



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 23, 2026 – 08:41 PM UTC

PDB ID : 5E7K / pdb_00005e7k
Title : Structure of T. thermophilus 70S ribosome complex with mRNA and cognate tRNA^{Lys} in the A-site
Authors : Rozov, A.; Demeshkina, N.; Khusainov, I.; Yusupov, M.; Yusupova, G.
Deposited on : 2015-10-12
Resolution : 3.20 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	FAILED
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

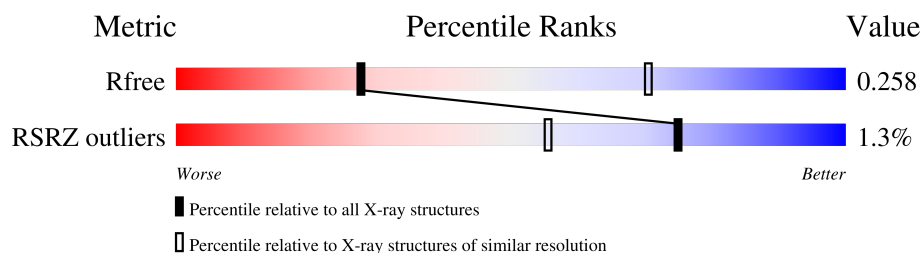
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.20 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	1466 (3.20-3.20)
RSRZ outliers	180081	1466 (3.20-3.20)

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
58	MG	14	3089	-	-	-	X
58	MG	1G	1603	-	-	-	X
58	MG	1G	1644	-	-	-	X

2 Entry composition

There are 61 unique types of molecules in this entry. The entry contains 294444 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 rRNA.

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	1507	Total	C	N	O	P	0	0	0
			32391	14418	6004	10463	1506			

There are 6 discrepancies between the modelled and reference sequences:

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	1E	231	Total	C	N	O	S	0	0	0
			1874	1199	334	336	5			
2	12	210	Total	C	N	O	S	0	0	0
			1721	1100	309	308	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	196	Total	C	N	O	S	0	0	0
			1541	975	298	267	1			

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	4E	149	Total	C	N	O	S	0	0	0
			1142	722	216	200	4			
5	42	148	Total	C	N	O	S	0	0	0
			1134	718	215	197	4			

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	1I	91	Total	C	N	O	S	0	0	0
			734	459	144	130	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	88	Total	C	N	O	S	0	0	0
			733	459	147	125	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	81	Total	C	N	O	S	0	0	0
			654	417	122	113	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			
20	BA	99	Total	C	N	O	S	0	0	0
			762	470	162	128	2			

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	1K	71	Total	C	N	O	P S	0	0	0
			1520	681	264	503	71 1			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
1K	?	-	G	deletion	GB 836716955

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	2K	77	Total	C	N	O	P S	0	0	0
			1646	735	297	536	77 1			
23	2L	77	Total	C	N	O	P S	0	0	0
			1646	735	297	536	77 1			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
24	3K	76	Total	C	N	O P	0	0	0
			1611	721	281	534 75			

- Molecule 25 is a RNA chain called mRNA.

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

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
25	4L	18	Total	C	N	O	P	0	0	0
			397	178	84	117	18			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	1H	2833	Total	C	N	O	P	0	0	0
			61028	27159	11418	19618	2833			
26	14	2861	Total	C	N	O	P	0	0	0
			61630	27429	11535	19806	2860			

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 rRNA.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
28	71	133	Total	C	N	O	S	0	0	0
			1033	651	194	187	1			

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
28	79	57	Total	C	N	O	0	0	0
			456	283	91	82			

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
30	21	203	Total	C	N	O	S	0	0	0
			1558	985	298	269	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	179	Total	C	N	O	S	0	0	0
			1458	931	266	257	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
33	51	171	Total	C	N	O	S	0	0	0
			1312	832	246	233	1			
33	59	73	Total	C	N	O		0	0	0
			568	356	116	96				

- 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			
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	138	Total	C	N	O	S	0	0	0
			1104	712	206	182	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
			1113	709	210	187	7			
38	45	138	Total	C	N	O	S	0	0	0
			1099	702	208	183	6			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
39	98	118	Total	C	N	O	S	0	0	0
			967	604	203	159	1			
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	S	0	0	0
			881	556	176	149				
40	65	110	Total	C	N	O	S	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	133	Total	C	N	O	S	0	0	0
			1109	691	228	189	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
			774	499	141	133	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
44	E8	112	Total	C	N	O	S	0	0	0
			890	560	175	153	2			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
44	A5	113	Total	C	N	O	S	0	0	0
			899	566	177	154	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		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	105	Total	C	N	O	S	0	0	0
			796	513	150	128	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	171	Total	C	N	O	S	0	0	0
			1373	876	247	247	3			
47	D5	132	Total	C	N	O	S	0	0	0
			1074	691	193	188	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
48	I8	76	Total	C	N	O	S	0	0	0
			606	376	128	101	1			
48	E5	77	Total	C	N	O	S	0	0	0
			608	375	129	103	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
			568	352	115	100	1			
50	G5	66	Total	C	N	O	S	0	0	0
			558	346	113	98	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	47	Total	C	N	O	S	0	0	0
			366	234	61	66	5			

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

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

- Molecule 54 is a protein called 50S ribosomal protein 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			

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

- Molecule 56 is a RNA chain called tRNA^{Lys}.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
56	1L	73	Total	C	N	O	P	S	0	0
			1563	700	271	518	73	1		

- Molecule 57 is a RNA chain called tRNA^{Lys}.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
57	3L	76	Total	C	N	O	P		0	0
			1612	722	281	534	75			

- Molecule 58 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

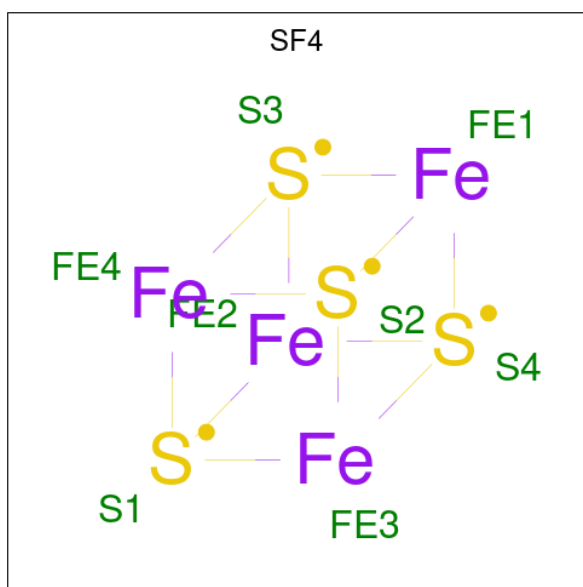
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
58	13	132	Total	Mg	0	0
			132	132		
58	1E	1	Total	Mg	0	0
			1	1		
58	5E	1	Total	Mg	0	0
			1	1		
58	1K	1	Total	Mg	0	0
			1	1		
58	2K	3	Total	Mg	0	0
			3	3		
58	3K	1	Total	Mg	0	0
			1	1		
58	1H	467	Total	Mg	0	0
			467	467		
58	16	9	Total	Mg	0	0
			9	9		
58	21	2	Total	Mg	0	0
			2	2		
58	41	1	Total	Mg	0	0
			1	1		
58	78	1	Total	Mg	0	0
			1	1		
58	88	1	Total	Mg	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
58	98	1	Total 1	Mg 1	0	0
58	I8	3	Total 3	Mg 3	0	0
58	J8	1	Total 1	Mg 1	0	0
58	L8	1	Total 1	Mg 1	0	0
58	P8	1	Total 1	Mg 1	0	0
58	Q8	1	Total 1	Mg 1	0	0
58	1G	90	Total 90	Mg 90	0	0
58	6A	1	Total 1	Mg 1	0	0
58	2L	2	Total 2	Mg 2	0	0
58	14	399	Total 399	Mg 399	0	0
58	1J	5	Total 5	Mg 5	0	0
58	29	4	Total 4	Mg 4	0	0
58	39	1	Total 1	Mg 1	0	0
58	25	1	Total 1	Mg 1	0	0
58	35	3	Total 3	Mg 3	0	0
58	45	2	Total 2	Mg 2	0	0
58	55	1	Total 1	Mg 1	0	0
58	E5	1	Total 1	Mg 1	0	0

- Molecule 59 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe₄S₄).



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	126	Total	O	0	0
			126	126		
61	3I	2	Total	O	0	0
			2	2		
61	5I	2	Total	O	0	0
			2	2		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
61	1K	8	Total 8	O 8	0	0
61	3K	1	Total 1	O 1	0	0
61	4K	2	Total 2	O 2	0	0
61	1H	629	Total 629	O 629	0	0
61	16	29	Total 29	O 29	0	0
61	11	7	Total 7	O 7	0	0
61	21	4	Total 4	O 4	0	0
61	31	9	Total 9	O 9	0	0
61	58	2	Total 2	O 2	0	0
61	78	7	Total 7	O 7	0	0
61	88	1	Total 1	O 1	0	0
61	B8	1	Total 1	O 1	0	0
61	E8	2	Total 2	O 2	0	0
61	F8	1	Total 1	O 1	0	0
61	G8	1	Total 1	O 1	0	0
61	I8	3	Total 3	O 3	0	0
61	L8	2	Total 2	O 2	0	0
61	1G	78	Total 78	O 78	0	0
61	32	1	Total 1	O 1	0	0
61	5A	2	Total 2	O 2	0	0
61	14	417	Total 417	O 417	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
61	1J	6	Total	O	0	0
			6	6		
61	19	8	Total	O	0	0
			8	8		
61	29	2	Total	O	0	0
			2	2		
61	39	5	Total	O	0	0
			5	5		
61	35	1	Total	O	0	0
			1	1		
61	55	1	Total	O	0	0
			1	1		
61	A5	1	Total	O	0	0
			1	1		
61	H5	2	Total	O	0	0
			2	2		

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 450.10Å 621.60Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	173.72 – 3.20 173.72 – 3.20	Depositor EDS
% Data completeness (in resolution range)	100.0 (173.72-3.20) 93.8 (173.72-3.20)	Depositor EDS
R_{merge}	0.38	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.81 (at 3.19Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.191 , 0.258 0.195 , 0.258	Depositor DCC
R_{free} test set	2000 reflections (0.21%)	wwPDB-VP
Wilson B-factor (Å ²)	92.5	Xtriage
Anisotropy	0.339	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.26 , 42.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	294444	wwPDB-VP
Average B, all atoms (Å ²)	107.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.48% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

4 Model quality [i](#)

4.1 Standard geometry [i](#)

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

4.2 Too-close contacts [i](#)

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

4.3 Torsion angles [i](#)

4.3.1 Protein backbone [i](#)

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

4.3.2 Protein sidechains [i](#)

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

4.3.3 RNA [i](#)

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

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

23 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	$\# Z > 2$
57	PSU	3L	39	57	18,21,22	1.28	1 (5%)	21,30,33	1.57	4 (19%)
23	5MU	2L	55	23	19,22,23	3.85	5 (26%)	27,32,35	3.41	8 (29%)
22	T6A	1K	37	22	31,34,35	2.00	10 (32%)	43,49,52	2.04	10 (23%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
56	T6A	1L	37	56	31,34,35	2.00	7 (22%)	43,49,52	2.28	15 (34%)
23	G7M	2L	47	23	23,26,27	4.71	7 (30%)	34,39,42	3.29	13 (38%)
23	PSU	2K	56	23	18,21,22	1.24	2 (11%)	21,30,33	2.06	5 (23%)
22	U8U	1K	34	22,25	20,24,25	2.28	5 (25%)	22,34,37	0.83	1 (4%)
23	OMC	2K	33	23	19,22,23	1.70	4 (21%)	25,31,34	0.96	2 (8%)
56	5MU	1L	54	56	19,22,23	3.90	5 (26%)	27,32,35	3.28	8 (29%)
56	PSU	1L	39	56	18,21,22	1.19	1 (5%)	21,30,33	1.69	4 (19%)
23	G7M	2K	47	23	23,26,27	4.62	8 (34%)	34,39,42	3.38	13 (38%)
22	5MU	1K	54	22	19,22,23	3.75	5 (26%)	27,32,35	3.14	6 (22%)
57	5MU	3L	54	57	19,22,23	4.12	6 (31%)	27,32,35	2.97	11 (40%)
22	PSU	1K	55	22	18,21,22	1.12	1 (5%)	21,30,33	1.68	4 (19%)
23	PSU	2L	56	23	18,21,22	1.32	1 (5%)	21,30,33	1.87	4 (19%)
22	PSU	1K	39	22	18,21,22	1.08	2 (11%)	21,30,33	1.75	4 (19%)
23	5MU	2K	55	23	19,22,23	3.85	5 (26%)	27,32,35	3.54	9 (33%)
23	4SU	2L	8	23	18,21,22	1.85	3 (16%)	25,30,33	2.74	4 (16%)
57	PSU	3L	55	57	18,21,22	1.26	1 (5%)	21,30,33	1.86	5 (23%)
56	U8U	1L	34	25,56	20,24,25	2.52	7 (35%)	22,34,37	0.84	1 (4%)
56	PSU	1L	55	56	18,21,22	1.13	1 (5%)	21,30,33	1.72	4 (19%)
23	OMC	2L	33	23	19,22,23	1.70	3 (15%)	25,31,34	1.06	2 (8%)
23	4SU	2K	8	23	18,21,22	1.91	4 (22%)	25,30,33	2.39	5 (20%)

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
57	PSU	3L	39	57	-	2/7/25/26	0/2/2/2
23	5MU	2L	55	23	-	0/7/25/26	0/2/2/2
22	T6A	1K	37	22	-	4/23/41/42	0/3/3/3
56	T6A	1L	37	56	-	4/23/41/42	0/3/3/3
23	G7M	2L	47	23	-	2/7/25/26	0/3/3/3
23	PSU	2K	56	23	-	2/7/25/26	0/2/2/2
22	U8U	1K	34	22,25	-	3/10/28/29	0/2/2/2
23	OMC	2K	33	23	-	1/9/27/28	0/2/2/2
56	5MU	1L	54	56	-	0/7/25/26	0/2/2/2
56	PSU	1L	39	56	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	G7M	2K	47	23	-	3/7/25/26	0/3/3/3
22	5MU	1K	54	22	-	0/7/25/26	0/2/2/2
57	5MU	3L	54	57	-	0/7/25/26	0/2/2/2
22	PSU	1K	55	22	-	0/7/25/26	0/2/2/2
23	PSU	2L	56	23	-	0/7/25/26	0/2/2/2
22	PSU	1K	39	22	-	1/7/25/26	0/2/2/2
23	5MU	2K	55	23	-	0/7/25/26	0/2/2/2
23	4SU	2L	8	23	-	0/7/25/26	0/2/2/2
57	PSU	3L	55	57	-	3/7/25/26	0/2/2/2
56	U8U	1L	34	25,56	-	3/10/28/29	0/2/2/2
56	PSU	1L	55	56	-	2/7/25/26	0/2/2/2
23	OMC	2L	33	23	-	0/9/27/28	0/2/2/2
23	4SU	2K	8	23	-	0/7/25/26	0/2/2/2

The worst 5 of 94 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	2L	47	G7M	C8-N7	18.96	1.65	1.33
23	2K	47	G7M	C8-N7	18.73	1.65	1.33
57	3L	54	5MU	C2-N1	12.89	1.58	1.38
56	1L	54	5MU	C2-N1	12.77	1.58	1.38
23	2L	55	5MU	C2-N1	12.49	1.58	1.38

The worst 5 of 142 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	2K	47	G7M	CN7-N7-C5	11.50	141.13	126.80
23	2L	47	G7M	CN7-N7-C5	11.28	140.86	126.80
23	2K	55	5MU	C5-C4-N3	11.08	124.95	115.32
22	1K	54	5MU	C5-C4-N3	10.71	124.63	115.32
23	2L	55	5MU	C5-C4-N3	10.68	124.61	115.32

There are no chirality outliers.

5 of 30 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
22	1K	34	U8U	C5-C-N-CA
22	1K	37	T6A	C13-C12-C14-O14
22	1K	37	T6A	C13-C12-C14-C15
56	1L	34	U8U	C5-C-N-CA
56	1L	37	T6A	C14-C12-N11-C10

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 1144 ligands modelled in this entry, 1142 are monoatomic - leaving 2 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
59	SF4	32	301	-	0,12,12	-	-	-		
59	SF4	3E	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
59	SF4	32	301	-	-	-	0/6/5/5
59	SF4	3E	301	4	-	-	0/6/5/5

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

4.7 Other polymers [i](#)

There are no such residues in this entry.

4.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

5 Fit of model and data ⓘ

5.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	13	1496/1522 (98%)	-0.80	0 100 100	62, 109, 164, 193	0
1	1G	1507/1522 (99%)	-0.77	6 (0%) 88 79	80, 127, 170, 197	0
2	12	210/256 (82%)	-0.11	2 (0%) 79 63	127, 152, 162, 177	0
2	1E	231/256 (90%)	-0.18	1 (0%) 88 79	117, 141, 159, 166	0
3	22	196/239 (82%)	-0.16	3 (1%) 72 52	129, 143, 156, 164	0
3	2E	205/239 (85%)	-0.28	1 (0%) 87 76	94, 114, 136, 145	0
4	32	208/209 (99%)	0.12	0 100 100	108, 128, 145, 152	0
4	3E	207/209 (99%)	0.04	3 (1%) 73 54	92, 114, 134, 139	0
5	42	148/162 (91%)	0.04	0 100 100	114, 129, 143, 152	0
5	4E	149/162 (91%)	-0.05	0 100 100	89, 108, 124, 140	0
6	52	101/101 (100%)	-0.14	1 (0%) 79 63	95, 111, 129, 137	0
6	5E	100/101 (99%)	-0.22	1 (1%) 79 63	87, 107, 126, 136	0
7	62	138/156 (88%)	0.21	8 (5%) 29 18	121, 134, 144, 148	0
7	6E	154/156 (98%)	0.25	2 (1%) 75 55	109, 125, 148, 166	0
8	72	137/138 (99%)	-0.27	0 100 100	111, 133, 142, 145	0
8	7E	138/138 (100%)	0.15	1 (0%) 84 69	97, 117, 128, 138	0
9	82	121/128 (94%)	-0.08	3 (2%) 58 39	117, 149, 158, 163	0
9	8E	126/128 (98%)	0.10	2 (1%) 70 51	96, 135, 152, 157	0
10	1A	80/105 (76%)	-0.12	1 (1%) 75 55	129, 146, 156, 161	0
10	1I	91/105 (86%)	-0.18	0 100 100	87, 128, 159, 165	0
11	2A	113/129 (87%)	0.42	5 (4%) 39 24	94, 117, 130, 138	0
11	2I	111/129 (86%)	0.26	3 (2%) 56 36	85, 113, 127, 142	0
12	3A	122/132 (92%)	0.45	12 (9%) 13 9	89, 107, 130, 146	0
12	3I	122/132 (92%)	-0.18	1 (0%) 82 67	73, 82, 106, 137	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	4A	111/126 (88%)	-0.22	2 (1%) 67 48	125, 145, 156, 160	0
13	4I	119/126 (94%)	-0.20	3 (2%) 58 39	93, 123, 136, 147	0
14	5A	59/61 (96%)	-0.07	2 (3%) 48 30	134, 143, 153, 154	0
14	5I	60/61 (98%)	-0.46	0 100 100	92, 103, 118, 131	0
15	6A	88/89 (98%)	-0.53	0 100 100	96, 119, 135, 139	0
15	6I	87/89 (97%)	-0.36	0 100 100	88, 104, 122, 127	0
16	7A	84/88 (95%)	-0.18	0 100 100	102, 117, 135, 152	0
16	7I	83/88 (94%)	-0.10	0 100 100	110, 119, 143, 150	0
17	8A	99/105 (94%)	-0.40	0 100 100	105, 120, 132, 133	0
17	8I	100/105 (95%)	-0.18	2 (2%) 65 45	98, 114, 124, 126	0
18	9A	67/88 (76%)	-0.18	2 (2%) 52 33	106, 121, 135, 142	0
18	9I	68/88 (77%)	-0.09	2 (2%) 53 35	94, 109, 133, 136	0
19	AA	62/93 (66%)	-0.03	2 (3%) 50 31	134, 149, 156, 158	0
19	AI	81/93 (87%)	-0.18	0 100 100	102, 122, 138, 151	0
20	BA	99/106 (93%)	-0.30	0 100 100	100, 118, 141, 152	0
20	BI	97/106 (91%)	-0.02	0 100 100	112, 125, 148, 157	0
21	1B	22/27 (81%)	-0.15	0 100 100	129, 137, 145, 148	0
21	1F	23/27 (85%)	-0.62	0 100 100	94, 112, 118, 122	0
22	1K	66/75 (88%)	-0.00	1 (1%) 72 52	85, 153, 177, 183	0
23	2K	72/77 (93%)	-0.52	1 (1%) 73 54	77, 104, 132, 146	0
23	2L	72/77 (93%)	-0.40	0 100 100	85, 122, 151, 162	0
24	3K	76/76 (100%)	0.50	4 (5%) 32 20	79, 178, 191, 196	0
25	4K	19/27 (70%)	0.41	1 (5%) 32 20	79, 152, 184, 184	0
25	4L	18/27 (66%)	0.05	0 100 100	101, 161, 187, 187	0
26	14	2861/2917 (98%)	-0.79	11 (0%) 88 79	55, 92, 180, 204	0
26	1H	2833/2917 (97%)	-0.94	3 (0%) 92 89	49, 79, 168, 203	0
27	16	122/122 (100%)	-1.10	0 100 100	74, 98, 119, 179	0
27	1J	122/122 (100%)	-0.74	1 (0%) 82 67	93, 125, 145, 177	0
28	71	133/229 (58%)	0.30	5 (3%) 44 27	143, 174, 185, 189	0
28	79	57/229 (24%)	0.16	1 (1%) 67 48	140, 165, 176, 179	0
29	11	273/276 (98%)	-0.14	1 (0%) 88 79	48, 71, 89, 113	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
29	19	274/276 (99%)	0.14	6 (2%) 62 42	58, 82, 101, 117	0
30	21	203/206 (98%)	0.38	14 (6%) 23 14	55, 93, 139, 153	0
30	29	204/206 (99%)	-0.15	1 (0%) 87 76	60, 99, 134, 144	0
31	31	202/210 (96%)	-0.40	0 100 100	54, 84, 118, 142	0
31	39	204/210 (97%)	-0.10	0 100 100	62, 111, 151, 168	0
32	41	179/182 (98%)	-0.43	2 (1%) 78 61	85, 107, 140, 156	0
32	49	179/182 (98%)	0.32	8 (4%) 38 24	122, 139, 155, 171	0
33	51	171/180 (95%)	-0.04	2 (1%) 76 58	89, 110, 127, 139	0
33	59	73/180 (40%)	0.83	10 (13%) 6 5	136, 154, 165, 177	0
34	61	146/148 (98%)	-0.39	1 (0%) 84 69	83, 130, 143, 150	0
34	69	145/148 (97%)	-0.06	3 (2%) 63 43	93, 129, 147, 152	0
35	15	138/140 (98%)	0.25	1 (0%) 84 69	86, 114, 139, 155	0
35	58	138/140 (98%)	0.19	1 (0%) 84 69	68, 97, 130, 145	0
36	25	122/122 (100%)	0.16	2 (1%) 70 51	77, 94, 114, 120	0
36	68	122/122 (100%)	0.18	5 (4%) 41 25	64, 81, 99, 104	0
37	35	147/150 (98%)	0.15	9 (6%) 27 17	65, 111, 138, 144	0
37	78	147/150 (98%)	-0.09	4 (2%) 56 36	53, 88, 113, 120	0
38	45	138/141 (97%)	0.24	13 (9%) 14 9	78, 108, 128, 142	0
38	88	141/141 (100%)	-0.41	1 (0%) 84 69	63, 83, 108, 129	0
39	55	118/118 (100%)	-0.48	0 100 100	69, 86, 108, 127	0
39	98	118/118 (100%)	-0.07	2 (1%) 69 49	67, 90, 109, 122	0
40	65	110/112 (98%)	-0.38	1 (0%) 81 64	92, 117, 135, 142	0
40	A8	111/112 (99%)	-0.51	0 100 100	71, 93, 115, 123	0
41	75	133/146 (91%)	-0.01	6 (4%) 38 24	87, 101, 129, 141	0
41	B8	133/146 (91%)	0.27	10 (7%) 20 13	78, 98, 133, 149	0
42	85	116/118 (98%)	0.12	3 (2%) 57 37	73, 100, 132, 138	0
42	C8	115/118 (97%)	0.12	6 (5%) 33 21	59, 86, 114, 118	0
43	95	100/101 (99%)	0.33	3 (3%) 52 33	69, 121, 139, 153	0
43	D8	100/101 (99%)	0.35	4 (4%) 42 26	62, 106, 126, 144	0
44	A5	113/113 (100%)	-0.07	1 (0%) 81 64	68, 82, 112, 158	0
44	E8	112/113 (99%)	-0.22	2 (1%) 67 48	63, 79, 106, 147	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
45	B5	94/96 (97%)	-0.27	0 100 100	77, 91, 118, 128	0
45	F8	95/96 (98%)	-0.23	0 100 100	60, 76, 104, 118	0
46	C5	104/110 (94%)	0.79	13 (12%) 8 6	91, 122, 149, 154	0
46	G8	105/110 (95%)	0.19	5 (4%) 35 22	75, 101, 131, 139	0
47	D5	132/206 (64%)	-0.27	2 (1%) 72 52	115, 135, 150, 158	0
47	H8	171/206 (83%)	-0.39	0 100 100	90, 122, 167, 172	0
48	E5	77/85 (90%)	0.02	3 (3%) 43 27	72, 94, 111, 131	0
48	I8	76/85 (89%)	-0.36	1 (1%) 75 55	61, 75, 90, 102	0
49	F5	94/98 (95%)	0.40	7 (7%) 20 13	67, 88, 121, 136	0
49	J8	94/98 (95%)	-0.06	3 (3%) 50 31	62, 77, 120, 122	0
50	G5	66/72 (91%)	-0.17	2 (3%) 52 33	87, 108, 126, 145	0
50	K8	68/72 (94%)	-0.14	1 (1%) 72 52	68, 84, 102, 124	0
51	H5	58/60 (96%)	-0.22	0 100 100	81, 106, 128, 135	0
51	L8	58/60 (96%)	-0.12	0 100 100	63, 85, 115, 127	0
52	M8	47/71 (66%)	-0.10	1 (2%) 63 43	109, 143, 158, 163	0
53	J5	56/60 (93%)	-0.19	0 100 100	66, 86, 141, 148	0
53	N8	48/60 (80%)	0.16	1 (2%) 63 43	56, 84, 140, 142	0
54	L5	47/49 (95%)	-0.38	1 (2%) 63 43	58, 66, 85, 91	0
54	P8	47/49 (95%)	-0.54	0 100 100	52, 57, 77, 88	0
55	M5	64/65 (98%)	0.11	2 (3%) 51 32	76, 85, 101, 117	0
55	Q8	64/65 (98%)	-0.29	0 100 100	61, 71, 88, 99	0
56	1L	68/76 (89%)	-0.16	4 (5%) 28 18	118, 173, 181, 188	0
57	3L	73/76 (96%)	0.21	3 (4%) 41 25	87, 172, 185, 190	0
All	All	20602/21966 (93%)	-0.39	270 (1%) 75 55	48, 107, 162, 204	0

The worst 5 of 270 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
41	B8	1	MET	8.5
12	3A	19	ARG	7.5
43	D8	37	VAL	7.0
41	75	104	ASN	6.5
41	75	106	SER	6.5

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
57	PSU	3L	55	20/21	0.66	0.08	166,169,175,175	0
57	5MU	3L	54	21/22	0.68	0.09	162,169,172,173	0
56	T6A	1L	37	32/33	0.82	0.09	102,120,127,130	0
22	PSU	1K	55	20/21	0.84	0.08	109,120,133,134	0
56	PSU	1L	55	20/21	0.85	0.07	134,150,156,159	0
23	5MU	2L	55	21/22	0.87	0.10	128,133,141,143	0
56	U8U	1L	34	23/24	0.87	0.10	110,126,134,138	0
23	G7M	2L	47	24/25	0.87	0.10	129,137,150,151	0
57	PSU	3L	39	20/21	0.89	0.08	153,162,166,168	0
23	PSU	2K	56	20/21	0.89	0.07	104,113,121,127	0
23	5MU	2K	55	21/22	0.89	0.08	112,118,125,127	0
23	PSU	2L	56	20/21	0.90	0.08	116,129,133,137	0
56	5MU	1L	54	21/22	0.90	0.06	138,147,154,155	0
23	4SU	2K	8	20/21	0.91	0.08	93,98,102,106	0
23	4SU	2L	8	20/21	0.91	0.08	112,125,130,135	0
56	PSU	1L	39	20/21	0.92	0.07	105,127,133,134	0
22	5MU	1K	54	21/22	0.92	0.06	114,122,134,142	0
23	OMC	2L	33	21/22	0.94	0.09	109,114,117,125	0
23	G7M	2K	47	24/25	0.95	0.07	104,115,129,135	0
22	PSU	1K	39	20/21	0.95	0.06	79,98,105,108	0
22	U8U	1K	34	23/24	0.96	0.06	78,88,93,105	0
22	T6A	1K	37	32/33	0.96	0.07	76,86,103,106	0
23	OMC	2K	33	21/22	0.97	0.07	82,87,92,96	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($\text{\AA}^2$)	Q<0.9
58	MG	3K	101	1/1	0.14	0.24	162,162,162,162	0
58	MG	1G	1668	1/1	0.41	0.33	116,116,116,116	0
58	MG	1G	1665	1/1	0.42	0.25	113,113,113,113	0
58	MG	14	3129	1/1	0.47	0.36	73,73,73,73	0
58	MG	14	3052	1/1	0.50	0.34	113,113,113,113	0
58	MG	14	3034	1/1	0.51	0.27	88,88,88,88	0
58	MG	1H	3287	1/1	0.52	0.28	104,104,104,104	0
58	MG	14	3316	1/1	0.53	0.28	122,122,122,122	0
58	MG	2K	103	1/1	0.55	0.26	114,114,114,114	0
58	MG	14	3293	1/1	0.56	0.37	91,91,91,91	0
58	MG	14	3310	1/1	0.56	0.23	114,114,114,114	0
58	MG	1H	3336	1/1	0.56	0.30	104,104,104,104	0
58	MG	14	3282	1/1	0.57	0.26	109,109,109,109	0
58	MG	14	3300	1/1	0.58	0.27	117,117,117,117	0
58	MG	14	3174	1/1	0.58	0.29	101,101,101,101	0
58	MG	14	3252	1/1	0.58	0.32	84,84,84,84	0
58	MG	1J	203	1/1	0.58	0.27	103,103,103,103	0
58	MG	14	3012	1/1	0.60	0.34	80,80,80,80	0
58	MG	13	1685	1/1	0.60	0.18	121,121,121,121	0
58	MG	1G	1664	1/1	0.61	0.26	100,100,100,100	0
58	MG	1H	3037	1/1	0.61	0.29	121,121,121,121	0
58	MG	1H	3342	1/1	0.61	0.37	92,92,92,92	0
58	MG	1G	1641	1/1	0.61	0.26	113,113,113,113	0
58	MG	14	3317	1/1	0.61	0.35	89,89,89,89	0
58	MG	1G	1644	1/1	0.61	0.41	92,92,92,92	0
58	MG	13	1657	1/1	0.62	0.24	103,103,103,103	0
58	MG	14	3184	1/1	0.62	0.24	98,98,98,98	0
58	MG	14	3288	1/1	0.62	0.31	86,86,86,86	0
58	MG	14	3238	1/1	0.63	0.22	99,99,99,99	0
58	MG	14	3108	1/1	0.63	0.30	92,92,92,92	0
58	MG	1H	3251	1/1	0.63	0.20	71,71,71,71	0
58	MG	1G	1634	1/1	0.63	0.24	112,112,112,112	0
58	MG	1G	1659	1/1	0.63	0.16	142,142,142,142	0
58	MG	14	3221	1/1	0.64	0.16	69,69,69,69	0
58	MG	14	3222	1/1	0.64	0.22	97,97,97,97	0
58	MG	1G	1635	1/1	0.64	0.26	107,107,107,107	0
58	MG	1H	3249	1/1	0.64	0.22	80,80,80,80	0
58	MG	1G	1661	1/1	0.64	0.26	123,123,123,123	0
58	MG	14	3057	1/1	0.64	0.28	101,101,101,101	0
58	MG	14	3303	1/1	0.65	0.22	106,106,106,106	0
58	MG	14	3308	1/1	0.65	0.28	106,106,106,106	0
58	MG	14	3017	1/1	0.65	0.28	90,90,90,90	0
58	MG	13	1688	1/1	0.65	0.28	101,101,101,101	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	1G	1602	1/1	0.65	0.32	79,79,79,79	0
58	MG	1H	3194	1/1	0.65	0.26	84,84,84,84	0
58	MG	14	3171	1/1	0.66	0.23	99,99,99,99	0
58	MG	1H	3308	1/1	0.66	0.32	90,90,90,90	0
58	MG	1H	3122	1/1	0.66	0.27	79,79,79,79	0
58	MG	1H	3255	1/1	0.66	0.34	73,73,73,73	0
58	MG	14	3290	1/1	0.66	0.22	92,92,92,92	0
58	MG	1H	3139	1/1	0.66	0.25	71,71,71,71	0
58	MG	14	3294	1/1	0.66	0.26	87,87,87,87	0
58	MG	1G	1611	1/1	0.67	0.27	104,104,104,104	0
58	MG	1H	3309	1/1	0.67	0.29	90,90,90,90	0
58	MG	14	3399	1/1	0.67	0.24	107,107,107,107	0
58	MG	13	1659	1/1	0.67	0.33	97,97,97,97	0
58	MG	13	1607	1/1	0.68	0.39	116,116,116,116	0
58	MG	14	3309	1/1	0.68	0.30	110,110,110,110	0
58	MG	1H	3222	1/1	0.68	0.25	98,98,98,98	0
58	MG	2K	102	1/1	0.68	0.39	94,94,94,94	0
58	MG	1G	1604	1/1	0.68	0.25	87,87,87,87	0
58	MG	1H	3016	1/1	0.68	0.36	75,75,75,75	0
58	MG	1G	1628	1/1	0.68	0.25	95,95,95,95	0
58	MG	13	1698	1/1	0.69	0.21	138,138,138,138	0
58	MG	14	3243	1/1	0.69	0.24	81,81,81,81	0
58	MG	1H	3279	1/1	0.69	0.20	67,67,67,67	0
58	MG	14	3255	1/1	0.69	0.22	78,78,78,78	0
58	MG	13	1623	1/1	0.69	0.28	108,108,108,108	0
58	MG	13	1672	1/1	0.69	0.20	109,109,109,109	0
58	MG	13	1699	1/1	0.70	0.30	94,94,94,94	0
58	MG	1H	3132	1/1	0.70	0.32	85,85,85,85	0
58	MG	14	3053	1/1	0.70	0.17	61,61,61,61	0
58	MG	14	3193	1/1	0.70	0.29	77,77,77,77	0
58	MG	13	1692	1/1	0.70	0.18	122,122,122,122	0
58	MG	1H	3171	1/1	0.70	0.30	83,83,83,83	0
58	MG	14	3292	1/1	0.70	0.11	113,113,113,113	0
58	MG	14	3231	1/1	0.70	0.28	86,86,86,86	0
58	MG	13	1678	1/1	0.70	0.26	93,93,93,93	0
58	MG	1H	3118	1/1	0.71	0.37	77,77,77,77	0
58	MG	1G	1674	1/1	0.71	0.22	102,102,102,102	0
58	MG	14	3242	1/1	0.71	0.27	67,67,67,67	0
58	MG	14	3168	1/1	0.71	0.32	106,106,106,106	0
58	MG	13	1615	1/1	0.71	0.32	77,77,77,77	0
58	MG	1H	3313	1/1	0.71	0.24	98,98,98,98	0
58	MG	14	3258	1/1	0.71	0.36	92,92,92,92	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	1H	3330	1/1	0.71	0.20	102,102,102,102	0
58	MG	1G	1614	1/1	0.71	0.27	107,107,107,107	0
58	MG	1H	3201	1/1	0.71	0.31	92,92,92,92	0
58	MG	1H	3341	1/1	0.71	0.20	79,79,79,79	0
58	MG	1G	1675	1/1	0.72	0.30	91,91,91,91	0
58	MG	14	3185	1/1	0.72	0.33	82,82,82,82	0
58	MG	2L	102	1/1	0.72	0.27	83,83,83,83	0
58	MG	14	3089	1/1	0.72	0.41	79,79,79,79	0
58	MG	1H	3236	1/1	0.72	0.19	99,99,99,99	0
58	MG	1G	1654	1/1	0.72	0.36	83,83,83,83	0
58	MG	14	3023	1/1	0.72	0.24	83,83,83,83	0
58	MG	13	1689	1/1	0.72	0.28	107,107,107,107	0
58	MG	1H	3292	1/1	0.72	0.21	77,77,77,77	0
58	MG	45	201	1/1	0.72	0.22	108,108,108,108	0
58	MG	13	1704	1/1	0.73	0.26	82,82,82,82	0
58	MG	14	3068	1/1	0.73	0.34	100,100,100,100	0
58	MG	1H	3286	1/1	0.73	0.26	94,94,94,94	0
58	MG	13	1604	1/1	0.73	0.28	87,87,87,87	0
58	MG	1H	3021	1/1	0.73	0.19	83,83,83,83	0
58	MG	14	3223	1/1	0.73	0.19	86,86,86,86	0
58	MG	14	3227	1/1	0.73	0.27	76,76,76,76	0
58	MG	13	1695	1/1	0.73	0.30	83,83,83,83	0
58	MG	1H	3265	1/1	0.73	0.26	78,78,78,78	0
58	MG	1H	3278	1/1	0.73	0.31	95,95,95,95	0
58	MG	14	3133	1/1	0.74	0.22	107,107,107,107	0
58	MG	14	3143	1/1	0.74	0.23	102,102,102,102	0
58	MG	13	1631	1/1	0.74	0.28	93,93,93,93	0
58	MG	1G	1638	1/1	0.74	0.28	93,93,93,93	0
58	MG	13	1632	1/1	0.74	0.28	107,107,107,107	0
58	MG	1G	1673	1/1	0.74	0.25	93,93,93,93	0
58	MG	13	1624	1/1	0.74	0.27	103,103,103,103	0
58	MG	1G	1629	1/1	0.74	0.35	104,104,104,104	0
58	MG	14	3211	1/1	0.74	0.26	91,91,91,91	0
58	MG	1G	1633	1/1	0.74	0.23	98,98,98,98	0
58	MG	1H	3217	1/1	0.74	0.28	71,71,71,71	0
58	MG	1J	204	1/1	0.74	0.26	101,101,101,101	0
58	MG	1G	1663	1/1	0.74	0.26	94,94,94,94	0
58	MG	1G	1660	1/1	0.75	0.23	85,85,85,85	0
58	MG	1H	3160	1/1	0.75	0.12	72,72,72,72	0
58	MG	1H	3167	1/1	0.75	0.31	93,93,93,93	0
58	MG	14	3217	1/1	0.75	0.19	83,83,83,83	0
58	MG	1H	3319	1/1	0.75	0.32	110,110,110,110	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	13	1681	1/1	0.75	0.18	116,116,116,116	0
58	MG	14	3301	1/1	0.75	0.20	109,109,109,109	0
58	MG	1H	3334	1/1	0.75	0.23	76,76,76,76	0
58	MG	13	1653	1/1	0.75	0.28	72,72,72,72	0
58	MG	1H	3044	1/1	0.75	0.20	82,82,82,82	0
58	MG	13	1696	1/1	0.75	0.29	92,92,92,92	0
58	MG	14	3135	1/1	0.75	0.23	95,95,95,95	0
58	MG	1G	1642	1/1	0.75	0.23	91,91,91,91	0
58	MG	13	1670	1/1	0.75	0.19	97,97,97,97	0
58	MG	1H	3013	1/1	0.75	0.27	82,82,82,82	0
58	MG	14	3020	1/1	0.75	0.29	75,75,75,75	0
58	MG	13	1680	1/1	0.75	0.23	96,96,96,96	0
58	MG	1H	3033	1/1	0.76	0.28	88,88,88,88	0
58	MG	1G	1605	1/1	0.76	0.27	101,101,101,101	0
58	MG	14	3283	1/1	0.76	0.11	69,69,69,69	0
58	MG	1H	3185	1/1	0.76	0.27	95,95,95,95	0
58	MG	13	1679	1/1	0.76	0.24	100,100,100,100	0
58	MG	14	3191	1/1	0.76	0.28	96,96,96,96	0
58	MG	1H	3316	1/1	0.76	0.38	92,92,92,92	0
58	MG	1H	3043	1/1	0.76	0.35	81,81,81,81	0
58	MG	14	3059	1/1	0.76	0.35	86,86,86,86	0
58	MG	1H	3321	1/1	0.76	0.19	67,67,67,67	0
58	MG	14	3302	1/1	0.76	0.29	66,66,66,66	0
58	MG	14	3080	1/1	0.76	0.33	82,82,82,82	0
58	MG	1H	3154	1/1	0.76	0.27	84,84,84,84	0
58	MG	14	3096	1/1	0.76	0.27	73,73,73,73	0
58	MG	13	1701	1/1	0.76	0.18	114,114,114,114	0
58	MG	14	3311	1/1	0.76	0.33	100,100,100,100	0
58	MG	14	3235	1/1	0.76	0.35	72,72,72,72	0
58	MG	13	1662	1/1	0.76	0.21	118,118,118,118	0
58	MG	1H	3170	1/1	0.76	0.18	65,65,65,65	0
58	MG	1H	3300	1/1	0.76	0.26	87,87,87,87	0
58	MG	1H	3306	1/1	0.76	0.20	91,91,91,91	0
58	MG	35	201	1/1	0.76	0.21	74,74,74,74	0
58	MG	1G	1653	1/1	0.76	0.26	97,97,97,97	0
58	MG	1H	3331	1/1	0.77	0.28	73,73,73,73	0
58	MG	14	3058	1/1	0.77	0.19	84,84,84,84	0
58	MG	13	1687	1/1	0.77	0.29	99,99,99,99	0
58	MG	1E	301	1/1	0.77	0.26	106,106,106,106	0
58	MG	1G	1655	1/1	0.77	0.20	100,100,100,100	0
58	MG	1G	1630	1/1	0.77	0.25	103,103,103,103	0
58	MG	14	3197	1/1	0.77	0.21	116,116,116,116	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	14	3265	1/1	0.77	0.27	98,98,98,98	0
58	MG	14	3313	1/1	0.77	0.19	92,92,92,92	0
58	MG	14	3315	1/1	0.77	0.28	93,93,93,93	0
58	MG	1H	3196	1/1	0.77	0.30	83,83,83,83	0
58	MG	1H	3027	1/1	0.77	0.20	81,81,81,81	0
58	MG	14	3022	1/1	0.77	0.20	64,64,64,64	0
58	MG	13	1702	1/1	0.77	0.34	98,98,98,98	0
58	MG	1H	3293	1/1	0.77	0.20	84,84,84,84	0
58	MG	1H	3220	1/1	0.77	0.15	82,82,82,82	0
58	MG	1H	3305	1/1	0.77	0.19	67,67,67,67	0
58	MG	1G	1603	1/1	0.78	0.41	102,102,102,102	0
58	MG	1H	3328	1/1	0.78	0.25	80,80,80,80	0
58	MG	1H	3152	1/1	0.78	0.30	100,100,100,100	0
58	MG	14	3099	1/1	0.78	0.27	87,87,87,87	0
58	MG	14	3295	1/1	0.78	0.20	85,85,85,85	0
58	MG	14	3299	1/1	0.78	0.22	98,98,98,98	0
58	MG	1G	1650	1/1	0.78	0.24	114,114,114,114	0
58	MG	1H	3219	1/1	0.78	0.17	103,103,103,103	0
58	MG	1H	3333	1/1	0.78	0.29	100,100,100,100	0
58	MG	1G	1615	1/1	0.78	0.26	125,125,125,125	0
58	MG	1H	3314	1/1	0.78	0.25	85,85,85,85	0
58	MG	14	3146	1/1	0.78	0.29	57,57,57,57	0
58	MG	14	3152	1/1	0.78	0.24	92,92,92,92	0
58	MG	14	3155	1/1	0.78	0.28	64,64,64,64	0
58	MG	14	3250	1/1	0.78	0.30	78,78,78,78	0
58	MG	14	3314	1/1	0.78	0.20	94,94,94,94	0
58	MG	1H	3335	1/1	0.78	0.31	74,74,74,74	0
58	MG	14	3254	1/1	0.78	0.18	111,111,111,111	0
58	MG	1H	3199	1/1	0.78	0.21	69,69,69,69	0
58	MG	13	1660	1/1	0.78	0.20	103,103,103,103	0
58	MG	1H	3224	1/1	0.78	0.32	73,73,73,73	0
58	MG	16	203	1/1	0.78	0.12	90,90,90,90	0
58	MG	1H	3324	1/1	0.78	0.34	89,89,89,89	0
58	MG	1G	1640	1/1	0.78	0.30	87,87,87,87	0
58	MG	14	3204	1/1	0.79	0.16	77,77,77,77	0
58	MG	14	3150	1/1	0.79	0.20	87,87,87,87	0
58	MG	14	3304	1/1	0.79	0.36	92,92,92,92	0
58	MG	1G	1617	1/1	0.79	0.15	135,135,135,135	0
58	MG	1H	3073	1/1	0.79	0.26	81,81,81,81	0
58	MG	14	3267	1/1	0.79	0.18	92,92,92,92	0
58	MG	1G	1646	1/1	0.79	0.23	100,100,100,100	0
58	MG	1G	1637	1/1	0.79	0.29	87,87,87,87	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	14	3224	1/1	0.79	0.26	90,90,90,90	0
58	MG	1H	3237	1/1	0.79	0.19	84,84,84,84	0
58	MG	1H	3327	1/1	0.79	0.35	82,82,82,82	0
58	MG	1H	3144	1/1	0.79	0.30	77,77,77,77	0
58	MG	14	3190	1/1	0.79	0.25	86,86,86,86	0
58	MG	14	3079	1/1	0.79	0.28	70,70,70,70	0
58	MG	1G	1657	1/1	0.79	0.29	92,92,92,92	0
58	MG	14	3147	1/1	0.79	0.20	95,95,95,95	0
58	MG	14	3203	1/1	0.79	0.22	56,56,56,56	0
58	MG	1H	3268	1/1	0.80	0.31	85,85,85,85	0
58	MG	1H	3107	1/1	0.80	0.22	71,71,71,71	0
58	MG	14	3251	1/1	0.80	0.29	69,69,69,69	0
58	MG	1H	3232	1/1	0.80	0.15	52,52,52,52	0
58	MG	1G	1662	1/1	0.80	0.24	72,72,72,72	0
58	MG	1H	3233	1/1	0.80	0.37	62,62,62,62	0
58	MG	1H	3028	1/1	0.80	0.19	68,68,68,68	0
58	MG	14	3262	1/1	0.80	0.29	96,96,96,96	0
58	MG	1G	1618	1/1	0.80	0.26	109,109,109,109	0
58	MG	14	3312	1/1	0.80	0.23	80,80,80,80	0
58	MG	13	1697	1/1	0.80	0.19	92,92,92,92	0
58	MG	1H	3071	1/1	0.80	0.33	61,61,61,61	0
58	MG	14	3067	1/1	0.80	0.19	87,87,87,87	0
58	MG	1H	3298	1/1	0.80	0.21	74,74,74,74	0
58	MG	1H	3072	1/1	0.80	0.24	77,77,77,77	0
58	MG	13	1706	1/1	0.80	0.26	109,109,109,109	0
58	MG	1H	3090	1/1	0.80	0.21	71,71,71,71	0
58	MG	14	3236	1/1	0.80	0.23	89,89,89,89	0
58	MG	39	301	1/1	0.80	0.17	96,96,96,96	0
58	MG	1G	1658	1/1	0.80	0.24	92,92,92,92	0
58	MG	14	3019	1/1	0.80	0.32	90,90,90,90	0
58	MG	14	3276	1/1	0.81	0.26	92,92,92,92	0
58	MG	1H	3239	1/1	0.81	0.19	75,75,75,75	0
58	MG	13	1605	1/1	0.81	0.24	76,76,76,76	0
58	MG	1H	3020	1/1	0.81	0.19	66,66,66,66	0
58	MG	1H	3254	1/1	0.81	0.29	99,99,99,99	0
58	MG	14	3291	1/1	0.81	0.27	87,87,87,87	0
58	MG	1H	3045	1/1	0.81	0.25	82,82,82,82	0
58	MG	13	1656	1/1	0.81	0.14	103,103,103,103	0
58	MG	1H	3204	1/1	0.81	0.28	69,69,69,69	0
58	MG	1H	3269	1/1	0.81	0.16	65,65,65,65	0
58	MG	1H	3211	1/1	0.81	0.18	83,83,83,83	0
58	MG	1H	3216	1/1	0.81	0.22	67,67,67,67	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	1H	3283	1/1	0.81	0.24	92,92,92,92	0
58	MG	1H	3024	1/1	0.81	0.44	82,82,82,82	0
58	MG	13	1700	1/1	0.81	0.18	94,94,94,94	0
58	MG	1H	3089	1/1	0.81	0.22	59,59,59,59	0
58	MG	13	1677	1/1	0.81	0.21	104,104,104,104	0
58	MG	14	3144	1/1	0.81	0.36	71,71,71,71	0
58	MG	14	3009	1/1	0.81	0.26	52,52,52,52	0
58	MG	1H	3337	1/1	0.81	0.19	89,89,89,89	0
58	MG	14	3247	1/1	0.81	0.20	67,67,67,67	0
58	MG	1H	3340	1/1	0.81	0.32	78,78,78,78	0
58	MG	13	1661	1/1	0.81	0.27	103,103,103,103	0
58	MG	1H	3116	1/1	0.81	0.26	55,55,55,55	0
58	MG	1H	3176	1/1	0.81	0.30	76,76,76,76	0
58	MG	1G	1647	1/1	0.81	0.27	83,83,83,83	0
58	MG	78	201	1/1	0.81	0.29	70,70,70,70	0
58	MG	14	3260	1/1	0.81	0.24	72,72,72,72	0
58	MG	14	3035	1/1	0.81	0.16	93,93,93,93	0
58	MG	13	1625	1/1	0.81	0.29	86,86,86,86	0
58	MG	1H	3187	1/1	0.81	0.20	69,69,69,69	0
58	MG	35	202	1/1	0.81	0.15	87,87,87,87	0
58	MG	35	203	1/1	0.81	0.38	75,75,75,75	0
58	MG	14	3271	1/1	0.81	0.16	81,81,81,81	0
58	MG	14	3192	1/1	0.82	0.30	63,63,63,63	0
58	MG	14	3279	1/1	0.82	0.17	104,104,104,104	0
58	MG	14	3280	1/1	0.82	0.25	86,86,86,86	0
58	MG	1G	1672	1/1	0.82	0.30	99,99,99,99	0
58	MG	1G	1607	1/1	0.82	0.19	73,73,73,73	0
58	MG	13	1629	1/1	0.82	0.21	96,96,96,96	0
58	MG	13	1705	1/1	0.82	0.28	90,90,90,90	0
58	MG	1H	3172	1/1	0.82	0.23	87,87,87,87	0
58	MG	14	3214	1/1	0.82	0.24	88,88,88,88	0
58	MG	14	3100	1/1	0.82	0.25	76,76,76,76	0
58	MG	14	3106	1/1	0.82	0.23	61,61,61,61	0
58	MG	14	3004	1/1	0.82	0.18	67,67,67,67	0
58	MG	14	3111	1/1	0.82	0.15	81,81,81,81	0
58	MG	14	3117	1/1	0.82	0.30	81,81,81,81	0
58	MG	1G	1616	1/1	0.82	0.28	87,87,87,87	0
58	MG	14	3229	1/1	0.82	0.51	88,88,88,88	0
58	MG	1G	1652	1/1	0.82	0.28	71,71,71,71	0
58	MG	1H	3079	1/1	0.82	0.20	79,79,79,79	0
58	MG	1H	3262	1/1	0.82	0.26	94,94,94,94	0
58	MG	1H	3184	1/1	0.82	0.28	82,82,82,82	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	1G	1656	1/1	0.82	0.31	78,78,78,78	0
58	MG	13	1648	1/1	0.82	0.21	95,95,95,95	0
58	MG	1H	3050	1/1	0.82	0.28	60,60,60,60	0
58	MG	1H	3190	1/1	0.82	0.20	73,73,73,73	0
58	MG	14	3153	1/1	0.82	0.29	89,89,89,89	0
58	MG	1H	3191	1/1	0.82	0.26	90,90,90,90	0
58	MG	14	3253	1/1	0.82	0.18	94,94,94,94	0
58	MG	1H	3101	1/1	0.82	0.18	59,59,59,59	0
58	MG	1G	1636	1/1	0.82	0.23	101,101,101,101	0
58	MG	1J	202	1/1	0.82	0.22	95,95,95,95	0
58	MG	1H	3056	1/1	0.82	0.27	56,56,56,56	0
58	MG	14	3179	1/1	0.82	0.21	60,60,60,60	0
58	MG	1H	3108	1/1	0.82	0.24	74,74,74,74	0
58	MG	13	1652	1/1	0.82	0.19	99,99,99,99	0
58	MG	1H	3247	1/1	0.82	0.20	81,81,81,81	0
58	MG	14	3269	1/1	0.82	0.41	88,88,88,88	0
58	MG	14	3074	1/1	0.82	0.41	79,79,79,79	0
58	MG	14	3029	1/1	0.83	0.24	78,78,78,78	0
58	MG	14	3139	1/1	0.83	0.14	99,99,99,99	0
58	MG	13	1676	1/1	0.83	0.23	76,76,76,76	0
58	MG	13	1646	1/1	0.83	0.24	75,75,75,75	0
58	MG	14	3044	1/1	0.83	0.28	64,64,64,64	0
58	MG	14	3048	1/1	0.83	0.19	90,90,90,90	0
58	MG	14	3050	1/1	0.83	0.37	59,59,59,59	0
58	MG	13	1658	1/1	0.83	0.17	83,83,83,83	0
58	MG	1H	3036	1/1	0.83	0.46	100,100,100,100	0
58	MG	1H	3297	1/1	0.83	0.14	99,99,99,99	0
58	MG	14	3165	1/1	0.83	0.27	77,77,77,77	0
58	MG	1H	3230	1/1	0.83	0.28	43,43,43,43	0
58	MG	14	3305	1/1	0.83	0.18	75,75,75,75	0
58	MG	1H	3264	1/1	0.83	0.16	76,76,76,76	0
58	MG	1H	3304	1/1	0.83	0.20	86,86,86,86	0
58	MG	1H	3019	1/1	0.83	0.39	92,92,92,92	0
58	MG	14	3181	1/1	0.83	0.25	89,89,89,89	0
58	MG	5E	201	1/1	0.83	0.17	89,89,89,89	0
58	MG	2L	101	1/1	0.83	0.30	73,73,73,73	0
58	MG	14	3259	1/1	0.83	0.66	98,98,98,98	0
58	MG	1H	3182	1/1	0.83	0.13	78,78,78,78	0
58	MG	1G	1625	1/1	0.83	0.20	93,93,93,93	0
58	MG	13	1647	1/1	0.83	0.21	89,89,89,89	0
58	MG	13	1602	1/1	0.83	0.16	86,86,86,86	0
58	MG	1J	201	1/1	0.83	0.22	94,94,94,94	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	14	3013	1/1	0.83	0.25	78,78,78,78	0
58	MG	14	3015	1/1	0.83	0.43	49,49,49,49	0
58	MG	1H	3282	1/1	0.83	0.39	88,88,88,88	0
58	MG	1G	1631	1/1	0.83	0.17	96,96,96,96	0
58	MG	14	3113	1/1	0.83	0.27	73,73,73,73	0
58	MG	16	202	1/1	0.83	0.11	64,64,64,64	0
58	MG	1H	3025	1/1	0.83	0.28	64,64,64,64	0
58	MG	1H	3284	1/1	0.83	0.29	81,81,81,81	0
58	MG	1H	3010	1/1	0.84	0.30	63,63,63,63	0
58	MG	1G	1606	1/1	0.84	0.24	88,88,88,88	0
58	MG	1H	3242	1/1	0.84	0.25	52,52,52,52	0
58	MG	14	3296	1/1	0.84	0.17	84,84,84,84	0
58	MG	14	3297	1/1	0.84	0.36	70,70,70,70	0
58	MG	14	3244	1/1	0.84	0.28	70,70,70,70	0
58	MG	14	3245	1/1	0.84	0.28	77,77,77,77	0
58	MG	14	3175	1/1	0.84	0.16	92,92,92,92	0
58	MG	1H	3011	1/1	0.84	0.28	51,51,51,51	0
58	MG	1G	1612	1/1	0.84	0.25	81,81,81,81	0
58	MG	13	1640	1/1	0.84	0.29	74,74,74,74	0
58	MG	1G	1667	1/1	0.84	0.23	109,109,109,109	0
58	MG	13	1671	1/1	0.84	0.18	87,87,87,87	0
58	MG	14	3038	1/1	0.84	0.19	71,71,71,71	0
58	MG	14	3121	1/1	0.84	0.28	78,78,78,78	0
58	MG	1G	1670	1/1	0.84	0.33	86,86,86,86	0
58	MG	14	3131	1/1	0.84	0.23	95,95,95,95	0
58	MG	14	3132	1/1	0.84	0.23	68,68,68,68	0
58	MG	1H	3205	1/1	0.84	0.13	81,81,81,81	0
58	MG	1H	3209	1/1	0.84	0.30	90,90,90,90	0
58	MG	1H	3258	1/1	0.84	0.19	59,59,59,59	0
58	MG	1H	3259	1/1	0.84	0.28	79,79,79,79	0
58	MG	14	3397	1/1	0.84	0.41	73,73,73,73	0
58	MG	14	3275	1/1	0.84	0.23	91,91,91,91	0
58	MG	1H	3376	1/1	0.84	0.14	76,76,76,76	0
58	MG	1H	3290	1/1	0.84	0.15	70,70,70,70	0
58	MG	1H	3291	1/1	0.84	0.10	73,73,73,73	0
58	MG	14	3007	1/1	0.84	0.20	54,54,54,54	0
58	MG	13	1669	1/1	0.84	0.27	68,68,68,68	0
58	MG	1H	3263	1/1	0.84	0.12	76,76,76,76	0
58	MG	1H	3007	1/1	0.84	0.20	54,54,54,54	0
58	MG	14	3163	1/1	0.84	0.21	90,90,90,90	0
58	MG	1H	3009	1/1	0.84	0.17	62,62,62,62	0
58	MG	14	3126	1/1	0.85	0.20	67,67,67,67	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	1H	3031	1/1	0.85	0.28	76,76,76,76	0
58	MG	14	3249	1/1	0.85	0.24	80,80,80,80	0
58	MG	14	3187	1/1	0.85	0.28	80,80,80,80	0
58	MG	14	3189	1/1	0.85	0.13	82,82,82,82	0
58	MG	14	3130	1/1	0.85	0.23	86,86,86,86	0
58	MG	98	201	1/1	0.85	0.23	72,72,72,72	0
58	MG	14	3065	1/1	0.85	0.26	67,67,67,67	0
58	MG	I8	101	1/1	0.85	0.34	73,73,73,73	0
58	MG	Q8	101	1/1	0.85	0.26	70,70,70,70	0
58	MG	1G	1601	1/1	0.85	0.21	91,91,91,91	0
58	MG	1H	3081	1/1	0.85	0.20	87,87,87,87	0
58	MG	13	1606	1/1	0.85	0.29	94,94,94,94	0
58	MG	14	3081	1/1	0.85	0.23	76,76,76,76	0
58	MG	14	3266	1/1	0.85	0.28	85,85,85,85	0
58	MG	13	1618	1/1	0.85	0.26	80,80,80,80	0
58	MG	14	3148	1/1	0.85	0.29	77,77,77,77	0
58	MG	14	3095	1/1	0.85	0.24	71,71,71,71	0
58	MG	1H	3174	1/1	0.85	0.24	88,88,88,88	0
58	MG	1H	3197	1/1	0.85	0.29	80,80,80,80	0
58	MG	1H	3065	1/1	0.85	0.24	61,61,61,61	0
58	MG	1H	3271	1/1	0.85	0.22	76,76,76,76	0
58	MG	14	3281	1/1	0.85	0.20	86,86,86,86	0
58	MG	13	1603	1/1	0.85	0.21	92,92,92,92	0
58	MG	1H	3226	1/1	0.85	0.26	85,85,85,85	0
58	MG	14	3112	1/1	0.85	0.26	65,65,65,65	0
58	MG	13	1608	1/1	0.85	0.31	90,90,90,90	0
58	MG	14	3239	1/1	0.85	0.14	80,80,80,80	0
58	MG	14	3054	1/1	0.85	0.24	70,70,70,70	0
58	MG	14	3120	1/1	0.85	0.23	82,82,82,82	0
58	MG	13	1609	1/1	0.85	0.18	75,75,75,75	0
58	MG	1H	3223	1/1	0.86	0.26	78,78,78,78	0
58	MG	14	3180	1/1	0.86	0.26	88,88,88,88	0
58	MG	13	1691	1/1	0.86	0.20	90,90,90,90	0
58	MG	1H	3307	1/1	0.86	0.28	94,94,94,94	0
58	MG	1H	3252	1/1	0.86	0.31	66,66,66,66	0
58	MG	1H	3225	1/1	0.86	0.22	78,78,78,78	0
58	MG	1H	3207	1/1	0.86	0.28	84,84,84,84	0
58	MG	1H	3227	1/1	0.86	0.40	85,85,85,85	0
58	MG	13	1654	1/1	0.86	0.19	74,74,74,74	0
58	MG	14	3060	1/1	0.86	0.16	73,73,73,73	0
58	MG	14	3008	1/1	0.86	0.23	65,65,65,65	0
58	MG	14	3194	1/1	0.86	0.21	81,81,81,81	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	1H	3260	1/1	0.86	0.26	72,72,72,72	0
58	MG	14	3201	1/1	0.86	0.14	59,59,59,59	0
58	MG	1G	1626	1/1	0.86	0.24	82,82,82,82	0
58	MG	14	3142	1/1	0.86	0.25	76,76,76,76	0
58	MG	16	204	1/1	0.86	0.15	73,73,73,73	0
58	MG	1H	3130	1/1	0.86	0.24	74,74,74,74	0
58	MG	1H	3323	1/1	0.86	0.28	80,80,80,80	0
58	MG	14	3018	1/1	0.86	0.25	72,72,72,72	0
58	MG	1H	3213	1/1	0.86	0.18	74,74,74,74	0
58	MG	14	3094	1/1	0.86	0.30	60,60,60,60	0
58	MG	I8	102	1/1	0.86	0.15	70,70,70,70	0
58	MG	1H	3162	1/1	0.86	0.23	88,88,88,88	0
58	MG	14	3098	1/1	0.86	0.13	93,93,93,93	0
58	MG	14	3230	1/1	0.86	0.16	64,64,64,64	0
58	MG	1H	3294	1/1	0.86	0.15	57,57,57,57	0
58	MG	1H	3060	1/1	0.86	0.21	61,61,61,61	0
58	MG	13	1667	1/1	0.86	0.22	71,71,71,71	0
58	MG	1H	3332	1/1	0.86	0.20	74,74,74,74	0
58	MG	1H	3003	1/1	0.86	0.19	64,64,64,64	0
58	MG	1H	3188	1/1	0.86	0.25	73,73,73,73	0
58	MG	14	3037	1/1	0.87	0.26	106,106,106,106	0
58	MG	1G	1666	1/1	0.87	0.32	84,84,84,84	0
58	MG	1H	3322	1/1	0.87	0.27	81,81,81,81	0
58	MG	1H	3093	1/1	0.87	0.24	72,72,72,72	0
58	MG	14	3049	1/1	0.87	0.16	70,70,70,70	0
58	MG	14	3278	1/1	0.87	0.28	75,75,75,75	0
58	MG	14	3196	1/1	0.87	0.31	75,75,75,75	0
58	MG	1H	3100	1/1	0.87	0.14	61,61,61,61	0
58	MG	1G	1639	1/1	0.87	0.17	74,74,74,74	0
58	MG	14	3122	1/1	0.87	0.18	88,88,88,88	0
58	MG	1H	3069	1/1	0.87	0.19	90,90,90,90	0
58	MG	14	3205	1/1	0.87	0.27	96,96,96,96	0
58	MG	14	3289	1/1	0.87	0.30	83,83,83,83	0
58	MG	1H	3256	1/1	0.87	0.11	61,61,61,61	0
58	MG	13	1668	1/1	0.87	0.14	90,90,90,90	0
58	MG	1H	3164	1/1	0.87	0.19	64,64,64,64	0
58	MG	1H	3004	1/1	0.87	0.20	57,57,57,57	0
58	MG	1H	3296	1/1	0.87	0.14	57,57,57,57	0
58	MG	14	3134	1/1	0.87	0.20	74,74,74,74	0
58	MG	13	1621	1/1	0.87	0.19	90,90,90,90	0
58	MG	1H	3075	1/1	0.87	0.18	43,43,43,43	0
58	MG	14	3140	1/1	0.87	0.23	82,82,82,82	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	1H	3203	1/1	0.87	0.29	79,79,79,79	0
58	MG	14	3070	1/1	0.87	0.23	60,60,60,60	0
58	MG	14	3232	1/1	0.87	0.17	81,81,81,81	0
58	MG	14	3234	1/1	0.87	0.27	70,70,70,70	0
58	MG	14	3071	1/1	0.87	0.21	68,68,68,68	0
58	MG	14	3073	1/1	0.87	0.44	83,83,83,83	0
58	MG	1H	3303	1/1	0.87	0.36	78,78,78,78	0
58	MG	14	3076	1/1	0.87	0.20	62,62,62,62	0
58	MG	14	3077	1/1	0.87	0.23	68,68,68,68	0
58	MG	1H	3058	1/1	0.87	0.24	46,46,46,46	0
58	MG	1H	3125	1/1	0.87	0.29	69,69,69,69	0
58	MG	1H	3206	1/1	0.87	0.31	77,77,77,77	0
58	MG	14	3082	1/1	0.87	0.30	61,61,61,61	0
58	MG	14	3248	1/1	0.87	0.15	79,79,79,79	0
58	MG	14	3083	1/1	0.87	0.28	72,72,72,72	0
58	MG	14	3084	1/1	0.87	0.28	80,80,80,80	0
58	MG	1H	3080	1/1	0.87	0.17	65,65,65,65	0
58	MG	14	3091	1/1	0.87	0.24	86,86,86,86	0
58	MG	1H	3275	1/1	0.87	0.24	75,75,75,75	0
58	MG	14	3177	1/1	0.87	0.26	72,72,72,72	0
58	MG	1H	3179	1/1	0.87	0.18	83,83,83,83	0
58	MG	1H	3059	1/1	0.87	0.19	49,49,49,49	0
58	MG	29	301	1/1	0.87	0.23	77,77,77,77	0
58	MG	13	1686	1/1	0.87	0.20	76,76,76,76	0
58	MG	1H	3032	1/1	0.87	0.28	79,79,79,79	0
58	MG	1H	3149	1/1	0.87	0.33	60,60,60,60	0
58	MG	1H	3285	1/1	0.87	0.28	68,68,68,68	0
58	MG	14	3107	1/1	0.87	0.30	77,77,77,77	0
58	MG	14	3285	1/1	0.88	0.10	68,68,68,68	0
58	MG	14	3287	1/1	0.88	0.13	82,82,82,82	0
58	MG	14	3055	1/1	0.88	0.16	81,81,81,81	0
58	MG	1H	3165	1/1	0.88	0.32	78,78,78,78	0
58	MG	1G	1627	1/1	0.88	0.16	94,94,94,94	0
58	MG	14	3233	1/1	0.88	0.13	86,86,86,86	0
58	MG	1H	3318	1/1	0.88	0.26	79,79,79,79	0
58	MG	13	1635	1/1	0.88	0.33	74,74,74,74	0
58	MG	1H	3168	1/1	0.88	0.21	69,69,69,69	0
58	MG	14	3118	1/1	0.88	0.27	69,69,69,69	0
58	MG	13	1703	1/1	0.88	0.34	77,77,77,77	0
58	MG	1H	3137	1/1	0.88	0.24	88,88,88,88	0
58	MG	14	3069	1/1	0.88	0.17	70,70,70,70	0
58	MG	14	3186	1/1	0.88	0.28	82,82,82,82	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	1H	3218	1/1	0.88	0.19	56,56,56,56	0
58	MG	14	3188	1/1	0.88	0.27	88,88,88,88	0
58	MG	1H	3295	1/1	0.88	0.27	93,93,93,93	0
58	MG	1H	3266	1/1	0.88	0.13	81,81,81,81	0
58	MG	13	1639	1/1	0.88	0.32	82,82,82,82	0
58	MG	14	3026	1/1	0.88	0.23	89,89,89,89	0
58	MG	14	3027	1/1	0.88	0.28	96,96,96,96	0
58	MG	1H	3243	1/1	0.88	0.24	65,65,65,65	0
58	MG	14	3030	1/1	0.88	0.23	86,86,86,86	0
58	MG	1H	3049	1/1	0.88	0.29	52,52,52,52	0
58	MG	1H	3302	1/1	0.88	0.19	92,92,92,92	0
58	MG	13	1627	1/1	0.88	0.30	69,69,69,69	0
58	MG	1H	3277	1/1	0.88	0.15	68,68,68,68	0
58	MG	14	3085	1/1	0.88	0.12	67,67,67,67	0
58	MG	14	3210	1/1	0.88	0.15	80,80,80,80	0
58	MG	14	3042	1/1	0.88	0.32	70,70,70,70	0
58	MG	13	1651	1/1	0.88	0.31	88,88,88,88	0
58	MG	14	3215	1/1	0.88	0.22	72,72,72,72	0
58	MG	14	3045	1/1	0.88	0.15	58,58,58,58	0
58	MG	1H	3038	1/1	0.88	0.18	92,92,92,92	0
58	MG	1H	3253	1/1	0.88	0.11	66,66,66,66	0
58	MG	1H	3094	1/1	0.88	0.21	64,64,64,64	0
58	MG	1H	3128	1/1	0.88	0.08	62,62,62,62	0
58	MG	14	3226	1/1	0.88	0.19	73,73,73,73	0
58	MG	1H	3129	1/1	0.88	0.30	85,85,85,85	0
58	MG	14	3228	1/1	0.88	0.12	101,101,101,101	0
58	MG	1H	3228	1/1	0.88	0.32	83,83,83,83	0
58	MG	13	1690	1/1	0.89	0.10	74,74,74,74	0
58	MG	1H	3023	1/1	0.89	0.28	56,56,56,56	0
58	MG	1H	3082	1/1	0.89	0.18	78,78,78,78	0
58	MG	1G	1609	1/1	0.89	0.20	94,94,94,94	0
58	MG	1G	1610	1/1	0.89	0.17	98,98,98,98	0
58	MG	1H	3133	1/1	0.89	0.22	71,71,71,71	0
58	MG	1H	3135	1/1	0.89	0.15	65,65,65,65	0
58	MG	1G	1613	1/1	0.89	0.11	98,98,98,98	0
58	MG	14	3125	1/1	0.89	0.27	72,72,72,72	0
58	MG	13	1675	1/1	0.89	0.22	73,73,73,73	0
58	MG	1H	3005	1/1	0.89	0.24	54,54,54,54	0
58	MG	1H	3141	1/1	0.89	0.24	61,61,61,61	0
58	MG	14	3286	1/1	0.89	0.27	80,80,80,80	0
58	MG	1H	3091	1/1	0.89	0.32	65,65,65,65	0
58	MG	1H	3146	1/1	0.89	0.25	72,72,72,72	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	1G	1619	1/1	0.89	0.21	101,101,101,101	0
58	MG	1G	1671	1/1	0.89	0.32	88,88,88,88	0
58	MG	1H	3198	1/1	0.89	0.20	69,69,69,69	0
58	MG	1H	3026	1/1	0.89	0.26	56,56,56,56	0
58	MG	1H	3200	1/1	0.89	0.36	81,81,81,81	0
58	MG	1H	3150	1/1	0.89	0.16	72,72,72,72	0
58	MG	1H	3248	1/1	0.89	0.26	74,74,74,74	0
58	MG	13	1682	1/1	0.89	0.35	88,88,88,88	0
58	MG	1H	3338	1/1	0.89	0.20	65,65,65,65	0
58	MG	1H	3096	1/1	0.89	0.19	60,60,60,60	0
58	MG	1H	3158	1/1	0.89	0.24	74,74,74,74	0
58	MG	1H	3008	1/1	0.89	0.23	81,81,81,81	0
58	MG	14	3011	1/1	0.89	0.28	48,48,48,48	0
58	MG	13	1683	1/1	0.89	0.17	94,94,94,94	0
58	MG	1H	3467	1/1	0.89	0.15	84,84,84,84	0
58	MG	14	3156	1/1	0.89	0.25	63,63,63,63	0
58	MG	14	3014	1/1	0.89	0.26	57,57,57,57	0
58	MG	13	1684	1/1	0.89	0.12	128,128,128,128	0
58	MG	14	3166	1/1	0.89	0.15	60,60,60,60	0
58	MG	13	1641	1/1	0.89	0.24	93,93,93,93	0
58	MG	1H	3111	1/1	0.89	0.31	74,74,74,74	0
58	MG	14	3173	1/1	0.89	0.16	66,66,66,66	0
58	MG	14	3086	1/1	0.89	0.28	83,83,83,83	0
58	MG	14	3088	1/1	0.89	0.20	52,52,52,52	0
58	MG	21	302	1/1	0.89	0.25	77,77,77,77	0
58	MG	14	3090	1/1	0.89	0.14	74,74,74,74	0
58	MG	1H	3215	1/1	0.89	0.24	63,63,63,63	0
58	MG	1H	3035	1/1	0.89	0.32	83,83,83,83	0
58	MG	1G	1645	1/1	0.89	0.25	74,74,74,74	0
58	MG	13	1636	1/1	0.89	0.11	64,64,64,64	0
58	MG	14	3257	1/1	0.89	0.45	86,86,86,86	0
58	MG	13	1634	1/1	0.89	0.37	93,93,93,93	0
58	MG	13	1663	1/1	0.89	0.20	82,82,82,82	0
58	MG	1H	3126	1/1	0.89	0.13	58,58,58,58	0
58	MG	1H	3221	1/1	0.89	0.24	89,89,89,89	0
58	MG	14	3264	1/1	0.89	0.33	85,85,85,85	0
58	MG	1H	3127	1/1	0.89	0.09	59,59,59,59	0
58	MG	13	1633	1/1	0.89	0.28	62,62,62,62	0
58	MG	1H	3241	1/1	0.90	0.23	66,66,66,66	0
58	MG	13	1628	1/1	0.90	0.28	65,65,65,65	0
58	MG	1H	3267	1/1	0.90	0.28	73,73,73,73	0
58	MG	1H	3051	1/1	0.90	0.19	45,45,45,45	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	2K	101	1/1	0.90	0.27	68,68,68,68	0
58	MG	13	1611	1/1	0.90	0.14	72,72,72,72	0
58	MG	1H	3273	1/1	0.90	0.18	68,68,68,68	0
58	MG	1H	3166	1/1	0.90	0.20	71,71,71,71	0
58	MG	1H	3276	1/1	0.90	0.23	75,75,75,75	0
58	MG	14	3195	1/1	0.90	0.29	68,68,68,68	0
58	MG	13	1664	1/1	0.90	0.13	89,89,89,89	0
58	MG	13	1630	1/1	0.90	0.24	80,80,80,80	0
58	MG	1H	3210	1/1	0.90	0.26	71,71,71,71	0
58	MG	1H	3192	1/1	0.90	0.16	80,80,80,80	0
58	MG	13	1730	1/1	0.90	0.16	86,86,86,86	0
58	MG	1H	3310	1/1	0.90	0.06	75,75,75,75	0
58	MG	14	3154	1/1	0.90	0.17	69,69,69,69	0
58	MG	1H	3311	1/1	0.90	0.20	75,75,75,75	0
58	MG	1G	1620	1/1	0.90	0.13	82,82,82,82	0
58	MG	14	3159	1/1	0.90	0.26	63,63,63,63	0
58	MG	14	3216	1/1	0.90	0.25	77,77,77,77	0
58	MG	14	3064	1/1	0.90	0.15	78,78,78,78	0
58	MG	14	3016	1/1	0.90	0.26	61,61,61,61	0
58	MG	1H	3231	1/1	0.90	0.24	58,58,58,58	0
58	MG	14	3167	1/1	0.90	0.26	87,87,87,87	0
58	MG	1H	3257	1/1	0.90	0.20	70,70,70,70	0
58	MG	14	3273	1/1	0.90	0.30	101,101,101,101	0
58	MG	14	3274	1/1	0.90	0.08	76,76,76,76	0
58	MG	1H	3066	1/1	0.90	0.22	59,59,59,59	0
58	MG	1H	3131	1/1	0.90	0.33	73,73,73,73	0
58	MG	1H	3288	1/1	0.90	0.37	93,93,93,93	0
58	MG	1H	3153	1/1	0.90	0.12	62,62,62,62	0
58	MG	14	3176	1/1	0.90	0.33	79,79,79,79	0
58	MG	1H	3068	1/1	0.90	0.20	86,86,86,86	0
58	MG	13	1637	1/1	0.90	0.17	56,56,56,56	0
58	MG	1H	3240	1/1	0.90	0.14	74,74,74,74	0
58	MG	1H	3325	1/1	0.90	0.24	71,71,71,71	0
58	MG	14	3033	1/1	0.90	0.16	77,77,77,77	0
58	MG	1H	3326	1/1	0.90	0.28	83,83,83,83	0
60	ZN	G8	201	1/1	0.90	0.14	149,149,149,149	0
58	MG	14	3002	1/1	0.91	0.20	57,57,57,57	0
58	MG	14	3092	1/1	0.91	0.15	76,76,76,76	0
58	MG	14	3003	1/1	0.91	0.16	62,62,62,62	0
58	MG	1G	1648	1/1	0.91	0.23	117,117,117,117	0
58	MG	14	3158	1/1	0.91	0.23	75,75,75,75	0
58	MG	14	3051	1/1	0.91	0.08	81,81,81,81	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	1H	3120	1/1	0.91	0.18	74,74,74,74	0
58	MG	1G	1651	1/1	0.91	0.15	104,104,104,104	0
58	MG	13	1666	1/1	0.91	0.10	78,78,78,78	0
58	MG	14	3101	1/1	0.91	0.20	64,64,64,64	0
58	MG	14	3104	1/1	0.91	0.19	86,86,86,86	0
58	MG	1H	3053	1/1	0.91	0.18	50,50,50,50	0
58	MG	14	3056	1/1	0.91	0.20	55,55,55,55	0
58	MG	1H	3173	1/1	0.91	0.33	84,84,84,84	0
58	MG	1H	3054	1/1	0.91	0.17	52,52,52,52	0
58	MG	1H	3202	1/1	0.91	0.28	70,70,70,70	0
58	MG	1H	3029	1/1	0.91	0.24	42,42,42,42	0
58	MG	14	3062	1/1	0.91	0.18	68,68,68,68	0
58	MG	1H	3074	1/1	0.91	0.16	64,64,64,64	0
58	MG	1H	3042	1/1	0.91	0.43	90,90,90,90	0
58	MG	14	3183	1/1	0.91	0.35	79,79,79,79	0
58	MG	1H	3183	1/1	0.91	0.24	67,67,67,67	0
58	MG	1H	3155	1/1	0.91	0.22	74,74,74,74	0
58	MG	1H	3208	1/1	0.91	0.31	88,88,88,88	0
58	MG	14	3021	1/1	0.91	0.22	52,52,52,52	0
58	MG	14	3306	1/1	0.91	0.22	88,88,88,88	0
58	MG	1H	3076	1/1	0.91	0.21	65,65,65,65	0
58	MG	1H	3186	1/1	0.91	0.22	75,75,75,75	0
58	MG	14	3024	1/1	0.91	0.28	77,77,77,77	0
58	MG	1H	3103	1/1	0.91	0.14	54,54,54,54	0
58	MG	1H	3015	1/1	0.91	0.27	63,63,63,63	0
58	MG	14	3078	1/1	0.91	0.21	64,64,64,64	0
58	MG	14	3028	1/1	0.91	0.24	69,69,69,69	0
58	MG	1H	3299	1/1	0.91	0.12	74,74,74,74	0
58	MG	1H	3214	1/1	0.91	0.45	76,76,76,76	0
58	MG	14	3141	1/1	0.91	0.14	93,93,93,93	0
58	MG	14	3261	1/1	0.91	0.17	77,77,77,77	0
58	MG	14	3198	1/1	0.91	0.09	107,107,107,107	0
58	MG	1H	3189	1/1	0.91	0.34	67,67,67,67	0
58	MG	14	3202	1/1	0.91	0.20	63,63,63,63	0
58	MG	13	1622	1/1	0.91	0.28	74,74,74,74	0
58	MG	1H	3246	1/1	0.91	0.13	54,54,54,54	0
58	MG	1H	3017	1/1	0.91	0.24	71,71,71,71	0
58	MG	29	303	1/1	0.91	0.25	52,52,52,52	0
58	MG	13	1650	1/1	0.91	0.27	94,94,94,94	0
58	MG	25	201	1/1	0.91	0.32	102,102,102,102	0
58	MG	1H	3117	1/1	0.91	0.18	48,48,48,48	0
58	MG	14	3213	1/1	0.91	0.24	64,64,64,64	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	14	3149	1/1	0.91	0.31	73,73,73,73	0
58	MG	13	1620	1/1	0.91	0.19	73,73,73,73	0
58	MG	E5	101	1/1	0.91	0.32	89,89,89,89	0
58	MG	1H	3280	1/1	0.91	0.20	77,77,77,77	0
58	MG	14	3043	1/1	0.92	0.20	57,57,57,57	0
58	MG	1H	3178	1/1	0.92	0.16	71,71,71,71	0
58	MG	1H	3061	1/1	0.92	0.22	48,48,48,48	0
58	MG	14	3047	1/1	0.92	0.10	74,74,74,74	0
58	MG	1H	3317	1/1	0.92	0.26	68,68,68,68	0
58	MG	14	3241	1/1	0.92	0.12	56,56,56,56	0
58	MG	1H	3180	1/1	0.92	0.29	75,75,75,75	0
58	MG	1H	3422	1/1	0.92	0.06	112,112,112,112	0
58	MG	1H	3438	1/1	0.92	0.08	83,83,83,83	0
58	MG	1H	3136	1/1	0.92	0.23	49,49,49,49	0
58	MG	16	201	1/1	0.92	0.11	85,85,85,85	0
58	MG	1H	3320	1/1	0.92	0.27	77,77,77,77	0
58	MG	13	1601	1/1	0.92	0.17	68,68,68,68	0
58	MG	1H	3250	1/1	0.92	0.23	74,74,74,74	0
58	MG	13	1612	1/1	0.92	0.18	63,63,63,63	0
58	MG	41	201	1/1	0.92	0.14	78,78,78,78	0
58	MG	14	3200	1/1	0.92	0.52	74,74,74,74	0
58	MG	1H	3163	1/1	0.92	0.30	50,50,50,50	0
58	MG	1H	3140	1/1	0.92	0.13	58,58,58,58	0
58	MG	1H	3018	1/1	0.92	0.30	71,71,71,71	0
58	MG	14	3307	1/1	0.92	0.28	101,101,101,101	0
58	MG	14	3105	1/1	0.92	0.16	67,67,67,67	0
58	MG	13	1732	1/1	0.92	0.16	65,65,65,65	0
58	MG	14	3209	1/1	0.92	0.14	66,66,66,66	0
58	MG	J8	101	1/1	0.92	0.19	66,66,66,66	0
58	MG	1H	3145	1/1	0.92	0.16	73,73,73,73	0
58	MG	14	3025	1/1	0.92	0.28	84,84,84,84	0
58	MG	1H	3329	1/1	0.92	0.32	81,81,81,81	0
58	MG	1H	3281	1/1	0.92	0.14	88,88,88,88	0
58	MG	14	3114	1/1	0.92	0.18	58,58,58,58	0
58	MG	14	3268	1/1	0.92	0.27	94,94,94,94	0
58	MG	1H	3039	1/1	0.92	0.15	68,68,68,68	0
58	MG	14	3169	1/1	0.92	0.18	58,58,58,58	0
58	MG	14	3272	1/1	0.92	0.25	76,76,76,76	0
58	MG	1H	3147	1/1	0.92	0.19	64,64,64,64	0
58	MG	14	3119	1/1	0.92	0.22	62,62,62,62	0
58	MG	13	1610	1/1	0.92	0.18	80,80,80,80	0
58	MG	14	3075	1/1	0.92	0.18	68,68,68,68	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	14	3277	1/1	0.92	0.21	85,85,85,85	0
58	MG	13	1694	1/1	0.92	0.30	64,64,64,64	0
58	MG	13	1617	1/1	0.92	0.12	83,83,83,83	0
58	MG	14	3178	1/1	0.92	0.20	84,84,84,84	0
58	MG	1G	1643	1/1	0.92	0.18	132,132,132,132	0
58	MG	1H	3006	1/1	0.92	0.21	46,46,46,46	0
58	MG	1H	3175	1/1	0.92	0.26	65,65,65,65	0
58	MG	14	3284	1/1	0.92	0.32	78,78,78,78	0
58	MG	1H	3119	1/1	0.92	0.13	69,69,69,69	0
58	MG	14	3207	1/1	0.93	0.16	80,80,80,80	0
58	MG	1H	3085	1/1	0.93	0.17	63,63,63,63	0
58	MG	1H	3159	1/1	0.93	0.24	67,67,67,67	0
58	MG	1H	3086	1/1	0.93	0.18	70,70,70,70	0
58	MG	14	3036	1/1	0.93	0.33	96,96,96,96	0
58	MG	1H	3161	1/1	0.93	0.21	84,84,84,84	0
58	MG	1H	3088	1/1	0.93	0.24	68,68,68,68	0
58	MG	1G	1669	1/1	0.93	0.19	107,107,107,107	0
58	MG	13	1642	1/1	0.93	0.17	74,74,74,74	0
58	MG	14	3219	1/1	0.93	0.12	48,48,48,48	0
58	MG	14	3220	1/1	0.93	0.39	76,76,76,76	0
58	MG	1H	3063	1/1	0.93	0.06	78,78,78,78	0
58	MG	1G	1632	1/1	0.93	0.23	75,75,75,75	0
58	MG	14	3046	1/1	0.93	0.12	66,66,66,66	0
58	MG	14	3097	1/1	0.93	0.14	65,65,65,65	0
58	MG	14	3161	1/1	0.93	0.21	70,70,70,70	0
58	MG	14	3162	1/1	0.93	0.31	70,70,70,70	0
58	MG	1H	3064	1/1	0.93	0.11	65,65,65,65	0
58	MG	21	301	1/1	0.93	0.33	54,54,54,54	0
58	MG	13	1731	1/1	0.93	0.18	84,84,84,84	0
58	MG	1G	1690	1/1	0.93	0.12	93,93,93,93	0
58	MG	1H	3030	1/1	0.93	0.11	67,67,67,67	0
58	MG	1H	3095	1/1	0.93	0.20	65,65,65,65	0
58	MG	1H	3169	1/1	0.93	0.18	85,85,85,85	0
58	MG	13	1645	1/1	0.93	0.30	64,64,64,64	0
58	MG	1H	3097	1/1	0.93	0.27	71,71,71,71	0
58	MG	14	3237	1/1	0.93	0.15	83,83,83,83	0
58	MG	1H	3048	1/1	0.93	0.17	56,56,56,56	0
58	MG	1H	3138	1/1	0.93	0.22	58,58,58,58	0
58	MG	14	3240	1/1	0.93	0.10	83,83,83,83	0
58	MG	1H	3001	1/1	0.93	0.16	43,43,43,43	0
58	MG	1H	3022	1/1	0.93	0.21	62,62,62,62	0
58	MG	14	3115	1/1	0.93	0.26	80,80,80,80	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	1H	3105	1/1	0.93	0.22	66,66,66,66	0
58	MG	14	3061	1/1	0.93	0.14	81,81,81,81	0
58	MG	14	3246	1/1	0.93	0.07	69,69,69,69	0
58	MG	1H	3177	1/1	0.93	0.17	74,74,74,74	0
58	MG	1H	3142	1/1	0.93	0.27	68,68,68,68	0
58	MG	1H	3106	1/1	0.93	0.21	63,63,63,63	0
58	MG	1G	1649	1/1	0.93	0.29	83,83,83,83	0
58	MG	14	3124	1/1	0.93	0.26	54,54,54,54	0
58	MG	1H	3002	1/1	0.93	0.13	38,38,38,38	0
58	MG	13	1655	1/1	0.93	0.29	87,87,87,87	0
58	MG	14	3127	1/1	0.93	0.19	69,69,69,69	0
58	MG	13	1616	1/1	0.93	0.04	88,88,88,88	0
58	MG	14	3398	1/1	0.93	0.06	108,108,108,108	0
58	MG	1H	3148	1/1	0.93	0.16	50,50,50,50	0
58	MG	1H	3055	1/1	0.93	0.21	49,49,49,49	0
58	MG	1K	101	1/1	0.93	0.06	145,145,145,145	0
58	MG	1H	3151	1/1	0.93	0.12	55,55,55,55	0
58	MG	1H	3301	1/1	0.93	0.35	84,84,84,84	0
58	MG	13	1619	1/1	0.93	0.14	91,91,91,91	0
58	MG	29	302	1/1	0.93	0.22	65,65,65,65	0
58	MG	1H	3040	1/1	0.93	0.28	70,70,70,70	0
58	MG	1H	3041	1/1	0.93	0.16	76,76,76,76	0
58	MG	1H	3083	1/1	0.93	0.23	67,67,67,67	0
58	MG	1H	3357	1/1	0.93	0.11	71,71,71,71	0
58	MG	1G	1621	1/1	0.93	0.10	92,92,92,92	0
58	MG	14	3031	1/1	0.93	0.27	68,68,68,68	0
58	MG	14	3270	1/1	0.93	0.19	63,63,63,63	0
58	MG	55	201	1/1	0.93	0.27	74,74,74,74	0
58	MG	14	3145	1/1	0.93	0.16	65,65,65,65	0
58	MG	14	3206	1/1	0.93	0.12	80,80,80,80	0
58	MG	1H	3375	1/1	0.94	0.15	60,60,60,60	0
58	MG	14	3006	1/1	0.94	0.32	56,56,56,56	0
58	MG	14	3109	1/1	0.94	0.24	73,73,73,73	0
58	MG	1H	3181	1/1	0.94	0.10	61,61,61,61	0
58	MG	14	3208	1/1	0.94	0.10	91,91,91,91	0
58	MG	1H	3312	1/1	0.94	0.15	67,67,67,67	0
58	MG	14	3032	1/1	0.94	0.29	75,75,75,75	0
58	MG	1H	3193	1/1	0.94	0.38	73,73,73,73	0
58	MG	1H	3441	1/1	0.94	0.06	89,89,89,89	0
58	MG	14	3087	1/1	0.94	0.18	40,40,40,40	0
58	MG	1H	3067	1/1	0.94	0.20	55,55,55,55	0
58	MG	1H	3315	1/1	0.94	0.24	76,76,76,76	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	1H	3052	1/1	0.94	0.12	53,53,53,53	0
58	MG	14	3358	1/1	0.94	0.13	91,91,91,91	0
58	MG	14	3396	1/1	0.94	0.08	108,108,108,108	0
58	MG	13	1614	1/1	0.94	0.16	78,78,78,78	0
58	MG	13	1644	1/1	0.94	0.25	96,96,96,96	0
58	MG	14	3093	1/1	0.94	0.18	42,42,42,42	0
58	MG	13	1719	1/1	0.94	0.06	71,71,71,71	0
58	MG	14	3157	1/1	0.94	0.10	57,57,57,57	0
58	MG	1H	3212	1/1	0.94	0.19	76,76,76,76	0
58	MG	14	3225	1/1	0.94	0.27	82,82,82,82	0
58	MG	13	1649	1/1	0.94	0.18	72,72,72,72	0
58	MG	14	3128	1/1	0.94	0.22	58,58,58,58	0
58	MG	1H	3244	1/1	0.94	0.17	62,62,62,62	0
58	MG	1G	1689	1/1	0.94	0.07	121,121,121,121	0
58	MG	1H	3057	1/1	0.94	0.22	66,66,66,66	0
58	MG	6A	101	1/1	0.94	0.24	93,93,93,93	0
58	MG	1H	3124	1/1	0.94	0.16	46,46,46,46	0
58	MG	14	3199	1/1	0.94	0.23	69,69,69,69	0
58	MG	1H	3012	1/1	0.94	0.37	83,83,83,83	0
58	MG	1H	3110	1/1	0.94	0.30	55,55,55,55	0
58	MG	1H	3364	1/1	0.94	0.06	98,98,98,98	0
58	MG	14	3172	1/1	0.94	0.37	70,70,70,70	0
58	MG	1H	3235	1/1	0.95	0.08	53,53,53,53	0
58	MG	13	1708	1/1	0.95	0.07	89,89,89,89	0
58	MG	14	3039	1/1	0.95	0.10	50,50,50,50	0
58	MG	L8	101	1/1	0.95	0.31	84,84,84,84	0
58	MG	1H	3134	1/1	0.95	0.08	69,69,69,69	0
58	MG	14	3110	1/1	0.95	0.19	57,57,57,57	0
58	MG	1H	3238	1/1	0.95	0.12	65,65,65,65	0
58	MG	1H	3034	1/1	0.95	0.28	80,80,80,80	0
58	MG	1H	3368	1/1	0.95	0.10	74,74,74,74	0
58	MG	1H	3014	1/1	0.95	0.23	70,70,70,70	0
58	MG	1H	3047	1/1	0.95	0.17	47,47,47,47	0
58	MG	1H	3084	1/1	0.95	0.14	94,94,94,94	0
58	MG	1H	3426	1/1	0.95	0.09	58,58,58,58	0
58	MG	1H	3261	1/1	0.95	0.15	69,69,69,69	0
58	MG	1H	3109	1/1	0.95	0.12	47,47,47,47	0
58	MG	1H	3446	1/1	0.95	0.10	84,84,84,84	0
58	MG	1H	3457	1/1	0.95	0.07	141,141,141,141	0
58	MG	14	3324	1/1	0.95	0.06	99,99,99,99	0
58	MG	14	3123	1/1	0.95	0.16	64,64,64,64	0
58	MG	14	3380	1/1	0.95	0.06	96,96,96,96	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	14	3391	1/1	0.95	0.13	104,104,104,104	0
58	MG	14	3392	1/1	0.95	0.05	128,128,128,128	0
58	MG	1H	3466	1/1	0.95	0.17	56,56,56,56	0
58	MG	14	3164	1/1	0.95	0.28	74,74,74,74	0
58	MG	13	1693	1/1	0.95	0.15	55,55,55,55	0
58	MG	1H	3245	1/1	0.95	0.34	62,62,62,62	0
58	MG	13	1613	1/1	0.95	0.08	81,81,81,81	0
58	MG	1G	1680	1/1	0.95	0.05	140,140,140,140	0
58	MG	1H	3156	1/1	0.95	0.25	67,67,67,67	0
58	MG	14	3170	1/1	0.95	0.14	83,83,83,83	0
58	MG	1H	3229	1/1	0.95	0.17	48,48,48,48	0
58	MG	16	205	1/1	0.95	0.08	81,81,81,81	0
58	MG	1H	3112	1/1	0.95	0.20	56,56,56,56	0
58	MG	14	3212	1/1	0.95	0.34	70,70,70,70	0
58	MG	1H	3098	1/1	0.95	0.14	53,53,53,53	0
58	MG	14	3066	1/1	0.95	0.28	62,62,62,62	0
58	MG	1H	3077	1/1	0.95	0.12	60,60,60,60	0
58	MG	14	3137	1/1	0.95	0.05	57,57,57,57	0
58	MG	1H	3272	1/1	0.95	0.13	64,64,64,64	0
58	MG	1H	3062	1/1	0.95	0.17	64,64,64,64	0
58	MG	14	3103	1/1	0.95	0.13	51,51,51,51	0
58	MG	1H	3274	1/1	0.95	0.17	59,59,59,59	0
58	MG	1H	3465	1/1	0.96	0.09	71,71,71,71	0
58	MG	1H	3121	1/1	0.96	0.20	62,62,62,62	0
58	MG	14	3063	1/1	0.96	0.12	58,58,58,58	0
58	MG	13	1720	1/1	0.96	0.06	90,90,90,90	0
58	MG	1H	3123	1/1	0.96	0.10	69,69,69,69	0
58	MG	13	1727	1/1	0.96	0.05	112,112,112,112	0
58	MG	1G	1608	1/1	0.96	0.09	89,89,89,89	0
58	MG	13	1729	1/1	0.96	0.05	113,113,113,113	0
58	MG	13	1707	1/1	0.96	0.07	76,76,76,76	0
58	MG	1H	3370	1/1	0.96	0.11	71,71,71,71	0
58	MG	14	3136	1/1	0.96	0.09	62,62,62,62	0
58	MG	14	3040	1/1	0.96	0.19	59,59,59,59	0
58	MG	14	3041	1/1	0.96	0.15	54,54,54,54	0
58	MG	14	3353	1/1	0.96	0.04	118,118,118,118	0
58	MG	14	3357	1/1	0.96	0.11	76,76,76,76	0
58	MG	16	209	1/1	0.96	0.08	100,100,100,100	0
58	MG	14	3363	1/1	0.96	0.06	72,72,72,72	0
58	MG	1H	3114	1/1	0.96	0.30	74,74,74,74	0
58	MG	14	3389	1/1	0.96	0.07	102,102,102,102	0
58	MG	1H	3104	1/1	0.96	0.22	69,69,69,69	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	1H	3381	1/1	0.96	0.06	63,63,63,63	0
58	MG	14	3393	1/1	0.96	0.06	127,127,127,127	0
58	MG	14	3395	1/1	0.96	0.05	103,103,103,103	0
58	MG	1H	3413	1/1	0.96	0.05	102,102,102,102	0
58	MG	1H	3078	1/1	0.96	0.24	67,67,67,67	0
58	MG	1H	3234	1/1	0.96	0.05	66,66,66,66	0
58	MG	13	1626	1/1	0.96	0.17	69,69,69,69	0
58	MG	1H	3087	1/1	0.96	0.31	70,70,70,70	0
58	MG	14	3218	1/1	0.96	0.28	62,62,62,62	0
58	MG	1H	3445	1/1	0.96	0.05	110,110,110,110	0
58	MG	1G	1622	1/1	0.96	0.38	92,92,92,92	0
58	MG	14	3256	1/1	0.96	0.28	83,83,83,83	0
58	MG	14	3151	1/1	0.96	0.27	79,79,79,79	0
58	MG	1G	1623	1/1	0.96	0.21	62,62,62,62	0
58	MG	1G	1678	1/1	0.96	0.06	128,128,128,128	0
58	MG	1G	1624	1/1	0.96	0.23	65,65,65,65	0
58	MG	1G	1681	1/1	0.96	0.06	78,78,78,78	0
58	MG	P8	101	1/1	0.96	0.31	77,77,77,77	0
58	MG	14	3263	1/1	0.96	0.17	75,75,75,75	0
58	MG	1H	3157	1/1	0.96	0.28	73,73,73,73	0
58	MG	13	1673	1/1	0.96	0.33	70,70,70,70	0
58	MG	1H	3463	1/1	0.96	0.05	112,112,112,112	0
58	MG	14	3160	1/1	0.96	0.17	72,72,72,72	0
58	MG	14	3182	1/1	0.97	0.30	75,75,75,75	0
58	MG	1G	1682	1/1	0.97	0.05	97,97,97,97	0
58	MG	1G	1686	1/1	0.97	0.07	125,125,125,125	0
58	MG	1G	1687	1/1	0.97	0.07	139,139,139,139	0
58	MG	1H	3339	1/1	0.97	0.17	48,48,48,48	0
58	MG	1H	3383	1/1	0.97	0.07	60,60,60,60	0
58	MG	1H	3399	1/1	0.97	0.07	62,62,62,62	0
58	MG	13	1665	1/1	0.97	0.04	82,82,82,82	0
58	MG	14	3364	1/1	0.97	0.08	85,85,85,85	0
58	MG	14	3376	1/1	0.97	0.04	94,94,94,94	0
58	MG	1H	3417	1/1	0.97	0.08	94,94,94,94	0
58	MG	14	3385	1/1	0.97	0.04	116,116,116,116	0
58	MG	1H	3113	1/1	0.97	0.23	51,51,51,51	0
58	MG	1H	3425	1/1	0.97	0.05	63,63,63,63	0
58	MG	1H	3195	1/1	0.97	0.27	62,62,62,62	0
58	MG	14	3005	1/1	0.97	0.24	48,48,48,48	0
58	MG	1H	3433	1/1	0.97	0.12	87,87,87,87	0
58	MG	1H	3343	1/1	0.97	0.06	54,54,54,54	0
58	MG	88	201	1/1	0.97	0.17	81,81,81,81	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	13	1674	1/1	0.97	0.06	91,91,91,91	0
58	MG	14	3298	1/1	0.97	0.37	64,64,64,64	0
58	MG	14	3010	1/1	0.97	0.23	41,41,41,41	0
58	MG	14	3102	1/1	0.97	0.07	61,61,61,61	0
58	MG	1H	3443	1/1	0.97	0.11	76,76,76,76	0
58	MG	1H	3115	1/1	0.97	0.13	43,43,43,43	0
58	MG	1H	3367	1/1	0.97	0.05	71,71,71,71	0
58	MG	1H	3447	1/1	0.97	0.07	86,86,86,86	0
58	MG	1H	3452	1/1	0.97	0.06	104,104,104,104	0
58	MG	29	304	1/1	0.97	0.26	81,81,81,81	0
58	MG	13	1725	1/1	0.97	0.05	94,94,94,94	0
58	MG	1H	3459	1/1	0.97	0.05	106,106,106,106	0
58	MG	1H	3070	1/1	0.97	0.21	58,58,58,58	0
58	MG	1H	3464	1/1	0.97	0.04	107,107,107,107	0
58	MG	13	1710	1/1	0.97	0.04	97,97,97,97	0
58	MG	1G	1679	1/1	0.97	0.08	119,119,119,119	0
58	MG	45	202	1/1	0.97	0.19	72,72,72,72	0
58	MG	1H	3046	1/1	0.97	0.17	47,47,47,47	0
58	MG	1H	3379	1/1	0.97	0.07	73,73,73,73	0
58	MG	14	3116	1/1	0.97	0.11	64,64,64,64	0
60	ZN	C5	201	1/1	0.97	0.07	165,165,165,165	0
58	MG	1H	3361	1/1	0.98	0.05	63,63,63,63	0
58	MG	1H	3442	1/1	0.98	0.05	69,69,69,69	0
58	MG	13	1715	1/1	0.98	0.07	109,109,109,109	0
58	MG	1H	3365	1/1	0.98	0.09	74,74,74,74	0
58	MG	1G	1676	1/1	0.98	0.05	90,90,90,90	0
58	MG	14	3319	1/1	0.98	0.09	59,59,59,59	0
58	MG	14	3321	1/1	0.98	0.04	78,78,78,78	0
58	MG	14	3322	1/1	0.98	0.05	65,65,65,65	0
58	MG	13	1638	1/1	0.98	0.08	59,59,59,59	0
58	MG	14	3325	1/1	0.98	0.04	63,63,63,63	0
58	MG	14	3326	1/1	0.98	0.05	90,90,90,90	0
58	MG	14	3327	1/1	0.98	0.04	59,59,59,59	0
58	MG	14	3333	1/1	0.98	0.06	74,74,74,74	0
58	MG	14	3335	1/1	0.98	0.04	61,61,61,61	0
58	MG	14	3336	1/1	0.98	0.04	62,62,62,62	0
58	MG	14	3345	1/1	0.98	0.04	90,90,90,90	0
58	MG	14	3347	1/1	0.98	0.03	108,108,108,108	0
58	MG	14	3349	1/1	0.98	0.04	83,83,83,83	0
58	MG	14	3352	1/1	0.98	0.08	97,97,97,97	0
58	MG	1H	3270	1/1	0.98	0.54	80,80,80,80	0
58	MG	14	3355	1/1	0.98	0.04	102,102,102,102	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	1H	3451	1/1	0.98	0.04	114,114,114,114	0
58	MG	13	1643	1/1	0.98	0.09	99,99,99,99	0
58	MG	14	3362	1/1	0.98	0.03	77,77,77,77	0
58	MG	1H	3454	1/1	0.98	0.04	96,96,96,96	0
58	MG	14	3072	1/1	0.98	0.10	45,45,45,45	0
58	MG	14	3365	1/1	0.98	0.06	94,94,94,94	0
58	MG	14	3369	1/1	0.98	0.06	59,59,59,59	0
58	MG	14	3372	1/1	0.98	0.04	70,70,70,70	0
58	MG	14	3374	1/1	0.98	0.09	76,76,76,76	0
58	MG	14	3375	1/1	0.98	0.05	97,97,97,97	0
58	MG	1G	1683	1/1	0.98	0.04	89,89,89,89	0
58	MG	14	3378	1/1	0.98	0.06	100,100,100,100	0
58	MG	1G	1685	1/1	0.98	0.05	87,87,87,87	0
58	MG	14	3381	1/1	0.98	0.04	81,81,81,81	0
58	MG	14	3382	1/1	0.98	0.06	87,87,87,87	0
58	MG	14	3383	1/1	0.98	0.05	86,86,86,86	0
58	MG	14	3384	1/1	0.98	0.06	83,83,83,83	0
58	MG	1H	3456	1/1	0.98	0.06	97,97,97,97	0
58	MG	14	3386	1/1	0.98	0.04	90,90,90,90	0
58	MG	14	3387	1/1	0.98	0.04	96,96,96,96	0
58	MG	1H	3099	1/1	0.98	0.06	55,55,55,55	0
58	MG	1G	1688	1/1	0.98	0.03	138,138,138,138	0
58	MG	13	1722	1/1	0.98	0.05	103,103,103,103	0
58	MG	1H	3461	1/1	0.98	0.11	92,92,92,92	0
58	MG	14	3394	1/1	0.98	0.07	109,109,109,109	0
58	MG	1H	3462	1/1	0.98	0.04	97,97,97,97	0
58	MG	1H	3092	1/1	0.98	0.07	49,49,49,49	0
58	MG	1H	3102	1/1	0.98	0.19	35,35,35,35	0
58	MG	1H	3143	1/1	0.98	0.06	56,56,56,56	0
58	MG	1H	3387	1/1	0.98	0.04	80,80,80,80	0
58	MG	1H	3393	1/1	0.98	0.10	54,54,54,54	0
58	MG	1H	3289	1/1	0.98	0.07	49,49,49,49	0
58	MG	1H	3403	1/1	0.98	0.04	76,76,76,76	0
58	MG	1H	3406	1/1	0.98	0.07	76,76,76,76	0
58	MG	1J	205	1/1	0.98	0.04	101,101,101,101	0
58	MG	1H	3412	1/1	0.98	0.05	78,78,78,78	0
58	MG	13	1711	1/1	0.98	0.04	97,97,97,97	0
58	MG	13	1712	1/1	0.98	0.05	83,83,83,83	0
58	MG	1H	3418	1/1	0.98	0.05	92,92,92,92	0
58	MG	1H	3345	1/1	0.98	0.06	61,61,61,61	0
58	MG	1H	3347	1/1	0.98	0.13	51,51,51,51	0
58	MG	1H	3354	1/1	0.98	0.04	49,49,49,49	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	1H	3429	1/1	0.98	0.04	71,71,71,71	0
58	MG	14	3138	1/1	0.98	0.16	45,45,45,45	0
58	MG	13	1728	1/1	0.98	0.03	118,118,118,118	0
58	MG	1H	3435	1/1	0.98	0.04	56,56,56,56	0
58	MG	1H	3436	1/1	0.98	0.10	73,73,73,73	0
58	MG	1H	3437	1/1	0.98	0.07	58,58,58,58	0
59	SF4	3E	301	8/8	0.98	0.03	86,99,103,105	0
58	MG	1H	3360	1/1	0.98	0.04	61,61,61,61	0
60	ZN	5A	101	1/1	0.98	0.04	142,142,142,142	0
58	MG	1H	3439	1/1	0.98	0.05	99,99,99,99	0
58	MG	1H	3371	1/1	0.99	0.04	59,59,59,59	0
58	MG	14	3320	1/1	0.99	0.06	64,64,64,64	0
58	MG	1G	1677	1/1	0.99	0.09	96,96,96,96	0
58	MG	1H	3372	1/1	0.99	0.03	62,62,62,62	0
58	MG	14	3323	1/1	0.99	0.04	64,64,64,64	0
58	MG	1H	3373	1/1	0.99	0.04	51,51,51,51	0
58	MG	13	1724	1/1	0.99	0.06	102,102,102,102	0
58	MG	1H	3348	1/1	0.99	0.05	50,50,50,50	0
58	MG	1H	3377	1/1	0.99	0.06	70,70,70,70	0
58	MG	14	3328	1/1	0.99	0.03	74,74,74,74	0
58	MG	14	3329	1/1	0.99	0.03	56,56,56,56	0
58	MG	14	3330	1/1	0.99	0.03	77,77,77,77	0
58	MG	14	3332	1/1	0.99	0.03	53,53,53,53	0
58	MG	1H	3349	1/1	0.99	0.05	64,64,64,64	0
58	MG	1G	1684	1/1	0.99	0.03	109,109,109,109	0
58	MG	1H	3380	1/1	0.99	0.03	59,59,59,59	0
58	MG	14	3337	1/1	0.99	0.03	66,66,66,66	0
58	MG	14	3338	1/1	0.99	0.10	60,60,60,60	0
58	MG	14	3340	1/1	0.99	0.03	79,79,79,79	0
58	MG	14	3341	1/1	0.99	0.08	68,68,68,68	0
58	MG	14	3342	1/1	0.99	0.05	80,80,80,80	0
58	MG	14	3343	1/1	0.99	0.07	82,82,82,82	0
58	MG	14	3344	1/1	0.99	0.08	81,81,81,81	0
58	MG	1H	3444	1/1	0.99	0.04	69,69,69,69	0
58	MG	14	3346	1/1	0.99	0.07	85,85,85,85	0
58	MG	1H	3350	1/1	0.99	0.03	48,48,48,48	0
58	MG	14	3348	1/1	0.99	0.06	70,70,70,70	0
58	MG	1H	3353	1/1	0.99	0.06	57,57,57,57	0
58	MG	14	3350	1/1	0.99	0.03	85,85,85,85	0
58	MG	14	3351	1/1	0.99	0.04	85,85,85,85	0
58	MG	1H	3384	1/1	0.99	0.04	58,58,58,58	0
58	MG	1H	3448	1/1	0.99	0.03	82,82,82,82	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	1H	3449	1/1	0.99	0.07	106,106,106,106	0
58	MG	14	3356	1/1	0.99	0.04	58,58,58,58	0
58	MG	1H	3450	1/1	0.99	0.02	54,54,54,54	0
58	MG	1H	3385	1/1	0.99	0.07	47,47,47,47	0
58	MG	14	3359	1/1	0.99	0.03	79,79,79,79	0
58	MG	14	3360	1/1	0.99	0.04	83,83,83,83	0
58	MG	14	3361	1/1	0.99	0.03	64,64,64,64	0
58	MG	14	3001	1/1	0.99	0.04	46,46,46,46	0
58	MG	13	1717	1/1	0.99	0.05	92,92,92,92	0
58	MG	1H	3453	1/1	0.99	0.03	84,84,84,84	0
58	MG	1H	3388	1/1	0.99	0.03	77,77,77,77	0
58	MG	14	3366	1/1	0.99	0.02	86,86,86,86	0
58	MG	14	3367	1/1	0.99	0.05	65,65,65,65	0
58	MG	14	3368	1/1	0.99	0.06	62,62,62,62	0
58	MG	1H	3455	1/1	0.99	0.05	59,59,59,59	0
58	MG	14	3370	1/1	0.99	0.04	64,64,64,64	0
58	MG	14	3371	1/1	0.99	0.04	53,53,53,53	0
58	MG	1H	3389	1/1	0.99	0.03	38,38,38,38	0
58	MG	14	3373	1/1	0.99	0.05	61,61,61,61	0
58	MG	1H	3391	1/1	0.99	0.03	61,61,61,61	0
58	MG	1H	3458	1/1	0.99	0.09	73,73,73,73	0
58	MG	1H	3392	1/1	0.99	0.03	68,68,68,68	0
58	MG	1H	3460	1/1	0.99	0.03	104,104,104,104	0
58	MG	1H	3355	1/1	0.99	0.06	48,48,48,48	0
58	MG	1H	3394	1/1	0.99	0.08	53,53,53,53	0
58	MG	1H	3395	1/1	0.99	0.03	77,77,77,77	0
58	MG	1H	3397	1/1	0.99	0.04	71,71,71,71	0
58	MG	13	1726	1/1	0.99	0.03	126,126,126,126	0
58	MG	1H	3400	1/1	0.99	0.03	72,72,72,72	0
58	MG	1H	3402	1/1	0.99	0.03	51,51,51,51	0
58	MG	1H	3358	1/1	0.99	0.04	45,45,45,45	0
58	MG	14	3388	1/1	0.99	0.10	68,68,68,68	0
58	MG	1H	3405	1/1	0.99	0.03	63,63,63,63	0
58	MG	14	3390	1/1	0.99	0.03	89,89,89,89	0
58	MG	1H	3359	1/1	0.99	0.06	59,59,59,59	0
58	MG	1H	3407	1/1	0.99	0.07	116,116,116,116	0
58	MG	1H	3408	1/1	0.99	0.07	82,82,82,82	0
58	MG	16	207	1/1	0.99	0.03	80,80,80,80	0
58	MG	16	208	1/1	0.99	0.04	86,86,86,86	0
58	MG	1H	3409	1/1	0.99	0.02	85,85,85,85	0
58	MG	1H	3410	1/1	0.99	0.03	58,58,58,58	0
58	MG	1H	3411	1/1	0.99	0.04	69,69,69,69	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	13	1718	1/1	0.99	0.07	83,83,83,83	0
58	MG	13	1714	1/1	0.99	0.03	73,73,73,73	0
58	MG	1H	3414	1/1	0.99	0.04	80,80,80,80	0
58	MG	1H	3415	1/1	0.99	0.05	73,73,73,73	0
58	MG	1H	3362	1/1	0.99	0.04	53,53,53,53	0
58	MG	13	1709	1/1	0.99	0.08	92,92,92,92	0
58	MG	I8	103	1/1	0.99	0.07	73,73,73,73	0
58	MG	1H	3419	1/1	0.99	0.04	101,101,101,101	0
58	MG	1H	3420	1/1	0.99	0.04	92,92,92,92	0
58	MG	1H	3421	1/1	0.99	0.03	64,64,64,64	0
58	MG	13	1716	1/1	0.99	0.03	76,76,76,76	0
58	MG	1H	3423	1/1	0.99	0.03	66,66,66,66	0
58	MG	1H	3424	1/1	0.99	0.04	48,48,48,48	0
58	MG	1H	3344	1/1	0.99	0.02	58,58,58,58	0
58	MG	13	1723	1/1	0.99	0.03	87,87,87,87	0
58	MG	1H	3428	1/1	0.99	0.06	51,51,51,51	0
58	MG	1H	3369	1/1	0.99	0.06	49,49,49,49	0
58	MG	1H	3430	1/1	0.99	0.08	49,49,49,49	0
58	MG	1H	3431	1/1	0.99	0.04	70,70,70,70	0
58	MG	1H	3432	1/1	0.99	0.03	50,50,50,50	0
59	SF4	32	301	8/8	0.99	0.03	115,123,133,136	0
58	MG	1H	3346	1/1	0.99	0.03	45,45,45,45	0
58	MG	1H	3434	1/1	0.99	0.05	51,51,51,51	0
58	MG	14	3318	1/1	0.99	0.10	64,64,64,64	0
58	MG	1H	3382	1/1	1.00	0.03	77,77,77,77	0
58	MG	1H	3366	1/1	1.00	0.04	76,76,76,76	0
58	MG	1H	3396	1/1	1.00	0.02	78,78,78,78	0
58	MG	1H	3374	1/1	1.00	0.04	53,53,53,53	0
58	MG	1H	3398	1/1	1.00	0.08	66,66,66,66	0
58	MG	1H	3351	1/1	1.00	0.03	46,46,46,46	0
58	MG	14	3377	1/1	1.00	0.03	52,52,52,52	0
58	MG	1H	3416	1/1	1.00	0.03	69,69,69,69	0
58	MG	14	3379	1/1	1.00	0.02	60,60,60,60	0
58	MG	14	3354	1/1	1.00	0.03	70,70,70,70	0
58	MG	14	3331	1/1	1.00	0.02	63,63,63,63	0
58	MG	16	206	1/1	1.00	0.01	73,73,73,73	0
58	MG	1H	3386	1/1	1.00	0.02	57,57,57,57	0
58	MG	14	3334	1/1	1.00	0.06	64,64,64,64	0
58	MG	1H	3401	1/1	1.00	0.03	69,69,69,69	0
58	MG	1H	3356	1/1	1.00	0.05	42,42,42,42	0
58	MG	1H	3352	1/1	1.00	0.02	61,61,61,61	0
58	MG	1H	3404	1/1	1.00	0.03	48,48,48,48	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	14	3339	1/1	1.00	0.03	82,82,82,82	0
58	MG	1H	3440	1/1	1.00	0.04	58,58,58,58	0
58	MG	1H	3378	1/1	1.00	0.04	53,53,53,53	0
58	MG	1H	3390	1/1	1.00	0.06	50,50,50,50	0
58	MG	1H	3363	1/1	1.00	0.02	68,68,68,68	0
60	ZN	5I	101	1/1	1.00	0.03	102,102,102,102	0
58	MG	13	1713	1/1	1.00	0.03	101,101,101,101	0
58	MG	13	1721	1/1	1.00	0.02	66,66,66,66	0
58	MG	1H	3427	1/1	1.00	0.02	72,72,72,72	0

5.5 Other polymers [i](#)

There are no such residues in this entry.