



wwPDB X-ray Structure Validation Summary Report ⓘ

Sep 16, 2026 – 06:14 am BST

PDB ID : 5IB7 / pdb_00005ib7
Title : Structure of T. thermophilus 70S ribosome complex with mRNA, tRNA^{fMet}, near-cognate tRNA^{Lys} with U-G mismatch in the A-site and antibiotic paromomycin
Authors : Rozov, A.; Demeshkina, N.; Yusupov, M.; Yusupova, G.
Deposited on : 2016-02-22
Resolution : 2.99 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	FAILED
Mogul	:	1.8.4, CSD as541be (2020)
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	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

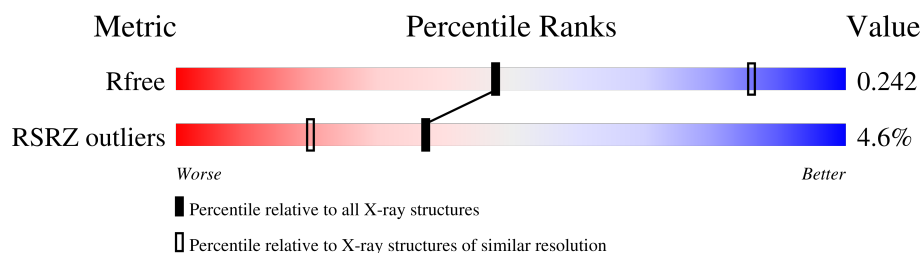
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.99 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	2672 (3.00-3.00)
RSRZ outliers	180081	2671 (3.00-3.00)

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

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
57	MG	13	1643	-	-	-	X
57	MG	13	1669	-	-	-	X
57	MG	13	1671	-	-	-	X
57	MG	13	1676	-	-	-	X
57	MG	14	3088	-	-	-	X
57	MG	14	3197	-	-	-	X
57	MG	14	3208	-	-	-	X
57	MG	1H	3151	-	-	-	X
57	MG	1H	3157	-	-	-	X
57	MG	1H	3206	-	-	-	X

2 Entry composition

There are 62 unique types of molecules in this entry. The entry contains 297444 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	13	1499	Total	C	N	O	P	0	0	0
			32223	14342	5973	10409	1499			
1	1G	1508	Total	C	N	O	P	0	0	0
			32414	14427	6005	10474	1508			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
13	1542	G	-	expression tag	GB 55771382
13	1543	C	-	expression tag	GB 55771382
13	1544	U	-	expression tag	GB 55771382
1G	1542	G	-	expression tag	GB 55771382
1G	1543	C	-	expression tag	GB 55771382
1G	1544	U	-	expression tag	GB 55771382

- Molecule 2 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	1E	231	Total	C	N	O	S	0	0	0
			1874	1199	334	336	5			
2	12	207	Total	C	N	O	S	0	0	0
			1696	1083	306	303	4			

- Molecule 3 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	2E	205	Total	C	N	O	S	0	0	0
			1605	1011	313	280	1			
3	22	195	Total	C	N	O	S	0	0	0
			1537	973	297	266	1			

- Molecule 4 is a protein called 30S ribosomal protein S4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	3E	207	Total	C	N	O	S	0	0	0
			1698	1064	338	289	7			
4	32	208	Total	C	N	O	S	0	0	0
			1702	1066	339	290	7			

- Molecule 5 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	4E	149	Total	C	N	O	S	0	0	0
			1142	722	216	200	4			
5	42	150	Total	C	N	O	S	0	0	0
			1141	719	217	201	4			

- Molecule 6 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	5E	100	Total	C	N	O	S	0	0	0
			837	528	154	152	3			
6	52	101	Total	C	N	O	S	0	0	0
			842	531	155	153	3			

- Molecule 7 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	6E	154	Total	C	N	O	S	0	0	0
			1242	770	250	216	6			
7	62	138	Total	C	N	O	S	0	0	0
			1110	689	221	194	6			

- Molecule 8 is a protein called 30S ribosomal protein S8.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	7E	138	Total	C	N	O	S	0	0	0
			1115	705	215	192	3			
8	72	137	Total	C	N	O	S	0	0	0
			1107	700	214	191	2			

- Molecule 9 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	8E	126	Total	C	N	O		0	0	0
			1000	634	196	170				

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
9	82	121	Total	C	N	O	0	0	0
			953	605	186	162			

- Molecule 10 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	1I	94	Total	C	N	O	S	0	0	0
			749	468	147	133	1			
10	1A	80	Total	C	N	O		0	0	0
			646	403	129	114				

- Molecule 11 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	2I	111	Total	C	N	O	S	0	0	0
			823	512	154	154	3			
11	2A	113	Total	C	N	O	S	0	0	0
			835	520	156	156	3			

- Molecule 12 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	3I	122	Total	C	N	O	S	0	0	0
			956	603	193	159	1			
12	3A	121	Total	C	N	O	S	0	0	0
			947	597	191	158	1			

- Molecule 13 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	4I	117	Total	C	N	O	S	0	0	0
			933	577	192	162	2			
13	4A	109	Total	C	N	O	S	0	0	0
			879	544	181	152	2			

- Molecule 14 is a protein called 30S ribosomal protein S14 type Z.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	5I	59	Total	C	N	O	S	0	0	0
			486	309	103	70	4			
14	5A	59	Total	C	N	O	S	0	0	0
			486	309	103	70	4			

- Molecule 15 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	6I	87	Total	C	N	O	S	0	0	0
			729	457	146	124	2			
15	6A	87	Total	C	N	O	S	0	0	0
			729	457	146	124	2			

- Molecule 16 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	7I	83	Total	C	N	O	S	0	0	0
			700	443	139	117	1			
16	7A	84	Total	C	N	O	S	0	0	0
			705	446	140	118	1			

- Molecule 17 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	8I	99	Total	C	N	O	S	0	0	0
			823	528	151	142	2			
17	8A	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	9I	68	Total	C	N	O	0	0	0
			549	352	105	92			
18	9A	67	Total	C	N	O	0	0	0
			544	349	104	91			

- Molecule 19 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	AI	82	Total	C	N	O	S	0	0	0
			661	422	123	114	2			
19	AA	65	Total	C	N	O	S	0	0	0
			510	324	92	92	2			

- Molecule 20 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	BI	97	Total	C	N	O	S	0	0	0
			746	461	157	126	2			
20	BA	99	Total	C	N	O	S	0	0	0
			762	470	162	128	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
21	1F	23	Total	C	N	O		0	0	0
			199	122	48	29				
21	1B	22	Total	C	N	O		0	0	0
			188	116	44	28				

- Molecule 22 is a RNA chain called tRNA^{Lys}.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
22	1K	72	Total	C	N	O	P	S	0	0	0
			1542	691	269	509	72	1			

- Molecule 23 is a RNA chain called tRNA^{fMet}.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
23	2K	77	Total	C	N	O	P	S	0	0	0
			1646	735	298	535	77	1			
23	2L	77	Total	C	N	O	P	S	0	0	0
			1646	735	298	535	77	1			

- Molecule 24 is a RNA chain called tRNA^{Lys}.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	3K	70	Total	C	N	O	P	0	0	0
			1483	664	260	490	69			
24	1L	66	Total	C	N	O	P	0	0	0
			1401	626	244	465	66			
24	3L	72	Total	C	N	O	P	0	0	0
			1528	684	270	503	71			

- Molecule 25 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
25	4K	19	Total	C	N	O	P	0	0	0
			420	188	89	124	19			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
25	4L	19	Total	C	N	O	P	0	0	0
			419	188	89	123	19			

- Molecule 26 is a RNA chain called 23S ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	1H	2860	Total	C	N	O	P	0	0	0
			61609	27418	11525	19806	2860			
26	14	2826	Total	C	N	O	P	0	0	0
			60877	27092	11393	19566	2826			

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
1H	161	U	UNK	conflict	GB 55771382
1H	654A	A	G	conflict	GB 55771382
1H	654E	C	G	conflict	GB 55771382
1H	654P	G	C	conflict	GB 55771382
1H	654T	A	C	conflict	GB 55771382
1H	1059B	U	G	conflict	GB 55771382
1H	1080	A	C	conflict	GB 55771382
14	158	U	UNK	conflict	GB 55771382
14	654A	A	G	conflict	GB 55771382
14	654E	C	G	conflict	GB 55771382
14	654P	G	C	conflict	GB 55771382
14	654T	A	C	conflict	GB 55771382
14	1058	U	G	conflict	GB 55771382
14	1080	A	C	conflict	GB 55771382

- Molecule 27 is a RNA chain called 5S ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
27	16	122	Total	C	N	O	P	0	0	0
			2617	1166	486	844	121			
27	1J	122	Total	C	N	O	P	0	0	0
			2617	1166	486	844	121			

- Molecule 28 is a protein called 50S ribosomal protein L1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
28	71	132	Total	C	N	O	S	0	0	0
			1027	648	193	185	1			

- Molecule 29 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
29	11	273	Total	C	N	O	S	0	0	0
			2120	1338	421	358	3			
29	19	274	Total	C	N	O	S	0	0	0
			2125	1341	422	359	3			

- Molecule 30 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
30	21	203	Total	C	N	O	S	0	0	0
			1546	978	295	267	6			
30	29	204	Total	C	N	O	S	0	0	0
			1563	988	299	270	6			

- Molecule 31 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
31	31	202	Total	C	N	O	S	0	0	0
			1585	1011	297	275	2			
31	39	204	Total	C	N	O	S	0	0	0
			1602	1022	299	279	2			

- Molecule 32 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
32	41	179	Total	C	N	O	S	0	0	0
			1457	931	265	257	4			
32	49	180	Total	C	N	O	S	0	0	0
			1459	931	266	258	4			

- Molecule 33 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
33	51	174	Total	C	N	O	S	0	0	0
			1328	842	249	236	1			
33	59	169	Total	C	N	O	S	0	0	0
			1295	823	241	230	1			

- Molecule 34 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
34	61	145	Total	C	N	O	S	0	0	0
			1131	723	200	207	1			
34	69	145	Total	C	N	O	S	0	0	0
			1131	723	200	207	1			

- Molecule 35 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
35	58	137	Total	C	N	O	S	0	0	0
			1096	706	205	181	4			
35	15	137	Total	C	N	O	S	0	0	0
			1096	707	205	181	3			

- Molecule 36 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
36	68	122	Total	C	N	O	S	0	0	0
			932	588	171	169	4			
36	25	122	Total	C	N	O	S	0	0	0
			932	588	171	169	4			

- Molecule 37 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
37	78	147	Total	C	N	O	S	0	0	0
			1122	698	229	192	3			
37	35	147	Total	C	N	O	S	0	0	0
			1122	698	229	192	3			

- Molecule 38 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
38	88	141	Total	C	N	O	S	0	0	0
			1117	712	211	187	7			
38	45	138	Total	C	N	O	S	0	0	0
			1099	702	208	183	6			

- Molecule 39 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
39	98	118	Total	C	N	O	S	0	0	0
			967	604	203	159	1			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
39	55	118	Total	C	N	O	S	0	0	0
			967	604	203	159	1			

- Molecule 40 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
40	A8	111	Total	C	N	O		0	0	0
			881	556	176	149				
40	65	110	Total	C	N	O		0	0	0
			876	553	175	148				

- Molecule 41 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
41	B8	135	Total	C	N	O	S	0	0	0
			1119	697	230	191	1			
41	75	133	Total	C	N	O	S	0	0	0
			1109	691	228	189	1			

- Molecule 42 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
42	C8	115	Total	C	N	O	S	0	0	0
			950	603	199	147	1			
42	85	116	Total	C	N	O	S	0	0	0
			959	608	201	149	1			

- Molecule 43 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
43	D8	100	Total	C	N	O	S	0	0	0
			774	499	141	133	1			
43	95	100	Total	C	N	O	S	0	0	0
			770	496	140	133	1			

- Molecule 44 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
44	E8	110	Total	C	N	O	S	0	0	0
			876	552	171	151	2			
44	A5	111	Total	C	N	O	S	0	0	0
			886	558	174	152	2			

- Molecule 45 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
45	F8	95	Total	C	N	O	S	0	0	0
			750	488	135	126	1			
45	B5	94	Total	C	N	O		0	0	0
			735	477	133	125				

- Molecule 46 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
46	G8	103	Total	C	N	O	S	0	0	0
			783	504	148	126	5			
46	C5	104	Total	C	N	O	S	0	0	0
			794	510	152	127	5			

- Molecule 47 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
47	H8	170	Total	C	N	O	S	0	0	0
			1365	870	246	246	3			
47	D5	177	Total	C	N	O	S	0	0	0
			1411	901	253	255	2			

- Molecule 48 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
48	I8	77	Total	C	N	O	S	0	0	0
			611	378	129	103	1			
48	E5	76	Total	C	N	O	S	0	0	0
			603	372	128	102	1			

- Molecule 49 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
49	J8	96	Total	C	N	O	S	0	0	0
			747	469	148	129	1			
49	F5	94	Total	C	N	O	S	0	0	0
			737	463	146	127	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
50	K8	68	Total	C	N	O	S	0	0	0
			575	358	116	100	1			
50	G5	69	Total	C	N	O	S	0	0	0
			576	358	116	101	1			

- Molecule 51 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
51	L8	58	Total	C	N	O	S	0	0	0
			459	293	89	77				
51	H5	58	Total	C	N	O	S	0	0	0
			459	293	89	77				

- Molecule 52 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
52	M8	60	Total	C	N	O	S	0	0	0
			475	300	84	86	5			

- Molecule 53 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
53	N8	48	Total	C	N	O	S	0	0	0
			369	229	75	60	5			
53	J5	56	Total	C	N	O	S	0	0	0
			434	272	87	70	5			

- Molecule 54 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
54	O8	45	Total	C	N	O	S	0	0	0
			389	241	79	65	4			

- Molecule 55 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
55	P8	47	Total	C	N	O	S	0	0	0
			401	246	99	54	2			
55	L5	47	Total	C	N	O	S	0	0	0
			401	246	99	54	2			

- Molecule 56 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
56	Q8	64	Total	C	N	O	S	0	0	0
			516	331	102	81	2			
56	M5	64	Total	C	N	O	S	0	0	0
			516	331	102	81	2			

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

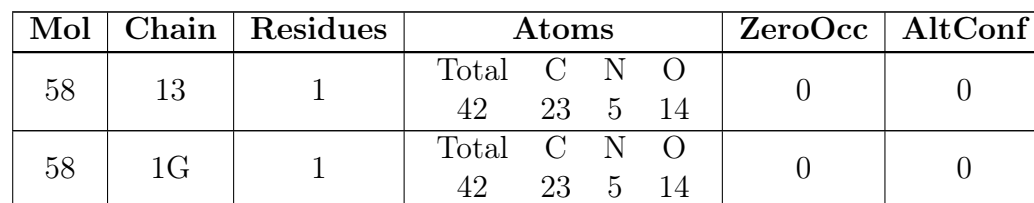
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	13	140	Total	Mg	0	0
			140	140		
57	3I	1	Total	Mg	0	0
			1	1		
57	4I	1	Total	Mg	0	0
			1	1		
57	5I	1	Total	Mg	0	0
			1	1		
57	2K	2	Total	Mg	0	0
			2	2		
57	1H	525	Total	Mg	0	0
			525	525		
57	16	11	Total	Mg	0	0
			11	11		
57	21	3	Total	Mg	0	0
			3	3		
57	31	2	Total	Mg	0	0
			2	2		
57	41	1	Total	Mg	0	0
			1	1		
57	78	1	Total	Mg	0	0
			1	1		
57	88	3	Total	Mg	0	0
			3	3		
57	I8	2	Total	Mg	0	0
			2	2		
57	P8	1	Total	Mg	0	0
			1	1		
57	Q8	1	Total	Mg	0	0
			1	1		
57	1G	102	Total	Mg	0	0
			102	102		
57	32	1	Total	Mg	0	0
			1	1		
57	42	1	Total	Mg	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	52	1	Total 1	Mg 1	0	0
57	7A	1	Total 1	Mg 1	0	0
57	2L	2	Total 2	Mg 2	0	0
57	4L	1	Total 1	Mg 1	0	0
57	14	435	Total 435	Mg 435	0	0
57	1J	8	Total 8	Mg 8	0	0
57	19	1	Total 1	Mg 1	0	0
57	29	1	Total 1	Mg 1	0	0
57	39	2	Total 2	Mg 2	0	0
57	25	1	Total 1	Mg 1	0	0
57	35	1	Total 1	Mg 1	0	0
57	45	2	Total 2	Mg 2	0	0
57	C5	1	Total 1	Mg 1	0	0
57	E5	1	Total 1	Mg 1	0	0
57	M5	1	Total 1	Mg 1	0	0

- Molecule 58 is PAROMOMYCIN (CCD ID: PAR) (formula: $C_{23}H_{45}N_5O_{14}$).



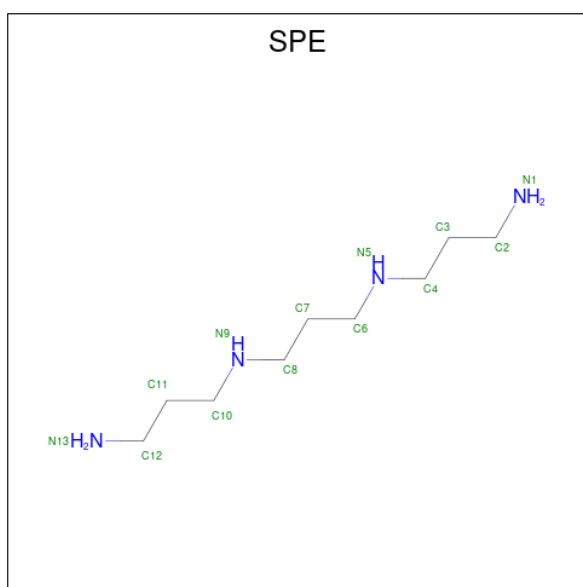
-
- The diagram shows a cubane-like complex with four iron (Fe) atoms at the corners of a cube and four sulfur (S) atoms at the centers of the edges. The sulfur atoms are labeled S1, S2, S3, and S4. The iron atoms are labeled FE1, FE2, FE3, and FE4. The sulfur atoms are shown with a charge of -2 (S⁻²). The iron atoms are shown with a charge of 0 (Fe). The bonds between the iron and sulfur atoms are represented by lines. The structure is shown in a perspective view.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
59	3E	1	Total 8	Fe 4	S 4	0	0
59	32	1	Total 8	Fe 4	S 4	0	0

- Molecule 60 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
60	5I	1	Total	Zn	0	0
			1	1		
60	G8	1	Total	Zn	0	0
			1	1		
60	5A	1	Total	Zn	0	0
			1	1		
60	C5	1	Total	Zn	0	0
			1	1		

- Molecule 61 is THERMINE (CCD ID: SPE) (formula: C₉H₂₄N₄).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
61	1G	1	Total	C	N	0	0
			13	9	4		
61	14	1	Total	C	N	0	0
			13	9	4		
61	14	1	Total	C	N	0	0
			13	9	4		

- Molecule 62 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
62	13	320	Total	O	0	0
			320	320		
62	4E	3	Total	O	0	0
			3	3		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
62	8E	2	Total 2	O 2	0	0
62	1I	2	Total 2	O 2	0	0
62	3I	2	Total 2	O 2	0	0
62	5I	2	Total 2	O 2	0	0
62	6I	3	Total 3	O 3	0	0
62	7I	1	Total 1	O 1	0	0
62	BI	2	Total 2	O 2	0	0
62	1F	1	Total 1	O 1	0	0
62	1K	2	Total 2	O 2	0	0
62	2K	8	Total 8	O 8	0	0
62	4K	5	Total 5	O 5	0	0
62	1H	1470	Total 1470	O 1470	0	0
62	16	12	Total 12	O 12	0	0
62	11	17	Total 17	O 17	0	0
62	21	7	Total 7	O 7	0	0
62	31	5	Total 5	O 5	0	0
62	41	1	Total 1	O 1	0	0
62	58	2	Total 2	O 2	0	0
62	78	10	Total 10	O 10	0	0
62	B8	1	Total 1	O 1	0	0
62	C8	3	Total 3	O 3	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
62	F8	2	Total 2	O 2	0	0
62	G8	2	Total 2	O 2	0	0
62	I8	6	Total 6	O 6	0	0
62	J8	4	Total 4	O 4	0	0
62	L8	3	Total 3	O 3	0	0
62	P8	1	Total 1	O 1	0	0
62	Q8	5	Total 5	O 5	0	0
62	1G	317	Total 317	O 317	0	0
62	32	1	Total 1	O 1	0	0
62	52	4	Total 4	O 4	0	0
62	1A	1	Total 1	O 1	0	0
62	6A	2	Total 2	O 2	0	0
62	7A	5	Total 5	O 5	0	0
62	9A	2	Total 2	O 2	0	0
62	BA	2	Total 2	O 2	0	0
62	2L	6	Total 6	O 6	0	0
62	4L	6	Total 6	O 6	0	0
62	14	1144	Total 1144	O 1144	0	0
62	1J	12	Total 12	O 12	0	0
62	19	15	Total 15	O 15	0	0
62	29	4	Total 4	O 4	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
62	39	5	Total	O	0	0
			5	5		
62	15	1	Total	O	0	0
			1	1		
62	25	6	Total	O	0	0
			6	6		
62	35	8	Total	O	0	0
			8	8		
62	55	3	Total	O	0	0
			3	3		
62	85	2	Total	O	0	0
			2	2		
62	A5	1	Total	O	0	0
			1	1		
62	B5	1	Total	O	0	0
			1	1		
62	C5	3	Total	O	0	0
			3	3		
62	F5	1	Total	O	0	0
			1	1		
62	H5	2	Total	O	0	0
			2	2		
62	M5	9	Total	O	0	0
			9	9		

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	209.30Å 448.80Å 620.20Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	147.08 – 2.99 147.08 – 2.99	Depositor EDS
% Data completeness (in resolution range)	99.9 (147.08-2.99) 90.8 (147.08-2.99)	Depositor EDS
R_{merge}	0.34	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.92 (at 3.01Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.202 , 0.241 0.204 , 0.242	Depositor DCC
R_{free} test set	2000 reflections (0.17%)	wwPDB-VP
Wilson B-factor (Å ²)	81.3	Xtriage
Anisotropy	0.342	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 70.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	297444	wwPDB-VP
Average B, all atoms (Å ²)	104.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.49% 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](#)

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
23	5MU	2L	55	23	19,22,23	4.00	5 (26%)	28,32,35	3.11	8 (28%)
23	5MU	2K	55	23	19,22,23	3.89	5 (26%)	28,32,35	3.15	9 (32%)
23	PSU	2K	56	23	18,21,22	1.32	2 (11%)	22,30,33	1.79	3 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
22	5MU	1K	54	22	19,22,23	3.94	5 (26%)	28,32,35	2.92	7 (25%)
22	U8U	1K	34	25,22	19,24,25	2.61	7 (36%)	23,34,37	1.18	2 (8%)
22	T6A	1K	37	22	31,34,35	2.14	8 (25%)	44,49,52	2.37	14 (31%)
22	PSU	1K	39	22	18,21,22	1.02	1 (5%)	22,30,33	1.53	4 (18%)
23	OMC	2K	33	23	19,22,23	1.82	3 (15%)	26,31,34	1.03	2 (7%)
22	PSU	1K	55	22	18,21,22	1.28	1 (5%)	22,30,33	1.56	4 (18%)
23	PSU	2L	56	23	18,21,22	1.25	2 (11%)	22,30,33	1.45	2 (9%)
23	4SU	2L	8	23	18,21,22	1.95	4 (22%)	26,30,33	2.36	5 (19%)
23	7MG	2K	47	23	22,26,27	2.88	7 (31%)	29,39,42	2.89	10 (34%)
23	4SU	2K	8	23	18,21,22	1.66	3 (16%)	26,30,33	2.38	4 (15%)
23	OMC	2L	33	23	19,22,23	1.78	4 (21%)	26,31,34	1.26	2 (7%)
23	7MG	2L	47	23	22,26,27	3.01	8 (36%)	29,39,42	2.86	10 (34%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	5MU	2L	55	23	-	0/7/25/26	0/2/2/2
23	5MU	2K	55	23	-	0/7/25/26	0/2/2/2
23	PSU	2K	56	23	-	0/7/25/26	0/2/2/2
22	5MU	1K	54	22	-	0/7/25/26	0/2/2/2
22	U8U	1K	34	25,22	-	0/9/28/29	0/2/2/2
22	T6A	1K	37	22	-	6/23/41/42	0/3/3/3
22	PSU	1K	39	22	-	0/7/25/26	0/2/2/2
23	OMC	2K	33	23	-	0/9/27/28	0/2/2/2
22	PSU	1K	55	22	-	2/7/25/26	0/2/2/2
23	PSU	2L	56	23	-	0/7/25/26	0/2/2/2
23	4SU	2L	8	23	-	3/7/25/26	0/2/2/2
23	7MG	2K	47	23	-	4/7/37/38	0/3/3/3
23	4SU	2K	8	23	-	2/7/25/26	0/2/2/2
23	OMC	2L	33	23	-	1/9/27/28	0/2/2/2
23	7MG	2L	47	23	-	2/7/37/38	0/3/3/3

The worst 5 of 65 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	2L	55	5MU	C2-N1	12.89	1.59	1.38
22	1K	54	5MU	C2-N1	12.63	1.58	1.38
23	2K	55	5MU	C2-N1	12.52	1.58	1.38
23	2L	47	7MG	C5-N7	8.90	1.45	1.35
23	2K	47	7MG	C5-N7	8.03	1.44	1.35

The worst 5 of 86 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	2L	55	5MU	C5-C4-N3	9.89	123.75	115.31
23	2K	55	5MU	C5-C4-N3	9.69	123.58	115.31
22	1K	54	5MU	C5-C4-N3	9.41	123.34	115.31
23	2L	8	4SU	C4-N3-C2	-8.13	119.44	127.34
23	2K	8	4SU	C4-N3-C2	-7.63	119.93	127.34

There are no chirality outliers.

5 of 20 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
22	1K	37	T6A	C14-C12-N11-C10
22	1K	37	T6A	N11-C12-C14-O14
22	1K	37	T6A	C13-C12-C14-O14
22	1K	37	T6A	C13-C12-C14-C15
23	2K	8	4SU	C3'-C4'-C5'-O5'

There are no ring outliers.

No monomer is involved in short contacts.

4.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

4.6 Ligand geometry [i](#)

Of 1269 ligands modelled in this entry, 1262 are monoatomic - leaving 7 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	$\# Z > 2$
59	SF4	3E	301	4	0,12,12	-	-	-		
61	SPE	14	3436	-	12,12,12	0.43	0	11,11,11	0.65	0
58	PAR	1G	1702	-	45,45,45	0.67	1 (2%)	64,67,67	1.39	9 (14%)
61	SPE	1G	1703	-	12,12,12	0.35	0	11,11,11	0.76	0
58	PAR	13	1741	1	45,45,45	0.68	0	64,67,67	1.48	10 (15%)
59	SF4	32	302	4	0,12,12	-	-	-		
61	SPE	14	3437	26	12,12,12	0.83	0	11,11,11	0.96	1 (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
59	SF4	3E	301	4	-	-	0/6/5/5
61	SPE	14	3436	-	-	5/10/10/10	-
58	PAR	1G	1702	-	-	1/18/94/94	0/4/4/4
61	SPE	1G	1703	-	-	3/10/10/10	-
58	PAR	13	1741	1	-	5/18/94/94	0/4/4/4
59	SF4	32	302	4	-	-	0/6/5/5
61	SPE	14	3437	26	-	5/10/10/10	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
58	1G	1702	PAR	C24-N24	-2.22	1.43	1.47

The worst 5 of 20 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
58	13	1741	PAR	C32-C22-C12	3.69	118.76	111.18
58	13	1741	PAR	C11-O51-C51	3.65	120.85	113.69
58	1G	1702	PAR	C14-O33-C33	-3.57	109.14	117.96
58	13	1741	PAR	C22-C12-C62	3.28	115.00	110.04
58	1G	1702	PAR	C13-O52-C52	-3.28	109.84	117.96

There are no chirality outliers.

5 of 19 torsion outliers are listed below:

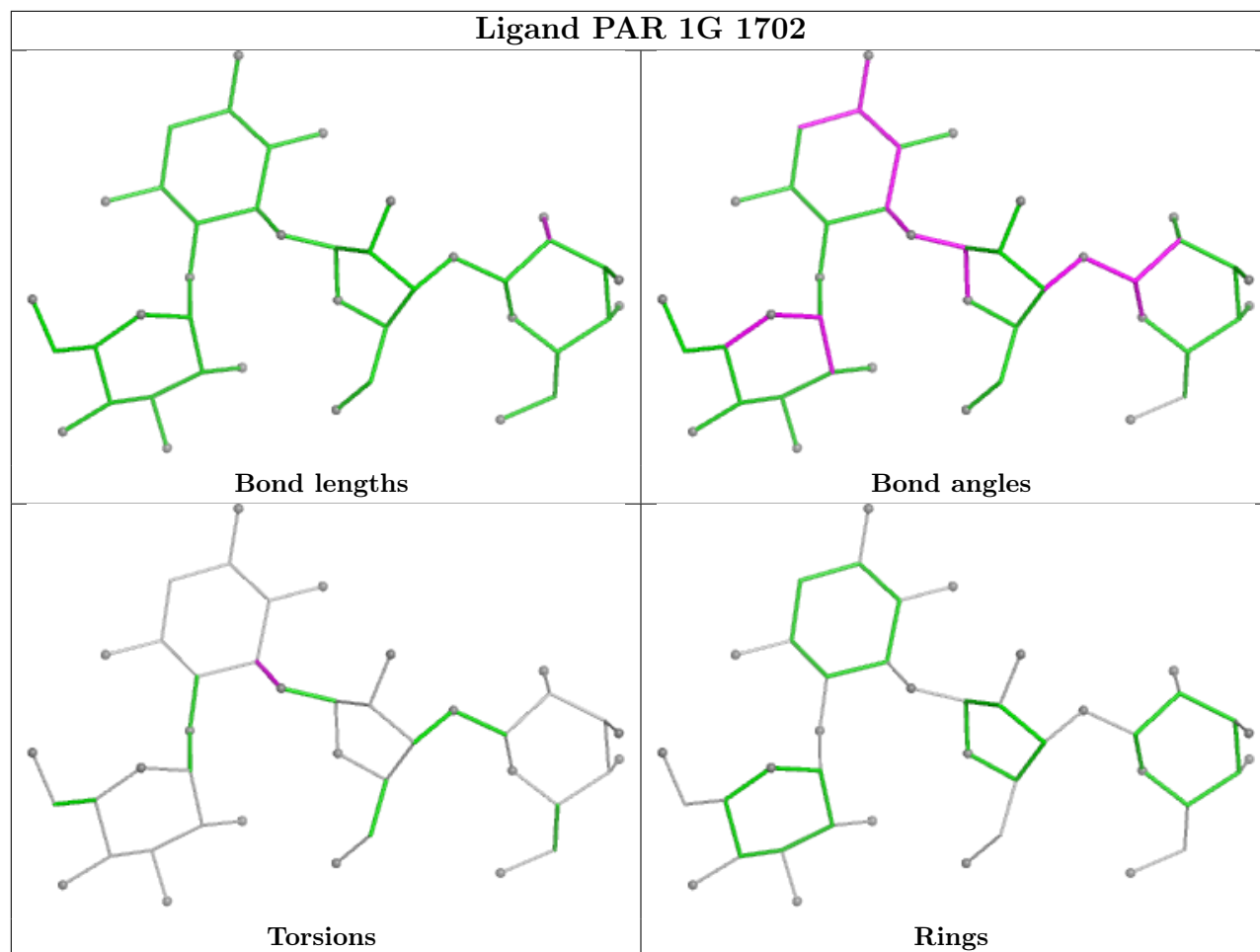
Mol	Chain	Res	Type	Atoms
58	13	1741	PAR	C44-C54-C64-N64
58	13	1741	PAR	O54-C54-C64-N64
61	1G	1703	SPE	C2-C3-C4-N5
61	14	3437	SPE	C6-C7-C8-N9
61	14	3437	SPE	N9-C10-C11-C12

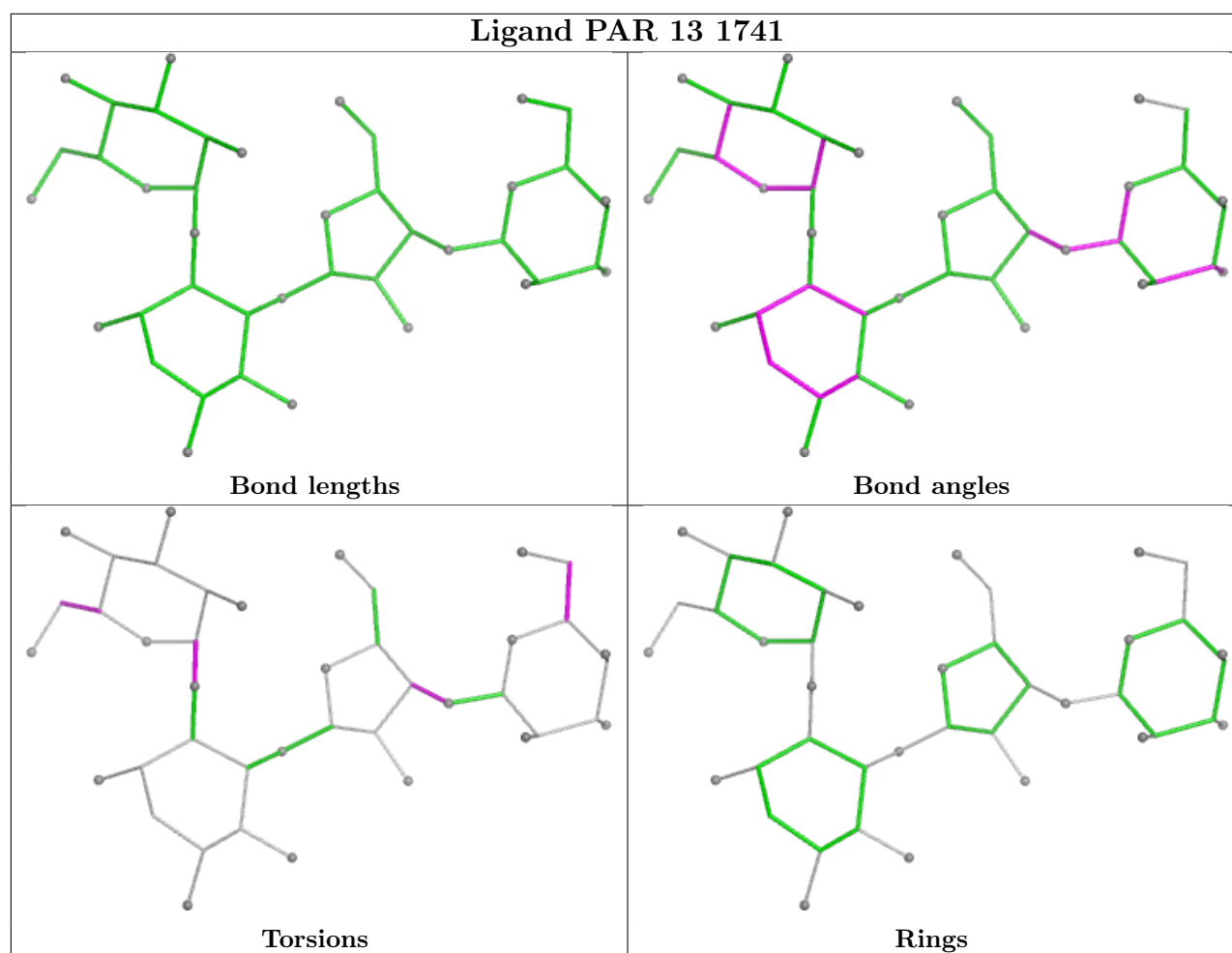
There are no ring outliers.

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.

Ligand PAR 1G 1702





4.7 Other polymers [i](#)

There are no such residues in this entry.

4.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
10	1A	2
26	1H	1
24	1L	1
47	D5	1
4	3E	1

The worst 5 of 6 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	1H	1055:G	O3'	1059:G	P	14.13
1	1L	72:C	O3'	73:A	P	3.25
1	1A	38:ILE	C	39:PRO	N	1.71
1	1A	76:ASN	C	77:PRO	N	1.61
1	D5	94:GLU	C	95:PRO	N	1.61

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	13	1499/1522 (98%)	-0.15	28 (1%) 66 43	57, 100, 176, 247	0
1	1G	1508/1522 (99%)	-0.01	39 (2%) 57 34	71, 119, 192, 267	0
2	12	207/256 (80%)	0.90	27 (13%) 7 4	131, 164, 184, 192	0
2	1E	231/256 (90%)	0.99	36 (15%) 5 3	112, 143, 169, 174	0
3	22	195/239 (81%)	0.80	18 (9%) 14 8	135, 160, 173, 178	0
3	2E	205/239 (85%)	0.45	8 (3%) 43 24	88, 111, 143, 151	0
4	32	208/209 (99%)	0.52	10 (4%) 35 19	92, 113, 136, 142	0
4	3E	207/209 (99%)	0.72	12 (5%) 29 15	84, 108, 132, 144	0
5	42	150/162 (92%)	0.83	11 (7%) 21 11	108, 128, 148, 160	0
5	4E	149/162 (91%)	0.61	7 (4%) 36 19	82, 103, 121, 131	0
6	52	101/101 (100%)	0.46	2 (1%) 65 41	85, 104, 121, 132	0
6	5E	100/101 (99%)	0.58	9 (9%) 15 8	85, 105, 120, 132	0
7	62	138/156 (88%)	0.52	12 (8%) 16 8	116, 130, 141, 147	0
7	6E	154/156 (98%)	0.30	4 (2%) 57 34	102, 120, 150, 171	0
8	72	137/138 (99%)	0.74	7 (5%) 33 17	100, 131, 142, 149	0
8	7E	138/138 (100%)	0.46	4 (2%) 53 31	93, 110, 122, 134	0
9	82	121/128 (94%)	0.96	16 (13%) 7 4	116, 163, 174, 182	0
9	8E	126/128 (98%)	0.64	14 (11%) 10 6	87, 138, 157, 163	0
10	1A	80/105 (76%)	2.02	30 (37%) 1 1	133, 156, 169, 174	0
10	1I	94/105 (89%)	0.59	4 (4%) 40 21	81, 131, 168, 173	0
11	2A	113/129 (87%)	0.72	10 (8%) 15 8	84, 109, 124, 135	0
11	2I	111/129 (86%)	0.51	3 (2%) 56 33	72, 107, 123, 133	0
12	3A	121/132 (91%)	1.24	19 (15%) 5 3	90, 112, 135, 151	0
12	3I	122/132 (92%)	0.43	11 (9%) 15 8	66, 76, 102, 135	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	4A	109/126 (86%)	0.76	17 (15%) 5 3	123, 150, 180, 194	0
13	4I	117/126 (92%)	0.57	10 (8%) 16 8	88, 116, 131, 138	0
14	5A	59/61 (96%)	1.29	12 (20%) 3 2	137, 158, 180, 183	0
14	5I	59/61 (96%)	0.23	2 (3%) 48 27	81, 96, 114, 122	0
15	6A	87/89 (97%)	0.03	2 (2%) 61 38	84, 113, 128, 131	0
15	6I	87/89 (97%)	0.09	1 (1%) 78 57	80, 98, 113, 123	0
16	7A	84/88 (95%)	0.63	8 (9%) 14 7	92, 105, 129, 155	0
16	7I	83/88 (94%)	0.97	10 (12%) 9 5	96, 111, 137, 155	0
17	8A	99/105 (94%)	0.37	2 (2%) 65 41	97, 113, 130, 135	0
17	8I	99/105 (94%)	0.35	5 (5%) 33 17	89, 106, 115, 124	0
18	9A	67/88 (76%)	0.91	8 (11%) 9 5	92, 112, 132, 138	0
18	9I	68/88 (77%)	0.47	3 (4%) 39 21	88, 107, 131, 135	0
19	AA	65/93 (69%)	1.31	14 (21%) 2 1	162, 178, 187, 192	0
19	AI	82/93 (88%)	0.45	5 (6%) 27 14	96, 117, 138, 151	0
20	BA	99/106 (93%)	0.24	2 (2%) 65 41	90, 114, 140, 152	0
20	BI	97/106 (91%)	0.26	3 (3%) 51 30	106, 119, 145, 151	0
21	1B	22/27 (81%)	0.57	1 (4%) 38 20	127, 141, 145, 148	0
21	1F	23/27 (85%)	-0.16	0 100 100	92, 99, 107, 115	0
22	1K	67/76 (88%)	1.52	17 (25%) 1 1	90, 193, 226, 233	0
23	2K	72/77 (93%)	0.11	1 (1%) 73 51	67, 92, 124, 140	0
23	2L	72/77 (93%)	0.72	5 (6%) 23 12	80, 116, 152, 163	0
24	1L	66/76 (86%)	1.67	22 (33%) 1 1	145, 224, 245, 249	0
24	3K	70/76 (92%)	0.98	9 (12%) 7 5	76, 229, 251, 253	0
24	3L	72/76 (94%)	1.63	20 (27%) 1 1	85, 220, 238, 240	0
25	4K	19/30 (63%)	0.93	3 (15%) 5 3	71, 140, 219, 219	0
25	4L	19/30 (63%)	1.09	4 (21%) 2 1	98, 158, 230, 230	0
26	14	2826/2917 (96%)	-0.29	23 (0%) 82 64	50, 85, 199, 264	0
26	1H	2860/2917 (98%)	-0.47	28 (0%) 79 59	40, 69, 186, 257	0
27	16	122/122 (100%)	-0.62	0 100 100	61, 88, 107, 197	0
27	1J	122/122 (100%)	-0.08	2 (1%) 70 47	85, 119, 145, 205	0
28	7I	132/229 (57%)	0.51	6 (4%) 38 20	146, 210, 235, 243	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
29	11	273/276 (98%)	-0.00	6 (2%) 62 39	41, 63, 79, 93	0
29	19	274/276 (99%)	0.38	19 (6%) 23 12	47, 73, 88, 107	0
30	21	203/206 (98%)	0.40	11 (5%) 31 16	48, 84, 120, 130	0
30	29	204/206 (99%)	0.46	16 (7%) 19 10	60, 95, 134, 149	0
31	31	202/210 (96%)	-0.10	3 (1%) 72 49	46, 76, 112, 127	0
31	39	204/210 (97%)	0.35	11 (5%) 31 16	57, 101, 148, 177	0
32	41	179/182 (98%)	0.28	10 (5%) 30 15	79, 100, 134, 146	0
32	49	180/182 (98%)	0.56	10 (5%) 30 15	117, 138, 156, 174	0
33	51	174/180 (96%)	0.51	12 (6%) 23 12	77, 102, 119, 130	0
33	59	169/180 (93%)	1.35	39 (23%) 2 1	152, 196, 220, 233	0
34	61	145/148 (97%)	0.40	10 (6%) 23 12	76, 131, 149, 157	0
34	69	145/148 (97%)	0.43	13 (8%) 15 8	86, 122, 149, 156	0
35	15	137/140 (97%)	1.06	18 (13%) 7 4	81, 108, 135, 151	0
35	58	137/140 (97%)	0.54	8 (5%) 29 15	63, 85, 121, 138	0
36	25	122/122 (100%)	0.18	1 (0%) 82 64	69, 88, 105, 117	0
36	68	122/122 (100%)	0.05	2 (1%) 70 47	56, 72, 90, 99	0
37	35	147/150 (98%)	0.45	6 (4%) 41 23	58, 102, 135, 152	0
37	78	147/150 (98%)	-0.04	2 (1%) 73 51	47, 80, 104, 115	0
38	45	138/141 (97%)	0.86	15 (10%) 10 6	76, 105, 124, 155	0
38	88	141/141 (100%)	0.01	2 (1%) 73 51	54, 75, 95, 123	0
39	55	118/118 (100%)	-0.07	1 (0%) 82 64	65, 80, 97, 112	0
39	98	118/118 (100%)	0.02	0 100 100	60, 78, 94, 106	0
40	65	110/112 (98%)	0.60	5 (4%) 38 20	89, 112, 132, 137	0
40	A8	111/112 (99%)	0.05	3 (2%) 56 33	72, 85, 105, 116	0
41	75	133/146 (91%)	0.23	5 (3%) 44 24	80, 96, 128, 151	0
41	B8	135/146 (92%)	0.63	12 (8%) 15 8	67, 84, 128, 139	0
42	85	116/118 (98%)	0.66	8 (6%) 23 12	63, 96, 127, 134	0
42	C8	115/118 (97%)	0.40	4 (3%) 47 27	53, 77, 102, 108	0
43	95	100/101 (99%)	0.73	4 (4%) 42 23	65, 116, 135, 142	0
43	D8	100/101 (99%)	0.48	3 (3%) 52 30	53, 101, 119, 126	0
44	A5	111/113 (98%)	0.23	2 (1%) 67 44	57, 75, 101, 137	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
44	E8	110/113 (97%)	0.27	5 (4%) 38 20	53, 70, 94, 106	0
45	B5	94/96 (97%)	0.23	4 (4%) 40 21	68, 83, 104, 118	0
45	F8	95/96 (98%)	0.09	2 (2%) 63 40	49, 66, 97, 110	0
46	C5	104/110 (94%)	1.57	32 (30%) 1 1	92, 118, 156, 164	0
46	G8	103/110 (93%)	0.81	13 (12%) 8 5	73, 95, 122, 130	0
47	D5	177/206 (85%)	0.49	5 (2%) 55 32	108, 148, 226, 236	0
47	H8	170/206 (82%)	0.14	1 (0%) 85 69	80, 116, 202, 210	0
48	E5	76/85 (89%)	0.33	4 (5%) 32 16	66, 88, 102, 115	0
48	I8	77/85 (90%)	-0.10	4 (5%) 33 17	54, 69, 91, 102	0
49	F5	94/98 (95%)	0.54	4 (4%) 40 21	60, 83, 122, 136	0
49	J8	96/98 (97%)	0.43	6 (6%) 26 13	51, 71, 126, 138	0
50	G5	69/72 (95%)	0.46	5 (7%) 21 11	81, 104, 124, 138	0
50	K8	68/72 (94%)	0.19	2 (2%) 53 31	59, 79, 96, 120	0
51	H5	58/60 (96%)	0.32	0 100 100	77, 99, 122, 135	0
51	L8	58/60 (96%)	-0.17	0 100 100	60, 77, 103, 110	0
52	M8	60/71 (84%)	0.78	5 (8%) 17 9	102, 143, 168, 171	0
53	J5	56/60 (93%)	0.42	6 (10%) 11 6	58, 85, 131, 141	0
53	N8	48/60 (80%)	0.02	1 (2%) 63 40	46, 78, 119, 127	0
54	O8	45/54 (83%)	1.28	10 (22%) 2 1	117, 153, 171, 177	0
55	L5	47/49 (95%)	-0.27	1 (2%) 63 40	47, 60, 87, 97	0
55	P8	47/49 (95%)	-0.43	1 (2%) 63 40	42, 50, 72, 87	0
56	M5	64/65 (98%)	0.44	4 (6%) 26 13	68, 80, 97, 117	0
56	Q8	64/65 (98%)	0.01	1 (1%) 70 47	51, 65, 80, 98	0
All	All	20730/21798 (95%)	0.17	963 (4%) 37 20	40, 99, 184, 267	0

The worst 5 of 963 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
41	B8	104	ASN	9.4
9	82	115	GLY	8.7
24	3L	35	U	8.3
22	1K	76	A	7.7
24	3L	34	U	7.6

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
22	PSU	1K	55	20/21	0.83	0.10	107,127,140,145	0
23	7MG	2L	47	24/25	0.85	0.11	118,128,137,141	0
23	PSU	2L	56	20/21	0.85	0.08	109,121,126,126	0
22	5MU	1K	54	21/22	0.86	0.09	104,125,133,143	0
23	4SU	2L	8	20/21	0.86	0.12	107,118,124,125	0
23	5MU	2L	55	21/22	0.87	0.10	115,122,127,130	0
23	OMC	2L	33	21/22	0.87	0.13	94,103,107,109	0
23	7MG	2K	47	24/25	0.89	0.10	96,101,113,116	0
23	PSU	2K	56	20/21	0.89	0.07	91,101,110,117	0
23	5MU	2K	55	21/22	0.89	0.09	98,105,112,114	0
23	4SU	2K	8	20/21	0.90	0.12	89,95,101,103	0
22	U8U	1K	34	23/24	0.93	0.12	83,98,108,110	0
22	T6A	1K	37	32/33	0.94	0.16	81,92,114,116	0
22	PSU	1K	39	20/21	0.94	0.20	94,112,118,120	0
23	OMC	2K	33	21/22	0.95	0.15	73,79,82,94	0

5.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
57	MG	14	3017	1/1	0.31	0.30	119,119,119,119	0
57	MG	14	3187	1/1	0.40	0.28	117,117,117,117	0
57	MG	13	1678	1/1	0.46	0.24	112,112,112,112	0
57	MG	14	3072	1/1	0.49	0.29	94,94,94,94	0
57	MG	14	3129	1/1	0.57	0.31	118,118,118,118	0
57	MG	14	3060	1/1	0.59	0.33	98,98,98,98	0
57	MG	1H	3136	1/1	0.59	0.32	116,116,116,116	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	14	3154	1/1	0.61	0.26	95,95,95,95	0
57	MG	14	3177	1/1	0.61	0.33	101,101,101,101	0
57	MG	1H	3081	1/1	0.61	0.33	83,83,83,83	0
57	MG	13	1659	1/1	0.62	0.21	126,126,126,126	0
57	MG	1J	202	1/1	0.62	0.32	92,92,92,92	0
57	MG	1G	1640	1/1	0.63	0.29	108,108,108,108	0
57	MG	1H	3119	1/1	0.63	0.35	83,83,83,83	0
57	MG	1G	1623	1/1	0.63	0.26	115,115,115,115	0
57	MG	1H	3216	1/1	0.64	0.36	82,82,82,82	0
57	MG	1H	3204	1/1	0.65	0.25	91,91,91,91	0
57	MG	1G	1642	1/1	0.65	0.28	99,99,99,99	0
57	MG	1G	1628	1/1	0.65	0.26	113,113,113,113	0
57	MG	14	3153	1/1	0.65	0.35	90,90,90,90	0
57	MG	13	1671	1/1	0.66	0.41	79,79,79,79	0
57	MG	1H	3148	1/1	0.66	0.39	83,83,83,83	0
57	MG	14	3163	1/1	0.66	0.26	93,93,93,93	0
57	MG	1H	3237	1/1	0.67	0.25	81,81,81,81	0
57	MG	14	3144	1/1	0.67	0.29	102,102,102,102	0
57	MG	1G	1602	1/1	0.67	0.28	106,106,106,106	0
57	MG	13	1675	1/1	0.67	0.35	101,101,101,101	0
57	MG	1H	3221	1/1	0.68	0.18	73,73,73,73	0
57	MG	1H	3157	1/1	0.68	0.41	89,89,89,89	0
57	MG	4L	101	1/1	0.68	0.16	131,131,131,131	0
57	MG	1H	3242	1/1	0.68	0.34	90,90,90,90	0
57	MG	1H	3144	1/1	0.68	0.38	102,102,102,102	0
57	MG	1H	3206	1/1	0.68	0.42	93,93,93,93	0
57	MG	14	3208	1/1	0.68	0.41	88,88,88,88	0
57	MG	13	1651	1/1	0.68	0.31	98,98,98,98	0
57	MG	14	3136	1/1	0.69	0.37	92,92,92,92	0
57	MG	13	1676	1/1	0.69	0.41	93,93,93,93	0
57	MG	14	3183	1/1	0.69	0.23	103,103,103,103	0
57	MG	1G	1631	1/1	0.70	0.32	92,92,92,92	0
57	MG	1H	3043	1/1	0.70	0.26	75,75,75,75	0
57	MG	1H	3151	1/1	0.70	0.41	80,80,80,80	0
57	MG	1G	1609	1/1	0.71	0.38	92,92,92,92	0
57	MG	14	3101	1/1	0.72	0.27	87,87,87,87	0
57	MG	16	203	1/1	0.72	0.17	82,82,82,82	0
57	MG	14	3201	1/1	0.72	0.28	88,88,88,88	0
57	MG	13	1645	1/1	0.72	0.31	92,92,92,92	0
57	MG	1H	3172	1/1	0.72	0.18	83,83,83,83	0
57	MG	1H	3088	1/1	0.73	0.34	80,80,80,80	0
57	MG	14	3157	1/1	0.73	0.31	92,92,92,92	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	1H	3061	1/1	0.73	0.14	53,53,53,53	0
57	MG	14	3175	1/1	0.73	0.25	88,88,88,88	0
57	MG	14	3430	1/1	0.73	0.12	107,107,107,107	0
57	MG	1G	1608	1/1	0.73	0.21	93,93,93,93	0
57	MG	35	201	1/1	0.74	0.17	75,75,75,75	0
57	MG	1H	3044	1/1	0.75	0.29	67,67,67,67	0
57	MG	1H	3174	1/1	0.75	0.13	55,55,55,55	0
57	MG	1H	3201	1/1	0.75	0.29	104,104,104,104	0
57	MG	1G	1641	1/1	0.75	0.34	103,103,103,103	0
57	MG	13	1626	1/1	0.75	0.28	84,84,84,84	0
57	MG	1H	3150	1/1	0.75	0.34	98,98,98,98	0
57	MG	1H	3120	1/1	0.75	0.31	88,88,88,88	0
57	MG	14	3046	1/1	0.75	0.25	79,79,79,79	0
57	MG	13	1643	1/1	0.75	0.41	101,101,101,101	0
57	MG	13	1668	1/1	0.76	0.22	66,66,66,66	0
57	MG	1H	3106	1/1	0.76	0.32	87,87,87,87	0
57	MG	1H	3008	1/1	0.76	0.27	82,82,82,82	0
57	MG	13	1661	1/1	0.76	0.23	90,90,90,90	0
57	MG	1G	1605	1/1	0.76	0.31	104,104,104,104	0
57	MG	1H	3180	1/1	0.76	0.35	90,90,90,90	0
57	MG	1H	3235	1/1	0.76	0.27	71,71,71,71	0
57	MG	88	201	1/1	0.77	0.26	76,76,76,76	0
57	MG	1G	1635	1/1	0.77	0.20	105,105,105,105	0
57	MG	1H	3129	1/1	0.77	0.14	76,76,76,76	0
57	MG	1H	3230	1/1	0.77	0.25	82,82,82,82	0
57	MG	13	1641	1/1	0.77	0.18	81,81,81,81	0
57	MG	14	3197	1/1	0.77	0.48	77,77,77,77	0
57	MG	1H	3141	1/1	0.77	0.26	83,83,83,83	0
57	MG	14	3152	1/1	0.77	0.19	78,78,78,78	0
57	MG	14	3008	1/1	0.77	0.23	77,77,77,77	0
57	MG	13	1679	1/1	0.77	0.33	99,99,99,99	0
57	MG	4I	200	1/1	0.77	0.30	95,95,95,95	0
57	MG	45	201	1/1	0.77	0.20	101,101,101,101	0
57	MG	1H	3321	1/1	0.78	0.14	86,86,86,86	0
57	MG	1H	3085	1/1	0.78	0.31	70,70,70,70	0
57	MG	14	3169	1/1	0.78	0.28	85,85,85,85	0
57	MG	14	3097	1/1	0.78	0.22	97,97,97,97	0
57	MG	1H	3130	1/1	0.78	0.10	63,63,63,63	0
57	MG	14	3112	1/1	0.78	0.18	83,83,83,83	0
57	MG	14	3122	1/1	0.78	0.18	75,75,75,75	0
57	MG	1H	3006	1/1	0.78	0.16	74,74,74,74	0
57	MG	14	3134	1/1	0.78	0.27	85,85,85,85	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	1H	3222	1/1	0.78	0.22	69,69,69,69	0
57	MG	13	1628	1/1	0.78	0.23	91,91,91,91	0
57	MG	1H	3024	1/1	0.78	0.24	83,83,83,83	0
57	MG	1J	206	1/1	0.78	0.26	94,94,94,94	0
57	MG	1H	3029	1/1	0.78	0.26	77,77,77,77	0
57	MG	1H	3127	1/1	0.78	0.23	91,91,91,91	0
57	MG	14	3195	1/1	0.79	0.17	78,78,78,78	0
57	MG	1H	3156	1/1	0.79	0.28	83,83,83,83	0
57	MG	14	3198	1/1	0.79	0.31	81,81,81,81	0
57	MG	1H	3113	1/1	0.79	0.21	81,81,81,81	0
57	MG	13	1602	1/1	0.79	0.24	120,120,120,120	0
57	MG	1H	3205	1/1	0.79	0.35	79,79,79,79	0
57	MG	14	3102	1/1	0.79	0.28	85,85,85,85	0
57	MG	14	3025	1/1	0.79	0.25	80,80,80,80	0
57	MG	14	3186	1/1	0.79	0.14	108,108,108,108	0
57	MG	1H	3154	1/1	0.79	0.13	58,58,58,58	0
57	MG	E5	101	1/1	0.79	0.37	89,89,89,89	0
57	MG	14	3161	1/1	0.80	0.25	78,78,78,78	0
57	MG	14	3064	1/1	0.80	0.22	63,63,63,63	0
57	MG	14	3168	1/1	0.80	0.17	89,89,89,89	0
57	MG	1H	3197	1/1	0.80	0.30	77,77,77,77	0
57	MG	14	3088	1/1	0.80	0.41	87,87,87,87	0
57	MG	13	1709	1/1	0.80	0.19	99,99,99,99	0
57	MG	14	3181	1/1	0.80	0.25	75,75,75,75	0
57	MG	1H	3203	1/1	0.80	0.26	74,74,74,74	0
57	MG	1H	3075	1/1	0.80	0.24	76,76,76,76	0
57	MG	1H	3114	1/1	0.80	0.25	71,71,71,71	0
57	MG	13	1669	1/1	0.80	0.45	95,95,95,95	0
57	MG	14	3127	1/1	0.80	0.39	87,87,87,87	0
57	MG	1H	3207	1/1	0.80	0.29	92,92,92,92	0
57	MG	1H	3209	1/1	0.80	0.34	76,76,76,76	0
57	MG	13	1630	1/1	0.80	0.25	96,96,96,96	0
57	MG	14	3391	1/1	0.80	0.17	99,99,99,99	0
57	MG	1H	3126	1/1	0.80	0.31	86,86,86,86	0
57	MG	14	3146	1/1	0.80	0.18	75,75,75,75	0
57	MG	14	3023	1/1	0.80	0.20	76,76,76,76	0
57	MG	13	1660	1/1	0.80	0.31	88,88,88,88	0
57	MG	1G	1620	1/1	0.80	0.22	91,91,91,91	0
57	MG	1G	1622	1/1	0.80	0.13	125,125,125,125	0
57	MG	13	1633	1/1	0.81	0.19	73,73,73,73	0
57	MG	16	208	1/1	0.81	0.28	85,85,85,85	0
57	MG	1H	3077	1/1	0.81	0.29	80,80,80,80	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	1H	3231	1/1	0.81	0.30	66,66,66,66	0
57	MG	14	3132	1/1	0.81	0.26	82,82,82,82	0
57	MG	14	3133	1/1	0.81	0.36	88,88,88,88	0
57	MG	14	3058	1/1	0.81	0.20	84,84,84,84	0
57	MG	14	3135	1/1	0.81	0.30	79,79,79,79	0
57	MG	1H	3234	1/1	0.81	0.19	79,79,79,79	0
57	MG	13	1665	1/1	0.81	0.30	82,82,82,82	0
57	MG	14	3145	1/1	0.81	0.20	90,90,90,90	0
57	MG	14	3207	1/1	0.81	0.25	70,70,70,70	0
57	MG	13	1674	1/1	0.81	0.34	92,92,92,92	0
57	MG	14	3082	1/1	0.81	0.33	79,79,79,79	0
57	MG	1G	1654	1/1	0.81	0.13	108,108,108,108	0
57	MG	2L	102	1/1	0.81	0.11	132,132,132,132	0
57	MG	14	3099	1/1	0.81	0.21	78,78,78,78	0
57	MG	39	302	1/1	0.81	0.14	74,74,74,74	0
57	MG	1H	3050	1/1	0.81	0.33	72,72,72,72	0
57	MG	13	1656	1/1	0.81	0.26	74,74,74,74	0
57	MG	14	3103	1/1	0.81	0.41	96,96,96,96	0
57	MG	14	3093	1/1	0.82	0.23	84,84,84,84	0
57	MG	14	3015	1/1	0.82	0.32	63,63,63,63	0
57	MG	14	3138	1/1	0.82	0.28	78,78,78,78	0
57	MG	1H	3488	1/1	0.82	0.12	105,105,105,105	0
57	MG	1H	3145	1/1	0.82	0.30	80,80,80,80	0
57	MG	1G	1616	1/1	0.82	0.23	94,94,94,94	0
57	MG	1H	3193	1/1	0.82	0.27	61,61,61,61	0
57	MG	14	3109	1/1	0.82	0.20	67,67,67,67	0
57	MG	14	3048	1/1	0.82	0.25	51,51,51,51	0
57	MG	14	3119	1/1	0.82	0.28	81,81,81,81	0
57	MG	13	1647	1/1	0.82	0.25	88,88,88,88	0
57	MG	13	1654	1/1	0.82	0.42	101,101,101,101	0
57	MG	14	3128	1/1	0.82	0.37	89,89,89,89	0
57	MG	2L	101	1/1	0.82	0.33	91,91,91,91	0
57	MG	1G	1625	1/1	0.82	0.17	99,99,99,99	0
57	MG	1H	3176	1/1	0.82	0.23	83,83,83,83	0
57	MG	1G	1630	1/1	0.82	0.28	72,72,72,72	0
57	MG	13	1640	1/1	0.83	0.22	92,92,92,92	0
57	MG	16	205	1/1	0.83	0.16	69,69,69,69	0
57	MG	14	3054	1/1	0.83	0.31	79,79,79,79	0
57	MG	1H	3220	1/1	0.83	0.39	89,89,89,89	0
57	MG	1G	1637	1/1	0.83	0.31	103,103,103,103	0
57	MG	1H	3189	1/1	0.83	0.23	68,68,68,68	0
57	MG	14	3069	1/1	0.83	0.25	86,86,86,86	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	14	3192	1/1	0.83	0.22	74,74,74,74	0
57	MG	1H	3052	1/1	0.83	0.28	59,59,59,59	0
57	MG	1H	3055	1/1	0.83	0.12	48,48,48,48	0
57	MG	14	3084	1/1	0.83	0.24	79,79,79,79	0
57	MG	1H	3084	1/1	0.83	0.23	62,62,62,62	0
57	MG	14	3203	1/1	0.83	0.30	79,79,79,79	0
57	MG	13	1610	1/1	0.83	0.33	82,82,82,82	0
57	MG	1G	1612	1/1	0.83	0.16	106,106,106,106	0
57	MG	1H	3158	1/1	0.83	0.18	71,71,71,71	0
57	MG	1H	3169	1/1	0.83	0.22	91,91,91,91	0
57	MG	1H	3070	1/1	0.83	0.26	75,75,75,75	0
57	MG	1H	3147	1/1	0.83	0.44	84,84,84,84	0
57	MG	1H	3089	1/1	0.83	0.20	38,38,38,38	0
57	MG	16	202	1/1	0.83	0.23	82,82,82,82	0
57	MG	14	3113	1/1	0.83	0.12	52,52,52,52	0
57	MG	14	3114	1/1	0.83	0.12	70,70,70,70	0
61	SPE	14	3437	13/13	0.83	0.19	59,68,73,74	0
57	MG	1H	3095	1/1	0.84	0.25	70,70,70,70	0
57	MG	14	3032	1/1	0.84	0.20	64,64,64,64	0
57	MG	13	1667	1/1	0.84	0.43	89,89,89,89	0
57	MG	1H	3224	1/1	0.84	0.23	85,85,85,85	0
57	MG	14	3053	1/1	0.84	0.23	95,95,95,95	0
57	MG	1G	1613	1/1	0.84	0.38	89,89,89,89	0
57	MG	1H	3226	1/1	0.84	0.30	71,71,71,71	0
57	MG	1G	1617	1/1	0.84	0.13	116,116,116,116	0
57	MG	1H	3007	1/1	0.84	0.23	81,81,81,81	0
57	MG	14	3155	1/1	0.84	0.20	78,78,78,78	0
57	MG	13	1637	1/1	0.84	0.34	74,74,74,74	0
57	MG	1H	3233	1/1	0.84	0.20	93,93,93,93	0
57	MG	14	3076	1/1	0.84	0.36	81,81,81,81	0
57	MG	14	3165	1/1	0.84	0.33	77,77,77,77	0
57	MG	1H	3079	1/1	0.84	0.17	63,63,63,63	0
57	MG	1H	3009	1/1	0.84	0.31	71,71,71,71	0
57	MG	1H	3198	1/1	0.84	0.28	79,79,79,79	0
57	MG	13	1639	1/1	0.84	0.35	70,70,70,70	0
57	MG	1G	1633	1/1	0.84	0.13	118,118,118,118	0
57	MG	1G	1634	1/1	0.84	0.31	85,85,85,85	0
57	MG	1H	3057	1/1	0.84	0.28	75,75,75,75	0
57	MG	1H	3445	1/1	0.84	0.11	92,92,92,92	0
57	MG	1H	3087	1/1	0.84	0.14	71,71,71,71	0
57	MG	14	3107	1/1	0.84	0.23	54,54,54,54	0
57	MG	1H	3521	1/1	0.84	0.08	82,82,82,82	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	14	3111	1/1	0.84	0.12	58,58,58,58	0
57	MG	13	1670	1/1	0.84	0.34	82,82,82,82	0
57	MG	1H	3134	1/1	0.84	0.15	57,57,57,57	0
57	MG	32	301	1/1	0.84	0.28	113,113,113,113	0
57	MG	14	3115	1/1	0.84	0.32	87,87,87,87	0
57	MG	1H	3160	1/1	0.84	0.26	71,71,71,71	0
57	MG	14	3393	1/1	0.84	0.13	165,165,165,165	0
57	MG	1H	3165	1/1	0.84	0.21	64,64,64,64	0
57	MG	14	3125	1/1	0.84	0.22	81,81,81,81	0
57	MG	1J	204	1/1	0.84	0.11	89,89,89,89	0
57	MG	31	302	1/1	0.84	0.17	77,77,77,77	0
57	MG	1H	3135	1/1	0.84	0.34	79,79,79,79	0
57	MG	1H	3217	1/1	0.84	0.33	82,82,82,82	0
57	MG	1G	1604	1/1	0.84	0.16	127,127,127,127	0
57	MG	14	3018	1/1	0.84	0.12	44,44,44,44	0
57	MG	1H	3066	1/1	0.84	0.24	60,60,60,60	0
57	MG	1H	3117	1/1	0.85	0.14	60,60,60,60	0
57	MG	14	3156	1/1	0.85	0.29	87,87,87,87	0
57	MG	14	3199	1/1	0.85	0.24	76,76,76,76	0
57	MG	14	3059	1/1	0.85	0.19	89,89,89,89	0
57	MG	1H	3187	1/1	0.85	0.28	44,44,44,44	0
57	MG	14	3020	1/1	0.85	0.15	75,75,75,75	0
57	MG	13	1635	1/1	0.85	0.24	81,81,81,81	0
57	MG	1H	3170	1/1	0.85	0.29	80,80,80,80	0
57	MG	1H	3137	1/1	0.85	0.25	70,70,70,70	0
57	MG	14	3035	1/1	0.85	0.24	58,58,58,58	0
57	MG	14	3142	1/1	0.85	0.30	80,80,80,80	0
57	MG	1H	3086	1/1	0.85	0.23	53,53,53,53	0
57	MG	1H	3102	1/1	0.85	0.20	60,60,60,60	0
57	MG	14	3051	1/1	0.85	0.21	61,61,61,61	0
57	MG	14	3094	1/1	0.85	0.26	73,73,73,73	0
57	MG	1G	1639	1/1	0.85	0.21	78,78,78,78	0
57	MG	1G	1610	1/1	0.85	0.28	91,91,91,91	0
57	MG	14	3196	1/1	0.85	0.29	71,71,71,71	0
57	MG	1H	3109	1/1	0.86	0.23	59,59,59,59	0
57	MG	1H	3163	1/1	0.86	0.36	91,91,91,91	0
57	MG	1G	1644	1/1	0.86	0.12	106,106,106,106	0
57	MG	13	1615	1/1	0.86	0.25	88,88,88,88	0
57	MG	14	3123	1/1	0.86	0.34	83,83,83,83	0
57	MG	14	3178	1/1	0.86	0.31	78,78,78,78	0
57	MG	14	3124	1/1	0.86	0.16	97,97,97,97	0
57	MG	1G	1663	1/1	0.86	0.10	98,98,98,98	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	1G	1673	1/1	0.86	0.09	115,115,115,115	0
57	MG	1H	3033	1/1	0.86	0.19	70,70,70,70	0
57	MG	1G	1614	1/1	0.86	0.30	88,88,88,88	0
57	MG	14	3077	1/1	0.86	0.16	52,52,52,52	0
57	MG	1H	3243	1/1	0.86	0.24	82,82,82,82	0
57	MG	14	3083	1/1	0.86	0.13	72,72,72,72	0
57	MG	13	1616	1/1	0.86	0.27	74,74,74,74	0
57	MG	1H	3067	1/1	0.86	0.21	58,58,58,58	0
57	MG	1H	3069	1/1	0.86	0.26	69,69,69,69	0
57	MG	13	1620	1/1	0.86	0.36	86,86,86,86	0
57	MG	1H	3177	1/1	0.86	0.36	82,82,82,82	0
57	MG	1H	3071	1/1	0.86	0.30	79,79,79,79	0
57	MG	14	3213	1/1	0.86	0.31	87,87,87,87	0
57	MG	14	3366	1/1	0.86	0.21	82,82,82,82	0
57	MG	13	1677	1/1	0.86	0.32	77,77,77,77	0
57	MG	14	3149	1/1	0.86	0.14	72,72,72,72	0
57	MG	1H	3012	1/1	0.86	0.27	58,58,58,58	0
57	MG	1H	3223	1/1	0.86	0.30	85,85,85,85	0
57	MG	14	3104	1/1	0.86	0.20	78,78,78,78	0
57	MG	1H	3191	1/1	0.86	0.24	58,58,58,58	0
57	MG	1H	3192	1/1	0.86	0.37	75,75,75,75	0
57	MG	1H	3132	1/1	0.86	0.22	65,65,65,65	0
57	MG	14	3159	1/1	0.86	0.20	79,79,79,79	0
57	MG	1H	3004	1/1	0.86	0.45	89,89,89,89	0
61	SPE	14	3436	13/13	0.86	0.20	83,88,93,94	0
57	MG	1H	3108	1/1	0.86	0.22	64,64,64,64	0
57	MG	14	3080	1/1	0.87	0.19	68,68,68,68	0
57	MG	1H	3101	1/1	0.87	0.32	78,78,78,78	0
57	MG	1H	3166	1/1	0.87	0.30	78,78,78,78	0
57	MG	1G	1627	1/1	0.87	0.21	87,87,87,87	0
57	MG	16	206	1/1	0.87	0.13	77,77,77,77	0
57	MG	16	207	1/1	0.87	0.25	74,74,74,74	0
57	MG	1H	3195	1/1	0.87	0.15	55,55,55,55	0
57	MG	16	209	1/1	0.87	0.22	76,76,76,76	0
57	MG	14	3031	1/1	0.87	0.20	73,73,73,73	0
57	MG	13	1650	1/1	0.87	0.30	75,75,75,75	0
57	MG	1H	3068	1/1	0.87	0.28	72,72,72,72	0
57	MG	14	3148	1/1	0.87	0.27	85,85,85,85	0
57	MG	14	3036	1/1	0.87	0.20	85,85,85,85	0
57	MG	14	3043	1/1	0.87	0.18	71,71,71,71	0
57	MG	14	3209	1/1	0.87	0.30	83,83,83,83	0
57	MG	14	3211	1/1	0.87	0.24	81,81,81,81	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	1H	3171	1/1	0.87	0.29	73,73,73,73	0
57	MG	1H	3202	1/1	0.87	0.27	73,73,73,73	0
57	MG	14	3381	1/1	0.87	0.23	79,79,79,79	0
57	MG	1H	3051	1/1	0.87	0.21	60,60,60,60	0
57	MG	1H	3173	1/1	0.87	0.10	59,59,59,59	0
57	MG	14	3428	1/1	0.87	0.14	119,119,119,119	0
57	MG	13	1601	1/1	0.87	0.28	80,80,80,80	0
57	MG	1H	3111	1/1	0.87	0.29	79,79,79,79	0
57	MG	1H	3011	1/1	0.87	0.23	56,56,56,56	0
57	MG	1H	3038	1/1	0.87	0.23	50,50,50,50	0
57	MG	1H	3212	1/1	0.87	0.10	65,65,65,65	0
57	MG	14	3066	1/1	0.87	0.25	61,61,61,61	0
57	MG	1H	3213	1/1	0.87	0.23	71,71,71,71	0
57	MG	13	1644	1/1	0.87	0.32	85,85,85,85	0
57	MG	1H	3093	1/1	0.87	0.10	56,56,56,56	0
57	MG	1H	3020	1/1	0.87	0.16	73,73,73,73	0
57	MG	1G	1621	1/1	0.88	0.28	82,82,82,82	0
57	MG	14	3063	1/1	0.88	0.18	67,67,67,67	0
57	MG	13	1662	1/1	0.88	0.35	89,89,89,89	0
57	MG	14	3180	1/1	0.88	0.30	91,91,91,91	0
57	MG	1H	3098	1/1	0.88	0.23	46,46,46,46	0
57	MG	14	3003	1/1	0.88	0.21	78,78,78,78	0
57	MG	14	3006	1/1	0.88	0.28	75,75,75,75	0
57	MG	14	3074	1/1	0.88	0.13	69,69,69,69	0
57	MG	5I	101	1/1	0.88	0.12	79,79,79,79	0
57	MG	14	3194	1/1	0.88	0.36	80,80,80,80	0
57	MG	14	3130	1/1	0.88	0.23	66,66,66,66	0
57	MG	1H	3225	1/1	0.88	0.28	71,71,71,71	0
57	MG	1H	3001	1/1	0.88	0.38	84,84,84,84	0
57	MG	1H	3013	1/1	0.88	0.19	40,40,40,40	0
57	MG	1H	3002	1/1	0.88	0.17	48,48,48,48	0
57	MG	14	3200	1/1	0.88	0.12	89,89,89,89	0
57	MG	13	1624	1/1	0.88	0.16	59,59,59,59	0
57	MG	14	3087	1/1	0.88	0.22	76,76,76,76	0
57	MG	1H	3025	1/1	0.88	0.24	75,75,75,75	0
57	MG	14	3090	1/1	0.88	0.23	86,86,86,86	0
57	MG	1H	3005	1/1	0.88	0.13	68,68,68,68	0
57	MG	14	3210	1/1	0.88	0.32	91,91,91,91	0
57	MG	1H	3211	1/1	0.88	0.30	78,78,78,78	0
57	MG	14	3033	1/1	0.88	0.26	80,80,80,80	0
57	MG	14	3350	1/1	0.88	0.12	101,101,101,101	0
57	MG	14	3098	1/1	0.88	0.25	77,77,77,77	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	1H	3240	1/1	0.88	0.24	73,73,73,73	0
57	MG	13	1666	1/1	0.88	0.22	85,85,85,85	0
57	MG	1H	3034	1/1	0.88	0.13	46,46,46,46	0
57	MG	14	3395	1/1	0.88	0.08	118,118,118,118	0
57	MG	1H	3214	1/1	0.88	0.32	77,77,77,77	0
57	MG	1H	3168	1/1	0.88	0.29	80,80,80,80	0
57	MG	14	3433	1/1	0.88	0.15	114,114,114,114	0
57	MG	14	3049	1/1	0.88	0.53	83,83,83,83	0
57	MG	13	1631	1/1	0.88	0.12	78,78,78,78	0
57	MG	1H	3196	1/1	0.88	0.17	77,77,77,77	0
57	MG	14	3162	1/1	0.88	0.41	74,74,74,74	0
57	MG	1H	3522	1/1	0.88	0.07	110,110,110,110	0
57	MG	14	3057	1/1	0.88	0.19	49,49,49,49	0
57	MG	14	3167	1/1	0.88	0.13	78,78,78,78	0
57	MG	13	1636	1/1	0.88	0.21	74,74,74,74	0
57	MG	42	201	1/1	0.88	0.23	120,120,120,120	0
57	MG	1H	3078	1/1	0.89	0.10	58,58,58,58	0
57	MG	13	1617	1/1	0.89	0.09	51,51,51,51	0
57	MG	88	203	1/1	0.89	0.22	79,79,79,79	0
57	MG	1H	3178	1/1	0.89	0.23	63,63,63,63	0
57	MG	1H	3161	1/1	0.89	0.20	67,67,67,67	0
57	MG	1H	3182	1/1	0.89	0.25	60,60,60,60	0
57	MG	1H	3238	1/1	0.89	0.31	80,80,80,80	0
57	MG	1H	3040	1/1	0.89	0.31	44,44,44,44	0
57	MG	14	3100	1/1	0.89	0.19	71,71,71,71	0
57	MG	1H	3188	1/1	0.89	0.23	49,49,49,49	0
57	MG	1H	3164	1/1	0.89	0.26	69,69,69,69	0
57	MG	14	3151	1/1	0.89	0.09	70,70,70,70	0
57	MG	14	3052	1/1	0.89	0.13	54,54,54,54	0
57	MG	1H	3041	1/1	0.89	0.14	51,51,51,51	0
57	MG	1G	1695	1/1	0.89	0.10	107,107,107,107	0
57	MG	1H	3376	1/1	0.89	0.15	66,66,66,66	0
57	MG	1H	3105	1/1	0.89	0.16	72,72,72,72	0
57	MG	1H	3167	1/1	0.89	0.41	98,98,98,98	0
57	MG	1G	1618	1/1	0.89	0.27	78,78,78,78	0
57	MG	13	1622	1/1	0.89	0.23	63,63,63,63	0
57	MG	14	3390	1/1	0.89	0.12	94,94,94,94	0
57	MG	1H	3056	1/1	0.89	0.23	49,49,49,49	0
57	MG	16	201	1/1	0.89	0.20	62,62,62,62	0
57	MG	14	3121	1/1	0.89	0.17	61,61,61,61	0
57	MG	13	1653	1/1	0.89	0.33	73,73,73,73	0
57	MG	14	3429	1/1	0.89	0.24	95,95,95,95	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	14	3013	1/1	0.89	0.16	47,47,47,47	0
57	MG	1H	3153	1/1	0.89	0.24	77,77,77,77	0
57	MG	14	3170	1/1	0.89	0.24	81,81,81,81	0
57	MG	1J	203	1/1	0.89	0.22	73,73,73,73	0
57	MG	14	3172	1/1	0.89	0.19	77,77,77,77	0
57	MG	1H	3200	1/1	0.89	0.37	71,71,71,71	0
57	MG	14	3126	1/1	0.89	0.17	72,72,72,72	0
57	MG	1H	3072	1/1	0.89	0.19	58,58,58,58	0
57	MG	1H	3049	1/1	0.89	0.14	62,62,62,62	0
57	MG	14	3022	1/1	0.89	0.15	81,81,81,81	0
61	SPE	1G	1703	13/13	0.89	0.12	90,107,113,114	0
57	MG	1H	3229	1/1	0.89	0.44	90,90,90,90	0
57	MG	1H	3063	1/1	0.89	0.21	100,100,100,100	0
57	MG	13	1704	1/1	0.90	0.10	106,106,106,106	0
57	MG	1H	3100	1/1	0.90	0.37	68,68,68,68	0
57	MG	14	3002	1/1	0.90	0.22	57,57,57,57	0
57	MG	13	1642	1/1	0.90	0.15	103,103,103,103	0
57	MG	13	1724	1/1	0.90	0.08	117,117,117,117	0
57	MG	14	3007	1/1	0.90	0.12	60,60,60,60	0
57	MG	14	3166	1/1	0.90	0.28	79,79,79,79	0
57	MG	14	3096	1/1	0.90	0.15	65,65,65,65	0
57	MG	1H	3139	1/1	0.90	0.21	71,71,71,71	0
57	MG	1G	1611	1/1	0.90	0.26	76,76,76,76	0
57	MG	13	1655	1/1	0.90	0.27	82,82,82,82	0
57	MG	1H	3017	1/1	0.90	0.19	62,62,62,62	0
57	MG	13	1672	1/1	0.90	0.20	88,88,88,88	0
57	MG	1H	3023	1/1	0.90	0.15	50,50,50,50	0
57	MG	1H	3244	1/1	0.90	0.27	74,74,74,74	0
57	MG	1H	3309	1/1	0.90	0.10	54,54,54,54	0
57	MG	14	3024	1/1	0.90	0.13	81,81,81,81	0
57	MG	14	3108	1/1	0.90	0.11	72,72,72,72	0
57	MG	14	3184	1/1	0.90	0.29	78,78,78,78	0
57	MG	1H	3175	1/1	0.90	0.20	64,64,64,64	0
57	MG	14	3026	1/1	0.90	0.18	56,56,56,56	0
57	MG	14	3027	1/1	0.90	0.23	66,66,66,66	0
57	MG	1H	3339	1/1	0.90	0.09	106,106,106,106	0
57	MG	1H	3367	1/1	0.90	0.08	66,66,66,66	0
57	MG	1H	3374	1/1	0.90	0.12	83,83,83,83	0
57	MG	14	3116	1/1	0.90	0.17	88,88,88,88	0
57	MG	14	3117	1/1	0.90	0.17	64,64,64,64	0
57	MG	1G	1624	1/1	0.90	0.19	95,95,95,95	0
57	MG	1H	3080	1/1	0.90	0.14	80,80,80,80	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	14	3039	1/1	0.90	0.18	89,89,89,89	0
57	MG	1H	3434	1/1	0.90	0.12	95,95,95,95	0
57	MG	13	1673	1/1	0.90	0.24	84,84,84,84	0
57	MG	1H	3082	1/1	0.90	0.20	71,71,71,71	0
57	MG	1H	3496	1/1	0.90	0.10	89,89,89,89	0
57	MG	1H	3116	1/1	0.90	0.20	53,53,53,53	0
57	MG	1H	3215	1/1	0.90	0.18	63,63,63,63	0
57	MG	13	1664	1/1	0.90	0.32	78,78,78,78	0
57	MG	14	3243	1/1	0.90	0.09	58,58,58,58	0
57	MG	14	3252	1/1	0.90	0.17	90,90,90,90	0
57	MG	14	3297	1/1	0.90	0.10	71,71,71,71	0
57	MG	14	3347	1/1	0.90	0.10	88,88,88,88	0
57	MG	1G	1636	1/1	0.90	0.19	90,90,90,90	0
57	MG	1H	3003	1/1	0.90	0.24	65,65,65,65	0
57	MG	14	3376	1/1	0.90	0.11	102,102,102,102	0
57	MG	14	3379	1/1	0.90	0.10	84,84,84,84	0
57	MG	13	1625	1/1	0.90	0.21	82,82,82,82	0
57	MG	1H	3124	1/1	0.90	0.16	61,61,61,61	0
57	MG	1H	3065	1/1	0.90	0.24	65,65,65,65	0
57	MG	13	1657	1/1	0.90	0.14	68,68,68,68	0
57	MG	14	3137	1/1	0.90	0.33	99,99,99,99	0
57	MG	14	3421	1/1	0.90	0.09	97,97,97,97	0
57	MG	1H	3162	1/1	0.90	0.10	60,60,60,60	0
57	MG	1H	3194	1/1	0.90	0.09	63,63,63,63	0
57	MG	14	3143	1/1	0.90	0.08	57,57,57,57	0
57	MG	14	3431	1/1	0.90	0.12	116,116,116,116	0
57	MG	14	3067	1/1	0.90	0.21	78,78,78,78	0
57	MG	13	1658	1/1	0.90	0.35	82,82,82,82	0
57	MG	14	3070	1/1	0.90	0.15	52,52,52,52	0
57	MG	14	3147	1/1	0.90	0.17	69,69,69,69	0
57	MG	1G	1671	1/1	0.90	0.14	112,112,112,112	0
57	MG	78	201	1/1	0.90	0.12	66,66,66,66	0
57	MG	1G	1678	1/1	0.90	0.12	111,111,111,111	0
57	MG	1H	3227	1/1	0.90	0.22	72,72,72,72	0
57	MG	14	3079	1/1	0.90	0.18	48,48,48,48	0
57	MG	88	202	1/1	0.90	0.18	66,66,66,66	0
57	MG	13	1603	1/1	0.90	0.16	74,74,74,74	0
57	MG	13	1614	1/1	0.90	0.24	84,84,84,84	0
57	MG	1H	3219	1/1	0.91	0.22	71,71,71,71	0
57	MG	13	1663	1/1	0.91	0.14	107,107,107,107	0
57	MG	14	3202	1/1	0.91	0.29	84,84,84,84	0
57	MG	14	3061	1/1	0.91	0.25	61,61,61,61	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	14	3204	1/1	0.91	0.14	72,72,72,72	0
57	MG	13	1613	1/1	0.91	0.16	87,87,87,87	0
57	MG	14	3110	1/1	0.91	0.14	69,69,69,69	0
57	MG	1H	3074	1/1	0.91	0.21	64,64,64,64	0
57	MG	1H	3143	1/1	0.91	0.20	50,50,50,50	0
57	MG	13	1627	1/1	0.91	0.37	71,71,71,71	0
57	MG	1H	3125	1/1	0.91	0.15	56,56,56,56	0
57	MG	14	3214	1/1	0.91	0.42	80,80,80,80	0
57	MG	1G	1674	1/1	0.91	0.10	107,107,107,107	0
57	MG	1H	3186	1/1	0.91	0.27	62,62,62,62	0
57	MG	14	3277	1/1	0.91	0.17	84,84,84,84	0
57	MG	14	3291	1/1	0.91	0.08	85,85,85,85	0
57	MG	14	3029	1/1	0.91	0.18	57,57,57,57	0
57	MG	14	3030	1/1	0.91	0.26	57,57,57,57	0
57	MG	14	3120	1/1	0.91	0.23	78,78,78,78	0
57	MG	1H	3146	1/1	0.91	0.15	52,52,52,52	0
57	MG	1H	3392	1/1	0.91	0.09	48,48,48,48	0
57	MG	1H	3423	1/1	0.91	0.18	84,84,84,84	0
57	MG	14	3081	1/1	0.91	0.16	56,56,56,56	0
57	MG	14	3384	1/1	0.91	0.15	78,78,78,78	0
57	MG	1H	3076	1/1	0.91	0.23	72,72,72,72	0
57	MG	1H	3053	1/1	0.91	0.27	75,75,75,75	0
57	MG	1H	3149	1/1	0.91	0.19	55,55,55,55	0
57	MG	14	3085	1/1	0.91	0.19	88,88,88,88	0
57	MG	14	3417	1/1	0.91	0.10	108,108,108,108	0
57	MG	13	1608	1/1	0.91	0.13	76,76,76,76	0
57	MG	1H	3110	1/1	0.91	0.12	79,79,79,79	0
57	MG	14	3131	1/1	0.91	0.12	64,64,64,64	0
57	MG	14	3047	1/1	0.91	0.17	65,65,65,65	0
57	MG	1H	3092	1/1	0.91	0.19	61,61,61,61	0
57	MG	13	1629	1/1	0.91	0.15	72,72,72,72	0
57	MG	14	3434	1/1	0.91	0.11	110,110,110,110	0
57	MG	14	3050	1/1	0.91	0.18	57,57,57,57	0
57	MG	1G	1638	1/1	0.91	0.13	127,127,127,127	0
57	MG	14	3010	1/1	0.91	0.18	57,57,57,57	0
57	MG	1J	205	1/1	0.91	0.13	73,73,73,73	0
57	MG	14	3191	1/1	0.91	0.18	67,67,67,67	0
57	MG	19	301	1/1	0.91	0.19	48,48,48,48	0
57	MG	29	301	1/1	0.91	0.23	58,58,58,58	0
57	MG	14	3012	1/1	0.91	0.18	57,57,57,57	0
57	MG	14	3139	1/1	0.91	0.13	68,68,68,68	0
57	MG	14	3141	1/1	0.91	0.22	95,95,95,95	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	13	1607	1/1	0.91	0.18	72,72,72,72	0
60	ZN	G8	201	1/1	0.91	0.17	139,139,139,139	0
57	MG	14	3055	1/1	0.91	0.18	60,60,60,60	0
57	MG	1H	3058	1/1	0.91	0.15	60,60,60,60	0
57	MG	14	3016	1/1	0.91	0.21	74,74,74,74	0
57	MG	1G	1704	1/1	0.92	0.18	84,84,84,84	0
57	MG	1H	3348	1/1	0.92	0.10	111,111,111,111	0
57	MG	13	1723	1/1	0.92	0.07	128,128,128,128	0
57	MG	7A	101	1/1	0.92	0.19	114,114,114,114	0
57	MG	1G	1606	1/1	0.92	0.09	73,73,73,73	0
57	MG	1H	3181	1/1	0.92	0.17	65,65,65,65	0
57	MG	1H	3014	1/1	0.92	0.13	53,53,53,53	0
57	MG	1H	3037	1/1	0.92	0.34	75,75,75,75	0
57	MG	1H	3396	1/1	0.92	0.09	59,59,59,59	0
57	MG	1H	3414	1/1	0.92	0.10	105,105,105,105	0
57	MG	1H	3415	1/1	0.92	0.10	72,72,72,72	0
57	MG	14	3206	1/1	0.92	0.16	85,85,85,85	0
57	MG	14	3075	1/1	0.92	0.19	73,73,73,73	0
57	MG	1H	3419	1/1	0.92	0.14	86,86,86,86	0
57	MG	1G	1615	1/1	0.92	0.16	86,86,86,86	0
57	MG	1H	3422	1/1	0.92	0.26	65,65,65,65	0
57	MG	1H	3083	1/1	0.92	0.63	83,83,83,83	0
57	MG	1H	3096	1/1	0.92	0.12	64,64,64,64	0
57	MG	1H	3444	1/1	0.92	0.09	74,74,74,74	0
57	MG	1H	3210	1/1	0.92	0.12	56,56,56,56	0
57	MG	1H	3458	1/1	0.92	0.17	82,82,82,82	0
57	MG	14	3019	1/1	0.92	0.21	57,57,57,57	0
57	MG	14	3281	1/1	0.92	0.07	69,69,69,69	0
57	MG	1H	3468	1/1	0.92	0.16	82,82,82,82	0
57	MG	1H	3232	1/1	0.92	0.11	48,48,48,48	0
57	MG	14	3312	1/1	0.92	0.08	92,92,92,92	0
57	MG	1H	3112	1/1	0.92	0.21	55,55,55,55	0
57	MG	1H	3503	1/1	0.92	0.11	91,91,91,91	0
57	MG	14	3355	1/1	0.92	0.07	104,104,104,104	0
57	MG	1H	3516	1/1	0.92	0.10	102,102,102,102	0
57	MG	1H	3054	1/1	0.92	0.22	52,52,52,52	0
57	MG	1H	3152	1/1	0.92	0.22	70,70,70,70	0
57	MG	1H	3236	1/1	0.92	0.27	67,67,67,67	0
57	MG	1H	3045	1/1	0.92	0.19	46,46,46,46	0
57	MG	14	3387	1/1	0.92	0.11	83,83,83,83	0
57	MG	1H	3048	1/1	0.92	0.08	45,45,45,45	0
57	MG	16	204	1/1	0.92	0.09	59,59,59,59	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	1H	3155	1/1	0.92	0.18	55,55,55,55	0
57	MG	13	1649	1/1	0.92	0.28	75,75,75,75	0
57	MG	14	3398	1/1	0.92	0.07	76,76,76,76	0
57	MG	14	3409	1/1	0.92	0.19	88,88,88,88	0
57	MG	14	3416	1/1	0.92	0.10	102,102,102,102	0
57	MG	1H	3118	1/1	0.92	0.09	69,69,69,69	0
57	MG	14	3164	1/1	0.92	0.24	78,78,78,78	0
57	MG	14	3424	1/1	0.92	0.08	109,109,109,109	0
57	MG	14	3037	1/1	0.92	0.13	65,65,65,65	0
57	MG	1H	3103	1/1	0.92	0.23	61,61,61,61	0
57	MG	14	3040	1/1	0.92	0.13	68,68,68,68	0
57	MG	14	3042	1/1	0.92	0.12	65,65,65,65	0
57	MG	1H	3249	1/1	0.92	0.11	63,63,63,63	0
57	MG	21	302	1/1	0.92	0.13	72,72,72,72	0
57	MG	14	3171	1/1	0.92	0.18	56,56,56,56	0
57	MG	31	301	1/1	0.92	0.05	63,63,63,63	0
57	MG	14	3173	1/1	0.92	0.25	79,79,79,79	0
57	MG	1H	3270	1/1	0.92	0.09	50,50,50,50	0
57	MG	1H	3271	1/1	0.92	0.10	51,51,51,51	0
57	MG	1G	1667	1/1	0.92	0.07	103,103,103,103	0
57	MG	1H	3159	1/1	0.92	0.22	80,80,80,80	0
57	MG	14	3118	1/1	0.92	0.28	61,61,61,61	0
57	MG	1H	3310	1/1	0.92	0.09	70,70,70,70	0
57	MG	1H	3104	1/1	0.92	0.09	43,43,43,43	0
57	MG	13	1605	1/1	0.92	0.14	71,71,71,71	0
57	MG	1G	1693	1/1	0.92	0.06	129,129,129,129	0
57	MG	14	3190	1/1	0.92	0.22	59,59,59,59	0
57	MG	1G	1603	1/1	0.92	0.09	88,88,88,88	0
57	MG	1G	1698	1/1	0.92	0.09	123,123,123,123	0
57	MG	1H	3274	1/1	0.93	0.09	97,97,97,97	0
57	MG	1H	3489	1/1	0.93	0.21	73,73,73,73	0
57	MG	14	3150	1/1	0.93	0.07	63,63,63,63	0
57	MG	14	3044	1/1	0.93	0.12	57,57,57,57	0
57	MG	14	3212	1/1	0.93	0.32	75,75,75,75	0
57	MG	1G	1699	1/1	0.93	0.05	133,133,133,133	0
57	MG	1H	3208	1/1	0.93	0.22	72,72,72,72	0
57	MG	14	3215	1/1	0.93	0.59	86,86,86,86	0
57	MG	1H	3497	1/1	0.93	0.07	107,107,107,107	0
57	MG	14	3105	1/1	0.93	0.12	73,73,73,73	0
57	MG	14	3106	1/1	0.93	0.25	57,57,57,57	0
57	MG	1H	3228	1/1	0.93	0.11	60,60,60,60	0
57	MG	1H	3505	1/1	0.93	0.14	100,100,100,100	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	14	3160	1/1	0.93	0.12	65,65,65,65	0
57	MG	13	1611	1/1	0.93	0.21	70,70,70,70	0
57	MG	14	3316	1/1	0.93	0.08	69,69,69,69	0
57	MG	1H	3059	1/1	0.93	0.18	56,56,56,56	0
57	MG	1H	3341	1/1	0.93	0.07	78,78,78,78	0
57	MG	13	1612	1/1	0.93	0.10	86,86,86,86	0
57	MG	1H	3352	1/1	0.93	0.08	57,57,57,57	0
57	MG	14	3005	1/1	0.93	0.17	54,54,54,54	0
57	MG	14	3377	1/1	0.93	0.09	131,131,131,131	0
57	MG	1H	3366	1/1	0.93	0.07	68,68,68,68	0
57	MG	1H	3140	1/1	0.93	0.18	54,54,54,54	0
57	MG	1H	3368	1/1	0.93	0.11	69,69,69,69	0
57	MG	14	3009	1/1	0.93	0.20	57,57,57,57	0
57	MG	13	1717	1/1	0.93	0.09	99,99,99,99	0
57	MG	14	3011	1/1	0.93	0.09	44,44,44,44	0
57	MG	1H	3142	1/1	0.93	0.24	68,68,68,68	0
57	MG	14	3174	1/1	0.93	0.09	89,89,89,89	0
57	MG	1H	3388	1/1	0.93	0.08	55,55,55,55	0
57	MG	14	3176	1/1	0.93	0.16	82,82,82,82	0
57	MG	14	3413	1/1	0.93	0.09	107,107,107,107	0
57	MG	1H	3391	1/1	0.93	0.09	89,89,89,89	0
57	MG	1H	3064	1/1	0.93	0.05	51,51,51,51	0
57	MG	1H	3395	1/1	0.93	0.17	68,68,68,68	0
57	MG	14	3073	1/1	0.93	0.15	78,78,78,78	0
57	MG	13	1652	1/1	0.93	0.37	71,71,71,71	0
57	MG	13	1606	1/1	0.93	0.15	72,72,72,72	0
57	MG	13	1728	1/1	0.93	0.06	117,117,117,117	0
57	MG	1H	3179	1/1	0.93	0.15	80,80,80,80	0
57	MG	14	3189	1/1	0.93	0.18	51,51,51,51	0
57	MG	1H	3241	1/1	0.93	0.14	58,58,58,58	0
57	MG	1J	201	1/1	0.93	0.24	73,73,73,73	0
57	MG	1H	3022	1/1	0.93	0.15	49,49,49,49	0
57	MG	1G	1643	1/1	0.93	0.35	83,83,83,83	0
57	MG	13	1732	1/1	0.93	0.07	114,114,114,114	0
57	MG	1H	3131	1/1	0.93	0.29	83,83,83,83	0
57	MG	1H	3099	1/1	0.93	0.20	56,56,56,56	0
57	MG	1H	3447	1/1	0.93	0.22	70,70,70,70	0
57	MG	1G	1669	1/1	0.93	0.10	105,105,105,105	0
57	MG	1H	3453	1/1	0.93	0.13	93,93,93,93	0
57	MG	13	1634	1/1	0.93	0.21	75,75,75,75	0
57	MG	13	1701	1/1	0.93	0.10	108,108,108,108	0
57	MG	1H	3484	1/1	0.93	0.08	105,105,105,105	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	14	3095	1/1	0.93	0.09	62,62,62,62	0
57	MG	1G	1685	1/1	0.93	0.09	110,110,110,110	0
57	MG	1G	1686	1/1	0.93	0.07	106,106,106,106	0
57	MG	1H	3487	1/1	0.93	0.11	85,85,85,85	0
57	MG	1H	3300	1/1	0.94	0.09	62,62,62,62	0
57	MG	1H	3090	1/1	0.94	0.12	42,42,42,42	0
57	MG	1G	1668	1/1	0.94	0.06	124,124,124,124	0
57	MG	1H	3047	1/1	0.94	0.12	55,55,55,55	0
57	MG	1H	3026	1/1	0.94	0.18	55,55,55,55	0
57	MG	13	1727	1/1	0.94	0.13	90,90,90,90	0
57	MG	14	3221	1/1	0.94	0.07	62,62,62,62	0
57	MG	1H	3133	1/1	0.94	0.06	55,55,55,55	0
57	MG	1G	1676	1/1	0.94	0.07	93,93,93,93	0
57	MG	14	3254	1/1	0.94	0.07	77,77,77,77	0
57	MG	14	3264	1/1	0.94	0.07	93,93,93,93	0
57	MG	14	3276	1/1	0.94	0.10	120,120,120,120	0
57	MG	14	3038	1/1	0.94	0.15	52,52,52,52	0
57	MG	14	3279	1/1	0.94	0.07	58,58,58,58	0
57	MG	1H	3476	1/1	0.94	0.17	82,82,82,82	0
57	MG	1H	3477	1/1	0.94	0.10	83,83,83,83	0
57	MG	14	3041	1/1	0.94	0.17	55,55,55,55	0
57	MG	14	3298	1/1	0.94	0.07	86,86,86,86	0
57	MG	14	3307	1/1	0.94	0.07	66,66,66,66	0
57	MG	1H	3483	1/1	0.94	0.15	91,91,91,91	0
57	MG	1G	1688	1/1	0.94	0.16	113,113,113,113	0
57	MG	14	3318	1/1	0.94	0.08	89,89,89,89	0
57	MG	14	3346	1/1	0.94	0.07	99,99,99,99	0
57	MG	1G	1692	1/1	0.94	0.11	101,101,101,101	0
57	MG	13	1682	1/1	0.94	0.06	93,93,93,93	0
57	MG	14	3354	1/1	0.94	0.17	60,60,60,60	0
57	MG	13	1731	1/1	0.94	0.06	112,112,112,112	0
57	MG	1G	1697	1/1	0.94	0.05	128,128,128,128	0
57	MG	1H	3354	1/1	0.94	0.08	60,60,60,60	0
57	MG	1H	3362	1/1	0.94	0.10	100,100,100,100	0
57	MG	1H	3363	1/1	0.94	0.09	96,96,96,96	0
57	MG	1H	3015	1/1	0.94	0.17	51,51,51,51	0
57	MG	1H	3498	1/1	0.94	0.10	98,98,98,98	0
57	MG	14	3385	1/1	0.94	0.14	67,67,67,67	0
57	MG	52	201	1/1	0.94	0.06	129,129,129,129	0
57	MG	13	1714	1/1	0.94	0.06	122,122,122,122	0
57	MG	13	1736	1/1	0.94	0.07	101,101,101,101	0
57	MG	1H	3511	1/1	0.94	0.11	101,101,101,101	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	1H	3515	1/1	0.94	0.11	58,58,58,58	0
57	MG	1H	3372	1/1	0.94	0.06	89,89,89,89	0
57	MG	14	3407	1/1	0.94	0.07	123,123,123,123	0
57	MG	14	3408	1/1	0.94	0.10	92,92,92,92	0
57	MG	1H	3520	1/1	0.94	0.08	105,105,105,105	0
57	MG	14	3004	1/1	0.94	0.15	63,63,63,63	0
57	MG	14	3414	1/1	0.94	0.07	97,97,97,97	0
57	MG	1H	3218	1/1	0.94	0.17	37,37,37,37	0
57	MG	1H	3239	1/1	0.94	0.20	67,67,67,67	0
57	MG	14	3185	1/1	0.94	0.31	86,86,86,86	0
57	MG	14	3422	1/1	0.94	0.17	108,108,108,108	0
57	MG	1H	3524	1/1	0.94	0.14	81,81,81,81	0
57	MG	14	3425	1/1	0.94	0.19	91,91,91,91	0
57	MG	1H	3525	1/1	0.94	0.10	68,68,68,68	0
57	MG	14	3188	1/1	0.94	0.25	72,72,72,72	0
57	MG	1G	1629	1/1	0.94	0.21	85,85,85,85	0
57	MG	1H	3386	1/1	0.94	0.07	42,42,42,42	0
57	MG	14	3432	1/1	0.94	0.12	116,116,116,116	0
57	MG	3I	201	1/1	0.94	0.16	60,60,60,60	0
57	MG	1H	3389	1/1	0.94	0.12	88,88,88,88	0
57	MG	14	3193	1/1	0.94	0.06	45,45,45,45	0
57	MG	13	1700	1/1	0.94	0.11	102,102,102,102	0
57	MG	1H	3122	1/1	0.94	0.05	52,52,52,52	0
57	MG	13	1648	1/1	0.94	0.12	67,67,67,67	0
57	MG	1H	3073	1/1	0.94	0.16	66,66,66,66	0
57	MG	13	1646	1/1	0.94	0.14	71,71,71,71	0
57	MG	1H	3261	1/1	0.94	0.08	63,63,63,63	0
57	MG	1H	3268	1/1	0.94	0.07	59,59,59,59	0
57	MG	1H	3046	1/1	0.94	0.08	33,33,33,33	0
57	MG	1H	3184	1/1	0.94	0.14	70,70,70,70	0
57	MG	4I	201	1/1	0.94	0.09	69,69,69,69	0
57	MG	1H	3128	1/1	0.94	0.34	85,85,85,85	0
58	PAR	1G	1702	42/42	0.94	0.10	83,92,100,103	0
57	MG	1H	3443	1/1	0.94	0.14	75,75,75,75	0
57	MG	1G	1655	1/1	0.94	0.09	110,110,110,110	0
57	MG	14	3091	1/1	0.94	0.12	78,78,78,78	0
57	MG	14	3028	1/1	0.94	0.19	45,45,45,45	0
57	MG	1H	3344	1/1	0.95	0.06	103,103,103,103	0
57	MG	14	3295	1/1	0.95	0.07	60,60,60,60	0
57	MG	2K	102	1/1	0.95	0.10	78,78,78,78	0
57	MG	14	3001	1/1	0.95	0.06	57,57,57,57	0
57	MG	1H	3350	1/1	0.95	0.10	74,74,74,74	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	1H	3042	1/1	0.95	0.16	65,65,65,65	0
57	MG	1H	3457	1/1	0.95	0.16	84,84,84,84	0
57	MG	2I	301	1/1	0.95	0.14	59,59,59,59	0
57	MG	14	3328	1/1	0.95	0.06	81,81,81,81	0
57	MG	14	3334	1/1	0.95	0.06	60,60,60,60	0
57	MG	14	3342	1/1	0.95	0.05	113,113,113,113	0
57	MG	1H	3021	1/1	0.95	0.09	49,49,49,49	0
57	MG	1H	3462	1/1	0.95	0.10	94,94,94,94	0
57	MG	13	1623	1/1	0.95	0.14	76,76,76,76	0
57	MG	1H	3010	1/1	0.95	0.28	39,39,39,39	0
57	MG	14	3179	1/1	0.95	0.06	77,77,77,77	0
57	MG	14	3362	1/1	0.95	0.05	114,114,114,114	0
57	MG	13	1712	1/1	0.95	0.09	89,89,89,89	0
57	MG	14	3372	1/1	0.95	0.07	86,86,86,86	0
57	MG	14	3373	1/1	0.95	0.10	65,65,65,65	0
57	MG	1H	3479	1/1	0.95	0.15	83,83,83,83	0
57	MG	14	3182	1/1	0.95	0.13	74,74,74,74	0
57	MG	14	3068	1/1	0.95	0.27	53,53,53,53	0
57	MG	13	1726	1/1	0.95	0.10	74,74,74,74	0
57	MG	13	1739	1/1	0.95	0.05	121,121,121,121	0
57	MG	14	3014	1/1	0.95	0.13	59,59,59,59	0
57	MG	P8	101	1/1	0.95	0.32	71,71,71,71	0
57	MG	14	3388	1/1	0.95	0.05	85,85,85,85	0
57	MG	1G	1645	1/1	0.95	0.08	81,81,81,81	0
57	MG	1G	1650	1/1	0.95	0.09	101,101,101,101	0
57	MG	1H	3267	1/1	0.95	0.14	56,56,56,56	0
57	MG	1H	3373	1/1	0.95	0.07	80,80,80,80	0
57	MG	14	3078	1/1	0.95	0.21	56,56,56,56	0
57	MG	14	3402	1/1	0.95	0.06	78,78,78,78	0
57	MG	1G	1662	1/1	0.95	0.07	91,91,91,91	0
57	MG	13	1632	1/1	0.95	0.08	78,78,78,78	0
57	MG	1G	1666	1/1	0.95	0.08	100,100,100,100	0
57	MG	1H	3492	1/1	0.95	0.15	78,78,78,78	0
57	MG	1H	3375	1/1	0.95	0.07	79,79,79,79	0
57	MG	1H	3032	1/1	0.95	0.11	47,47,47,47	0
57	MG	1H	3123	1/1	0.95	0.25	65,65,65,65	0
57	MG	1H	3500	1/1	0.95	0.10	94,94,94,94	0
57	MG	13	1708	1/1	0.95	0.08	65,65,65,65	0
57	MG	14	3423	1/1	0.95	0.06	120,120,120,120	0
57	MG	1H	3277	1/1	0.95	0.07	71,71,71,71	0
57	MG	1G	1677	1/1	0.95	0.14	92,92,92,92	0
57	MG	14	3426	1/1	0.95	0.13	104,104,104,104	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	14	3427	1/1	0.95	0.08	65,65,65,65	0
57	MG	14	3092	1/1	0.95	0.16	66,66,66,66	0
57	MG	14	3205	1/1	0.95	0.23	59,59,59,59	0
57	MG	1H	3508	1/1	0.95	0.06	117,117,117,117	0
57	MG	1H	3390	1/1	0.95	0.12	64,64,64,64	0
57	MG	14	3034	1/1	0.95	0.22	40,40,40,40	0
57	MG	1H	3283	1/1	0.95	0.10	71,71,71,71	0
57	MG	1H	3293	1/1	0.95	0.08	73,73,73,73	0
57	MG	14	3435	1/1	0.95	0.12	92,92,92,92	0
57	MG	1G	1690	1/1	0.95	0.05	117,117,117,117	0
57	MG	1H	3519	1/1	0.95	0.06	116,116,116,116	0
57	MG	1H	3298	1/1	0.95	0.07	51,51,51,51	0
57	MG	1G	1619	1/1	0.95	0.08	102,102,102,102	0
57	MG	1G	1696	1/1	0.95	0.07	128,128,128,128	0
57	MG	1H	3016	1/1	0.95	0.13	44,44,44,44	0
57	MG	1J	207	1/1	0.95	0.08	97,97,97,97	0
57	MG	1J	208	1/1	0.95	0.07	103,103,103,103	0
57	MG	14	3233	1/1	0.95	0.12	65,65,65,65	0
57	MG	14	3236	1/1	0.95	0.11	44,44,44,44	0
57	MG	39	301	1/1	0.95	0.15	89,89,89,89	0
57	MG	1H	3036	1/1	0.95	0.06	37,37,37,37	0
57	MG	1H	3199	1/1	0.95	0.07	61,61,61,61	0
57	MG	13	1729	1/1	0.95	0.07	110,110,110,110	0
57	MG	1H	3331	1/1	0.95	0.10	70,70,70,70	0
58	PAR	13	1741	42/42	0.95	0.08	64,71,75,82	0
57	MG	1H	3334	1/1	0.95	0.07	77,77,77,77	0
57	MG	1G	1626	1/1	0.95	0.12	83,83,83,83	0
57	MG	1H	3018	1/1	0.95	0.15	41,41,41,41	0
57	MG	1H	3019	1/1	0.95	0.13	32,32,32,32	0
57	MG	14	3285	1/1	0.95	0.09	108,108,108,108	0
57	MG	13	1604	1/1	0.96	0.09	62,62,62,62	0
57	MG	14	3317	1/1	0.96	0.11	82,82,82,82	0
57	MG	1G	1632	1/1	0.96	0.06	91,91,91,91	0
57	MG	14	3326	1/1	0.96	0.05	77,77,77,77	0
57	MG	1H	3380	1/1	0.96	0.13	55,55,55,55	0
57	MG	14	3329	1/1	0.96	0.05	105,105,105,105	0
57	MG	14	3330	1/1	0.96	0.07	94,94,94,94	0
57	MG	14	3332	1/1	0.96	0.05	102,102,102,102	0
57	MG	1H	3383	1/1	0.96	0.13	68,68,68,68	0
57	MG	14	3335	1/1	0.96	0.06	81,81,81,81	0
57	MG	14	3339	1/1	0.96	0.07	107,107,107,107	0
57	MG	16	210	1/1	0.96	0.06	73,73,73,73	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	14	3343	1/1	0.96	0.07	80,80,80,80	0
57	MG	1H	3121	1/1	0.96	0.18	39,39,39,39	0
57	MG	1H	3469	1/1	0.96	0.08	58,58,58,58	0
57	MG	1H	3470	1/1	0.96	0.08	83,83,83,83	0
57	MG	1H	3475	1/1	0.96	0.09	97,97,97,97	0
57	MG	13	1609	1/1	0.96	0.13	70,70,70,70	0
57	MG	14	3357	1/1	0.96	0.06	105,105,105,105	0
57	MG	14	3065	1/1	0.96	0.07	47,47,47,47	0
57	MG	14	3363	1/1	0.96	0.06	107,107,107,107	0
57	MG	13	1638	1/1	0.96	0.07	85,85,85,85	0
57	MG	14	3367	1/1	0.96	0.07	106,106,106,106	0
57	MG	14	3368	1/1	0.96	0.08	88,88,88,88	0
57	MG	14	3369	1/1	0.96	0.07	91,91,91,91	0
57	MG	1H	3138	1/1	0.96	0.12	54,54,54,54	0
57	MG	1H	3481	1/1	0.96	0.07	103,103,103,103	0
57	MG	1H	3185	1/1	0.96	0.28	64,64,64,64	0
57	MG	1H	3351	1/1	0.96	0.06	68,68,68,68	0
57	MG	1G	1646	1/1	0.96	0.06	86,86,86,86	0
57	MG	Q8	300	1/1	0.96	0.15	80,80,80,80	0
57	MG	14	3382	1/1	0.96	0.10	66,66,66,66	0
57	MG	1G	1653	1/1	0.96	0.06	97,97,97,97	0
57	MG	1G	1601	1/1	0.96	0.09	77,77,77,77	0
57	MG	14	3386	1/1	0.96	0.10	74,74,74,74	0
57	MG	13	1619	1/1	0.96	0.10	52,52,52,52	0
57	MG	1G	1660	1/1	0.96	0.07	74,74,74,74	0
57	MG	1G	1661	1/1	0.96	0.06	95,95,95,95	0
57	MG	13	1730	1/1	0.96	0.08	94,94,94,94	0
57	MG	1H	3400	1/1	0.96	0.06	53,53,53,53	0
57	MG	14	3021	1/1	0.96	0.20	38,38,38,38	0
57	MG	14	3140	1/1	0.96	0.04	51,51,51,51	0
57	MG	14	3399	1/1	0.96	0.08	123,123,123,123	0
57	MG	14	3400	1/1	0.96	0.06	108,108,108,108	0
57	MG	14	3401	1/1	0.96	0.11	110,110,110,110	0
57	MG	1H	3405	1/1	0.96	0.05	66,66,66,66	0
57	MG	14	3403	1/1	0.96	0.14	84,84,84,84	0
57	MG	14	3404	1/1	0.96	0.13	97,97,97,97	0
57	MG	14	3406	1/1	0.96	0.11	101,101,101,101	0
57	MG	1H	3407	1/1	0.96	0.09	72,72,72,72	0
57	MG	1H	3357	1/1	0.96	0.06	52,52,52,52	0
57	MG	1H	3358	1/1	0.96	0.10	45,45,45,45	0
57	MG	14	3412	1/1	0.96	0.06	97,97,97,97	0
57	MG	14	3086	1/1	0.96	0.12	56,56,56,56	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	1H	3416	1/1	0.96	0.06	89,89,89,89	0
57	MG	1G	1672	1/1	0.96	0.08	110,110,110,110	0
57	MG	14	3089	1/1	0.96	0.21	54,54,54,54	0
57	MG	14	3418	1/1	0.96	0.05	90,90,90,90	0
57	MG	14	3420	1/1	0.96	0.05	107,107,107,107	0
57	MG	1H	3417	1/1	0.96	0.16	83,83,83,83	0
57	MG	1H	3418	1/1	0.96	0.05	46,46,46,46	0
57	MG	13	1720	1/1	0.96	0.10	109,109,109,109	0
57	MG	1H	3421	1/1	0.96	0.06	82,82,82,82	0
57	MG	1H	3512	1/1	0.96	0.09	87,87,87,87	0
57	MG	1G	1682	1/1	0.96	0.05	123,123,123,123	0
57	MG	1G	1684	1/1	0.96	0.10	96,96,96,96	0
57	MG	1H	3285	1/1	0.96	0.14	55,55,55,55	0
57	MG	14	3222	1/1	0.96	0.11	59,59,59,59	0
57	MG	14	3230	1/1	0.96	0.07	63,63,63,63	0
57	MG	13	1721	1/1	0.96	0.09	106,106,106,106	0
57	MG	14	3158	1/1	0.96	0.06	66,66,66,66	0
57	MG	14	3237	1/1	0.96	0.10	51,51,51,51	0
57	MG	1H	3425	1/1	0.96	0.08	64,64,64,64	0
57	MG	1H	3428	1/1	0.96	0.08	89,89,89,89	0
57	MG	1G	1691	1/1	0.96	0.05	133,133,133,133	0
57	MG	14	3257	1/1	0.96	0.07	69,69,69,69	0
57	MG	14	3259	1/1	0.96	0.10	71,71,71,71	0
57	MG	14	3263	1/1	0.96	0.09	71,71,71,71	0
57	MG	1H	3431	1/1	0.96	0.06	98,98,98,98	0
57	MG	14	3271	1/1	0.96	0.05	94,94,94,94	0
57	MG	13	1722	1/1	0.96	0.06	87,87,87,87	0
57	MG	1H	3523	1/1	0.96	0.11	82,82,82,82	0
57	MG	1H	3440	1/1	0.96	0.06	92,92,92,92	0
57	MG	13	1737	1/1	0.96	0.12	99,99,99,99	0
57	MG	14	3284	1/1	0.96	0.07	72,72,72,72	0
57	MG	13	1706	1/1	0.96	0.05	117,117,117,117	0
57	MG	14	3286	1/1	0.96	0.08	73,73,73,73	0
57	MG	13	1680	1/1	0.96	0.08	64,64,64,64	0
57	MG	45	202	1/1	0.96	0.23	64,64,64,64	0
57	MG	C5	201	1/1	0.96	0.07	113,113,113,113	0
57	MG	14	3292	1/1	0.96	0.09	74,74,74,74	0
57	MG	M5	101	1/1	0.96	0.17	88,88,88,88	0
57	MG	1G	1700	1/1	0.96	0.06	109,109,109,109	0
57	MG	14	3296	1/1	0.96	0.06	72,72,72,72	0
57	MG	1H	3035	1/1	0.96	0.05	40,40,40,40	0
57	MG	1H	3062	1/1	0.96	0.12	38,38,38,38	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	1H	3454	1/1	0.96	0.05	111,111,111,111	0
57	MG	1H	3455	1/1	0.96	0.07	76,76,76,76	0
57	MG	13	1710	1/1	0.97	0.05	96,96,96,96	0
57	MG	1H	3343	1/1	0.97	0.05	78,78,78,78	0
57	MG	14	3313	1/1	0.97	0.04	105,105,105,105	0
57	MG	14	3314	1/1	0.97	0.09	69,69,69,69	0
57	MG	1H	3499	1/1	0.97	0.04	112,112,112,112	0
57	MG	1H	3408	1/1	0.97	0.07	67,67,67,67	0
57	MG	1H	3501	1/1	0.97	0.09	90,90,90,90	0
57	MG	14	3319	1/1	0.97	0.06	95,95,95,95	0
57	MG	14	3322	1/1	0.97	0.08	58,58,58,58	0
57	MG	14	3323	1/1	0.97	0.07	81,81,81,81	0
57	MG	1H	3502	1/1	0.97	0.18	141,141,141,141	0
57	MG	1H	3410	1/1	0.97	0.11	83,83,83,83	0
57	MG	1H	3504	1/1	0.97	0.04	109,109,109,109	0
57	MG	1H	3412	1/1	0.97	0.10	75,75,75,75	0
57	MG	1H	3506	1/1	0.97	0.07	106,106,106,106	0
57	MG	13	1711	1/1	0.97	0.07	74,74,74,74	0
57	MG	1H	3346	1/1	0.97	0.05	92,92,92,92	0
57	MG	14	3336	1/1	0.97	0.06	94,94,94,94	0
57	MG	14	3337	1/1	0.97	0.09	104,104,104,104	0
57	MG	13	1698	1/1	0.97	0.06	83,83,83,83	0
57	MG	1H	3513	1/1	0.97	0.06	53,53,53,53	0
57	MG	1H	3245	1/1	0.97	0.06	47,47,47,47	0
57	MG	14	3344	1/1	0.97	0.06	93,93,93,93	0
57	MG	14	3345	1/1	0.97	0.09	99,99,99,99	0
57	MG	1H	3115	1/1	0.97	0.06	61,61,61,61	0
57	MG	1H	3251	1/1	0.97	0.07	48,48,48,48	0
57	MG	14	3348	1/1	0.97	0.06	96,96,96,96	0
57	MG	1H	3420	1/1	0.97	0.04	69,69,69,69	0
57	MG	1H	3256	1/1	0.97	0.06	47,47,47,47	0
57	MG	1H	3355	1/1	0.97	0.06	59,59,59,59	0
57	MG	1H	3356	1/1	0.97	0.06	54,54,54,54	0
57	MG	14	3359	1/1	0.97	0.05	93,93,93,93	0
57	MG	14	3360	1/1	0.97	0.05	96,96,96,96	0
57	MG	1H	3094	1/1	0.97	0.03	33,33,33,33	0
57	MG	13	1618	1/1	0.97	0.09	48,48,48,48	0
57	MG	13	1621	1/1	0.97	0.13	85,85,85,85	0
57	MG	1H	3432	1/1	0.97	0.06	93,93,93,93	0
57	MG	1H	3433	1/1	0.97	0.14	72,72,72,72	0
57	MG	1H	3097	1/1	0.97	0.05	65,65,65,65	0
57	MG	14	3370	1/1	0.97	0.07	97,97,97,97	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	1G	1647	1/1	0.97	0.06	97,97,97,97	0
57	MG	1G	1648	1/1	0.97	0.09	115,115,115,115	0
57	MG	14	3375	1/1	0.97	0.04	93,93,93,93	0
57	MG	1G	1649	1/1	0.97	0.08	113,113,113,113	0
57	MG	1H	3435	1/1	0.97	0.10	62,62,62,62	0
57	MG	1G	1652	1/1	0.97	0.08	81,81,81,81	0
57	MG	14	3380	1/1	0.97	0.04	78,78,78,78	0
57	MG	1H	3437	1/1	0.97	0.07	92,92,92,92	0
57	MG	13	1703	1/1	0.97	0.06	70,70,70,70	0
57	MG	14	3383	1/1	0.97	0.06	90,90,90,90	0
57	MG	1H	3441	1/1	0.97	0.07	105,105,105,105	0
57	MG	1G	1656	1/1	0.97	0.06	100,100,100,100	0
57	MG	1G	1657	1/1	0.97	0.04	121,121,121,121	0
57	MG	1G	1659	1/1	0.97	0.05	115,115,115,115	0
57	MG	1H	3442	1/1	0.97	0.07	103,103,103,103	0
57	MG	13	1733	1/1	0.97	0.09	101,101,101,101	0
57	MG	13	1683	1/1	0.97	0.05	93,93,93,93	0
57	MG	13	1685	1/1	0.97	0.06	90,90,90,90	0
57	MG	13	1738	1/1	0.97	0.04	133,133,133,133	0
57	MG	14	3396	1/1	0.97	0.04	126,126,126,126	0
57	MG	14	3397	1/1	0.97	0.11	96,96,96,96	0
57	MG	13	1707	1/1	0.97	0.05	56,56,56,56	0
57	MG	1H	3190	1/1	0.97	0.35	91,91,91,91	0
57	MG	1H	3299	1/1	0.97	0.06	48,48,48,48	0
57	MG	1G	1670	1/1	0.97	0.05	134,134,134,134	0
57	MG	1H	3378	1/1	0.97	0.07	50,50,50,50	0
57	MG	1H	3379	1/1	0.97	0.05	73,73,73,73	0
57	MG	13	1740	1/1	0.97	0.05	98,98,98,98	0
57	MG	14	3405	1/1	0.97	0.04	108,108,108,108	0
57	MG	I8	101	1/1	0.97	0.05	85,85,85,85	0
57	MG	1G	1675	1/1	0.97	0.05	103,103,103,103	0
57	MG	1H	3301	1/1	0.97	0.05	45,45,45,45	0
57	MG	1H	3384	1/1	0.97	0.10	67,67,67,67	0
57	MG	14	3410	1/1	0.97	0.05	85,85,85,85	0
57	MG	1H	3027	1/1	0.97	0.10	52,52,52,52	0
57	MG	14	3218	1/1	0.97	0.05	65,65,65,65	0
57	MG	1G	1679	1/1	0.97	0.09	94,94,94,94	0
57	MG	14	3415	1/1	0.97	0.12	103,103,103,103	0
57	MG	1G	1680	1/1	0.97	0.05	123,123,123,123	0
57	MG	14	3223	1/1	0.97	0.10	87,87,87,87	0
57	MG	14	3225	1/1	0.97	0.05	73,73,73,73	0
57	MG	14	3419	1/1	0.97	0.04	110,110,110,110	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	14	3228	1/1	0.97	0.07	56,56,56,56	0
57	MG	1H	3474	1/1	0.97	0.07	93,93,93,93	0
57	MG	13	1691	1/1	0.97	0.07	92,92,92,92	0
57	MG	14	3056	1/1	0.97	0.09	54,54,54,54	0
57	MG	1H	3316	1/1	0.97	0.08	78,78,78,78	0
57	MG	14	3238	1/1	0.97	0.06	50,50,50,50	0
57	MG	1H	3317	1/1	0.97	0.06	66,66,66,66	0
57	MG	14	3244	1/1	0.97	0.06	54,54,54,54	0
57	MG	14	3245	1/1	0.97	0.05	63,63,63,63	0
57	MG	1G	1687	1/1	0.97	0.04	111,111,111,111	0
57	MG	1H	3478	1/1	0.97	0.04	101,101,101,101	0
57	MG	14	3255	1/1	0.97	0.13	79,79,79,79	0
57	MG	14	3256	1/1	0.97	0.08	83,83,83,83	0
57	MG	1G	1689	1/1	0.97	0.05	116,116,116,116	0
57	MG	14	3258	1/1	0.97	0.05	79,79,79,79	0
57	MG	14	3062	1/1	0.97	0.13	59,59,59,59	0
57	MG	1G	1607	1/1	0.97	0.10	86,86,86,86	0
57	MG	1H	3030	1/1	0.97	0.05	39,39,39,39	0
57	MG	14	3265	1/1	0.97	0.08	91,91,91,91	0
57	MG	14	3266	1/1	0.97	0.04	107,107,107,107	0
57	MG	14	3268	1/1	0.97	0.07	82,82,82,82	0
57	MG	1H	3329	1/1	0.97	0.05	85,85,85,85	0
57	MG	14	3275	1/1	0.97	0.06	65,65,65,65	0
57	MG	1H	3482	1/1	0.97	0.05	94,94,94,94	0
57	MG	1G	1694	1/1	0.97	0.06	113,113,113,113	0
57	MG	14	3278	1/1	0.97	0.04	102,102,102,102	0
57	MG	1H	3394	1/1	0.97	0.06	49,49,49,49	0
57	MG	1H	3031	1/1	0.97	0.06	51,51,51,51	0
57	MG	1H	3486	1/1	0.97	0.08	95,95,95,95	0
57	MG	14	3071	1/1	0.97	0.11	74,74,74,74	0
57	MG	13	1725	1/1	0.97	0.04	115,115,115,115	0
57	MG	1H	3397	1/1	0.97	0.08	51,51,51,51	0
57	MG	13	1694	1/1	0.97	0.12	82,82,82,82	0
57	MG	14	3293	1/1	0.97	0.06	63,63,63,63	0
57	MG	1G	1701	1/1	0.97	0.04	111,111,111,111	0
57	MG	1H	3490	1/1	0.97	0.07	89,89,89,89	0
57	MG	1H	3403	1/1	0.97	0.05	99,99,99,99	0
60	ZN	C5	202	1/1	0.97	0.04	165,165,165,165	0
57	MG	1H	3404	1/1	0.97	0.06	71,71,71,71	0
57	MG	14	3299	1/1	0.97	0.05	79,79,79,79	0
57	MG	14	3304	1/1	0.97	0.07	74,74,74,74	0
57	MG	14	3325	1/1	0.98	0.06	79,79,79,79	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	13	1735	1/1	0.98	0.06	100,100,100,100	0
57	MG	13	1688	1/1	0.98	0.05	109,109,109,109	0
57	MG	1H	3303	1/1	0.98	0.05	48,48,48,48	0
57	MG	1H	3307	1/1	0.98	0.06	44,44,44,44	0
57	MG	14	3331	1/1	0.98	0.11	90,90,90,90	0
57	MG	1H	3308	1/1	0.98	0.05	50,50,50,50	0
57	MG	13	1684	1/1	0.98	0.04	85,85,85,85	0
57	MG	1H	3393	1/1	0.98	0.04	50,50,50,50	0
57	MG	1H	3491	1/1	0.98	0.12	70,70,70,70	0
57	MG	13	1681	1/1	0.98	0.05	59,59,59,59	0
57	MG	14	3338	1/1	0.98	0.04	107,107,107,107	0
57	MG	1H	3494	1/1	0.98	0.09	72,72,72,72	0
57	MG	1H	3314	1/1	0.98	0.05	68,68,68,68	0
57	MG	1H	3246	1/1	0.98	0.04	55,55,55,55	0
57	MG	1H	3248	1/1	0.98	0.05	44,44,44,44	0
57	MG	1H	3318	1/1	0.98	0.07	59,59,59,59	0
57	MG	1H	3401	1/1	0.98	0.05	64,64,64,64	0
57	MG	13	1713	1/1	0.98	0.04	86,86,86,86	0
57	MG	1H	3323	1/1	0.98	0.10	57,57,57,57	0
57	MG	14	3349	1/1	0.98	0.05	83,83,83,83	0
57	MG	1H	3324	1/1	0.98	0.07	70,70,70,70	0
57	MG	14	3351	1/1	0.98	0.05	78,78,78,78	0
57	MG	14	3353	1/1	0.98	0.05	83,83,83,83	0
57	MG	1H	3250	1/1	0.98	0.06	41,41,41,41	0
57	MG	1H	3330	1/1	0.98	0.06	71,71,71,71	0
57	MG	1H	3409	1/1	0.98	0.04	85,85,85,85	0
57	MG	1H	3507	1/1	0.98	0.04	57,57,57,57	0
57	MG	13	1695	1/1	0.98	0.04	106,106,106,106	0
57	MG	1H	3509	1/1	0.98	0.04	47,47,47,47	0
57	MG	1H	3332	1/1	0.98	0.11	102,102,102,102	0
57	MG	14	3364	1/1	0.98	0.07	92,92,92,92	0
57	MG	14	3365	1/1	0.98	0.04	78,78,78,78	0
57	MG	1H	3253	1/1	0.98	0.05	42,42,42,42	0
57	MG	1H	3335	1/1	0.98	0.04	48,48,48,48	0
57	MG	1G	1651	1/1	0.98	0.06	76,76,76,76	0
57	MG	1H	3514	1/1	0.98	0.04	98,98,98,98	0
57	MG	1H	3336	1/1	0.98	0.04	62,62,62,62	0
57	MG	14	3371	1/1	0.98	0.05	107,107,107,107	0
57	MG	13	1716	1/1	0.98	0.05	71,71,71,71	0
57	MG	1H	3518	1/1	0.98	0.05	96,96,96,96	0
57	MG	14	3374	1/1	0.98	0.06	92,92,92,92	0
57	MG	1H	3340	1/1	0.98	0.05	76,76,76,76	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	1H	3260	1/1	0.98	0.06	42,42,42,42	0
57	MG	1G	1658	1/1	0.98	0.03	104,104,104,104	0
57	MG	14	3378	1/1	0.98	0.07	92,92,92,92	0
57	MG	14	3219	1/1	0.98	0.04	57,57,57,57	0
57	MG	14	3220	1/1	0.98	0.05	54,54,54,54	0
57	MG	13	1696	1/1	0.98	0.07	93,93,93,93	0
57	MG	1H	3264	1/1	0.98	0.15	50,50,50,50	0
57	MG	1H	3266	1/1	0.98	0.04	54,54,54,54	0
57	MG	14	3224	1/1	0.98	0.06	45,45,45,45	0
57	MG	1H	3347	1/1	0.98	0.10	67,67,67,67	0
57	MG	14	3227	1/1	0.98	0.04	58,58,58,58	0
57	MG	1H	3424	1/1	0.98	0.04	101,101,101,101	0
57	MG	1G	1664	1/1	0.98	0.08	80,80,80,80	0
57	MG	14	3389	1/1	0.98	0.04	93,93,93,93	0
57	MG	14	3231	1/1	0.98	0.07	55,55,55,55	0
57	MG	14	3045	1/1	0.98	0.15	53,53,53,53	0
57	MG	14	3392	1/1	0.98	0.04	63,63,63,63	0
57	MG	14	3234	1/1	0.98	0.06	57,57,57,57	0
57	MG	13	1718	1/1	0.98	0.07	90,90,90,90	0
57	MG	1H	3427	1/1	0.98	0.11	67,67,67,67	0
57	MG	1H	3039	1/1	0.98	0.13	33,33,33,33	0
57	MG	14	3241	1/1	0.98	0.05	78,78,78,78	0
57	MG	1H	3430	1/1	0.98	0.07	73,73,73,73	0
57	MG	2K	101	1/1	0.98	0.09	100,100,100,100	0
57	MG	13	1697	1/1	0.98	0.07	84,84,84,84	0
57	MG	14	3249	1/1	0.98	0.06	52,52,52,52	0
57	MG	14	3251	1/1	0.98	0.05	80,80,80,80	0
57	MG	1H	3273	1/1	0.98	0.10	78,78,78,78	0
57	MG	13	1687	1/1	0.98	0.04	103,103,103,103	0
57	MG	1H	3276	1/1	0.98	0.03	78,78,78,78	0
57	MG	1H	3107	1/1	0.98	0.06	60,60,60,60	0
57	MG	1H	3281	1/1	0.98	0.09	61,61,61,61	0
57	MG	1H	3359	1/1	0.98	0.06	44,44,44,44	0
57	MG	1H	3360	1/1	0.98	0.04	78,78,78,78	0
57	MG	14	3260	1/1	0.98	0.08	106,106,106,106	0
57	MG	1H	3361	1/1	0.98	0.04	52,52,52,52	0
57	MG	1H	3028	1/1	0.98	0.10	67,67,67,67	0
57	MG	1G	1681	1/1	0.98	0.05	96,96,96,96	0
57	MG	1H	3284	1/1	0.98	0.04	83,83,83,83	0
57	MG	14	3267	1/1	0.98	0.06	82,82,82,82	0
57	MG	1G	1683	1/1	0.98	0.10	121,121,121,121	0
57	MG	14	3269	1/1	0.98	0.10	78,78,78,78	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	14	3270	1/1	0.98	0.05	67,67,67,67	0
57	MG	1H	3446	1/1	0.98	0.05	98,98,98,98	0
57	MG	1H	3091	1/1	0.98	0.17	41,41,41,41	0
57	MG	1H	3449	1/1	0.98	0.05	80,80,80,80	0
57	MG	1H	3451	1/1	0.98	0.03	102,102,102,102	0
57	MG	1H	3452	1/1	0.98	0.09	72,72,72,72	0
57	MG	1H	3287	1/1	0.98	0.05	71,71,71,71	0
57	MG	1H	3289	1/1	0.98	0.05	59,59,59,59	0
57	MG	14	3282	1/1	0.98	0.06	90,90,90,90	0
57	MG	14	3283	1/1	0.98	0.08	68,68,68,68	0
57	MG	1H	3369	1/1	0.98	0.04	44,44,44,44	0
57	MG	1H	3370	1/1	0.98	0.09	68,68,68,68	0
57	MG	1H	3371	1/1	0.98	0.07	56,56,56,56	0
57	MG	14	3287	1/1	0.98	0.04	88,88,88,88	0
57	MG	14	3288	1/1	0.98	0.07	49,49,49,49	0
57	MG	14	3289	1/1	0.98	0.04	74,74,74,74	0
57	MG	14	3290	1/1	0.98	0.07	59,59,59,59	0
57	MG	1H	3459	1/1	0.98	0.05	75,75,75,75	0
57	MG	1H	3460	1/1	0.98	0.04	96,96,96,96	0
57	MG	1H	3461	1/1	0.98	0.04	45,45,45,45	0
57	MG	1H	3290	1/1	0.98	0.05	55,55,55,55	0
57	MG	1H	3465	1/1	0.98	0.11	67,67,67,67	0
57	MG	1H	3467	1/1	0.98	0.06	84,84,84,84	0
57	MG	1H	3291	1/1	0.98	0.04	59,59,59,59	0
57	MG	1H	3292	1/1	0.98	0.11	43,43,43,43	0
57	MG	14	3303	1/1	0.98	0.07	74,74,74,74	0
57	MG	13	1699	1/1	0.98	0.04	83,83,83,83	0
57	MG	1H	3471	1/1	0.98	0.09	90,90,90,90	0
57	MG	25	201	1/1	0.98	0.04	115,115,115,115	0
57	MG	14	3308	1/1	0.98	0.05	94,94,94,94	0
57	MG	14	3311	1/1	0.98	0.04	67,67,67,67	0
57	MG	1H	3473	1/1	0.98	0.10	95,95,95,95	0
57	MG	1H	3294	1/1	0.98	0.07	54,54,54,54	0
57	MG	1H	3377	1/1	0.98	0.12	76,76,76,76	0
57	MG	14	3315	1/1	0.98	0.06	68,68,68,68	0
57	MG	1H	3295	1/1	0.98	0.04	89,89,89,89	0
57	MG	1H	3296	1/1	0.98	0.08	91,91,91,91	0
59	SF4	3E	301	8/8	0.98	0.04	82,91,95,98	0
57	MG	1H	3297	1/1	0.98	0.06	49,49,49,49	0
60	ZN	5A	101	1/1	0.98	0.04	146,146,146,146	0
57	MG	1H	3381	1/1	0.98	0.09	74,74,74,74	0
57	MG	14	3320	1/1	0.98	0.06	53,53,53,53	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	1H	3183	1/1	0.98	0.15	70,70,70,70	0
57	MG	1H	3060	1/1	0.98	0.09	35,35,35,35	0
57	MG	14	3356	1/1	0.99	0.07	75,75,75,75	0
57	MG	1H	3411	1/1	0.99	0.03	63,63,63,63	0
57	MG	14	3358	1/1	0.99	0.04	86,86,86,86	0
57	MG	1G	1665	1/1	0.99	0.03	91,91,91,91	0
57	MG	13	1734	1/1	0.99	0.03	94,94,94,94	0
57	MG	14	3361	1/1	0.99	0.09	79,79,79,79	0
57	MG	1H	3413	1/1	0.99	0.08	78,78,78,78	0
57	MG	13	1693	1/1	0.99	0.03	85,85,85,85	0
57	MG	I8	102	1/1	0.99	0.07	62,62,62,62	0
57	MG	1H	3320	1/1	0.99	0.02	58,58,58,58	0
57	MG	1H	3364	1/1	0.99	0.03	44,44,44,44	0
57	MG	14	3261	1/1	0.99	0.05	59,59,59,59	0
57	MG	14	3262	1/1	0.99	0.04	83,83,83,83	0
57	MG	1H	3480	1/1	0.99	0.06	87,87,87,87	0
57	MG	1H	3365	1/1	0.99	0.09	67,67,67,67	0
57	MG	1H	3286	1/1	0.99	0.03	40,40,40,40	0
57	MG	1H	3262	1/1	0.99	0.07	43,43,43,43	0
57	MG	1H	3288	1/1	0.99	0.05	54,54,54,54	0
57	MG	1H	3485	1/1	0.99	0.04	77,77,77,77	0
57	MG	1H	3326	1/1	0.99	0.02	62,62,62,62	0
57	MG	1H	3327	1/1	0.99	0.05	50,50,50,50	0
57	MG	1H	3328	1/1	0.99	0.03	47,47,47,47	0
57	MG	14	3272	1/1	0.99	0.08	71,71,71,71	0
57	MG	14	3273	1/1	0.99	0.05	86,86,86,86	0
57	MG	14	3274	1/1	0.99	0.08	85,85,85,85	0
57	MG	1H	3263	1/1	0.99	0.05	46,46,46,46	0
57	MG	1H	3247	1/1	0.99	0.06	36,36,36,36	0
57	MG	1H	3426	1/1	0.99	0.06	74,74,74,74	0
57	MG	13	1690	1/1	0.99	0.09	70,70,70,70	0
57	MG	1H	3493	1/1	0.99	0.03	101,101,101,101	0
57	MG	14	3280	1/1	0.99	0.04	61,61,61,61	0
57	MG	13	1715	1/1	0.99	0.06	76,76,76,76	0
57	MG	1H	3495	1/1	0.99	0.03	97,97,97,97	0
57	MG	1H	3429	1/1	0.99	0.08	88,88,88,88	0
57	MG	1H	3333	1/1	0.99	0.09	77,77,77,77	0
57	MG	13	1705	1/1	0.99	0.08	97,97,97,97	0
57	MG	1H	3269	1/1	0.99	0.04	41,41,41,41	0
57	MG	13	1689	1/1	0.99	0.06	88,88,88,88	0
57	MG	14	3394	1/1	0.99	0.04	91,91,91,91	0
57	MG	1H	3337	1/1	0.99	0.04	86,86,86,86	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	1H	3338	1/1	0.99	0.03	66,66,66,66	0
57	MG	1H	3436	1/1	0.99	0.03	70,70,70,70	0
57	MG	1H	3382	1/1	0.99	0.03	49,49,49,49	0
57	MG	1H	3438	1/1	0.99	0.07	62,62,62,62	0
57	MG	1H	3439	1/1	0.99	0.06	67,67,67,67	0
57	MG	14	3294	1/1	0.99	0.09	75,75,75,75	0
57	MG	1H	3252	1/1	0.99	0.04	65,65,65,65	0
57	MG	1H	3272	1/1	0.99	0.05	63,63,63,63	0
57	MG	13	1702	1/1	0.99	0.14	85,85,85,85	0
57	MG	1H	3510	1/1	0.99	0.07	39,39,39,39	0
57	MG	1H	3387	1/1	0.99	0.03	33,33,33,33	0
57	MG	14	3300	1/1	0.99	0.07	89,89,89,89	0
57	MG	14	3301	1/1	0.99	0.03	85,85,85,85	0
57	MG	14	3302	1/1	0.99	0.03	58,58,58,58	0
57	MG	1H	3342	1/1	0.99	0.03	86,86,86,86	0
57	MG	14	3411	1/1	0.99	0.04	105,105,105,105	0
57	MG	1H	3254	1/1	0.99	0.02	46,46,46,46	0
57	MG	14	3305	1/1	0.99	0.03	49,49,49,49	0
57	MG	14	3306	1/1	0.99	0.04	58,58,58,58	0
57	MG	1H	3275	1/1	0.99	0.11	57,57,57,57	0
57	MG	1H	3345	1/1	0.99	0.03	102,102,102,102	0
57	MG	14	3309	1/1	0.99	0.05	55,55,55,55	0
57	MG	14	3310	1/1	0.99	0.05	54,54,54,54	0
57	MG	1H	3448	1/1	0.99	0.06	80,80,80,80	0
57	MG	1H	3517	1/1	0.99	0.06	91,91,91,91	0
57	MG	1H	3255	1/1	0.99	0.02	49,49,49,49	0
57	MG	13	1719	1/1	0.99	0.06	81,81,81,81	0
57	MG	14	3217	1/1	0.99	0.06	56,56,56,56	0
57	MG	1H	3304	1/1	0.99	0.03	58,58,58,58	0
57	MG	1H	3349	1/1	0.99	0.03	50,50,50,50	0
57	MG	1H	3305	1/1	0.99	0.05	63,63,63,63	0
57	MG	1H	3278	1/1	0.99	0.03	75,75,75,75	0
57	MG	1H	3456	1/1	0.99	0.03	94,94,94,94	0
57	MG	14	3321	1/1	0.99	0.09	69,69,69,69	0
57	MG	1H	3398	1/1	0.99	0.07	78,78,78,78	0
57	MG	1H	3399	1/1	0.99	0.07	73,73,73,73	0
57	MG	14	3324	1/1	0.99	0.03	48,48,48,48	0
57	MG	1H	3279	1/1	0.99	0.06	48,48,48,48	0
57	MG	14	3226	1/1	0.99	0.05	51,51,51,51	0
57	MG	14	3327	1/1	0.99	0.03	82,82,82,82	0
57	MG	1H	3353	1/1	0.99	0.06	48,48,48,48	0
57	MG	1H	3402	1/1	0.99	0.04	85,85,85,85	0

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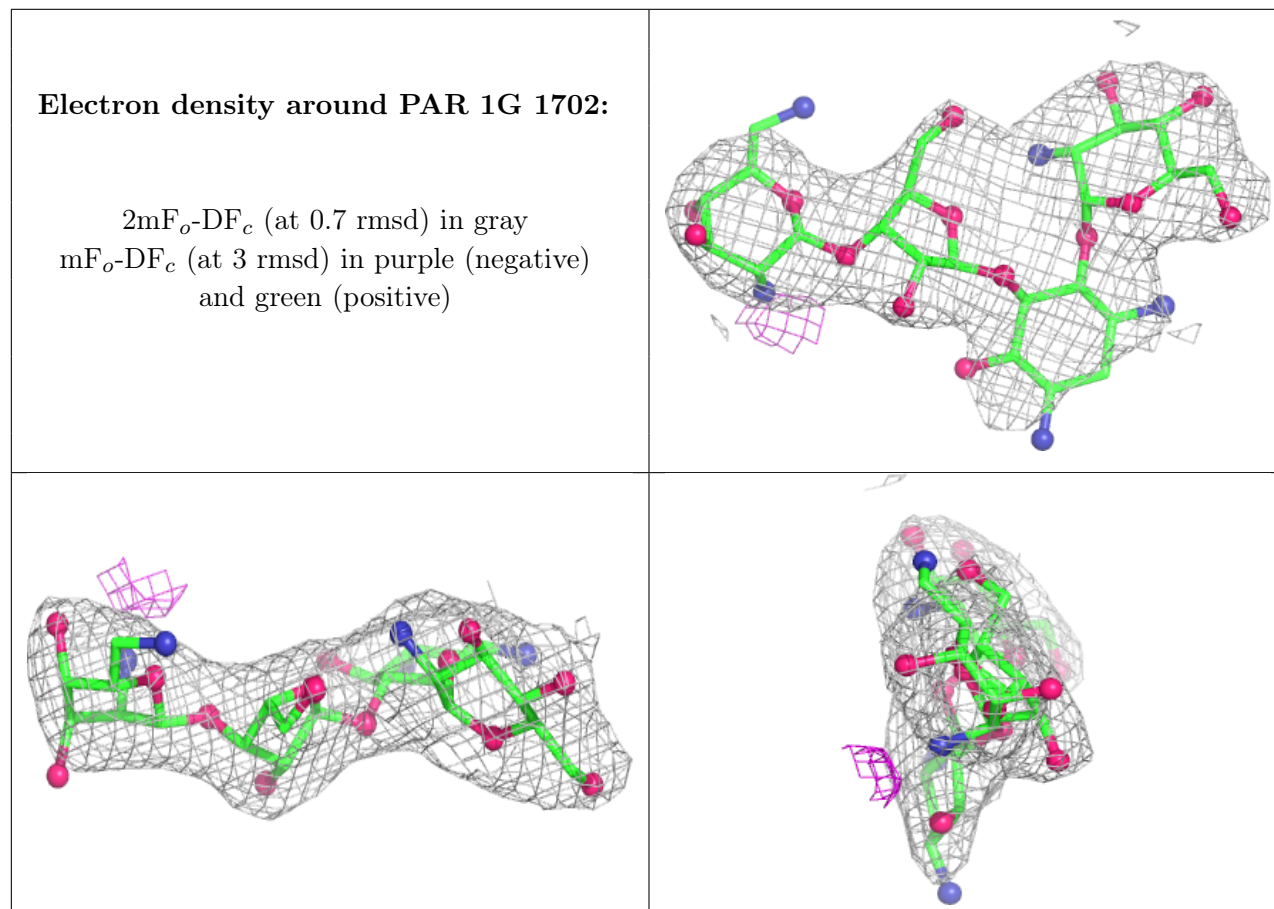
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	14	3229	1/1	0.99	0.02	59,59,59,59	0
57	MG	1H	3280	1/1	0.99	0.04	36,36,36,36	0
57	MG	1H	3463	1/1	0.99	0.06	81,81,81,81	0
57	MG	14	3333	1/1	0.99	0.04	50,50,50,50	0
57	MG	14	3232	1/1	0.99	0.03	66,66,66,66	0
57	MG	1H	3464	1/1	0.99	0.06	63,63,63,63	0
57	MG	1H	3258	1/1	0.99	0.03	47,47,47,47	0
57	MG	14	3235	1/1	0.99	0.09	48,48,48,48	0
57	MG	1H	3466	1/1	0.99	0.03	72,72,72,72	0
57	MG	1H	3312	1/1	0.99	0.05	44,44,44,44	0
57	MG	14	3340	1/1	0.99	0.07	107,107,107,107	0
57	MG	14	3341	1/1	0.99	0.03	66,66,66,66	0
57	MG	16	211	1/1	0.99	0.08	73,73,73,73	0
57	MG	14	3239	1/1	0.99	0.04	77,77,77,77	0
57	MG	14	3240	1/1	0.99	0.04	73,73,73,73	0
57	MG	1H	3406	1/1	0.99	0.08	85,85,85,85	0
57	MG	1H	3313	1/1	0.99	0.07	47,47,47,47	0
57	MG	1H	3282	1/1	0.99	0.08	71,71,71,71	0
57	MG	1H	3315	1/1	0.99	0.02	63,63,63,63	0
57	MG	14	3246	1/1	0.99	0.03	61,61,61,61	0
59	SF4	32	302	8/8	0.99	0.04	100,109,118,124	0
60	ZN	5I	102	1/1	0.99	0.02	86,86,86,86	0
57	MG	14	3247	1/1	0.99	0.05	52,52,52,52	0
57	MG	14	3248	1/1	0.99	0.11	47,47,47,47	0
57	MG	14	3352	1/1	0.99	0.09	82,82,82,82	0
57	MG	1H	3472	1/1	0.99	0.03	83,83,83,83	0
57	MG	14	3250	1/1	0.99	0.03	79,79,79,79	0
57	MG	1H	3259	1/1	0.99	0.07	54,54,54,54	0
57	MG	14	3242	1/1	1.00	0.02	62,62,62,62	0
57	MG	1H	3302	1/1	1.00	0.02	51,51,51,51	0
57	MG	1H	3385	1/1	1.00	0.04	25,25,25,25	0
57	MG	14	3216	1/1	1.00	0.05	52,52,52,52	0
57	MG	1H	3325	1/1	1.00	0.04	46,46,46,46	0
57	MG	13	1686	1/1	1.00	0.05	76,76,76,76	0
57	MG	21	303	1/1	1.00	0.03	46,46,46,46	0
57	MG	1H	3257	1/1	1.00	0.02	43,43,43,43	0
57	MG	1H	3311	1/1	1.00	0.02	53,53,53,53	0
57	MG	1H	3319	1/1	1.00	0.08	57,57,57,57	0
57	MG	13	1692	1/1	1.00	0.06	72,72,72,72	0
57	MG	14	3253	1/1	1.00	0.03	58,58,58,58	0
57	MG	1H	3306	1/1	1.00	0.03	75,75,75,75	0
57	MG	1H	3322	1/1	1.00	0.04	58,58,58,58	0

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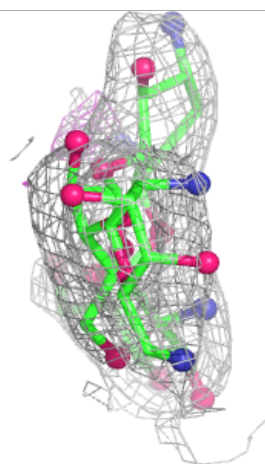
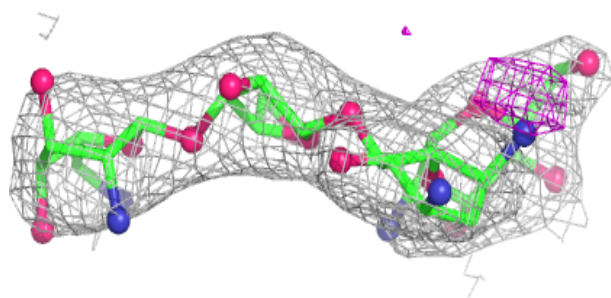
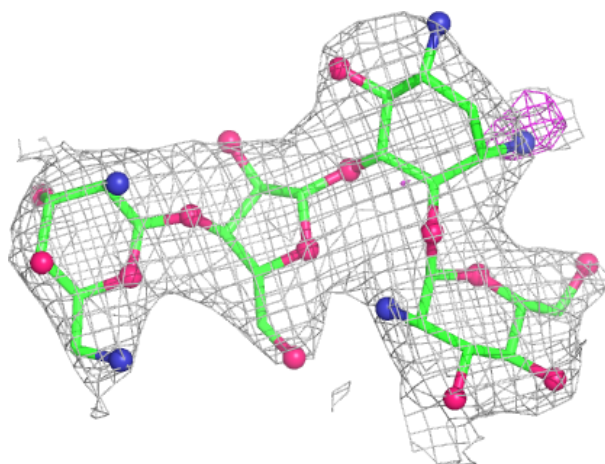
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	1H	3265	1/1	1.00	0.01	46,46,46,46	0
57	MG	1H	3450	1/1	1.00	0.01	44,44,44,44	0

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



Electron density around PAR 13 1741:

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



5.5 Other polymers [i](#)

There are no such residues in this entry.