



wwPDB X-ray Structure Validation Summary Report ⓘ

Sep 16, 2026 – 04:18 am BST

PDB ID : 5IBB / pdb_00005ibb
Title : Structure of T. thermophilus 70S ribosome complex with mRNA, tRNA^{fMet} and cognate tRNA^{Val} in the A-site
Authors : Rozov, A.; Demeshkina, N.; Yusupov, M.; Yusupova, G.
Deposited on : 2016-02-22
Resolution : 2.96 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
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

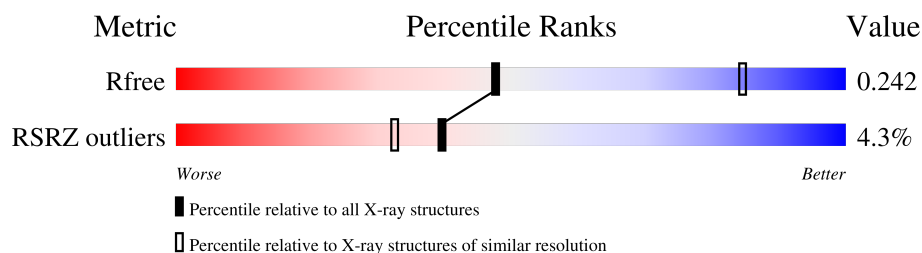
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.96 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	1130 (2.98-2.94)
RSRZ outliers	180081	1130 (2.98-2.94)

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	1653	-	-	-	X
57	MG	13	1660	-	-	-	X
57	MG	13	1671	-	-	-	X
57	MG	13	1676	-	-	-	X
57	MG	13	1685	-	-	-	X
57	MG	13	1687	-	-	-	X
57	MG	13	1690	-	-	-	X
57	MG	14	3157	-	-	-	X
57	MG	14	3178	-	-	-	X
57	MG	14	3214	-	-	-	X
57	MG	1G	1624	-	-	-	X
57	MG	1G	1630	-	-	-	X
57	MG	1G	1648	-	-	-	X
57	MG	1H	3008	-	-	-	X
57	MG	1H	3087	-	-	-	X
57	MG	1H	3097	-	-	-	X
57	MG	1H	3120	-	-	-	X
57	MG	1H	3133	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
57	MG	1H	3188	-	-	-	X
57	MG	1H	3224	-	-	-	X
57	MG	1H	3239	-	-	-	X
57	MG	1H	3248	-	-	-	X
57	MG	1H	3250	-	-	-	X
57	MG	1H	3260	-	-	-	X
57	MG	1H	3269	-	-	-	X
57	MG	1H	3274	-	-	-	X
57	MG	1H	3285	-	-	-	X
57	MG	4E	201	-	-	-	X
57	MG	J8	101	-	-	-	X

2 Entry composition

There are 61 unique types of molecules in this entry. The entry contains 296743 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	1496	Total	C	N	O	P	0	0	0
			32157	14313	5960	10388	1496			
1	1G	1506	Total	C	N	O	P	0	0	0
			32371	14409	6001	10456	1505			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
13	1542	G	U	conflict	GB 55771382
1G	1542	G	U	conflict	GB 55771382

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	1E	235	Total	C	N	O	S	0	0	0
			1902	1215	340	342	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			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
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	149	Total	C	N	O	S	0	0	0
			1139	721	216	198	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	140	Total	C	N	O	S	0	0	0
			1120	695	223	196	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			
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	95	Total	C	N	O	S	0	0	0
			754	471	148	134	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	122	Total	C	N	O	S	0	0	0
			956	603	193	159	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	4I	119	Total	C	N	O	S	0	0	0
			942	582	194	164	2			
13	4A	111	Total	C	N	O	S	0	0	0
			893	552	183	156	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	5I	60	Total	C	N	O	S	0	0	0
			491	312	104	71	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	100	Total	C	N	O	S	0	0	0
			834	534	155	143	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	62	Total	C	N	O	S	0	0	0
			481	306	85	88	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			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
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 tRNAVal.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	1K	72	Total	C	N	O	P	0	0	0
			1540	688	274	506	72			

- Molecule 23 is a RNA chain called tRNAfMet.

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	76	Total	C	N	O	P	S	0	0	0
			1626	726	296	527	76	1			

- Molecule 24 is a RNA chain called tRNAVal.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	3K	70	Total	C	N	O	P	0	0	0
			1491	665	268	488	70			
24	3L	71	Total	C	N	O	P	0	0	0
			1513	675	272	495	71			

- Molecule 25 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
25	4K	21	Total	C	N	O	P	0	0	0
			462	207	96	138	21			
25	4L	19	Total	C	N	O	P	0	0	0
			417	187	86	125	19			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	1H	2841	Total 61195	C 27234	N 11446	O 19674	P 2841	0	0	0
26	14	2810	Total 60535	C 26940	N 11330	O 19455	P 2810	0	0	0

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	1058	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 2617	C 1166	N 486	O 844	P 121	0	0	0
27	1J	122	Total 2617	C 1166	N 486	O 844	P 121	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
28	71	133	Total 1033	C 651	N 194	O 187	S 1	0	0	0
28	79	57	Total 456	C 283	N 91	O 82		0	0	0

- 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	202	Total	C	N	O	S	0	0	0
			1505	951	281	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	181	Total	C	N	O	S	0	0	0
			1468	937	268	259	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	167	Total	C	N	O	S	0	0	0
			1283	815	239	228	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
34	61	146	Total	C	N	O	S	0	0	0
			1136	726	201	208	1			

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

- 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	139	Total	C	N	O	S	0	0	0
			1104	705	209	184	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			
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	136	Total	C	N	O	S	0	0	0
			1124	700	231	192	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
			743	482	134	126	1			
45	B5	94	Total	C	N	O	S	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
			777	501	145	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	133	Total	C	N	O	S	0	0	0
			1079	694	194	189	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	94	Total	C	N	O	S	0	0	0
			737	463	146	127	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			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
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		0	0	0
			459	293	89	77				
51	H5	58	Total	C	N	O		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	61	Total	C	N	O	S	0	0	0
			479	299	86	89	5			
52	I5	63	Total	C	N	O	S	0	0	0
			515	326	93	91	5			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
53	N8	56	Total	C	N	O	S	0	0	0
			437	275	87	70	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 L34.

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

- Molecule 55 is a protein called 50S ribosomal protein L35.

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

- Molecule 56 is a RNA chain called tRNAVal.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
56	1L	69	Total	C	N	O	P	0	0	0
			1469	656	262	482	69			

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	13	148	Total	Mg	0	0
			148	148		
57	4E	1	Total	Mg	0	0
			1	1		
57	5E	1	Total	Mg	0	0
			1	1		
57	3I	1	Total	Mg	0	0
			1	1		
57	5I	1	Total	Mg	0	0
			1	1		
57	2K	4	Total	Mg	0	0
			4	4		
57	4K	2	Total	Mg	0	0
			2	2		
57	1H	548	Total	Mg	0	0
			548	548		
57	16	11	Total	Mg	0	0
			11	11		
57	11	2	Total	Mg	0	0
			2	2		
57	21	2	Total	Mg	0	0
			2	2		
57	31	2	Total	Mg	0	0
			2	2		
57	41	1	Total	Mg	0	0
			1	1		
57	68	2	Total	Mg	0	0
			2	2		
57	78	1	Total	Mg	0	0
			1	1		
57	88	3	Total	Mg	0	0
			3	3		
57	F8	1	Total	Mg	0	0
			1	1		
57	I8	1	Total	Mg	0	0
			1	1		

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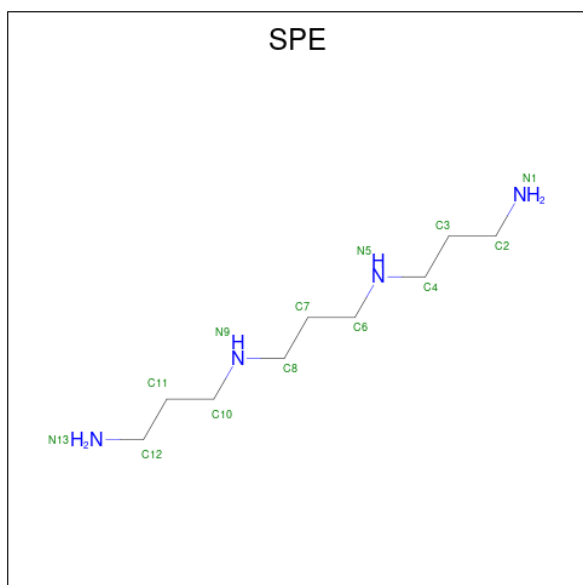
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	J8	1	Total 1	Mg 1	0	0
57	L8	1	Total 1	Mg 1	0	0
57	P8	1	Total 1	Mg 1	0	0
57	Q8	1	Total 1	Mg 1	0	0
57	1G	133	Total 133	Mg 133	0	0
57	42	1	Total 1	Mg 1	0	0
57	3A	1	Total 1	Mg 1	0	0
57	4A	1	Total 1	Mg 1	0	0
57	9A	1	Total 1	Mg 1	0	0
57	2L	3	Total 3	Mg 3	0	0
57	4L	2	Total 2	Mg 2	0	0
57	14	445	Total 445	Mg 445	0	0
57	1J	7	Total 7	Mg 7	0	0
57	19	1	Total 1	Mg 1	0	0
57	29	2	Total 2	Mg 2	0	0
57	39	2	Total 2	Mg 2	0	0
57	25	2	Total 2	Mg 2	0	0
57	35	2	Total 2	Mg 2	0	0
57	45	1	Total 1	Mg 1	0	0
57	B5	1	Total 1	Mg 1	0	0
57	C5	1	Total 1	Mg 1	0	0

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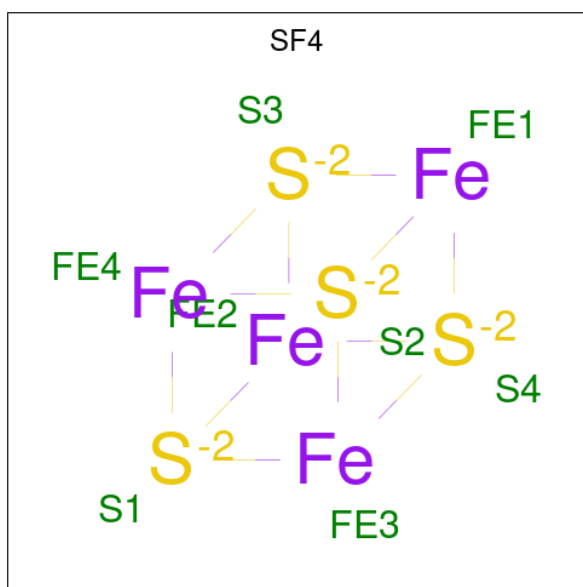
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
57	E5	1	Total Mg 1 1	0	0
57	M5	1	Total Mg 1 1	0	0

- Molecule 58 is THERMINE (CCD ID: SPE) (formula: $C_9H_{24}N_4$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
58	13	1	Total C N 13 9 4	0	0
58	1G	1	Total C N 13 9 4	0	0
58	14	1	Total C N 13 9 4	0	0
58	14	1	Total C N 13 9 4	0	0
58	1J	1	Total C N 13 9 4	0	0

- Molecule 59 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4).



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

- 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 water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
61	13	304	Total	O	0	0
			304	304		
61	3E	1	Total	O	0	0
			1	1		
61	4E	1	Total	O	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
61	1I	2	Total 2	O 2	0	0
61	2I	1	Total 1	O 1	0	0
61	3I	2	Total 2	O 2	0	0
61	5I	2	Total 2	O 2	0	0
61	7I	2	Total 2	O 2	0	0
61	1K	1	Total 1	O 1	0	0
61	2K	6	Total 6	O 6	0	0
61	3K	1	Total 1	O 1	0	0
61	4K	11	Total 11	O 11	0	0
61	1H	1133	Total 1133	O 1133	0	0
61	16	15	Total 15	O 15	0	0
61	11	16	Total 16	O 16	0	0
61	21	8	Total 8	O 8	0	0
61	31	4	Total 4	O 4	0	0
61	58	1	Total 1	O 1	0	0
61	78	11	Total 11	O 11	0	0
61	98	2	Total 2	O 2	0	0
61	A8	3	Total 3	O 3	0	0
61	B8	1	Total 1	O 1	0	0
61	E8	1	Total 1	O 1	0	0
61	F8	1	Total 1	O 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
61	I8	6	Total 6	O 6	0	0
61	K8	1	Total 1	O 1	0	0
61	L8	1	Total 1	O 1	0	0
61	P8	1	Total 1	O 1	0	0
61	Q8	5	Total 5	O 5	0	0
61	1G	391	Total 391	O 391	0	0
61	22	1	Total 1	O 1	0	0
61	42	1	Total 1	O 1	0	0
61	52	3	Total 3	O 3	0	0
61	3A	1	Total 1	O 1	0	0
61	7A	1	Total 1	O 1	0	0
61	9A	3	Total 3	O 3	0	0
61	BA	2	Total 2	O 2	0	0
61	4L	14	Total 14	O 14	0	0
61	14	1135	Total 1135	O 1135	0	0
61	1J	18	Total 18	O 18	0	0
61	19	8	Total 8	O 8	0	0
61	29	6	Total 6	O 6	0	0
61	39	6	Total 6	O 6	0	0
61	25	11	Total 11	O 11	0	0
61	35	9	Total 9	O 9	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
61	45	3	Total	O	0	0
			3	3		
61	55	1	Total	O	0	0
			1	1		
61	75	1	Total	O	0	0
			1	1		
61	85	1	Total	O	0	0
			1	1		
61	A5	1	Total	O	0	0
			1	1		
61	C5	3	Total	O	0	0
			3	3		
61	E5	5	Total	O	0	0
			5	5		
61	F5	3	Total	O	0	0
			3	3		
61	H5	1	Total	O	0	0
			1	1		
61	M5	7	Total	O	0	0
			7	7		

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	209.50Å 448.90Å 620.80Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	146.68 – 2.96 146.68 – 2.96	Depositor EDS
% Data completeness (in resolution range)	99.8 (146.68-2.96) 89.3 (146.68-2.96)	Depositor EDS
R_{merge}	0.44	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.84 (at 2.96Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.201 , 0.243 0.203 , 0.242	Depositor DCC
R_{free} test set	2000 reflections (0.17%)	wwPDB-VP
Wilson B-factor (Å ²)	75.4	Xtriage
Anisotropy	0.336	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 50.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	296743	wwPDB-VP
Average B, all atoms (Å ²)	97.0	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](#)

17 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	$\# Z > 2$
22	6MZ	1K	37	22	22,25,26	3.00	5 (22%)	30,36,39	2.61	11 (36%)
23	5MU	2L	55	23	19,22,23	3.93	5 (26%)	28,32,35	3.04	9 (32%)
22	PSU	1K	55	22	18,21,22	1.36	1 (5%)	22,30,33	1.75	4 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
23	OMC	2L	33	23	19,22,23	1.80	4 (21%)	26,31,34	1.03	1 (3%)
56	PSU	1L	55	56	18,21,22	1.38	1 (5%)	22,30,33	1.51	4 (18%)
23	7MG	2L	47	23	22,26,27	2.83	8 (36%)	29,39,42	3.00	10 (34%)
23	5MU	2K	55	57,23	19,22,23	3.85	5 (26%)	28,32,35	3.22	8 (28%)
23	OMC	2K	33	23	19,22,23	1.81	3 (15%)	26,31,34	1.09	3 (11%)
22	CM0	1K	34	22	22,26,27	3.97	7 (31%)	28,37,40	1.54	4 (14%)
23	7MG	2K	47	23	22,26,27	3.09	6 (27%)	29,39,42	2.81	11 (37%)
23	PSU	2L	56	23	18,21,22	1.14	1 (5%)	22,30,33	1.58	2 (9%)
23	4SU	2L	8	23	18,21,22	1.94	3 (16%)	26,30,33	2.59	4 (15%)
56	5MU	1L	54	56	19,22,23	3.87	5 (26%)	28,32,35	3.17	9 (32%)
23	4SU	2K	8	23	18,21,22	1.91	3 (16%)	26,30,33	2.56	4 (15%)
23	PSU	2K	56	23	18,21,22	1.16	2 (11%)	22,30,33	2.02	4 (18%)
22	5MU	1K	54	22	19,22,23	3.90	5 (26%)	28,32,35	2.99	7 (25%)
22	H2U	1K	17	22	18,21,22	2.13	4 (22%)	21,30,33	2.38	5 (23%)

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
22	6MZ	1K	37	22	-	2/9/27/28	0/3/3/3
23	5MU	2L	55	23	-	0/7/25/26	0/2/2/2
22	PSU	1K	55	22	-	2/7/25/26	0/2/2/2
23	OMC	2L	33	23	-	0/9/27/28	0/2/2/2
56	PSU	1L	55	56	-	2/7/25/26	0/2/2/2
23	7MG	2L	47	23	-	3/7/37/38	0/3/3/3
23	5MU	2K	55	57,23	-	0/7/25/26	0/2/2/2
23	OMC	2K	33	23	-	0/9/27/28	0/2/2/2
22	CM0	1K	34	22	-	6/12/30/31	0/2/2/2
23	7MG	2K	47	23	-	0/7/37/38	0/3/3/3
23	PSU	2L	56	23	-	0/7/25/26	0/2/2/2
23	4SU	2L	8	23	-	0/7/25/26	0/2/2/2
56	5MU	1L	54	56	-	0/7/25/26	0/2/2/2
23	4SU	2K	8	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	H2U	1K	17	22	-	1/7/38/39	0/2/2/2

The worst 5 of 68 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	1K	34	CM0	C6-C5	14.10	1.50	1.34
22	1K	54	5MU	C2-N1	12.81	1.59	1.38
23	2L	55	5MU	C2-N1	12.78	1.59	1.38
56	1L	54	5MU	C2-N1	12.69	1.58	1.38
23	2K	55	5MU	C2-N1	12.54	1.58	1.38

The worst 5 of 100 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	2K	55	5MU	C5-C4-N3	10.74	124.48	115.31
56	1L	54	5MU	C5-C4-N3	10.28	124.09	115.31
22	1K	54	5MU	C5-C4-N3	10.26	124.07	115.31
23	2L	55	5MU	C5-C4-N3	9.92	123.78	115.31
23	2K	8	4SU	C4-N3-C2	-8.58	119.00	127.34

There are no chirality outliers.

5 of 16 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
22	1K	34	CM0	O4'-C4'-C5'-O5'
23	2L	47	7MG	C2'-C1'-N9-C8
22	1K	34	CM0	C3'-C4'-C5'-O5'
22	1K	34	CM0	O5-C7-C8-O8
22	1K	34	CM0	C6-C5-O5-C7

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 1355 ligands modelled in this entry, 1348 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	$\# Z > 2$
58	SPE	14	3445	26,57	12,12,12	0.58	0	11,11,11	0.89	0
58	SPE	1J	208	-	12,12,12	0.40	0	11,11,11	0.88	0
58	SPE	14	3446	-	12,12,12	0.73	0	11,11,11	0.98	1 (9%)
59	SF4	3E	301	4	0,12,12	-	-	-		
58	SPE	1G	1733	-	12,12,12	0.40	0	11,11,11	0.91	0
58	SPE	13	1748	1,57	12,12,12	0.49	0	11,11,11	0.97	1 (9%)
59	SF4	32	301	4	0,12,12	-	-	-		

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
58	SPE	14	3445	26,57	-	6/10/10/10	-
58	SPE	1J	208	-	-	5/10/10/10	-
58	SPE	14	3446	-	-	5/10/10/10	-
59	SF4	3E	301	4	-	-	0/6/5/5
58	SPE	1G	1733	-	-	4/10/10/10	-
58	SPE	13	1748	1,57	-	7/10/10/10	-
59	SF4	32	301	4	-	-	0/6/5/5

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
58	13	1748	SPE	C11-C10-N9	-2.43	105.58	112.14
58	14	3446	SPE	C11-C10-N9	-2.39	105.69	112.14

There are no chirality outliers.

5 of 27 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
58	14	3445	SPE	C2-C3-C4-N5
58	14	3446	SPE	N9-C10-C11-C12
58	13	1748	SPE	C2-C3-C4-N5

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Mol	Chain	Res	Type	Atoms
58	13	1748	SPE	N9-C10-C11-C12
58	13	1748	SPE	C7-C6-N5-C4

There are no ring outliers.

No monomer is involved in short contacts.

4.7 Other polymers [i](#)

There are no such residues in this entry.

4.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
2	1E	1
25	4K	1
3	22	1
10	1A	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	1E	78:GLN	C	79:ASP	N	4.14
1	4K	25:A	O3'	26:A	P	3.23
1	22	173:VAL	C	174:PRO	N	1.71
1	1A	38:ILE	C	39:PRO	N	1.62

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	1496/1522 (98%)	-0.14	14 (0%) 81 76	57, 98, 164, 235	0
1	1G	1506/1522 (98%)	-0.01	24 (1%) 70 63	68, 105, 166, 238	0
2	12	207/256 (80%)	0.92	24 (11%) 9 8	121, 148, 168, 185	0
2	1E	235/256 (91%)	0.61	9 (3%) 44 36	108, 135, 160, 171	0
3	22	195/239 (81%)	0.94	21 (10%) 11 10	113, 131, 152, 164	0
3	2E	205/239 (85%)	0.30	2 (0%) 79 74	85, 107, 142, 149	0
4	32	208/209 (99%)	0.38	4 (1%) 66 58	84, 101, 123, 132	0
4	3E	207/209 (99%)	0.64	12 (5%) 29 24	77, 103, 125, 132	0
5	42	149/162 (91%)	0.62	4 (2%) 56 48	91, 111, 128, 149	0
5	4E	149/162 (91%)	0.50	3 (2%) 65 57	79, 98, 118, 135	0
6	52	101/101 (100%)	0.01	0 100 100	81, 97, 110, 131	0
6	5E	100/101 (99%)	0.20	1 (1%) 79 74	83, 99, 113, 123	0
7	62	140/156 (89%)	0.54	14 (10%) 12 11	103, 119, 131, 138	0
7	6E	154/156 (98%)	0.36	8 (5%) 33 28	98, 113, 138, 162	0
8	72	137/138 (99%)	0.65	4 (2%) 53 46	90, 114, 125, 128	0
8	7E	138/138 (100%)	0.66	5 (3%) 46 38	87, 102, 113, 120	0
9	82	121/128 (94%)	1.48	24 (19%) 3 3	101, 144, 160, 164	0
9	8E	126/128 (98%)	0.76	8 (6%) 26 22	84, 133, 153, 157	0
10	1A	80/105 (76%)	1.70	31 (38%) 1 0	111, 138, 152, 156	0
10	1I	95/105 (90%)	0.58	4 (4%) 40 33	80, 127, 155, 159	0
11	2A	113/129 (87%)	0.60	10 (8%) 15 14	78, 103, 117, 120	0
11	2I	111/129 (86%)	0.54	5 (4%) 38 31	70, 99, 115, 125	0
12	3A	122/132 (92%)	1.01	20 (16%) 4 4	74, 91, 116, 132	0
12	3I	122/132 (92%)	0.31	9 (7%) 20 18	65, 76, 103, 112	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	4A	111/126 (88%)	0.66	10 (9%) 15 13	102, 129, 143, 152	0
13	4I	119/126 (94%)	0.66	15 (12%) 8 7	87, 111, 129, 139	0
14	5A	59/61 (96%)	2.04	25 (42%) 0 0	118, 129, 141, 142	0
14	5I	60/61 (98%)	0.67	3 (5%) 34 28	83, 97, 112, 119	0
15	6A	87/89 (97%)	0.01	1 (1%) 78 73	79, 100, 115, 117	0
15	6I	87/89 (97%)	0.19	3 (3%) 48 41	75, 94, 109, 116	0
16	7A	84/88 (95%)	0.47	3 (3%) 46 38	85, 98, 119, 145	0
16	7I	83/88 (94%)	1.37	23 (27%) 1 1	91, 107, 132, 147	0
17	8A	99/105 (94%)	0.50	5 (5%) 33 28	89, 100, 117, 120	0
17	8I	100/105 (95%)	0.65	8 (8%) 18 16	81, 98, 108, 115	0
18	9A	67/88 (76%)	0.35	1 (1%) 72 65	87, 101, 125, 129	0
18	9I	68/88 (77%)	0.33	2 (2%) 53 46	85, 100, 125, 128	0
19	AA	62/93 (66%)	1.13	7 (11%) 10 9	118, 142, 155, 158	0
19	AI	82/93 (88%)	0.42	3 (3%) 45 37	95, 110, 128, 136	0
20	BA	99/106 (93%)	0.54	5 (5%) 33 28	85, 104, 128, 140	0
20	BI	97/106 (91%)	1.04	13 (13%) 7 7	103, 117, 138, 145	0
21	1B	22/27 (81%)	1.44	7 (31%) 1 1	110, 116, 124, 134	0
21	1F	23/27 (85%)	0.40	1 (4%) 40 32	90, 98, 106, 108	0
22	1K	67/76 (88%)	0.54	4 (5%) 27 23	80, 167, 196, 203	0
23	2K	72/77 (93%)	0.15	1 (1%) 73 67	68, 89, 116, 129	0
23	2L	71/77 (92%)	0.20	1 (1%) 73 67	78, 100, 132, 145	0
24	3K	70/76 (92%)	1.26	14 (20%) 3 3	71, 198, 222, 224	0
24	3L	71/76 (93%)	0.86	11 (15%) 5 5	78, 191, 215, 218	0
25	4K	21/30 (70%)	1.37	8 (38%) 1 0	69, 129, 212, 213	0
25	4L	19/30 (63%)	1.35	7 (36%) 1 1	85, 144, 210, 210	0
26	14	2810/2917 (96%)	-0.36	18 (0%) 85 82	54, 81, 180, 237	0
26	1H	2841/2917 (97%)	-0.49	10 (0%) 88 86	44, 70, 166, 244	0
27	16	122/122 (100%)	-0.45	0 100 100	65, 87, 105, 180	0
27	1J	122/122 (100%)	-0.07	3 (2%) 58 50	79, 106, 125, 185	0
28	71	133/229 (58%)	0.76	11 (8%) 17 15	136, 194, 219, 229	0
28	79	57/229 (24%)	1.92	24 (42%) 0 0	136, 178, 198, 205	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
29	11	273/276 (98%)	0.12	7 (2%) 57 49	44, 62, 78, 94	0
29	19	274/276 (99%)	0.44	23 (8%) 17 15	50, 72, 87, 102	0
30	21	202/206 (98%)	0.45	13 (6%) 25 21	49, 82, 115, 123	0
30	29	204/206 (99%)	0.56	16 (7%) 19 17	57, 88, 124, 135	0
31	31	202/210 (96%)	0.00	2 (0%) 79 74	46, 75, 108, 123	0
31	39	204/210 (97%)	0.26	5 (2%) 58 50	57, 95, 139, 164	0
32	41	179/182 (98%)	0.57	10 (5%) 30 25	75, 95, 124, 138	0
32	49	181/182 (99%)	0.55	7 (3%) 43 35	99, 118, 142, 156	0
33	51	174/180 (96%)	0.46	8 (4%) 37 31	76, 99, 116, 128	0
33	59	167/180 (92%)	1.65	49 (29%) 1 1	123, 190, 216, 225	0
34	61	146/148 (98%)	0.43	6 (4%) 41 34	75, 119, 134, 148	0
34	69	145/148 (97%)	0.60	10 (6%) 23 19	80, 115, 138, 144	0
35	15	138/140 (98%)	1.00	12 (8%) 16 14	76, 98, 124, 139	0
35	58	137/140 (97%)	0.54	6 (4%) 39 32	64, 84, 113, 134	0
36	25	122/122 (100%)	0.27	1 (0%) 82 78	68, 81, 97, 107	0
36	68	122/122 (100%)	0.12	1 (0%) 82 78	57, 72, 87, 93	0
37	35	147/150 (98%)	0.53	9 (6%) 27 22	58, 93, 121, 133	0
37	78	147/150 (98%)	0.23	6 (4%) 41 34	46, 77, 98, 106	0
38	45	139/141 (98%)	0.45	9 (6%) 25 21	70, 94, 112, 126	0
38	88	141/141 (100%)	-0.02	1 (0%) 84 80	57, 74, 97, 117	0
39	55	118/118 (100%)	0.17	2 (1%) 69 62	61, 77, 92, 109	0
39	98	118/118 (100%)	0.27	2 (1%) 69 62	58, 76, 94, 104	0
40	65	110/112 (98%)	0.66	5 (4%) 38 31	82, 100, 119, 130	0
40	A8	111/112 (99%)	0.17	2 (1%) 67 59	73, 86, 104, 112	0
41	75	133/146 (91%)	0.48	4 (3%) 52 45	76, 88, 117, 142	0
41	B8	136/146 (93%)	0.36	8 (5%) 28 23	66, 83, 121, 152	0
42	85	116/118 (98%)	0.46	4 (3%) 48 41	65, 91, 116, 123	0
42	C8	115/118 (97%)	0.32	2 (1%) 69 62	57, 75, 96, 106	0
43	95	100/101 (99%)	0.73	7 (7%) 22 19	65, 108, 126, 132	0
43	D8	100/101 (99%)	0.53	7 (7%) 22 19	56, 92, 111, 125	0
44	A5	111/113 (98%)	0.11	0 100 100	62, 73, 95, 128	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
44	E8	110/113 (97%)	0.18	4 (3%) 46 38	57, 69, 90, 101	0
45	B5	94/96 (97%)	0.57	5 (5%) 32 27	66, 80, 103, 111	0
45	F8	95/96 (98%)	0.24	0 100 100	50, 66, 91, 99	0
46	C5	104/110 (94%)	1.62	32 (30%) 1 1	84, 110, 143, 150	0
46	G8	103/110 (93%)	0.62	8 (7%) 19 17	74, 91, 118, 125	0
47	D5	133/206 (64%)	0.51	5 (3%) 44 36	93, 123, 150, 159	0
47	H8	170/206 (82%)	0.28	2 (1%) 76 71	77, 112, 191, 198	0
48	E5	76/85 (89%)	0.61	8 (10%) 11 10	58, 82, 94, 108	0
48	I8	77/85 (90%)	0.22	4 (5%) 33 28	54, 70, 87, 98	0
49	F5	94/98 (95%)	0.70	7 (7%) 20 18	61, 76, 117, 123	0
49	J8	94/98 (95%)	0.56	6 (6%) 25 21	49, 70, 115, 135	0
50	G5	69/72 (95%)	0.46	3 (4%) 40 32	77, 96, 113, 130	0
50	K8	68/72 (94%)	0.06	1 (1%) 72 65	60, 76, 94, 124	0
51	H5	58/60 (96%)	0.56	3 (5%) 33 28	73, 90, 118, 123	0
51	L8	58/60 (96%)	0.21	1 (1%) 69 62	59, 75, 94, 101	0
52	I5	63/71 (88%)	0.77	7 (11%) 10 9	132, 174, 191, 195	0
52	M8	61/71 (85%)	1.07	8 (13%) 7 7	96, 137, 167, 174	0
53	J5	56/60 (93%)	0.44	3 (5%) 31 26	57, 81, 130, 140	0
53	N8	56/60 (93%)	0.48	7 (12%) 8 7	50, 83, 145, 155	0
54	L5	47/49 (95%)	0.17	4 (8%) 16 15	51, 61, 82, 96	0
54	P8	47/49 (95%)	-0.10	2 (4%) 40 32	44, 53, 68, 89	0
55	M5	64/65 (98%)	0.62	3 (4%) 36 30	64, 76, 89, 114	0
55	Q8	64/65 (98%)	0.23	2 (3%) 51 44	52, 64, 78, 91	0
56	1L	67/76 (88%)	0.70	6 (8%) 15 13	98, 180, 207, 210	0
All	All	20742/22044 (94%)	0.18	882 (4%) 40 32	44, 93, 167, 244	0

The worst 5 of 882 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
33	59	131	VAL	9.3
14	5A	38	GLY	8.5
9	82	115	GLY	7.7
30	29	76	ARG	7.3
10	1A	63	PHE	7.2

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	H2U	1K	17	20/21	0.71	0.09	119,145,154,154	0
23	7MG	2L	47	24/25	0.72	0.15	92,112,117,118	0
56	PSU	1L	55	20/21	0.73	0.10	118,133,146,147	0
22	PSU	1K	55	20/21	0.76	0.11	102,116,131,132	0
56	5MU	1L	54	21/22	0.83	0.08	117,124,131,143	0
23	OMC	2L	33	21/22	0.83	0.16	83,94,97,100	0
23	PSU	2L	56	20/21	0.87	0.09	105,114,120,120	0
22	5MU	1K	54	21/22	0.87	0.07	100,106,117,129	0
23	PSU	2K	56	20/21	0.87	0.08	93,98,106,114	0
23	5MU	2L	55	21/22	0.88	0.08	111,115,122,127	0
23	5MU	2K	55	21/22	0.89	0.10	99,102,106,113	0
23	4SU	2L	8	20/21	0.90	0.08	104,106,109,112	0
23	4SU	2K	8	20/21	0.94	0.10	84,88,92,94	0
23	7MG	2K	47	24/25	0.94	0.09	90,98,109,111	0
22	CM0	1K	34	25/26	0.94	0.10	72,89,106,107	0
23	OMC	2K	33	21/22	0.96	0.12	72,79,82,89	0
22	6MZ	1K	37	23/24	0.98	0.06	61,79,86,90	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	1G	1653	1/1	0.11	0.35	103,103,103,103	0
57	MG	14	3189	1/1	0.48	0.27	85,85,85,85	0
57	MG	1G	1604	1/1	0.49	0.40	103,103,103,103	0
57	MG	1H	3322	1/1	0.51	0.29	100,100,100,100	0
57	MG	1H	3235	1/1	0.51	0.26	99,99,99,99	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	1G	1630	1/1	0.52	0.43	106,106,106,106	0
57	MG	13	1690	1/1	0.55	0.44	100,100,100,100	0
57	MG	1H	3104	1/1	0.55	0.31	88,88,88,88	0
57	MG	1H	3233	1/1	0.55	0.25	110,110,110,110	0
57	MG	14	3173	1/1	0.56	0.27	98,98,98,98	0
57	MG	1H	3227	1/1	0.57	0.22	79,79,79,79	0
57	MG	1H	3283	1/1	0.57	0.26	146,146,146,146	0
57	MG	1H	3247	1/1	0.58	0.33	101,101,101,101	0
57	MG	1H	3058	1/1	0.58	0.31	77,77,77,77	0
57	MG	1H	3120	1/1	0.59	0.41	96,96,96,96	0
57	MG	13	1645	1/1	0.59	0.20	78,78,78,78	0
57	MG	1H	3006	1/1	0.59	0.17	71,71,71,71	0
57	MG	14	3225	1/1	0.59	0.20	95,95,95,95	0
57	MG	14	3031	1/1	0.60	0.30	86,86,86,86	0
57	MG	1G	1644	1/1	0.61	0.37	107,107,107,107	0
57	MG	1G	1615	1/1	0.61	0.37	91,91,91,91	0
57	MG	1H	3155	1/1	0.61	0.32	91,91,91,91	0
57	MG	1G	1650	1/1	0.62	0.22	114,114,114,114	0
57	MG	1H	3248	1/1	0.62	0.43	96,96,96,96	0
57	MG	13	1646	1/1	0.63	0.37	97,97,97,97	0
57	MG	1H	3206	1/1	0.64	0.31	91,91,91,91	0
57	MG	1H	3205	1/1	0.65	0.22	90,90,90,90	0
57	MG	1G	1710	1/1	0.65	0.20	102,102,102,102	0
57	MG	1H	3118	1/1	0.65	0.27	83,83,83,83	0
57	MG	1H	3224	1/1	0.65	0.40	90,90,90,90	0
57	MG	13	1654	1/1	0.65	0.11	113,113,113,113	0
57	MG	13	1660	1/1	0.65	0.52	96,96,96,96	0
57	MG	14	3110	1/1	0.66	0.36	72,72,72,72	0
57	MG	13	1653	1/1	0.66	0.46	94,94,94,94	0
57	MG	13	1677	1/1	0.67	0.40	92,92,92,92	0
57	MG	2K	103	1/1	0.67	0.30	89,89,89,89	0
57	MG	1H	3260	1/1	0.68	0.45	98,98,98,98	0
57	MG	1H	3188	1/1	0.68	0.53	95,95,95,95	0
57	MG	14	3166	1/1	0.68	0.38	82,82,82,82	0
57	MG	1H	3246	1/1	0.68	0.23	72,72,72,72	0
57	MG	13	1686	1/1	0.68	0.31	104,104,104,104	0
57	MG	14	3224	1/1	0.68	0.23	113,113,113,113	0
57	MG	1H	3077	1/1	0.68	0.18	56,56,56,56	0
57	MG	1H	3161	1/1	0.69	0.36	93,93,93,93	0
57	MG	13	1687	1/1	0.69	0.41	82,82,82,82	0
57	MG	14	3190	1/1	0.69	0.27	79,79,79,79	0
57	MG	1H	3217	1/1	0.69	0.35	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	1G	1616	1/1	0.69	0.37	88,88,88,88	0
57	MG	13	1635	1/1	0.70	0.21	99,99,99,99	0
57	MG	14	3158	1/1	0.70	0.34	76,76,76,76	0
57	MG	1H	3295	1/1	0.70	0.17	70,70,70,70	0
57	MG	1G	1623	1/1	0.70	0.38	75,75,75,75	0
57	MG	14	3229	1/1	0.70	0.33	90,90,90,90	0
57	MG	1G	1608	1/1	0.71	0.17	111,111,111,111	0
57	MG	14	3101	1/1	0.71	0.29	90,90,90,90	0
57	MG	13	1668	1/1	0.71	0.21	121,121,121,121	0
57	MG	1H	3115	1/1	0.71	0.40	84,84,84,84	0
57	MG	1H	3282	1/1	0.71	0.32	89,89,89,89	0
57	MG	13	1656	1/1	0.71	0.31	87,87,87,87	0
57	MG	1H	3061	1/1	0.71	0.27	76,76,76,76	0
57	MG	1H	3321	1/1	0.71	0.37	90,90,90,90	0
57	MG	13	1622	1/1	0.71	0.38	74,74,74,74	0
57	MG	1H	3218	1/1	0.71	0.23	81,81,81,81	0
57	MG	14	3030	1/1	0.71	0.34	89,89,89,89	0
57	MG	1J	201	1/1	0.71	0.30	86,86,86,86	0
57	MG	1G	1635	1/1	0.72	0.24	102,102,102,102	0
57	MG	13	1603	1/1	0.72	0.23	116,116,116,116	0
57	MG	13	1682	1/1	0.72	0.34	85,85,85,85	0
57	MG	1H	3296	1/1	0.72	0.34	81,81,81,81	0
57	MG	1H	3276	1/1	0.72	0.33	90,90,90,90	0
57	MG	14	3217	1/1	0.72	0.16	77,77,77,77	0
57	MG	1G	1617	1/1	0.72	0.29	86,86,86,86	0
57	MG	13	1670	1/1	0.72	0.21	100,100,100,100	0
57	MG	1G	1624	1/1	0.72	0.41	76,76,76,76	0
57	MG	16	201	1/1	0.72	0.25	83,83,83,83	0
57	MG	29	301	1/1	0.72	0.29	75,75,75,75	0
57	MG	39	302	1/1	0.72	0.25	67,67,67,67	0
57	MG	14	3174	1/1	0.73	0.25	83,83,83,83	0
57	MG	1H	3274	1/1	0.73	0.43	83,83,83,83	0
57	MG	14	3023	1/1	0.73	0.36	82,82,82,82	0
57	MG	14	3214	1/1	0.73	0.45	93,93,93,93	0
57	MG	14	3216	1/1	0.73	0.20	106,106,106,106	0
57	MG	13	1614	1/1	0.73	0.29	88,88,88,88	0
57	MG	14	3220	1/1	0.73	0.32	73,73,73,73	0
57	MG	1H	3080	1/1	0.73	0.39	103,103,103,103	0
57	MG	1H	3170	1/1	0.73	0.27	79,79,79,79	0
57	MG	1H	3183	1/1	0.73	0.21	73,73,73,73	0
57	MG	14	3394	1/1	0.73	0.14	63,63,63,63	0
57	MG	1H	3185	1/1	0.73	0.36	90,90,90,90	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	13	1678	1/1	0.73	0.26	94,94,94,94	0
57	MG	1G	1661	1/1	0.73	0.29	99,99,99,99	0
57	MG	14	3199	1/1	0.74	0.28	68,68,68,68	0
57	MG	13	1636	1/1	0.74	0.25	103,103,103,103	0
57	MG	13	1669	1/1	0.74	0.33	92,92,92,92	0
57	MG	14	3138	1/1	0.74	0.30	86,86,86,86	0
57	MG	1H	3008	1/1	0.74	0.44	75,75,75,75	0
57	MG	14	3164	1/1	0.74	0.24	80,80,80,80	0
57	MG	1G	1680	1/1	0.74	0.19	91,91,91,91	0
57	MG	14	3226	1/1	0.74	0.39	83,83,83,83	0
57	MG	13	1683	1/1	0.74	0.27	72,72,72,72	0
57	MG	4E	201	1/1	0.74	0.46	85,85,85,85	0
57	MG	14	3177	1/1	0.74	0.28	82,82,82,82	0
57	MG	2K	102	1/1	0.74	0.31	92,92,92,92	0
57	MG	1G	1647	1/1	0.74	0.30	102,102,102,102	0
57	MG	1H	3239	1/1	0.75	0.41	92,92,92,92	0
57	MG	1H	3315	1/1	0.75	0.31	99,99,99,99	0
57	MG	14	3014	1/1	0.75	0.19	62,62,62,62	0
57	MG	1G	1629	1/1	0.75	0.36	97,97,97,97	0
57	MG	J8	101	1/1	0.75	0.46	79,79,79,79	0
57	MG	13	1675	1/1	0.75	0.21	104,104,104,104	0
57	MG	14	3035	1/1	0.75	0.34	79,79,79,79	0
57	MG	14	3097	1/1	0.75	0.38	90,90,90,90	0
57	MG	1H	3269	1/1	0.76	0.43	86,86,86,86	0
57	MG	14	3178	1/1	0.76	0.48	92,92,92,92	0
57	MG	1H	3523	1/1	0.76	0.21	84,84,84,84	0
57	MG	13	1649	1/1	0.76	0.20	72,72,72,72	0
57	MG	13	1662	1/1	0.76	0.15	76,76,76,76	0
57	MG	14	3058	1/1	0.76	0.21	83,83,83,83	0
57	MG	14	3081	1/1	0.76	0.36	81,81,81,81	0
57	MG	13	1625	1/1	0.76	0.36	93,93,93,93	0
57	MG	1H	3078	1/1	0.76	0.26	79,79,79,79	0
57	MG	1G	1652	1/1	0.76	0.36	94,94,94,94	0
57	MG	1H	3286	1/1	0.76	0.33	87,87,87,87	0
57	MG	1H	3133	1/1	0.76	0.43	78,78,78,78	0
57	MG	1H	3010	1/1	0.76	0.23	78,78,78,78	0
57	MG	1H	3086	1/1	0.76	0.29	66,66,66,66	0
57	MG	14	3170	1/1	0.76	0.29	87,87,87,87	0
57	MG	1G	1712	1/1	0.76	0.10	142,142,142,142	0
57	MG	1H	3103	1/1	0.76	0.33	82,82,82,82	0
57	MG	1H	3212	1/1	0.77	0.18	65,65,65,65	0
57	MG	14	3198	1/1	0.77	0.24	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	3535	1/1	0.77	0.18	93,93,93,93	0
57	MG	1H	3214	1/1	0.77	0.36	86,86,86,86	0
57	MG	16	206	1/1	0.77	0.27	77,77,77,77	0
57	MG	2L	103	1/1	0.77	0.28	75,75,75,75	0
57	MG	1H	3094	1/1	0.77	0.36	68,68,68,68	0
57	MG	1H	3095	1/1	0.77	0.25	69,69,69,69	0
57	MG	1H	3125	1/1	0.77	0.25	63,63,63,63	0
57	MG	13	1679	1/1	0.77	0.33	86,86,86,86	0
57	MG	13	1676	1/1	0.77	0.41	92,92,92,92	0
57	MG	1H	3031	1/1	0.77	0.36	74,74,74,74	0
57	MG	14	3063	1/1	0.77	0.23	52,52,52,52	0
57	MG	14	3074	1/1	0.77	0.24	81,81,81,81	0
57	MG	14	3077	1/1	0.77	0.27	84,84,84,84	0
57	MG	35	201	1/1	0.77	0.21	86,86,86,86	0
57	MG	13	1671	1/1	0.78	0.40	91,91,91,91	0
57	MG	14	3218	1/1	0.78	0.18	84,84,84,84	0
57	MG	1H	3250	1/1	0.78	0.45	93,93,93,93	0
57	MG	13	1606	1/1	0.78	0.26	77,77,77,77	0
57	MG	14	3104	1/1	0.78	0.24	84,84,84,84	0
57	MG	1H	3171	1/1	0.78	0.33	90,90,90,90	0
57	MG	14	3057	1/1	0.78	0.34	84,84,84,84	0
57	MG	1G	1648	1/1	0.78	0.40	79,79,79,79	0
57	MG	3A	201	1/1	0.78	0.27	77,77,77,77	0
57	MG	14	3210	1/1	0.78	0.17	80,80,80,80	0
57	MG	1H	3325	1/1	0.78	0.32	88,88,88,88	0
57	MG	1H	3182	1/1	0.78	0.27	90,90,90,90	0
58	SPE	1J	208	13/13	0.78	0.17	94,98,105,105	0
57	MG	14	3053	1/1	0.79	0.12	72,72,72,72	0
57	MG	1G	1632	1/1	0.79	0.15	99,99,99,99	0
57	MG	1H	3097	1/1	0.79	0.43	83,83,83,83	0
57	MG	14	3060	1/1	0.79	0.36	56,56,56,56	0
57	MG	1H	3087	1/1	0.79	0.41	79,79,79,79	0
57	MG	1H	3285	1/1	0.79	0.45	96,96,96,96	0
57	MG	1H	3124	1/1	0.79	0.35	73,73,73,73	0
57	MG	1G	1649	1/1	0.79	0.36	89,89,89,89	0
57	MG	14	3291	1/1	0.79	0.14	90,90,90,90	0
57	MG	1H	3207	1/1	0.79	0.38	87,87,87,87	0
57	MG	14	3025	1/1	0.79	0.35	80,80,80,80	0
57	MG	13	1624	1/1	0.79	0.19	93,93,93,93	0
57	MG	1H	3105	1/1	0.79	0.28	79,79,79,79	0
57	MG	13	1685	1/1	0.79	0.42	91,91,91,91	0
57	MG	14	3157	1/1	0.79	0.48	89,89,89,89	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	14	3085	1/1	0.80	0.44	81,81,81,81	0
57	MG	1H	3122	1/1	0.80	0.22	67,67,67,67	0
57	MG	1G	1609	1/1	0.80	0.40	96,96,96,96	0
57	MG	14	3103	1/1	0.80	0.37	75,75,75,75	0
57	MG	1G	1613	1/1	0.80	0.36	83,83,83,83	0
57	MG	1H	3112	1/1	0.80	0.23	79,79,79,79	0
57	MG	14	3112	1/1	0.80	0.32	99,99,99,99	0
57	MG	14	3124	1/1	0.80	0.30	82,82,82,82	0
57	MG	14	3032	1/1	0.80	0.29	80,80,80,80	0
57	MG	1H	3180	1/1	0.80	0.35	88,88,88,88	0
57	MG	1H	3450	1/1	0.80	0.16	59,59,59,59	0
57	MG	1H	3198	1/1	0.80	0.26	108,108,108,108	0
57	MG	1H	3216	1/1	0.80	0.32	89,89,89,89	0
57	MG	1H	3266	1/1	0.80	0.32	89,89,89,89	0
57	MG	14	3061	1/1	0.80	0.38	56,56,56,56	0
57	MG	1H	3027	1/1	0.80	0.27	84,84,84,84	0
57	MG	14	3175	1/1	0.80	0.17	107,107,107,107	0
57	MG	1H	3302	1/1	0.80	0.32	81,81,81,81	0
57	MG	1H	3245	1/1	0.80	0.28	78,78,78,78	0
57	MG	1G	1607	1/1	0.80	0.26	92,92,92,92	0
57	MG	13	1726	1/1	0.81	0.14	103,103,103,103	0
57	MG	1H	3091	1/1	0.81	0.38	77,77,77,77	0
57	MG	4K	101	1/1	0.81	0.28	86,86,86,86	0
57	MG	1H	3312	1/1	0.81	0.22	94,94,94,94	0
57	MG	13	1688	1/1	0.81	0.33	72,72,72,72	0
57	MG	1H	3317	1/1	0.81	0.41	83,83,83,83	0
57	MG	14	3194	1/1	0.81	0.33	87,87,87,87	0
57	MG	1H	3134	1/1	0.81	0.22	44,44,44,44	0
57	MG	14	3082	1/1	0.81	0.30	90,90,90,90	0
57	MG	14	3206	1/1	0.81	0.23	101,101,101,101	0
57	MG	1G	1620	1/1	0.81	0.30	79,79,79,79	0
57	MG	14	3212	1/1	0.81	0.37	94,94,94,94	0
57	MG	14	3213	1/1	0.81	0.31	76,76,76,76	0
57	MG	14	3095	1/1	0.81	0.29	74,74,74,74	0
57	MG	1H	3145	1/1	0.81	0.30	62,62,62,62	0
57	MG	4L	101	1/1	0.81	0.10	110,110,110,110	0
57	MG	14	3007	1/1	0.81	0.36	72,72,72,72	0
57	MG	14	3013	1/1	0.81	0.30	63,63,63,63	0
57	MG	1H	3149	1/1	0.81	0.30	86,86,86,86	0
57	MG	1H	3270	1/1	0.81	0.31	61,61,61,61	0
57	MG	1H	3189	1/1	0.81	0.28	78,78,78,78	0
57	MG	1H	3232	1/1	0.81	0.37	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	3036	1/1	0.81	0.31	70,70,70,70	0
57	MG	14	3295	1/1	0.81	0.21	90,90,90,90	0
57	MG	16	203	1/1	0.81	0.16	78,78,78,78	0
57	MG	14	3423	1/1	0.81	0.30	92,92,92,92	0
57	MG	14	3159	1/1	0.81	0.34	93,93,93,93	0
57	MG	1H	3202	1/1	0.81	0.35	82,82,82,82	0
57	MG	14	3042	1/1	0.81	0.26	69,69,69,69	0
57	MG	1H	3157	1/1	0.81	0.13	73,73,73,73	0
57	MG	13	1651	1/1	0.81	0.39	97,97,97,97	0
57	MG	14	3134	1/1	0.82	0.16	71,71,71,71	0
57	MG	13	1616	1/1	0.82	0.25	82,82,82,82	0
57	MG	14	3141	1/1	0.82	0.19	76,76,76,76	0
57	MG	14	3145	1/1	0.82	0.15	85,85,85,85	0
57	MG	1H	3259	1/1	0.82	0.32	92,92,92,92	0
57	MG	1H	3313	1/1	0.82	0.21	74,74,74,74	0
57	MG	1H	3012	1/1	0.82	0.23	84,84,84,84	0
57	MG	13	1707	1/1	0.82	0.16	92,92,92,92	0
57	MG	1H	3067	1/1	0.82	0.26	62,62,62,62	0
57	MG	1G	1659	1/1	0.82	0.24	72,72,72,72	0
57	MG	14	3223	1/1	0.82	0.32	87,87,87,87	0
57	MG	14	3172	1/1	0.82	0.29	82,82,82,82	0
57	MG	1H	3200	1/1	0.82	0.32	73,73,73,73	0
57	MG	13	1630	1/1	0.82	0.33	87,87,87,87	0
57	MG	1H	3340	1/1	0.82	0.17	70,70,70,70	0
57	MG	14	3176	1/1	0.82	0.19	69,69,69,69	0
57	MG	1H	3377	1/1	0.82	0.17	75,75,75,75	0
57	MG	1G	1715	1/1	0.82	0.15	119,119,119,119	0
57	MG	14	3411	1/1	0.82	0.16	93,93,93,93	0
57	MG	1G	1643	1/1	0.82	0.25	83,83,83,83	0
57	MG	2L	102	1/1	0.82	0.49	90,90,90,90	0
57	MG	1J	204	1/1	0.82	0.20	88,88,88,88	0
57	MG	14	3191	1/1	0.82	0.17	82,82,82,82	0
57	MG	14	3193	1/1	0.82	0.27	95,95,95,95	0
57	MG	1H	3300	1/1	0.82	0.22	87,87,87,87	0
57	MG	14	3131	1/1	0.82	0.28	70,70,70,70	0
57	MG	14	3128	1/1	0.83	0.24	88,88,88,88	0
57	MG	13	1659	1/1	0.83	0.46	85,85,85,85	0
57	MG	1H	3141	1/1	0.83	0.22	66,66,66,66	0
57	MG	14	3136	1/1	0.83	0.17	127,127,127,127	0
57	MG	1G	1619	1/1	0.83	0.31	86,86,86,86	0
57	MG	14	3008	1/1	0.83	0.35	90,90,90,90	0
57	MG	14	3064	1/1	0.83	0.23	62,62,62,62	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	14	3151	1/1	0.83	0.33	87,87,87,87	0
57	MG	14	3068	1/1	0.83	0.24	64,64,64,64	0
57	MG	1H	3144	1/1	0.83	0.26	64,64,64,64	0
57	MG	13	1627	1/1	0.83	0.28	85,85,85,85	0
57	MG	14	3222	1/1	0.83	0.29	88,88,88,88	0
57	MG	1G	1657	1/1	0.83	0.26	82,82,82,82	0
57	MG	14	3024	1/1	0.83	0.22	77,77,77,77	0
57	MG	1H	3320	1/1	0.83	0.33	80,80,80,80	0
57	MG	14	3027	1/1	0.83	0.27	76,76,76,76	0
57	MG	1H	3287	1/1	0.83	0.29	78,78,78,78	0
57	MG	14	3100	1/1	0.83	0.21	61,61,61,61	0
57	MG	1H	3289	1/1	0.83	0.29	78,78,78,78	0
57	MG	14	3386	1/1	0.83	0.14	93,93,93,93	0
57	MG	13	1618	1/1	0.83	0.28	60,60,60,60	0
57	MG	1H	3204	1/1	0.83	0.36	81,81,81,81	0
57	MG	14	3106	1/1	0.83	0.45	94,94,94,94	0
57	MG	13	1633	1/1	0.83	0.22	87,87,87,87	0
57	MG	1J	202	1/1	0.83	0.13	84,84,84,84	0
57	MG	1J	203	1/1	0.83	0.26	91,91,91,91	0
57	MG	1H	3434	1/1	0.83	0.15	68,68,68,68	0
57	MG	14	3115	1/1	0.83	0.21	48,48,48,48	0
57	MG	14	3192	1/1	0.83	0.34	82,82,82,82	0
57	MG	14	3117	1/1	0.83	0.17	58,58,58,58	0
57	MG	1H	3088	1/1	0.83	0.22	61,61,61,61	0
57	MG	14	3171	1/1	0.84	0.10	57,57,57,57	0
57	MG	1G	1654	1/1	0.84	0.37	94,94,94,94	0
57	MG	1H	3261	1/1	0.84	0.30	77,77,77,77	0
57	MG	1H	3265	1/1	0.84	0.22	77,77,77,77	0
57	MG	1H	3220	1/1	0.84	0.18	89,89,89,89	0
57	MG	1H	3316	1/1	0.84	0.39	89,89,89,89	0
57	MG	14	3070	1/1	0.84	0.34	82,82,82,82	0
57	MG	1G	1707	1/1	0.84	0.17	108,108,108,108	0
57	MG	14	3187	1/1	0.84	0.25	90,90,90,90	0
57	MG	1G	1614	1/1	0.84	0.27	82,82,82,82	0
57	MG	1H	3126	1/1	0.84	0.15	75,75,75,75	0
57	MG	1G	1714	1/1	0.84	0.15	99,99,99,99	0
57	MG	1H	3128	1/1	0.84	0.18	79,79,79,79	0
57	MG	14	3087	1/1	0.84	0.21	58,58,58,58	0
57	MG	42	201	1/1	0.84	0.17	116,116,116,116	0
57	MG	1H	3272	1/1	0.84	0.36	80,80,80,80	0
57	MG	14	3099	1/1	0.84	0.26	77,77,77,77	0
57	MG	14	3200	1/1	0.84	0.34	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	1H	3132	1/1	0.84	0.23	88,88,88,88	0
57	MG	14	3208	1/1	0.84	0.25	78,78,78,78	0
57	MG	13	1648	1/1	0.84	0.20	77,77,77,77	0
57	MG	14	3211	1/1	0.84	0.44	85,85,85,85	0
57	MG	1H	3172	1/1	0.84	0.29	84,84,84,84	0
57	MG	14	3004	1/1	0.84	0.15	73,73,73,73	0
57	MG	1H	3364	1/1	0.84	0.10	72,72,72,72	0
57	MG	1H	3100	1/1	0.84	0.16	62,62,62,62	0
57	MG	1H	3240	1/1	0.84	0.26	67,67,67,67	0
57	MG	14	3114	1/1	0.84	0.35	63,63,63,63	0
57	MG	1H	3449	1/1	0.84	0.21	80,80,80,80	0
57	MG	14	3116	1/1	0.84	0.27	66,66,66,66	0
57	MG	14	3018	1/1	0.84	0.25	78,78,78,78	0
57	MG	14	3021	1/1	0.84	0.21	76,76,76,76	0
57	MG	14	3126	1/1	0.84	0.28	75,75,75,75	0
57	MG	1G	1633	1/1	0.84	0.20	89,89,89,89	0
57	MG	14	3228	1/1	0.84	0.40	86,86,86,86	0
57	MG	13	1623	1/1	0.84	0.34	80,80,80,80	0
57	MG	1G	1637	1/1	0.84	0.14	113,113,113,113	0
57	MG	1G	1640	1/1	0.84	0.12	92,92,92,92	0
57	MG	14	3298	1/1	0.84	0.13	56,56,56,56	0
57	MG	14	3029	1/1	0.84	0.25	73,73,73,73	0
57	MG	14	3388	1/1	0.84	0.14	89,89,89,89	0
57	MG	1H	3210	1/1	0.84	0.14	83,83,83,83	0
57	MG	14	3396	1/1	0.84	0.18	109,109,109,109	0
57	MG	1H	3070	1/1	0.84	0.26	56,56,56,56	0
57	MG	14	3147	1/1	0.84	0.10	69,69,69,69	0
57	MG	13	1647	1/1	0.84	0.33	91,91,91,91	0
57	MG	14	3155	1/1	0.84	0.20	80,80,80,80	0
57	MG	1H	3106	1/1	0.84	0.17	68,68,68,68	0
57	MG	14	3040	1/1	0.84	0.18	72,72,72,72	0
57	MG	1H	3108	1/1	0.84	0.23	69,69,69,69	0
57	MG	31	301	1/1	0.84	0.11	63,63,63,63	0
57	MG	1H	3190	1/1	0.84	0.30	75,75,75,75	0
57	MG	1H	3311	1/1	0.84	0.24	93,93,93,93	0
57	MG	14	3009	1/1	0.85	0.24	68,68,68,68	0
57	MG	1H	3127	1/1	0.85	0.27	84,84,84,84	0
57	MG	1H	3184	1/1	0.85	0.36	93,93,93,93	0
57	MG	2K	101	1/1	0.85	0.22	63,63,63,63	0
57	MG	1H	3186	1/1	0.85	0.37	94,94,94,94	0
57	MG	1H	3066	1/1	0.85	0.21	65,65,65,65	0
57	MG	1H	3504	1/1	0.85	0.11	93,93,93,93	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	1H	3509	1/1	0.85	0.16	88,88,88,88	0
57	MG	13	1626	1/1	0.85	0.29	67,67,67,67	0
57	MG	1H	3018	1/1	0.85	0.28	55,55,55,55	0
57	MG	1H	3238	1/1	0.85	0.28	87,87,87,87	0
57	MG	14	3120	1/1	0.85	0.27	75,75,75,75	0
57	MG	14	3122	1/1	0.85	0.23	84,84,84,84	0
57	MG	16	202	1/1	0.85	0.29	78,78,78,78	0
57	MG	1H	3196	1/1	0.85	0.14	56,56,56,56	0
57	MG	1H	3073	1/1	0.85	0.34	59,59,59,59	0
57	MG	13	1661	1/1	0.85	0.20	92,92,92,92	0
57	MG	68	202	1/1	0.85	0.22	83,83,83,83	0
57	MG	14	3043	1/1	0.85	0.30	83,83,83,83	0
57	MG	88	202	1/1	0.85	0.30	72,72,72,72	0
57	MG	14	3056	1/1	0.85	0.20	80,80,80,80	0
57	MG	1H	3297	1/1	0.85	0.16	78,78,78,78	0
57	MG	13	1634	1/1	0.85	0.26	78,78,78,78	0
57	MG	14	3148	1/1	0.85	0.15	63,63,63,63	0
57	MG	14	3150	1/1	0.85	0.34	81,81,81,81	0
57	MG	1G	1675	1/1	0.85	0.12	107,107,107,107	0
57	MG	14	3154	1/1	0.85	0.15	87,87,87,87	0
57	MG	14	3230	1/1	0.85	0.26	81,81,81,81	0
57	MG	1G	1605	1/1	0.85	0.30	82,82,82,82	0
57	MG	1H	3203	1/1	0.85	0.33	74,74,74,74	0
57	MG	1H	3303	1/1	0.85	0.29	76,76,76,76	0
57	MG	1H	3033	1/1	0.85	0.21	73,73,73,73	0
57	MG	1H	3034	1/1	0.85	0.24	72,72,72,72	0
57	MG	1H	3252	1/1	0.85	0.38	81,81,81,81	0
57	MG	1H	3117	1/1	0.85	0.26	54,54,54,54	0
57	MG	1H	3035	1/1	0.85	0.28	80,80,80,80	0
57	MG	13	1667	1/1	0.85	0.41	96,96,96,96	0
57	MG	14	3083	1/1	0.85	0.39	87,87,87,87	0
57	MG	1H	3089	1/1	0.85	0.21	66,66,66,66	0
57	MG	14	3086	1/1	0.85	0.22	64,64,64,64	0
57	MG	1H	3038	1/1	0.85	0.35	65,65,65,65	0
57	MG	1H	3268	1/1	0.85	0.42	92,92,92,92	0
57	MG	1H	3048	1/1	0.85	0.13	43,43,43,43	0
57	MG	14	3181	1/1	0.85	0.25	81,81,81,81	0
57	MG	13	1673	1/1	0.85	0.37	80,80,80,80	0
57	MG	1H	3197	1/1	0.86	0.33	80,80,80,80	0
57	MG	1H	3069	1/1	0.86	0.23	60,60,60,60	0
57	MG	1H	3199	1/1	0.86	0.19	78,78,78,78	0
57	MG	1G	1662	1/1	0.86	0.42	94,94,94,94	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	1H	3256	1/1	0.86	0.24	67,67,67,67	0
57	MG	1H	3309	1/1	0.86	0.24	74,74,74,74	0
57	MG	1H	3004	1/1	0.86	0.31	79,79,79,79	0
57	MG	14	3293	1/1	0.86	0.13	72,72,72,72	0
57	MG	1H	3016	1/1	0.86	0.21	47,47,47,47	0
57	MG	1H	3284	1/1	0.86	0.20	71,71,71,71	0
57	MG	1G	1611	1/1	0.86	0.38	77,77,77,77	0
57	MG	14	3168	1/1	0.86	0.16	87,87,87,87	0
57	MG	13	1650	1/1	0.86	0.39	85,85,85,85	0
57	MG	13	1643	1/1	0.86	0.33	86,86,86,86	0
57	MG	1H	3537	1/1	0.86	0.15	61,61,61,61	0
57	MG	14	3033	1/1	0.86	0.40	75,75,75,75	0
57	MG	1H	3191	1/1	0.86	0.18	72,72,72,72	0
57	MG	14	3215	1/1	0.86	0.10	72,72,72,72	0
57	MG	1H	3267	1/1	0.86	0.37	68,68,68,68	0
57	MG	1G	1651	1/1	0.86	0.24	105,105,105,105	0
57	MG	1H	3292	1/1	0.86	0.19	84,84,84,84	0
57	MG	14	3046	1/1	0.86	0.37	76,76,76,76	0
57	MG	1H	3221	1/1	0.86	0.27	64,64,64,64	0
57	MG	1H	3002	1/1	0.86	0.44	82,82,82,82	0
57	MG	14	3207	1/1	0.87	0.32	85,85,85,85	0
57	MG	14	3006	1/1	0.87	0.28	79,79,79,79	0
57	MG	88	203	1/1	0.87	0.26	76,76,76,76	0
57	MG	1H	3223	1/1	0.87	0.20	80,80,80,80	0
57	MG	14	3076	1/1	0.87	0.18	89,89,89,89	0
57	MG	1H	3055	1/1	0.87	0.20	60,60,60,60	0
57	MG	14	3012	1/1	0.87	0.31	60,60,60,60	0
57	MG	1H	3324	1/1	0.87	0.24	66,66,66,66	0
57	MG	1H	3098	1/1	0.87	0.36	78,78,78,78	0
57	MG	1H	3290	1/1	0.87	0.18	87,87,87,87	0
57	MG	1H	3291	1/1	0.87	0.23	78,78,78,78	0
57	MG	1H	3263	1/1	0.87	0.42	91,91,91,91	0
57	MG	1H	3402	1/1	0.87	0.11	79,79,79,79	0
57	MG	13	1631	1/1	0.87	0.25	78,78,78,78	0
57	MG	1H	3059	1/1	0.87	0.27	72,72,72,72	0
57	MG	1H	3153	1/1	0.87	0.24	82,82,82,82	0
57	MG	13	1601	1/1	0.87	0.27	74,74,74,74	0
57	MG	13	1607	1/1	0.87	0.29	80,80,80,80	0
57	MG	1H	3019	1/1	0.87	0.19	61,61,61,61	0
57	MG	1G	1622	1/1	0.87	0.41	85,85,85,85	0
57	MG	14	3261	1/1	0.87	0.12	67,67,67,67	0
57	MG	1H	3307	1/1	0.87	0.44	72,72,72,72	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	14	3039	1/1	0.87	0.27	65,65,65,65	0
57	MG	1H	3271	1/1	0.87	0.14	77,77,77,77	0
57	MG	1H	3192	1/1	0.87	0.33	76,76,76,76	0
57	MG	13	1604	1/1	0.87	0.24	77,77,77,77	0
57	MG	14	3185	1/1	0.87	0.18	76,76,76,76	0
57	MG	14	3391	1/1	0.87	0.12	103,103,103,103	0
57	MG	1G	1631	1/1	0.87	0.17	82,82,82,82	0
57	MG	14	3047	1/1	0.87	0.21	81,81,81,81	0
57	MG	14	3409	1/1	0.87	0.12	95,95,95,95	0
57	MG	1H	3131	1/1	0.87	0.25	75,75,75,75	0
57	MG	1H	3042	1/1	0.87	0.28	67,67,67,67	0
57	MG	14	3428	1/1	0.87	0.12	109,109,109,109	0
57	MG	14	3435	1/1	0.87	0.11	93,93,93,93	0
57	MG	14	3443	1/1	0.87	0.18	92,92,92,92	0
57	MG	14	3447	1/1	0.87	0.40	69,69,69,69	0
57	MG	4A	201	1/1	0.87	0.22	96,96,96,96	0
57	MG	1G	1634	1/1	0.87	0.17	93,93,93,93	0
57	MG	1H	3072	1/1	0.87	0.33	72,72,72,72	0
57	MG	13	1605	1/1	0.87	0.23	70,70,70,70	0
57	MG	14	3002	1/1	0.87	0.34	68,68,68,68	0
57	MG	1H	3222	1/1	0.87	0.26	64,64,64,64	0
57	MG	14	3204	1/1	0.87	0.36	80,80,80,80	0
57	MG	14	3140	1/1	0.87	0.23	89,89,89,89	0
57	MG	14	3195	1/1	0.88	0.31	78,78,78,78	0
57	MG	68	201	1/1	0.88	0.24	78,78,78,78	0
57	MG	1H	3306	1/1	0.88	0.14	70,70,70,70	0
57	MG	13	1632	1/1	0.88	0.45	90,90,90,90	0
57	MG	1H	3150	1/1	0.88	0.31	67,67,67,67	0
57	MG	13	1613	1/1	0.88	0.26	81,81,81,81	0
57	MG	P8	101	1/1	0.88	0.27	71,71,71,71	0
57	MG	14	3038	1/1	0.88	0.16	69,69,69,69	0
57	MG	1H	3093	1/1	0.88	0.34	71,71,71,71	0
57	MG	1H	3231	1/1	0.88	0.23	67,67,67,67	0
57	MG	1H	3009	1/1	0.88	0.34	77,77,77,77	0
57	MG	1H	3158	1/1	0.88	0.37	71,71,71,71	0
57	MG	14	3133	1/1	0.88	0.15	58,58,58,58	0
57	MG	1H	3273	1/1	0.88	0.14	69,69,69,69	0
57	MG	1H	3234	1/1	0.88	0.33	76,76,76,76	0
57	MG	14	3137	1/1	0.88	0.20	68,68,68,68	0
57	MG	13	1663	1/1	0.88	0.41	90,90,90,90	0
57	MG	1H	3279	1/1	0.88	0.36	76,76,76,76	0
57	MG	14	3221	1/1	0.88	0.17	91,91,91,91	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	1H	3281	1/1	0.88	0.19	67,67,67,67	0
57	MG	1H	3096	1/1	0.88	0.14	53,53,53,53	0
57	MG	1G	1723	1/1	0.88	0.19	94,94,94,94	0
57	MG	13	1629	1/1	0.88	0.19	56,56,56,56	0
57	MG	13	1672	1/1	0.88	0.46	86,86,86,86	0
57	MG	1H	3242	1/1	0.88	0.14	74,74,74,74	0
57	MG	14	3066	1/1	0.88	0.24	59,59,59,59	0
57	MG	14	3067	1/1	0.88	0.26	69,69,69,69	0
57	MG	13	1736	1/1	0.88	0.12	104,104,104,104	0
57	MG	13	1743	1/1	0.88	0.07	153,153,153,153	0
57	MG	1H	3130	1/1	0.88	0.40	87,87,87,87	0
57	MG	14	3162	1/1	0.88	0.21	67,67,67,67	0
57	MG	14	3075	1/1	0.88	0.37	89,89,89,89	0
57	MG	1G	1626	1/1	0.88	0.25	68,68,68,68	0
57	MG	1H	3211	1/1	0.88	0.38	79,79,79,79	0
57	MG	1H	3052	1/1	0.88	0.21	50,50,50,50	0
57	MG	1H	3022	1/1	0.88	0.19	41,41,41,41	0
57	MG	1H	3519	1/1	0.88	0.17	83,83,83,83	0
57	MG	1H	3294	1/1	0.88	0.14	90,90,90,90	0
57	MG	1H	3056	1/1	0.88	0.44	73,73,73,73	0
57	MG	1H	3107	1/1	0.88	0.26	72,72,72,72	0
57	MG	14	3092	1/1	0.88	0.37	81,81,81,81	0
57	MG	14	3093	1/1	0.88	0.22	79,79,79,79	0
57	MG	1H	3005	1/1	0.88	0.40	74,74,74,74	0
57	MG	14	3015	1/1	0.88	0.22	73,73,73,73	0
57	MG	14	3016	1/1	0.88	0.28	63,63,63,63	0
57	MG	1H	3219	1/1	0.88	0.36	82,82,82,82	0
57	MG	1H	3109	1/1	0.88	0.27	79,79,79,79	0
57	MG	1H	3029	1/1	0.88	0.18	63,63,63,63	0
57	MG	16	207	1/1	0.88	0.10	84,84,84,84	0
57	MG	14	3105	1/1	0.88	0.26	73,73,73,73	0
57	MG	16	208	1/1	0.88	0.32	79,79,79,79	0
57	MG	35	202	1/1	0.88	0.33	84,84,84,84	0
58	SPE	13	1748	13/13	0.88	0.14	60,77,82,87	0
58	SPE	1G	1733	13/13	0.88	0.15	98,101,104,105	0
57	MG	1H	3304	1/1	0.88	0.37	85,85,85,85	0
57	MG	1H	3114	1/1	0.89	0.31	67,67,67,67	0
57	MG	13	1637	1/1	0.89	0.14	79,79,79,79	0
57	MG	1H	3373	1/1	0.89	0.11	89,89,89,89	0
57	MG	14	3118	1/1	0.89	0.08	73,73,73,73	0
57	MG	14	3201	1/1	0.89	0.55	95,95,95,95	0
57	MG	1H	3262	1/1	0.89	0.19	71,71,71,71	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	1H	3380	1/1	0.89	0.11	59,59,59,59	0
57	MG	1H	3194	1/1	0.89	0.36	71,71,71,71	0
57	MG	14	3050	1/1	0.89	0.29	77,77,77,77	0
57	MG	1H	3415	1/1	0.89	0.13	72,72,72,72	0
57	MG	1H	3152	1/1	0.89	0.18	51,51,51,51	0
57	MG	1H	3448	1/1	0.89	0.11	86,86,86,86	0
57	MG	13	1680	1/1	0.89	0.44	84,84,84,84	0
57	MG	1H	3092	1/1	0.89	0.08	74,74,74,74	0
57	MG	1H	3464	1/1	0.89	0.10	48,48,48,48	0
57	MG	14	3062	1/1	0.89	0.40	71,71,71,71	0
57	MG	14	3139	1/1	0.89	0.33	84,84,84,84	0
57	MG	2L	101	1/1	0.89	0.29	77,77,77,77	0
57	MG	1H	3017	1/1	0.89	0.22	53,53,53,53	0
57	MG	1H	3301	1/1	0.89	0.20	70,70,70,70	0
57	MG	1G	1625	1/1	0.89	0.12	98,98,98,98	0
57	MG	5I	101	1/1	0.89	0.12	80,80,80,80	0
57	MG	14	3069	1/1	0.89	0.21	93,93,93,93	0
57	MG	1H	3521	1/1	0.89	0.18	86,86,86,86	0
57	MG	14	3153	1/1	0.89	0.22	65,65,65,65	0
57	MG	14	3072	1/1	0.89	0.13	57,57,57,57	0
57	MG	14	3005	1/1	0.89	0.16	50,50,50,50	0
57	MG	14	3156	1/1	0.89	0.13	71,71,71,71	0
57	MG	13	1641	1/1	0.89	0.24	68,68,68,68	0
57	MG	1H	3524	1/1	0.89	0.16	96,96,96,96	0
57	MG	1H	3164	1/1	0.89	0.15	64,64,64,64	0
57	MG	14	3161	1/1	0.89	0.30	79,79,79,79	0
57	MG	1H	3037	1/1	0.89	0.26	71,71,71,71	0
57	MG	14	3351	1/1	0.89	0.10	104,104,104,104	0
57	MG	14	3380	1/1	0.89	0.10	85,85,85,85	0
57	MG	14	3381	1/1	0.89	0.19	74,74,74,74	0
57	MG	1H	3020	1/1	0.89	0.15	47,47,47,47	0
57	MG	1H	3308	1/1	0.89	0.20	56,56,56,56	0
57	MG	14	3167	1/1	0.89	0.20	76,76,76,76	0
57	MG	1H	3021	1/1	0.89	0.27	63,63,63,63	0
57	MG	16	205	1/1	0.89	0.10	66,66,66,66	0
57	MG	14	3405	1/1	0.89	0.10	91,91,91,91	0
57	MG	1G	1642	1/1	0.89	0.21	82,82,82,82	0
57	MG	14	3089	1/1	0.89	0.35	79,79,79,79	0
57	MG	14	3421	1/1	0.89	0.15	98,98,98,98	0
57	MG	14	3090	1/1	0.89	0.25	65,65,65,65	0
57	MG	14	3017	1/1	0.89	0.33	60,60,60,60	0
57	MG	1H	3043	1/1	0.89	0.24	66,66,66,66	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	1H	3278	1/1	0.89	0.23	83,83,83,83	0
57	MG	1H	3209	1/1	0.89	0.21	52,52,52,52	0
57	MG	1H	3314	1/1	0.89	0.20	88,88,88,88	0
57	MG	14	3179	1/1	0.89	0.23	71,71,71,71	0
57	MG	1H	3074	1/1	0.89	0.28	73,73,73,73	0
57	MG	1H	3044	1/1	0.89	0.44	81,81,81,81	0
57	MG	1J	206	1/1	0.89	0.11	109,109,109,109	0
57	MG	88	201	1/1	0.89	0.23	78,78,78,78	0
57	MG	13	1642	1/1	0.89	0.17	72,72,72,72	0
57	MG	1H	3051	1/1	0.89	0.30	76,76,76,76	0
57	MG	1H	3082	1/1	0.89	0.34	76,76,76,76	0
57	MG	13	1602	1/1	0.89	0.29	78,78,78,78	0
57	MG	1H	3028	1/1	0.89	0.25	62,62,62,62	0
58	SPE	14	3445	13/13	0.89	0.18	70,76,79,79	0
58	SPE	14	3446	13/13	0.89	0.24	68,79,87,89	0
57	MG	13	1620	1/1	0.89	0.20	57,57,57,57	0
57	MG	14	3078	1/1	0.90	0.37	64,64,64,64	0
57	MG	1H	3208	1/1	0.90	0.33	78,78,78,78	0
57	MG	13	1681	1/1	0.90	0.10	68,68,68,68	0
57	MG	13	1608	1/1	0.90	0.13	71,71,71,71	0
57	MG	13	1710	1/1	0.90	0.09	82,82,82,82	0
57	MG	13	1628	1/1	0.90	0.29	79,79,79,79	0
57	MG	1H	3244	1/1	0.90	0.35	77,77,77,77	0
57	MG	1G	1658	1/1	0.90	0.17	84,84,84,84	0
57	MG	1H	3085	1/1	0.90	0.39	75,75,75,75	0
57	MG	14	3091	1/1	0.90	0.32	66,66,66,66	0
57	MG	1H	3515	1/1	0.90	0.09	98,98,98,98	0
57	MG	13	1619	1/1	0.90	0.11	53,53,53,53	0
57	MG	14	3094	1/1	0.90	0.31	70,70,70,70	0
57	MG	1H	3310	1/1	0.90	0.51	87,87,87,87	0
57	MG	14	3165	1/1	0.90	0.25	74,74,74,74	0
57	MG	1H	3165	1/1	0.90	0.17	59,59,59,59	0
57	MG	1G	1696	1/1	0.90	0.09	91,91,91,91	0
57	MG	1G	1618	1/1	0.90	0.35	89,89,89,89	0
57	MG	1H	3168	1/1	0.90	0.12	80,80,80,80	0
57	MG	1H	3529	1/1	0.90	0.24	78,78,78,78	0
57	MG	1G	1621	1/1	0.90	0.32	86,86,86,86	0
57	MG	1H	3531	1/1	0.90	0.17	76,76,76,76	0
57	MG	14	3365	1/1	0.90	0.12	96,96,96,96	0
57	MG	14	3045	1/1	0.90	0.24	61,61,61,61	0
57	MG	14	3107	1/1	0.90	0.18	65,65,65,65	0
57	MG	1H	3068	1/1	0.90	0.36	71,71,71,71	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	1G	1729	1/1	0.90	0.09	104,104,104,104	0
57	MG	14	3113	1/1	0.90	0.21	57,57,57,57	0
57	MG	13	1610	1/1	0.90	0.33	73,73,73,73	0
57	MG	1H	3542	1/1	0.90	0.16	90,90,90,90	0
57	MG	14	3401	1/1	0.90	0.17	85,85,85,85	0
57	MG	14	3402	1/1	0.90	0.07	118,118,118,118	0
57	MG	14	3182	1/1	0.90	0.08	82,82,82,82	0
57	MG	1H	3253	1/1	0.90	0.37	71,71,71,71	0
57	MG	13	1665	1/1	0.90	0.44	88,88,88,88	0
57	MG	1H	3257	1/1	0.90	0.18	51,51,51,51	0
57	MG	14	3119	1/1	0.90	0.24	79,79,79,79	0
57	MG	1H	3258	1/1	0.90	0.33	84,84,84,84	0
57	MG	14	3434	1/1	0.90	0.08	115,115,115,115	0
57	MG	1H	3288	1/1	0.90	0.27	77,77,77,77	0
57	MG	1H	3173	1/1	0.90	0.49	89,89,89,89	0
57	MG	14	3003	1/1	0.90	0.28	54,54,54,54	0
57	MG	1H	3201	1/1	0.90	0.40	88,88,88,88	0
57	MG	14	3196	1/1	0.90	0.23	68,68,68,68	0
57	MG	1H	3176	1/1	0.90	0.14	62,62,62,62	0
57	MG	1H	3148	1/1	0.90	0.22	80,80,80,80	0
57	MG	1G	1639	1/1	0.90	0.17	103,103,103,103	0
57	MG	1H	3293	1/1	0.90	0.31	46,46,46,46	0
57	MG	14	3203	1/1	0.90	0.46	93,93,93,93	0
57	MG	25	201	1/1	0.90	0.07	118,118,118,118	0
57	MG	1H	3228	1/1	0.90	0.25	70,70,70,70	0
57	MG	1H	3053	1/1	0.90	0.35	66,66,66,66	0
57	MG	13	1612	1/1	0.90	0.24	76,76,76,76	0
57	MG	1H	3151	1/1	0.90	0.14	59,59,59,59	0
57	MG	13	1689	1/1	0.90	0.37	85,85,85,85	0
57	MG	1G	1602	1/1	0.90	0.17	81,81,81,81	0
57	MG	14	3146	1/1	0.90	0.14	51,51,51,51	0
57	MG	1H	3213	1/1	0.91	0.33	77,77,77,77	0
57	MG	13	1727	1/1	0.91	0.11	90,90,90,90	0
57	MG	13	1733	1/1	0.91	0.10	106,106,106,106	0
57	MG	1H	3323	1/1	0.91	0.21	75,75,75,75	0
57	MG	13	1609	1/1	0.91	0.20	71,71,71,71	0
57	MG	1H	3243	1/1	0.91	0.21	79,79,79,79	0
57	MG	1H	3547	1/1	0.91	0.23	61,61,61,61	0
57	MG	14	3282	1/1	0.91	0.10	105,105,105,105	0
57	MG	1H	3110	1/1	0.91	0.21	65,65,65,65	0
57	MG	14	3071	1/1	0.91	0.17	63,63,63,63	0
57	MG	1H	3179	1/1	0.91	0.28	67,67,67,67	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	14	3073	1/1	0.91	0.20	48,48,48,48	0
57	MG	14	3307	1/1	0.91	0.11	72,72,72,72	0
57	MG	14	3324	1/1	0.91	0.12	66,66,66,66	0
57	MG	14	3127	1/1	0.91	0.29	62,62,62,62	0
57	MG	14	3355	1/1	0.91	0.08	107,107,107,107	0
57	MG	1H	3111	1/1	0.91	0.50	73,73,73,73	0
57	MG	14	3130	1/1	0.91	0.31	70,70,70,70	0
57	MG	14	3019	1/1	0.91	0.10	53,53,53,53	0
57	MG	16	204	1/1	0.91	0.30	70,70,70,70	0
57	MG	1H	3129	1/1	0.91	0.32	69,69,69,69	0
57	MG	1G	1691	1/1	0.91	0.12	99,99,99,99	0
57	MG	1H	3154	1/1	0.91	0.16	66,66,66,66	0
57	MG	1G	1698	1/1	0.91	0.09	105,105,105,105	0
57	MG	1G	1701	1/1	0.91	0.08	101,101,101,101	0
57	MG	13	1737	1/1	0.91	0.12	98,98,98,98	0
57	MG	14	3404	1/1	0.91	0.12	100,100,100,100	0
57	MG	1H	3251	1/1	0.91	0.19	77,77,77,77	0
57	MG	1H	3421	1/1	0.91	0.09	99,99,99,99	0
57	MG	3I	302	1/1	0.91	0.18	73,73,73,73	0
57	MG	14	3419	1/1	0.91	0.08	110,110,110,110	0
57	MG	1H	3422	1/1	0.91	0.09	101,101,101,101	0
57	MG	1G	1717	1/1	0.91	0.09	99,99,99,99	0
57	MG	14	3202	1/1	0.91	0.18	83,83,83,83	0
57	MG	14	3431	1/1	0.91	0.11	60,60,60,60	0
57	MG	14	3149	1/1	0.91	0.31	71,71,71,71	0
57	MG	1H	3429	1/1	0.91	0.09	56,56,56,56	0
57	MG	14	3441	1/1	0.91	0.13	102,102,102,102	0
57	MG	13	1711	1/1	0.91	0.13	102,102,102,102	0
57	MG	14	3152	1/1	0.91	0.41	86,86,86,86	0
57	MG	14	3041	1/1	0.91	0.51	76,76,76,76	0
57	MG	1H	3011	1/1	0.91	0.16	73,73,73,73	0
57	MG	1H	3001	1/1	0.91	0.25	61,61,61,61	0
57	MG	1H	3229	1/1	0.91	0.25	64,64,64,64	0
57	MG	1H	3230	1/1	0.91	0.22	87,87,87,87	0
57	MG	1H	3162	1/1	0.91	0.32	68,68,68,68	0
57	MG	13	1745	1/1	0.91	0.07	111,111,111,111	0
57	MG	14	3160	1/1	0.91	0.42	92,92,92,92	0
57	MG	13	1640	1/1	0.91	0.29	77,77,77,77	0
57	MG	1H	3121	1/1	0.91	0.51	80,80,80,80	0
57	MG	B5	101	1/1	0.91	0.11	85,85,85,85	0
57	MG	14	3219	1/1	0.91	0.26	54,54,54,54	0
57	MG	1G	1645	1/1	0.91	0.12	93,93,93,93	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	1H	3064	1/1	0.91	0.22	63,63,63,63	0
57	MG	1H	3237	1/1	0.91	0.21	73,73,73,73	0
57	MG	1G	1610	1/1	0.91	0.18	69,69,69,69	0
57	MG	1G	1685	1/1	0.92	0.09	91,91,91,91	0
57	MG	1G	1689	1/1	0.92	0.10	89,89,89,89	0
57	MG	1H	3147	1/1	0.92	0.23	64,64,64,64	0
57	MG	1H	3350	1/1	0.92	0.10	57,57,57,57	0
57	MG	1H	3352	1/1	0.92	0.07	84,84,84,84	0
57	MG	14	3227	1/1	0.92	0.24	76,76,76,76	0
57	MG	14	3037	1/1	0.92	0.22	57,57,57,57	0
57	MG	14	3163	1/1	0.92	0.41	84,84,84,84	0
57	MG	1H	3298	1/1	0.92	0.11	83,83,83,83	0
57	MG	14	3246	1/1	0.92	0.10	72,72,72,72	0
57	MG	14	3256	1/1	0.92	0.08	54,54,54,54	0
57	MG	1H	3370	1/1	0.92	0.09	59,59,59,59	0
57	MG	13	1666	1/1	0.92	0.19	78,78,78,78	0
57	MG	13	1639	1/1	0.92	0.14	73,73,73,73	0
57	MG	1G	1713	1/1	0.92	0.11	113,113,113,113	0
57	MG	1G	1627	1/1	0.92	0.24	77,77,77,77	0
57	MG	14	3296	1/1	0.92	0.09	62,62,62,62	0
57	MG	1G	1628	1/1	0.92	0.34	76,76,76,76	0
57	MG	14	3109	1/1	0.92	0.42	74,74,74,74	0
57	MG	14	3313	1/1	0.92	0.10	87,87,87,87	0
57	MG	1H	3175	1/1	0.92	0.12	64,64,64,64	0
57	MG	14	3331	1/1	0.92	0.10	79,79,79,79	0
57	MG	14	3111	1/1	0.92	0.39	86,86,86,86	0
57	MG	13	1657	1/1	0.92	0.41	80,80,80,80	0
57	MG	1G	1725	1/1	0.92	0.08	113,113,113,113	0
57	MG	14	3378	1/1	0.92	0.07	86,86,86,86	0
57	MG	14	3052	1/1	0.92	0.40	79,79,79,79	0
57	MG	1H	3083	1/1	0.92	0.35	71,71,71,71	0
57	MG	14	3054	1/1	0.92	0.13	49,49,49,49	0
57	MG	21	301	1/1	0.92	0.20	62,62,62,62	0
57	MG	14	3390	1/1	0.92	0.13	108,108,108,108	0
57	MG	1H	3084	1/1	0.92	0.32	68,68,68,68	0
57	MG	1H	3280	1/1	0.92	0.22	68,68,68,68	0
57	MG	1H	3181	1/1	0.92	0.12	94,94,94,94	0
57	MG	1G	1636	1/1	0.92	0.09	91,91,91,91	0
57	MG	1H	3255	1/1	0.92	0.28	73,73,73,73	0
57	MG	14	3125	1/1	0.92	0.30	70,70,70,70	0
57	MG	1H	3113	1/1	0.92	0.26	64,64,64,64	0
57	MG	13	1715	1/1	0.92	0.07	114,114,114,114	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	1G	1641	1/1	0.92	0.09	88,88,88,88	0
57	MG	14	3413	1/1	0.92	0.17	81,81,81,81	0
57	MG	1H	3023	1/1	0.92	0.15	72,72,72,72	0
57	MG	1H	3156	1/1	0.92	0.13	66,66,66,66	0
57	MG	14	3422	1/1	0.92	0.14	100,100,100,100	0
57	MG	1H	3484	1/1	0.92	0.09	84,84,84,84	0
57	MG	14	3426	1/1	0.92	0.06	126,126,126,126	0
57	MG	1H	3498	1/1	0.92	0.13	85,85,85,85	0
57	MG	14	3135	1/1	0.92	0.18	69,69,69,69	0
57	MG	1H	3500	1/1	0.92	0.10	93,93,93,93	0
57	MG	1H	3071	1/1	0.92	0.23	57,57,57,57	0
57	MG	14	3010	1/1	0.92	0.14	50,50,50,50	0
57	MG	1H	3508	1/1	0.92	0.08	84,84,84,84	0
57	MG	14	3444	1/1	0.92	0.17	85,85,85,85	0
57	MG	14	3205	1/1	0.92	0.23	79,79,79,79	0
57	MG	13	1658	1/1	0.92	0.39	75,75,75,75	0
57	MG	1H	3062	1/1	0.92	0.13	40,40,40,40	0
57	MG	14	3142	1/1	0.92	0.19	76,76,76,76	0
57	MG	14	3209	1/1	0.92	0.20	65,65,65,65	0
57	MG	1H	3137	1/1	0.92	0.18	57,57,57,57	0
57	MG	19	301	1/1	0.92	0.21	57,57,57,57	0
57	MG	1H	3163	1/1	0.92	0.13	74,74,74,74	0
57	MG	1G	1612	1/1	0.92	0.17	82,82,82,82	0
57	MG	1H	3139	1/1	0.92	0.09	54,54,54,54	0
57	MG	1H	3241	1/1	0.92	0.09	64,64,64,64	0
57	MG	14	3084	1/1	0.92	0.28	87,87,87,87	0
57	MG	1H	3527	1/1	0.92	0.07	107,107,107,107	0
57	MG	13	1674	1/1	0.92	0.27	92,92,92,92	0
57	MG	1H	3065	1/1	0.92	0.16	50,50,50,50	0
57	MG	1H	3123	1/1	0.92	0.30	65,65,65,65	0
57	MG	1G	1678	1/1	0.92	0.10	73,73,73,73	0
57	MG	1H	3331	1/1	0.92	0.10	53,53,53,53	0
57	MG	14	3268	1/1	0.93	0.19	86,86,86,86	0
57	MG	1H	3024	1/1	0.93	0.09	51,51,51,51	0
57	MG	14	3284	1/1	0.93	0.07	72,72,72,72	0
57	MG	14	3051	1/1	0.93	0.20	72,72,72,72	0
57	MG	1H	3026	1/1	0.93	0.27	52,52,52,52	0
57	MG	1H	3045	1/1	0.93	0.13	42,42,42,42	0
57	MG	1H	3090	1/1	0.93	0.21	77,77,77,77	0
57	MG	13	1747	1/1	0.93	0.08	110,110,110,110	0
57	MG	1G	1638	1/1	0.93	0.15	93,93,93,93	0
57	MG	1H	3451	1/1	0.93	0.08	83,83,83,83	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	1H	3167	1/1	0.93	0.08	60,60,60,60	0
57	MG	14	3184	1/1	0.93	0.18	72,72,72,72	0
57	MG	14	3346	1/1	0.93	0.07	92,92,92,92	0
57	MG	1H	3473	1/1	0.93	0.08	76,76,76,76	0
57	MG	14	3352	1/1	0.93	0.10	84,84,84,84	0
57	MG	14	3353	1/1	0.93	0.08	90,90,90,90	0
57	MG	1H	3479	1/1	0.93	0.10	75,75,75,75	0
57	MG	14	3188	1/1	0.93	0.43	76,76,76,76	0
57	MG	14	3369	1/1	0.93	0.08	92,92,92,92	0
57	MG	14	3376	1/1	0.93	0.14	78,78,78,78	0
57	MG	1H	3480	1/1	0.93	0.11	53,53,53,53	0
57	MG	1H	3483	1/1	0.93	0.10	103,103,103,103	0
57	MG	14	3065	1/1	0.93	0.21	60,60,60,60	0
57	MG	1G	1603	1/1	0.93	0.18	79,79,79,79	0
57	MG	1G	1646	1/1	0.93	0.08	83,83,83,83	0
57	MG	1H	3014	1/1	0.93	0.18	43,43,43,43	0
57	MG	1H	3254	1/1	0.93	0.42	75,75,75,75	0
57	MG	1H	3226	1/1	0.93	0.32	60,60,60,60	0
57	MG	1H	3169	1/1	0.93	0.40	82,82,82,82	0
57	MG	1H	3015	1/1	0.93	0.22	65,65,65,65	0
57	MG	13	1749	1/1	0.93	0.10	78,78,78,78	0
57	MG	1H	3513	1/1	0.93	0.12	80,80,80,80	0
57	MG	1H	3032	1/1	0.93	0.11	56,56,56,56	0
57	MG	1H	3119	1/1	0.93	0.18	62,62,62,62	0
57	MG	13	1730	1/1	0.93	0.09	81,81,81,81	0
57	MG	1H	3522	1/1	0.93	0.10	91,91,91,91	0
57	MG	14	3415	1/1	0.93	0.06	101,101,101,101	0
57	MG	14	3144	1/1	0.93	0.17	56,56,56,56	0
57	MG	1G	1660	1/1	0.93	0.24	75,75,75,75	0
57	MG	1H	3057	1/1	0.93	0.15	72,72,72,72	0
57	MG	5E	201	1/1	0.93	0.19	75,75,75,75	0
57	MG	13	1684	1/1	0.93	0.24	74,74,74,74	0
57	MG	14	3022	1/1	0.93	0.19	44,44,44,44	0
57	MG	1H	3349	1/1	0.93	0.14	67,67,67,67	0
57	MG	1H	3236	1/1	0.93	0.27	70,70,70,70	0
57	MG	1H	3101	1/1	0.93	0.10	65,65,65,65	0
57	MG	14	3436	1/1	0.93	0.15	96,96,96,96	0
57	MG	14	3438	1/1	0.93	0.11	101,101,101,101	0
57	MG	1G	1686	1/1	0.93	0.06	107,107,107,107	0
57	MG	14	3442	1/1	0.93	0.24	75,75,75,75	0
57	MG	1H	3081	1/1	0.93	0.09	55,55,55,55	0
57	MG	1H	3299	1/1	0.93	0.11	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	1G	1695	1/1	0.93	0.07	112,112,112,112	0
57	MG	1H	3060	1/1	0.93	0.20	51,51,51,51	0
57	MG	13	1652	1/1	0.93	0.20	68,68,68,68	0
57	MG	14	3096	1/1	0.93	0.18	50,50,50,50	0
57	MG	1G	1700	1/1	0.93	0.07	109,109,109,109	0
57	MG	1H	3379	1/1	0.93	0.09	58,58,58,58	0
57	MG	1G	1702	1/1	0.93	0.07	95,95,95,95	0
57	MG	13	1664	1/1	0.93	0.17	69,69,69,69	0
57	MG	39	301	1/1	0.93	0.17	95,95,95,95	0
57	MG	1G	1709	1/1	0.93	0.09	87,87,87,87	0
57	MG	13	1702	1/1	0.93	0.07	107,107,107,107	0
57	MG	1G	1711	1/1	0.93	0.10	108,108,108,108	0
57	MG	1H	3187	1/1	0.93	0.38	81,81,81,81	0
57	MG	1H	3418	1/1	0.93	0.08	86,86,86,86	0
57	MG	14	3231	1/1	0.93	0.44	80,80,80,80	0
57	MG	14	3244	1/1	0.93	0.10	58,58,58,58	0
57	MG	13	1611	1/1	0.93	0.12	85,85,85,85	0
57	MG	1H	3159	1/1	0.93	0.13	74,74,74,74	0
57	MG	14	3049	1/1	0.93	0.19	57,57,57,57	0
57	MG	14	3048	1/1	0.94	0.13	67,67,67,67	0
57	MG	13	1732	1/1	0.94	0.07	118,118,118,118	0
57	MG	11	301	1/1	0.94	0.25	60,60,60,60	0
57	MG	13	1655	1/1	0.94	0.16	65,65,65,65	0
57	MG	1G	1664	1/1	0.94	0.10	73,73,73,73	0
57	MG	1G	1666	1/1	0.94	0.07	103,103,103,103	0
57	MG	14	3370	1/1	0.94	0.21	87,87,87,87	0
57	MG	1H	3025	1/1	0.94	0.19	48,48,48,48	0
57	MG	1H	3003	1/1	0.94	0.36	65,65,65,65	0
57	MG	1H	3138	1/1	0.94	0.24	41,41,41,41	0
57	MG	1G	1681	1/1	0.94	0.10	96,96,96,96	0
57	MG	1G	1684	1/1	0.94	0.06	120,120,120,120	0
57	MG	14	3387	1/1	0.94	0.06	89,89,89,89	0
57	MG	13	1617	1/1	0.94	0.41	78,78,78,78	0
57	MG	1H	3365	1/1	0.94	0.09	62,62,62,62	0
57	MG	3I	201	1/1	0.94	0.20	64,64,64,64	0
57	MG	14	3393	1/1	0.94	0.08	118,118,118,118	0
57	MG	13	1615	1/1	0.94	0.13	73,73,73,73	0
57	MG	1H	3264	1/1	0.94	0.08	59,59,59,59	0
57	MG	13	1728	1/1	0.94	0.06	112,112,112,112	0
57	MG	Q8	101	1/1	0.94	0.17	81,81,81,81	0
57	MG	14	3020	1/1	0.94	0.25	61,61,61,61	0
57	MG	1H	3146	1/1	0.94	0.25	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	3388	1/1	0.94	0.09	58,58,58,58	0
57	MG	14	3169	1/1	0.94	0.09	53,53,53,53	0
57	MG	1H	3397	1/1	0.94	0.08	58,58,58,58	0
57	MG	1H	3046	1/1	0.94	0.13	49,49,49,49	0
57	MG	14	3418	1/1	0.94	0.06	101,101,101,101	0
57	MG	14	3123	1/1	0.94	0.29	60,60,60,60	0
57	MG	1H	3166	1/1	0.94	0.23	56,56,56,56	0
57	MG	14	3026	1/1	0.94	0.15	69,69,69,69	0
57	MG	1H	3047	1/1	0.94	0.22	55,55,55,55	0
57	MG	14	3424	1/1	0.94	0.13	94,94,94,94	0
57	MG	14	3028	1/1	0.94	0.22	61,61,61,61	0
57	MG	14	3427	1/1	0.94	0.14	92,92,92,92	0
57	MG	1H	3526	1/1	0.94	0.07	113,113,113,113	0
57	MG	14	3429	1/1	0.94	0.07	99,99,99,99	0
57	MG	14	3430	1/1	0.94	0.10	88,88,88,88	0
57	MG	1H	3249	1/1	0.94	0.16	68,68,68,68	0
57	MG	14	3079	1/1	0.94	0.18	61,61,61,61	0
57	MG	14	3232	1/1	0.94	0.10	56,56,56,56	0
57	MG	14	3236	1/1	0.94	0.08	70,70,70,70	0
57	MG	14	3437	1/1	0.94	0.06	107,107,107,107	0
57	MG	14	3132	1/1	0.94	0.19	78,78,78,78	0
57	MG	13	1638	1/1	0.94	0.09	78,78,78,78	0
57	MG	14	3254	1/1	0.94	0.07	52,52,52,52	0
57	MG	1H	3425	1/1	0.94	0.09	74,74,74,74	0
57	MG	1H	3318	1/1	0.94	0.13	54,54,54,54	0
57	MG	14	3186	1/1	0.94	0.15	74,74,74,74	0
57	MG	14	3274	1/1	0.94	0.07	81,81,81,81	0
57	MG	14	3279	1/1	0.94	0.16	83,83,83,83	0
57	MG	14	3280	1/1	0.94	0.08	97,97,97,97	0
57	MG	14	3281	1/1	0.94	0.07	95,95,95,95	0
57	MG	1J	205	1/1	0.94	0.08	87,87,87,87	0
57	MG	1H	3431	1/1	0.94	0.08	60,60,60,60	0
57	MG	1H	3049	1/1	0.94	0.27	69,69,69,69	0
57	MG	1H	3436	1/1	0.94	0.08	65,65,65,65	0
57	MG	1H	3440	1/1	0.94	0.11	61,61,61,61	0
57	MG	13	1746	1/1	0.94	0.05	119,119,119,119	0
57	MG	13	1731	1/1	0.94	0.07	90,90,90,90	0
57	MG	1H	3275	1/1	0.94	0.26	67,67,67,67	0
57	MG	14	3143	1/1	0.94	0.26	54,54,54,54	0
57	MG	1G	1656	1/1	0.94	0.19	66,66,66,66	0
57	MG	C5	201	1/1	0.94	0.09	103,103,103,103	0
57	MG	1H	3193	1/1	0.94	0.43	93,93,93,93	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	14	3327	1/1	0.94	0.07	100,100,100,100	0
57	MG	1H	3458	1/1	0.94	0.11	82,82,82,82	0
57	MG	14	3335	1/1	0.94	0.11	63,63,63,63	0
57	MG	1H	3116	1/1	0.94	0.12	82,82,82,82	0
57	MG	14	3044	1/1	0.95	0.28	48,48,48,48	0
57	MG	13	1695	1/1	0.95	0.07	82,82,82,82	0
57	MG	14	3374	1/1	0.95	0.07	83,83,83,83	0
57	MG	9A	101	1/1	0.95	0.07	115,115,115,115	0
57	MG	1H	3452	1/1	0.95	0.07	75,75,75,75	0
57	MG	13	1723	1/1	0.95	0.07	83,83,83,83	0
57	MG	1H	3174	1/1	0.95	0.05	37,37,37,37	0
57	MG	1H	3079	1/1	0.95	0.17	45,45,45,45	0
57	MG	1H	3140	1/1	0.95	0.07	40,40,40,40	0
57	MG	1H	3374	1/1	0.95	0.09	86,86,86,86	0
57	MG	1H	3482	1/1	0.95	0.08	102,102,102,102	0
57	MG	13	1740	1/1	0.95	0.05	132,132,132,132	0
57	MG	14	3055	1/1	0.95	0.19	50,50,50,50	0
57	MG	1H	3160	1/1	0.95	0.36	68,68,68,68	0
57	MG	1H	3050	1/1	0.95	0.16	54,54,54,54	0
57	MG	41	201	1/1	0.95	0.09	62,62,62,62	0
57	MG	14	3059	1/1	0.95	0.16	70,70,70,70	0
57	MG	13	1741	1/1	0.95	0.06	110,110,110,110	0
57	MG	1H	3502	1/1	0.95	0.06	90,90,90,90	0
57	MG	14	3011	1/1	0.95	0.23	51,51,51,51	0
57	MG	1H	3395	1/1	0.95	0.06	84,84,84,84	0
57	MG	14	3412	1/1	0.95	0.07	101,101,101,101	0
57	MG	13	1742	1/1	0.95	0.06	98,98,98,98	0
57	MG	1G	1688	1/1	0.95	0.07	89,89,89,89	0
57	MG	14	3121	1/1	0.95	0.14	55,55,55,55	0
57	MG	1H	3401	1/1	0.95	0.11	63,63,63,63	0
57	MG	F8	101	1/1	0.95	0.14	86,86,86,86	0
57	MG	1H	3319	1/1	0.95	0.11	56,56,56,56	0
57	MG	14	3239	1/1	0.95	0.07	59,59,59,59	0
57	MG	14	3243	1/1	0.95	0.07	82,82,82,82	0
57	MG	L8	101	1/1	0.95	0.33	86,86,86,86	0
57	MG	1G	1697	1/1	0.95	0.06	110,110,110,110	0
57	MG	14	3180	1/1	0.95	0.11	65,65,65,65	0
57	MG	13	1724	1/1	0.95	0.06	73,73,73,73	0
57	MG	1H	3517	1/1	0.95	0.16	87,87,87,87	0
57	MG	14	3183	1/1	0.95	0.30	65,65,65,65	0
57	MG	14	3432	1/1	0.95	0.10	103,103,103,103	0
57	MG	14	3129	1/1	0.95	0.51	75,75,75,75	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	1H	3040	1/1	0.95	0.15	36,36,36,36	0
57	MG	1H	3007	1/1	0.95	0.05	58,58,58,58	0
57	MG	1H	3225	1/1	0.95	0.19	74,74,74,74	0
57	MG	13	1699	1/1	0.95	0.07	102,102,102,102	0
57	MG	1H	3428	1/1	0.95	0.10	68,68,68,68	0
57	MG	1H	3030	1/1	0.95	0.27	75,75,75,75	0
57	MG	1H	3330	1/1	0.95	0.07	47,47,47,47	0
57	MG	14	3294	1/1	0.95	0.06	114,114,114,114	0
57	MG	14	3080	1/1	0.95	0.19	51,51,51,51	0
57	MG	1H	3432	1/1	0.95	0.09	56,56,56,56	0
57	MG	1H	3305	1/1	0.95	0.27	71,71,71,71	0
57	MG	14	3303	1/1	0.95	0.10	70,70,70,70	0
57	MG	1H	3533	1/1	0.95	0.08	44,44,44,44	0
57	MG	14	3308	1/1	0.95	0.09	58,58,58,58	0
57	MG	1H	3339	1/1	0.95	0.08	43,43,43,43	0
57	MG	1J	207	1/1	0.95	0.06	92,92,92,92	0
57	MG	1G	1719	1/1	0.95	0.09	119,119,119,119	0
57	MG	14	3034	1/1	0.95	0.13	48,48,48,48	0
57	MG	1G	1722	1/1	0.95	0.08	101,101,101,101	0
57	MG	14	3332	1/1	0.95	0.08	80,80,80,80	0
57	MG	13	1644	1/1	0.95	0.07	82,82,82,82	0
57	MG	1G	1724	1/1	0.95	0.07	94,94,94,94	0
57	MG	14	3349	1/1	0.95	0.06	105,105,105,105	0
57	MG	1H	3348	1/1	0.95	0.07	49,49,49,49	0
57	MG	1G	1728	1/1	0.95	0.05	114,114,114,114	0
57	MG	M5	101	1/1	0.95	0.11	86,86,86,86	0
57	MG	13	1735	1/1	0.95	0.06	111,111,111,111	0
57	MG	1H	3135	1/1	0.95	0.12	42,42,42,42	0
57	MG	14	3362	1/1	0.95	0.06	97,97,97,97	0
57	MG	1G	1655	1/1	0.95	0.13	70,70,70,70	0
57	MG	14	3367	1/1	0.95	0.06	99,99,99,99	0
60	ZN	G8	201	1/1	0.95	0.14	131,131,131,131	0
57	MG	1H	3516	1/1	0.96	0.11	79,79,79,79	0
57	MG	14	3342	1/1	0.96	0.07	82,82,82,82	0
57	MG	14	3197	1/1	0.96	0.15	78,78,78,78	0
57	MG	14	3348	1/1	0.96	0.06	101,101,101,101	0
57	MG	1H	3357	1/1	0.96	0.12	62,62,62,62	0
57	MG	1G	1606	1/1	0.96	0.07	84,84,84,84	0
57	MG	1H	3518	1/1	0.96	0.12	101,101,101,101	0
57	MG	1H	3099	1/1	0.96	0.34	84,84,84,84	0
57	MG	1H	3520	1/1	0.96	0.07	97,97,97,97	0
57	MG	1H	3178	1/1	0.96	0.14	57,57,57,57	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	1H	3369	1/1	0.96	0.15	54,54,54,54	0
57	MG	13	1744	1/1	0.96	0.10	90,90,90,90	0
57	MG	14	3368	1/1	0.96	0.07	74,74,74,74	0
57	MG	1H	3372	1/1	0.96	0.07	76,76,76,76	0
57	MG	1G	1668	1/1	0.96	0.09	95,95,95,95	0
57	MG	14	3373	1/1	0.96	0.07	97,97,97,97	0
57	MG	1G	1674	1/1	0.96	0.08	78,78,78,78	0
57	MG	4K	102	1/1	0.96	0.07	93,93,93,93	0
57	MG	1H	3443	1/1	0.96	0.06	53,53,53,53	0
57	MG	1H	3528	1/1	0.96	0.10	96,96,96,96	0
57	MG	1H	3444	1/1	0.96	0.06	73,73,73,73	0
57	MG	14	3383	1/1	0.96	0.11	92,92,92,92	0
57	MG	1G	1683	1/1	0.96	0.05	113,113,113,113	0
57	MG	1H	3530	1/1	0.96	0.10	98,98,98,98	0
57	MG	1H	3447	1/1	0.96	0.09	66,66,66,66	0
57	MG	1H	3532	1/1	0.96	0.06	103,103,103,103	0
57	MG	1H	3102	1/1	0.96	0.29	66,66,66,66	0
57	MG	14	3392	1/1	0.96	0.05	112,112,112,112	0
57	MG	1H	3041	1/1	0.96	0.13	51,51,51,51	0
57	MG	1H	3327	1/1	0.96	0.06	65,65,65,65	0
57	MG	1H	3540	1/1	0.96	0.07	81,81,81,81	0
57	MG	14	3397	1/1	0.96	0.04	109,109,109,109	0
57	MG	13	1706	1/1	0.96	0.06	103,103,103,103	0
57	MG	1H	3544	1/1	0.96	0.11	84,84,84,84	0
57	MG	1H	3142	1/1	0.96	0.09	64,64,64,64	0
57	MG	1H	3548	1/1	0.96	0.10	70,70,70,70	0
57	MG	1H	3389	1/1	0.96	0.08	68,68,68,68	0
57	MG	14	3410	1/1	0.96	0.04	116,116,116,116	0
57	MG	1H	3459	1/1	0.96	0.10	64,64,64,64	0
57	MG	1G	1703	1/1	0.96	0.06	113,113,113,113	0
57	MG	1G	1704	1/1	0.96	0.04	107,107,107,107	0
57	MG	14	3098	1/1	0.96	0.40	62,62,62,62	0
57	MG	14	3416	1/1	0.96	0.07	89,89,89,89	0
57	MG	1H	3391	1/1	0.96	0.08	50,50,50,50	0
57	MG	1G	1708	1/1	0.96	0.05	140,140,140,140	0
57	MG	14	3420	1/1	0.96	0.09	96,96,96,96	0
57	MG	1H	3468	1/1	0.96	0.08	68,68,68,68	0
57	MG	14	3102	1/1	0.96	0.14	73,73,73,73	0
57	MG	14	3238	1/1	0.96	0.07	66,66,66,66	0
57	MG	1H	3469	1/1	0.96	0.05	93,93,93,93	0
57	MG	14	3241	1/1	0.96	0.06	100,100,100,100	0
57	MG	1H	3332	1/1	0.96	0.08	50,50,50,50	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	1H	3474	1/1	0.96	0.06	82,82,82,82	0
57	MG	1H	3334	1/1	0.96	0.10	42,42,42,42	0
57	MG	14	3251	1/1	0.96	0.08	63,63,63,63	0
57	MG	16	211	1/1	0.96	0.12	99,99,99,99	0
57	MG	14	3108	1/1	0.96	0.48	77,77,77,77	0
57	MG	1H	3399	1/1	0.96	0.07	54,54,54,54	0
57	MG	1H	3481	1/1	0.96	0.06	80,80,80,80	0
57	MG	13	1700	1/1	0.96	0.06	86,86,86,86	0
57	MG	1G	1720	1/1	0.96	0.05	106,106,106,106	0
57	MG	1G	1721	1/1	0.96	0.06	107,107,107,107	0
57	MG	14	3439	1/1	0.96	0.07	99,99,99,99	0
57	MG	14	3440	1/1	0.96	0.07	98,98,98,98	0
57	MG	13	1734	1/1	0.96	0.04	100,100,100,100	0
57	MG	1H	3409	1/1	0.96	0.06	55,55,55,55	0
57	MG	14	3283	1/1	0.96	0.08	71,71,71,71	0
57	MG	1H	3488	1/1	0.96	0.07	88,88,88,88	0
57	MG	14	3287	1/1	0.96	0.06	73,73,73,73	0
57	MG	14	3288	1/1	0.96	0.07	77,77,77,77	0
57	MG	1H	3493	1/1	0.96	0.06	102,102,102,102	0
57	MG	1G	1726	1/1	0.96	0.05	113,113,113,113	0
57	MG	1H	3496	1/1	0.96	0.08	98,98,98,98	0
57	MG	1H	3410	1/1	0.96	0.06	106,106,106,106	0
57	MG	1G	1731	1/1	0.96	0.06	114,114,114,114	0
57	MG	1H	3343	1/1	0.96	0.06	44,44,44,44	0
57	MG	14	3299	1/1	0.96	0.09	58,58,58,58	0
57	MG	1H	3417	1/1	0.96	0.05	74,74,74,74	0
57	MG	14	3305	1/1	0.96	0.07	78,78,78,78	0
57	MG	14	3306	1/1	0.96	0.08	86,86,86,86	0
57	MG	13	1691	1/1	0.96	0.07	65,65,65,65	0
57	MG	25	202	1/1	0.96	0.07	110,110,110,110	0
57	MG	1H	3075	1/1	0.96	0.11	61,61,61,61	0
57	MG	13	1705	1/1	0.96	0.16	83,83,83,83	0
57	MG	14	3316	1/1	0.96	0.06	90,90,90,90	0
57	MG	14	3317	1/1	0.96	0.07	64,64,64,64	0
57	MG	E5	101	1/1	0.96	0.07	100,100,100,100	0
57	MG	14	3319	1/1	0.96	0.06	78,78,78,78	0
57	MG	14	3322	1/1	0.96	0.07	64,64,64,64	0
57	MG	1H	3512	1/1	0.96	0.09	97,97,97,97	0
57	MG	1H	3013	1/1	0.96	0.20	37,37,37,37	0
57	MG	1H	3426	1/1	0.96	0.09	76,76,76,76	0
57	MG	4L	102	1/1	0.96	0.15	108,108,108,108	0
57	MG	14	3334	1/1	0.96	0.07	94,94,94,94	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	14	3347	1/1	0.97	0.04	101,101,101,101	0
57	MG	1H	3503	1/1	0.97	0.10	47,47,47,47	0
57	MG	1H	3326	1/1	0.97	0.06	47,47,47,47	0
57	MG	1H	3430	1/1	0.97	0.06	61,61,61,61	0
57	MG	1G	1601	1/1	0.97	0.10	70,70,70,70	0
57	MG	13	1693	1/1	0.97	0.05	84,84,84,84	0
57	MG	14	3001	1/1	0.97	0.07	52,52,52,52	0
57	MG	14	3356	1/1	0.97	0.06	67,67,67,67	0
57	MG	14	3357	1/1	0.97	0.05	96,96,96,96	0
57	MG	14	3358	1/1	0.97	0.05	88,88,88,88	0
57	MG	1H	3510	1/1	0.97	0.05	70,70,70,70	0
57	MG	1H	3329	1/1	0.97	0.07	50,50,50,50	0
57	MG	14	3366	1/1	0.97	0.12	98,98,98,98	0
57	MG	1H	3433	1/1	0.97	0.09	61,61,61,61	0
57	MG	1G	1663	1/1	0.97	0.12	76,76,76,76	0
57	MG	13	1716	1/1	0.97	0.05	55,55,55,55	0
57	MG	13	1719	1/1	0.97	0.05	71,71,71,71	0
57	MG	14	3371	1/1	0.97	0.07	90,90,90,90	0
57	MG	14	3372	1/1	0.97	0.11	79,79,79,79	0
57	MG	1H	3439	1/1	0.97	0.05	95,95,95,95	0
57	MG	1G	1670	1/1	0.97	0.13	88,88,88,88	0
57	MG	14	3375	1/1	0.97	0.04	84,84,84,84	0
57	MG	1G	1672	1/1	0.97	0.09	92,92,92,92	0
57	MG	1H	3039	1/1	0.97	0.14	40,40,40,40	0
57	MG	1H	3441	1/1	0.97	0.06	44,44,44,44	0
57	MG	1G	1676	1/1	0.97	0.05	100,100,100,100	0
57	MG	14	3382	1/1	0.97	0.06	72,72,72,72	0
57	MG	1H	3442	1/1	0.97	0.12	69,69,69,69	0
57	MG	1H	3054	1/1	0.97	0.17	37,37,37,37	0
57	MG	1H	3336	1/1	0.97	0.06	50,50,50,50	0
57	MG	1H	3445	1/1	0.97	0.06	44,44,44,44	0
57	MG	14	3389	1/1	0.97	0.14	94,94,94,94	0
57	MG	14	3088	1/1	0.97	0.07	53,53,53,53	0
57	MG	1H	3338	1/1	0.97	0.08	63,63,63,63	0
57	MG	1H	3525	1/1	0.97	0.12	134,134,134,134	0
57	MG	14	3235	1/1	0.97	0.09	65,65,65,65	0
57	MG	1H	3215	1/1	0.97	0.33	69,69,69,69	0
57	MG	1H	3390	1/1	0.97	0.07	68,68,68,68	0
57	MG	1H	3177	1/1	0.97	0.45	77,77,77,77	0
57	MG	14	3398	1/1	0.97	0.07	99,99,99,99	0
57	MG	14	3400	1/1	0.97	0.06	76,76,76,76	0
57	MG	1H	3392	1/1	0.97	0.10	52,52,52,52	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	1G	1692	1/1	0.97	0.06	105,105,105,105	0
57	MG	14	3403	1/1	0.97	0.09	83,83,83,83	0
57	MG	1G	1694	1/1	0.97	0.07	94,94,94,94	0
57	MG	1H	3063	1/1	0.97	0.13	53,53,53,53	0
57	MG	14	3407	1/1	0.97	0.05	83,83,83,83	0
57	MG	14	3408	1/1	0.97	0.04	111,111,111,111	0
57	MG	14	3248	1/1	0.97	0.05	57,57,57,57	0
57	MG	1H	3455	1/1	0.97	0.05	42,42,42,42	0
57	MG	1H	3344	1/1	0.97	0.04	46,46,46,46	0
57	MG	13	1621	1/1	0.97	0.10	56,56,56,56	0
57	MG	14	3257	1/1	0.97	0.06	69,69,69,69	0
57	MG	1G	1699	1/1	0.97	0.07	93,93,93,93	0
57	MG	14	3262	1/1	0.97	0.07	66,66,66,66	0
57	MG	14	3417	1/1	0.97	0.08	89,89,89,89	0
57	MG	1H	3462	1/1	0.97	0.06	53,53,53,53	0
57	MG	14	3272	1/1	0.97	0.06	78,78,78,78	0
57	MG	14	3273	1/1	0.97	0.10	70,70,70,70	0
57	MG	2K	104	1/1	0.97	0.10	89,89,89,89	0
57	MG	14	3275	1/1	0.97	0.06	74,74,74,74	0
57	MG	1H	3539	1/1	0.97	0.07	45,45,45,45	0
57	MG	1H	3465	1/1	0.97	0.07	63,63,63,63	0
57	MG	14	3425	1/1	0.97	0.11	91,91,91,91	0
57	MG	1H	3467	1/1	0.97	0.05	85,85,85,85	0
57	MG	14	3036	1/1	0.97	0.14	47,47,47,47	0
57	MG	13	1729	1/1	0.97	0.10	73,73,73,73	0
57	MG	1H	3404	1/1	0.97	0.05	65,65,65,65	0
57	MG	1H	3471	1/1	0.97	0.06	73,73,73,73	0
57	MG	1H	3472	1/1	0.97	0.14	62,62,62,62	0
57	MG	14	3289	1/1	0.97	0.05	90,90,90,90	0
57	MG	1H	3405	1/1	0.97	0.06	46,46,46,46	0
57	MG	14	3292	1/1	0.97	0.05	85,85,85,85	0
57	MG	1H	3277	1/1	0.97	0.30	82,82,82,82	0
57	MG	1H	3477	1/1	0.97	0.05	83,83,83,83	0
57	MG	1H	3353	1/1	0.97	0.11	64,64,64,64	0
57	MG	1H	3414	1/1	0.97	0.06	95,95,95,95	0
57	MG	14	3297	1/1	0.97	0.08	66,66,66,66	0
57	MG	1G	1716	1/1	0.97	0.05	92,92,92,92	0
57	MG	1H	3354	1/1	0.97	0.07	73,73,73,73	0
57	MG	14	3301	1/1	0.97	0.07	117,117,117,117	0
57	MG	14	3302	1/1	0.97	0.12	86,86,86,86	0
57	MG	1G	1718	1/1	0.97	0.07	91,91,91,91	0
57	MG	1H	3356	1/1	0.97	0.05	75,75,75,75	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	1H	3136	1/1	0.97	0.11	45,45,45,45	0
57	MG	1H	3420	1/1	0.97	0.06	102,102,102,102	0
57	MG	1H	3487	1/1	0.97	0.08	72,72,72,72	0
57	MG	14	3310	1/1	0.97	0.06	64,64,64,64	0
57	MG	14	3312	1/1	0.97	0.05	80,80,80,80	0
57	MG	1H	3360	1/1	0.97	0.10	76,76,76,76	0
57	MG	1H	3489	1/1	0.97	0.06	69,69,69,69	0
57	MG	1H	3491	1/1	0.97	0.14	62,62,62,62	0
57	MG	1H	3195	1/1	0.97	0.07	59,59,59,59	0
57	MG	14	3320	1/1	0.97	0.05	46,46,46,46	0
57	MG	1H	3495	1/1	0.97	0.05	94,94,94,94	0
57	MG	14	3323	1/1	0.97	0.05	83,83,83,83	0
57	MG	78	201	1/1	0.97	0.10	57,57,57,57	0
57	MG	1G	1730	1/1	0.97	0.08	94,94,94,94	0
57	MG	14	3330	1/1	0.97	0.06	64,64,64,64	0
57	MG	1H	3076	1/1	0.97	0.09	39,39,39,39	0
57	MG	1G	1734	1/1	0.97	0.10	84,84,84,84	0
57	MG	1H	3366	1/1	0.97	0.07	63,63,63,63	0
57	MG	1H	3427	1/1	0.97	0.05	66,66,66,66	0
57	MG	14	3337	1/1	0.97	0.05	57,57,57,57	0
57	MG	14	3338	1/1	0.97	0.07	81,81,81,81	0
57	MG	1H	3501	1/1	0.97	0.07	75,75,75,75	0
57	MG	14	3343	1/1	0.97	0.05	87,87,87,87	0
57	MG	1H	3368	1/1	0.97	0.08	59,59,59,59	0
57	MG	14	3379	1/1	0.98	0.07	99,99,99,99	0
57	MG	1H	3463	1/1	0.98	0.06	48,48,48,48	0
57	MG	1H	3396	1/1	0.98	0.05	64,64,64,64	0
57	MG	13	1718	1/1	0.98	0.04	88,88,88,88	0
57	MG	14	3285	1/1	0.98	0.09	79,79,79,79	0
57	MG	14	3384	1/1	0.98	0.05	88,88,88,88	0
57	MG	14	3385	1/1	0.98	0.08	80,80,80,80	0
57	MG	14	3286	1/1	0.98	0.04	93,93,93,93	0
57	MG	13	1697	1/1	0.98	0.05	78,78,78,78	0
57	MG	1G	1682	1/1	0.98	0.05	105,105,105,105	0
57	MG	1H	3400	1/1	0.98	0.04	59,59,59,59	0
57	MG	14	3290	1/1	0.98	0.06	66,66,66,66	0
57	MG	13	1720	1/1	0.98	0.04	100,100,100,100	0
57	MG	1H	3371	1/1	0.98	0.05	56,56,56,56	0
57	MG	13	1722	1/1	0.98	0.04	77,77,77,77	0
57	MG	1G	1687	1/1	0.98	0.04	95,95,95,95	0
57	MG	1H	3435	1/1	0.98	0.04	60,60,60,60	0
57	MG	1H	3333	1/1	0.98	0.10	67,67,67,67	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	1G	1690	1/1	0.98	0.05	114,114,114,114	0
57	MG	14	3399	1/1	0.98	0.12	95,95,95,95	0
57	MG	1H	3476	1/1	0.98	0.05	68,68,68,68	0
57	MG	1H	3437	1/1	0.98	0.07	46,46,46,46	0
57	MG	14	3300	1/1	0.98	0.10	73,73,73,73	0
57	MG	1G	1693	1/1	0.98	0.06	84,84,84,84	0
57	MG	1H	3478	1/1	0.98	0.08	78,78,78,78	0
57	MG	1H	3438	1/1	0.98	0.05	50,50,50,50	0
57	MG	14	3406	1/1	0.98	0.05	90,90,90,90	0
57	MG	14	3304	1/1	0.98	0.05	68,68,68,68	0
57	MG	1H	3407	1/1	0.98	0.07	77,77,77,77	0
57	MG	1H	3408	1/1	0.98	0.05	69,69,69,69	0
57	MG	13	1738	1/1	0.98	0.05	70,70,70,70	0
57	MG	1H	3143	1/1	0.98	0.08	66,66,66,66	0
57	MG	1H	3411	1/1	0.98	0.06	80,80,80,80	0
57	MG	14	3311	1/1	0.98	0.05	68,68,68,68	0
57	MG	14	3414	1/1	0.98	0.12	100,100,100,100	0
57	MG	1H	3486	1/1	0.98	0.06	89,89,89,89	0
57	MG	1H	3378	1/1	0.98	0.05	65,65,65,65	0
57	MG	14	3314	1/1	0.98	0.08	83,83,83,83	0
57	MG	1H	3534	1/1	0.98	0.08	92,92,92,92	0
57	MG	13	1739	1/1	0.98	0.03	92,92,92,92	0
57	MG	1G	1705	1/1	0.98	0.05	124,124,124,124	0
57	MG	1H	3536	1/1	0.98	0.05	60,60,60,60	0
57	MG	1H	3446	1/1	0.98	0.06	60,60,60,60	0
57	MG	14	3234	1/1	0.98	0.06	56,56,56,56	0
57	MG	1H	3416	1/1	0.98	0.04	89,89,89,89	0
57	MG	14	3325	1/1	0.98	0.10	52,52,52,52	0
57	MG	1H	3492	1/1	0.98	0.04	83,83,83,83	0
57	MG	14	3328	1/1	0.98	0.09	56,56,56,56	0
57	MG	1H	3541	1/1	0.98	0.05	67,67,67,67	0
57	MG	1H	3358	1/1	0.98	0.05	40,40,40,40	0
57	MG	14	3240	1/1	0.98	0.04	62,62,62,62	0
57	MG	1H	3543	1/1	0.98	0.07	70,70,70,70	0
57	MG	1H	3386	1/1	0.98	0.04	48,48,48,48	0
57	MG	1H	3545	1/1	0.98	0.03	116,116,116,116	0
57	MG	13	1708	1/1	0.98	0.07	95,95,95,95	0
57	MG	14	3339	1/1	0.98	0.04	49,49,49,49	0
57	MG	14	3341	1/1	0.98	0.05	91,91,91,91	0
57	MG	14	3247	1/1	0.98	0.07	60,60,60,60	0
57	MG	1H	3362	1/1	0.98	0.05	56,56,56,56	0
57	MG	14	3344	1/1	0.98	0.07	88,88,88,88	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	14	3250	1/1	0.98	0.05	76,76,76,76	0
57	MG	1H	3363	1/1	0.98	0.05	47,47,47,47	0
57	MG	14	3252	1/1	0.98	0.07	62,62,62,62	0
57	MG	1H	3453	1/1	0.98	0.10	58,58,58,58	0
57	MG	14	3255	1/1	0.98	0.06	52,52,52,52	0
57	MG	1H	3424	1/1	0.98	0.04	100,100,100,100	0
57	MG	1H	3456	1/1	0.98	0.05	41,41,41,41	0
57	MG	14	3260	1/1	0.98	0.05	55,55,55,55	0
57	MG	1G	1667	1/1	0.98	0.09	90,90,90,90	0
57	MG	13	1694	1/1	0.98	0.04	94,94,94,94	0
57	MG	14	3263	1/1	0.98	0.04	56,56,56,56	0
57	MG	14	3359	1/1	0.98	0.04	86,86,86,86	0
57	MG	14	3360	1/1	0.98	0.07	94,94,94,94	0
57	MG	14	3264	1/1	0.98	0.06	52,52,52,52	0
57	MG	29	302	1/1	0.98	0.04	52,52,52,52	0
57	MG	14	3363	1/1	0.98	0.05	102,102,102,102	0
57	MG	14	3364	1/1	0.98	0.08	85,85,85,85	0
57	MG	14	3265	1/1	0.98	0.06	52,52,52,52	0
57	MG	14	3267	1/1	0.98	0.04	86,86,86,86	0
57	MG	1G	1669	1/1	0.98	0.08	99,99,99,99	0
57	MG	14	3271	1/1	0.98	0.07	72,72,72,72	0
57	MG	13	1717	1/1	0.98	0.06	53,53,53,53	0
57	MG	1G	1671	1/1	0.98	0.06	86,86,86,86	0
57	MG	1G	1727	1/1	0.98	0.04	93,93,93,93	0
57	MG	1H	3461	1/1	0.98	0.05	48,48,48,48	0
57	MG	14	3276	1/1	0.98	0.05	95,95,95,95	0
57	MG	14	3277	1/1	0.98	0.06	59,59,59,59	0
57	MG	1G	1673	1/1	0.98	0.06	71,71,71,71	0
57	MG	1H	3328	1/1	0.98	0.06	46,46,46,46	0
57	MG	14	3377	1/1	0.98	0.05	64,64,64,64	0
57	MG	1H	3511	1/1	0.98	0.04	92,92,92,92	0
57	MG	I8	101	1/1	0.99	0.06	69,69,69,69	0
57	MG	14	3242	1/1	0.99	0.05	44,44,44,44	0
57	MG	1H	3341	1/1	0.99	0.07	48,48,48,48	0
57	MG	1H	3342	1/1	0.99	0.04	42,42,42,42	0
57	MG	14	3245	1/1	0.99	0.06	56,56,56,56	0
57	MG	14	3395	1/1	0.99	0.05	91,91,91,91	0
57	MG	14	3315	1/1	0.99	0.09	86,86,86,86	0
57	MG	1H	3381	1/1	0.99	0.05	48,48,48,48	0
57	MG	1H	3382	1/1	0.99	0.09	54,54,54,54	0
57	MG	14	3318	1/1	0.99	0.04	75,75,75,75	0
57	MG	1G	1706	1/1	0.99	0.04	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	14	3249	1/1	0.99	0.06	60,60,60,60	0
57	MG	14	3321	1/1	0.99	0.05	64,64,64,64	0
57	MG	1H	3413	1/1	0.99	0.04	59,59,59,59	0
57	MG	1H	3384	1/1	0.99	0.02	61,61,61,61	0
57	MG	1H	3385	1/1	0.99	0.04	77,77,77,77	0
57	MG	14	3253	1/1	0.99	0.09	53,53,53,53	0
57	MG	14	3326	1/1	0.99	0.04	60,60,60,60	0
57	MG	13	1701	1/1	0.99	0.08	69,69,69,69	0
57	MG	1H	3485	1/1	0.99	0.03	83,83,83,83	0
57	MG	14	3329	1/1	0.99	0.03	60,60,60,60	0
57	MG	1H	3387	1/1	0.99	0.04	53,53,53,53	0
57	MG	13	1698	1/1	0.99	0.03	94,94,94,94	0
57	MG	14	3258	1/1	0.99	0.03	71,71,71,71	0
57	MG	14	3333	1/1	0.99	0.05	66,66,66,66	0
57	MG	14	3259	1/1	0.99	0.05	63,63,63,63	0
57	MG	1H	3419	1/1	0.99	0.04	78,78,78,78	0
57	MG	14	3336	1/1	0.99	0.09	65,65,65,65	0
57	MG	1H	3346	1/1	0.99	0.05	53,53,53,53	0
57	MG	1H	3490	1/1	0.99	0.03	65,65,65,65	0
57	MG	1H	3347	1/1	0.99	0.07	56,56,56,56	0
57	MG	14	3340	1/1	0.99	0.06	69,69,69,69	0
57	MG	1H	3538	1/1	0.99	0.11	58,58,58,58	0
57	MG	1H	3367	1/1	0.99	0.05	56,56,56,56	0
57	MG	14	3266	1/1	0.99	0.04	72,72,72,72	0
57	MG	1G	1665	1/1	0.99	0.10	78,78,78,78	0
57	MG	14	3345	1/1	0.99	0.07	83,83,83,83	0
57	MG	1H	3454	1/1	0.99	0.02	48,48,48,48	0
57	MG	14	3269	1/1	0.99	0.03	63,63,63,63	0
57	MG	1H	3494	1/1	0.99	0.05	98,98,98,98	0
57	MG	1H	3423	1/1	0.99	0.04	66,66,66,66	0
57	MG	14	3350	1/1	0.99	0.04	61,61,61,61	0
57	MG	13	1709	1/1	0.99	0.06	69,69,69,69	0
57	MG	14	3433	1/1	0.99	0.04	69,69,69,69	0
57	MG	1H	3497	1/1	0.99	0.03	79,79,79,79	0
57	MG	1H	3457	1/1	0.99	0.03	45,45,45,45	0
57	MG	14	3354	1/1	0.99	0.04	73,73,73,73	0
57	MG	1H	3546	1/1	0.99	0.03	41,41,41,41	0
57	MG	1H	3393	1/1	0.99	0.03	69,69,69,69	0
57	MG	14	3278	1/1	0.99	0.05	80,80,80,80	0
57	MG	1H	3394	1/1	0.99	0.05	74,74,74,74	0
57	MG	1H	3460	1/1	0.99	0.03	48,48,48,48	0
57	MG	13	1704	1/1	0.99	0.05	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	14	3361	1/1	0.99	0.04	80,80,80,80	0
57	MG	1G	1732	1/1	0.99	0.04	114,114,114,114	0
57	MG	1G	1677	1/1	0.99	0.07	97,97,97,97	0
57	MG	13	1696	1/1	0.99	0.07	83,83,83,83	0
57	MG	1G	1679	1/1	0.99	0.05	93,93,93,93	0
57	MG	1H	3505	1/1	0.99	0.04	79,79,79,79	0
57	MG	1H	3506	1/1	0.99	0.06	61,61,61,61	0
57	MG	1H	3507	1/1	0.99	0.05	74,74,74,74	0
57	MG	13	1712	1/1	0.99	0.08	101,101,101,101	0
57	MG	1H	3398	1/1	0.99	0.06	61,61,61,61	0
57	MG	16	209	1/1	0.99	0.06	68,68,68,68	0
57	MG	16	210	1/1	0.99	0.04	78,78,78,78	0
57	MG	13	1713	1/1	0.99	0.04	65,65,65,65	0
57	MG	1H	3466	1/1	0.99	0.03	89,89,89,89	0
57	MG	1H	3337	1/1	0.99	0.07	44,44,44,44	0
57	MG	21	302	1/1	0.99	0.03	46,46,46,46	0
57	MG	13	1714	1/1	0.99	0.06	100,100,100,100	0
57	MG	1H	3514	1/1	0.99	0.07	76,76,76,76	0
57	MG	1H	3375	1/1	0.99	0.07	48,48,48,48	0
57	MG	45	201	1/1	0.99	0.14	74,74,74,74	0
57	MG	1H	3470	1/1	0.99	0.07	73,73,73,73	0
57	MG	14	3233	1/1	0.99	0.10	54,54,54,54	0
57	MG	1H	3403	1/1	0.99	0.04	50,50,50,50	0
57	MG	1H	3376	1/1	0.99	0.04	45,45,45,45	0
57	MG	13	1725	1/1	0.99	0.06	90,90,90,90	0
57	MG	14	3237	1/1	0.99	0.06	56,56,56,56	0
57	MG	1H	3406	1/1	0.99	0.04	46,46,46,46	0
57	MG	1H	3475	1/1	0.99	0.04	83,83,83,83	0
57	MG	13	1692	1/1	0.99	0.05	61,61,61,61	0
59	SF4	3E	301	8/8	0.99	0.03	86,90,100,103	0
59	SF4	32	301	8/8	0.99	0.04	90,99,108,116	0
60	ZN	5I	102	1/1	0.99	0.03	98,98,98,98	0
57	MG	14	3309	1/1	0.99	0.05	71,71,71,71	0
60	ZN	5A	101	1/1	0.99	0.04	123,123,123,123	0
60	ZN	C5	202	1/1	0.99	0.06	151,151,151,151	0
57	MG	14	3270	1/1	1.00	0.03	65,65,65,65	0
57	MG	1H	3412	1/1	1.00	0.03	51,51,51,51	0
57	MG	1H	3335	1/1	1.00	0.03	53,53,53,53	0
57	MG	1H	3361	1/1	1.00	0.02	74,74,74,74	0
57	MG	11	302	1/1	1.00	0.05	47,47,47,47	0
57	MG	1H	3345	1/1	1.00	0.04	51,51,51,51	0
57	MG	1H	3355	1/1	1.00	0.05	67,67,67,67	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	13	1721	1/1	1.00	0.07	62,62,62,62	0
57	MG	1H	3351	1/1	1.00	0.04	59,59,59,59	0
57	MG	1H	3499	1/1	1.00	0.02	52,52,52,52	0
57	MG	13	1703	1/1	1.00	0.07	66,66,66,66	0
57	MG	1H	3383	1/1	1.00	0.02	53,53,53,53	0
57	MG	1H	3359	1/1	1.00	0.04	60,60,60,60	0

5.5 Other polymers [i](#)

There are no such residues in this entry.