DA	2137	C	2.5
54	D8	34	TRP	2.5
2	CB	152	PHE	2.5
3	CC	47	LEU	2.5
9	CI	96	LEU	2.5
14	AN	16	PHE	2.5
16	AP	74	LEU	2.5
30	BG	139	LEU	2.5
31	BH	171	LEU	2.5
4	AD	86	LYS	2.5
13	CM	92	HIS	2.5
3	AC	98	ASN	2.5
14	AN	33	VAL	2.5
25	BA	2818	U	2.5
1	AA	1001(A)	G	2.5
1	CA	1030(C)	G	2.5
1	CA	1033	G	2.5
23	AY	24	G	2.5
25	DA	2207	G	2.5
25	DA	2793	G	2.5
3	CC	60	ALA	2.5
7	CG	2	ALA	2.5
13	CM	28	ALA	2.5
49	D3	29	ARG	2.5
8	CH	67	PRO	2.5
3	CC	25	GLY	2.5
4	AD	180	GLY	2.5
4	CD	192	GLU	2.5
12	AL	14	GLY	2.5
20	CT	101	GLY	2.5
29	DF	131	GLY	2.5
8	AH	134	ILE	2.5
20	AT	55	ILE	2.5
27	BD	71	ASP	2.5
2	CB	51	LEU	2.5
4	CD	78	LEU	2.5
43	BX	95	LEU	2.5
44	DY	34	LYS	2.5
16	AP	80	PHE	2.5
2	CB	136	VAL	2.5
3	AC	76	VAL	2.5
4	CD	198	VAL	2.5

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Mol	Chain	Res	Type	RSRZ
7	CG	21	VAL	2.5
8	CH	51	VAL	2.5
3	AC	190	ARG	2.5
14	AN	3	ARG	2.5
9	AI	119	ALA	2.5
18	CR	60	ALA	2.5
14	CN	22	THR	2.5
17	AQ	99	SER	2.5
25	BA	162	G	2.5
25	DA	2165	G	2.5
31	DH	10	PRO	2.4
5	CE	114	GLY	2.4
7	AG	8	GLU	2.4
35	BP	82	GLY	2.4
38	DS	109	GLY	2.4
55	D9	21	GLY	2.4
8	CH	48	TYR	2.4
9	CI	75	ASP	2.4
9	CI	97	LYS	2.4
11	CK	59	TYR	2.4
19	CS	52	TYR	2.4
31	DH	25	LYS	2.4
47	D1	78	LYS	2.4
2	CB	145	LEU	2.4
3	AC	47	LEU	2.4
4	CD	194	LEU	2.4
35	BP	148	LEU	2.4
3	CC	186	PHE	2.4
9	CI	101	PHE	2.4
10	CJ	13	HIS	2.4
19	CS	81	ARG	2.4
3	AC	151	VAL	2.4
3	CC	99	VAL	2.4
9	AI	65	VAL	2.4
17	CQ	9	VAL	2.4
31	DH	79	VAL	2.4
1	CA	1150	U	2.4
4	AD	195	ALA	2.4
9	AI	15	ALA	2.4
9	CI	119	ALA	2.4
10	CJ	27	ALA	2.4
17	CQ	82	MET	2.4

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Mol	Chain	Res	Type	RSRZ
18	AR	20	ALA	2.4
18	CR	20	ALA	2.4
30	BG	2	PRO	2.4
48	D2	66	GLU	2.4
1	CA	1117	G	2.4
1	CA	1202	G	2.4
4	CD	87	GLY	2.4
19	CS	46	GLY	2.4
20	CT	96	GLY	2.4
25	BA	694	G	2.4
25	DA	2112	G	2.4
45	DZ	160	GLY	2.4
46	D0	42	GLY	2.4
9	CI	63	ILE	2.4
11	AK	36	ASP	2.4
2	CB	102	LEU	2.4
18	AR	31	LEU	2.4
20	CT	62	LEU	2.4
30	DG	146	TYR	2.4
31	DH	88	LEU	2.4
50	D4	25	TYR	2.4
4	CD	73	ARG	2.4
4	CD	115	ARG	2.4
10	AJ	63	PHE	2.4
53	D7	47	ARG	2.4
1	AA	1005	A	2.4
25	BA	1091	A	2.4
25	BA	1878	A	2.4
25	BA	2136	A	2.4
25	DA	2126	A	2.4
5	AE	67	VAL	2.4
13	CM	40	ASN	2.4
20	CT	26	ASN	2.4
1	CA	1019	C	2.4
4	CD	48	ALA	2.4
11	AK	15	ALA	2.4
23	CY	13	C	2.4
1	AA	65	U	2.4
1	CA	1126	U	2.4
4	AD	89	THR	2.4
3	AC	206	GLU	2.4
9	CI	110	GLU	2.4

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Mol	Chain	Res	Type	RSRZ
16	AP	41	PRO	2.4
30	DG	2	PRO	2.4
13	CM	65	LYS	2.4
14	CN	11	LYS	2.4
27	DD	276	LYS	2.4
30	DG	30	GLU	2.4
35	DP	76	LYS	2.4
9	CI	57	GLY	2.4
12	AL	95	GLY	2.4
13	CM	68	GLY	2.4
29	BF	16	GLY	2.4
29	BF	131	GLY	2.4
2	AB	222	ILE	2.4
1	CA	976	G	2.4
2	AB	221	LEU	2.4
15	CO	9	GLN	2.4
25	BA	2178	G	2.4
25	BA	2187	G	2.4
25	DA	2148	G	2.4
47	B1	82	LEU	2.4
13	CM	87	TYR	2.4
10	AJ	47	PHE	2.4
4	AD	165	MET	2.4
13	CM	53	VAL	2.4
17	CQ	23	VAL	2.4
31	DH	76	VAL	2.4
45	BZ	141	VAL	2.4
51	B5	60	VAL	2.4
1	AA	1035	A	2.4
22	AV	13	A	2.4
29	DF	160	ASN	2.4
3	CC	100	ALA	2.4
2	CB	47	THR	2.4
8	AH	3	THR	2.4
9	CI	98	PRO	2.4
14	CN	17	LYS	2.4
28	BE	73	GLU	2.4
31	BH	32	GLU	2.4
43	DX	33	LYS	2.4
50	D4	52	THR	2.4
1	AA	343	U	2.4
1	AA	1029	C	2.4

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Mol	Chain	Res	Type	RSRZ
1	AA	1030	C	2.4
1	CA	1045	C	2.4
23	AY	12	U	2.4
25	BA	2152	U	2.4
25	DA	886	C	2.4
28	DE	74	PRO	2.4
45	DZ	129	SER	2.4
7	AG	81	GLY	2.4
4	AD	191	ARG	2.4
6	AF	14	LEU	2.4
10	AJ	85	LEU	2.4
10	CJ	46	ARG	2.4
10	CJ	70	ARG	2.4
14	AN	35	ARG	2.4
30	DG	136	ARG	2.4
30	DG	147	ASP	2.4
38	DS	17	ARG	2.4
45	BZ	125	LEU	2.4
53	B7	47	ARG	2.4
1	CA	973	G	2.4
1	CA	1385	G	2.4
2	CB	148	TYR	2.4
25	DA	2127	G	2.4
36	DQ	104	PHE	2.4
10	CJ	44	VAL	2.4
13	CM	54	VAL	2.4
31	DH	45	VAL	2.4
40	DU	90	VAL	2.4
44	DY	3	VAL	2.4
45	DZ	90	VAL	2.4
10	CJ	69	ASN	2.4
3	AC	53	ALA	2.4
22	AV	12	A	2.4
22	CV	14	A	2.4
25	BA	937	A	2.4
25	BA	2812	A	2.4
27	BD	2	ALA	2.4
2	CB	126	GLU	2.4
9	AI	90	PRO	2.3
10	CJ	48	THR	2.3
14	AN	14	PRO	2.3
32	DI	137	PRO	2.3

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Mol	Chain	Res	Type	RSRZ
44	DY	82	PRO	2.3
23	AW	20	U	2.3
25	BA	941	U	2.3
2	AB	227	GLY	2.3
9	CI	115	GLY	2.3
23	AY	67	C	2.3
24	AX	69	C	2.3
2	CB	80	ILE	2.3
4	AD	131	ARG	2.3
14	CN	23	ARG	2.3
30	DG	115	ARG	2.3
35	BP	79	ARG	2.3
45	DZ	81	ARG	2.3
45	DZ	103	ARG	2.3
13	CM	70	LEU	2.3
29	DF	12	LEU	2.3
30	BG	3	LEU	2.3
45	BZ	151	HIS	2.3
45	BZ	155	LEU	2.3
48	B2	70	GLN	2.3
28	BE	1	MET	2.3
2	AB	28	PHE	2.3
28	DE	151	TYR	2.3
44	DY	35	TYR	2.3
45	DZ	9	TYR	2.3
45	DZ	89	PHE	2.3
9	CI	26	VAL	2.3
20	AT	74	LYS	2.3
1	CA	1032	G	2.3
4	AD	154	ASN	2.3
10	AJ	76	ASN	2.3
23	AW	70	G	2.3
25	BA	11	G	2.3
25	BA	1152	G	2.3
25	DA	881	G	2.3
10	AJ	83	GLU	2.3
12	AL	94	PRO	2.3
1	CA	1041	A	2.3
7	CG	3	ARG	2.3
7	CG	115	ARG	2.3
9	AI	128	ARG	2.3
13	AM	26	GLY	2.3

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Mol	Chain	Res	Type	RSRZ
29	DF	16	GLY	2.3
31	BH	14	GLY	2.3
31	DH	48	GLY	2.3
49	B3	55	ARG	2.3
1	CA	1148	U	2.3
9	CI	124	GLN	2.3
25	DA	2132	U	2.3
20	AT	100	ILE	2.3
40	BU	117	GLN	2.3
3	AC	87	LEU	2.3
10	AJ	90	LEU	2.3
32	DI	75	LEU	2.3
44	DY	44	ILE	2.3
44	DY	75	ILE	2.3
45	DZ	163	LEU	2.3
1	CA	999	C	2.3
23	AW	2	C	2.3
25	BA	670	C	2.3
25	BA	940	C	2.3
45	DZ	1	MET	2.3
11	CK	124	LYS	2.3
14	CN	40	CYS	2.3
36	DQ	22	LYS	2.3
50	D4	38	LYS	2.3
3	AC	207	VAL	2.3
3	CC	23	TYR	2.3
7	CG	151	TYR	2.3
8	AH	53	VAL	2.3
10	CJ	72	VAL	2.3
45	BZ	161	VAL	2.3
7	CG	40	ALA	2.3
31	BH	168	PRO	2.3
33	DN	44	PRO	2.3
1	AA	104	G	2.3
1	CA	1024	G	2.3
13	AM	49	THR	2.3
13	CM	49	THR	2.3
9	AI	9	ARG	2.3
10	AJ	79	ARG	2.3
1	CA	1183	A	2.3
3	CC	41	GLY	2.3
19	CS	34	TRP	2.3

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Mol	Chain	Res	Type	RSRZ
38	DS	45	GLY	2.3
2	CB	42	ILE	2.3
4	AD	96	LEU	2.3
4	CD	5	ILE	2.3
4	CD	19	LEU	2.3
20	CT	100	ILE	2.3
31	DH	7	LEU	2.3
31	DH	103	LEU	2.3
40	DU	88	ILE	2.3
44	DY	61	ILE	2.3
45	BZ	171	ILE	2.3
45	DZ	120	ILE	2.3
25	BA	12	U	2.3
25	BA	1220	U	2.3
25	DA	2167	U	2.3
25	DA	1509	C	2.3
25	DA	2789	C	2.3
50	B4	69	LYS	2.3
9	AI	33	PHE	2.3
16	AP	9	PHE	2.3
2	AB	126	GLU	2.3
2	CB	93	VAL	2.3
16	AP	21	VAL	2.3
45	DZ	119	GLU	2.3
30	BG	25	TYR	2.3
49	D3	59	VAL	2.3
54	D8	64	TYR	2.3
2	CB	88	ALA	2.3
3	CC	129	ALA	2.3
4	CD	154	ASN	2.3
9	AI	46	ALA	2.3
13	CM	72	ALA	2.3
31	BH	20	ALA	2.3
31	DH	39	PRO	2.3
32	DI	146	ALA	2.3
34	DO	29	ASN	2.3
13	CM	110	ARG	2.3
39	DT	111	ARG	2.3
50	B4	55	ARG	2.3
12	AL	6	THR	2.3
16	AP	22	THR	2.3
21	CU	17	THR	2.3

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Mol	Chain	Res	Type	RSRZ
3	CC	31	HIS	2.3
5	CE	20	GLN	2.3
7	AG	110	GLN	2.3
15	CO	61	GLY	2.3
19	AS	4	SER	2.3
1	AA	607	A	2.3
3	CC	18	TRP	2.3
9	AI	74	ILE	2.3
20	CT	99	LEU	2.3
25	BA	569	G	2.3
25	BA	2188	G	2.3
35	DP	1	MET	2.3
45	DZ	28	MET	2.3
2	AB	27	LYS	2.3
25	BA	9	U	2.3
17	CQ	96	GLU	2.3
25	BA	696	C	2.3
25	BA	2197	C	2.3
30	DG	48	GLU	2.3
3	CC	88	ARG	2.3
5	AE	96	PRO	2.3
5	CE	133	TYR	2.3
16	AP	75	ARG	2.3
31	DH	112	PRO	2.3
9	AI	76	ALA	2.2
9	CI	13	ALA	2.2
9	CI	45	ALA	2.2
9	CI	82	ALA	2.2
11	CK	74	ALA	2.2
43	DX	18	TYR	2.3
50	B4	67	TYR	2.3
2	CB	16	HIS	2.2
9	CI	39	GLY	2.2
11	CK	102	GLY	2.2
35	BP	116	GLY	2.2
36	DQ	33	GLY	2.2
46	D0	80	HIS	2.2
2	AB	39	ILE	2.2
3	CC	202	ILE	2.2
8	AH	111	ILE	2.2
10	AJ	74	ILE	2.2
10	CJ	82	ILE	2.2

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Mol	Chain	Res	Type	RSRZ
12	AL	17	LYS	2.2
13	AM	27	LYS	2.2
19	CS	15	LEU	2.2
30	BG	43	LEU	2.2
38	DS	58	LEU	2.2
44	DY	46	LYS	2.2
46	D0	37	LEU	2.2
1	CA	1044	A	2.2
27	DD	200	ASP	2.2
39	DT	124	ASP	2.2
1	CA	1036	G	2.2
23	AY	53	G	2.2
25	BA	2173	G	2.2
25	BA	2174	G	2.2
23	CY	45	U	2.2
25	DA	2118	U	2.2
2	CB	12	GLU	2.2
10	AJ	64	GLU	2.2
31	BH	34	GLU	2.2
9	AI	18	PHE	2.2
36	DQ	65	PHE	2.2
1	CA	1260	C	2.2
3	CC	68	VAL	2.2
3	CC	151	VAL	2.2
4	AD	3	ARG	2.2
4	AD	139	ARG	2.2
5	CE	25	ARG	2.2
7	CG	155	ARG	2.2
9	AI	14	VAL	2.2
10	AJ	66	ARG	2.2
13	CM	41	PRO	2.2
14	AN	23	ARG	2.2
19	CS	58	VAL	2.2
27	BD	262	ARG	2.2
28	BE	72	VAL	2.2
31	BH	113	VAL	2.2
39	BT	125	ARG	2.2
5	AE	48	ALA	2.2
9	CI	94	ALA	2.2
13	CM	51	ALA	2.2
52	D6	20	ASN	2.2
4	AD	138	TYR	2.2

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Mol	Chain	Res	Type	RSRZ
11	AK	104	GLN	2.2
48	D2	43	GLN	2.2
4	CD	2	GLY	2.2
9	CI	67	GLY	2.2
10	CJ	31	GLY	2.2
12	CL	126	LYS	2.2
14	AN	51	GLY	2.2
21	AU	2	GLY	2.2
21	CU	11	GLY	2.2
37	DR	7	GLY	2.2
2	CB	118	LEU	2.2
4	CD	196	LEU	2.2
5	CE	53	LEU	2.2
5	CE	71	LEU	2.2
9	AI	19	LEU	2.2
13	CM	34	LEU	2.2
19	CS	71	LEU	2.2
29	DF	196	LEU	2.2
8	CH	29	SER	2.2
45	DZ	137	ILE	2.2
2	AB	193	ASP	2.2
4	AD	53	ASP	2.2
9	AI	32	ASP	2.2
16	CP	59	TRP	2.2
3	CC	19	GLU	2.2
5	CE	50	GLU	2.2
44	BY	91	GLU	2.2
1	AA	1026	G	2.2
4	AD	118	ARG	2.2
7	CG	32	ARG	2.2
10	CJ	5	ARG	2.2
23	AY	22	G	2.2
23	CY	5	G	2.2
24	CX	2	G	2.2
24	CX	70	G	2.2
25	DA	10	G	2.2
25	DA	879	G	2.2
25	DA	880	G	2.2
8	AH	31	PHE	2.2
15	AO	19	PRO	2.2
36	DQ	109	VAL	2.2
45	DZ	96	VAL	2.2

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Mol	Chain	Res	Type	RSRZ
45	DZ	128	VAL	2.2
50	D4	29	PRO	2.2
55	D9	3	VAL	2.2
2	CB	225	ALA	2.2
9	CI	46	ALA	2.2
14	CN	30	ALA	2.2
25	DA	2140	C	2.2
34	BO	89	ASN	2.2
3	CC	107	GLN	2.2
16	AP	17	TYR	2.2
19	AS	83	HIS	2.2
32	DI	129	THR	2.2
36	DQ	113	GLN	2.2
38	DS	33	LYS	2.2
2	CB	48	MET	2.2
2	AB	196	LEU	2.2
4	AD	2	GLY	2.2
4	AD	108	LEU	2.2
4	AD	202	LEU	2.2
9	CI	50	LEU	2.2
30	DG	119	GLY	2.2
31	BH	5	GLY	2.2
38	DS	24	LEU	2.2
44	DY	25	GLY	2.2
44	DY	104	GLY	2.2
21	CU	13	ILE	2.2
30	BG	77	ILE	2.2
16	AP	23	ASP	2.2
29	BF	23	ASP	2.2
42	DW	63	ASP	2.2
29	DF	161	GLU	2.2
45	DZ	2	GLU	2.2
2	CB	36	ARG	2.2
2	CB	130	ARG	2.2
5	CE	24	ARG	2.2
13	CM	88	ARG	2.2
16	AP	25	ARG	2.2
47	D1	26	ARG	2.2
23	AY	20	U	2.2
25	BA	1072	U	2.2
25	DA	899	A	2.2
9	CI	21	PRO	2.2

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Mol	Chain	Res	Type	RSRZ
31	DH	123	PHE	2.2
39	DT	57	PHE	2.2
43	DX	21	PHE	2.2
8	AH	61	VAL	2.2
13	AM	117	VAL	2.2
55	D9	16	VAL	2.2
1	CA	485	G	2.2
23	CY	57	G	2.2
24	AX	2	G	2.2
25	DA	2149	G	2.2
4	CD	195	ALA	2.2
43	DX	22	ALA	2.2
44	DY	6	HIS	2.2
3	CC	196	LEU	2.2
4	AD	162	LEU	2.2
8	AH	47	GLY	2.2
9	AI	102	LEU	2.2
19	AS	82	GLY	2.2
19	CS	22	LEU	2.2
24	AX	67	C	2.2
25	BA	939	C	2.2
25	BA	2129	C	2.2
25	BA	2158	C	2.2
25	DA	2111	C	2.2
30	DG	25	TYR	2.2
35	DP	93	GLY	2.2
45	DZ	110	GLY	2.2
2	AB	182	ILE	2.2
3	AC	124	ILE	2.2
14	AN	7	ILE	2.2
31	BH	4	ILE	2.2
2	CB	192	SER	2.2
27	DD	22	SER	2.2
8	AH	54	ASP	2.2
45	BZ	145	GLU	2.2
5	AE	18	ARG	2.2
8	CH	30	ARG	2.2
15	CO	68	ARG	2.2
21	AU	24	ARG	2.2
32	DI	103	ARG	2.2
50	D4	48	ARG	2.2
19	CS	59	PRO	2.2

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Mol	Chain	Res	Type	RSRZ
30	DG	29	TRP	2.2
1	AA	160	A	2.1
3	CC	4	LYS	2.2
13	CM	31	LYS	2.2
15	AO	5	LYS	2.2
17	CQ	14	LYS	2.2
25	BA	1554	A	2.1
25	BA	2172	U	2.2
27	DD	15	PHE	2.2
30	DG	180	PHE	2.2
45	DZ	104	PHE	2.2
2	AB	93	VAL	2.1
16	AP	51	VAL	2.1
31	BH	24	VAL	2.1
31	BH	37	VAL	2.1
31	DH	114	VAL	2.1
32	BI	127	VAL	2.1
2	AB	120	ALA	2.1
2	CB	40	HIS	2.1
2	CB	77	ALA	2.1
19	CS	47	HIS	2.1
3	CC	162	GLN	2.1
3	CC	170	GLN	2.1
34	DO	51	ALA	2.1
1	AA	1024	G	2.1
1	CA	1127	G	2.1
8	CH	10	LEU	2.1
13	CM	105	THR	2.1
14	CN	47	LEU	2.1
25	BA	938	G	2.1
25	BA	2177	G	2.1
25	BA	2190	G	2.1
25	DA	545	G	2.1
25	DA	2893	G	2.1
31	DH	171	LEU	2.1
32	BI	72	LEU	2.1
50	D4	44	THR	2.1
2	AB	31	TYR	2.1
4	AD	70	ILE	2.1
10	AJ	82	ILE	2.1
11	AK	25	TYR	2.1
19	CS	31	ILE	2.1

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Mol	Chain	Res	Type	RSRZ
30	BG	140	ILE	2.1
23	AY	48	C	2.1
25	BA	2130	C	2.1
25	DA	2128	C	2.1
2	AB	30	ARG	2.1
15	AO	64	ARG	2.1
30	DG	54	GLU	2.1
50	D4	30	GLU	2.1
6	AF	55	ASP	2.1
39	DT	107	ASP	2.1
2	CB	91	PRO	2.1
4	AD	169	LYS	2.1
9	AI	21	PRO	2.1
10	AJ	80	LYS	2.1
10	CJ	91	PRO	2.1
3	CC	128	PHE	2.1
14	AN	18	VAL	2.1
45	DZ	141	VAL	2.1
4	AD	181	MET	2.1
23	CY	60	U	2.1
25	DA	12	U	2.1
25	DA	157	U	2.1
25	DA	1026	U	2.1
25	DA	2113	U	2.1
2	AB	207	ALA	2.1
16	AP	70	ALA	2.1
25	BA	2198	A	2.1
3	CC	32	LEU	2.1
7	CG	130	GLY	2.1
8	AH	59	LEU	2.1
31	DH	82	GLY	2.1
35	DP	44	GLY	2.1
41	DV	17	GLY	2.1
45	BZ	160	GLY	2.1
2	AB	214	ILE	2.1
3	CC	57	ILE	2.1
3	CC	124	ILE	2.1
5	AE	11	ILE	2.1
7	AG	50	ILE	2.1
17	CQ	90	ILE	2.1
31	BH	92	ILE	2.1
32	DI	109	ILE	2.1

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Mol	Chain	Res	Type	RSRZ
1	AA	346	G	2.1
2	AB	231	GLU	2.1
9	AI	88	TYR	2.1
10	AJ	29	ARG	2.1
12	CL	64	TYR	2.1
16	CP	26	ARG	2.1
17	CQ	49	GLU	2.1
20	CT	86	ARG	2.1
32	BI	57	ARG	2.1
25	BA	269	G	2.1
25	BA	299	G	2.1
25	BA	2176	G	2.1
45	BZ	135	GLU	2.1
1	CA	1244	C	2.1
4	CD	71	SER	2.1
5	CE	5	ASP	2.1
10	CJ	19	SER	2.1
10	CJ	59	SER	2.1
25	BA	2210	C	2.1
25	DA	2164	C	2.1
30	BG	156	ASP	2.1
31	BH	25	LYS	2.1
47	D1	48	LYS	2.1
10	CJ	39	PRO	2.1
41	DV	50	PRO	2.1
16	CP	9	PHE	2.1
4	AD	104	VAL	2.1
7	AG	86	GLN	2.1
11	CK	105	VAL	2.1
27	DD	112	GLN	2.1
32	BI	136	VAL	2.1
33	DN	5	VAL	2.1
1	CA	981	U	2.1
3	AC	50	ALA	2.1
3	CC	92	ALA	2.1
8	AH	138	TRP	2.1
21	AU	14	TRP	2.1
49	D3	21	ALA	2.1
1	AA	1286	A	2.1
2	CB	138	LEU	2.1
4	AD	157	LEU	2.1
10	CJ	15	THR	2.1

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Mol	Chain	Res	Type	RSRZ
15	AO	89	GLY	2.1
16	CP	74	LEU	2.1
25	BA	554	A	2.1
25	DA	2173	A	2.1
45	BZ	163	LEU	2.1
15	CO	4	THR	2.1
21	CU	24	ARG	2.1
3	CC	134	ILE	2.1
4	AD	5	ILE	2.1
13	AM	25	ILE	2.1
15	CO	3	ILE	2.1
39	DT	52	ILE	2.1
45	DZ	133	ILE	2.1
4	AD	68	TYR	2.1
4	AD	207	TYR	2.1
12	AL	64	TYR	2.1
49	D3	15	TYR	2.1
50	D4	43	TYR	2.1
10	AJ	57	LYS	2.1
28	DE	69	LYS	2.1
52	D6	53	LYS	2.1
34	DO	28	SER	2.1
23	CY	6	G	2.1
23	CY	53	G	2.1
23	CY	69	G	2.1
1	AA	91	C	2.1
1	CA	1006	C	2.1
1	CA	1007	C	2.1
25	BA	2185	C	2.1
25	DA	2175	C	2.1
2	CB	83	MET	2.1
3	AC	10	PHE	2.1
8	AH	70	GLN	2.1
4	CD	88	VAL	2.1
7	CG	69	VAL	2.1
8	AH	93	VAL	2.1
11	AK	125	PHE	2.1
27	DD	18	VAL	2.1
31	DH	49	VAL	2.1
45	DZ	139	VAL	2.1
28	DE	131	ALA	2.1
29	DF	130	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
31	DH	156	ALA	2.1
1	CA	1000	U	2.1
2	AB	24	TRP	2.1
2	CB	137	ARG	2.1
4	CD	21	LEU	2.1
7	CG	103	TRP	2.1
3	AC	96	GLY	2.1
9	CI	111	ARG	2.1
23	CY	33	U	2.1
23	CY	59	U	2.1
25	BA	2194	U	2.1
25	DA	2172	U	2.1
44	DY	50	ARG	2.1
44	DY	106	LEU	2.1
2	AB	129	GLU	2.1
4	AD	80	GLU	2.1
30	BG	54	GLU	2.1
41	DV	32	THR	2.1
45	DZ	145	GLU	2.1
1	AA	1001	A	2.1
3	CC	5	ILE	2.1
4	AD	204	ILE	2.1
25	BA	702	A	2.1
25	DA	887	A	2.1
35	BP	75	ILE	2.1
13	CM	46	LYS	2.1
30	BG	75	LYS	2.1
6	CF	55	ASP	2.1
10	CJ	73	ASP	2.1
35	DP	110	TYR	2.1
17	AQ	28	PRO	2.1
21	AU	23	PRO	2.1
31	BH	36	PRO	2.1
32	DI	8	PRO	2.1
5	CE	10	MET	2.1
23	CW	15	G	2.0
25	BA	2903	G	2.0
9	AI	37	PHE	2.0
28	DE	72	VAL	2.0
30	DG	80	PHE	2.0
35	DP	146	VAL	2.0
41	DV	51	VAL	2.0

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Mol	Chain	Res	Type	RSRZ
45	BZ	165	VAL	2.0
46	D0	57	PHE	2.0
46	D0	79	VAL	2.0
51	D5	60	VAL	2.0
3	CC	187	ALA	2.0
4	AD	47	ARG	2.0
5	CE	146	ALA	2.0
7	AG	127	ALA	2.0
7	CG	79	ARG	2.0
9	AI	10	ARG	2.0
19	CS	3	ARG	2.0
30	BG	136	ARG	2.0
30	DG	83	ARG	2.0
33	BN	115	ARG	2.0
44	DY	48	ALA	2.0
45	DZ	4	ARG	2.0
3	CC	12	LEU	2.0
48	D2	10	LEU	2.0
49	D3	23	LEU	2.0
2	CB	65	GLY	2.0
3	AC	19	GLU	2.0
4	CD	69	GLY	2.0
32	DI	16	GLY	2.0
47	D1	31	GLY	2.0
1	CA	992	U	2.0
3	CC	8	ILE	2.0
7	CG	42	ILE	2.0
9	CI	78	LYS	2.0
12	CL	61	THR	2.0
13	AM	4	ILE	2.0
16	CP	45	THR	2.0
19	AS	79	THR	2.0
19	CS	48	THR	2.0
23	AY	45	U	2.0
23	CW	45	U	2.0
32	BI	79	ILE	2.0
39	DT	102	ILE	2.0
22	CV	24	A	2.0
2	CB	232	PRO	2.0
2	AB	48	MET	2.0
3	AC	49	SER	2.0
5	CE	70	PRO	2.0

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Mol	Chain	Res	Type	RSRZ
20	CT	82	SER	2.0
31	BH	112	PRO	2.0
31	DH	21	PRO	2.0
16	AP	1	MET	2.0
31	BH	41	MET	2.0
7	CG	86	GLN	2.0
1	AA	345	C	2.0
1	CA	962	C	2.0
2	CB	7	VAL	2.0
2	CB	144	ARG	2.0
2	CB	226	ARG	2.0
3	CC	86	VAL	2.0
9	AI	26	VAL	2.0
9	CI	65	VAL	2.0
13	CM	17	VAL	2.0
13	CM	98	VAL	2.0
16	AP	79	VAL	2.0
23	AY	56	C	2.0
25	DA	2794	C	2.0
31	BH	23	ARG	2.0
35	BP	83	VAL	2.0
43	DX	81	VAL	2.0
44	DY	89	PHE	2.0
48	D2	25	VAL	2.0
1	AA	78	G	2.0
1	AA	1002	G	2.0
1	CA	1154	G	2.0
25	BA	1218	G	2.0
25	DA	271(M)	G	2.0
25	DA	2153	G	2.0
4	AD	78	LEU	2.0
36	DQ	53	ALA	2.0
45	DZ	67	LEU	2.0
2	CB	38	GLY	2.0
3	CC	51	GLY	2.0
3	CC	72	LYS	2.0
27	DD	238	GLY	2.0
44	BY	92	ASN	2.0
44	DY	95	LYS	2.0
2	CB	200	ILE	2.0
8	AH	24	THR	2.0
20	CT	63	ILE	2.0

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Mol	Chain	Res	Type	RSRZ
35	DP	75	ILE	2.0
36	DQ	75	THR	2.0
40	DU	62	ILE	2.0
1	CA	1040	U	2.0
1	CA	1281	U	2.0
23	CY	47	U	2.0
1	CA	969	A	2.0
1	CA	1250	A	2.0
3	CC	62	ASP	2.0
25	BA	925	A	2.0
25	BA	946	A	2.0
34	BO	112	MET	2.0
13	CM	23	TYR	2.0
20	CT	11	SER	2.0
31	BH	63	SER	2.0
32	DI	130	TYR	2.0
47	D1	86	SER	2.0

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
23	PSU	CY	55	20/21	0.64	0.15	92,98,105,119	0
23	MIA	CY	37	22/30	0.65	0.19	82,93,117,140	0
23	7MG	AY	46	24/25	0.66	0.17	80,94,107,121	0
23	PSU	AY	55	20/21	0.69	0.17	93,99,105,118	0
23	4SU	AY	8	20/21	0.70	0.15	92,98,108,126	0
23	7MG	CY	46	24/25	0.71	0.17	86,95,102,125	0
23	5MU	CY	54	21/22	0.72	0.19	78,92,113,136	0
23	5MU	AY	54	21/22	0.73	0.16	81,91,102,125	0
23	7MG	AW	46	24/25	0.73	0.14	70,83,111,120	0
23	4SU	CY	8	20/21	0.73	0.16	83,99,114,124	0
23	PSU	CY	32	20/21	0.73	0.16	83,92,99,105	0
23	7MG	CW	46	24/25	0.75	0.14	85,98,110,126	0
23	MIA	AY	37	22/30	0.76	0.14	72,87,104,128	0
23	4SU	CW	8	20/21	0.78	0.12	88,94,105,122	0
23	PSU	CY	39	20/21	0.80	0.14	80,88,99,111	0
23	PSU	AY	32	20/21	0.81	0.15	83,91,98,100	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
23	4SU	AW	8	20/21	0.83	0.13	73,85,96,105	0
23	PSU	CW	55	20/21	0.84	0.12	61,83,94,94	0
23	PSU	AY	39	20/21	0.84	0.14	77,86,97,100	0
23	PSU	CW	32	20/21	0.85	0.15	70,85,92,95	0
24	5MU	CX	54	21/22	0.87	0.13	71,80,88,94	0
24	PSU	CX	55	20/21	0.87	0.12	63,69,89,97	0
24	4SU	CX	8	20/21	0.87	0.12	54,78,85,86	0
23	5MU	CW	54	21/22	0.89	0.11	60,72,84,86	0
24	5MC	CX	32	21/22	0.90	0.16	66,71,81,83	0
24	5MU	AX	54	21/22	0.91	0.12	58,65,74,81	0
24	PSU	AX	55	20/21	0.92	0.10	60,67,93,94	0
23	MIA	CW	37	22/30	0.92	0.09	55,66,75,81	0
23	PSU	AW	32	20/21	0.93	0.10	50,60,69,69	0
23	PSU	AW	55	20/21	0.93	0.08	50,70,80,81	0
24	5MC	AX	32	21/22	0.95	0.13	48,54,58,72	0
23	PSU	CW	39	20/21	0.95	0.08	63,72,81,82	0
23	5MU	AW	54	21/22	0.95	0.07	42,58,69,76	0
24	4SU	AX	8	20/21	0.95	0.10	51,64,80,88	0
23	MIA	AW	37	29/30	0.96	0.11	40,49,63,75	0
23	PSU	AW	39	20/21	0.96	0.08	49,59,65,65	0

5.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	CA	3121	1/1	0.51	0.26	75,75,75,75	0
56	MG	DA	3607	1/1	0.61	0.28	53,53,53,53	0
56	MG	CJ	5001	1/1	0.62	0.23	76,76,76,76	0
56	MG	DA	3565	1/1	0.63	0.20	70,70,70,70	0
56	MG	BA	3367	1/1	0.64	0.31	53,53,53,53	0
56	MG	B8	101	1/1	0.64	0.14	42,42,42,42	0
56	MG	BA	3470	1/1	0.68	0.19	48,48,48,48	0
56	MG	AA	3204	1/1	0.68	0.27	71,71,71,71	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	BA	3571	1/1	0.69	0.13	66,66,66,66	0
56	MG	BA	3548	1/1	0.69	0.26	48,48,48,48	0
56	MG	BA	3726	1/1	0.70	0.19	70,70,70,70	0
56	MG	BA	3221	1/1	0.70	0.16	54,54,54,54	0
56	MG	BA	3692	1/1	0.71	0.23	57,57,57,57	0
56	MG	DA	3241	1/1	0.72	0.17	50,50,50,50	0
56	MG	AA	3190	1/1	0.72	0.21	65,65,65,65	0
56	MG	DA	3580	1/1	0.72	0.22	64,64,64,64	0
56	MG	BA	3553	1/1	0.72	0.16	42,42,42,42	0
56	MG	AA	3198	1/1	0.73	0.24	70,70,70,70	0
56	MG	DA	3002	1/1	0.73	0.16	68,68,68,68	0
56	MG	BA	3728	1/1	0.73	0.15	72,72,72,72	0
56	MG	BA	3333	1/1	0.74	0.16	61,61,61,61	0
56	MG	AA	3192	1/1	0.74	0.30	69,69,69,69	0
56	MG	DA	3521	1/1	0.74	0.14	51,51,51,51	0
56	MG	DA	3547	1/1	0.75	0.17	65,65,65,65	0
56	MG	BA	3720	1/1	0.75	0.14	46,46,46,46	0
56	MG	BA	3585	1/1	0.75	0.25	55,55,55,55	0
56	MG	BA	3105	1/1	0.75	0.33	69,69,69,69	0
56	MG	DA	3466	1/1	0.76	0.17	62,62,62,62	0
56	MG	BA	3605	1/1	0.76	0.14	61,61,61,61	0
56	MG	BA	3618	1/1	0.76	0.21	63,63,63,63	0
56	MG	BA	3637	1/1	0.76	0.17	59,59,59,59	0
56	MG	BA	3079	1/1	0.76	0.19	57,57,57,57	0
56	MG	DA	3404	1/1	0.76	0.15	51,51,51,51	0
56	MG	DA	3508	1/1	0.77	0.14	59,59,59,59	0
56	MG	BA	3435	1/1	0.77	0.16	57,57,57,57	0
56	MG	DA	3538	1/1	0.77	0.12	56,56,56,56	0
56	MG	DA	3066	1/1	0.77	0.19	65,65,65,65	0
56	MG	BA	3725	1/1	0.77	0.28	67,67,67,67	0
56	MG	BE	307	1/1	0.77	0.21	70,70,70,70	0
56	MG	CX	3006	1/1	0.77	0.21	70,70,70,70	0
56	MG	AA	3095	1/1	0.78	0.28	68,68,68,68	0
56	MG	DA	3408	1/1	0.78	0.19	48,48,48,48	0
56	MG	AA	3069	1/1	0.78	0.31	67,67,67,67	0
56	MG	BA	3527	1/1	0.78	0.14	52,52,52,52	0
56	MG	BA	3531	1/1	0.78	0.26	61,61,61,61	0
56	MG	BA	3639	1/1	0.79	0.29	59,59,59,59	0
56	MG	CA	3122	1/1	0.79	0.19	70,70,70,70	0
56	MG	CA	3169	1/1	0.79	0.21	65,65,65,65	0
56	MG	BA	3753	1/1	0.79	0.15	44,44,44,44	0
56	MG	BB	3018	1/1	0.79	0.18	77,77,77,77	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	BA	3516	1/1	0.79	0.21	65,65,65,65	0
56	MG	B1	102	1/1	0.79	0.26	68,68,68,68	0
56	MG	BA	3712	1/1	0.79	0.18	64,64,64,64	0
56	MG	DA	3312	1/1	0.79	0.14	52,52,52,52	0
56	MG	DA	3583	1/1	0.79	0.13	60,60,60,60	0
56	MG	DA	3401	1/1	0.79	0.10	36,36,36,36	0
56	MG	BA	3431	1/1	0.80	0.18	55,55,55,55	0
56	MG	BA	3503	1/1	0.80	0.18	58,58,58,58	0
56	MG	CA	3060	1/1	0.80	0.35	68,68,68,68	0
56	MG	CA	3070	1/1	0.80	0.17	71,71,71,71	0
56	MG	BA	3734	1/1	0.80	0.23	60,60,60,60	0
56	MG	DA	3549	1/1	0.80	0.19	57,57,57,57	0
56	MG	DA	3323	1/1	0.80	0.19	53,53,53,53	0
56	MG	BA	3204	1/1	0.80	0.35	66,66,66,66	0
56	MG	DA	3581	1/1	0.80	0.23	63,63,63,63	0
56	MG	BA	3633	1/1	0.80	0.15	45,45,45,45	0
56	MG	DA	3596	1/1	0.80	0.28	63,63,63,63	0
56	MG	BA	3442	1/1	0.80	0.13	59,59,59,59	0
56	MG	DA	3505	1/1	0.81	0.12	66,66,66,66	0
56	MG	AA	3222	1/1	0.81	0.25	67,67,67,67	0
56	MG	DA	3286	1/1	0.81	0.14	64,64,64,64	0
56	MG	BA	3760	1/1	0.81	0.26	68,68,68,68	0
56	MG	DA	3319	1/1	0.81	0.19	43,43,43,43	0
56	MG	CA	3012	1/1	0.81	0.26	68,68,68,68	0
56	MG	DA	3556	1/1	0.81	0.15	64,64,64,64	0
56	MG	DA	3564	1/1	0.81	0.18	53,53,53,53	0
56	MG	DA	3393	1/1	0.81	0.14	52,52,52,52	0
56	MG	BB	3005	1/1	0.81	0.25	64,64,64,64	0
56	MG	BA	3358	1/1	0.81	0.20	64,64,64,64	0
56	MG	BA	3291	1/1	0.81	0.18	71,71,71,71	0
56	MG	DA	3424	1/1	0.81	0.19	63,63,63,63	0
56	MG	DA	3102	1/1	0.81	0.13	57,57,57,57	0
56	MG	DB	3001	1/1	0.81	0.19	73,73,73,73	0
56	MG	BA	3625	1/1	0.82	0.17	57,57,57,57	0
56	MG	BA	3298	1/1	0.82	0.28	68,68,68,68	0
56	MG	CA	3140	1/1	0.82	0.29	79,79,79,79	0
56	MG	BA	3743	1/1	0.82	0.10	21,21,21,21	0
56	MG	AW	3005	1/1	0.82	0.25	68,68,68,68	0
56	MG	BA	3638	1/1	0.82	0.13	38,38,38,38	0
56	MG	CA	3027	1/1	0.82	0.34	70,70,70,70	0
56	MG	DA	3041	1/1	0.82	0.13	55,55,55,55	0
56	MG	BA	3825	1/1	0.82	0.21	65,65,65,65	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	DA	3420	1/1	0.82	0.13	46,46,46,46	0
56	MG	AA	3033	1/1	0.82	0.18	57,57,57,57	0
56	MG	DA	3436	1/1	0.82	0.11	54,54,54,54	0
56	MG	DA	3155	1/1	0.82	0.21	40,40,40,40	0
56	MG	DA	3199	1/1	0.82	0.23	52,52,52,52	0
56	MG	BA	3511	1/1	0.83	0.17	54,54,54,54	0
56	MG	DA	3528	1/1	0.83	0.18	57,57,57,57	0
56	MG	DA	3028	1/1	0.83	0.20	70,70,70,70	0
56	MG	DA	3400	1/1	0.83	0.17	39,39,39,39	0
56	MG	CA	3051	1/1	0.83	0.18	66,66,66,66	0
56	MG	BA	3831	1/1	0.83	0.51	52,52,52,52	0
56	MG	AA	3139	1/1	0.83	0.19	58,58,58,58	0
56	MG	AA	3125	1/1	0.83	0.13	71,71,71,71	0
56	MG	BA	3685	1/1	0.83	0.14	59,59,59,59	0
56	MG	BA	3449	1/1	0.83	0.27	60,60,60,60	0
56	MG	DA	3452	1/1	0.83	0.21	61,61,61,61	0
56	MG	BA	3409	1/1	0.83	0.22	62,62,62,62	0
56	MG	CA	3007	1/1	0.83	0.21	69,69,69,69	0
56	MG	BA	3347	1/1	0.83	0.14	48,48,48,48	0
60	K	CX	3001	1/1	0.83	0.18	74,74,74,74	0
56	MG	BA	3683	1/1	0.84	0.18	61,61,61,61	0
56	MG	BA	3446	1/1	0.84	0.18	52,52,52,52	0
56	MG	AA	3183	1/1	0.84	0.16	71,71,71,71	0
56	MG	DA	3460	1/1	0.84	0.25	65,65,65,65	0
56	MG	BA	3699	1/1	0.84	0.18	42,42,42,42	0
56	MG	DA	3504	1/1	0.84	0.17	60,60,60,60	0
56	MG	BA	3464	1/1	0.84	0.21	56,56,56,56	0
56	MG	BA	3716	1/1	0.84	0.15	54,54,54,54	0
56	MG	BA	3593	1/1	0.84	0.15	42,42,42,42	0
56	MG	BA	3224	1/1	0.84	0.20	64,64,64,64	0
56	MG	BA	3606	1/1	0.84	0.12	34,34,34,34	0
56	MG	DA	3540	1/1	0.84	0.13	67,67,67,67	0
56	MG	DA	3542	1/1	0.84	0.13	63,63,63,63	0
56	MG	DA	3297	1/1	0.84	0.13	66,66,66,66	0
56	MG	DA	3300	1/1	0.84	0.22	60,60,60,60	0
56	MG	CA	3054	1/1	0.84	0.31	71,71,71,71	0
56	MG	BA	3249	1/1	0.84	0.29	74,74,74,74	0
56	MG	AA	3038	1/1	0.84	0.16	51,51,51,51	0
56	MG	DA	3568	1/1	0.84	0.15	54,54,54,54	0
56	MG	DA	3347	1/1	0.84	0.10	44,44,44,44	0
56	MG	BA	3740	1/1	0.84	0.17	51,51,51,51	0
56	MG	AA	3210	1/1	0.84	0.20	69,69,69,69	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	BA	3315	1/1	0.84	0.16	56,56,56,56	0
56	MG	DA	3605	1/1	0.84	0.12	52,52,52,52	0
56	MG	BA	3439	1/1	0.84	0.20	58,58,58,58	0
56	MG	DA	3614	1/1	0.84	0.12	50,50,50,50	0
56	MG	AA	3098	1/1	0.84	0.23	68,68,68,68	0
56	MG	BA	3681	1/1	0.84	0.18	53,53,53,53	0
56	MG	BA	3030	1/1	0.85	0.12	50,50,50,50	0
56	MG	AA	3213	1/1	0.85	0.11	69,69,69,69	0
56	MG	DA	3105	1/1	0.85	0.19	60,60,60,60	0
56	MG	BA	3101	1/1	0.85	0.18	60,60,60,60	0
56	MG	BA	3311	1/1	0.85	0.12	37,37,37,37	0
56	MG	CA	3036	1/1	0.85	0.09	60,60,60,60	0
56	MG	AA	3216	1/1	0.85	0.18	72,72,72,72	0
56	MG	BA	3320	1/1	0.85	0.18	60,60,60,60	0
56	MG	BA	3186	1/1	0.85	0.23	51,51,51,51	0
56	MG	BA	3746	1/1	0.85	0.12	25,25,25,25	0
56	MG	CA	3103	1/1	0.85	0.15	75,75,75,75	0
56	MG	AA	3134	1/1	0.85	0.17	69,69,69,69	0
56	MG	DA	3342	1/1	0.85	0.14	56,56,56,56	0
56	MG	DA	3562	1/1	0.85	0.14	58,58,58,58	0
56	MG	BA	3689	1/1	0.85	0.18	57,57,57,57	0
56	MG	DA	3359	1/1	0.85	0.19	57,57,57,57	0
56	MG	CA	3125	1/1	0.85	0.11	64,64,64,64	0
56	MG	AN	502	1/1	0.85	0.10	52,52,52,52	0
56	MG	BA	3490	1/1	0.85	0.09	44,44,44,44	0
56	MG	BA	3708	1/1	0.85	0.32	63,63,63,63	0
56	MG	BA	3492	1/1	0.85	0.14	55,55,55,55	0
56	MG	DA	3598	1/1	0.85	0.19	63,63,63,63	0
56	MG	BB	3020	1/1	0.85	0.14	54,54,54,54	0
56	MG	AA	3082	1/1	0.85	0.29	68,68,68,68	0
56	MG	DA	3434	1/1	0.85	0.20	51,51,51,51	0
56	MG	DA	3632	1/1	0.85	0.15	58,58,58,58	0
56	MG	DA	3645	1/1	0.85	0.10	44,44,44,44	0
56	MG	BA	3718	1/1	0.85	0.12	46,46,46,46	0
56	MG	DB	3005	1/1	0.85	0.28	64,64,64,64	0
57	PCY	CA	3178	40/40	0.85	0.19	58,78,89,91	0
56	MG	DA	3051	1/1	0.85	0.15	56,56,56,56	0
56	MG	CA	3067	1/1	0.86	0.31	79,79,79,79	0
56	MG	BA	3577	1/1	0.86	0.18	60,60,60,60	0
56	MG	AA	3024	1/1	0.86	0.14	58,58,58,58	0
56	MG	CA	3109	1/1	0.86	0.23	68,68,68,68	0
56	MG	AX	3003	1/1	0.86	0.13	66,66,66,66	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	BA	3594	1/1	0.86	0.12	24,24,24,24	0
56	MG	DA	3454	1/1	0.86	0.14	54,54,54,54	0
56	MG	DA	3457	1/1	0.86	0.09	47,47,47,47	0
56	MG	BA	3595	1/1	0.86	0.15	32,32,32,32	0
56	MG	AY	3002	1/1	0.86	0.14	68,68,68,68	0
56	MG	DA	3468	1/1	0.86	0.14	44,44,44,44	0
56	MG	BA	3028	1/1	0.86	0.17	59,59,59,59	0
56	MG	BA	3617	1/1	0.86	0.20	64,64,64,64	0
56	MG	AA	3153	1/1	0.86	0.15	55,55,55,55	0
56	MG	DA	3518	1/1	0.86	0.14	50,50,50,50	0
56	MG	AA	3176	1/1	0.86	0.17	54,54,54,54	0
56	MG	BA	3089	1/1	0.86	0.16	45,45,45,45	0
56	MG	DA	3536	1/1	0.86	0.11	54,54,54,54	0
56	MG	BA	3787	1/1	0.86	0.20	59,59,59,59	0
56	MG	BA	3472	1/1	0.86	0.16	70,70,70,70	0
56	MG	AA	3073	1/1	0.86	0.26	58,58,58,58	0
56	MG	AA	3062	1/1	0.86	0.14	60,60,60,60	0
56	MG	BA	3651	1/1	0.86	0.18	56,56,56,56	0
56	MG	BA	3659	1/1	0.86	0.15	53,53,53,53	0
56	MG	DA	3163	1/1	0.86	0.16	49,49,49,49	0
56	MG	BB	3022	1/1	0.86	0.18	62,62,62,62	0
56	MG	BE	305	1/1	0.86	0.17	59,59,59,59	0
56	MG	BA	3357	1/1	0.86	0.12	46,46,46,46	0
56	MG	BA	3114	1/1	0.86	0.12	52,52,52,52	0
56	MG	AA	3094	1/1	0.86	0.21	44,44,44,44	0
56	MG	BA	3523	1/1	0.86	0.13	64,64,64,64	0
56	MG	BA	3370	1/1	0.86	0.16	60,60,60,60	0
56	MG	BA	3393	1/1	0.86	0.12	54,54,54,54	0
56	MG	CA	3028	1/1	0.86	0.13	60,60,60,60	0
56	MG	BA	3706	1/1	0.86	0.10	50,50,50,50	0
56	MG	BA	3404	1/1	0.86	0.12	36,36,36,36	0
56	MG	DA	3365	1/1	0.86	0.21	57,57,57,57	0
56	MG	CA	3053	1/1	0.86	0.18	74,74,74,74	0
56	MG	DA	3398	1/1	0.86	0.17	57,57,57,57	0
56	MG	AA	3194	1/1	0.86	0.17	58,58,58,58	0
56	MG	DB	3007	1/1	0.86	0.14	59,59,59,59	0
56	MG	CA	3056	1/1	0.86	0.20	60,60,60,60	0
56	MG	AW	3001	1/1	0.86	0.12	55,55,55,55	0
56	MG	DA	3410	1/1	0.87	0.12	62,62,62,62	0
56	MG	BA	3115	1/1	0.87	0.12	67,67,67,67	0
56	MG	BA	3701	1/1	0.87	0.14	51,51,51,51	0
56	MG	DA	3428	1/1	0.87	0.18	61,61,61,61	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	DA	3433	1/1	0.87	0.18	61,61,61,61	0
56	MG	AA	3003	1/1	0.87	0.14	66,66,66,66	0
56	MG	BA	3200	1/1	0.87	0.24	56,56,56,56	0
56	MG	DA	3451	1/1	0.87	0.14	56,56,56,56	0
56	MG	DA	3014	1/1	0.87	0.12	50,50,50,50	0
56	MG	AA	3068	1/1	0.87	0.17	60,60,60,60	0
56	MG	BR	202	1/1	0.87	0.23	53,53,53,53	0
56	MG	BR	203	1/1	0.87	0.14	44,44,44,44	0
56	MG	DA	3064	1/1	0.87	0.20	64,64,64,64	0
56	MG	BY	502	1/1	0.87	0.20	50,50,50,50	0
56	MG	DA	3079	1/1	0.87	0.08	48,48,48,48	0
56	MG	BA	3491	1/1	0.87	0.17	47,47,47,47	0
56	MG	AA	3145	1/1	0.87	0.18	58,58,58,58	0
56	MG	DA	3513	1/1	0.87	0.14	50,50,50,50	0
56	MG	DA	3117	1/1	0.87	0.23	60,60,60,60	0
56	MG	DA	3127	1/1	0.87	0.12	38,38,38,38	0
56	MG	DA	3144	1/1	0.87	0.17	63,63,63,63	0
56	MG	BA	3031	1/1	0.87	0.23	56,56,56,56	0
56	MG	AA	3150	1/1	0.87	0.23	55,55,55,55	0
56	MG	DA	3182	1/1	0.87	0.17	64,64,64,64	0
56	MG	BA	3278	1/1	0.87	0.20	55,55,55,55	0
56	MG	AA	3100	1/1	0.87	0.15	68,68,68,68	0
56	MG	DA	3243	1/1	0.87	0.13	54,54,54,54	0
56	MG	DA	3260	1/1	0.87	0.10	41,41,41,41	0
56	MG	BA	3729	1/1	0.87	0.15	52,52,52,52	0
56	MG	BA	3433	1/1	0.87	0.15	57,57,57,57	0
56	MG	BA	3095	1/1	0.87	0.16	53,53,53,53	0
56	MG	DA	3303	1/1	0.87	0.12	42,42,42,42	0
56	MG	BA	3652	1/1	0.87	0.12	46,46,46,46	0
56	MG	BA	3438	1/1	0.87	0.09	47,47,47,47	0
56	MG	BA	3672	1/1	0.87	0.17	61,61,61,61	0
56	MG	DA	3584	1/1	0.87	0.24	58,58,58,58	0
56	MG	BA	3758	1/1	0.87	0.10	34,34,34,34	0
56	MG	AA	3156	1/1	0.87	0.14	52,52,52,52	0
56	MG	CA	3090	1/1	0.87	0.19	62,62,62,62	0
56	MG	BA	3784	1/1	0.87	0.23	52,52,52,52	0
56	MG	DA	3610	1/1	0.87	0.16	48,48,48,48	0
56	MG	DA	3387	1/1	0.87	0.15	56,56,56,56	0
56	MG	AA	3042	1/1	0.87	0.13	57,57,57,57	0
56	MG	DA	3642	1/1	0.87	0.14	49,49,49,49	0
56	MG	BA	3113	1/1	0.87	0.28	58,58,58,58	0
56	MG	DA	3674	1/1	0.87	0.18	73,73,73,73	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	AX	3010	1/1	0.87	0.17	62,62,62,62	0
56	MG	BA	3838	1/1	0.87	0.15	50,50,50,50	0
56	MG	CA	3133	1/1	0.87	0.13	65,65,65,65	0
56	MG	DB	3008	1/1	0.87	0.14	68,68,68,68	0
56	MG	DF	301	1/1	0.87	0.08	47,47,47,47	0
56	MG	DA	3405	1/1	0.87	0.15	52,52,52,52	0
56	MG	BA	3457	1/1	0.87	0.13	44,44,44,44	0
56	MG	AX	3007	1/1	0.88	0.28	72,72,72,72	0
56	MG	CA	3059	1/1	0.88	0.38	67,67,67,67	0
56	MG	BA	3588	1/1	0.88	0.08	47,47,47,47	0
56	MG	BA	3441	1/1	0.88	0.22	46,46,46,46	0
56	MG	AA	3209	1/1	0.88	0.16	51,51,51,51	0
56	MG	CA	3072	1/1	0.88	0.19	62,62,62,62	0
56	MG	CA	3083	1/1	0.88	0.09	58,58,58,58	0
56	MG	CA	3085	1/1	0.88	0.32	71,71,71,71	0
56	MG	AA	3174	1/1	0.88	0.17	60,60,60,60	0
56	MG	BA	3603	1/1	0.88	0.10	54,54,54,54	0
56	MG	DA	3415	1/1	0.88	0.12	50,50,50,50	0
56	MG	DA	3419	1/1	0.88	0.12	44,44,44,44	0
56	MG	BA	3181	1/1	0.88	0.11	41,41,41,41	0
56	MG	DA	3421	1/1	0.88	0.11	53,53,53,53	0
56	MG	CA	3113	1/1	0.88	0.10	55,55,55,55	0
56	MG	BA	3023	1/1	0.88	0.22	55,55,55,55	0
56	MG	BA	3356	1/1	0.88	0.15	55,55,55,55	0
56	MG	BA	3199	1/1	0.88	0.15	53,53,53,53	0
56	MG	CA	3126	1/1	0.88	0.18	72,72,72,72	0
56	MG	AA	3067	1/1	0.88	0.20	59,59,59,59	0
56	MG	BA	3626	1/1	0.88	0.10	49,49,49,49	0
56	MG	CA	3151	1/1	0.88	0.18	65,65,65,65	0
56	MG	CA	3158	1/1	0.88	0.15	53,53,53,53	0
56	MG	BA	3769	1/1	0.88	0.10	56,56,56,56	0
56	MG	CA	3177	1/1	0.88	0.16	62,62,62,62	0
56	MG	BA	3773	1/1	0.88	0.17	49,49,49,49	0
56	MG	DA	3493	1/1	0.88	0.15	58,58,58,58	0
56	MG	DA	3500	1/1	0.88	0.09	45,45,45,45	0
56	MG	CX	3002	1/1	0.88	0.13	81,81,81,81	0
56	MG	BA	3779	1/1	0.88	0.14	59,59,59,59	0
56	MG	BA	3478	1/1	0.88	0.13	59,59,59,59	0
56	MG	BA	3483	1/1	0.88	0.10	38,38,38,38	0
56	MG	BA	3797	1/1	0.88	0.13	52,52,52,52	0
56	MG	AA	3017	1/1	0.88	0.13	62,62,62,62	0
56	MG	AA	3221	1/1	0.88	0.13	49,49,49,49	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	BA	3376	1/1	0.88	0.12	34,34,34,34	0
56	MG	DA	3065	1/1	0.88	0.12	56,56,56,56	0
56	MG	AA	3084	1/1	0.88	0.10	49,49,49,49	0
56	MG	DA	3072	1/1	0.88	0.15	36,36,36,36	0
56	MG	BA	3654	1/1	0.88	0.17	55,55,55,55	0
56	MG	BA	3401	1/1	0.88	0.13	48,48,48,48	0
56	MG	AA	3109	1/1	0.88	0.26	64,64,64,64	0
56	MG	BA	3676	1/1	0.88	0.22	53,53,53,53	0
56	MG	BA	3680	1/1	0.88	0.11	52,52,52,52	0
56	MG	BO	5001	1/1	0.88	0.09	55,55,55,55	0
56	MG	BA	3254	1/1	0.88	0.09	30,30,30,30	0
56	MG	DA	3569	1/1	0.88	0.13	57,57,57,57	0
56	MG	BA	3413	1/1	0.88	0.14	41,41,41,41	0
56	MG	BX	101	1/1	0.88	0.15	65,65,65,65	0
56	MG	DA	3184	1/1	0.88	0.18	49,49,49,49	0
56	MG	BA	3429	1/1	0.88	0.13	47,47,47,47	0
56	MG	DA	3589	1/1	0.88	0.09	63,63,63,63	0
56	MG	BA	3534	1/1	0.88	0.14	31,31,31,31	0
56	MG	BA	3539	1/1	0.88	0.12	23,23,23,23	0
56	MG	DA	3604	1/1	0.88	0.17	57,57,57,57	0
56	MG	DA	3244	1/1	0.88	0.10	48,48,48,48	0
56	MG	CA	3005	1/1	0.88	0.12	58,58,58,58	0
56	MG	BA	3693	1/1	0.88	0.15	70,70,70,70	0
56	MG	BA	3547	1/1	0.88	0.15	41,41,41,41	0
56	MG	DA	3615	1/1	0.88	0.12	47,47,47,47	0
56	MG	CA	3026	1/1	0.88	0.17	64,64,64,64	0
56	MG	DA	3636	1/1	0.88	0.11	56,56,56,56	0
56	MG	AA	3120	1/1	0.88	0.21	59,59,59,59	0
56	MG	DA	3310	1/1	0.88	0.11	55,55,55,55	0
56	MG	BA	3290	1/1	0.88	0.24	58,58,58,58	0
56	MG	CA	3034	1/1	0.88	0.14	61,61,61,61	0
56	MG	BA	3560	1/1	0.88	0.14	35,35,35,35	0
56	MG	DA	3325	1/1	0.88	0.15	57,57,57,57	0
56	MG	BA	3563	1/1	0.88	0.12	60,60,60,60	0
56	MG	AA	3155	1/1	0.88	0.13	53,53,53,53	0
56	MG	D8	5001	1/1	0.88	0.23	55,55,55,55	0
56	MG	DA	3354	1/1	0.88	0.15	46,46,46,46	0
56	MG	AA	3040	1/1	0.88	0.26	59,59,59,59	0
56	MG	CA	3163	1/1	0.89	0.16	53,53,53,53	0
56	MG	AA	3046	1/1	0.89	0.18	56,56,56,56	0
56	MG	BA	3392	1/1	0.89	0.11	46,46,46,46	0
56	MG	BA	3241	1/1	0.89	0.16	52,52,52,52	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	AA	3136	1/1	0.89	0.11	53,53,53,53	0
56	MG	BA	3504	1/1	0.89	0.17	58,58,58,58	0
56	MG	DA	3422	1/1	0.89	0.21	43,43,43,43	0
56	MG	DA	3423	1/1	0.89	0.14	51,51,51,51	0
56	MG	AA	3050	1/1	0.89	0.28	70,70,70,70	0
56	MG	BA	3408	1/1	0.89	0.12	55,55,55,55	0
56	MG	DA	3432	1/1	0.89	0.12	56,56,56,56	0
56	MG	BA	3635	1/1	0.89	0.17	62,62,62,62	0
56	MG	DA	3039	1/1	0.89	0.18	56,56,56,56	0
56	MG	B9	502	1/1	0.89	0.18	57,57,57,57	0
56	MG	BA	3275	1/1	0.89	0.11	46,46,46,46	0
56	MG	AA	3162	1/1	0.89	0.24	59,59,59,59	0
56	MG	DA	3453	1/1	0.89	0.12	45,45,45,45	0
56	MG	AA	3203	1/1	0.89	0.19	57,57,57,57	0
56	MG	CA	3025	1/1	0.89	0.21	61,61,61,61	0
56	MG	BA	3111	1/1	0.89	0.17	47,47,47,47	0
56	MG	AX	3006	1/1	0.89	0.20	74,74,74,74	0
56	MG	BA	3544	1/1	0.89	0.13	35,35,35,35	0
56	MG	DA	3487	1/1	0.89	0.22	65,65,65,65	0
56	MG	CA	3029	1/1	0.89	0.25	61,61,61,61	0
56	MG	DA	3110	1/1	0.89	0.10	50,50,50,50	0
56	MG	BA	3755	1/1	0.89	0.10	52,52,52,52	0
56	MG	AA	3165	1/1	0.89	0.16	60,60,60,60	0
56	MG	CA	3046	1/1	0.89	0.17	56,56,56,56	0
56	MG	DA	3509	1/1	0.89	0.09	53,53,53,53	0
56	MG	BA	3663	1/1	0.89	0.11	50,50,50,50	0
56	MG	BA	3761	1/1	0.89	0.14	54,54,54,54	0
56	MG	BA	3763	1/1	0.89	0.23	34,34,34,34	0
56	MG	BA	3313	1/1	0.89	0.12	46,46,46,46	0
56	MG	DA	3197	1/1	0.89	0.09	48,48,48,48	0
56	MG	AA	3205	1/1	0.89	0.08	51,51,51,51	0
56	MG	DA	3213	1/1	0.89	0.14	61,61,61,61	0
56	MG	DA	3238	1/1	0.89	0.21	61,61,61,61	0
56	MG	BA	3778	1/1	0.89	0.12	35,35,35,35	0
56	MG	BA	3170	1/1	0.89	0.12	48,48,48,48	0
56	MG	BA	3322	1/1	0.89	0.10	32,32,32,32	0
56	MG	DA	3248	1/1	0.89	0.15	33,33,33,33	0
56	MG	BA	3171	1/1	0.89	0.21	53,53,53,53	0
56	MG	DA	3284	1/1	0.89	0.13	40,40,40,40	0
56	MG	BA	3794	1/1	0.89	0.13	33,33,33,33	0
56	MG	DA	3293	1/1	0.89	0.13	60,60,60,60	0
56	MG	CA	3084	1/1	0.89	0.41	69,69,69,69	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	AA	3143	1/1	0.89	0.21	73,73,73,73	0
56	MG	BA	3802	1/1	0.89	0.15	56,56,56,56	0
56	MG	CA	3092	1/1	0.89	0.12	44,44,44,44	0
56	MG	AA	3096	1/1	0.89	0.24	48,48,48,48	0
56	MG	CA	3107	1/1	0.89	0.21	66,66,66,66	0
56	MG	DA	3320	1/1	0.89	0.09	40,40,40,40	0
56	MG	DA	3600	1/1	0.89	0.09	53,53,53,53	0
56	MG	BA	3828	1/1	0.89	0.12	37,37,37,37	0
56	MG	AA	3179	1/1	0.89	0.14	79,79,79,79	0
56	MG	CA	3120	1/1	0.89	0.13	64,64,64,64	0
56	MG	AA	3182	1/1	0.89	0.18	52,52,52,52	0
56	MG	BB	3001	1/1	0.89	0.20	50,50,50,50	0
56	MG	BA	3364	1/1	0.89	0.11	42,42,42,42	0
56	MG	DA	3620	1/1	0.89	0.16	62,62,62,62	0
56	MG	BB	3012	1/1	0.89	0.09	59,59,59,59	0
56	MG	DA	3633	1/1	0.89	0.14	61,61,61,61	0
56	MG	DA	3366	1/1	0.89	0.11	50,50,50,50	0
56	MG	DA	3639	1/1	0.89	0.11	64,64,64,64	0
56	MG	DA	3370	1/1	0.89	0.08	46,46,46,46	0
56	MG	DA	3380	1/1	0.89	0.09	55,55,55,55	0
56	MG	DA	3649	1/1	0.89	0.12	64,64,64,64	0
56	MG	DA	3672	1/1	0.89	0.13	52,52,52,52	0
56	MG	CA	3128	1/1	0.89	0.14	63,63,63,63	0
56	MG	AA	3032	1/1	0.89	0.25	75,75,75,75	0
56	MG	DB	3002	1/1	0.89	0.15	56,56,56,56	0
56	MG	DA	3395	1/1	0.89	0.10	42,42,42,42	0
56	MG	BA	3702	1/1	0.89	0.10	51,51,51,51	0
56	MG	CA	3143	1/1	0.89	0.19	62,62,62,62	0
56	MG	BA	3704	1/1	0.89	0.13	55,55,55,55	0
56	MG	DA	3402	1/1	0.89	0.26	65,65,65,65	0
56	MG	CA	3154	1/1	0.89	0.24	62,62,62,62	0
56	MG	BA	3067	1/1	0.89	0.18	49,49,49,49	0
56	MG	AA	3103	1/1	0.90	0.24	59,59,59,59	0
56	MG	DA	3403	1/1	0.90	0.17	57,57,57,57	0
56	MG	BA	3586	1/1	0.90	0.14	65,65,65,65	0
56	MG	BW	201	1/1	0.90	0.10	46,46,46,46	0
56	MG	BA	3116	1/1	0.90	0.07	29,29,29,29	0
56	MG	AX	3009	1/1	0.90	0.14	71,71,71,71	0
56	MG	BA	3451	1/1	0.90	0.09	64,64,64,64	0
56	MG	DA	3005	1/1	0.90	0.18	58,58,58,58	0
56	MG	AA	3140	1/1	0.90	0.12	71,71,71,71	0
56	MG	AA	3141	1/1	0.90	0.10	55,55,55,55	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	BA	3020	1/1	0.90	0.14	61,61,61,61	0
56	MG	BA	3193	1/1	0.90	0.20	57,57,57,57	0
56	MG	BA	3608	1/1	0.90	0.23	60,60,60,60	0
56	MG	CA	3016	1/1	0.90	0.11	61,61,61,61	0
56	MG	CA	3020	1/1	0.90	0.22	73,73,73,73	0
56	MG	BA	3477	1/1	0.90	0.10	55,55,55,55	0
56	MG	AA	3027	1/1	0.90	0.24	54,54,54,54	0
56	MG	BA	3481	1/1	0.90	0.13	45,45,45,45	0
56	MG	DA	3448	1/1	0.90	0.08	41,41,41,41	0
56	MG	DA	3098	1/1	0.90	0.11	43,43,43,43	0
56	MG	BA	3748	1/1	0.90	0.10	63,63,63,63	0
56	MG	DA	3103	1/1	0.90	0.14	50,50,50,50	0
56	MG	BA	3482	1/1	0.90	0.13	59,59,59,59	0
56	MG	AA	3116	1/1	0.90	0.14	61,61,61,61	0
56	MG	BA	3486	1/1	0.90	0.21	48,48,48,48	0
56	MG	AA	3218	1/1	0.90	0.23	53,53,53,53	0
56	MG	DA	3131	1/1	0.90	0.18	52,52,52,52	0
56	MG	DA	3135	1/1	0.90	0.13	50,50,50,50	0
56	MG	BA	3220	1/1	0.90	0.20	55,55,55,55	0
56	MG	DA	3497	1/1	0.90	0.38	51,51,51,51	0
56	MG	BA	3762	1/1	0.90	0.19	40,40,40,40	0
56	MG	BA	3371	1/1	0.90	0.12	54,54,54,54	0
56	MG	CA	3055	1/1	0.90	0.10	53,53,53,53	0
56	MG	BA	3768	1/1	0.90	0.10	56,56,56,56	0
56	MG	AA	3020	1/1	0.90	0.17	59,59,59,59	0
56	MG	BA	3044	1/1	0.90	0.20	49,49,49,49	0
56	MG	DA	3516	1/1	0.90	0.14	59,59,59,59	0
56	MG	DA	3201	1/1	0.90	0.26	52,52,52,52	0
56	MG	DA	3206	1/1	0.90	0.09	39,39,39,39	0
56	MG	AA	3022	1/1	0.90	0.15	55,55,55,55	0
56	MG	DA	3534	1/1	0.90	0.16	74,74,74,74	0
56	MG	CA	3068	1/1	0.90	0.28	55,55,55,55	0
56	MG	DA	3537	1/1	0.90	0.11	55,55,55,55	0
56	MG	BA	3658	1/1	0.90	0.13	45,45,45,45	0
56	MG	AA	3223	1/1	0.90	0.29	59,59,59,59	0
56	MG	AA	3127	1/1	0.90	0.10	48,48,48,48	0
56	MG	BA	3270	1/1	0.90	0.21	57,57,57,57	0
56	MG	DA	3250	1/1	0.90	0.15	61,61,61,61	0
56	MG	BA	3795	1/1	0.90	0.11	53,53,53,53	0
56	MG	DA	3557	1/1	0.90	0.10	34,34,34,34	0
56	MG	DA	3263	1/1	0.90	0.16	61,61,61,61	0
56	MG	DA	3272	1/1	0.90	0.10	44,44,44,44	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	DA	3282	1/1	0.90	0.09	42,42,42,42	0
56	MG	DA	3566	1/1	0.90	0.08	48,48,48,48	0
56	MG	BA	3274	1/1	0.90	0.15	49,49,49,49	0
56	MG	BA	3679	1/1	0.90	0.15	61,61,61,61	0
56	MG	DA	3579	1/1	0.90	0.09	55,55,55,55	0
56	MG	DA	3288	1/1	0.90	0.18	61,61,61,61	0
56	MG	CA	3102	1/1	0.90	0.13	54,54,54,54	0
56	MG	BA	3808	1/1	0.90	0.15	34,34,34,34	0
56	MG	AA	3130	1/1	0.90	0.08	43,43,43,43	0
56	MG	BA	3427	1/1	0.90	0.12	32,32,32,32	0
56	MG	DA	3591	1/1	0.90	0.09	56,56,56,56	0
56	MG	BA	3428	1/1	0.90	0.11	38,38,38,38	0
56	MG	DA	3597	1/1	0.90	0.08	51,51,51,51	0
56	MG	BA	3277	1/1	0.90	0.20	54,54,54,54	0
56	MG	DA	3317	1/1	0.90	0.11	55,55,55,55	0
56	MG	AW	3002	1/1	0.90	0.12	69,69,69,69	0
56	MG	BB	3004	1/1	0.90	0.10	47,47,47,47	0
56	MG	CA	3124	1/1	0.90	0.09	79,79,79,79	0
56	MG	BA	3102	1/1	0.90	0.22	54,54,54,54	0
56	MG	DA	3327	1/1	0.90	0.14	59,59,59,59	0
56	MG	BB	3009	1/1	0.90	0.22	58,58,58,58	0
56	MG	AA	3202	1/1	0.90	0.11	57,57,57,57	0
56	MG	DA	3628	1/1	0.90	0.09	56,56,56,56	0
56	MG	DA	3631	1/1	0.90	0.14	56,56,56,56	0
56	MG	DA	3349	1/1	0.90	0.08	44,44,44,44	0
56	MG	AX	3002	1/1	0.90	0.11	53,53,53,53	0
56	MG	DA	3635	1/1	0.90	0.11	52,52,52,52	0
56	MG	DA	3357	1/1	0.90	0.08	44,44,44,44	0
56	MG	CA	3136	1/1	0.90	0.17	65,65,65,65	0
56	MG	CA	3139	1/1	0.90	0.10	61,61,61,61	0
56	MG	BA	3700	1/1	0.90	0.14	54,54,54,54	0
56	MG	BA	3567	1/1	0.90	0.13	50,50,50,50	0
56	MG	DA	3650	1/1	0.90	0.12	44,44,44,44	0
56	MG	DA	3655	1/1	0.90	0.14	57,57,57,57	0
56	MG	DA	3657	1/1	0.90	0.16	67,67,67,67	0
56	MG	DA	3378	1/1	0.90	0.10	45,45,45,45	0
56	MG	CA	3147	1/1	0.90	0.18	72,72,72,72	0
56	MG	DA	3386	1/1	0.90	0.12	48,48,48,48	0
56	MG	CA	3150	1/1	0.90	0.21	62,62,62,62	0
56	MG	AA	3019	1/1	0.90	0.09	48,48,48,48	0
56	MG	AA	3102	1/1	0.90	0.19	51,51,51,51	0
56	MG	DA	3396	1/1	0.90	0.13	45,45,45,45	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	DA	3397	1/1	0.90	0.09	49,49,49,49	0
56	MG	DR	5001	1/1	0.90	0.12	58,58,58,58	0
56	MG	CA	3156	1/1	0.90	0.15	68,68,68,68	0
56	MG	BA	3583	1/1	0.90	0.09	45,45,45,45	0
56	MG	BQ	3005	1/1	0.90	0.18	50,50,50,50	0
56	MG	DA	3335	1/1	0.91	0.12	32,32,32,32	0
56	MG	DA	3338	1/1	0.91	0.07	40,40,40,40	0
56	MG	DA	3341	1/1	0.91	0.11	31,31,31,31	0
56	MG	BA	3634	1/1	0.91	0.11	64,64,64,64	0
56	MG	DA	3343	1/1	0.91	0.12	40,40,40,40	0
56	MG	AA	3079	1/1	0.91	0.14	47,47,47,47	0
56	MG	CA	3105	1/1	0.91	0.08	49,49,49,49	0
56	MG	BA	3363	1/1	0.91	0.12	50,50,50,50	0
56	MG	DA	3355	1/1	0.91	0.11	50,50,50,50	0
56	MG	AA	3101	1/1	0.91	0.11	54,54,54,54	0
56	MG	CA	3111	1/1	0.91	0.19	61,61,61,61	0
56	MG	BA	3365	1/1	0.91	0.11	49,49,49,49	0
56	MG	BA	3647	1/1	0.91	0.08	45,45,45,45	0
56	MG	BA	3798	1/1	0.91	0.12	61,61,61,61	0
56	MG	BA	3799	1/1	0.91	0.14	47,47,47,47	0
56	MG	AA	3188	1/1	0.91	0.13	56,56,56,56	0
56	MG	DA	3385	1/1	0.91	0.14	55,55,55,55	0
56	MG	BA	3804	1/1	0.91	0.09	58,58,58,58	0
56	MG	AA	3080	1/1	0.91	0.09	47,47,47,47	0
56	MG	BA	3818	1/1	0.91	0.13	32,32,32,32	0
56	MG	BA	3060	1/1	0.91	0.11	56,56,56,56	0
56	MG	BA	3229	1/1	0.91	0.20	51,51,51,51	0
56	MG	CA	3137	1/1	0.91	0.11	52,52,52,52	0
56	MG	BA	3508	1/1	0.91	0.08	54,54,54,54	0
56	MG	BA	3382	1/1	0.91	0.09	55,55,55,55	0
56	MG	BA	3670	1/1	0.91	0.10	47,47,47,47	0
56	MG	BA	3512	1/1	0.91	0.11	27,27,27,27	0
56	MG	CA	3148	1/1	0.91	0.17	67,67,67,67	0
56	MG	BA	3233	1/1	0.91	0.18	48,48,48,48	0
56	MG	BA	3678	1/1	0.91	0.09	58,58,58,58	0
56	MG	BB	3011	1/1	0.91	0.08	59,59,59,59	0
56	MG	BA	3519	1/1	0.91	0.08	44,44,44,44	0
56	MG	DA	3412	1/1	0.91	0.17	63,63,63,63	0
56	MG	BA	3520	1/1	0.91	0.23	47,47,47,47	0
56	MG	DA	3418	1/1	0.91	0.11	37,37,37,37	0
56	MG	CA	3160	1/1	0.91	0.25	65,65,65,65	0
56	MG	CA	3162	1/1	0.91	0.23	67,67,67,67	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	BA	3237	1/1	0.91	0.14	36,36,36,36	0
56	MG	BA	3524	1/1	0.91	0.16	53,53,53,53	0
56	MG	CA	3171	1/1	0.91	0.19	63,63,63,63	0
56	MG	CA	3172	1/1	0.91	0.19	64,64,64,64	0
56	MG	CA	3173	1/1	0.91	0.19	69,69,69,69	0
56	MG	BE	304	1/1	0.91	0.20	40,40,40,40	0
56	MG	CE	201	1/1	0.91	0.19	50,50,50,50	0
56	MG	AA	3228	1/1	0.91	0.13	68,68,68,68	0
56	MG	CV	3001	1/1	0.91	0.18	58,58,58,58	0
56	MG	DA	3442	1/1	0.91	0.12	44,44,44,44	0
56	MG	DA	3445	1/1	0.91	0.11	72,72,72,72	0
56	MG	DA	3446	1/1	0.91	0.20	47,47,47,47	0
56	MG	BA	3686	1/1	0.91	0.12	30,30,30,30	0
56	MG	BF	305	1/1	0.91	0.14	47,47,47,47	0
56	MG	BA	3688	1/1	0.91	0.12	45,45,45,45	0
56	MG	AA	3229	1/1	0.91	0.30	62,62,62,62	0
56	MG	DA	3010	1/1	0.91	0.08	43,43,43,43	0
56	MG	DA	3456	1/1	0.91	0.19	49,49,49,49	0
56	MG	BA	3690	1/1	0.91	0.14	63,63,63,63	0
56	MG	BA	3532	1/1	0.91	0.20	49,49,49,49	0
56	MG	DA	3029	1/1	0.91	0.09	51,51,51,51	0
56	MG	AK	201	1/1	0.91	0.13	61,61,61,61	0
56	MG	DA	3477	1/1	0.91	0.10	55,55,55,55	0
56	MG	DA	3040	1/1	0.91	0.14	53,53,53,53	0
56	MG	BA	3268	1/1	0.91	0.27	58,58,58,58	0
56	MG	DA	3043	1/1	0.91	0.15	48,48,48,48	0
56	MG	DA	3044	1/1	0.91	0.11	58,58,58,58	0
56	MG	BA	3543	1/1	0.91	0.11	26,26,26,26	0
56	MG	DA	3063	1/1	0.91	0.19	46,46,46,46	0
56	MG	AA	3004	1/1	0.91	0.13	67,67,67,67	0
56	MG	B4	502	1/1	0.91	0.23	72,72,72,72	0
56	MG	DA	3512	1/1	0.91	0.12	46,46,46,46	0
56	MG	BA	3424	1/1	0.91	0.14	24,24,24,24	0
56	MG	BA	3273	1/1	0.91	0.20	53,53,53,53	0
56	MG	CA	3001	1/1	0.91	0.23	73,73,73,73	0
56	MG	DA	3081	1/1	0.91	0.13	45,45,45,45	0
56	MG	BA	3705	1/1	0.91	0.12	54,54,54,54	0
56	MG	DA	3099	1/1	0.91	0.09	60,60,60,60	0
56	MG	DA	3535	1/1	0.91	0.12	54,54,54,54	0
56	MG	DA	3101	1/1	0.91	0.11	53,53,53,53	0
56	MG	AV	101	1/1	0.91	0.17	59,59,59,59	0
56	MG	CA	3010	1/1	0.91	0.14	53,53,53,53	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	BA	3557	1/1	0.91	0.16	56,56,56,56	0
56	MG	DA	3109	1/1	0.91	0.22	66,66,66,66	0
56	MG	CA	3015	1/1	0.91	0.16	58,58,58,58	0
56	MG	DA	3548	1/1	0.91	0.20	65,65,65,65	0
56	MG	AA	3025	1/1	0.91	0.16	43,43,43,43	0
56	MG	BA	3714	1/1	0.91	0.09	47,47,47,47	0
56	MG	CA	3023	1/1	0.91	0.29	55,55,55,55	0
56	MG	DA	3560	1/1	0.91	0.12	34,34,34,34	0
56	MG	CA	3024	1/1	0.91	0.19	63,63,63,63	0
56	MG	BA	3430	1/1	0.91	0.11	32,32,32,32	0
56	MG	DA	3153	1/1	0.91	0.12	44,44,44,44	0
56	MG	AA	3085	1/1	0.91	0.15	55,55,55,55	0
56	MG	BA	3432	1/1	0.91	0.16	52,52,52,52	0
56	MG	DA	3169	1/1	0.91	0.17	49,49,49,49	0
56	MG	DA	3575	1/1	0.91	0.07	47,47,47,47	0
56	MG	DA	3178	1/1	0.91	0.09	54,54,54,54	0
56	MG	DA	3181	1/1	0.91	0.14	45,45,45,45	0
56	MG	AA	3088	1/1	0.91	0.22	56,56,56,56	0
56	MG	DA	3582	1/1	0.91	0.08	39,39,39,39	0
56	MG	BA	3112	1/1	0.91	0.08	57,57,57,57	0
56	MG	DA	3186	1/1	0.91	0.10	40,40,40,40	0
56	MG	DA	3588	1/1	0.91	0.12	39,39,39,39	0
56	MG	DA	3195	1/1	0.91	0.11	57,57,57,57	0
56	MG	CA	3032	1/1	0.91	0.21	52,52,52,52	0
56	MG	CA	3033	1/1	0.91	0.18	56,56,56,56	0
56	MG	BA	3436	1/1	0.91	0.08	46,46,46,46	0
56	MG	AA	3091	1/1	0.91	0.26	70,70,70,70	0
56	MG	DA	3207	1/1	0.91	0.16	57,57,57,57	0
56	MG	CA	3037	1/1	0.91	0.19	55,55,55,55	0
56	MG	DA	3220	1/1	0.91	0.10	46,46,46,46	0
56	MG	DA	3223	1/1	0.91	0.15	54,54,54,54	0
56	MG	DA	3229	1/1	0.91	0.07	55,55,55,55	0
56	MG	DA	3611	1/1	0.91	0.14	55,55,55,55	0
56	MG	BA	3292	1/1	0.91	0.07	42,42,42,42	0
56	MG	CA	3049	1/1	0.91	0.16	68,68,68,68	0
56	MG	AA	3044	1/1	0.91	0.35	71,71,71,71	0
56	MG	BA	3309	1/1	0.91	0.09	55,55,55,55	0
56	MG	DA	3247	1/1	0.91	0.27	57,57,57,57	0
56	MG	AA	3034	1/1	0.91	0.22	48,48,48,48	0
56	MG	AA	3207	1/1	0.91	0.13	68,68,68,68	0
56	MG	BA	3604	1/1	0.91	0.17	72,72,72,72	0
56	MG	CA	3058	1/1	0.91	0.20	70,70,70,70	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	BA	3158	1/1	0.91	0.25	44,44,44,44	0
56	MG	DA	3277	1/1	0.91	0.18	56,56,56,56	0
56	MG	DA	3643	1/1	0.91	0.13	60,60,60,60	0
56	MG	DA	3278	1/1	0.91	0.16	53,53,53,53	0
56	MG	BA	3317	1/1	0.91	0.12	64,64,64,64	0
56	MG	CA	3061	1/1	0.91	0.26	56,56,56,56	0
56	MG	CA	3063	1/1	0.91	0.13	59,59,59,59	0
56	MG	CA	3064	1/1	0.91	0.14	57,57,57,57	0
56	MG	DA	3667	1/1	0.91	0.34	73,73,73,73	0
56	MG	AA	3011	1/1	0.91	0.07	64,64,64,64	0
56	MG	BA	3612	1/1	0.91	0.13	62,62,62,62	0
56	MG	AA	3076	1/1	0.91	0.20	55,55,55,55	0
56	MG	AA	3212	1/1	0.91	0.16	59,59,59,59	0
56	MG	DB	3003	1/1	0.91	0.20	68,68,68,68	0
56	MG	BA	3619	1/1	0.91	0.16	51,51,51,51	0
56	MG	AA	3099	1/1	0.91	0.34	63,63,63,63	0
56	MG	BA	3770	1/1	0.91	0.16	37,37,37,37	0
56	MG	DE	301	1/1	0.91	0.25	45,45,45,45	0
56	MG	DE	304	1/1	0.91	0.12	47,47,47,47	0
56	MG	CA	3086	1/1	0.91	0.22	61,61,61,61	0
56	MG	DG	3001	1/1	0.91	0.11	56,56,56,56	0
56	MG	BA	3022	1/1	0.91	0.09	40,40,40,40	0
56	MG	DW	3002	1/1	0.91	0.21	65,65,65,65	0
56	MG	DW	3003	1/1	0.91	0.14	47,47,47,47	0
56	MG	AA	3181	1/1	0.91	0.13	75,75,75,75	0
56	MG	CA	3094	1/1	0.91	0.22	72,72,72,72	0
56	MG	CA	3101	1/1	0.91	0.17	54,54,54,54	0
56	MG	CA	3022	1/1	0.92	0.11	53,53,53,53	0
56	MG	BA	3747	1/1	0.92	0.10	42,42,42,42	0
56	MG	DA	3012	1/1	0.92	0.09	39,39,39,39	0
56	MG	BA	3192	1/1	0.92	0.11	48,48,48,48	0
56	MG	DA	3020	1/1	0.92	0.13	50,50,50,50	0
56	MG	DA	3027	1/1	0.92	0.15	53,53,53,53	0
56	MG	BA	3752	1/1	0.92	0.09	19,19,19,19	0
56	MG	BA	3005	1/1	0.92	0.17	51,51,51,51	0
56	MG	DA	3034	1/1	0.92	0.14	43,43,43,43	0
56	MG	DA	3037	1/1	0.92	0.08	54,54,54,54	0
56	MG	BA	3197	1/1	0.92	0.12	36,36,36,36	0
56	MG	BA	3757	1/1	0.92	0.07	25,25,25,25	0
56	MG	BA	3630	1/1	0.92	0.09	30,30,30,30	0
56	MG	DA	3406	1/1	0.92	0.08	40,40,40,40	0
56	MG	BA	3359	1/1	0.92	0.08	46,46,46,46	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	BA	3360	1/1	0.92	0.09	50,50,50,50	0
56	MG	DA	3411	1/1	0.92	0.13	46,46,46,46	0
56	MG	DA	3046	1/1	0.92	0.36	57,57,57,57	0
56	MG	DA	3047	1/1	0.92	0.17	49,49,49,49	0
56	MG	BA	3007	1/1	0.92	0.10	51,51,51,51	0
56	MG	DA	3056	1/1	0.92	0.16	44,44,44,44	0
56	MG	BA	3636	1/1	0.92	0.10	53,53,53,53	0
56	MG	BA	3765	1/1	0.92	0.11	33,33,33,33	0
56	MG	CA	3044	1/1	0.92	0.22	55,55,55,55	0
56	MG	AA	3167	1/1	0.92	0.20	47,47,47,47	0
56	MG	DA	3068	1/1	0.92	0.10	58,58,58,58	0
56	MG	DA	3426	1/1	0.92	0.10	41,41,41,41	0
56	MG	BA	3203	1/1	0.92	0.09	39,39,39,39	0
56	MG	DA	3078	1/1	0.92	0.07	45,45,45,45	0
56	MG	AA	3169	1/1	0.92	0.12	64,64,64,64	0
56	MG	BA	3645	1/1	0.92	0.12	32,32,32,32	0
56	MG	DA	3087	1/1	0.92	0.17	49,49,49,49	0
56	MG	DA	3093	1/1	0.92	0.13	57,57,57,57	0
56	MG	DA	3096	1/1	0.92	0.11	51,51,51,51	0
56	MG	BA	3775	1/1	0.92	0.09	43,43,43,43	0
56	MG	BA	3369	1/1	0.92	0.11	55,55,55,55	0
56	MG	DA	3449	1/1	0.92	0.12	47,47,47,47	0
56	MG	BA	3648	1/1	0.92	0.17	53,53,53,53	0
56	MG	CA	3057	1/1	0.92	0.29	58,58,58,58	0
56	MG	BA	3781	1/1	0.92	0.15	52,52,52,52	0
56	MG	AA	3055	1/1	0.92	0.26	58,58,58,58	0
56	MG	DA	3106	1/1	0.92	0.28	61,61,61,61	0
56	MG	BA	3510	1/1	0.92	0.08	48,48,48,48	0
56	MG	AA	3057	1/1	0.92	0.21	61,61,61,61	0
56	MG	DA	3463	1/1	0.92	0.12	37,37,37,37	0
56	MG	BA	3656	1/1	0.92	0.12	45,45,45,45	0
56	MG	DA	3118	1/1	0.92	0.20	52,52,52,52	0
56	MG	DA	3469	1/1	0.92	0.12	54,54,54,54	0
56	MG	AA	3002	1/1	0.92	0.10	62,62,62,62	0
56	MG	BA	3227	1/1	0.92	0.10	57,57,57,57	0
56	MG	DA	3132	1/1	0.92	0.19	41,41,41,41	0
56	MG	BA	3385	1/1	0.92	0.10	39,39,39,39	0
56	MG	DA	3138	1/1	0.92	0.26	59,59,59,59	0
56	MG	DA	3143	1/1	0.92	0.20	50,50,50,50	0
56	MG	BA	3666	1/1	0.92	0.16	58,58,58,58	0
56	MG	DA	3145	1/1	0.92	0.31	49,49,49,49	0
56	MG	AA	3030	1/1	0.92	0.12	57,57,57,57	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	DA	3511	1/1	0.92	0.10	45,45,45,45	0
56	MG	CA	3076	1/1	0.92	0.20	56,56,56,56	0
56	MG	BA	3807	1/1	0.92	0.10	67,67,67,67	0
56	MG	DA	3515	1/1	0.92	0.11	57,57,57,57	0
56	MG	AA	3014	1/1	0.92	0.08	69,69,69,69	0
56	MG	BA	3812	1/1	0.92	0.09	52,52,52,52	0
56	MG	AA	3005	1/1	0.92	0.10	53,53,53,53	0
56	MG	DA	3523	1/1	0.92	0.10	57,57,57,57	0
56	MG	BA	3525	1/1	0.92	0.11	52,52,52,52	0
56	MG	DA	3533	1/1	0.92	0.21	53,53,53,53	0
56	MG	BA	3403	1/1	0.92	0.14	31,31,31,31	0
56	MG	DA	3185	1/1	0.92	0.23	54,54,54,54	0
56	MG	BA	3066	1/1	0.92	0.21	51,51,51,51	0
56	MG	DA	3188	1/1	0.92	0.19	50,50,50,50	0
56	MG	DA	3190	1/1	0.92	0.08	45,45,45,45	0
56	MG	DA	3191	1/1	0.92	0.08	44,44,44,44	0
56	MG	CA	3097	1/1	0.92	0.19	57,57,57,57	0
56	MG	DA	3545	1/1	0.92	0.09	37,37,37,37	0
56	MG	CA	3100	1/1	0.92	0.11	62,62,62,62	0
56	MG	AA	3187	1/1	0.92	0.12	62,62,62,62	0
56	MG	BA	3070	1/1	0.92	0.19	55,55,55,55	0
56	MG	DA	3204	1/1	0.92	0.12	51,51,51,51	0
56	MG	BA	3262	1/1	0.92	0.15	47,47,47,47	0
56	MG	AA	3230	1/1	0.92	0.18	68,68,68,68	0
56	MG	DA	3561	1/1	0.92	0.08	48,48,48,48	0
56	MG	DA	3211	1/1	0.92	0.09	48,48,48,48	0
56	MG	AA	3110	1/1	0.92	0.21	61,61,61,61	0
56	MG	DA	3216	1/1	0.92	0.16	46,46,46,46	0
56	MG	AA	3112	1/1	0.92	0.10	57,57,57,57	0
56	MG	CA	3110	1/1	0.92	0.11	48,48,48,48	0
56	MG	DA	3226	1/1	0.92	0.16	54,54,54,54	0
56	MG	DA	3574	1/1	0.92	0.09	51,51,51,51	0
56	MG	BA	3096	1/1	0.92	0.08	41,41,41,41	0
56	MG	DA	3235	1/1	0.92	0.24	61,61,61,61	0
56	MG	BA	3099	1/1	0.92	0.16	50,50,50,50	0
56	MG	AA	3148	1/1	0.92	0.20	63,63,63,63	0
56	MG	AA	3113	1/1	0.92	0.13	59,59,59,59	0
56	MG	BD	305	1/1	0.92	0.10	37,37,37,37	0
56	MG	CA	3123	1/1	0.92	0.14	80,80,80,80	0
56	MG	DA	3587	1/1	0.92	0.08	61,61,61,61	0
56	MG	BA	3284	1/1	0.92	0.23	51,51,51,51	0
56	MG	AA	3195	1/1	0.92	0.14	59,59,59,59	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	DA	3251	1/1	0.92	0.09	51,51,51,51	0
56	MG	DA	3594	1/1	0.92	0.07	44,44,44,44	0
56	MG	DA	3595	1/1	0.92	0.12	61,61,61,61	0
56	MG	AA	3071	1/1	0.92	0.32	62,62,62,62	0
56	MG	BA	3576	1/1	0.92	0.12	48,48,48,48	0
56	MG	CA	3132	1/1	0.92	0.21	70,70,70,70	0
56	MG	BF	306	1/1	0.92	0.16	40,40,40,40	0
56	MG	DA	3601	1/1	0.92	0.13	54,54,54,54	0
56	MG	CA	3134	1/1	0.92	0.23	70,70,70,70	0
56	MG	DA	3279	1/1	0.92	0.08	48,48,48,48	0
56	MG	DA	3280	1/1	0.92	0.07	43,43,43,43	0
56	MG	DA	3609	1/1	0.92	0.10	60,60,60,60	0
56	MG	BF	311	1/1	0.92	0.08	43,43,43,43	0
56	MG	AA	3010	1/1	0.92	0.20	59,59,59,59	0
56	MG	DA	3612	1/1	0.92	0.14	56,56,56,56	0
56	MG	AA	3121	1/1	0.92	0.17	66,66,66,66	0
56	MG	DA	3287	1/1	0.92	0.13	47,47,47,47	0
56	MG	DA	3618	1/1	0.92	0.14	54,54,54,54	0
56	MG	AX	3004	1/1	0.92	0.23	70,70,70,70	0
56	MG	CA	3141	1/1	0.92	0.18	49,49,49,49	0
56	MG	AA	3158	1/1	0.92	0.14	59,59,59,59	0
56	MG	CA	3145	1/1	0.92	0.13	63,63,63,63	0
56	MG	DA	3302	1/1	0.92	0.07	33,33,33,33	0
56	MG	CA	3146	1/1	0.92	0.10	69,69,69,69	0
56	MG	AA	3159	1/1	0.92	0.09	59,59,59,59	0
56	MG	BA	3447	1/1	0.92	0.14	26,26,26,26	0
56	MG	CA	3149	1/1	0.92	0.17	65,65,65,65	0
56	MG	BA	3133	1/1	0.92	0.22	47,47,47,47	0
56	MG	B0	101	1/1	0.92	0.11	39,39,39,39	0
56	MG	DA	3648	1/1	0.92	0.18	60,60,60,60	0
56	MG	AA	3047	1/1	0.92	0.08	47,47,47,47	0
56	MG	DA	3324	1/1	0.92	0.11	39,39,39,39	0
56	MG	DA	3653	1/1	0.92	0.18	58,58,58,58	0
56	MG	BA	3724	1/1	0.92	0.16	44,44,44,44	0
56	MG	B5	105	1/1	0.92	0.07	49,49,49,49	0
56	MG	DA	3658	1/1	0.92	0.08	37,37,37,37	0
56	MG	DA	3663	1/1	0.92	0.19	60,60,60,60	0
56	MG	B6	101	1/1	0.92	0.12	48,48,48,48	0
56	MG	CA	3161	1/1	0.92	0.15	70,70,70,70	0
56	MG	BA	3452	1/1	0.92	0.12	27,27,27,27	0
56	MG	AA	3037	1/1	0.92	0.12	44,44,44,44	0
56	MG	CA	3165	1/1	0.92	0.13	56,56,56,56	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	BA	3727	1/1	0.92	0.14	39,39,39,39	0
56	MG	BA	3459	1/1	0.92	0.13	48,48,48,48	0
56	MG	AA	3166	1/1	0.92	0.08	65,65,65,65	0
56	MG	BA	3467	1/1	0.92	0.15	39,39,39,39	0
56	MG	DB	3010	1/1	0.92	0.11	55,55,55,55	0
56	MG	CA	3011	1/1	0.92	0.16	63,63,63,63	0
56	MG	DE	303	1/1	0.92	0.14	44,44,44,44	0
56	MG	BA	3328	1/1	0.92	0.12	60,60,60,60	0
56	MG	CA	3013	1/1	0.92	0.16	63,63,63,63	0
56	MG	BA	3742	1/1	0.92	0.08	51,51,51,51	0
56	MG	DA	3367	1/1	0.92	0.08	51,51,51,51	0
56	MG	DV	3002	1/1	0.92	0.26	57,57,57,57	0
56	MG	AY	3003	1/1	0.92	0.08	48,48,48,48	0
56	MG	DA	3377	1/1	0.92	0.07	42,42,42,42	0
56	MG	CX	3004	1/1	0.92	0.16	54,54,54,54	0
57	PCY	AA	3231	40/40	0.92	0.13	45,69,81,87	0
56	MG	CA	3019	1/1	0.92	0.22	58,58,58,58	0
56	MG	BA	3002	1/1	0.92	0.18	62,62,62,62	0
56	MG	BA	3783	1/1	0.93	0.13	53,53,53,53	0
56	MG	BA	3198	1/1	0.93	0.18	55,55,55,55	0
56	MG	BA	3352	1/1	0.93	0.09	29,29,29,29	0
56	MG	BA	3641	1/1	0.93	0.10	49,49,49,49	0
56	MG	BA	3643	1/1	0.93	0.07	30,30,30,30	0
56	MG	BA	3796	1/1	0.93	0.09	40,40,40,40	0
56	MG	DA	3086	1/1	0.93	0.14	62,62,62,62	0
56	MG	CA	3066	1/1	0.93	0.20	66,66,66,66	0
56	MG	DA	3091	1/1	0.93	0.10	43,43,43,43	0
56	MG	DA	3092	1/1	0.93	0.14	48,48,48,48	0
56	MG	DA	3413	1/1	0.93	0.14	36,36,36,36	0
56	MG	BA	3354	1/1	0.93	0.11	31,31,31,31	0
56	MG	DA	3416	1/1	0.93	0.15	40,40,40,40	0
56	MG	AA	3168	1/1	0.93	0.09	62,62,62,62	0
56	MG	DA	3097	1/1	0.93	0.18	43,43,43,43	0
56	MG	BA	3057	1/1	0.93	0.20	53,53,53,53	0
56	MG	AA	3072	1/1	0.93	0.20	68,68,68,68	0
56	MG	CA	3073	1/1	0.93	0.13	48,48,48,48	0
56	MG	BA	3064	1/1	0.93	0.29	61,61,61,61	0
56	MG	CA	3079	1/1	0.93	0.24	54,54,54,54	0
56	MG	BA	3806	1/1	0.93	0.14	51,51,51,51	0
56	MG	BA	3218	1/1	0.93	0.10	44,44,44,44	0
56	MG	DA	3429	1/1	0.93	0.10	40,40,40,40	0
56	MG	BA	3655	1/1	0.93	0.12	50,50,50,50	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	BA	3810	1/1	0.93	0.17	50,50,50,50	0
56	MG	CA	3088	1/1	0.93	0.29	53,53,53,53	0
56	MG	BA	3811	1/1	0.93	0.27	38,38,38,38	0
56	MG	DA	3119	1/1	0.93	0.30	62,62,62,62	0
56	MG	AA	3170	1/1	0.93	0.14	57,57,57,57	0
56	MG	BA	3493	1/1	0.93	0.07	46,46,46,46	0
56	MG	CA	3095	1/1	0.93	0.15	61,61,61,61	0
56	MG	BA	3820	1/1	0.93	0.11	45,45,45,45	0
56	MG	AW	3003	1/1	0.93	0.30	59,59,59,59	0
56	MG	DA	3142	1/1	0.93	0.10	45,45,45,45	0
56	MG	AW	3004	1/1	0.93	0.07	51,51,51,51	0
56	MG	BA	3366	1/1	0.93	0.09	45,45,45,45	0
56	MG	BA	3833	1/1	0.93	0.08	43,43,43,43	0
56	MG	DA	3150	1/1	0.93	0.08	41,41,41,41	0
56	MG	DA	3458	1/1	0.93	0.09	42,42,42,42	0
56	MG	AA	3172	1/1	0.93	0.09	47,47,47,47	0
56	MG	DA	3154	1/1	0.93	0.22	52,52,52,52	0
56	MG	BA	3228	1/1	0.93	0.11	50,50,50,50	0
56	MG	DA	3159	1/1	0.93	0.08	41,41,41,41	0
56	MG	AA	3086	1/1	0.93	0.18	52,52,52,52	0
56	MG	DA	3474	1/1	0.93	0.08	53,53,53,53	0
56	MG	BA	3230	1/1	0.93	0.13	62,62,62,62	0
56	MG	DA	3485	1/1	0.93	0.08	44,44,44,44	0
56	MG	DA	3486	1/1	0.93	0.13	44,44,44,44	0
56	MG	BA	3374	1/1	0.93	0.06	37,37,37,37	0
56	MG	BA	3093	1/1	0.93	0.11	38,38,38,38	0
56	MG	CA	3114	1/1	0.93	0.17	56,56,56,56	0
56	MG	DA	3499	1/1	0.93	0.16	60,60,60,60	0
56	MG	BA	3522	1/1	0.93	0.15	36,36,36,36	0
56	MG	DA	3502	1/1	0.93	0.11	64,64,64,64	0
56	MG	BB	3014	1/1	0.93	0.17	69,69,69,69	0
56	MG	BA	3377	1/1	0.93	0.07	30,30,30,30	0
56	MG	DA	3507	1/1	0.93	0.16	60,60,60,60	0
56	MG	DA	3187	1/1	0.93	0.12	56,56,56,56	0
56	MG	BB	3019	1/1	0.93	0.10	49,49,49,49	0
56	MG	DA	3510	1/1	0.93	0.10	50,50,50,50	0
56	MG	BA	3235	1/1	0.93	0.13	37,37,37,37	0
56	MG	BB	3021	1/1	0.93	0.13	54,54,54,54	0
56	MG	DA	3192	1/1	0.93	0.15	51,51,51,51	0
56	MG	AA	3175	1/1	0.93	0.11	54,54,54,54	0
56	MG	DA	3196	1/1	0.93	0.10	53,53,53,53	0
56	MG	CA	3127	1/1	0.93	0.15	44,44,44,44	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	BA	3390	1/1	0.93	0.16	52,52,52,52	0
56	MG	DA	3200	1/1	0.93	0.19	43,43,43,43	0
56	MG	DA	3527	1/1	0.93	0.18	53,53,53,53	0
56	MG	BA	3530	1/1	0.93	0.09	51,51,51,51	0
56	MG	DA	3531	1/1	0.93	0.10	54,54,54,54	0
56	MG	AA	3149	1/1	0.93	0.06	41,41,41,41	0
56	MG	BA	3244	1/1	0.93	0.10	63,63,63,63	0
56	MG	BA	3396	1/1	0.93	0.18	55,55,55,55	0
56	MG	BA	3535	1/1	0.93	0.08	18,18,18,18	0
56	MG	BA	3397	1/1	0.93	0.15	53,53,53,53	0
56	MG	BN	3001	1/1	0.93	0.20	51,51,51,51	0
56	MG	DA	3217	1/1	0.93	0.17	50,50,50,50	0
56	MG	DA	3218	1/1	0.93	0.13	47,47,47,47	0
56	MG	BA	3541	1/1	0.93	0.07	29,29,29,29	0
56	MG	AA	3051	1/1	0.93	0.22	62,62,62,62	0
56	MG	DA	3224	1/1	0.93	0.21	48,48,48,48	0
56	MG	CA	3144	1/1	0.93	0.14	59,59,59,59	0
56	MG	BA	3252	1/1	0.93	0.08	45,45,45,45	0
56	MG	AA	3211	1/1	0.93	0.13	59,59,59,59	0
56	MG	DA	3558	1/1	0.93	0.12	34,34,34,34	0
56	MG	BA	3256	1/1	0.93	0.11	49,49,49,49	0
56	MG	DA	3239	1/1	0.93	0.12	54,54,54,54	0
56	MG	DA	3240	1/1	0.93	0.12	51,51,51,51	0
56	MG	BA	3260	1/1	0.93	0.32	57,57,57,57	0
56	MG	BA	3711	1/1	0.93	0.09	45,45,45,45	0
56	MG	AA	3180	1/1	0.93	0.09	57,57,57,57	0
56	MG	BA	3558	1/1	0.93	0.08	29,29,29,29	0
56	MG	CA	3152	1/1	0.93	0.16	79,79,79,79	0
56	MG	DA	3573	1/1	0.93	0.12	46,46,46,46	0
56	MG	B3	101	1/1	0.93	0.15	48,48,48,48	0
56	MG	CA	3155	1/1	0.93	0.14	50,50,50,50	0
56	MG	DA	3256	1/1	0.93	0.09	47,47,47,47	0
56	MG	BA	3715	1/1	0.93	0.10	53,53,53,53	0
56	MG	DA	3262	1/1	0.93	0.07	43,43,43,43	0
56	MG	CA	3157	1/1	0.93	0.27	64,64,64,64	0
56	MG	DA	3268	1/1	0.93	0.10	60,60,60,60	0
56	MG	DA	3271	1/1	0.93	0.08	47,47,47,47	0
56	MG	BA	3559	1/1	0.93	0.08	30,30,30,30	0
56	MG	DA	3276	1/1	0.93	0.07	33,33,33,33	0
56	MG	BA	3414	1/1	0.93	0.08	29,29,29,29	0
56	MG	DA	3590	1/1	0.93	0.13	60,60,60,60	0
56	MG	B7	102	1/1	0.93	0.13	58,58,58,58	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	AA	3066	1/1	0.93	0.07	44,44,44,44	0
56	MG	AX	3011	1/1	0.93	0.12	50,50,50,50	0
56	MG	AA	3106	1/1	0.93	0.20	51,51,51,51	0
56	MG	CA	3167	1/1	0.93	0.09	48,48,48,48	0
56	MG	CA	3168	1/1	0.93	0.11	72,72,72,72	0
56	MG	BA	3575	1/1	0.93	0.09	64,64,64,64	0
56	MG	AA	3018	1/1	0.93	0.06	51,51,51,51	0
56	MG	AA	3185	1/1	0.93	0.23	53,53,53,53	0
56	MG	BA	3578	1/1	0.93	0.14	47,47,47,47	0
56	MG	DA	3298	1/1	0.93	0.05	33,33,33,33	0
56	MG	BA	3004	1/1	0.93	0.10	36,36,36,36	0
56	MG	BA	3739	1/1	0.93	0.14	46,46,46,46	0
56	MG	AA	3028	1/1	0.93	0.23	56,56,56,56	0
56	MG	DA	3305	1/1	0.93	0.06	28,28,28,28	0
56	MG	DA	3306	1/1	0.93	0.08	42,42,42,42	0
56	MG	DA	3309	1/1	0.93	0.07	42,42,42,42	0
56	MG	DA	3616	1/1	0.93	0.07	45,45,45,45	0
56	MG	DA	3617	1/1	0.93	0.11	53,53,53,53	0
56	MG	BA	3130	1/1	0.93	0.09	48,48,48,48	0
56	MG	DA	3619	1/1	0.93	0.10	58,58,58,58	0
56	MG	BA	3434	1/1	0.93	0.07	34,34,34,34	0
56	MG	DA	3627	1/1	0.93	0.07	48,48,48,48	0
56	MG	BA	3289	1/1	0.93	0.18	55,55,55,55	0
56	MG	AA	3111	1/1	0.93	0.20	52,52,52,52	0
56	MG	DA	3001	1/1	0.93	0.11	58,58,58,58	0
56	MG	BA	3136	1/1	0.93	0.14	58,58,58,58	0
56	MG	BA	3017	1/1	0.93	0.09	50,50,50,50	0
56	MG	DA	3006	1/1	0.93	0.10	43,43,43,43	0
56	MG	DA	3007	1/1	0.93	0.13	54,54,54,54	0
56	MG	DA	3332	1/1	0.93	0.09	41,41,41,41	0
56	MG	DA	3333	1/1	0.93	0.08	50,50,50,50	0
56	MG	BA	3167	1/1	0.93	0.11	50,50,50,50	0
56	MG	DA	3646	1/1	0.93	0.10	49,49,49,49	0
56	MG	AA	3189	1/1	0.93	0.13	59,59,59,59	0
56	MG	BA	3756	1/1	0.93	0.10	27,27,27,27	0
56	MG	DA	3019	1/1	0.93	0.13	57,57,57,57	0
56	MG	BA	3444	1/1	0.93	0.10	48,48,48,48	0
56	MG	BA	3021	1/1	0.93	0.15	60,60,60,60	0
56	MG	BA	3176	1/1	0.93	0.21	55,55,55,55	0
56	MG	AA	3081	1/1	0.93	0.25	58,58,58,58	0
56	MG	AA	3058	1/1	0.93	0.26	57,57,57,57	0
56	MG	DA	3665	1/1	0.93	0.13	58,58,58,58	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	DA	3666	1/1	0.93	0.27	41,41,41,41	0
56	MG	BA	3190	1/1	0.93	0.17	45,45,45,45	0
56	MG	BA	3620	1/1	0.93	0.08	47,47,47,47	0
56	MG	DA	3361	1/1	0.93	0.21	55,55,55,55	0
56	MG	CA	3043	1/1	0.93	0.19	54,54,54,54	0
56	MG	AE	3001	1/1	0.93	0.07	66,66,66,66	0
56	MG	CA	3045	1/1	0.93	0.27	58,58,58,58	0
56	MG	DB	3004	1/1	0.93	0.11	51,51,51,51	0
56	MG	BA	3323	1/1	0.93	0.12	39,39,39,39	0
56	MG	DA	3371	1/1	0.93	0.16	55,55,55,55	0
56	MG	BA	3463	1/1	0.93	0.09	37,37,37,37	0
56	MG	AA	3142	1/1	0.93	0.09	62,62,62,62	0
56	MG	DB	3011	1/1	0.93	0.14	52,52,52,52	0
56	MG	DA	3379	1/1	0.93	0.13	59,59,59,59	0
56	MG	AA	3059	1/1	0.93	0.25	59,59,59,59	0
56	MG	DA	3381	1/1	0.93	0.17	60,60,60,60	0
56	MG	DA	3053	1/1	0.93	0.09	45,45,45,45	0
56	MG	BA	3339	1/1	0.93	0.11	40,40,40,40	0
56	MG	DQ	3003	1/1	0.93	0.08	58,58,58,58	0
56	MG	DA	3057	1/1	0.93	0.09	47,47,47,47	0
56	MG	DU	3002	1/1	0.93	0.09	50,50,50,50	0
56	MG	DA	3060	1/1	0.93	0.09	47,47,47,47	0
56	MG	DA	3061	1/1	0.93	0.15	56,56,56,56	0
56	MG	DA	3062	1/1	0.93	0.16	53,53,53,53	0
56	MG	BA	3471	1/1	0.93	0.07	45,45,45,45	0
56	MG	BA	3346	1/1	0.93	0.05	32,32,32,32	0
56	MG	DA	3399	1/1	0.93	0.13	47,47,47,47	0
56	MG	BA	3782	1/1	0.93	0.08	51,51,51,51	0
56	MG	BA	3206	1/1	0.94	0.10	29,29,29,29	0
56	MG	BA	3698	1/1	0.94	0.09	48,48,48,48	0
56	MG	BA	3215	1/1	0.94	0.13	45,45,45,45	0
56	MG	DA	3383	1/1	0.94	0.07	37,37,37,37	0
56	MG	DA	3384	1/1	0.94	0.08	52,52,52,52	0
56	MG	BA	3514	1/1	0.94	0.10	41,41,41,41	0
56	MG	CA	3002	1/1	0.94	0.08	51,51,51,51	0
56	MG	CA	3004	1/1	0.94	0.09	71,71,71,71	0
56	MG	DA	3389	1/1	0.94	0.11	53,53,53,53	0
56	MG	BA	3515	1/1	0.94	0.07	20,20,20,20	0
56	MG	BA	3087	1/1	0.94	0.14	37,37,37,37	0
56	MG	CA	3009	1/1	0.94	0.17	50,50,50,50	0
56	MG	BA	3219	1/1	0.94	0.09	29,29,29,29	0
56	MG	BA	3361	1/1	0.94	0.12	35,35,35,35	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	AA	3041	1/1	0.94	0.24	52,52,52,52	0
56	MG	BA	3707	1/1	0.94	0.13	66,66,66,66	0
56	MG	AA	3087	1/1	0.94	0.24	52,52,52,52	0
56	MG	DA	3059	1/1	0.94	0.20	53,53,53,53	0
56	MG	BA	3709	1/1	0.94	0.23	44,44,44,44	0
56	MG	AA	3215	1/1	0.94	0.21	57,57,57,57	0
56	MG	AA	3184	1/1	0.94	0.11	55,55,55,55	0
56	MG	AA	3128	1/1	0.94	0.09	41,41,41,41	0
56	MG	DA	3407	1/1	0.94	0.06	46,46,46,46	0
56	MG	AX	3013	1/1	0.94	0.13	39,39,39,39	0
56	MG	AA	3105	1/1	0.94	0.09	49,49,49,49	0
56	MG	BA	3103	1/1	0.94	0.12	48,48,48,48	0
56	MG	DA	3067	1/1	0.94	0.08	49,49,49,49	0
56	MG	BA	3234	1/1	0.94	0.12	48,48,48,48	0
56	MG	DA	3414	1/1	0.94	0.14	41,41,41,41	0
56	MG	BA	3723	1/1	0.94	0.11	47,47,47,47	0
56	MG	DA	3074	1/1	0.94	0.15	50,50,50,50	0
56	MG	AA	3131	1/1	0.94	0.25	63,63,63,63	0
56	MG	BA	3236	1/1	0.94	0.14	43,43,43,43	0
56	MG	BA	3380	1/1	0.94	0.09	60,60,60,60	0
56	MG	DA	3085	1/1	0.94	0.10	52,52,52,52	0
56	MG	AA	3048	1/1	0.94	0.09	51,51,51,51	0
56	MG	AA	3226	1/1	0.94	0.27	58,58,58,58	0
56	MG	DA	3089	1/1	0.94	0.10	46,46,46,46	0
56	MG	DA	3090	1/1	0.94	0.09	45,45,45,45	0
56	MG	DA	3427	1/1	0.94	0.06	38,38,38,38	0
56	MG	CA	3035	1/1	0.94	0.13	60,60,60,60	0
56	MG	BA	3386	1/1	0.94	0.09	42,42,42,42	0
56	MG	AA	3060	1/1	0.94	0.25	59,59,59,59	0
56	MG	DA	3094	1/1	0.94	0.09	52,52,52,52	0
56	MG	BA	3248	1/1	0.94	0.08	45,45,45,45	0
56	MG	DA	3435	1/1	0.94	0.07	44,44,44,44	0
56	MG	BA	3554	1/1	0.94	0.13	37,37,37,37	0
56	MG	DA	3440	1/1	0.94	0.07	39,39,39,39	0
56	MG	AA	3061	1/1	0.94	0.11	54,54,54,54	0
56	MG	BA	3394	1/1	0.94	0.11	52,52,52,52	0
56	MG	BA	3744	1/1	0.94	0.06	20,20,20,20	0
56	MG	CA	3050	1/1	0.94	0.20	60,60,60,60	0
56	MG	BA	3251	1/1	0.94	0.10	52,52,52,52	0
56	MG	BA	3015	1/1	0.94	0.12	47,47,47,47	0
56	MG	BA	3561	1/1	0.94	0.06	27,27,27,27	0
56	MG	BA	3751	1/1	0.94	0.11	45,45,45,45	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	BA	3562	1/1	0.94	0.12	35,35,35,35	0
56	MG	DA	3113	1/1	0.94	0.20	44,44,44,44	0
56	MG	BA	3399	1/1	0.94	0.06	25,25,25,25	0
56	MG	BA	3754	1/1	0.94	0.18	60,60,60,60	0
56	MG	DA	3459	1/1	0.94	0.07	57,57,57,57	0
56	MG	BA	3564	1/1	0.94	0.07	41,41,41,41	0
56	MG	DA	3461	1/1	0.94	0.07	56,56,56,56	0
56	MG	DA	3462	1/1	0.94	0.14	43,43,43,43	0
56	MG	DA	3124	1/1	0.94	0.09	34,34,34,34	0
56	MG	DA	3464	1/1	0.94	0.06	44,44,44,44	0
56	MG	BA	3253	1/1	0.94	0.11	40,40,40,40	0
56	MG	DA	3467	1/1	0.94	0.18	43,43,43,43	0
56	MG	BA	3402	1/1	0.94	0.08	30,30,30,30	0
56	MG	AA	3016	1/1	0.94	0.15	46,46,46,46	0
56	MG	DA	3133	1/1	0.94	0.12	40,40,40,40	0
56	MG	BA	3255	1/1	0.94	0.28	58,58,58,58	0
56	MG	DA	3483	1/1	0.94	0.10	48,48,48,48	0
56	MG	DA	3484	1/1	0.94	0.08	45,45,45,45	0
56	MG	BA	3117	1/1	0.94	0.25	42,42,42,42	0
56	MG	DA	3139	1/1	0.94	0.05	40,40,40,40	0
56	MG	BA	3259	1/1	0.94	0.16	52,52,52,52	0
56	MG	DA	3488	1/1	0.94	0.10	37,37,37,37	0
56	MG	DA	3491	1/1	0.94	0.08	45,45,45,45	0
56	MG	BA	3581	1/1	0.94	0.06	38,38,38,38	0
56	MG	CA	3069	1/1	0.94	0.23	68,68,68,68	0
56	MG	BA	3582	1/1	0.94	0.11	44,44,44,44	0
56	MG	CA	3071	1/1	0.94	0.07	50,50,50,50	0
56	MG	DA	3152	1/1	0.94	0.14	42,42,42,42	0
56	MG	DA	3503	1/1	0.94	0.07	37,37,37,37	0
56	MG	BA	3410	1/1	0.94	0.09	46,46,46,46	0
56	MG	BA	3584	1/1	0.94	0.08	27,27,27,27	0
56	MG	CA	3074	1/1	0.94	0.32	55,55,55,55	0
56	MG	BA	3119	1/1	0.94	0.11	36,36,36,36	0
56	MG	DA	3160	1/1	0.94	0.21	59,59,59,59	0
56	MG	CA	3078	1/1	0.94	0.15	48,48,48,48	0
56	MG	DA	3168	1/1	0.94	0.17	53,53,53,53	0
56	MG	AD	502	1/1	0.94	0.28	56,56,56,56	0
56	MG	DA	3170	1/1	0.94	0.06	50,50,50,50	0
56	MG	DA	3171	1/1	0.94	0.17	38,38,38,38	0
56	MG	DA	3172	1/1	0.94	0.09	51,51,51,51	0
56	MG	DA	3174	1/1	0.94	0.12	48,48,48,48	0
56	MG	CA	3082	1/1	0.94	0.24	63,63,63,63	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	BA	3422	1/1	0.94	0.08	32,32,32,32	0
56	MG	DA	3526	1/1	0.94	0.10	47,47,47,47	0
56	MG	BA	3777	1/1	0.94	0.07	49,49,49,49	0
56	MG	DA	3183	1/1	0.94	0.27	58,58,58,58	0
56	MG	BA	3591	1/1	0.94	0.12	23,23,23,23	0
56	MG	BA	3592	1/1	0.94	0.10	29,29,29,29	0
56	MG	BA	3266	1/1	0.94	0.32	64,64,64,64	0
56	MG	CA	3089	1/1	0.94	0.07	58,58,58,58	0
56	MG	BA	3131	1/1	0.94	0.08	38,38,38,38	0
56	MG	CA	3091	1/1	0.94	0.13	48,48,48,48	0
56	MG	BA	3269	1/1	0.94	0.25	53,53,53,53	0
56	MG	DA	3539	1/1	0.94	0.06	46,46,46,46	0
56	MG	CA	3093	1/1	0.94	0.07	34,34,34,34	0
56	MG	DA	3541	1/1	0.94	0.07	54,54,54,54	0
56	MG	BA	3596	1/1	0.94	0.13	45,45,45,45	0
56	MG	BA	3601	1/1	0.94	0.07	42,42,42,42	0
56	MG	AA	3063	1/1	0.94	0.12	63,63,63,63	0
56	MG	CA	3098	1/1	0.94	0.12	43,43,43,43	0
56	MG	CA	3099	1/1	0.94	0.13	62,62,62,62	0
56	MG	AA	3197	1/1	0.94	0.12	56,56,56,56	0
56	MG	BA	3138	1/1	0.94	0.10	48,48,48,48	0
56	MG	BA	3140	1/1	0.94	0.11	46,46,46,46	0
56	MG	BA	3149	1/1	0.94	0.11	53,53,53,53	0
56	MG	DA	3210	1/1	0.94	0.11	44,44,44,44	0
56	MG	BA	3150	1/1	0.94	0.08	48,48,48,48	0
56	MG	BA	3616	1/1	0.94	0.11	53,53,53,53	0
56	MG	BA	3279	1/1	0.94	0.07	43,43,43,43	0
56	MG	BA	3280	1/1	0.94	0.08	49,49,49,49	0
56	MG	DA	3567	1/1	0.94	0.08	46,46,46,46	0
56	MG	BA	3152	1/1	0.94	0.08	43,43,43,43	0
56	MG	DA	3219	1/1	0.94	0.18	54,54,54,54	0
56	MG	DA	3571	1/1	0.94	0.12	57,57,57,57	0
56	MG	BA	3287	1/1	0.94	0.27	54,54,54,54	0
56	MG	DA	3221	1/1	0.94	0.12	49,49,49,49	0
56	MG	BA	3156	1/1	0.94	0.08	41,41,41,41	0
56	MG	DA	3577	1/1	0.94	0.07	49,49,49,49	0
56	MG	CA	3119	1/1	0.94	0.15	58,58,58,58	0
56	MG	DA	3225	1/1	0.94	0.15	54,54,54,54	0
56	MG	AA	3039	1/1	0.94	0.14	61,61,61,61	0
56	MG	BA	3628	1/1	0.94	0.10	30,30,30,30	0
56	MG	DA	3231	1/1	0.94	0.14	57,57,57,57	0
56	MG	DA	3234	1/1	0.94	0.09	45,45,45,45	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	BA	3815	1/1	0.94	0.18	50,50,50,50	0
56	MG	BA	3166	1/1	0.94	0.08	40,40,40,40	0
56	MG	AA	3114	1/1	0.94	0.13	51,51,51,51	0
56	MG	BA	3824	1/1	0.94	0.08	43,43,43,43	0
56	MG	BA	3293	1/1	0.94	0.20	52,52,52,52	0
56	MG	DA	3592	1/1	0.94	0.10	52,52,52,52	0
56	MG	BA	3448	1/1	0.94	0.09	28,28,28,28	0
56	MG	BA	3295	1/1	0.94	0.08	42,42,42,42	0
56	MG	DA	3245	1/1	0.94	0.12	62,62,62,62	0
56	MG	AA	3054	1/1	0.94	0.25	52,52,52,52	0
56	MG	AA	3147	1/1	0.94	0.09	55,55,55,55	0
56	MG	BA	3453	1/1	0.94	0.10	42,42,42,42	0
56	MG	CA	3135	1/1	0.94	0.12	53,53,53,53	0
56	MG	DA	3602	1/1	0.94	0.12	51,51,51,51	0
56	MG	BB	3002	1/1	0.94	0.19	52,52,52,52	0
56	MG	BB	3003	1/1	0.94	0.07	40,40,40,40	0
56	MG	BA	3455	1/1	0.94	0.12	39,39,39,39	0
56	MG	AA	3119	1/1	0.94	0.09	58,58,58,58	0
56	MG	BB	3008	1/1	0.94	0.21	54,54,54,54	0
56	MG	BA	3180	1/1	0.94	0.10	58,58,58,58	0
56	MG	BA	3052	1/1	0.94	0.10	43,43,43,43	0
56	MG	DA	3613	1/1	0.94	0.10	50,50,50,50	0
56	MG	AA	3206	1/1	0.94	0.12	47,47,47,47	0
56	MG	BA	3650	1/1	0.94	0.09	57,57,57,57	0
56	MG	BA	3319	1/1	0.94	0.11	20,20,20,20	0
56	MG	BA	3469	1/1	0.94	0.14	37,37,37,37	0
56	MG	BA	3059	1/1	0.94	0.07	55,55,55,55	0
56	MG	AA	3177	1/1	0.94	0.20	57,57,57,57	0
56	MG	BA	3063	1/1	0.94	0.09	47,47,47,47	0
56	MG	DA	3623	1/1	0.94	0.09	70,70,70,70	0
56	MG	DA	3625	1/1	0.94	0.09	53,53,53,53	0
56	MG	BD	301	1/1	0.94	0.18	49,49,49,49	0
56	MG	BD	303	1/1	0.94	0.25	44,44,44,44	0
56	MG	DA	3630	1/1	0.94	0.14	49,49,49,49	0
56	MG	BA	3473	1/1	0.94	0.09	57,57,57,57	0
56	MG	DA	3289	1/1	0.94	0.10	42,42,42,42	0
56	MG	BA	3475	1/1	0.94	0.15	53,53,53,53	0
56	MG	BA	3661	1/1	0.94	0.10	53,53,53,53	0
56	MG	BA	3662	1/1	0.94	0.12	50,50,50,50	0
56	MG	BF	302	1/1	0.94	0.06	39,39,39,39	0
56	MG	DA	3301	1/1	0.94	0.13	48,48,48,48	0
56	MG	BA	3476	1/1	0.94	0.07	24,24,24,24	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	DA	3644	1/1	0.94	0.14	55,55,55,55	0
56	MG	BA	3325	1/1	0.94	0.12	56,56,56,56	0
56	MG	BA	3668	1/1	0.94	0.08	56,56,56,56	0
56	MG	CA	3164	1/1	0.94	0.10	54,54,54,54	0
56	MG	BA	3326	1/1	0.94	0.10	38,38,38,38	0
56	MG	BN	3002	1/1	0.94	0.07	46,46,46,46	0
56	MG	BN	3005	1/1	0.94	0.21	51,51,51,51	0
56	MG	DA	3654	1/1	0.94	0.09	55,55,55,55	0
56	MG	BA	3196	1/1	0.94	0.21	51,51,51,51	0
56	MG	BP	201	1/1	0.94	0.38	41,41,41,41	0
56	MG	AW	3006	1/1	0.94	0.16	50,50,50,50	0
56	MG	DA	3661	1/1	0.94	0.15	42,42,42,42	0
56	MG	BR	201	1/1	0.94	0.14	44,44,44,44	0
56	MG	DA	3664	1/1	0.94	0.10	38,38,38,38	0
56	MG	AW	3007	1/1	0.94	0.10	64,64,64,64	0
56	MG	BA	3340	1/1	0.94	0.09	45,45,45,45	0
56	MG	CE	202	1/1	0.94	0.11	66,66,66,66	0
56	MG	DA	3671	1/1	0.94	0.13	59,59,59,59	0
56	MG	BU	201	1/1	0.94	0.09	39,39,39,39	0
56	MG	CT	3001	1/1	0.94	0.08	47,47,47,47	0
56	MG	BA	3488	1/1	0.94	0.09	50,50,50,50	0
56	MG	CW	3001	1/1	0.94	0.20	63,63,63,63	0
56	MG	AA	3045	1/1	0.94	0.26	59,59,59,59	0
56	MG	BX	102	1/1	0.94	0.17	41,41,41,41	0
56	MG	CX	3005	1/1	0.94	0.23	58,58,58,58	0
56	MG	DB	3006	1/1	0.94	0.21	62,62,62,62	0
56	MG	BA	3068	1/1	0.94	0.18	51,51,51,51	0
56	MG	BZ	3001	1/1	0.94	0.20	52,52,52,52	0
56	MG	DA	3351	1/1	0.94	0.06	39,39,39,39	0
56	MG	DA	3353	1/1	0.94	0.09	37,37,37,37	0
56	MG	DD	307	1/1	0.94	0.11	56,56,56,56	0
56	MG	BA	3348	1/1	0.94	0.12	54,54,54,54	0
56	MG	B0	102	1/1	0.94	0.13	68,68,68,68	0
56	MG	B0	103	1/1	0.94	0.07	54,54,54,54	0
56	MG	BA	3349	1/1	0.94	0.11	34,34,34,34	0
56	MG	DA	3360	1/1	0.94	0.09	51,51,51,51	0
56	MG	DN	5001	1/1	0.94	0.06	62,62,62,62	0
56	MG	DA	3009	1/1	0.94	0.07	38,38,38,38	0
56	MG	B2	3001	1/1	0.94	0.10	45,45,45,45	0
56	MG	BA	3351	1/1	0.94	0.08	34,34,34,34	0
56	MG	BA	3201	1/1	0.94	0.09	40,40,40,40	0
56	MG	DA	3369	1/1	0.94	0.10	61,61,61,61	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	B5	103	1/1	0.94	0.09	44,44,44,44	0
56	MG	AA	3021	1/1	0.94	0.09	45,45,45,45	0
56	MG	DA	3372	1/1	0.94	0.06	47,47,47,47	0
56	MG	AA	3123	1/1	0.94	0.16	57,57,57,57	0
56	MG	B6	102	1/1	0.94	0.27	55,55,55,55	0
56	MG	DA	3167	1/1	0.95	0.14	47,47,47,47	0
56	MG	BN	3004	1/1	0.95	0.24	50,50,50,50	0
56	MG	BA	3240	1/1	0.95	0.12	45,45,45,45	0
56	MG	BA	3062	1/1	0.95	0.30	57,57,57,57	0
56	MG	DA	3438	1/1	0.95	0.13	60,60,60,60	0
56	MG	BA	3139	1/1	0.95	0.10	61,61,61,61	0
56	MG	CA	3129	1/1	0.95	0.19	61,61,61,61	0
56	MG	DA	3443	1/1	0.95	0.07	51,51,51,51	0
56	MG	BQ	3003	1/1	0.95	0.11	54,54,54,54	0
56	MG	DA	3176	1/1	0.95	0.09	52,52,52,52	0
56	MG	DA	3177	1/1	0.95	0.09	54,54,54,54	0
56	MG	BQ	3004	1/1	0.95	0.13	35,35,35,35	0
56	MG	DA	3179	1/1	0.95	0.05	46,46,46,46	0
56	MG	BA	3717	1/1	0.95	0.12	58,58,58,58	0
56	MG	AX	3012	1/1	0.95	0.14	59,59,59,59	0
56	MG	BA	3719	1/1	0.95	0.07	42,42,42,42	0
56	MG	BA	3456	1/1	0.95	0.16	41,41,41,41	0
56	MG	BA	3141	1/1	0.95	0.06	38,38,38,38	0
56	MG	BU	208	1/1	0.95	0.14	41,41,41,41	0
56	MG	BA	3143	1/1	0.95	0.13	42,42,42,42	0
56	MG	CA	3142	1/1	0.95	0.16	61,61,61,61	0
56	MG	AA	3036	1/1	0.95	0.16	52,52,52,52	0
56	MG	AY	3001	1/1	0.95	0.24	70,70,70,70	0
56	MG	BA	3465	1/1	0.95	0.09	42,42,42,42	0
56	MG	DA	3194	1/1	0.95	0.15	35,35,35,35	0
56	MG	DA	3465	1/1	0.95	0.12	55,55,55,55	0
56	MG	AA	3007	1/1	0.95	0.25	65,65,65,65	0
56	MG	BA	3362	1/1	0.95	0.09	19,19,19,19	0
56	MG	BA	3733	1/1	0.95	0.14	41,41,41,41	0
56	MG	BA	3153	1/1	0.95	0.07	39,39,39,39	0
56	MG	DA	3470	1/1	0.95	0.10	42,42,42,42	0
56	MG	DA	3471	1/1	0.95	0.10	50,50,50,50	0
56	MG	B1	101	1/1	0.95	0.24	44,44,44,44	0
56	MG	BA	3736	1/1	0.95	0.10	56,56,56,56	0
56	MG	DA	3480	1/1	0.95	0.07	48,48,48,48	0
56	MG	DA	3481	1/1	0.95	0.06	30,30,30,30	0
56	MG	DA	3482	1/1	0.95	0.09	50,50,50,50	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	DA	3203	1/1	0.95	0.13	37,37,37,37	0
56	MG	BA	3738	1/1	0.95	0.14	58,58,58,58	0
56	MG	BA	3597	1/1	0.95	0.07	44,44,44,44	0
56	MG	BA	3598	1/1	0.95	0.07	47,47,47,47	0
56	MG	DA	3209	1/1	0.95	0.07	52,52,52,52	0
56	MG	BA	3741	1/1	0.95	0.06	28,28,28,28	0
56	MG	BA	3599	1/1	0.95	0.12	23,23,23,23	0
56	MG	BA	3600	1/1	0.95	0.11	56,56,56,56	0
56	MG	DA	3496	1/1	0.95	0.09	48,48,48,48	0
56	MG	DA	3214	1/1	0.95	0.09	47,47,47,47	0
56	MG	DA	3498	1/1	0.95	0.13	57,57,57,57	0
56	MG	CA	3159	1/1	0.95	0.14	57,57,57,57	0
56	MG	AA	3052	1/1	0.95	0.34	68,68,68,68	0
56	MG	DA	3501	1/1	0.95	0.21	59,59,59,59	0
56	MG	BA	3602	1/1	0.95	0.17	46,46,46,46	0
56	MG	AA	3164	1/1	0.95	0.19	50,50,50,50	0
56	MG	BA	3073	1/1	0.95	0.13	41,41,41,41	0
56	MG	BA	3749	1/1	0.95	0.15	45,45,45,45	0
56	MG	DA	3506	1/1	0.95	0.07	48,48,48,48	0
56	MG	DA	3222	1/1	0.95	0.14	54,54,54,54	0
56	MG	AA	3208	1/1	0.95	0.07	45,45,45,45	0
56	MG	CA	3003	1/1	0.95	0.23	58,58,58,58	0
56	MG	BA	3264	1/1	0.95	0.08	39,39,39,39	0
56	MG	BA	3169	1/1	0.95	0.16	47,47,47,47	0
56	MG	DA	3227	1/1	0.95	0.12	38,38,38,38	0
56	MG	CA	3170	1/1	0.95	0.13	64,64,64,64	0
56	MG	DA	3514	1/1	0.95	0.09	41,41,41,41	0
56	MG	CA	3006	1/1	0.95	0.24	53,53,53,53	0
56	MG	DA	3232	1/1	0.95	0.13	53,53,53,53	0
56	MG	BA	3610	1/1	0.95	0.12	64,64,64,64	0
56	MG	CA	3008	1/1	0.95	0.06	50,50,50,50	0
56	MG	CA	3174	1/1	0.95	0.11	46,46,46,46	0
56	MG	CA	3176	1/1	0.95	0.08	43,43,43,43	0
56	MG	BA	3081	1/1	0.95	0.19	49,49,49,49	0
56	MG	BA	3613	1/1	0.95	0.08	45,45,45,45	0
56	MG	DA	3529	1/1	0.95	0.07	41,41,41,41	0
56	MG	DA	3530	1/1	0.95	0.09	55,55,55,55	0
56	MG	BA	3082	1/1	0.95	0.09	59,59,59,59	0
56	MG	DA	3532	1/1	0.95	0.11	57,57,57,57	0
56	MG	BA	3375	1/1	0.95	0.06	35,35,35,35	0
56	MG	BA	3759	1/1	0.95	0.06	9,9,9,9	0
56	MG	CA	3014	1/1	0.95	0.14	47,47,47,47	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	BA	3172	1/1	0.95	0.13	45,45,45,45	0
56	MG	BA	3085	1/1	0.95	0.06	31,31,31,31	0
56	MG	CX	3003	1/1	0.95	0.24	50,50,50,50	0
56	MG	DA	3253	1/1	0.95	0.10	38,38,38,38	0
56	MG	BA	3379	1/1	0.95	0.13	45,45,45,45	0
56	MG	BA	3622	1/1	0.95	0.07	31,31,31,31	0
56	MG	BA	3764	1/1	0.95	0.11	58,58,58,58	0
56	MG	DA	3543	1/1	0.95	0.05	55,55,55,55	0
56	MG	CY	3001	1/1	0.95	0.23	58,58,58,58	0
56	MG	DA	3546	1/1	0.95	0.09	53,53,53,53	0
56	MG	DA	3266	1/1	0.95	0.07	47,47,47,47	0
56	MG	DA	3267	1/1	0.95	0.09	38,38,38,38	0
56	MG	BA	3623	1/1	0.95	0.09	52,52,52,52	0
56	MG	DA	3555	1/1	0.95	0.08	54,54,54,54	0
56	MG	DA	3270	1/1	0.95	0.09	49,49,49,49	0
56	MG	BA	3766	1/1	0.95	0.07	31,31,31,31	0
56	MG	BA	3767	1/1	0.95	0.16	29,29,29,29	0
56	MG	DA	3559	1/1	0.95	0.09	48,48,48,48	0
56	MG	DA	3273	1/1	0.95	0.06	45,45,45,45	0
56	MG	AA	3144	1/1	0.95	0.06	50,50,50,50	0
56	MG	BA	3006	1/1	0.95	0.09	52,52,52,52	0
56	MG	AA	3097	1/1	0.95	0.11	50,50,50,50	0
56	MG	BA	3094	1/1	0.95	0.06	43,43,43,43	0
56	MG	CA	3031	1/1	0.95	0.08	53,53,53,53	0
56	MG	BA	3496	1/1	0.95	0.13	39,39,39,39	0
56	MG	DA	3283	1/1	0.95	0.16	46,46,46,46	0
56	MG	BA	3388	1/1	0.95	0.07	52,52,52,52	0
56	MG	BA	3191	1/1	0.95	0.15	40,40,40,40	0
56	MG	BA	3505	1/1	0.95	0.08	54,54,54,54	0
56	MG	AA	3186	1/1	0.95	0.11	52,52,52,52	0
56	MG	BA	3509	1/1	0.95	0.07	39,39,39,39	0
56	MG	DA	3031	1/1	0.95	0.20	51,51,51,51	0
56	MG	DA	3578	1/1	0.95	0.10	55,55,55,55	0
56	MG	DA	3295	1/1	0.95	0.11	58,58,58,58	0
56	MG	CA	3038	1/1	0.95	0.13	46,46,46,46	0
56	MG	CA	3039	1/1	0.95	0.17	50,50,50,50	0
56	MG	DA	3038	1/1	0.95	0.13	47,47,47,47	0
56	MG	CA	3040	1/1	0.95	0.16	58,58,58,58	0
56	MG	CA	3041	1/1	0.95	0.14	58,58,58,58	0
56	MG	DA	3585	1/1	0.95	0.06	51,51,51,51	0
56	MG	BA	3281	1/1	0.95	0.07	49,49,49,49	0
56	MG	BA	3283	1/1	0.95	0.10	36,36,36,36	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	BA	3785	1/1	0.95	0.11	41,41,41,41	0
56	MG	DA	3045	1/1	0.95	0.09	47,47,47,47	0
56	MG	AA	3146	1/1	0.95	0.08	53,53,53,53	0
56	MG	CA	3048	1/1	0.95	0.24	52,52,52,52	0
56	MG	DA	3593	1/1	0.95	0.07	39,39,39,39	0
56	MG	DA	3048	1/1	0.95	0.07	45,45,45,45	0
56	MG	AA	3115	1/1	0.95	0.08	51,51,51,51	0
56	MG	BA	3100	1/1	0.95	0.08	45,45,45,45	0
56	MG	DA	3321	1/1	0.95	0.09	35,35,35,35	0
56	MG	DA	3054	1/1	0.95	0.07	43,43,43,43	0
56	MG	DA	3599	1/1	0.95	0.28	38,38,38,38	0
56	MG	DA	3055	1/1	0.95	0.10	36,36,36,36	0
56	MG	AA	3074	1/1	0.95	0.09	47,47,47,47	0
56	MG	BA	3649	1/1	0.95	0.07	43,43,43,43	0
56	MG	DA	3603	1/1	0.95	0.11	52,52,52,52	0
56	MG	DA	3328	1/1	0.95	0.08	47,47,47,47	0
56	MG	DA	3058	1/1	0.95	0.09	46,46,46,46	0
56	MG	AA	3108	1/1	0.95	0.16	55,55,55,55	0
56	MG	AA	3135	1/1	0.95	0.12	65,65,65,65	0
56	MG	BA	3521	1/1	0.95	0.09	36,36,36,36	0
56	MG	DA	3340	1/1	0.95	0.11	42,42,42,42	0
56	MG	BA	3653	1/1	0.95	0.19	49,49,49,49	0
56	MG	AA	3152	1/1	0.95	0.13	45,45,45,45	0
56	MG	BA	3202	1/1	0.95	0.09	46,46,46,46	0
56	MG	BA	3106	1/1	0.95	0.21	50,50,50,50	0
56	MG	BA	3300	1/1	0.95	0.17	22,22,22,22	0
56	MG	BA	3411	1/1	0.95	0.07	36,36,36,36	0
56	MG	BA	3302	1/1	0.95	0.10	35,35,35,35	0
56	MG	DA	3070	1/1	0.95	0.08	48,48,48,48	0
56	MG	CA	3065	1/1	0.95	0.15	65,65,65,65	0
56	MG	BA	3109	1/1	0.95	0.08	42,42,42,42	0
56	MG	DA	3076	1/1	0.95	0.11	43,43,43,43	0
56	MG	DA	3626	1/1	0.95	0.06	54,54,54,54	0
56	MG	DA	3077	1/1	0.95	0.09	43,43,43,43	0
56	MG	BA	3416	1/1	0.95	0.06	21,21,21,21	0
56	MG	DA	3629	1/1	0.95	0.08	52,52,52,52	0
56	MG	DA	3362	1/1	0.95	0.10	43,43,43,43	0
56	MG	BA	3533	1/1	0.95	0.12	50,50,50,50	0
56	MG	BA	3822	1/1	0.95	0.09	21,21,21,21	0
56	MG	DA	3084	1/1	0.95	0.10	27,27,27,27	0
56	MG	DA	3634	1/1	0.95	0.12	53,53,53,53	0
56	MG	BA	3823	1/1	0.95	0.09	53,53,53,53	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	BA	3418	1/1	0.95	0.07	32,32,32,32	0
56	MG	BA	3110	1/1	0.95	0.06	41,41,41,41	0
56	MG	BA	3826	1/1	0.95	0.17	33,33,33,33	0
56	MG	BA	3538	1/1	0.95	0.13	45,45,45,45	0
56	MG	CA	3075	1/1	0.95	0.10	44,44,44,44	0
56	MG	BA	3829	1/1	0.95	0.24	45,45,45,45	0
56	MG	BA	3673	1/1	0.95	0.14	47,47,47,47	0
56	MG	BA	3423	1/1	0.95	0.06	23,23,23,23	0
56	MG	CA	3081	1/1	0.95	0.21	58,58,58,58	0
56	MG	BA	3677	1/1	0.95	0.05	62,62,62,62	0
56	MG	DA	3652	1/1	0.95	0.09	49,49,49,49	0
56	MG	BA	3540	1/1	0.95	0.11	44,44,44,44	0
56	MG	BA	3029	1/1	0.95	0.12	46,46,46,46	0
56	MG	BA	3314	1/1	0.95	0.07	47,47,47,47	0
56	MG	AA	3089	1/1	0.95	0.28	57,57,57,57	0
56	MG	DA	3392	1/1	0.95	0.08	36,36,36,36	0
56	MG	AA	3154	1/1	0.95	0.11	59,59,59,59	0
56	MG	BB	3006	1/1	0.95	0.10	38,38,38,38	0
56	MG	BA	3032	1/1	0.95	0.11	38,38,38,38	0
56	MG	BA	3552	1/1	0.95	0.11	34,34,34,34	0
56	MG	BA	3038	1/1	0.95	0.22	47,47,47,47	0
56	MG	BA	3223	1/1	0.95	0.07	29,29,29,29	0
56	MG	DA	3668	1/1	0.95	0.17	79,79,79,79	0
56	MG	DA	3115	1/1	0.95	0.16	41,41,41,41	0
56	MG	AA	3029	1/1	0.95	0.15	53,53,53,53	0
56	MG	DA	3673	1/1	0.95	0.09	61,61,61,61	0
56	MG	BA	3047	1/1	0.95	0.05	27,27,27,27	0
56	MG	AX	3008	1/1	0.95	0.28	57,57,57,57	0
56	MG	DA	3122	1/1	0.95	0.08	36,36,36,36	0
56	MG	BA	3695	1/1	0.95	0.14	48,48,48,48	0
56	MG	BA	3124	1/1	0.95	0.12	38,38,38,38	0
56	MG	DA	3129	1/1	0.95	0.05	45,45,45,45	0
56	MG	BA	3128	1/1	0.95	0.13	27,27,27,27	0
56	MG	DA	3409	1/1	0.95	0.08	47,47,47,47	0
56	MG	BA	3055	1/1	0.95	0.14	31,31,31,31	0
56	MG	DB	3009	1/1	0.95	0.15	47,47,47,47	0
56	MG	AA	3201	1/1	0.95	0.06	59,59,59,59	0
56	MG	BA	3341	1/1	0.95	0.12	57,57,57,57	0
56	MG	BD	306	1/1	0.95	0.13	22,22,22,22	0
56	MG	AA	3178	1/1	0.95	0.10	54,54,54,54	0
56	MG	BA	3568	1/1	0.95	0.13	52,52,52,52	0
56	MG	BE	306	1/1	0.95	0.08	25,25,25,25	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	BA	3570	1/1	0.95	0.13	30,30,30,30	0
56	MG	BF	301	1/1	0.95	0.11	38,38,38,38	0
56	MG	DA	3149	1/1	0.95	0.14	48,48,48,48	0
56	MG	BA	3135	1/1	0.95	0.18	35,35,35,35	0
56	MG	CA	3115	1/1	0.95	0.10	62,62,62,62	0
56	MG	DU	3001	1/1	0.95	0.14	50,50,50,50	0
56	MG	AA	3122	1/1	0.95	0.23	60,60,60,60	0
56	MG	BA	3238	1/1	0.95	0.09	43,43,43,43	0
56	MG	BF	307	1/1	0.95	0.08	39,39,39,39	0
56	MG	BA	3710	1/1	0.95	0.06	28,28,28,28	0
56	MG	D7	102	1/1	0.95	0.26	43,43,43,43	0
56	MG	BA	3350	1/1	0.95	0.11	27,27,27,27	0
56	MG	BA	3450	1/1	0.95	0.13	34,34,34,34	0
56	MG	DA	3430	1/1	0.95	0.07	28,28,28,28	0
59	ZN	D4	501	1/1	0.95	0.07	119,119,119,119	0
56	MG	DA	3164	1/1	0.95	0.17	33,33,33,33	0
56	MG	BV	203	1/1	0.96	0.31	32,32,32,32	0
56	MG	BA	3587	1/1	0.96	0.08	44,44,44,44	0
56	MG	BA	3145	1/1	0.96	0.27	32,32,32,32	0
56	MG	BA	3019	1/1	0.96	0.17	42,42,42,42	0
56	MG	BA	3083	1/1	0.96	0.29	47,47,47,47	0
56	MG	BA	3242	1/1	0.96	0.30	42,42,42,42	0
56	MG	BA	3460	1/1	0.96	0.12	35,35,35,35	0
56	MG	BA	3461	1/1	0.96	0.09	31,31,31,31	0
56	MG	CA	3153	1/1	0.96	0.10	61,61,61,61	0
56	MG	BA	3737	1/1	0.96	0.13	36,36,36,36	0
56	MG	AA	3023	1/1	0.96	0.07	37,37,37,37	0
56	MG	AA	3191	1/1	0.96	0.07	48,48,48,48	0
56	MG	BA	3154	1/1	0.96	0.15	29,29,29,29	0
56	MG	BA	3355	1/1	0.96	0.07	24,24,24,24	0
56	MG	DA	3198	1/1	0.96	0.05	51,51,51,51	0
56	MG	BA	3468	1/1	0.96	0.10	49,49,49,49	0
56	MG	B5	102	1/1	0.96	0.24	45,45,45,45	0
56	MG	AA	3214	1/1	0.96	0.08	44,44,44,44	0
56	MG	DA	3202	1/1	0.96	0.19	50,50,50,50	0
56	MG	BA	3090	1/1	0.96	0.16	37,37,37,37	0
56	MG	AA	3118	1/1	0.96	0.16	53,53,53,53	0
56	MG	DA	3205	1/1	0.96	0.11	47,47,47,47	0
56	MG	BA	3025	1/1	0.96	0.06	38,38,38,38	0
56	MG	BA	3027	1/1	0.96	0.14	42,42,42,42	0
56	MG	DA	3478	1/1	0.96	0.08	47,47,47,47	0
56	MG	DA	3208	1/1	0.96	0.06	59,59,59,59	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	CA	3166	1/1	0.96	0.09	66,66,66,66	0
56	MG	AA	3043	1/1	0.96	0.08	26,26,26,26	0
56	MG	BA	3750	1/1	0.96	0.10	49,49,49,49	0
56	MG	BA	3258	1/1	0.96	0.20	41,41,41,41	0
56	MG	AA	3107	1/1	0.96	0.18	51,51,51,51	0
56	MG	AA	3219	1/1	0.96	0.21	65,65,65,65	0
56	MG	BA	3479	1/1	0.96	0.10	37,37,37,37	0
56	MG	BA	3615	1/1	0.96	0.28	35,35,35,35	0
56	MG	DA	3489	1/1	0.96	0.10	37,37,37,37	0
56	MG	DA	3490	1/1	0.96	0.06	39,39,39,39	0
56	MG	BA	3261	1/1	0.96	0.17	44,44,44,44	0
56	MG	CA	3175	1/1	0.96	0.08	39,39,39,39	0
56	MG	DA	3495	1/1	0.96	0.11	62,62,62,62	0
56	MG	BA	3175	1/1	0.96	0.05	35,35,35,35	0
56	MG	AA	3196	1/1	0.96	0.10	32,32,32,32	0
56	MG	BA	3178	1/1	0.96	0.17	38,38,38,38	0
56	MG	BA	3267	1/1	0.96	0.06	37,37,37,37	0
56	MG	CF	3001	1/1	0.96	0.14	38,38,38,38	0
56	MG	BA	3621	1/1	0.96	0.13	52,52,52,52	0
56	MG	BA	3179	1/1	0.96	0.07	39,39,39,39	0
56	MG	DA	3228	1/1	0.96	0.07	42,42,42,42	0
56	MG	BA	3372	1/1	0.96	0.11	24,24,24,24	0
56	MG	BA	3624	1/1	0.96	0.07	29,29,29,29	0
56	MG	CW	3002	1/1	0.96	0.13	74,74,74,74	0
56	MG	DA	3233	1/1	0.96	0.09	43,43,43,43	0
56	MG	BA	3373	1/1	0.96	0.10	38,38,38,38	0
56	MG	AA	3078	1/1	0.96	0.08	48,48,48,48	0
56	MG	DA	3237	1/1	0.96	0.07	51,51,51,51	0
56	MG	CA	3018	1/1	0.96	0.13	45,45,45,45	0
56	MG	BA	3034	1/1	0.96	0.10	28,28,28,28	0
56	MG	BA	3629	1/1	0.96	0.09	56,56,56,56	0
56	MG	BA	3502	1/1	0.96	0.18	45,45,45,45	0
56	MG	BA	3631	1/1	0.96	0.07	43,43,43,43	0
56	MG	BA	3771	1/1	0.96	0.07	41,41,41,41	0
56	MG	DA	3517	1/1	0.96	0.06	47,47,47,47	0
56	MG	BA	3632	1/1	0.96	0.10	55,55,55,55	0
56	MG	BA	3774	1/1	0.96	0.06	43,43,43,43	0
56	MG	BA	3271	1/1	0.96	0.05	26,26,26,26	0
56	MG	DA	3525	1/1	0.96	0.08	41,41,41,41	0
56	MG	AA	3157	1/1	0.96	0.06	46,46,46,46	0
56	MG	AA	3199	1/1	0.96	0.12	59,59,59,59	0
56	MG	BA	3507	1/1	0.96	0.07	39,39,39,39	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	BA	3046	1/1	0.96	0.07	43,43,43,43	0
56	MG	DA	3258	1/1	0.96	0.20	59,59,59,59	0
56	MG	AA	3200	1/1	0.96	0.17	45,45,45,45	0
56	MG	DA	3261	1/1	0.96	0.06	44,44,44,44	0
56	MG	BA	3049	1/1	0.96	0.12	37,37,37,37	0
56	MG	DA	3023	1/1	0.96	0.09	30,30,30,30	0
56	MG	DA	3025	1/1	0.96	0.08	44,44,44,44	0
56	MG	DA	3026	1/1	0.96	0.06	42,42,42,42	0
56	MG	BA	3640	1/1	0.96	0.20	39,39,39,39	0
56	MG	BA	3194	1/1	0.96	0.09	37,37,37,37	0
56	MG	BA	3786	1/1	0.96	0.07	37,37,37,37	0
56	MG	DA	3030	1/1	0.96	0.11	40,40,40,40	0
56	MG	BA	3195	1/1	0.96	0.19	50,50,50,50	0
56	MG	BA	3788	1/1	0.96	0.07	41,41,41,41	0
56	MG	DA	3035	1/1	0.96	0.07	38,38,38,38	0
56	MG	DA	3036	1/1	0.96	0.06	29,29,29,29	0
56	MG	BA	3789	1/1	0.96	0.16	39,39,39,39	0
56	MG	BA	3791	1/1	0.96	0.08	47,47,47,47	0
56	MG	DA	3281	1/1	0.96	0.11	33,33,33,33	0
56	MG	CA	3042	1/1	0.96	0.10	58,58,58,58	0
56	MG	DA	3550	1/1	0.96	0.06	51,51,51,51	0
56	MG	DA	3553	1/1	0.96	0.09	54,54,54,54	0
56	MG	BA	3793	1/1	0.96	0.07	38,38,38,38	0
56	MG	BA	3051	1/1	0.96	0.07	25,25,25,25	0
56	MG	DA	3285	1/1	0.96	0.07	28,28,28,28	0
56	MG	BA	3646	1/1	0.96	0.07	38,38,38,38	0
56	MG	BA	3391	1/1	0.96	0.09	41,41,41,41	0
56	MG	AA	3006	1/1	0.96	0.05	37,37,37,37	0
56	MG	AA	3015	1/1	0.96	0.16	60,60,60,60	0
56	MG	BA	3285	1/1	0.96	0.23	49,49,49,49	0
56	MG	DA	3294	1/1	0.96	0.06	42,42,42,42	0
56	MG	BA	3286	1/1	0.96	0.18	46,46,46,46	0
56	MG	DA	3296	1/1	0.96	0.07	48,48,48,48	0
56	MG	DA	3049	1/1	0.96	0.06	24,24,24,24	0
56	MG	CA	3052	1/1	0.96	0.15	65,65,65,65	0
56	MG	DA	3052	1/1	0.96	0.07	38,38,38,38	0
56	MG	BA	3056	1/1	0.96	0.15	33,33,33,33	0
56	MG	BA	3288	1/1	0.96	0.29	40,40,40,40	0
56	MG	AA	3161	1/1	0.96	0.18	46,46,46,46	0
56	MG	BA	3058	1/1	0.96	0.14	36,36,36,36	0
56	MG	BA	3809	1/1	0.96	0.07	29,29,29,29	0
56	MG	BA	3118	1/1	0.96	0.13	38,38,38,38	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	AA	3124	1/1	0.96	0.08	53,53,53,53	0
56	MG	DA	3311	1/1	0.96	0.09	42,42,42,42	0
56	MG	BA	3406	1/1	0.96	0.06	32,32,32,32	0
56	MG	DA	3314	1/1	0.96	0.06	33,33,33,33	0
56	MG	BA	3407	1/1	0.96	0.09	37,37,37,37	0
56	MG	DA	3318	1/1	0.96	0.08	42,42,42,42	0
56	MG	CA	3062	1/1	0.96	0.18	44,44,44,44	0
56	MG	DA	3586	1/1	0.96	0.08	44,44,44,44	0
56	MG	AA	3064	1/1	0.96	0.07	61,61,61,61	0
56	MG	BA	3126	1/1	0.96	0.08	43,43,43,43	0
56	MG	BA	3209	1/1	0.96	0.12	41,41,41,41	0
56	MG	BA	3667	1/1	0.96	0.08	52,52,52,52	0
56	MG	BA	3536	1/1	0.96	0.12	48,48,48,48	0
56	MG	DA	3326	1/1	0.96	0.09	46,46,46,46	0
56	MG	BA	3669	1/1	0.96	0.06	42,42,42,42	0
56	MG	BA	3213	1/1	0.96	0.06	45,45,45,45	0
56	MG	DA	3330	1/1	0.96	0.06	46,46,46,46	0
56	MG	DA	3071	1/1	0.96	0.13	44,44,44,44	0
56	MG	BA	3671	1/1	0.96	0.09	45,45,45,45	0
56	MG	DA	3073	1/1	0.96	0.15	54,54,54,54	0
56	MG	DA	3336	1/1	0.96	0.06	47,47,47,47	0
56	MG	BA	3214	1/1	0.96	0.08	49,49,49,49	0
56	MG	BA	3303	1/1	0.96	0.13	35,35,35,35	0
56	MG	BA	3832	1/1	0.96	0.05	37,37,37,37	0
56	MG	BA	3674	1/1	0.96	0.07	47,47,47,47	0
56	MG	BA	3308	1/1	0.96	0.08	39,39,39,39	0
56	MG	DA	3080	1/1	0.96	0.16	45,45,45,45	0
56	MG	DA	3606	1/1	0.96	0.09	54,54,54,54	0
56	MG	BA	3127	1/1	0.96	0.09	41,41,41,41	0
56	MG	DA	3608	1/1	0.96	0.09	53,53,53,53	0
56	MG	DA	3083	1/1	0.96	0.06	51,51,51,51	0
56	MG	DA	3352	1/1	0.96	0.07	35,35,35,35	0
56	MG	BA	3001	1/1	0.96	0.15	43,43,43,43	0
56	MG	BA	3545	1/1	0.96	0.12	41,41,41,41	0
56	MG	CA	3080	1/1	0.96	0.23	52,52,52,52	0
56	MG	BA	3546	1/1	0.96	0.14	30,30,30,30	0
56	MG	DA	3358	1/1	0.96	0.16	45,45,45,45	0
56	MG	BA	3312	1/1	0.96	0.11	33,33,33,33	0
56	MG	BA	3682	1/1	0.96	0.14	50,50,50,50	0
56	MG	AK	202	1/1	0.96	0.14	38,38,38,38	0
56	MG	BA	3684	1/1	0.96	0.15	49,49,49,49	0
56	MG	BB	3010	1/1	0.96	0.09	48,48,48,48	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	DA	3621	1/1	0.96	0.09	45,45,45,45	0
56	MG	CA	3087	1/1	0.96	0.17	63,63,63,63	0
56	MG	DA	3624	1/1	0.96	0.07	47,47,47,47	0
56	MG	BA	3550	1/1	0.96	0.13	34,34,34,34	0
56	MG	BA	3551	1/1	0.96	0.07	33,33,33,33	0
56	MG	AA	3126	1/1	0.96	0.07	46,46,46,46	0
56	MG	BA	3132	1/1	0.96	0.06	42,42,42,42	0
56	MG	DA	3100	1/1	0.96	0.05	36,36,36,36	0
56	MG	AA	3090	1/1	0.96	0.29	53,53,53,53	0
56	MG	BA	3318	1/1	0.96	0.07	37,37,37,37	0
56	MG	BA	3134	1/1	0.96	0.13	35,35,35,35	0
56	MG	BA	3694	1/1	0.96	0.08	27,27,27,27	0
56	MG	CA	3096	1/1	0.96	0.15	61,61,61,61	0
56	MG	BA	3225	1/1	0.96	0.10	42,42,42,42	0
56	MG	BD	302	1/1	0.96	0.13	23,23,23,23	0
56	MG	DA	3638	1/1	0.96	0.11	60,60,60,60	0
56	MG	DA	3111	1/1	0.96	0.08	33,33,33,33	0
56	MG	BA	3696	1/1	0.96	0.08	33,33,33,33	0
56	MG	BA	3697	1/1	0.96	0.06	35,35,35,35	0
56	MG	BA	3321	1/1	0.96	0.06	54,54,54,54	0
56	MG	DA	3390	1/1	0.96	0.05	54,54,54,54	0
56	MG	BD	307	1/1	0.96	0.14	35,35,35,35	0
56	MG	DA	3647	1/1	0.96	0.10	47,47,47,47	0
56	MG	BD	308	1/1	0.96	0.07	39,39,39,39	0
56	MG	DA	3121	1/1	0.96	0.08	41,41,41,41	0
56	MG	CA	3104	1/1	0.96	0.14	64,64,64,64	0
56	MG	DA	3123	1/1	0.96	0.13	47,47,47,47	0
56	MG	BE	301	1/1	0.96	0.06	23,23,23,23	0
56	MG	AA	3008	1/1	0.96	0.07	54,54,54,54	0
56	MG	DA	3128	1/1	0.96	0.05	45,45,45,45	0
56	MG	CA	3108	1/1	0.96	0.10	51,51,51,51	0
56	MG	AA	3129	1/1	0.96	0.07	73,73,73,73	0
56	MG	DA	3659	1/1	0.96	0.24	67,67,67,67	0
56	MG	BA	3137	1/1	0.96	0.13	45,45,45,45	0
56	MG	DA	3662	1/1	0.96	0.05	27,27,27,27	0
56	MG	BA	3437	1/1	0.96	0.07	28,28,28,28	0
56	MG	BA	3565	1/1	0.96	0.12	42,42,42,42	0
56	MG	DA	3137	1/1	0.96	0.09	54,54,54,54	0
56	MG	BA	3566	1/1	0.96	0.07	30,30,30,30	0
56	MG	BA	3011	1/1	0.96	0.12	40,40,40,40	0
56	MG	DA	3141	1/1	0.96	0.13	56,56,56,56	0
56	MG	DA	3669	1/1	0.96	0.09	49,49,49,49	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	CA	3117	1/1	0.96	0.10	48,48,48,48	0
56	MG	CA	3118	1/1	0.96	0.07	47,47,47,47	0
56	MG	BA	3327	1/1	0.96	0.09	25,25,25,25	0
56	MG	BA	3569	1/1	0.96	0.12	57,57,57,57	0
56	MG	BA	3232	1/1	0.96	0.06	37,37,37,37	0
56	MG	BF	312	1/1	0.96	0.07	47,47,47,47	0
56	MG	BG	201	1/1	0.96	0.11	57,57,57,57	0
56	MG	DA	3417	1/1	0.96	0.10	33,33,33,33	0
56	MG	BG	203	1/1	0.96	0.05	36,36,36,36	0
56	MG	BA	3072	1/1	0.96	0.06	30,30,30,30	0
56	MG	BA	3574	1/1	0.96	0.08	63,63,63,63	0
56	MG	DA	3157	1/1	0.96	0.15	44,44,44,44	0
56	MG	DA	3158	1/1	0.96	0.13	40,40,40,40	0
56	MG	BA	3335	1/1	0.96	0.14	50,50,50,50	0
56	MG	BA	3338	1/1	0.96	0.09	41,41,41,41	0
56	MG	DD	302	1/1	0.96	0.09	49,49,49,49	0
56	MG	DD	303	1/1	0.96	0.12	49,49,49,49	0
56	MG	DA	3425	1/1	0.96	0.07	45,45,45,45	0
56	MG	DA	3161	1/1	0.96	0.21	49,49,49,49	0
56	MG	DE	302	1/1	0.96	0.10	39,39,39,39	0
56	MG	AA	3083	1/1	0.96	0.20	52,52,52,52	0
56	MG	CA	3130	1/1	0.96	0.14	60,60,60,60	0
56	MG	DA	3166	1/1	0.96	0.10	46,46,46,46	0
56	MG	DF	303	1/1	0.96	0.06	46,46,46,46	0
56	MG	DF	305	1/1	0.96	0.18	43,43,43,43	0
56	MG	BA	3016	1/1	0.96	0.12	44,44,44,44	0
56	MG	BA	3579	1/1	0.96	0.05	47,47,47,47	0
56	MG	DQ	3002	1/1	0.96	0.06	42,42,42,42	0
56	MG	AA	3104	1/1	0.96	0.14	50,50,50,50	0
56	MG	BA	3342	1/1	0.96	0.06	51,51,51,51	0
56	MG	BA	3344	1/1	0.96	0.06	37,37,37,37	0
56	MG	BA	3721	1/1	0.96	0.08	47,47,47,47	0
56	MG	DV	3001	1/1	0.96	0.10	71,71,71,71	0
56	MG	DA	3437	1/1	0.96	0.10	39,39,39,39	0
56	MG	BA	3345	1/1	0.96	0.08	44,44,44,44	0
56	MG	DA	3439	1/1	0.96	0.18	50,50,50,50	0
56	MG	D0	102	1/1	0.96	0.12	62,62,62,62	0
56	MG	BA	3144	1/1	0.96	0.06	43,43,43,43	0
56	MG	BU	202	1/1	0.96	0.13	40,40,40,40	0
56	MG	BU	204	1/1	0.96	0.13	38,38,38,38	0
56	MG	BU	206	1/1	0.96	0.27	43,43,43,43	0
56	MG	BA	3454	1/1	0.96	0.07	31,31,31,31	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	DA	3447	1/1	0.96	0.07	35,35,35,35	0
56	MG	DA	3257	1/1	0.97	0.09	34,34,34,34	0
56	MG	BE	308	1/1	0.97	0.04	21,21,21,21	0
56	MG	BA	3500	1/1	0.97	0.05	26,26,26,26	0
56	MG	BA	3732	1/1	0.97	0.26	40,40,40,40	0
56	MG	BF	303	1/1	0.97	0.22	42,42,42,42	0
56	MG	BA	3501	1/1	0.97	0.05	20,20,20,20	0
56	MG	DA	3265	1/1	0.97	0.17	52,52,52,52	0
56	MG	DA	3069	1/1	0.97	0.10	53,53,53,53	0
56	MG	BA	3123	1/1	0.97	0.09	35,35,35,35	0
56	MG	BA	3614	1/1	0.97	0.05	26,26,26,26	0
56	MG	DA	3269	1/1	0.97	0.07	32,32,32,32	0
56	MG	BF	309	1/1	0.97	0.14	30,30,30,30	0
56	MG	BF	310	1/1	0.97	0.22	38,38,38,38	0
56	MG	BA	3398	1/1	0.97	0.06	42,42,42,42	0
56	MG	DA	3075	1/1	0.97	0.11	39,39,39,39	0
56	MG	DA	3274	1/1	0.97	0.07	33,33,33,33	0
56	MG	DA	3275	1/1	0.97	0.06	52,52,52,52	0
56	MG	BA	3033	1/1	0.97	0.06	33,33,33,33	0
56	MG	BA	3316	1/1	0.97	0.08	23,23,23,23	0
56	MG	BA	3506	1/1	0.97	0.12	51,51,51,51	0
56	MG	BA	3125	1/1	0.97	0.07	42,42,42,42	0
56	MG	BA	3246	1/1	0.97	0.09	27,27,27,27	0
56	MG	BA	3247	1/1	0.97	0.04	28,28,28,28	0
56	MG	DA	3082	1/1	0.97	0.16	34,34,34,34	0
56	MG	BA	3182	1/1	0.97	0.12	41,41,41,41	0
56	MG	BA	3745	1/1	0.97	0.08	30,30,30,30	0
56	MG	BA	3184	1/1	0.97	0.17	30,30,30,30	0
56	MG	BP	202	1/1	0.97	0.17	34,34,34,34	0
56	MG	BP	203	1/1	0.97	0.06	32,32,32,32	0
56	MG	DA	3088	1/1	0.97	0.06	42,42,42,42	0
56	MG	BQ	3002	1/1	0.97	0.08	37,37,37,37	0
56	MG	DA	3291	1/1	0.97	0.05	42,42,42,42	0
56	MG	BA	3250	1/1	0.97	0.12	40,40,40,40	0
56	MG	DA	3519	1/1	0.97	0.04	24,24,24,24	0
56	MG	BA	3513	1/1	0.97	0.07	34,34,34,34	0
56	MG	AA	3026	1/1	0.97	0.23	53,53,53,53	0
56	MG	CA	3116	1/1	0.97	0.12	55,55,55,55	0
56	MG	BA	3035	1/1	0.97	0.12	31,31,31,31	0
56	MG	DA	3095	1/1	0.97	0.20	47,47,47,47	0
56	MG	DA	3299	1/1	0.97	0.08	43,43,43,43	0
56	MG	BA	3036	1/1	0.97	0.13	26,26,26,26	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	BA	3517	1/1	0.97	0.08	51,51,51,51	0
56	MG	BA	3518	1/1	0.97	0.10	43,43,43,43	0
56	MG	BA	3084	1/1	0.97	0.16	45,45,45,45	0
56	MG	AA	3220	1/1	0.97	0.05	64,64,64,64	0
56	MG	BA	3329	1/1	0.97	0.06	29,29,29,29	0
56	MG	DA	3308	1/1	0.97	0.10	45,45,45,45	0
56	MG	BA	3417	1/1	0.97	0.13	33,33,33,33	0
56	MG	BA	3086	1/1	0.97	0.09	41,41,41,41	0
56	MG	BV	204	1/1	0.97	0.17	50,50,50,50	0
56	MG	BA	3419	1/1	0.97	0.08	39,39,39,39	0
56	MG	DA	3313	1/1	0.97	0.07	23,23,23,23	0
56	MG	DA	3107	1/1	0.97	0.16	49,49,49,49	0
56	MG	DA	3315	1/1	0.97	0.07	41,41,41,41	0
56	MG	DA	3316	1/1	0.97	0.05	44,44,44,44	0
56	MG	DA	3544	1/1	0.97	0.12	37,37,37,37	0
56	MG	BW	202	1/1	0.97	0.14	49,49,49,49	0
56	MG	BW	203	1/1	0.97	0.16	34,34,34,34	0
56	MG	BA	3420	1/1	0.97	0.06	22,22,22,22	0
56	MG	BA	3421	1/1	0.97	0.09	33,33,33,33	0
56	MG	BA	3528	1/1	0.97	0.05	43,43,43,43	0
56	MG	DA	3322	1/1	0.97	0.13	43,43,43,43	0
56	MG	DA	3552	1/1	0.97	0.06	43,43,43,43	0
56	MG	DA	3116	1/1	0.97	0.15	57,57,57,57	0
56	MG	BA	3529	1/1	0.97	0.07	33,33,33,33	0
56	MG	BA	3642	1/1	0.97	0.10	37,37,37,37	0
56	MG	BA	3334	1/1	0.97	0.10	30,30,30,30	0
56	MG	DA	3120	1/1	0.97	0.15	45,45,45,45	0
56	MG	BA	3644	1/1	0.97	0.04	36,36,36,36	0
56	MG	DA	3329	1/1	0.97	0.04	29,29,29,29	0
56	MG	BA	3257	1/1	0.97	0.17	41,41,41,41	0
56	MG	DA	3331	1/1	0.97	0.08	39,39,39,39	0
56	MG	BA	3040	1/1	0.97	0.05	47,47,47,47	0
56	MG	BA	3042	1/1	0.97	0.18	40,40,40,40	0
56	MG	DA	3125	1/1	0.97	0.12	45,45,45,45	0
56	MG	DA	3126	1/1	0.97	0.12	44,44,44,44	0
56	MG	DA	3337	1/1	0.97	0.05	43,43,43,43	0
56	MG	BA	3043	1/1	0.97	0.21	39,39,39,39	0
56	MG	DA	3570	1/1	0.97	0.05	49,49,49,49	0
56	MG	DA	3339	1/1	0.97	0.07	52,52,52,52	0
56	MG	AA	3092	1/1	0.97	0.13	39,39,39,39	0
56	MG	B5	101	1/1	0.97	0.15	31,31,31,31	0
56	MG	DA	3130	1/1	0.97	0.13	47,47,47,47	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	AA	3093	1/1	0.97	0.14	50,50,50,50	0
56	MG	DA	3344	1/1	0.97	0.08	44,44,44,44	0
56	MG	DA	3345	1/1	0.97	0.05	35,35,35,35	0
56	MG	DA	3346	1/1	0.97	0.05	35,35,35,35	0
56	MG	BA	3537	1/1	0.97	0.07	49,49,49,49	0
56	MG	DA	3348	1/1	0.97	0.05	38,38,38,38	0
56	MG	BA	3343	1/1	0.97	0.08	33,33,33,33	0
56	MG	DA	3350	1/1	0.97	0.10	29,29,29,29	0
56	MG	DA	3134	1/1	0.97	0.09	49,49,49,49	0
56	MG	BA	3263	1/1	0.97	0.19	32,32,32,32	0
56	MG	DA	3136	1/1	0.97	0.16	44,44,44,44	0
56	MG	BA	3008	1/1	0.97	0.14	27,27,27,27	0
56	MG	AA	3065	1/1	0.97	0.14	58,58,58,58	0
56	MG	BA	3780	1/1	0.97	0.06	41,41,41,41	0
56	MG	B8	103	1/1	0.97	0.14	48,48,48,48	0
56	MG	BA	3542	1/1	0.97	0.09	48,48,48,48	0
56	MG	BA	3657	1/1	0.97	0.18	47,47,47,47	0
56	MG	BA	3097	1/1	0.97	0.15	52,52,52,52	0
56	MG	BA	3098	1/1	0.97	0.14	26,26,26,26	0
56	MG	DA	3363	1/1	0.97	0.15	54,54,54,54	0
56	MG	DA	3147	1/1	0.97	0.05	44,44,44,44	0
56	MG	DA	3148	1/1	0.97	0.08	29,29,29,29	0
56	MG	BA	3660	1/1	0.97	0.06	51,51,51,51	0
56	MG	BA	3142	1/1	0.97	0.18	34,34,34,34	0
56	MG	DA	3151	1/1	0.97	0.19	44,44,44,44	0
56	MG	BA	3205	1/1	0.97	0.16	41,41,41,41	0
56	MG	BA	3013	1/1	0.97	0.07	34,34,34,34	0
56	MG	DA	3375	1/1	0.97	0.07	40,40,40,40	0
56	MG	DA	3376	1/1	0.97	0.13	54,54,54,54	0
56	MG	BA	3665	1/1	0.97	0.12	49,49,49,49	0
56	MG	BA	3207	1/1	0.97	0.09	38,38,38,38	0
56	MG	BA	3353	1/1	0.97	0.07	49,49,49,49	0
56	MG	BA	3208	1/1	0.97	0.15	48,48,48,48	0
56	MG	BA	3445	1/1	0.97	0.06	32,32,32,32	0
56	MG	DA	3382	1/1	0.97	0.10	44,44,44,44	0
56	MG	BA	3014	1/1	0.97	0.07	33,33,33,33	0
56	MG	BA	3210	1/1	0.97	0.23	31,31,31,31	0
56	MG	DA	3162	1/1	0.97	0.12	43,43,43,43	0
56	MG	BA	3555	1/1	0.97	0.15	33,33,33,33	0
56	MG	BA	3053	1/1	0.97	0.12	22,22,22,22	0
56	MG	BA	3801	1/1	0.97	0.07	53,53,53,53	0
56	MG	BA	3146	1/1	0.97	0.06	42,42,42,42	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	DA	3391	1/1	0.97	0.05	44,44,44,44	0
56	MG	BA	3803	1/1	0.97	0.05	47,47,47,47	0
56	MG	CA	3021	1/1	0.97	0.05	42,42,42,42	0
56	MG	DA	3394	1/1	0.97	0.09	49,49,49,49	0
56	MG	AA	3009	1/1	0.97	0.10	46,46,46,46	0
56	MG	BA	3805	1/1	0.97	0.05	21,21,21,21	0
56	MG	BA	3216	1/1	0.97	0.05	34,34,34,34	0
56	MG	AA	3227	1/1	0.97	0.15	48,48,48,48	0
56	MG	BA	3151	1/1	0.97	0.07	42,42,42,42	0
56	MG	AA	3053	1/1	0.97	0.24	49,49,49,49	0
56	MG	AA	3160	1/1	0.97	0.14	57,57,57,57	0
56	MG	BA	3222	1/1	0.97	0.11	27,27,27,27	0
56	MG	DA	3180	1/1	0.97	0.10	51,51,51,51	0
56	MG	CA	3030	1/1	0.97	0.06	59,59,59,59	0
56	MG	AA	3193	1/1	0.97	0.08	43,43,43,43	0
56	MG	BA	3458	1/1	0.97	0.13	19,19,19,19	0
56	MG	BA	3816	1/1	0.97	0.06	21,21,21,21	0
56	MG	DA	3637	1/1	0.97	0.06	44,44,44,44	0
56	MG	BA	3817	1/1	0.97	0.10	47,47,47,47	0
56	MG	AA	3077	1/1	0.97	0.12	49,49,49,49	0
56	MG	DA	3641	1/1	0.97	0.06	44,44,44,44	0
56	MG	AA	3132	1/1	0.97	0.05	22,22,22,22	0
56	MG	BA	3821	1/1	0.97	0.08	50,50,50,50	0
56	MG	DA	3189	1/1	0.97	0.19	48,48,48,48	0
56	MG	BA	3687	1/1	0.97	0.05	36,36,36,36	0
56	MG	BA	3226	1/1	0.97	0.09	41,41,41,41	0
56	MG	BA	3161	1/1	0.97	0.21	37,37,37,37	0
56	MG	DA	3193	1/1	0.97	0.32	40,40,40,40	0
56	MG	BA	3572	1/1	0.97	0.10	63,63,63,63	0
56	MG	DA	3004	1/1	0.97	0.11	42,42,42,42	0
56	MG	BA	3162	1/1	0.97	0.15	46,46,46,46	0
56	MG	BA	3165	1/1	0.97	0.16	40,40,40,40	0
56	MG	BA	3296	1/1	0.97	0.12	31,31,31,31	0
56	MG	BA	3297	1/1	0.97	0.31	55,55,55,55	0
56	MG	DA	3656	1/1	0.97	0.16	62,62,62,62	0
56	MG	AF	3001	1/1	0.97	0.14	40,40,40,40	0
56	MG	BA	3299	1/1	0.97	0.09	32,32,32,32	0
56	MG	BA	3835	1/1	0.97	0.14	46,46,46,46	0
56	MG	DA	3018	1/1	0.97	0.12	41,41,41,41	0
56	MG	BA	3836	1/1	0.97	0.22	45,45,45,45	0
56	MG	BA	3837	1/1	0.97	0.09	40,40,40,40	0
56	MG	DA	3021	1/1	0.97	0.14	48,48,48,48	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	BA	3580	1/1	0.97	0.10	42,42,42,42	0
56	MG	DA	3024	1/1	0.97	0.31	40,40,40,40	0
56	MG	BA	3839	1/1	0.97	0.10	38,38,38,38	0
56	MG	BA	3378	1/1	0.97	0.05	34,34,34,34	0
56	MG	AA	3163	1/1	0.97	0.11	37,37,37,37	0
56	MG	AA	3031	1/1	0.97	0.05	44,44,44,44	0
56	MG	BA	3474	1/1	0.97	0.06	61,61,61,61	0
56	MG	DA	3215	1/1	0.97	0.09	37,37,37,37	0
56	MG	BA	3703	1/1	0.97	0.07	48,48,48,48	0
56	MG	DA	3675	1/1	0.97	0.17	44,44,44,44	0
56	MG	BA	3381	1/1	0.97	0.08	43,43,43,43	0
56	MG	DA	3032	1/1	0.97	0.05	40,40,40,40	0
56	MG	AA	3049	1/1	0.97	0.15	52,52,52,52	0
56	MG	BA	3384	1/1	0.97	0.04	30,30,30,30	0
56	MG	BA	3304	1/1	0.97	0.06	39,39,39,39	0
56	MG	BA	3589	1/1	0.97	0.05	17,17,17,17	0
56	MG	BA	3590	1/1	0.97	0.07	32,32,32,32	0
56	MG	BB	3013	1/1	0.97	0.07	42,42,42,42	0
56	MG	DA	3450	1/1	0.97	0.08	36,36,36,36	0
56	MG	BA	3306	1/1	0.97	0.18	31,31,31,31	0
56	MG	BB	3015	1/1	0.97	0.05	51,51,51,51	0
56	MG	DD	301	1/1	0.97	0.09	39,39,39,39	0
56	MG	DA	3042	1/1	0.97	0.05	41,41,41,41	0
56	MG	BB	3016	1/1	0.97	0.12	43,43,43,43	0
56	MG	DD	305	1/1	0.97	0.25	38,38,38,38	0
56	MG	DD	306	1/1	0.97	0.15	44,44,44,44	0
56	MG	DA	3455	1/1	0.97	0.06	27,27,27,27	0
56	MG	BA	3480	1/1	0.97	0.08	56,56,56,56	0
56	MG	BA	3387	1/1	0.97	0.07	65,65,65,65	0
56	MG	BA	3713	1/1	0.97	0.07	54,54,54,54	0
56	MG	BA	3307	1/1	0.97	0.10	37,37,37,37	0
56	MG	BA	3389	1/1	0.97	0.07	37,37,37,37	0
56	MG	DF	302	1/1	0.97	0.06	43,43,43,43	0
56	MG	BB	3023	1/1	0.97	0.08	46,46,46,46	0
56	MG	DF	304	1/1	0.97	0.15	39,39,39,39	0
56	MG	DA	3050	1/1	0.97	0.18	40,40,40,40	0
56	MG	BA	3484	1/1	0.97	0.12	36,36,36,36	0
56	MG	BA	3485	1/1	0.97	0.09	46,46,46,46	0
56	MG	DO	5001	1/1	0.97	0.07	51,51,51,51	0
56	MG	DQ	3001	1/1	0.97	0.06	48,48,48,48	0
56	MG	AA	3070	1/1	0.97	0.19	49,49,49,49	0
56	MG	AA	3137	1/1	0.97	0.11	42,42,42,42	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	DQ	3004	1/1	0.97	0.08	51,51,51,51	0
56	MG	BA	3489	1/1	0.97	0.06	44,44,44,44	0
56	MG	BA	3310	1/1	0.97	0.07	57,57,57,57	0
56	MG	AA	3217	1/1	0.97	0.14	55,55,55,55	0
56	MG	DA	3246	1/1	0.97	0.08	39,39,39,39	0
56	MG	AA	3013	1/1	0.97	0.06	51,51,51,51	0
56	MG	DV	3003	1/1	0.97	0.07	52,52,52,52	0
56	MG	DW	3001	1/1	0.97	0.18	43,43,43,43	0
56	MG	DA	3472	1/1	0.97	0.05	33,33,33,33	0
56	MG	BE	303	1/1	0.97	0.15	27,27,27,27	0
56	MG	DY	502	1/1	0.97	0.09	52,52,52,52	0
56	MG	DA	3249	1/1	0.97	0.10	41,41,41,41	0
56	MG	D7	101	1/1	0.97	0.18	39,39,39,39	0
56	MG	BA	3395	1/1	0.97	0.11	44,44,44,44	0
56	MG	DA	3479	1/1	0.97	0.08	50,50,50,50	0
56	MG	BA	3494	1/1	0.97	0.17	57,57,57,57	0
56	MG	DA	3252	1/1	0.97	0.05	29,29,29,29	0
59	ZN	CN	501	1/1	0.97	0.07	92,92,92,92	0
59	ZN	DY	501	1/1	0.97	0.07	106,106,106,106	0
56	MG	BA	3120	1/1	0.97	0.07	32,32,32,32	0
60	K	AX	3001	1/1	0.97	0.08	57,57,57,57	0
56	MG	BA	3497	1/1	0.97	0.14	41,41,41,41	0
56	MG	BA	3573	1/1	0.98	0.04	32,32,32,32	0
56	MG	DA	3011	1/1	0.98	0.07	40,40,40,40	0
56	MG	BA	3735	1/1	0.98	0.13	35,35,35,35	0
56	MG	DA	3013	1/1	0.98	0.07	40,40,40,40	0
56	MG	BA	3498	1/1	0.98	0.07	54,54,54,54	0
56	MG	DA	3140	1/1	0.98	0.10	34,34,34,34	0
56	MG	DA	3016	1/1	0.98	0.04	53,53,53,53	0
56	MG	BA	3827	1/1	0.98	0.12	30,30,30,30	0
56	MG	BA	3425	1/1	0.98	0.09	29,29,29,29	0
56	MG	BA	3426	1/1	0.98	0.04	22,22,22,22	0
56	MG	BA	3830	1/1	0.98	0.10	21,21,21,21	0
56	MG	DA	3146	1/1	0.98	0.10	46,46,46,46	0
56	MG	BA	3189	1/1	0.98	0.08	30,30,30,30	0
56	MG	AA	3117	1/1	0.98	0.07	48,48,48,48	0
56	MG	B3	102	1/1	0.98	0.10	35,35,35,35	0
56	MG	B3	103	1/1	0.98	0.05	45,45,45,45	0
56	MG	DA	3431	1/1	0.98	0.03	25,25,25,25	0
56	MG	BA	3108	1/1	0.98	0.11	24,24,24,24	0
56	MG	BA	3834	1/1	0.98	0.06	35,35,35,35	0
56	MG	BA	3243	1/1	0.98	0.07	44,44,44,44	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	DA	3290	1/1	0.98	0.09	44,44,44,44	0
56	MG	BA	3301	1/1	0.98	0.08	26,26,26,26	0
56	MG	DA	3292	1/1	0.98	0.06	37,37,37,37	0
56	MG	BA	3074	1/1	0.98	0.12	32,32,32,32	0
56	MG	DA	3156	1/1	0.98	0.11	43,43,43,43	0
56	MG	BA	3245	1/1	0.98	0.14	29,29,29,29	0
56	MG	DA	3441	1/1	0.98	0.07	43,43,43,43	0
56	MG	DA	3033	1/1	0.98	0.04	31,31,31,31	0
56	MG	BA	3076	1/1	0.98	0.07	23,23,23,23	0
56	MG	B7	101	1/1	0.98	0.08	33,33,33,33	0
56	MG	BA	3305	1/1	0.98	0.09	33,33,33,33	0
56	MG	CA	3106	1/1	0.98	0.10	50,50,50,50	0
56	MG	BA	3664	1/1	0.98	0.04	43,43,43,43	0
56	MG	B8	102	1/1	0.98	0.07	50,50,50,50	0
56	MG	DA	3165	1/1	0.98	0.09	33,33,33,33	0
56	MG	DA	3304	1/1	0.98	0.04	40,40,40,40	0
56	MG	BA	3368	1/1	0.98	0.05	12,12,12,12	0
56	MG	BA	3050	1/1	0.98	0.06	31,31,31,31	0
56	MG	DA	3307	1/1	0.98	0.07	45,45,45,45	0
56	MG	BA	3080	1/1	0.98	0.04	24,24,24,24	0
56	MG	CA	3112	1/1	0.98	0.05	59,59,59,59	0
56	MG	AA	3056	1/1	0.98	0.10	46,46,46,46	0
56	MG	BA	3440	1/1	0.98	0.09	29,29,29,29	0
56	MG	BA	3147	1/1	0.98	0.10	30,30,30,30	0
56	MG	DA	3173	1/1	0.98	0.05	30,30,30,30	0
56	MG	BA	3148	1/1	0.98	0.07	15,15,15,15	0
56	MG	DA	3175	1/1	0.98	0.08	53,53,53,53	0
56	MG	BA	3443	1/1	0.98	0.03	25,25,25,25	0
56	MG	AA	3138	1/1	0.98	0.07	34,34,34,34	0
56	MG	DA	3622	1/1	0.98	0.04	53,53,53,53	0
56	MG	AX	3005	1/1	0.98	0.04	44,44,44,44	0
56	MG	BA	3054	1/1	0.98	0.09	30,30,30,30	0
56	MG	BA	3009	1/1	0.98	0.05	25,25,25,25	0
56	MG	AA	3035	1/1	0.98	0.06	46,46,46,46	0
56	MG	BB	3017	1/1	0.98	0.04	33,33,33,33	0
56	MG	BA	3037	1/1	0.98	0.20	37,37,37,37	0
56	MG	BA	3088	1/1	0.98	0.14	50,50,50,50	0
56	MG	BA	3157	1/1	0.98	0.11	36,36,36,36	0
56	MG	DA	3473	1/1	0.98	0.05	49,49,49,49	0
56	MG	BA	3121	1/1	0.98	0.20	41,41,41,41	0
56	MG	DA	3475	1/1	0.98	0.05	42,42,42,42	0
56	MG	DA	3476	1/1	0.98	0.10	45,45,45,45	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	CA	3017	1/1	0.98	0.06	49,49,49,49	0
56	MG	BA	3383	1/1	0.98	0.05	24,24,24,24	0
56	MG	BA	3159	1/1	0.98	0.12	30,30,30,30	0
56	MG	CA	3131	1/1	0.98	0.06	55,55,55,55	0
56	MG	BA	3160	1/1	0.98	0.09	32,32,32,32	0
56	MG	DA	3640	1/1	0.98	0.07	52,52,52,52	0
56	MG	BA	3122	1/1	0.98	0.20	26,26,26,26	0
56	MG	BA	3607	1/1	0.98	0.07	40,40,40,40	0
56	MG	DA	3334	1/1	0.98	0.06	32,32,32,32	0
56	MG	BD	304	1/1	0.98	0.06	48,48,48,48	0
56	MG	BA	3211	1/1	0.98	0.25	36,36,36,36	0
56	MG	BA	3772	1/1	0.98	0.04	31,31,31,31	0
56	MG	BA	3609	1/1	0.98	0.06	20,20,20,20	0
56	MG	BA	3212	1/1	0.98	0.20	42,42,42,42	0
56	MG	BD	310	1/1	0.98	0.07	31,31,31,31	0
56	MG	BD	311	1/1	0.98	0.09	51,51,51,51	0
56	MG	DA	3492	1/1	0.98	0.07	47,47,47,47	0
56	MG	BA	3691	1/1	0.98	0.04	38,38,38,38	0
56	MG	DA	3494	1/1	0.98	0.11	30,30,30,30	0
56	MG	BE	302	1/1	0.98	0.09	34,34,34,34	0
56	MG	BA	3776	1/1	0.98	0.05	49,49,49,49	0
56	MG	BA	3024	1/1	0.98	0.05	22,22,22,22	0
56	MG	BA	3163	1/1	0.98	0.11	45,45,45,45	0
56	MG	BA	3164	1/1	0.98	0.07	43,43,43,43	0
56	MG	DA	3660	1/1	0.98	0.09	40,40,40,40	0
56	MG	BA	3039	1/1	0.98	0.22	47,47,47,47	0
56	MG	BA	3330	1/1	0.98	0.14	29,29,29,29	0
56	MG	BA	3332	1/1	0.98	0.09	30,30,30,30	0
56	MG	BA	3217	1/1	0.98	0.12	20,20,20,20	0
56	MG	BA	3092	1/1	0.98	0.22	41,41,41,41	0
56	MG	DA	3212	1/1	0.98	0.15	44,44,44,44	0
56	MG	BF	304	1/1	0.98	0.12	32,32,32,32	0
56	MG	BA	3012	1/1	0.98	0.09	26,26,26,26	0
56	MG	DA	3356	1/1	0.98	0.08	20,20,20,20	0
56	MG	DA	3670	1/1	0.98	0.15	38,38,38,38	0
56	MG	BA	3336	1/1	0.98	0.06	35,35,35,35	0
56	MG	BA	3337	1/1	0.98	0.05	35,35,35,35	0
56	MG	BA	3400	1/1	0.98	0.05	25,25,25,25	0
56	MG	BA	3061	1/1	0.98	0.05	40,40,40,40	0
56	MG	CA	3047	1/1	0.98	0.13	35,35,35,35	0
56	MG	BA	3276	1/1	0.98	0.12	41,41,41,41	0
56	MG	BA	3792	1/1	0.98	0.14	32,32,32,32	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	BA	3549	1/1	0.98	0.12	37,37,37,37	0
56	MG	BA	3627	1/1	0.98	0.09	45,45,45,45	0
56	MG	BA	3041	1/1	0.98	0.16	18,18,18,18	0
56	MG	DA	3368	1/1	0.98	0.10	50,50,50,50	0
56	MG	DA	3520	1/1	0.98	0.07	48,48,48,48	0
56	MG	BA	3129	1/1	0.98	0.06	36,36,36,36	0
56	MG	DA	3522	1/1	0.98	0.08	25,25,25,25	0
56	MG	BN	3003	1/1	0.98	0.04	38,38,38,38	0
56	MG	BA	3405	1/1	0.98	0.09	33,33,33,33	0
56	MG	BA	3026	1/1	0.98	0.04	19,19,19,19	0
56	MG	DA	3373	1/1	0.98	0.04	31,31,31,31	0
56	MG	BA	3173	1/1	0.98	0.09	36,36,36,36	0
56	MG	DD	304	1/1	0.98	0.10	31,31,31,31	0
56	MG	DA	3230	1/1	0.98	0.06	33,33,33,33	0
56	MG	BA	3800	1/1	0.98	0.06	39,39,39,39	0
56	MG	BA	3174	1/1	0.98	0.07	34,34,34,34	0
56	MG	BA	3556	1/1	0.98	0.06	45,45,45,45	0
56	MG	DA	3104	1/1	0.98	0.08	46,46,46,46	0
56	MG	BQ	3001	1/1	0.98	0.15	40,40,40,40	0
56	MG	DA	3236	1/1	0.98	0.09	48,48,48,48	0
56	MG	AA	3001	1/1	0.98	0.07	34,34,34,34	0
56	MG	BA	3065	1/1	0.98	0.04	37,37,37,37	0
56	MG	DA	3108	1/1	0.98	0.07	30,30,30,30	0
56	MG	BA	3177	1/1	0.98	0.11	44,44,44,44	0
56	MG	BA	3412	1/1	0.98	0.10	41,41,41,41	0
56	MG	DA	3388	1/1	0.98	0.04	35,35,35,35	0
56	MG	DA	3242	1/1	0.98	0.04	43,43,43,43	0
56	MG	AA	3133	1/1	0.98	0.09	30,30,30,30	0
56	MG	DA	3112	1/1	0.98	0.16	42,42,42,42	0
56	MG	BA	3045	1/1	0.98	0.07	42,42,42,42	0
56	MG	DA	3114	1/1	0.98	0.03	28,28,28,28	0
56	MG	BA	3231	1/1	0.98	0.16	37,37,37,37	0
56	MG	BR	204	1/1	0.98	0.20	42,42,42,42	0
56	MG	BA	3722	1/1	0.98	0.08	50,50,50,50	0
56	MG	AA	3075	1/1	0.98	0.09	33,33,33,33	0
56	MG	DA	3551	1/1	0.98	0.12	55,55,55,55	0
56	MG	AA	3012	1/1	0.98	0.05	33,33,33,33	0
56	MG	BU	205	1/1	0.98	0.20	38,38,38,38	0
56	MG	BA	3814	1/1	0.98	0.11	26,26,26,26	0
56	MG	DA	3255	1/1	0.98	0.06	59,59,59,59	0
56	MG	BU	207	1/1	0.98	0.07	29,29,29,29	0
56	MG	BA	3071	1/1	0.98	0.17	42,42,42,42	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	D0	101	1/1	0.98	0.07	56,56,56,56	0
56	MG	CA	3077	1/1	0.98	0.04	48,48,48,48	0
56	MG	D3	3001	1/1	0.98	0.06	58,58,58,58	0
56	MG	BA	3183	1/1	0.98	0.06	40,40,40,40	0
56	MG	BA	3104	1/1	0.98	0.07	27,27,27,27	0
56	MG	BV	205	1/1	0.98	0.07	32,32,32,32	0
56	MG	DA	3003	1/1	0.98	0.08	20,20,20,20	0
56	MG	BA	3294	1/1	0.98	0.15	45,45,45,45	0
58	SF4	AD	501	8/8	0.98	0.06	56,62,64,76	0
58	SF4	CD	501	8/8	0.98	0.04	54,64,76,87	0
56	MG	BA	3495	1/1	0.98	0.07	34,34,34,34	0
56	MG	BA	3730	1/1	0.98	0.10	27,27,27,27	0
56	MG	BA	3048	1/1	0.98	0.12	28,28,28,28	0
59	ZN	D9	501	1/1	0.98	0.04	63,63,63,63	0
56	MG	DA	3008	1/1	0.98	0.06	33,33,33,33	0
56	MG	BA	3188	1/1	0.98	0.09	19,19,19,19	0
56	MG	BA	3526	1/1	0.99	0.04	32,32,32,32	0
56	MG	DA	3259	1/1	0.99	0.03	34,34,34,34	0
56	MG	BB	3007	1/1	0.99	0.03	36,36,36,36	0
56	MG	BA	3813	1/1	0.99	0.03	4,4,4,4	0
56	MG	BA	3168	1/1	0.99	0.08	27,27,27,27	0
56	MG	BA	3155	1/1	0.99	0.07	54,54,54,54	0
56	MG	DA	3572	1/1	0.99	0.04	28,28,28,28	0
56	MG	DA	3264	1/1	0.99	0.04	31,31,31,31	0
56	MG	BU	209	1/1	0.99	0.11	27,27,27,27	0
56	MG	DA	3364	1/1	0.99	0.04	38,38,38,38	0
56	MG	DA	3576	1/1	0.99	0.04	37,37,37,37	0
56	MG	BV	201	1/1	0.99	0.14	29,29,29,29	0
56	MG	BV	202	1/1	0.99	0.04	26,26,26,26	0
56	MG	BA	3324	1/1	0.99	0.04	34,34,34,34	0
56	MG	CA	3138	1/1	0.99	0.10	59,59,59,59	0
56	MG	DA	3524	1/1	0.99	0.07	38,38,38,38	0
56	MG	BA	3611	1/1	0.99	0.04	42,42,42,42	0
56	MG	BA	3107	1/1	0.99	0.09	20,20,20,20	0
56	MG	BA	3819	1/1	0.99	0.08	32,32,32,32	0
56	MG	BF	308	1/1	0.99	0.05	36,36,36,36	0
56	MG	BA	3185	1/1	0.99	0.03	32,32,32,32	0
56	MG	DA	3374	1/1	0.99	0.05	37,37,37,37	0
56	MG	AA	3173	1/1	0.99	0.04	47,47,47,47	0
56	MG	BA	3187	1/1	0.99	0.12	36,36,36,36	0
56	MG	BA	3790	1/1	0.99	0.06	32,32,32,32	0
56	MG	BA	3075	1/1	0.99	0.08	27,27,27,27	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	BG	202	1/1	0.99	0.06	46,46,46,46	0
56	MG	BA	3731	1/1	0.99	0.09	23,23,23,23	0
56	MG	BA	3272	1/1	0.99	0.13	11,11,11,11	0
56	MG	DA	3651	1/1	0.99	0.08	47,47,47,47	0
56	MG	BA	3415	1/1	0.99	0.08	29,29,29,29	0
56	MG	BA	3675	1/1	0.99	0.12	37,37,37,37	0
56	MG	BA	3331	1/1	0.99	0.09	32,32,32,32	0
56	MG	BA	3018	1/1	0.99	0.09	34,34,34,34	0
56	MG	BA	3462	1/1	0.99	0.03	11,11,11,11	0
56	MG	BA	3487	1/1	0.99	0.08	25,25,25,25	0
56	MG	BA	3077	1/1	0.99	0.23	34,34,34,34	0
56	MG	BA	3239	1/1	0.99	0.12	31,31,31,31	0
56	MG	AA	3171	1/1	0.99	0.04	48,48,48,48	0
56	MG	BA	3466	1/1	0.99	0.06	28,28,28,28	0
56	MG	BD	309	1/1	0.99	0.15	37,37,37,37	0
56	MG	DA	3444	1/1	0.99	0.05	30,30,30,30	0
56	MG	BA	3069	1/1	0.99	0.08	31,31,31,31	0
56	MG	DA	3015	1/1	0.99	0.09	31,31,31,31	0
56	MG	BA	3091	1/1	0.99	0.13	38,38,38,38	0
56	MG	DA	3017	1/1	0.99	0.08	28,28,28,28	0
56	MG	AM	201	1/1	0.99	0.03	50,50,50,50	0
56	MG	AA	3151	1/1	0.99	0.04	41,41,41,41	0
56	MG	AA	3225	1/1	0.99	0.05	26,26,26,26	0
56	MG	BA	3282	1/1	0.99	0.07	24,24,24,24	0
56	MG	DA	3022	1/1	0.99	0.09	40,40,40,40	0
59	ZN	BY	501	1/1	0.99	0.03	58,58,58,58	0
59	ZN	B4	501	1/1	0.99	0.06	73,73,73,73	0
59	ZN	B6	103	1/1	0.99	0.03	29,29,29,29	0
59	ZN	B9	501	1/1	0.99	0.07	49,49,49,49	0
56	MG	BR	205	1/1	0.99	0.08	29,29,29,29	0
56	MG	DA	3254	1/1	0.99	0.10	21,21,21,21	0
56	MG	BA	3010	1/1	0.99	0.05	29,29,29,29	0
59	ZN	D5	501	1/1	0.99	0.04	53,53,53,53	0
59	ZN	D6	501	1/1	0.99	0.04	73,73,73,73	0
56	MG	DA	3563	1/1	0.99	0.03	42,42,42,42	0
56	MG	BA	3499	1/1	0.99	0.11	33,33,33,33	0
56	MG	BU	203	1/1	0.99	0.04	31,31,31,31	0
59	ZN	AN	501	1/1	1.00	0.02	58,58,58,58	0
56	MG	BA	3003	1/1	1.00	0.05	20,20,20,20	0
56	MG	BA	3078	1/1	1.00	0.04	17,17,17,17	0
59	ZN	B5	104	1/1	1.00	0.02	38,38,38,38	0
56	MG	BA	3265	1/1	1.00	0.12	29,29,29,29	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	AA	3224	1/1	1.00	0.05	33,33,33,33	0
56	MG	DA	3554	1/1	1.00	0.02	23,23,23,23	0

5.5 Other polymers [i](#)

There are no such residues in this entry.