



Full wwPDB X-ray Structure Validation Report ⓘ

Sep 16, 2026 – 09:05 am BST

PDB ID : 5EL5 / pdb_00005el5
Title : Structure of T. thermophilus 70S ribosome complex with mRNA and tRNA^{Lys} in the A-site with a U-U mismatch in the second position
Authors : Rozov, A.; Demeshkina, N.; Khusainov, I.; Yusupov, M.; Yusupova, G.
Deposited on : 2015-11-04
Resolution : 3.15 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	FAILED
Mogul	:	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

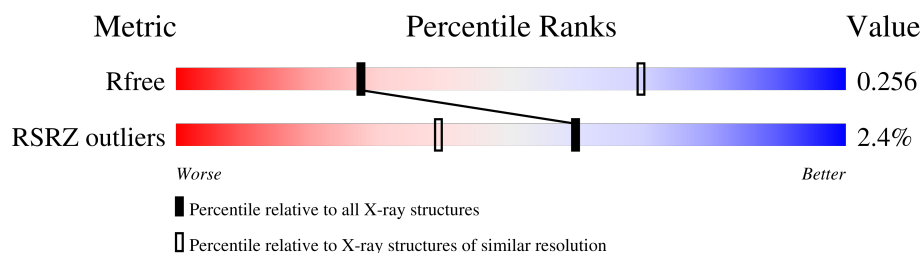
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.15 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	2361 (3.20-3.12)
RSRZ outliers	180081	2361 (3.20-3.12)

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	13	1648	-	-	-	X
58	MG	14	3089	-	-	-	X
58	MG	14	3188	-	-	-	X
58	MG	14	3247	-	-	-	X
58	MG	14	3260	-	-	-	X
58	MG	14	3294	-	-	-	X
58	MG	1H	3141	-	-	-	X
58	MG	1H	3235	-	-	-	X
58	MG	1H	3289	-	-	-	X

2 Entry composition

There are 61 unique types of molecules in this entry. The entry contains 292607 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	1493	Total	C	N	O	P	0	0	0
			32097	14286	5951	10367	1493			
1	1G	1496	Total	C	N	O	P	0	0	0
			32152	14311	5953	10392	1496			

- 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	206	Total	C	N	O	S	0	0	0
			1695	1082	305	304	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	194	Total	C	N	O	S	0	0	0
			1529	967	296	265	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
			1696	1062	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	149	Total	C	N	O	S	0	0	0
			1136	716	216	200	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	151	Total	C	N	O	S	0	0	0
			1229	763	247	213	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				
9	82	105	Total	C	N	O		0	0	0
			820	523	158	139				

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	1I	72	Total	C	N	O	S	0	0	0
			593	373	115	104	1			

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
10	1A	60	Total	C	N	O	0	0	0
			474	298	91	85			

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

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

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

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

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

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

- 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	0	0	0
			491	312	104	71			
14	5A	48	Total	C	N	O	0	0	0
			388	245	82	57			

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	7I	80	Total	C	N	O	S	0	0	0
			671	427	132	111	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	67	Total	C	N	O	0	0	0
			544	349	104	91			
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	36	Total	C	N	O	S	0	0	0
			283	182	49	51	1			

- 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	98	Total	C	N	O	S	0	0	0
			757	467	161	127	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	23	Total	C	N	O	0	0	0
			204	126	49	29			

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

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
22	1K	69	Total	C	N	O	P	S	0	0	0
			1477	662	257	488	69	1			

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	3K	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	20	Total	C	N	O	P	0	0	0
			439	197	91	131	20			
25	4L	17	Total	C	N	O	P	0	0	0
			373	167	76	113	17			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	1H	2830	Total	C	N	O	P	0	0	0
			60960	27129	11403	19598	2830			
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 ribosomal RNA.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
28	71	135	Total	C	N	O	S	0	0	0
			1050	662	197	190	1			

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

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

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
30	29	203	Total	C	N	O	S	0	0	0
			1558	985	298	269	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
			1457	931	265	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	69	Total	C	N	O		0	0	0
			539	339	109	91				

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
35	58	138	Total	C	N	O	S	0	0	0
			1104	712	206	182	4			
35	15	137	Total	C	N	O	S	0	0	0
			1096	707	205	181	3			

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
37	78	147	Total	C	N	O	S	0	0	0
			1122	698	229	192	3			
37	35	148	Total	C	N	O	S	0	0	0
			1130	704	230	193	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	0	0	0
			881	556	176	149			
40	65	110	Total	C	N	O	0	0	0
			876	553	175	148			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
41	B8	135	Total	C	N	O	S	0	0	0
			1123	699	230	193	1			
41	75	136	Total	C	N	O		0	0	0
			1133	705	233	195				

- 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	101	Total	C	N	O	S	0	0	0
			778	501	142	134	1			
43	95	99	Total	C	N	O		0	0	0
			766	494	140	132				

- 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	110	Total	C	N	O	S	0	0	0
			876	552	171	151	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	0	0	0
			740	480	134	126			
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	104	Total	C	N	O	S	0	0	0
			788	507	149	127	5			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
46	C5	105	Total	C	N	O	S	0	0	0
			799	513	153	128	5			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
47	H8	148	Total	C	N	O	S	0	0	0
			1218	779	220	217	2			
47	D5	130	Total	C	N	O	S	0	0	0
			1064	685	191	186	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	78	Total	C	N	O	S	0	0	0
			616	381	130	104	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	67	Total	C	N	O	S	0	0	0
			563	349	114	99	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	45	Total	C	N	O	S	0	0	0
			391	240	97	52	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 tRNA^{Lys}.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
56	1L	74	Total	C	N	O	P	0	0	0
			1570	702	271	523	74			

- 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	0
			1611	721	281	534	75			

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

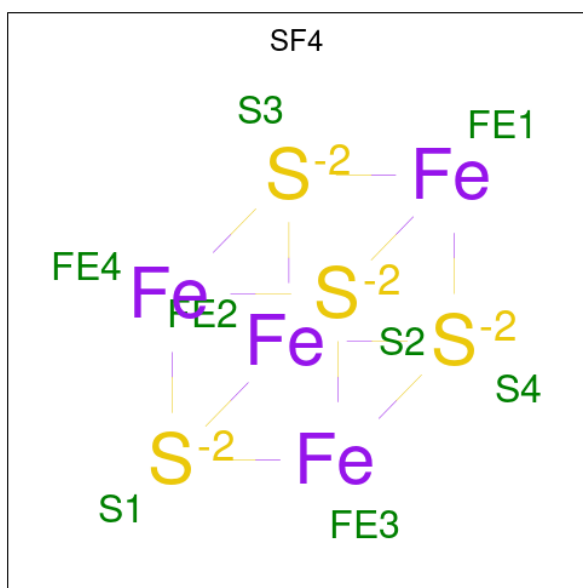
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
58	13	139	Total Mg 139 139	0	0
58	5E	2	Total Mg 2 2	0	0
58	5I	1	Total Mg 1 1	0	0
58	BI	1	Total Mg 1 1	0	0
58	1F	1	Total Mg 1 1	0	0
58	2K	3	Total Mg 3 3	0	0
58	4K	1	Total Mg 1 1	0	0
58	1H	489	Total Mg 489 489	0	0
58	16	12	Total Mg 12 12	0	0
58	11	1	Total Mg 1 1	0	0
58	21	2	Total Mg 2 2	0	0
58	41	1	Total Mg 1 1	0	0
58	78	1	Total Mg 1 1	0	0
58	88	2	Total Mg 2 2	0	0
58	D8	1	Total Mg 1 1	0	0
58	I8	1	Total Mg 1 1	0	0
58	P8	1	Total Mg 1 1	0	0
58	Q8	1	Total Mg 1 1	0	0
58	1G	77	Total Mg 77 77	0	0
58	32	1	Total Mg 1 1	0	0
58	2A	1	Total Mg 1 1	0	0
58	7A	1	Total Mg 1 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
58	2L	3	Total 3	Mg 3	0	0
58	14	419	Total 419	Mg 419	0	0
58	1J	6	Total 6	Mg 6	0	0
58	29	4	Total 4	Mg 4	0	0
58	39	1	Total 1	Mg 1	0	0
58	35	1	Total 1	Mg 1	0	0
58	45	3	Total 3	Mg 3	0	0
58	55	1	Total 1	Mg 1	0	0
58	85	1	Total 1	Mg 1	0	0
58	C5	1	Total 1	Mg 1	0	0
58	E5	1	Total 1	Mg 1	0	0
58	L5	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	148	Total	O	0	0
			148	148		
61	3E	2	Total	O	0	0
			2	2		
61	3I	2	Total	O	0	0
			2	2		
61	5I	1	Total	O	0	0
			1	1		
61	6I	1	Total	O	0	0
			1	1		
61	1K	1	Total	O	0	0
			1	1		
61	4K	6	Total	O	0	0
			6	6		
61	1H	670	Total	O	0	0
			670	670		
61	16	18	Total	O	0	0
			18	18		
61	11	9	Total	O	0	0
			9	9		
61	21	5	Total	O	0	0
			5	5		
61	31	6	Total	O	0	0
			6	6		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
61	58	2	Total 2	O 2	0	0
61	78	3	Total 3	O 3	0	0
61	B8	1	Total 1	O 1	0	0
61	D8	1	Total 1	O 1	0	0
61	E8	1	Total 1	O 1	0	0
61	G8	1	Total 1	O 1	0	0
61	I8	1	Total 1	O 1	0	0
61	Q8	1	Total 1	O 1	0	0
61	1G	44	Total 44	O 44	0	0
61	5A	3	Total 3	O 3	0	0
61	BA	1	Total 1	O 1	0	0
61	14	411	Total 411	O 411	0	0
61	1J	11	Total 11	O 11	0	0
61	19	4	Total 4	O 4	0	0
61	29	3	Total 3	O 3	0	0
61	39	8	Total 8	O 8	0	0
61	35	2	Total 2	O 2	0	0
61	55	1	Total 1	O 1	0	0
61	E5	1	Total 1	O 1	0	0
61	F5	2	Total 2	O 2	0	0
61	L5	1	Total 1	O 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
61	M5	2	Total	O	0	0
			2	2		

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3 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	208.40Å 447.10Å 616.90Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	152.44 – 3.15 152.44 – 3.15	Depositor EDS
% Data completeness (in resolution range)	100.0 (152.44-3.15) 92.0 (152.44-3.15)	Depositor EDS
R_{merge}	0.23	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.84 (at 3.13Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.198 , 0.254 0.196 , 0.256	Depositor DCC
R_{free} test set	2000 reflections (0.20%)	wwPDB-VP
Wilson B-factor (Å ²)	107.7	Xtriage
Anisotropy	0.223	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.26 , 55.8	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	292607	wwPDB-VP
Average B, all atoms (Å ²)	131.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.47% 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](#)

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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](#)

19 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	U8U	1K	34	22,25	19,24,25	2.66	6 (31%)	23,34,37	1.52	4 (17%)
22	T6A	1K	37	22	31,34,35	2.47	10 (32%)	44,49,52	3.27	19 (43%)
56	5MU	1L	54	56	19,22,23	3.81	5 (26%)	28,32,35	3.23	11 (39%)

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	1.96	3 (15%)	26,31,34	1.56	4 (15%)
22	PSU	1K	55	22	18,21,22	1.23	1 (5%)	22,30,33	1.83	4 (18%)
23	4SU	2K	8	23	18,21,22	1.84	3 (16%)	26,30,33	2.38	7 (26%)
23	4SU	2L	8	23	18,21,22	1.87	4 (22%)	26,30,33	2.83	7 (26%)
57	PSU	3L	39	57	18,21,22	1.11	1 (5%)	22,30,33	1.53	3 (13%)
23	5MU	2L	55	23	19,22,23	4.07	5 (26%)	28,32,35	3.14	11 (39%)
23	PSU	2L	56	23	18,21,22	1.28	2 (11%)	22,30,33	1.83	4 (18%)
56	PSU	1L	55	56	18,21,22	1.32	1 (5%)	22,30,33	1.82	4 (18%)
23	G7M	2L	47	23	23,26,27	2.45	8 (34%)	35,39,42	1.79	9 (25%)
23	G7M	2K	47	23	23,26,27	2.53	7 (30%)	35,39,42	1.60	8 (22%)
23	OMC	2K	33	23	19,22,23	1.67	3 (15%)	26,31,34	1.39	3 (11%)
23	5MU	2K	55	23	19,22,23	3.95	5 (26%)	28,32,35	3.43	9 (32%)
23	PSU	2K	56	23	18,21,22	1.37	2 (11%)	22,30,33	2.43	5 (22%)
22	5MU	1K	54	22	19,22,23	3.95	5 (26%)	28,32,35	2.86	9 (32%)
56	PSU	1L	39	56	18,21,22	1.11	2 (11%)	22,30,33	1.50	4 (18%)
22	PSU	1K	39	22	18,21,22	1.11	2 (11%)	22,30,33	1.78	5 (22%)

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	U8U	1K	34	22,25	–	4/9/28/29	0/2/2/2
22	T6A	1K	37	22	–	3/23/41/42	0/3/3/3
56	5MU	1L	54	56	–	0/7/25/26	0/2/2/2
23	OMC	2L	33	23	–	2/9/27/28	0/2/2/2
22	PSU	1K	55	22	–	0/7/25/26	0/2/2/2
23	4SU	2K	8	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	39	57	–	0/7/25/26	0/2/2/2
23	5MU	2L	55	23	–	0/7/25/26	0/2/2/2
23	PSU	2L	56	23	–	0/7/25/26	0/2/2/2
56	PSU	1L	55	56	–	2/7/25/26	0/2/2/2
23	G7M	2L	47	23	–	2/7/25/26	0/3/3/3
23	G7M	2K	47	23	–	3/7/25/26	0/3/3/3
23	OMC	2K	33	23	–	3/9/27/28	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	5MU	2K	55	23	-	2/7/25/26	0/2/2/2
23	PSU	2K	56	23	-	0/7/25/26	0/2/2/2
22	5MU	1K	54	22	-	2/7/25/26	0/2/2/2
56	PSU	1L	39	56	-	2/7/25/26	0/2/2/2
22	PSU	1K	39	22	-	0/7/25/26	0/2/2/2

All (75) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	2L	55	5MU	C2-N1	13.10	1.59	1.38
23	2K	55	5MU	C2-N1	12.95	1.59	1.38
22	1K	54	5MU	C2-N1	12.38	1.58	1.38
56	1L	54	5MU	C2-N1	11.97	1.57	1.38
22	1K	37	T6A	C10-N11	7.71	1.52	1.35
23	2K	55	5MU	C2-N3	6.87	1.50	1.38
23	2L	55	5MU	C2-N3	6.45	1.49	1.38
22	1K	54	5MU	C2-N3	6.33	1.49	1.38
22	1K	54	5MU	C6-N1	6.20	1.48	1.38
23	2L	47	G7M	C4-N3	6.13	1.48	1.34
23	2K	8	4SU	C5-C4	6.12	1.50	1.42
22	1K	37	T6A	C10-N6	6.08	1.50	1.37
56	1L	54	5MU	C4-N3	-6.04	1.27	1.38
23	2K	55	5MU	C6-N1	5.96	1.48	1.38
23	2L	55	5MU	C4-C5	5.88	1.54	1.44
56	1L	54	5MU	C6-N1	5.87	1.48	1.38
22	1K	34	U8U	C2-S2	-5.80	1.58	1.67
23	2L	55	5MU	C6-N1	5.69	1.47	1.38
23	2L	33	OMC	C2-N3	5.57	1.47	1.36
56	1L	54	5MU	C2-N3	5.50	1.47	1.38
23	2K	47	G7M	C4-N3	5.43	1.47	1.34
23	2L	8	4SU	C5-C4	5.42	1.49	1.42
22	1K	34	U8U	C6-C5	5.41	1.50	1.34
22	1K	54	5MU	C4-C5	5.37	1.53	1.44
22	1K	54	5MU	C4-N3	-5.34	1.28	1.38
23	2L	55	5MU	C4-N3	-5.34	1.28	1.38
23	2K	47	G7M	C2-N3	5.24	1.45	1.33
23	2L	47	G7M	C2-N3	5.10	1.45	1.33
56	1L	54	5MU	C4-C5	5.06	1.53	1.44
23	2L	33	OMC	C4-N4	5.00	1.45	1.33
23	2K	33	OMC	C2-N3	4.85	1.46	1.36
56	1L	55	PSU	C6-C5	4.79	1.40	1.35
23	2K	47	G7M	C5-N7	-4.73	1.33	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	2K	55	5MU	C4-N3	-4.72	1.30	1.38
23	2K	56	PSU	C6-C5	4.55	1.40	1.35
22	1K	37	T6A	C6-N6	4.52	1.48	1.39
22	1K	34	U8U	C6-N1	4.51	1.45	1.38
23	2K	55	5MU	C4-C5	4.51	1.52	1.44
23	2K	47	G7M	C5-C6	4.44	1.55	1.43
22	1K	34	U8U	C2-N3	4.38	1.47	1.37
22	1K	55	PSU	C6-C5	4.29	1.40	1.35
23	2L	47	G7M	C5-N7	-4.22	1.34	1.39
23	2L	47	G7M	C2-N2	4.14	1.44	1.34
23	2K	33	OMC	C4-N4	3.98	1.43	1.33
23	2L	47	G7M	C5-C6	3.96	1.54	1.43
23	2K	47	G7M	C2-N2	3.95	1.43	1.34
23	2K	47	G7M	C6-N1	3.76	1.45	1.38
23	2L	56	PSU	C6-C5	3.75	1.39	1.35
23	2L	8	4SU	C2-N1	3.59	1.44	1.38
57	3L	39	PSU	C6-C5	3.52	1.39	1.35
22	1K	37	T6A	C12-C13	3.41	1.57	1.52
56	1L	39	PSU	C6-C5	3.40	1.39	1.35
22	1K	34	U8U	C4-C5	3.39	1.52	1.45
22	1K	37	T6A	C12-N11	3.17	1.52	1.45
23	2K	47	G7M	C2-N1	3.03	1.45	1.37
22	1K	34	U8U	C4-N3	2.99	1.44	1.38
23	2L	33	OMC	C5-C4	2.88	1.49	1.42
23	2K	8	4SU	C2-N1	2.78	1.42	1.38
23	2L	56	PSU	C2-N1	2.76	1.40	1.36
22	1K	37	T6A	C4-N3	2.76	1.39	1.34
23	2L	8	4SU	C6-N1	2.71	1.44	1.38
22	1K	39	PSU	C6-C5	2.67	1.38	1.35
22	1K	37	T6A	C5-N7	-2.61	1.34	1.39
23	2K	33	OMC	C5-C4	2.56	1.48	1.42
23	2L	47	G7M	C2-N1	2.54	1.44	1.37
22	1K	37	T6A	C5-C6	-2.53	1.35	1.41
23	2L	47	G7M	O6-C6	-2.45	1.18	1.23
22	1K	37	T6A	C5-C4	-2.43	1.34	1.39
23	2K	56	PSU	C4-C5	-2.34	1.37	1.44
23	2K	8	4SU	C6-N1	2.32	1.43	1.38
22	1K	39	PSU	O4'-C1'	-2.19	1.40	1.43
23	2L	8	4SU	C4-S4	-2.19	1.64	1.68
56	1L	39	PSU	C4-C5	-2.17	1.38	1.44
23	2L	47	G7M	C6-N1	2.10	1.42	1.38
22	1K	37	T6A	ODA-C13	2.02	1.28	1.22

All (130) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
56	1L	54	5MU	C5-C4-N3	10.94	124.65	115.31
22	1K	37	T6A	N3-C2-N1	-9.80	113.27	128.60
23	2K	55	5MU	C5-C4-N3	9.59	123.50	115.31
22	1K	54	5MU	C5-C4-N3	9.15	123.12	115.31
23	2L	8	4SU	C4-N3-C2	-9.09	118.50	127.34
23	2L	55	5MU	C5-C4-N3	8.97	122.97	115.31
23	2K	55	5MU	O4-C4-C5	-8.56	114.98	124.90
23	2L	8	4SU	C5-C4-N3	8.53	122.60	114.69
22	1K	37	T6A	C12-N11-C10	8.17	135.56	121.94
23	2K	8	4SU	C4-N3-C2	-8.15	119.42	127.34
23	2K	56	PSU	C6-N1-C2	-6.64	115.89	122.68
23	2K	55	5MU	C6-C5-C4	6.60	123.55	118.03
22	1K	37	T6A	C5-C4-N3	-6.49	118.29	126.75
23	2K	55	5MU	C4-N3-C2	-6.48	118.96	127.35
56	1L	54	5MU	C4-N3-C2	-6.42	119.04	127.35
22	1K	37	T6A	N6-C10-N11	6.37	122.66	113.76
56	1L	54	5MU	C5-C6-N1	-6.37	116.79	123.34
23	2K	56	PSU	N1-C2-N3	6.30	122.27	115.13
22	1K	37	T6A	N3-C4-N9	6.17	137.25	127.08
23	2L	55	5MU	C4-N3-C2	-6.07	119.50	127.35
23	2L	55	5MU	C6-C5-C4	5.76	122.85	118.03
22	1K	54	5MU	O4-C4-C5	-5.40	118.64	124.90
22	1K	37	T6A	C2-N3-C4	5.36	124.41	111.75
23	2L	55	5MU	C5M-C5-C6	-5.27	115.81	122.85
23	2K	55	5MU	C5-C6-N1	-5.22	117.97	123.34
56	1L	54	5MU	C6-C5-C4	5.17	122.35	118.03
22	1K	54	5MU	C4-N3-C2	-5.14	120.70	127.35
23	2L	33	OMC	N4-C4-N3	5.07	126.86	117.97
22	1K	37	T6A	O10-C10-N6	-5.06	115.07	123.62
23	2L	56	PSU	C4-N3-C2	-4.94	119.22	126.34
56	1L	54	5MU	O4-C4-C5	-4.89	119.24	124.90
56	1L	55	PSU	N1-C2-N3	4.72	120.47	115.13
23	2L	55	5MU	C5-C6-N1	-4.70	118.50	123.34
22	1K	34	U8U	S2-C2-N3	-4.55	111.20	119.96
22	1K	37	T6A	N9-C8-N7	-4.54	107.71	113.91
22	1K	39	PSU	C4-N3-C2	-4.51	119.83	126.34
22	1K	54	5MU	C6-C5-C4	4.51	121.80	118.03
23	2L	55	5MU	O4-C4-C5	-4.37	119.83	124.90
23	2L	55	5MU	C6-N1-C2	-4.28	116.96	121.30
23	2K	8	4SU	N3-C2-N1	4.27	120.56	114.89
22	1K	54	5MU	C5-C6-N1	-4.25	118.97	123.34
23	2L	8	4SU	C5-C4-S4	-4.22	119.03	124.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	1K	55	PSU	N1-C2-N3	4.21	119.90	115.13
23	2K	8	4SU	C5-C4-N3	4.12	118.51	114.69
22	1K	55	PSU	O2-C2-N1	-4.08	118.30	122.79
57	3L	39	PSU	C4-N3-C2	-4.07	120.47	126.34
23	2K	33	OMC	N4-C4-N3	4.06	125.09	117.97
22	1K	39	PSU	N1-C2-N3	4.03	119.70	115.13
23	2K	47	G7M	C5-C4-N3	-4.02	120.44	128.15
23	2L	47	G7M	CN7-N7-C5	4.00	131.74	126.77
22	1K	55	PSU	C6-N1-C2	-3.96	118.63	122.68
22	1K	54	5MU	C5M-C5-C6	-3.94	117.58	122.85
23	2L	56	PSU	N1-C2-N3	3.92	119.57	115.13
56	1L	39	PSU	C4-N3-C2	-3.85	120.79	126.34
23	2K	8	4SU	O2-C2-N1	-3.80	117.73	122.79
22	1K	54	5MU	C6-N1-C2	-3.77	117.48	121.30
56	1L	55	PSU	C6-N1-C2	-3.76	118.84	122.68
56	1L	55	PSU	C4-N3-C2	-3.74	120.95	126.34
23	2L	47	G7M	C5-C4-N3	-3.74	120.98	128.15
23	2L	47	G7M	C2-N3-C4	3.72	118.92	112.30
23	2K	55	5MU	C6-N1-C2	-3.59	117.66	121.30
22	1K	37	T6A	C13-C12-N11	3.56	118.05	110.28
23	2K	55	5MU	C5M-C5-C6	-3.55	118.11	122.85
22	1K	37	T6A	ODB-C13-ODA	-3.54	116.04	124.09
23	2L	33	OMC	C5-C4-N4	-3.51	115.05	120.57
23	2L	47	G7M	C5-C6-N1	3.50	119.10	111.79
23	2K	56	PSU	C4-N3-C2	-3.49	121.31	126.34
56	1L	55	PSU	O2-C2-N1	-3.31	119.14	122.79
23	2K	8	4SU	C5-C4-S4	-3.30	120.21	124.47
23	2L	47	G7M	CN7-N7-C8	-3.27	119.79	124.84
22	1K	55	PSU	C4-N3-C2	-3.23	121.69	126.34
23	2L	55	5MU	N3-C2-N1	3.22	119.16	114.89
23	2K	56	PSU	O2-C2-N1	-3.16	119.31	122.79
23	2K	33	OMC	C5-C4-N4	-3.15	115.61	120.57
23	2L	8	4SU	N3-C2-N1	3.14	119.05	114.89
23	2K	55	5MU	O2-C2-N1	-3.11	118.65	122.79
23	2K	47	G7M	C2-N3-C4	3.03	117.69	112.30
22	1K	37	T6A	C4-N9-C8	3.02	109.00	105.73
22	1K	37	T6A	C5-N7-C8	3.01	107.79	103.51
57	3L	39	PSU	N1-C2-N3	2.98	118.50	115.13
22	1K	39	PSU	O2-C2-N1	-2.95	119.55	122.79
56	1L	54	5MU	C5M-C5-C6	-2.93	118.94	122.85
22	1K	37	T6A	ODB-C13-C12	2.92	124.50	114.21
22	1K	34	U8U	C5-C4-N3	2.89	119.03	114.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	1K	37	T6A	C14-C12-C13	2.88	115.11	110.19
23	2L	47	G7M	C2-N1-C6	-2.84	119.91	125.10
23	2K	47	G7M	O6-C6-C5	-2.83	121.67	128.06
22	1K	37	T6A	C4-C5-C6	2.78	118.96	116.81
23	2L	56	PSU	C6-C5-C4	2.75	120.12	118.20
23	2K	47	G7M	C2-N1-C6	-2.72	120.14	125.10
22	1K	37	T6A	N6-C6-N1	2.71	124.42	117.45
23	2K	8	4SU	C6-C5-C4	2.68	122.28	119.95
22	1K	37	T6A	C2-N1-C6	2.67	124.21	115.25
56	1L	39	PSU	N1-C2-N3	2.66	118.14	115.13
23	2L	55	5MU	O2-C2-N1	-2.63	119.29	122.79
23	2K	55	5MU	N3-C2-N1	2.60	118.34	114.89
23	2L	47	G7M	O6-C6-C5	-2.60	122.19	128.06
23	2L	47	G7M	C1'-N9-C4	-2.60	118.78	126.50
23	2L	33	OMC	C1'-N1-C2	2.57	124.16	118.42
56	1L	54	5MU	N3-C2-N1	2.55	118.28	114.89
23	2K	47	G7M	CN7-N7-C5	2.55	129.93	126.77
23	2K	47	G7M	N9-C4-N3	2.48	130.92	125.94
22	1K	54	5MU	O2-C2-N1	-2.46	119.52	122.79
56	1L	39	PSU	O2-C2-N1	-2.39	120.16	122.79
56	1L	54	5MU	C6-N1-C2	-2.38	118.89	121.30
22	1K	37	T6A	C5-C6-N1	2.36	120.71	118.20
56	1L	39	PSU	O4-C4-C5	-2.36	117.89	124.05
22	1K	34	U8U	O4-C4-N3	-2.34	115.63	120.12
56	1L	54	5MU	O2-C2-N1	-2.34	119.68	122.79
23	2L	55	5MU	C5M-C5-C4	2.34	121.34	118.77
23	2K	8	4SU	C5-C6-N1	-2.34	117.90	121.81
23	2L	47	G7M	N9-C4-N3	2.29	130.54	125.94
22	1K	54	5MU	N3-C2-N1	2.28	117.92	114.89
23	2K	47	G7M	C6-C5-C4	2.26	122.98	119.02
56	1L	54	5MU	C1'-N1-C6	2.26	124.88	121.12
22	1K	37	T6A	C6-C5-N7	-2.24	129.96	132.39
23	2K	33	OMC	C1'-N1-C6	-2.24	115.95	120.84
23	2K	47	G7M	CN7-N7-C8	-2.24	121.38	124.84
22	1K	39	PSU	C6-C5-C4	2.22	119.75	118.20
22	1K	34	U8U	C-C5-C6	-2.19	117.92	121.21
23	2K	56	PSU	C6-C5-C4	2.17	119.71	118.20
23	2L	8	4SU	C1'-N1-C2	2.13	121.42	117.57
23	2L	56	PSU	C5-C6-N1	-2.12	118.93	122.11
23	2L	33	OMC	C6-N1-C2	-2.11	116.83	120.49
23	2L	55	5MU	C1'-N1-C2	2.09	121.36	117.57
56	1L	54	5MU	O4-C4-N3	-2.09	116.11	120.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	2L	8	4SU	C1'-N1-C6	-2.08	116.31	120.84
57	3L	39	PSU	O4-C4-N3	-2.08	116.13	120.12
22	1K	39	PSU	C6-N1-C2	-2.06	120.58	122.68
23	2L	8	4SU	O2-C2-N3	-2.02	117.73	121.50

There are no chirality outliers.

All (25) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
22	1K	34	U8U	N-C-C5-C4
22	1K	34	U8U	N-C-C5-C6
22	1K	37	T6A	C13-C12-C14-O14
22	1K	37	T6A	C13-C12-C14-C15
23	2L	47	G7M	O4'-C4'-C5'-O5'
23	2K	55	5MU	C3'-C4'-C5'-O5'
22	1K	34	U8U	O4'-C4'-C5'-O5'
23	2L	47	G7M	C3'-C4'-C5'-O5'
23	2K	55	5MU	O4'-C4'-C5'-O5'
22	1K	54	5MU	O4'-C4'-C5'-O5'
22	1K	54	5MU	C3'-C4'-C5'-O5'
56	1L	39	PSU	O4'-C4'-C5'-O5'
22	1K	37	T6A	N11-C12-C14-C15
23	2L	33	OMC	O4'-C4'-C5'-O5'
23	2K	47	G7M	C2'-C1'-N9-C4
23	2L	33	OMC	C3'-C4'-C5'-O5'
56	1L	55	PSU	O4'-C1'-C5-C4
23	2K	33	OMC	C3'-C2'-O2'-CM2
23	2K	47	G7M	C2'-C1'-N9-C8
23	2K	47	G7M	C4'-C5'-O5'-P
56	1L	39	PSU	C3'-C4'-C5'-O5'
23	2K	33	OMC	C1'-C2'-O2'-CM2
56	1L	55	PSU	O4'-C1'-C5-C6
22	1K	34	U8U	C3'-C4'-C5'-O5'
23	2K	33	OMC	C2'-C1'-N1-C2

There are no ring outliers.

No monomer is involved in short contacts.

4.5 Carbohydrates

There are no oligosaccharides in this entry.

4.6 Ligand geometry [i](#)

Of 1188 ligands modelled in this entry, 1186 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	3E	301	4	0,12,12	-	-	-		
59	SF4	32	302	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	3E	301	4	-	-	0/6/5/5
59	SF4	32	302	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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
25	4K	1
37	35	1
38	45	1
5	4E	1
38	88	1
4	3E	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	4K	24:A	O3'	25:A	P	4.44
1	35	121:LYS	C	122:PRO	N	1.77
1	45	124:LYS	C	125:LEU	N	1.15
1	4E	69:VAL	C	70:PRO	N	1.12
1	88	124:LYS	C	125:LEU	N	1.12
1	3E	36:ARG	C	37:PRO	N	1.07

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	1493/1522 (98%)	-0.64	47 (3%) 51 31	83, 129, 202, 287	0
1	1G	1496/1522 (98%)	-0.60	37 (2%) 58 37	100, 152, 223, 279	0
2	12	206/256 (80%)	-0.03	1 (0%) 87 75	173, 206, 218, 228	0
2	1E	231/256 (90%)	-0.39	0 100 100	140, 173, 197, 207	0
3	22	194/239 (81%)	-0.27	2 (1%) 79 62	172, 196, 209, 214	0
3	2E	205/239 (85%)	-0.24	6 (2%) 53 34	115, 136, 165, 176	0
4	32	208/209 (99%)	-0.08	5 (2%) 59 39	129, 152, 173, 183	0
4	3E	207/209 (99%)	-0.19	2 (0%) 79 62	104, 131, 154, 164	0
5	42	149/162 (91%)	0.00	0 100 100	138, 160, 177, 190	0
5	4E	149/162 (91%)	-0.05	5 (3%) 48 28	104, 125, 147, 155	0
6	52	101/101 (100%)	-0.42	0 100 100	119, 135, 156, 163	0
6	5E	100/101 (99%)	-0.40	0 100 100	103, 129, 149, 159	0
7	62	138/156 (88%)	0.21	8 (5%) 29 16	150, 164, 173, 181	0
7	6E	151/156 (96%)	0.03	11 (7%) 21 12	134, 150, 170, 179	0
8	72	137/138 (99%)	-0.10	0 100 100	136, 164, 180, 190	0
8	7E	138/138 (100%)	-0.08	3 (2%) 62 41	112, 138, 152, 161	0
9	82	105/128 (82%)	-0.09	1 (0%) 79 62	149, 196, 209, 221	0
9	8E	126/128 (98%)	-0.18	4 (3%) 50 30	111, 170, 192, 200	0
10	1A	60/105 (57%)	-0.28	1 (1%) 69 48	166, 193, 204, 205	0
10	1I	72/105 (68%)	-0.09	2 (2%) 55 34	112, 150, 193, 204	0
11	2A	113/129 (87%)	0.27	4 (3%) 47 28	118, 143, 157, 167	0
11	2I	111/129 (86%)	0.13	5 (4%) 38 22	102, 136, 151, 164	0
12	3A	121/132 (91%)	0.44	10 (8%) 17 10	119, 142, 165, 179	0
12	3I	122/132 (92%)	-0.02	5 (4%) 41 24	91, 102, 126, 160	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	4A	111/126 (88%)	0.26	10 (9%) 15 9	162, 187, 202, 212	0
13	4I	119/126 (94%)	-0.23	4 (3%) 48 28	111, 146, 162, 173	0
14	5A	48/61 (78%)	0.05	1 (2%) 63 42	170, 191, 208, 218	0
14	5I	60/61 (98%)	-0.63	0 100 100	107, 124, 141, 155	0
15	6A	87/89 (97%)	-0.40	0 100 100	123, 148, 167, 174	0
15	6I	87/89 (97%)	-0.71	0 100 100	106, 127, 148, 153	0
16	7A	84/88 (95%)	-0.30	1 (1%) 76 57	120, 139, 161, 184	0
16	7I	80/88 (90%)	-0.22	0 100 100	127, 140, 169, 180	0
17	8A	99/105 (94%)	-0.52	0 100 100	121, 143, 156, 159	0
17	8I	100/105 (95%)	-0.64	1 (1%) 79 62	117, 136, 148, 154	0
18	9A	67/88 (76%)	-0.24	0 100 100	128, 145, 163, 171	0
18	9I	67/88 (76%)	-0.30	1 (1%) 72 52	115, 134, 159, 164	0
19	AA	36/93 (38%)	0.39	2 (5%) 30 17	191, 209, 217, 223	0
19	AI	81/93 (87%)	-0.43	0 100 100	125, 148, 173, 183	0
20	BA	98/106 (92%)	-0.64	1 (1%) 79 62	107, 139, 163, 176	0
20	BI	97/106 (91%)	-0.29	0 100 100	135, 152, 181, 193	0
21	1B	23/27 (85%)	-0.71	0 100 100	157, 179, 187, 189	0
21	1F	23/27 (85%)	-0.86	0 100 100	119, 134, 143, 145	0
22	1K	64/76 (84%)	1.04	12 (18%) 3 2	112, 226, 251, 253	0
23	2K	72/77 (93%)	-0.65	0 100 100	94, 125, 153, 169	0
23	2L	72/77 (93%)	0.55	8 (11%) 10 6	100, 151, 178, 198	0
24	3K	76/76 (100%)	-0.59	0 100 100	96, 189, 207, 218	0
25	4K	20/27 (74%)	0.65	4 (20%) 3 2	96, 156, 196, 199	0
25	4L	17/27 (62%)	0.93	3 (17%) 4 2	131, 170, 208, 211	0
26	14	2861/2912 (98%)	-0.79	44 (1%) 72 52	72, 111, 235, 276	0
26	1H	2830/2912 (97%)	-0.92	24 (0%) 82 66	65, 97, 204, 287	0
27	16	122/122 (100%)	-1.10	0 100 100	92, 117, 143, 228	0
27	1J	122/122 (100%)	-0.85	0 100 100	117, 155, 179, 225	0
28	7I	135/229 (58%)	-0.37	0 100 100	149, 167, 190, 202	0
29	11	273/276 (98%)	0.18	22 (8%) 18 10	65, 90, 111, 122	0
29	19	273/276 (98%)	0.13	17 (6%) 26 15	74, 100, 121, 136	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
30	21	203/206 (98%)	0.12	4 (1%) 65 44	73, 112, 157, 172	0
30	29	203/206 (98%)	-0.38	2 (0%) 79 62	79, 116, 162, 178	0
31	31	202/210 (96%)	-0.37	3 (1%) 72 52	70, 102, 136, 155	0
31	39	204/210 (97%)	-0.18	8 (3%) 43 25	83, 128, 181, 201	0
32	41	179/182 (98%)	-0.50	4 (2%) 62 41	107, 128, 164, 174	0
32	49	179/182 (98%)	0.22	10 (5%) 30 17	151, 171, 195, 204	0
33	51	171/180 (95%)	0.13	7 (4%) 41 24	102, 128, 146, 157	0
33	59	69/180 (38%)	0.44	7 (10%) 12 7	170, 198, 213, 220	0
34	61	145/148 (97%)	-0.17	2 (1%) 73 53	102, 163, 188, 199	0
34	69	145/148 (97%)	-0.27	9 (6%) 26 15	111, 152, 176, 189	0
35	15	137/140 (97%)	0.14	7 (5%) 33 19	106, 134, 162, 179	0
35	58	138/140 (98%)	0.12	9 (6%) 25 14	86, 112, 154, 172	0
36	25	122/122 (100%)	-0.09	0 100 100	92, 113, 132, 142	0
36	68	122/122 (100%)	0.07	2 (1%) 70 50	81, 98, 118, 131	0
37	35	148/150 (98%)	0.15	11 (7%) 20 12	84, 135, 174, 190	0
37	78	147/150 (98%)	-0.23	4 (2%) 56 35	72, 104, 136, 144	0
38	45	138/141 (97%)	0.07	13 (9%) 14 8	99, 131, 151, 168	0
38	88	141/141 (100%)	-0.38	0 100 100	76, 101, 123, 153	0
39	55	118/118 (100%)	-0.72	0 100 100	87, 102, 118, 138	0
39	98	118/118 (100%)	-0.46	0 100 100	87, 109, 131, 147	0
40	65	110/112 (98%)	-0.56	0 100 100	116, 145, 164, 172	0
40	A8	111/112 (99%)	-0.66	0 100 100	93, 112, 135, 144	0
41	75	136/146 (93%)	-0.28	5 (3%) 45 26	102, 120, 169, 198	0
41	B8	135/146 (92%)	0.10	6 (4%) 39 22	92, 116, 166, 185	0
42	85	116/118 (98%)	-0.05	2 (1%) 69 48	90, 121, 154, 166	0
42	C8	115/118 (97%)	0.10	5 (4%) 40 23	77, 102, 130, 141	0
43	95	99/101 (98%)	0.22	5 (5%) 33 19	91, 152, 166, 174	0
43	D8	101/101 (100%)	-0.30	1 (0%) 79 62	78, 124, 149, 160	0
44	A5	110/113 (97%)	0.11	5 (4%) 38 22	84, 96, 127, 133	0
44	E8	110/113 (97%)	0.09	6 (5%) 30 17	79, 95, 125, 140	0
45	B5	94/96 (97%)	-0.28	3 (3%) 50 30	94, 110, 134, 144	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
45	F8	95/96 (98%)	-0.34	0 100 100	78, 93, 120, 133	0
46	C5	105/110 (95%)	0.56	7 (6%) 24 13	110, 143, 175, 185	0
46	G8	104/110 (94%)	0.27	2 (1%) 66 45	88, 116, 148, 161	0
47	D5	130/206 (63%)	-0.38	1 (0%) 82 66	138, 163, 188, 194	0
47	H8	148/206 (71%)	-0.39	1 (0%) 84 69	106, 140, 195, 207	0
48	E5	78/85 (91%)	-0.08	4 (5%) 33 19	99, 116, 136, 149	0
48	I8	76/85 (89%)	-0.66	1 (1%) 75 55	79, 95, 111, 130	0
49	F5	94/98 (95%)	0.06	3 (3%) 50 30	86, 109, 144, 159	0
49	J8	94/98 (95%)	-0.31	1 (1%) 78 60	79, 96, 143, 153	0
50	G5	67/72 (93%)	-0.31	0 100 100	113, 134, 152, 171	0
50	K8	68/72 (94%)	-0.12	0 100 100	82, 105, 124, 151	0
51	H5	58/60 (96%)	-0.49	0 100 100	103, 128, 155, 180	0
51	L8	58/60 (96%)	-0.47	0 100 100	83, 104, 140, 152	0
52	M8	47/71 (66%)	-0.17	0 100 100	131, 172, 183, 188	0
53	J5	56/60 (93%)	-0.31	0 100 100	82, 108, 155, 165	0
53	N8	48/60 (80%)	-0.30	0 100 100	72, 108, 153, 164	0
54	L5	45/49 (91%)	-0.24	2 (4%) 39 22	75, 83, 95, 107	0
54	P8	47/49 (95%)	-0.50	1 (2%) 63 42	68, 74, 98, 108	0
55	M5	64/65 (98%)	-0.07	1 (1%) 70 50	90, 105, 123, 143	0
55	Q8	64/65 (98%)	-0.27	1 (1%) 70 50	80, 91, 108, 123	0
56	1L	71/76 (93%)	0.09	3 (4%) 40 23	140, 257, 274, 277	0
57	3L	75/76 (98%)	1.11	13 (17%) 4 2	107, 259, 277, 285	0
All	All	20395/21728 (93%)	-0.41	495 (2%) 59 39	65, 127, 204, 287	0

All (495) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
57	3L	34	U	15.7
57	3L	35	U	11.8
9	8E	126	SER	7.8
48	E5	7	LEU	7.3
9	8E	127	LYS	7.2
12	3A	64	TYR	7.1
23	2L	40	C	7.0

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Mol	Chain	Res	Type	RSRZ
57	3L	33	U	7.0
41	B8	1	MET	6.8
32	49	23	PHE	6.7
13	4A	117	VAL	6.7
29	19	5	LYS	6.2
29	19	274	ARG	6.0
46	C5	29	GLU	5.9
1	13	701	C	5.7
29	19	55	GLY	5.6
13	4A	111	LYS	5.6
41	B8	104	ASN	5.5
34	69	20	ASP	5.4
57	3L	36	U	5.3
23	2L	39	A	5.3
12	3I	19	ARG	5.3
13	4A	118	ALA	5.2
1	13	688	G	5.2
31	39	72	ARG	5.2
22	1K	73	A	5.1
1	13	698	G	5.1
42	C8	116	ALA	5.0
1	13	700	G	5.0
20	BA	9	ASN	4.9
33	59	169	VAL	4.7
1	13	702	A	4.7
32	49	34	LEU	4.6
26	14	766	C	4.5
5	4E	23	GLY	4.5
1	13	687	A	4.5
29	11	274	ARG	4.5
38	45	90	VAL	4.4
23	2L	29	C	4.4
1	1G	791	G	4.4
1	13	699	C	4.4
44	A5	110	LYS	4.4
46	G8	105	ALA	4.3
26	14	767	U	4.2
22	1K	75	C	4.2
29	11	270	ILE	4.1
48	E5	8	GLY	4.1
3	2E	201	TYR	4.1
13	4A	113	PRO	4.1

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Mol	Chain	Res	Type	RSRZ
35	58	138	LEU	4.1
12	3A	21	LYS	4.0
1	13	685	G	4.0
1	1G	790	A	4.0
8	7E	93	VAL	4.0
1	13	686	U	4.0
32	41	23	PHE	4.0
12	3I	28	LYS	4.0
22	1K	74	C	4.0
1	1G	1341	U	4.0
26	14	765	G	4.0
44	A5	85	VAL	3.9
41	75	104	ASN	3.9
1	13	1394	A	3.9
22	1K	76	A	3.9
56	1L	40	C	3.9
33	51	86	GLU	3.9
1	13	703	G	3.9
23	2L	41	C	3.9
57	3L	70	C	3.9
1	1G	1377	A	3.9
26	1H	2712(A)	A	3.9
33	51	164	TYR	3.8
57	3L	37	A	3.8
13	4I	118	ALA	3.8
33	51	87	LEU	3.8
1	1G	1227	A	3.8
26	14	229	A	3.8
1	1G	789	U	3.8
13	4A	116	THR	3.8
1	1G	966	G	3.8
26	1H	1106	G	3.8
54	L5	45	ALA	3.8
22	1K	72	C	3.7
41	B8	135	ALA	3.7
44	A5	93	ALA	3.7
29	11	166	GLN	3.7
57	3L	32	C	3.7
12	3A	62	SER	3.7
7	6E	153	HIS	3.7
1	1G	1497	G	3.7
35	15	87	LEU	3.7

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Mol	Chain	Res	Type	RSRZ
7	62	8	GLU	3.7
1	13	681	C	3.7
1	1G	1340	A	3.6
25	4K	13	A	3.6
44	E8	85	VAL	3.6
43	95	73	SER	3.6
11	2I	48	ILE	3.6
44	A5	82	LEU	3.6
9	8E	128	ARG	3.6
4	32	29	PRO	3.6
1	13	800	G	3.5
26	14	1555	G	3.5
1	13	1403	C	3.5
7	6E	78	ARG	3.5
44	E8	92	ARG	3.5
34	69	3	VAL	3.5
57	3L	7	U	3.5
29	11	262	ARG	3.5
14	5A	44	LEU	3.5
29	11	112	GLN	3.4
23	2L	1	C	3.4
13	4A	107	ALA	3.4
22	1K	71	C	3.4
1	1G	693	G	3.4
30	29	71	GLY	3.4
37	35	75	ILE	3.4
13	4I	120	LYS	3.3
37	35	58	THR	3.3
35	58	74	ARG	3.3
35	58	84	LYS	3.3
1	13	679	C	3.3
34	69	12	LEU	3.3
34	69	18	VAL	3.3
26	14	896	A	3.3
4	3E	138	TYR	3.2
7	62	87	VAL	3.2
29	11	138	VAL	3.2
13	4I	119	GLY	3.2
48	I8	9	SER	3.2
29	11	169	GLU	3.2
12	3I	64	TYR	3.2
33	51	21	PRO	3.2

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Mol	Chain	Res	Type	RSRZ
1	13	680	C	3.2
42	C8	18	LEU	3.2
35	58	75	TYR	3.2
11	2I	91	ARG	3.2
29	19	54	ARG	3.2
26	14	530	G	3.2
26	14	879	G	3.2
1	1G	1496	C	3.2
26	14	1963	U	3.1
49	F5	85	LEU	3.1
26	14	691	C	3.1
26	14	1566	A	3.1
26	14	654(R)	C	3.0
26	14	1625	C	3.0
26	1H	2003	G	3.0
1	1G	792	A	3.0
26	14	764	A	3.0
34	69	2	LYS	3.0
29	11	38	LYS	3.0
35	15	92	ALA	3.0
11	2A	36	ASP	3.0
49	J8	91	LYS	3.0
1	13	791	G	3.0
22	1K	1	G	3.0
8	7E	91	ARG	2.9
26	14	654(D)	G	2.9
26	14	878	A	2.9
49	F5	84	GLY	2.9
7	6E	86	GLN	2.9
26	14	2901	C	2.9
43	D8	70	ILE	2.9
1	13	1381	U	2.9
12	3A	27	LEU	2.9
34	61	140	LEU	2.9
7	6E	85	TYR	2.9
33	59	79	VAL	2.9
1	13	799	G	2.9
26	1H	2002	G	2.9
26	1H	1847	A	2.9
41	B8	6	LEU	2.9
3	22	162	GLN	2.9
57	3L	38	A	2.9

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Mol	Chain	Res	Type	RSRZ
1	13	796	C	2.9
22	1K	40	C	2.9
29	11	271	ILE	2.9
35	58	68	GLU	2.9
1	1G	1494	G	2.9
25	4K	25	A	2.9
32	49	25	TYR	2.9
38	45	93	TYR	2.9
26	1H	882	G	2.9
1	13	697	U	2.8
26	1H	895	U	2.8
26	1H	1273	U	2.8
48	E5	9	SER	2.8
25	4L	15	A	2.8
12	3A	68	ALA	2.8
26	14	2833	G	2.8
35	58	22	THR	2.8
5	4E	24	ARG	2.8
2	12	102	LEU	2.8
41	75	50	ILE	2.8
54	L5	1	MET	2.8
32	41	26	GLN	2.8
42	85	48	ALA	2.8
29	19	6	PHE	2.8
41	75	105	LEU	2.8
42	85	40	PHE	2.8
29	11	167	GLY	2.8
43	95	70	ILE	2.8
1	13	1384	C	2.8
7	6E	154	TYR	2.8
44	A5	92	ARG	2.8
47	H8	142	SER	2.8
34	69	1	MET	2.8
23	2L	28	U	2.8
1	1G	1228	C	2.8
3	2E	200	ALA	2.8
7	6E	80	VAL	2.8
46	C5	106	LEU	2.8
38	45	78	PRO	2.7
35	58	85	ILE	2.7
35	58	73	THR	2.7
26	14	1816	G	2.7

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Mol	Chain	Res	Type	RSRZ
29	11	184	LYS	2.7
32	41	25	TYR	2.7
7	62	7	ALA	2.7
37	78	135	LEU	2.7
37	35	48	PRO	2.7
45	B5	70	LEU	2.7
29	19	216	GLY	2.7
41	75	106	SER	2.7
31	39	65	TRP	2.7
26	1H	1657	C	2.7
3	22	43	LEU	2.7
29	11	175	LEU	2.7
1	1G	1405	G	2.7
33	59	12	PRO	2.7
29	11	105	ILE	2.7
46	C5	63	LYS	2.7
26	14	1553	A	2.7
13	4I	96	LEU	2.7
1	1G	1226	C	2.7
29	11	170	GLY	2.7
46	C5	22	GLY	2.7
55	M5	34	TRP	2.7
29	11	182	LEU	2.7
29	19	215	LEU	2.7
1	13	792	A	2.6
31	39	56	GLU	2.6
13	4A	114	ARG	2.6
26	1H	1653	G	2.6
22	1K	44	U	2.6
26	14	2797	U	2.6
1	1G	787	A	2.6
1	1G	1400	C	2.6
26	1H	893	C	2.6
7	6E	148	ASN	2.6
1	1G	1381	U	2.6
11	2A	89	ALA	2.6
37	35	71	VAL	2.6
26	14	2902	C	2.6
9	82	115	GLY	2.6
7	6E	152	ALA	2.6
26	1H	1659	U	2.6
55	Q8	52	LYS	2.6

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Mol	Chain	Res	Type	RSRZ
1	13	711	G	2.6
26	1H	1846	G	2.6
31	39	83	PHE	2.6
1	1G	1519	A	2.6
26	1H	1848	A	2.6
12	3I	29	GLY	2.6
1	13	241	C	2.6
5	4E	13	ILE	2.5
4	32	189	PRO	2.5
29	11	37	LEU	2.5
38	45	2	LEU	2.5
29	11	168	ARG	2.5
37	78	36	LYS	2.5
57	3L	68	G	2.5
33	59	148	ILE	2.5
7	62	89	MET	2.5
1	1G	1383	C	2.5
41	75	101	PHE	2.5
33	59	168	PRO	2.5
29	19	212	SER	2.5
12	3A	28	LYS	2.5
29	19	211	ARG	2.5
1	13	76	G	2.5
25	4K	6	G	2.5
26	14	1906	G	2.5
4	32	188	LEU	2.5
26	14	1556	C	2.5
31	39	69	HIS	2.5
37	35	35	HIS	2.5
29	11	41	GLY	2.5
33	51	22	GLY	2.5
1	1G	941	G	2.5
1	1G	954	G	2.5
1	1G	1407	C	2.5
10	1A	58	ASP	2.5
1	13	93	U	2.5
37	35	30	THR	2.5
7	62	88	PRO	2.5
11	2I	25	TYR	2.5
32	49	108	ASN	2.4
22	1K	49	G	2.4
32	41	3	LEU	2.4

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Mol	Chain	Res	Type	RSRZ
35	15	73	THR	2.4
1	13	678	U	2.4
1	13	1196	U	2.4
11	2A	25	TYR	2.4
26	14	1917	U	2.4
12	3A	55	VAL	2.4
31	39	82	ILE	2.4
1	13	1500	A	2.4
1	13	239	U	2.4
1	1G	1338	G	2.4
3	2E	128	PHE	2.4
5	4E	18	ARG	2.4
30	29	73	GLU	2.4
37	35	74	GLU	2.4
38	45	79	LEU	2.4
29	11	200	ASP	2.4
29	19	56	GLY	2.4
26	14	1913	A	2.4
41	B8	132	LYS	2.4
23	2L	35	C	2.4
32	49	82	LEU	2.4
1	13	1508	G	2.4
25	4L	7	G	2.4
26	14	654(S)	G	2.4
26	14	2023	G	2.4
12	3A	61	THR	2.4
38	45	70	PRO	2.4
29	19	111	LEU	2.4
1	13	815	A	2.4
26	1H	2001	A	2.4
26	1H	2688	U	2.4
35	15	98	VAL	2.4
1	13	1195	C	2.3
26	1H	2690	C	2.3
38	45	88	GLY	2.3
31	31	64	ILE	2.3
19	AA	66	MET	2.3
35	15	90	MET	2.3
1	1G	1379	G	2.3
4	32	94	LEU	2.3
29	19	181	GLU	2.3
35	58	88	GLU	2.3

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Mol	Chain	Res	Type	RSRZ
29	11	258	LYS	2.3
7	6E	151	TYR	2.3
1	1G	1382	C	2.3
4	3E	110	PHE	2.3
1	1G	1343	G	2.3
26	1H	145	G	2.3
26	1H	1651	G	2.3
32	49	109	VAL	2.3
34	69	21	VAL	2.3
31	39	79	GLY	2.3
29	19	27	THR	2.3
17	8I	29	HIS	2.3
46	C5	43	ASN	2.3
26	14	1932	A	2.3
38	45	69	PHE	2.3
44	E8	94	ASP	2.3
1	13	1400	C	2.3
1	1G	1384	C	2.3
7	62	141	VAL	2.3
29	11	174	ILE	2.3
13	4A	103	THR	2.3
36	68	117	LEU	2.3
43	95	91	TYR	2.3
11	2A	122	LYS	2.3
3	2E	166	GLU	2.3
26	14	688	U	2.3
7	6E	147	ALA	2.3
49	F5	21	ARG	2.3
37	35	119	GLU	2.2
38	45	91	GLU	2.2
19	AA	62	ILE	2.2
34	61	138	ILE	2.2
12	3A	26	ALA	2.2
37	78	130	PHE	2.2
22	1K	32	C	2.2
26	14	698	C	2.2
26	14	737	C	2.2
57	3L	75	C	2.2
46	G8	98	VAL	2.2
16	7A	54	GLU	2.2
26	14	975	G	2.2
30	21	132	HIS	2.2

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Mol	Chain	Res	Type	RSRZ
1	1G	1406	U	2.2
1	13	965	A	2.2
1	1G	1339	A	2.2
1	1G	1518	A	2.2
56	1L	38	A	2.2
7	62	9	VAL	2.2
11	2I	47	VAL	2.2
12	3A	24	VAL	2.2
47	D5	138	GLU	2.2
26	1H	1218	C	2.2
7	62	2	ALA	2.2
12	3I	26	ALA	2.2
31	39	80	ALA	2.2
42	C8	15	LYS	2.2
43	95	81	TYR	2.2
9	8E	81	ILE	2.2
1	13	968	A	2.2
35	15	91	LEU	2.2
45	B5	61	GLY	2.2
37	35	50	ARG	2.2
29	19	3	VAL	2.2
46	C5	42	VAL	2.2
33	59	162	ILE	2.2
34	69	17	GLN	2.2
30	21	63	LEU	2.2
35	15	129	PRO	2.2
38	45	8	LYS	2.2
26	1H	1130	U	2.2
54	P8	47	ARG	2.2
23	2L	38	A	2.2
25	4K	23	A	2.2
26	1H	146	G	2.2
26	14	880	G	2.2
26	14	1929	G	2.2
3	2E	153	VAL	2.1
38	45	102	VAL	2.1
33	59	151	ILE	2.1
44	E8	96	ILE	2.1
10	1I	58	ASP	2.1
37	35	47	ASP	2.1
37	78	19	VAL	2.1
1	13	1398	A	2.1

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Mol	Chain	Res	Type	RSRZ
26	14	735	A	2.1
26	14	1439	A	2.1
42	C8	39	LEU	2.1
1	1G	1517	G	2.1
10	1I	60	ARG	2.1
13	4A	93	ARG	2.1
25	4L	6	G	2.1
8	7E	131	GLY	2.1
32	49	177	GLY	2.1
26	14	754	C	2.1
32	49	160	VAL	2.1
46	C5	39	VAL	2.1
32	49	161	THR	2.1
44	E8	82	LEU	2.1
43	95	83	ARG	2.1
36	68	84	ALA	2.1
42	C8	35	ALA	2.1
1	13	712	A	2.1
1	13	790	A	2.1
26	14	1762	A	2.1
1	13	709	G	2.1
26	14	763	G	2.1
57	3L	6	G	2.1
56	1L	56	C	2.1
29	19	214	TRP	2.1
45	B5	63	LYS	2.1
13	4A	9	ILE	2.1
18	9I	76	LEU	2.1
1	13	1498	U	2.1
1	13	706	A	2.1
22	1K	31	A	2.1
26	14	734	A	2.1
44	E8	98	LYS	2.1
48	E5	71	ASP	2.1
3	2E	193	TYR	2.1
1	13	806	C	2.1
26	1H	2008	C	2.1
1	1G	953	G	2.1
5	4E	21	ALA	2.1
26	1H	1650	G	2.1
26	14	561	G	2.1
29	19	2	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
32	49	169	ALA	2.1
31	31	56	GLU	2.1
26	14	1926	U	2.0
33	51	172	LYS	2.0
11	2I	42	TRP	2.0
29	19	16	MET	2.0
38	45	7	MET	2.0
1	1G	938	A	2.0
30	21	171	GLU	2.0
1	13	708	C	2.0
1	1G	75	C	2.0
1	1G	1533	C	2.0
30	21	7	VAL	2.0
33	51	19	VAL	2.0
34	69	19	VAL	2.0
57	3L	74	C	2.0
1	13	966	G	2.0
37	35	77	ARG	2.0
4	32	91	SER	2.0
1	13	788	U	2.0
26	14	1438	U	2.0
7	6E	103	TRP	2.0
29	11	39	LYS	2.0
31	31	66	PRO	2.0
38	45	80	GLU	2.0
41	B8	114	LEU	2.0

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
56	PSU	1L	55	20/21	0.61	0.08	176,201,207,207	0
22	PSU	1K	55	20/21	0.79	0.08	143,175,183,183	0
56	5MU	1L	54	21/22	0.80	0.07	184,194,212,217	0
23	PSU	2L	56	20/21	0.81	0.08	143,152,158,162	0
22	5MU	1K	54	21/22	0.85	0.07	155,171,185,188	0
23	5MU	2K	55	21/22	0.87	0.05	122,135,144,159	0
23	4SU	2L	8	20/21	0.88	0.09	131,155,165,169	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	PSU	1L	39	20/21	0.88	0.17	155,179,185,187	0
23	PSU	2K	56	20/21	0.88	0.05	122,127,139,140	0
57	PSU	3L	39	20/21	0.88	0.24	160,164,169,170	0
23	G7M	2L	47	24/25	0.89	0.08	161,169,178,179	0
23	4SU	2K	8	20/21	0.90	0.09	111,120,124,128	0
23	5MU	2L	55	21/22	0.90	0.07	146,159,164,166	0
23	G7M	2K	47	24/25	0.93	0.06	124,132,139,146	0
23	OMC	2L	33	21/22	0.93	0.15	132,140,144,151	0
22	T6A	1K	37	32/33	0.94	0.26	100,113,152,156	0
22	U8U	1K	34	23/24	0.95	0.15	116,123,130,131	0
23	OMC	2K	33	21/22	0.96	0.10	95,105,111,117	0
22	PSU	1K	39	20/21	0.96	0.15	98,124,139,139	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	1G	1602	1/1	-0.02	0.33	133,133,133,133	0
58	MG	1G	1627	1/1	0.14	0.38	142,142,142,142	0
58	MG	14	3062	1/1	0.18	0.28	129,129,129,129	0
58	MG	1H	3327	1/1	0.19	0.33	120,120,120,120	0
58	MG	32	301	1/1	0.20	0.33	128,128,128,128	0
58	MG	14	3310	1/1	0.22	0.34	124,124,124,124	0
58	MG	14	3051	1/1	0.23	0.26	158,158,158,158	0
58	MG	1H	3264	1/1	0.24	0.29	122,122,122,122	0
58	MG	1H	3318	1/1	0.25	0.35	116,116,116,116	0
58	MG	1H	3272	1/1	0.26	0.29	118,118,118,118	0
58	MG	1H	3337	1/1	0.26	0.31	140,140,140,140	0
58	MG	13	1705	1/1	0.28	0.29	150,150,150,150	0
58	MG	14	3168	1/1	0.29	0.27	122,122,122,122	0
58	MG	1H	3343	1/1	0.29	0.18	137,137,137,137	0
58	MG	1H	3317	1/1	0.32	0.37	106,106,106,106	0
58	MG	14	3324	1/1	0.32	0.27	104,104,104,104	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	1G	1642	1/1	0.33	0.32	114,114,114,114	0
58	MG	1H	3035	1/1	0.35	0.28	123,123,123,123	0
58	MG	13	1704	1/1	0.36	0.21	134,134,134,134	0
58	MG	14	3301	1/1	0.37	0.18	115,115,115,115	0
58	MG	2K	103	1/1	0.37	0.19	134,134,134,134	0
58	MG	1G	1669	1/1	0.37	0.20	151,151,151,151	0
58	MG	14	3303	1/1	0.38	0.33	115,115,115,115	0
58	MG	14	3293	1/1	0.39	0.36	109,109,109,109	0
58	MG	1H	3323	1/1	0.40	0.29	122,122,122,122	0
58	MG	C5	201	1/1	0.40	0.28	137,137,137,137	0
58	MG	14	3284	1/1	0.41	0.40	112,112,112,112	0
58	MG	13	1650	1/1	0.42	0.24	134,134,134,134	0
58	MG	1H	3033	1/1	0.43	0.23	109,109,109,109	0
58	MG	29	304	1/1	0.44	0.15	106,106,106,106	0
58	MG	1H	3257	1/1	0.44	0.37	97,97,97,97	0
58	MG	13	1652	1/1	0.45	0.20	138,138,138,138	0
58	MG	1H	3261	1/1	0.46	0.28	115,115,115,115	0
58	MG	14	3335	1/1	0.46	0.29	124,124,124,124	0
58	MG	1H	3313	1/1	0.47	0.29	114,114,114,114	0
58	MG	1H	3291	1/1	0.48	0.36	116,116,116,116	0
58	MG	13	1644	1/1	0.48	0.21	120,120,120,120	0
58	MG	1H	3322	1/1	0.48	0.27	121,121,121,121	0
58	MG	1H	3247	1/1	0.49	0.24	101,101,101,101	0
58	MG	1H	3187	1/1	0.50	0.26	105,105,105,105	0
58	MG	14	3089	1/1	0.50	0.43	104,104,104,104	0
58	MG	1G	1666	1/1	0.51	0.33	121,121,121,121	0
58	MG	1G	1635	1/1	0.51	0.34	111,111,111,111	0
58	MG	1H	3288	1/1	0.52	0.26	99,99,99,99	0
58	MG	14	3057	1/1	0.52	0.25	119,119,119,119	0
58	MG	14	3195	1/1	0.52	0.30	107,107,107,107	0
58	MG	14	3022	1/1	0.52	0.31	101,101,101,101	0
58	MG	1H	3314	1/1	0.53	0.20	107,107,107,107	0
58	MG	1G	1667	1/1	0.53	0.23	111,111,111,111	0
58	MG	13	1709	1/1	0.53	0.26	112,112,112,112	0
58	MG	1H	3350	1/1	0.53	0.33	113,113,113,113	0
58	MG	1H	3351	1/1	0.53	0.20	122,122,122,122	0
58	MG	14	3028	1/1	0.54	0.33	124,124,124,124	0
58	MG	1H	3161	1/1	0.54	0.24	115,115,115,115	0
58	MG	1H	3331	1/1	0.55	0.21	120,120,120,120	0
58	MG	13	1678	1/1	0.55	0.22	121,121,121,121	0
58	MG	1H	3230	1/1	0.55	0.20	104,104,104,104	0
58	MG	1G	1640	1/1	0.55	0.33	115,115,115,115	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	14	3319	1/1	0.55	0.18	128,128,128,128	0
58	MG	13	1703	1/1	0.55	0.20	128,128,128,128	0
58	MG	14	3199	1/1	0.55	0.36	91,91,91,91	0
58	MG	13	1645	1/1	0.55	0.26	113,113,113,113	0
58	MG	14	3289	1/1	0.55	0.24	116,116,116,116	0
58	MG	1H	3330	1/1	0.56	0.23	105,105,105,105	0
58	MG	1H	3112	1/1	0.56	0.29	101,101,101,101	0
58	MG	14	3328	1/1	0.56	0.39	107,107,107,107	0
58	MG	1G	1643	1/1	0.56	0.36	102,102,102,102	0
58	MG	14	3058	1/1	0.56	0.23	107,107,107,107	0
58	MG	2K	102	1/1	0.56	0.29	109,109,109,109	0
58	MG	1H	3069	1/1	0.57	0.19	101,101,101,101	0
58	MG	1H	3070	1/1	0.57	0.28	100,100,100,100	0
58	MG	14	3255	1/1	0.57	0.29	105,105,105,105	0
58	MG	13	1675	1/1	0.57	0.21	149,149,149,149	0
58	MG	14	3286	1/1	0.57	0.34	117,117,117,117	0
58	MG	1H	3154	1/1	0.57	0.32	106,106,106,106	0
58	MG	1H	3256	1/1	0.57	0.29	104,104,104,104	0
58	MG	1G	1659	1/1	0.57	0.23	142,142,142,142	0
58	MG	14	3267	1/1	0.58	0.37	104,104,104,104	0
58	MG	1H	3286	1/1	0.58	0.34	109,109,109,109	0
58	MG	14	3018	1/1	0.58	0.25	111,111,111,111	0
58	MG	1H	3338	1/1	0.58	0.18	112,112,112,112	0
58	MG	1G	1611	1/1	0.58	0.29	129,129,129,129	0
58	MG	14	3068	1/1	0.58	0.37	108,108,108,108	0
58	MG	14	3260	1/1	0.58	0.42	115,115,115,115	0
58	MG	1H	3244	1/1	0.59	0.37	103,103,103,103	0
58	MG	14	3182	1/1	0.59	0.21	105,105,105,105	0
58	MG	1H	3309	1/1	0.59	0.22	126,126,126,126	0
58	MG	1H	3285	1/1	0.59	0.19	115,115,115,115	0
58	MG	14	3232	1/1	0.59	0.24	89,89,89,89	0
58	MG	14	3234	1/1	0.59	0.21	85,85,85,85	0
58	MG	2L	103	1/1	0.59	0.31	128,128,128,128	0
58	MG	14	3005	1/1	0.59	0.25	101,101,101,101	0
58	MG	1H	3016	1/1	0.59	0.26	105,105,105,105	0
58	MG	1H	3269	1/1	0.59	0.32	99,99,99,99	0
58	MG	14	3150	1/1	0.59	0.37	102,102,102,102	0
58	MG	1G	1616	1/1	0.60	0.26	118,118,118,118	0
58	MG	14	3223	1/1	0.60	0.16	116,116,116,116	0
58	MG	14	3033	1/1	0.60	0.30	95,95,95,95	0
58	MG	1H	3289	1/1	0.60	0.45	86,86,86,86	0
58	MG	14	3152	1/1	0.60	0.31	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	3282	1/1	0.60	0.24	106,106,106,106	0
58	MG	1H	3340	1/1	0.60	0.38	101,101,101,101	0
58	MG	14	3185	1/1	0.60	0.27	113,113,113,113	0
58	MG	14	3193	1/1	0.60	0.28	79,79,79,79	0
58	MG	1H	3212	1/1	0.60	0.27	93,93,93,93	0
58	MG	14	3316	1/1	0.61	0.25	111,111,111,111	0
58	MG	14	3026	1/1	0.61	0.20	115,115,115,115	0
58	MG	14	3322	1/1	0.61	0.30	117,117,117,117	0
58	MG	1H	3301	1/1	0.61	0.38	99,99,99,99	0
58	MG	14	3295	1/1	0.61	0.37	96,96,96,96	0
58	MG	1H	3328	1/1	0.61	0.28	119,119,119,119	0
58	MG	14	3339	1/1	0.61	0.31	120,120,120,120	0
58	MG	1G	1628	1/1	0.61	0.31	120,120,120,120	0
58	MG	1H	3105	1/1	0.61	0.34	86,86,86,86	0
58	MG	1H	3297	1/1	0.62	0.22	133,133,133,133	0
58	MG	1H	3320	1/1	0.62	0.28	107,107,107,107	0
58	MG	14	3233	1/1	0.62	0.29	108,108,108,108	0
58	MG	1H	3054	1/1	0.62	0.19	110,110,110,110	0
58	MG	14	3163	1/1	0.62	0.30	104,104,104,104	0
58	MG	1H	3198	1/1	0.62	0.28	119,119,119,119	0
58	MG	14	3258	1/1	0.63	0.24	93,93,93,93	0
58	MG	1H	3300	1/1	0.63	0.29	99,99,99,99	0
58	MG	13	1710	1/1	0.63	0.23	118,118,118,118	0
58	MG	13	1681	1/1	0.63	0.20	124,124,124,124	0
58	MG	13	1684	1/1	0.63	0.21	141,141,141,141	0
58	MG	1H	3146	1/1	0.63	0.27	103,103,103,103	0
58	MG	14	3170	1/1	0.63	0.22	119,119,119,119	0
58	MG	13	1637	1/1	0.63	0.23	123,123,123,123	0
58	MG	14	3245	1/1	0.63	0.22	97,97,97,97	0
58	MG	1H	3346	1/1	0.63	0.29	113,113,113,113	0
58	MG	14	3337	1/1	0.64	0.37	125,125,125,125	0
58	MG	14	3272	1/1	0.64	0.30	96,96,96,96	0
58	MG	14	3321	1/1	0.64	0.25	109,109,109,109	0
58	MG	13	1653	1/1	0.64	0.20	144,144,144,144	0
58	MG	1H	3319	1/1	0.65	0.29	102,102,102,102	0
58	MG	13	1694	1/1	0.65	0.25	114,114,114,114	0
58	MG	1H	3120	1/1	0.65	0.26	107,107,107,107	0
58	MG	1H	3290	1/1	0.65	0.32	103,103,103,103	0
58	MG	1G	1644	1/1	0.65	0.30	110,110,110,110	0
58	MG	1H	3220	1/1	0.65	0.21	115,115,115,115	0
58	MG	1G	1665	1/1	0.65	0.25	122,122,122,122	0
58	MG	1H	3060	1/1	0.66	0.29	111,111,111,111	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	1H	3023	1/1	0.66	0.27	92,92,92,92	0
58	MG	14	3269	1/1	0.66	0.14	115,115,115,115	0
58	MG	14	3325	1/1	0.66	0.23	110,110,110,110	0
58	MG	14	3240	1/1	0.66	0.19	111,111,111,111	0
58	MG	14	3304	1/1	0.66	0.28	87,87,87,87	0
58	MG	14	3200	1/1	0.66	0.25	94,94,94,94	0
58	MG	14	3315	1/1	0.66	0.23	114,114,114,114	0
58	MG	13	1692	1/1	0.66	0.37	99,99,99,99	0
58	MG	1H	3176	1/1	0.66	0.30	110,110,110,110	0
58	MG	14	3192	1/1	0.67	0.27	104,104,104,104	0
58	MG	13	1625	1/1	0.67	0.36	102,102,102,102	0
58	MG	13	1670	1/1	0.67	0.19	119,119,119,119	0
58	MG	7A	101	1/1	0.67	0.27	104,104,104,104	0
58	MG	1H	3011	1/1	0.67	0.36	71,71,71,71	0
58	MG	1H	3268	1/1	0.67	0.30	104,104,104,104	0
58	MG	1H	3315	1/1	0.67	0.19	99,99,99,99	0
58	MG	1G	1645	1/1	0.67	0.31	122,122,122,122	0
58	MG	14	3024	1/1	0.67	0.37	106,106,106,106	0
58	MG	13	1702	1/1	0.67	0.30	114,114,114,114	0
58	MG	13	1690	1/1	0.67	0.35	113,113,113,113	0
58	MG	1H	3281	1/1	0.67	0.34	108,108,108,108	0
58	MG	1H	3206	1/1	0.67	0.28	100,100,100,100	0
58	MG	14	3165	1/1	0.68	0.29	102,102,102,102	0
58	MG	14	3331	1/1	0.68	0.32	108,108,108,108	0
58	MG	14	3101	1/1	0.68	0.21	108,108,108,108	0
58	MG	1H	3165	1/1	0.68	0.19	99,99,99,99	0
58	MG	14	3338	1/1	0.68	0.13	114,114,114,114	0
58	MG	14	3309	1/1	0.68	0.20	109,109,109,109	0
58	MG	14	3179	1/1	0.68	0.26	102,102,102,102	0
58	MG	14	3297	1/1	0.68	0.29	91,91,91,91	0
58	MG	1H	3062	1/1	0.69	0.19	103,103,103,103	0
58	MG	1H	3255	1/1	0.69	0.38	94,94,94,94	0
58	MG	14	3263	1/1	0.69	0.28	102,102,102,102	0
58	MG	14	3265	1/1	0.69	0.16	110,110,110,110	0
58	MG	14	3056	1/1	0.69	0.22	109,109,109,109	0
58	MG	1H	3262	1/1	0.69	0.25	100,100,100,100	0
58	MG	14	3271	1/1	0.69	0.20	101,101,101,101	0
58	MG	13	1606	1/1	0.69	0.20	119,119,119,119	0
58	MG	14	3059	1/1	0.69	0.24	92,92,92,92	0
58	MG	14	3215	1/1	0.69	0.31	89,89,89,89	0
58	MG	14	3318	1/1	0.69	0.24	102,102,102,102	0
58	MG	14	3257	1/1	0.69	0.17	143,143,143,143	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	1H	3182	1/1	0.70	0.20	91,91,91,91	0
58	MG	1G	1630	1/1	0.70	0.23	120,120,120,120	0
58	MG	1H	3202	1/1	0.70	0.27	95,95,95,95	0
58	MG	1G	1652	1/1	0.70	0.27	110,110,110,110	0
58	MG	14	3129	1/1	0.70	0.25	84,84,84,84	0
58	MG	14	3290	1/1	0.70	0.19	113,113,113,113	0
58	MG	14	3143	1/1	0.70	0.26	110,110,110,110	0
58	MG	1H	3141	1/1	0.70	0.41	83,83,83,83	0
58	MG	1H	3341	1/1	0.70	0.16	110,110,110,110	0
58	MG	14	3153	1/1	0.70	0.24	102,102,102,102	0
58	MG	E5	101	1/1	0.70	0.39	100,100,100,100	0
58	MG	14	3262	1/1	0.71	0.26	109,109,109,109	0
58	MG	1H	3194	1/1	0.71	0.19	91,91,91,91	0
58	MG	14	3052	1/1	0.71	0.16	83,83,83,83	0
58	MG	1H	3347	1/1	0.71	0.12	102,102,102,102	0
58	MG	1H	3149	1/1	0.71	0.29	102,102,102,102	0
58	MG	14	3227	1/1	0.71	0.32	104,104,104,104	0
58	MG	13	1626	1/1	0.71	0.25	113,113,113,113	0
58	MG	14	3281	1/1	0.71	0.34	103,103,103,103	0
58	MG	16	208	1/1	0.71	0.13	111,111,111,111	0
58	MG	13	1698	1/1	0.71	0.21	96,96,96,96	0
58	MG	14	3239	1/1	0.71	0.30	90,90,90,90	0
58	MG	1H	3119	1/1	0.71	0.31	81,81,81,81	0
58	MG	14	3333	1/1	0.71	0.28	102,102,102,102	0
58	MG	13	1679	1/1	0.71	0.24	122,122,122,122	0
58	MG	13	1663	1/1	0.71	0.29	86,86,86,86	0
58	MG	14	3256	1/1	0.71	0.25	110,110,110,110	0
58	MG	14	3299	1/1	0.71	0.26	118,118,118,118	0
58	MG	14	3112	1/1	0.71	0.14	108,108,108,108	0
58	MG	1H	3342	1/1	0.71	0.24	105,105,105,105	0
58	MG	1H	3090	1/1	0.71	0.23	76,76,76,76	0
58	MG	14	3283	1/1	0.72	0.32	98,98,98,98	0
58	MG	14	3247	1/1	0.72	0.42	104,104,104,104	0
58	MG	1H	3082	1/1	0.72	0.22	79,79,79,79	0
58	MG	1F	101	1/1	0.72	0.22	107,107,107,107	0
58	MG	13	1680	1/1	0.72	0.25	125,125,125,125	0
58	MG	14	3202	1/1	0.72	0.21	79,79,79,79	0
58	MG	14	3294	1/1	0.72	0.45	100,100,100,100	0
58	MG	1H	3310	1/1	0.72	0.30	95,95,95,95	0
58	MG	1H	3208	1/1	0.72	0.37	99,99,99,99	0
58	MG	13	1708	1/1	0.72	0.32	102,102,102,102	0
58	MG	14	3300	1/1	0.72	0.15	118,118,118,118	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	0.72	0.36	115,115,115,115	0
58	MG	1H	3008	1/1	0.72	0.28	99,99,99,99	0
58	MG	1G	1612	1/1	0.72	0.28	105,105,105,105	0
58	MG	1H	3034	1/1	0.72	0.21	145,145,145,145	0
58	MG	35	201	1/1	0.72	0.37	90,90,90,90	0
58	MG	1H	3296	1/1	0.72	0.33	86,86,86,86	0
58	MG	1H	3081	1/1	0.72	0.15	88,88,88,88	0
58	MG	13	1612	1/1	0.73	0.29	108,108,108,108	0
58	MG	1G	1604	1/1	0.73	0.21	119,119,119,119	0
58	MG	1H	3132	1/1	0.73	0.25	87,87,87,87	0
58	MG	14	3320	1/1	0.73	0.17	119,119,119,119	0
58	MG	1G	1647	1/1	0.73	0.25	101,101,101,101	0
58	MG	1H	3274	1/1	0.73	0.28	105,105,105,105	0
58	MG	1H	3235	1/1	0.73	0.43	112,112,112,112	0
58	MG	1H	3152	1/1	0.73	0.30	108,108,108,108	0
58	MG	14	3113	1/1	0.73	0.23	102,102,102,102	0
58	MG	14	3030	1/1	0.73	0.14	104,104,104,104	0
58	MG	14	3132	1/1	0.73	0.33	86,86,86,86	0
58	MG	14	3135	1/1	0.73	0.23	115,115,115,115	0
58	MG	1H	3263	1/1	0.73	0.34	92,92,92,92	0
58	MG	14	3045	1/1	0.73	0.23	89,89,89,89	0
58	MG	13	1647	1/1	0.73	0.23	108,108,108,108	0
58	MG	1J	201	1/1	0.73	0.29	100,100,100,100	0
58	MG	1H	3143	1/1	0.73	0.27	101,101,101,101	0
58	MG	1H	3339	1/1	0.73	0.35	104,104,104,104	0
58	MG	45	202	1/1	0.73	0.17	122,122,122,122	0
58	MG	14	3311	1/1	0.73	0.26	105,105,105,105	0
58	MG	78	201	1/1	0.73	0.27	92,92,92,92	0
58	MG	13	1621	1/1	0.74	0.26	99,99,99,99	0
58	MG	14	3241	1/1	0.74	0.20	115,115,115,115	0
58	MG	1G	1634	1/1	0.74	0.22	127,127,127,127	0
58	MG	1H	3086	1/1	0.74	0.33	89,89,89,89	0
58	MG	1H	3316	1/1	0.74	0.18	91,91,91,91	0
58	MG	1H	3210	1/1	0.74	0.25	101,101,101,101	0
58	MG	1H	3077	1/1	0.74	0.24	65,65,65,65	0
58	MG	14	3218	1/1	0.74	0.23	97,97,97,97	0
58	MG	13	1700	1/1	0.74	0.21	123,123,123,123	0
58	MG	1H	3348	1/1	0.74	0.26	111,111,111,111	0
58	MG	14	3117	1/1	0.74	0.26	91,91,91,91	0
58	MG	14	3001	1/1	0.74	0.36	97,97,97,97	0
58	MG	1H	3169	1/1	0.74	0.18	95,95,95,95	0
58	MG	1H	3173	1/1	0.74	0.23	108,108,108,108	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	16	205	1/1	0.75	0.17	106,106,106,106	0
58	MG	1H	3324	1/1	0.75	0.18	97,97,97,97	0
58	MG	14	3231	1/1	0.75	0.21	107,107,107,107	0
58	MG	13	1673	1/1	0.75	0.34	106,106,106,106	0
58	MG	1G	1636	1/1	0.75	0.29	111,111,111,111	0
58	MG	1H	3229	1/1	0.75	0.30	89,89,89,89	0
58	MG	14	3235	1/1	0.75	0.18	102,102,102,102	0
58	MG	1G	1603	1/1	0.75	0.26	132,132,132,132	0
58	MG	13	1648	1/1	0.75	0.42	108,108,108,108	0
58	MG	14	3134	1/1	0.75	0.31	100,100,100,100	0
58	MG	13	1660	1/1	0.75	0.21	104,104,104,104	0
58	MG	1H	3333	1/1	0.75	0.24	93,93,93,93	0
58	MG	1H	3240	1/1	0.75	0.32	96,96,96,96	0
58	MG	13	1605	1/1	0.75	0.21	134,134,134,134	0
58	MG	14	3023	1/1	0.75	0.31	103,103,103,103	0
58	MG	13	1603	1/1	0.75	0.29	102,102,102,102	0
58	MG	1G	1664	1/1	0.76	0.21	122,122,122,122	0
58	MG	13	1662	1/1	0.76	0.15	116,116,116,116	0
58	MG	1H	3155	1/1	0.76	0.14	86,86,86,86	0
58	MG	14	3054	1/1	0.76	0.12	99,99,99,99	0
58	MG	1G	1605	1/1	0.76	0.20	125,125,125,125	0
58	MG	1H	3128	1/1	0.76	0.22	90,90,90,90	0
58	MG	14	3274	1/1	0.76	0.18	97,97,97,97	0
58	MG	14	3313	1/1	0.76	0.22	107,107,107,107	0
58	MG	14	3032	1/1	0.76	0.20	109,109,109,109	0
58	MG	1H	3205	1/1	0.76	0.39	114,114,114,114	0
58	MG	14	3317	1/1	0.77	0.18	122,122,122,122	0
58	MG	1H	3312	1/1	0.77	0.28	103,103,103,103	0
58	MG	1H	3030	1/1	0.77	0.34	85,85,85,85	0
58	MG	1G	1606	1/1	0.77	0.26	93,93,93,93	0
58	MG	1H	3036	1/1	0.77	0.14	118,118,118,118	0
58	MG	14	3146	1/1	0.77	0.24	77,77,77,77	0
58	MG	1H	3071	1/1	0.77	0.21	94,94,94,94	0
58	MG	1G	1614	1/1	0.77	0.17	127,127,127,127	0
58	MG	14	3261	1/1	0.77	0.17	101,101,101,101	0
58	MG	13	1634	1/1	0.77	0.27	104,104,104,104	0
58	MG	1G	1621	1/1	0.77	0.27	110,110,110,110	0
58	MG	1H	3116	1/1	0.77	0.32	88,88,88,88	0
58	MG	14	3302	1/1	0.77	0.37	95,95,95,95	0
58	MG	1G	1663	1/1	0.77	0.16	133,133,133,133	0
58	MG	16	209	1/1	0.77	0.14	106,106,106,106	0
58	MG	14	3174	1/1	0.77	0.26	98,98,98,98	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	13	1707	1/1	0.77	0.33	114,114,114,114	0
58	MG	1G	1632	1/1	0.77	0.22	130,130,130,130	0
58	MG	14	3275	1/1	0.77	0.23	90,90,90,90	0
58	MG	13	1688	1/1	0.77	0.23	96,96,96,96	0
58	MG	1H	3332	1/1	0.77	0.34	93,93,93,93	0
58	MG	13	1685	1/1	0.78	0.26	107,107,107,107	0
58	MG	1H	3349	1/1	0.78	0.14	119,119,119,119	0
58	MG	13	1627	1/1	0.78	0.33	105,105,105,105	0
58	MG	1H	3295	1/1	0.78	0.22	110,110,110,110	0
58	MG	1H	3355	1/1	0.78	0.35	88,88,88,88	0
58	MG	1H	3488	1/1	0.78	0.23	89,89,89,89	0
58	MG	14	3031	1/1	0.78	0.21	89,89,89,89	0
58	MG	1H	3005	1/1	0.78	0.25	79,79,79,79	0
58	MG	16	207	1/1	0.78	0.17	92,92,92,92	0
58	MG	14	3326	1/1	0.78	0.31	104,104,104,104	0
58	MG	13	1695	1/1	0.78	0.17	122,122,122,122	0
58	MG	1H	3175	1/1	0.78	0.17	92,92,92,92	0
58	MG	1H	3209	1/1	0.78	0.31	99,99,99,99	0
58	MG	14	3053	1/1	0.78	0.29	82,82,82,82	0
58	MG	14	3216	1/1	0.78	0.21	101,101,101,101	0
58	MG	14	3217	1/1	0.78	0.30	89,89,89,89	0
58	MG	14	3264	1/1	0.78	0.23	106,106,106,106	0
58	MG	1H	3150	1/1	0.78	0.30	63,63,63,63	0
58	MG	1J	204	1/1	0.78	0.13	119,119,119,119	0
58	MG	13	1646	1/1	0.78	0.18	129,129,129,129	0
58	MG	13	1699	1/1	0.78	0.29	97,97,97,97	0
58	MG	14	3156	1/1	0.78	0.32	88,88,88,88	0
58	MG	1H	3226	1/1	0.78	0.23	88,88,88,88	0
58	MG	1H	3102	1/1	0.78	0.31	73,73,73,73	0
58	MG	14	3298	1/1	0.79	0.29	104,104,104,104	0
58	MG	1H	3242	1/1	0.79	0.17	90,90,90,90	0
58	MG	14	3110	1/1	0.79	0.25	94,94,94,94	0
58	MG	1H	3049	1/1	0.79	0.23	82,82,82,82	0
58	MG	1G	1620	1/1	0.79	0.28	91,91,91,91	0
58	MG	1H	3167	1/1	0.79	0.34	96,96,96,96	0
58	MG	14	3277	1/1	0.79	0.23	111,111,111,111	0
58	MG	1H	3178	1/1	0.79	0.26	93,93,93,93	0
58	MG	1H	3486	1/1	0.79	0.28	106,106,106,106	0
58	MG	1H	3129	1/1	0.79	0.36	85,85,85,85	0
58	MG	2L	101	1/1	0.79	0.23	97,97,97,97	0
58	MG	14	3136	1/1	0.79	0.27	93,93,93,93	0
58	MG	1J	202	1/1	0.79	0.28	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	1H	3336	1/1	0.79	0.17	93,93,93,93	0
58	MG	14	3292	1/1	0.79	0.32	83,83,83,83	0
58	MG	14	3188	1/1	0.79	0.42	93,93,93,93	0
58	MG	1H	3237	1/1	0.79	0.16	88,88,88,88	0
58	MG	13	1676	1/1	0.79	0.17	130,130,130,130	0
58	MG	14	3151	1/1	0.79	0.24	109,109,109,109	0
58	MG	13	1661	1/1	0.80	0.21	90,90,90,90	0
58	MG	1G	1633	1/1	0.80	0.08	137,137,137,137	0
58	MG	14	3105	1/1	0.80	0.29	110,110,110,110	0
58	MG	13	1671	1/1	0.80	0.12	107,107,107,107	0
58	MG	1H	3275	1/1	0.80	0.15	83,83,83,83	0
58	MG	13	1604	1/1	0.80	0.29	90,90,90,90	0
58	MG	14	3171	1/1	0.80	0.35	91,91,91,91	0
58	MG	1G	1638	1/1	0.80	0.33	102,102,102,102	0
58	MG	1H	3038	1/1	0.80	0.18	102,102,102,102	0
58	MG	1H	3024	1/1	0.80	0.19	99,99,99,99	0
58	MG	14	3183	1/1	0.80	0.26	89,89,89,89	0
58	MG	14	3238	1/1	0.80	0.36	83,83,83,83	0
58	MG	1H	3196	1/1	0.80	0.26	102,102,102,102	0
58	MG	14	3342	1/1	0.80	0.14	120,120,120,120	0
58	MG	13	1674	1/1	0.80	0.18	121,121,121,121	0
58	MG	13	1691	1/1	0.80	0.35	94,94,94,94	0
58	MG	1J	203	1/1	0.80	0.22	124,124,124,124	0
58	MG	1G	1622	1/1	0.80	0.24	103,103,103,103	0
58	MG	1H	3032	1/1	0.80	0.27	110,110,110,110	0
58	MG	1G	1656	1/1	0.80	0.20	102,102,102,102	0
58	MG	14	3287	1/1	0.80	0.20	101,101,101,101	0
58	MG	1H	3063	1/1	0.80	0.23	57,57,57,57	0
58	MG	13	1624	1/1	0.80	0.20	118,118,118,118	0
58	MG	14	3166	1/1	0.81	0.16	79,79,79,79	0
58	MG	13	1641	1/1	0.81	0.13	112,112,112,112	0
58	MG	14	3224	1/1	0.81	0.05	105,105,105,105	0
58	MG	1H	3219	1/1	0.81	0.17	120,120,120,120	0
58	MG	14	3327	1/1	0.81	0.23	83,83,83,83	0
58	MG	13	1635	1/1	0.81	0.27	111,111,111,111	0
58	MG	1G	1654	1/1	0.81	0.24	110,110,110,110	0
58	MG	14	3011	1/1	0.81	0.32	85,85,85,85	0
58	MG	1H	3222	1/1	0.81	0.19	94,94,94,94	0
58	MG	1H	3003	1/1	0.81	0.24	72,72,72,72	0
58	MG	13	1623	1/1	0.81	0.21	88,88,88,88	0
58	MG	5E	201	1/1	0.81	0.12	107,107,107,107	0
58	MG	1H	3207	1/1	0.81	0.24	93,93,93,93	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	1H	3039	1/1	0.81	0.27	100,100,100,100	0
58	MG	14	3075	1/1	0.81	0.29	96,96,96,96	0
58	MG	14	3080	1/1	0.81	0.28	105,105,105,105	0
58	MG	14	3251	1/1	0.81	0.12	90,90,90,90	0
58	MG	1G	1641	1/1	0.81	0.21	131,131,131,131	0
58	MG	1H	3043	1/1	0.81	0.18	75,75,75,75	0
58	MG	14	3162	1/1	0.81	0.36	90,90,90,90	0
58	MG	85	201	1/1	0.81	0.47	100,100,100,100	0
58	MG	13	1672	1/1	0.81	0.14	133,133,133,133	0
58	MG	1H	3294	1/1	0.81	0.16	103,103,103,103	0
58	MG	5I	101	1/1	0.82	0.11	110,110,110,110	0
58	MG	14	3106	1/1	0.82	0.21	85,85,85,85	0
58	MG	14	3108	1/1	0.82	0.18	88,88,88,88	0
58	MG	1H	3051	1/1	0.82	0.18	90,90,90,90	0
58	MG	1H	3303	1/1	0.82	0.21	102,102,102,102	0
58	MG	1H	3277	1/1	0.82	0.09	122,122,122,122	0
58	MG	1H	3118	1/1	0.82	0.26	104,104,104,104	0
58	MG	1H	3066	1/1	0.82	0.29	86,86,86,86	0
58	MG	1H	3179	1/1	0.82	0.23	101,101,101,101	0
58	MG	14	3288	1/1	0.82	0.18	120,120,120,120	0
58	MG	14	3133	1/1	0.82	0.23	98,98,98,98	0
58	MG	13	1666	1/1	0.82	0.11	99,99,99,99	0
58	MG	14	3291	1/1	0.82	0.21	96,96,96,96	0
58	MG	14	3246	1/1	0.82	0.15	95,95,95,95	0
58	MG	1H	3057	1/1	0.82	0.20	75,75,75,75	0
58	MG	14	3191	1/1	0.82	0.26	93,93,93,93	0
58	MG	1H	3158	1/1	0.82	0.16	105,105,105,105	0
58	MG	1H	3093	1/1	0.82	0.35	88,88,88,88	0
58	MG	14	3144	1/1	0.82	0.16	112,112,112,112	0
58	MG	1H	3162	1/1	0.82	0.29	106,106,106,106	0
58	MG	14	3147	1/1	0.82	0.24	110,110,110,110	0
58	MG	14	3149	1/1	0.82	0.32	94,94,94,94	0
58	MG	14	3213	1/1	0.82	0.15	114,114,114,114	0
58	MG	13	1696	1/1	0.82	0.25	95,95,95,95	0
58	MG	1G	1660	1/1	0.82	0.20	111,111,111,111	0
58	MG	14	3308	1/1	0.82	0.41	104,104,104,104	0
58	MG	1H	3232	1/1	0.82	0.20	98,98,98,98	0
58	MG	1H	3072	1/1	0.82	0.15	120,120,120,120	0
58	MG	14	3029	1/1	0.82	0.22	90,90,90,90	0
58	MG	1H	3109	1/1	0.82	0.25	102,102,102,102	0
58	MG	1H	3231	1/1	0.83	0.25	85,85,85,85	0
58	MG	1H	3097	1/1	0.83	0.20	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	14	3296	1/1	0.83	0.16	110,110,110,110	0
58	MG	1H	3280	1/1	0.83	0.13	114,114,114,114	0
58	MG	14	3098	1/1	0.83	0.20	86,86,86,86	0
58	MG	1H	3215	1/1	0.83	0.25	69,69,69,69	0
58	MG	1H	3166	1/1	0.83	0.28	95,95,95,95	0
58	MG	14	3148	1/1	0.83	0.27	94,94,94,94	0
58	MG	13	1687	1/1	0.83	0.42	100,100,100,100	0
58	MG	1G	1662	1/1	0.83	0.19	118,118,118,118	0
58	MG	14	3109	1/1	0.83	0.27	94,94,94,94	0
58	MG	1H	3321	1/1	0.83	0.23	84,84,84,84	0
58	MG	1H	3145	1/1	0.83	0.25	117,117,117,117	0
58	MG	14	3196	1/1	0.83	0.20	98,98,98,98	0
58	MG	14	3197	1/1	0.83	0.23	124,124,124,124	0
58	MG	14	3155	1/1	0.83	0.18	101,101,101,101	0
58	MG	1H	3073	1/1	0.83	0.33	84,84,84,84	0
58	MG	14	3161	1/1	0.83	0.21	80,80,80,80	0
58	MG	1H	3074	1/1	0.83	0.24	94,94,94,94	0
58	MG	1H	3250	1/1	0.83	0.13	94,94,94,94	0
58	MG	14	3061	1/1	0.83	0.15	102,102,102,102	0
58	MG	1H	3134	1/1	0.83	0.21	103,103,103,103	0
58	MG	1H	3292	1/1	0.83	0.17	82,82,82,82	0
58	MG	14	3201	1/1	0.84	0.31	91,91,91,91	0
58	MG	14	3016	1/1	0.84	0.40	68,68,68,68	0
58	MG	14	3065	1/1	0.84	0.20	80,80,80,80	0
58	MG	13	1668	1/1	0.84	0.12	117,117,117,117	0
58	MG	1H	3203	1/1	0.84	0.20	91,91,91,91	0
58	MG	14	3078	1/1	0.84	0.19	82,82,82,82	0
58	MG	1G	1658	1/1	0.84	0.20	99,99,99,99	0
58	MG	1H	3017	1/1	0.84	0.21	79,79,79,79	0
58	MG	14	3096	1/1	0.84	0.26	57,57,57,57	0
58	MG	14	3278	1/1	0.84	0.18	86,86,86,86	0
58	MG	14	3279	1/1	0.84	0.20	103,103,103,103	0
58	MG	13	1667	1/1	0.84	0.23	91,91,91,91	0
58	MG	1H	3117	1/1	0.84	0.14	75,75,75,75	0
58	MG	1H	3075	1/1	0.84	0.39	82,82,82,82	0
58	MG	1H	3076	1/1	0.84	0.25	78,78,78,78	0
58	MG	1H	3184	1/1	0.84	0.34	94,94,94,94	0
58	MG	1H	3010	1/1	0.84	0.24	98,98,98,98	0
58	MG	16	203	1/1	0.84	0.13	112,112,112,112	0
58	MG	14	3035	1/1	0.84	0.18	89,89,89,89	0
58	MG	14	3039	1/1	0.84	0.28	86,86,86,86	0
58	MG	14	3116	1/1	0.84	0.30	75,75,75,75	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	1H	3148	1/1	0.84	0.20	92,92,92,92	0
58	MG	14	3049	1/1	0.84	0.28	74,74,74,74	0
58	MG	14	3130	1/1	0.84	0.18	93,93,93,93	0
58	MG	14	3250	1/1	0.84	0.20	79,79,79,79	0
58	MG	1H	3127	1/1	0.84	0.19	79,79,79,79	0
58	MG	13	1683	1/1	0.84	0.26	119,119,119,119	0
58	MG	1G	1623	1/1	0.84	0.23	100,100,100,100	0
58	MG	1G	1626	1/1	0.84	0.19	118,118,118,118	0
58	MG	1G	1648	1/1	0.84	0.24	128,128,128,128	0
58	MG	14	3004	1/1	0.84	0.29	76,76,76,76	0
58	MG	1G	1649	1/1	0.84	0.18	128,128,128,128	0
58	MG	1H	3344	1/1	0.84	0.20	81,81,81,81	0
58	MG	14	3013	1/1	0.84	0.19	98,98,98,98	0
58	MG	1H	3020	1/1	0.85	0.26	84,84,84,84	0
58	MG	14	3120	1/1	0.85	0.09	94,94,94,94	0
58	MG	13	1617	1/1	0.85	0.22	97,97,97,97	0
58	MG	13	1693	1/1	0.85	0.28	108,108,108,108	0
58	MG	14	3076	1/1	0.85	0.17	83,83,83,83	0
58	MG	14	3205	1/1	0.85	0.12	97,97,97,97	0
58	MG	1H	3236	1/1	0.85	0.19	89,89,89,89	0
58	MG	14	3167	1/1	0.85	0.15	105,105,105,105	0
58	MG	1H	3048	1/1	0.85	0.21	80,80,80,80	0
58	MG	41	201	1/1	0.85	0.14	102,102,102,102	0
58	MG	14	3015	1/1	0.85	0.32	82,82,82,82	0
58	MG	14	3220	1/1	0.85	0.20	97,97,97,97	0
58	MG	14	3332	1/1	0.85	0.23	98,98,98,98	0
58	MG	1H	3180	1/1	0.85	0.12	97,97,97,97	0
58	MG	14	3334	1/1	0.85	0.19	92,92,92,92	0
58	MG	14	3177	1/1	0.85	0.33	87,87,87,87	0
58	MG	13	1659	1/1	0.85	0.06	116,116,116,116	0
58	MG	14	3181	1/1	0.85	0.41	91,91,91,91	0
58	MG	14	3270	1/1	0.85	0.23	97,97,97,97	0
58	MG	14	3102	1/1	0.85	0.15	92,92,92,92	0
58	MG	1H	3137	1/1	0.85	0.22	93,93,93,93	0
58	MG	1H	3307	1/1	0.85	0.23	97,97,97,97	0
58	MG	1G	1646	1/1	0.85	0.14	126,126,126,126	0
58	MG	1G	1629	1/1	0.85	0.16	121,121,121,121	0
58	MG	14	3027	1/1	0.85	0.20	79,79,79,79	0
58	MG	13	1649	1/1	0.85	0.12	118,118,118,118	0
58	MG	14	3312	1/1	0.85	0.17	97,97,97,97	0
58	MG	55	201	1/1	0.85	0.31	96,96,96,96	0
58	MG	14	3280	1/1	0.85	0.29	98,98,98,98	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	1H	3126	1/1	0.85	0.14	83,83,83,83	0
58	MG	1H	3253	1/1	0.85	0.25	84,84,84,84	0
58	MG	14	3021	1/1	0.86	0.20	73,73,73,73	0
58	MG	1H	3009	1/1	0.86	0.13	98,98,98,98	0
58	MG	1G	1625	1/1	0.86	0.12	136,136,136,136	0
58	MG	1H	3157	1/1	0.86	0.24	88,88,88,88	0
58	MG	1H	3100	1/1	0.86	0.36	82,82,82,82	0
58	MG	14	3111	1/1	0.86	0.25	82,82,82,82	0
58	MG	14	3158	1/1	0.86	0.20	92,92,92,92	0
58	MG	1H	3329	1/1	0.86	0.12	105,105,105,105	0
58	MG	1H	3243	1/1	0.86	0.10	96,96,96,96	0
58	MG	14	3206	1/1	0.86	0.09	88,88,88,88	0
58	MG	14	3330	1/1	0.86	0.27	104,104,104,104	0
58	MG	1H	3002	1/1	0.86	0.24	64,64,64,64	0
58	MG	1H	3224	1/1	0.86	0.18	76,76,76,76	0
58	MG	13	1677	1/1	0.86	0.49	113,113,113,113	0
58	MG	1H	3085	1/1	0.86	0.21	92,92,92,92	0
58	MG	13	1618	1/1	0.86	0.15	108,108,108,108	0
58	MG	1H	3089	1/1	0.86	0.20	83,83,83,83	0
58	MG	13	1620	1/1	0.86	0.21	117,117,117,117	0
58	MG	14	3041	1/1	0.86	0.20	80,80,80,80	0
58	MG	14	3084	1/1	0.86	0.19	92,92,92,92	0
58	MG	14	3230	1/1	0.86	0.10	122,122,122,122	0
58	MG	14	3042	1/1	0.86	0.15	74,74,74,74	0
58	MG	14	3273	1/1	0.86	0.15	110,110,110,110	0
58	MG	14	3138	1/1	0.86	0.12	96,96,96,96	0
58	MG	29	302	1/1	0.86	0.20	69,69,69,69	0
58	MG	14	3091	1/1	0.86	0.22	92,92,92,92	0
58	MG	14	3044	1/1	0.86	0.12	88,88,88,88	0
58	MG	45	201	1/1	0.86	0.28	101,101,101,101	0
58	MG	1H	3019	1/1	0.86	0.28	65,65,65,65	0
58	MG	1H	3305	1/1	0.86	0.27	96,96,96,96	0
58	MG	1H	3214	1/1	0.86	0.19	65,65,65,65	0
58	MG	14	3103	1/1	0.86	0.15	81,81,81,81	0
58	MG	14	3282	1/1	0.86	0.13	96,96,96,96	0
58	MG	14	3266	1/1	0.87	0.16	99,99,99,99	0
58	MG	1H	3065	1/1	0.87	0.21	77,77,77,77	0
58	MG	1H	3489	1/1	0.87	0.23	77,77,77,77	0
58	MG	14	3208	1/1	0.87	0.11	93,93,93,93	0
58	MG	16	201	1/1	0.87	0.10	114,114,114,114	0
58	MG	1H	3110	1/1	0.87	0.16	83,83,83,83	0
58	MG	1H	3053	1/1	0.87	0.20	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	BI	201	1/1	0.87	0.21	113,113,113,113	0
58	MG	1H	3177	1/1	0.87	0.37	93,93,93,93	0
58	MG	1H	3136	1/1	0.87	0.31	80,80,80,80	0
58	MG	1H	3156	1/1	0.87	0.11	121,121,121,121	0
58	MG	14	3323	1/1	0.87	0.08	159,159,159,159	0
58	MG	14	3107	1/1	0.87	0.21	80,80,80,80	0
58	MG	1H	3311	1/1	0.87	0.11	77,77,77,77	0
58	MG	Q8	101	1/1	0.87	0.28	89,89,89,89	0
58	MG	1H	3047	1/1	0.87	0.33	71,71,71,71	0
58	MG	1H	3213	1/1	0.87	0.13	81,81,81,81	0
58	MG	1H	3283	1/1	0.87	0.51	95,95,95,95	0
58	MG	14	3007	1/1	0.87	0.26	81,81,81,81	0
58	MG	14	3115	1/1	0.87	0.20	88,88,88,88	0
58	MG	14	3055	1/1	0.87	0.18	77,77,77,77	0
58	MG	1H	3139	1/1	0.87	0.13	75,75,75,75	0
58	MG	1H	3248	1/1	0.87	0.44	93,93,93,93	0
58	MG	14	3336	1/1	0.87	0.29	120,120,120,120	0
58	MG	14	3124	1/1	0.87	0.24	90,90,90,90	0
58	MG	1H	3037	1/1	0.87	0.19	87,87,87,87	0
58	MG	13	1657	1/1	0.87	0.14	103,103,103,103	0
58	MG	14	3341	1/1	0.87	0.14	105,105,105,105	0
58	MG	1H	3189	1/1	0.87	0.31	93,93,93,93	0
58	MG	1H	3163	1/1	0.87	0.31	84,84,84,84	0
58	MG	1G	1650	1/1	0.87	0.24	98,98,98,98	0
58	MG	14	3253	1/1	0.87	0.10	90,90,90,90	0
58	MG	1H	3083	1/1	0.87	0.14	74,74,74,74	0
58	MG	1J	205	1/1	0.87	0.19	122,122,122,122	0
58	MG	1J	206	1/1	0.87	0.11	130,130,130,130	0
58	MG	1H	3225	1/1	0.87	0.27	70,70,70,70	0
58	MG	14	3137	1/1	0.87	0.08	119,119,119,119	0
58	MG	2K	101	1/1	0.87	0.23	84,84,84,84	0
58	MG	1H	3199	1/1	0.87	0.27	87,87,87,87	0
58	MG	1H	3326	1/1	0.87	0.24	97,97,97,97	0
58	MG	1H	3107	1/1	0.87	0.20	95,95,95,95	0
58	MG	14	3085	1/1	0.87	0.20	85,85,85,85	0
58	MG	14	3088	1/1	0.87	0.22	78,78,78,78	0
58	MG	14	3204	1/1	0.87	0.20	73,73,73,73	0
58	MG	1H	3027	1/1	0.88	0.12	95,95,95,95	0
58	MG	1H	3056	1/1	0.88	0.13	89,89,89,89	0
58	MG	14	3066	1/1	0.88	0.17	95,95,95,95	0
58	MG	1G	1610	1/1	0.88	0.14	118,118,118,118	0
58	MG	1H	3298	1/1	0.88	0.29	95,95,95,95	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	14	3019	1/1	0.88	0.19	87,87,87,87	0
58	MG	1H	3217	1/1	0.88	0.09	81,81,81,81	0
58	MG	1H	3200	1/1	0.88	0.21	79,79,79,79	0
58	MG	1H	3029	1/1	0.88	0.21	92,92,92,92	0
58	MG	1G	1618	1/1	0.88	0.15	131,131,131,131	0
58	MG	1G	1619	1/1	0.88	0.12	109,109,109,109	0
58	MG	1H	3304	1/1	0.88	0.26	94,94,94,94	0
58	MG	1H	3481	1/1	0.88	0.07	133,133,133,133	0
58	MG	14	3094	1/1	0.88	0.26	82,82,82,82	0
58	MG	14	3095	1/1	0.88	0.25	75,75,75,75	0
58	MG	1H	3121	1/1	0.88	0.25	93,93,93,93	0
58	MG	1H	3204	1/1	0.88	0.10	87,87,87,87	0
58	MG	1G	1624	1/1	0.88	0.20	92,92,92,92	0
58	MG	14	3157	1/1	0.88	0.10	81,81,81,81	0
58	MG	14	3228	1/1	0.88	0.14	96,96,96,96	0
58	MG	1H	3124	1/1	0.88	0.19	77,77,77,77	0
58	MG	1H	3252	1/1	0.88	0.17	75,75,75,75	0
58	MG	14	3104	1/1	0.88	0.21	78,78,78,78	0
58	MG	13	1609	1/1	0.88	0.14	99,99,99,99	0
58	MG	1H	3334	1/1	0.88	0.15	77,77,77,77	0
58	MG	1H	3227	1/1	0.88	0.19	92,92,92,92	0
58	MG	1H	3021	1/1	0.88	0.19	86,86,86,86	0
58	MG	1G	1631	1/1	0.88	0.28	97,97,97,97	0
58	MG	1H	3172	1/1	0.88	0.18	89,89,89,89	0
58	MG	2I	301	1/1	0.88	0.23	69,69,69,69	0
58	MG	1H	3260	1/1	0.88	0.35	95,95,95,95	0
58	MG	1H	3188	1/1	0.88	0.27	84,84,84,84	0
58	MG	D8	201	1/1	0.88	0.07	92,92,92,92	0
58	MG	14	3003	1/1	0.88	0.13	76,76,76,76	0
58	MG	1H	3006	1/1	0.88	0.17	71,71,71,71	0
58	MG	1H	3174	1/1	0.88	0.24	99,99,99,99	0
58	MG	14	3122	1/1	0.88	0.26	95,95,95,95	0
58	MG	14	3186	1/1	0.88	0.29	100,100,100,100	0
58	MG	14	3123	1/1	0.88	0.19	109,109,109,109	0
58	MG	13	1631	1/1	0.88	0.12	82,82,82,82	0
58	MG	14	3009	1/1	0.88	0.18	74,74,74,74	0
58	MG	14	3010	1/1	0.88	0.19	73,73,73,73	0
58	MG	1H	3267	1/1	0.88	0.14	85,85,85,85	0
58	MG	14	3259	1/1	0.89	0.30	111,111,111,111	0
58	MG	14	3141	1/1	0.89	0.17	76,76,76,76	0
58	MG	1H	3125	1/1	0.89	0.16	75,75,75,75	0
58	MG	1H	3181	1/1	0.89	0.17	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	1G	1668	1/1	0.89	0.09	138,138,138,138	0
58	MG	13	1669	1/1	0.89	0.13	120,120,120,120	0
58	MG	14	3034	1/1	0.89	0.18	96,96,96,96	0
58	MG	1H	3013	1/1	0.89	0.23	71,71,71,71	0
58	MG	1H	3186	1/1	0.89	0.18	96,96,96,96	0
58	MG	1G	1637	1/1	0.89	0.11	101,101,101,101	0
58	MG	13	1651	1/1	0.89	0.17	96,96,96,96	0
58	MG	14	3212	1/1	0.89	0.11	105,105,105,105	0
58	MG	14	3043	1/1	0.89	0.16	69,69,69,69	0
58	MG	13	1706	1/1	0.89	0.30	91,91,91,91	0
58	MG	1G	1609	1/1	0.89	0.10	113,113,113,113	0
58	MG	1H	3094	1/1	0.89	0.18	77,77,77,77	0
58	MG	1H	3190	1/1	0.89	0.14	108,108,108,108	0
58	MG	1H	3354	1/1	0.89	0.09	98,98,98,98	0
58	MG	14	3222	1/1	0.89	0.37	95,95,95,95	0
58	MG	1H	3193	1/1	0.89	0.26	104,104,104,104	0
58	MG	1H	3302	1/1	0.89	0.21	89,89,89,89	0
58	MG	1H	3095	1/1	0.89	0.40	95,95,95,95	0
58	MG	13	1602	1/1	0.89	0.20	98,98,98,98	0
58	MG	14	3014	1/1	0.89	0.22	82,82,82,82	0
58	MG	1H	3278	1/1	0.89	0.30	90,90,90,90	0
58	MG	1H	3098	1/1	0.89	0.34	70,70,70,70	0
58	MG	1H	3221	1/1	0.89	0.19	81,81,81,81	0
58	MG	16	204	1/1	0.89	0.09	106,106,106,106	0
58	MG	14	3175	1/1	0.89	0.20	93,93,93,93	0
58	MG	14	3237	1/1	0.89	0.14	181,181,181,181	0
58	MG	14	3406	1/1	0.89	0.06	121,121,121,121	0
58	MG	14	3176	1/1	0.89	0.19	96,96,96,96	0
58	MG	14	3020	1/1	0.89	0.23	93,93,93,93	0
58	MG	1H	3251	1/1	0.89	0.15	75,75,75,75	0
58	MG	13	1701	1/1	0.89	0.17	103,103,103,103	0
58	MG	14	3069	1/1	0.89	0.15	106,106,106,106	0
58	MG	14	3074	1/1	0.89	0.27	70,70,70,70	0
58	MG	13	1642	1/1	0.89	0.14	104,104,104,104	0
58	MG	14	3248	1/1	0.89	0.23	89,89,89,89	0
58	MG	1H	3159	1/1	0.89	0.16	89,89,89,89	0
58	MG	1H	3287	1/1	0.89	0.28	96,96,96,96	0
58	MG	1H	3160	1/1	0.89	0.21	88,88,88,88	0
58	MG	13	1628	1/1	0.89	0.18	94,94,94,94	0
58	MG	88	201	1/1	0.89	0.12	96,96,96,96	0
58	MG	14	3194	1/1	0.89	0.17	93,93,93,93	0
58	MG	14	3086	1/1	0.89	0.30	95,95,95,95	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
58	MG	13	1633	1/1	0.90	0.34	88,88,88,88	0
58	MG	1G	1655	1/1	0.90	0.07	176,176,176,176	0
58	MG	14	3017	1/1	0.90	0.25	68,68,68,68	0
58	MG	1H	3335	1/1	0.90	0.17	100,100,100,100	0
58	MG	1G	1657	1/1	0.90	0.07	163,163,163,163	0
58	MG	14	3221	1/1	0.90	0.10	80,80,80,80	0
58	MG	1H	3028	1/1	0.90	0.17	82,82,82,82	0
58	MG	14	3114	1/1	0.90	0.25	66,66,66,66	0
58	MG	14	3276	1/1	0.90	0.10	130,130,130,130	0
58	MG	1H	3144	1/1	0.90	0.27	89,89,89,89	0
58	MG	14	3169	1/1	0.90	0.19	69,69,69,69	0
58	MG	1H	3254	1/1	0.90	0.32	91,91,91,91	0
58	MG	13	1658	1/1	0.90	0.16	89,89,89,89	0
58	MG	14	3067	1/1	0.90	0.12	100,100,100,100	0
58	MG	1H	3092	1/1	0.90	0.19	76,76,76,76	0
58	MG	1H	3164	1/1	0.90	0.09	86,86,86,86	0
58	MG	1H	3108	1/1	0.90	0.33	92,92,92,92	0
58	MG	14	3178	1/1	0.90	0.21	94,94,94,94	0
58	MG	13	1638	1/1	0.90	0.27	82,82,82,82	0
58	MG	1H	3234	1/1	0.90	0.38	90,90,90,90	0
58	MG	14	3131	1/1	0.90	0.20	79,79,79,79	0
58	MG	5E	202	1/1	0.90	0.06	111,111,111,111	0
58	MG	1H	3151	1/1	0.90	0.07	90,90,90,90	0
58	MG	14	3081	1/1	0.90	0.17	89,89,89,89	0
58	MG	1H	3111	1/1	0.90	0.14	64,64,64,64	0
58	MG	1H	3153	1/1	0.90	0.12	86,86,86,86	0
58	MG	1H	3001	1/1	0.90	0.22	66,66,66,66	0
58	MG	14	3087	1/1	0.90	0.23	68,68,68,68	0
58	MG	2L	102	1/1	0.90	0.39	95,95,95,95	0
58	MG	1H	3270	1/1	0.90	0.20	87,87,87,87	0
58	MG	14	3040	1/1	0.90	0.20	72,72,72,72	0
58	MG	1H	3325	1/1	0.90	0.20	100,100,100,100	0
58	MG	1H	3299	1/1	0.90	0.25	94,94,94,94	0
58	MG	1H	3218	1/1	0.90	0.14	68,68,68,68	0
58	MG	29	303	1/1	0.90	0.17	94,94,94,94	0
58	MG	1H	3273	1/1	0.90	0.12	85,85,85,85	0
58	MG	39	301	1/1	0.90	0.11	118,118,118,118	0
58	MG	1H	3096	1/1	0.90	0.23	76,76,76,76	0
58	MG	14	3048	1/1	0.90	0.17	90,90,90,90	0
58	MG	1H	3246	1/1	0.90	0.25	87,87,87,87	0
58	MG	13	1697	1/1	0.90	0.30	98,98,98,98	0
58	MG	16	202	1/1	0.90	0.11	102,102,102,102	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	13	1639	1/1	0.90	0.16	87,87,87,87	0
58	MG	1H	3099	1/1	0.90	0.20	74,74,74,74	0
58	MG	1G	1651	1/1	0.91	0.07	128,128,128,128	0
58	MG	1H	3284	1/1	0.91	0.08	97,97,97,97	0
58	MG	14	3097	1/1	0.91	0.14	83,83,83,83	0
58	MG	14	3184	1/1	0.91	0.16	92,92,92,92	0
58	MG	1H	3044	1/1	0.91	0.15	68,68,68,68	0
58	MG	1H	3259	1/1	0.91	0.07	106,106,106,106	0
58	MG	14	3187	1/1	0.91	0.15	96,96,96,96	0
58	MG	1H	3026	1/1	0.91	0.18	80,80,80,80	0
58	MG	11	301	1/1	0.91	0.15	73,73,73,73	0
58	MG	1H	3170	1/1	0.91	0.07	92,92,92,92	0
58	MG	1H	3123	1/1	0.91	0.11	85,85,85,85	0
58	MG	1H	3140	1/1	0.91	0.20	89,89,89,89	0
58	MG	1H	3239	1/1	0.91	0.17	71,71,71,71	0
58	MG	13	1630	1/1	0.91	0.07	74,74,74,74	0
58	MG	I8	101	1/1	0.91	0.21	70,70,70,70	0
58	MG	1H	3293	1/1	0.91	0.25	94,94,94,94	0
58	MG	1G	1601	1/1	0.91	0.14	115,115,115,115	0
58	MG	14	3252	1/1	0.91	0.09	106,106,106,106	0
58	MG	1H	3142	1/1	0.91	0.23	89,89,89,89	0
58	MG	4K	101	1/1	0.91	0.15	88,88,88,88	0
58	MG	14	3159	1/1	0.91	0.17	81,81,81,81	0
58	MG	1H	3018	1/1	0.91	0.26	66,66,66,66	0
58	MG	1H	3052	1/1	0.91	0.19	69,69,69,69	0
58	MG	1G	1639	1/1	0.91	0.31	93,93,93,93	0
58	MG	14	3210	1/1	0.91	0.11	113,113,113,113	0
58	MG	1H	3042	1/1	0.91	0.20	59,59,59,59	0
58	MG	1H	3223	1/1	0.91	0.08	96,96,96,96	0
58	MG	1H	3147	1/1	0.91	0.32	93,93,93,93	0
58	MG	1H	3276	1/1	0.91	0.17	91,91,91,91	0
58	MG	14	3082	1/1	0.91	0.33	92,92,92,92	0
58	MG	1H	3014	1/1	0.91	0.11	65,65,65,65	0
58	MG	1H	3131	1/1	0.91	0.22	88,88,88,88	0
58	MG	1H	3279	1/1	0.91	0.13	106,106,106,106	0
58	MG	1H	3183	1/1	0.91	0.32	94,94,94,94	0
58	MG	1H	3104	1/1	0.91	0.18	66,66,66,66	0
58	MG	1H	3185	1/1	0.91	0.13	68,68,68,68	0
58	MG	14	3046	1/1	0.91	0.17	86,86,86,86	0
58	MG	1H	3078	1/1	0.91	0.15	80,80,80,80	0
58	MG	14	3229	1/1	0.91	0.14	93,93,93,93	0
58	MG	1H	3168	1/1	0.92	0.27	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	1675	1/1	0.92	0.09	150,150,150,150	0
58	MG	14	3236	1/1	0.92	0.07	121,121,121,121	0
58	MG	14	3072	1/1	0.92	0.24	84,84,84,84	0
58	MG	14	3164	1/1	0.92	0.16	93,93,93,93	0
58	MG	1G	1676	1/1	0.92	0.13	134,134,134,134	0
58	MG	1H	3050	1/1	0.92	0.14	74,74,74,74	0
58	MG	1H	3258	1/1	0.92	0.18	99,99,99,99	0
58	MG	1H	3059	1/1	0.92	0.09	110,110,110,110	0
58	MG	14	3203	1/1	0.92	0.18	84,84,84,84	0
58	MG	21	302	1/1	0.92	0.08	91,91,91,91	0
58	MG	14	3140	1/1	0.92	0.09	79,79,79,79	0
58	MG	1H	3171	1/1	0.92	0.46	83,83,83,83	0
58	MG	14	3173	1/1	0.92	0.10	96,96,96,96	0
58	MG	14	3209	1/1	0.92	0.16	90,90,90,90	0
58	MG	1H	3079	1/1	0.92	0.28	68,68,68,68	0
58	MG	14	3211	1/1	0.92	0.10	78,78,78,78	0
58	MG	1H	3133	1/1	0.92	0.07	83,83,83,83	0
58	MG	1H	3106	1/1	0.92	0.08	82,82,82,82	0
58	MG	14	3214	1/1	0.92	0.24	94,94,94,94	0
58	MG	1H	3012	1/1	0.92	0.35	93,93,93,93	0
58	MG	14	3358	1/1	0.92	0.08	107,107,107,107	0
58	MG	1H	3045	1/1	0.92	0.15	68,68,68,68	0
58	MG	14	3008	1/1	0.92	0.27	77,77,77,77	0
58	MG	1H	3192	1/1	0.92	0.25	85,85,85,85	0
58	MG	1H	3211	1/1	0.92	0.29	90,90,90,90	0
58	MG	1H	3041	1/1	0.92	0.14	73,73,73,73	0
58	MG	13	1654	1/1	0.92	0.15	111,111,111,111	0
58	MG	14	3305	1/1	0.92	0.10	127,127,127,127	0
58	MG	14	3154	1/1	0.92	0.09	84,84,84,84	0
58	MG	13	1607	1/1	0.92	0.08	101,101,101,101	0
58	MG	14	3268	1/1	0.92	0.23	84,84,84,84	0
58	MG	14	3225	1/1	0.92	0.21	95,95,95,95	0
58	MG	1H	3087	1/1	0.92	0.17	69,69,69,69	0
58	MG	14	3125	1/1	0.92	0.09	102,102,102,102	0
58	MG	14	3189	1/1	0.92	0.15	87,87,87,87	0
58	MG	14	3190	1/1	0.92	0.15	91,91,91,91	0
58	MG	1H	3068	1/1	0.92	0.24	70,70,70,70	0
58	MG	14	3099	1/1	0.92	0.12	91,91,91,91	0
58	MG	14	3160	1/1	0.92	0.14	98,98,98,98	0
58	MG	1H	3130	1/1	0.93	0.12	79,79,79,79	0
58	MG	13	1643	1/1	0.93	0.13	80,80,80,80	0
58	MG	1H	3266	1/1	0.93	0.12	65,65,65,65	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	14	3242	1/1	0.93	0.06	92,92,92,92	0
58	MG	14	3243	1/1	0.93	0.15	102,102,102,102	0
58	MG	13	1611	1/1	0.93	0.14	91,91,91,91	0
58	MG	13	1739	1/1	0.93	0.10	87,87,87,87	0
58	MG	1H	3007	1/1	0.93	0.13	65,65,65,65	0
58	MG	14	3219	1/1	0.93	0.13	83,83,83,83	0
58	MG	14	3090	1/1	0.93	0.08	83,83,83,83	0
58	MG	14	3063	1/1	0.93	0.17	79,79,79,79	0
58	MG	1H	3135	1/1	0.93	0.10	69,69,69,69	0
58	MG	14	3401	1/1	0.93	0.05	127,127,127,127	0
58	MG	1H	3352	1/1	0.93	0.19	75,75,75,75	0
58	MG	14	3419	1/1	0.93	0.13	85,85,85,85	0
58	MG	14	3314	1/1	0.93	0.27	99,99,99,99	0
58	MG	1H	3271	1/1	0.93	0.32	87,87,87,87	0
58	MG	1G	1661	1/1	0.93	0.10	169,169,169,169	0
58	MG	14	3226	1/1	0.93	0.23	88,88,88,88	0
58	MG	1H	3103	1/1	0.93	0.35	72,72,72,72	0
58	MG	13	1610	1/1	0.93	0.12	92,92,92,92	0
58	MG	14	3128	1/1	0.93	0.36	80,80,80,80	0
58	MG	14	3025	1/1	0.93	0.25	87,87,87,87	0
58	MG	14	3006	1/1	0.93	0.17	72,72,72,72	0
58	MG	13	1682	1/1	0.93	0.08	93,93,93,93	0
58	MG	14	3207	1/1	0.93	0.12	107,107,107,107	0
58	MG	1G	1613	1/1	0.93	0.12	114,114,114,114	0
58	MG	14	3079	1/1	0.93	0.11	87,87,87,87	0
58	MG	1H	3487	1/1	0.93	0.24	74,74,74,74	0
58	MG	13	1689	1/1	0.93	0.18	182,182,182,182	0
58	MG	14	3329	1/1	0.93	0.34	91,91,91,91	0
58	MG	13	1655	1/1	0.93	0.06	106,106,106,106	0
58	MG	L5	101	1/1	0.93	0.32	96,96,96,96	0
60	ZN	G8	201	1/1	0.93	0.14	171,171,171,171	0
58	MG	2A	201	1/1	0.94	0.09	119,119,119,119	0
58	MG	14	3340	1/1	0.94	0.15	91,91,91,91	0
58	MG	14	3077	1/1	0.94	0.10	83,83,83,83	0
58	MG	1H	3046	1/1	0.94	0.18	61,61,61,61	0
58	MG	1H	3442	1/1	0.94	0.13	63,63,63,63	0
58	MG	1H	3091	1/1	0.94	0.24	58,58,58,58	0
58	MG	14	3404	1/1	0.94	0.06	101,101,101,101	0
58	MG	13	1640	1/1	0.94	0.26	73,73,73,73	0
58	MG	13	1619	1/1	0.94	0.18	81,81,81,81	0
58	MG	14	3083	1/1	0.94	0.12	94,94,94,94	0
58	MG	14	3060	1/1	0.94	0.11	103,103,103,103	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	1H	3197	1/1	0.94	0.35	68,68,68,68	0
58	MG	1H	3122	1/1	0.94	0.07	83,83,83,83	0
58	MG	1H	3114	1/1	0.94	0.08	77,77,77,77	0
58	MG	14	3064	1/1	0.94	0.11	86,86,86,86	0
58	MG	1H	3115	1/1	0.94	0.16	70,70,70,70	0
58	MG	1H	3238	1/1	0.94	0.07	83,83,83,83	0
58	MG	1H	3064	1/1	0.94	0.12	82,82,82,82	0
58	MG	14	3093	1/1	0.94	0.23	71,71,71,71	0
58	MG	14	3249	1/1	0.94	0.07	102,102,102,102	0
58	MG	13	1629	1/1	0.94	0.17	79,79,79,79	0
58	MG	1G	1653	1/1	0.94	0.07	118,118,118,118	0
58	MG	14	3070	1/1	0.94	0.10	94,94,94,94	0
58	MG	1H	3191	1/1	0.94	0.33	95,95,95,95	0
58	MG	14	3254	1/1	0.94	0.17	83,83,83,83	0
58	MG	1H	3353	1/1	0.94	0.14	96,96,96,96	0
58	MG	14	3127	1/1	0.94	0.20	67,67,67,67	0
58	MG	1H	3228	1/1	0.94	0.31	74,74,74,74	0
58	MG	1G	1607	1/1	0.95	0.07	109,109,109,109	0
58	MG	1H	3067	1/1	0.95	0.09	74,74,74,74	0
58	MG	14	3126	1/1	0.95	0.08	95,95,95,95	0
58	MG	14	3244	1/1	0.95	0.10	79,79,79,79	0
58	MG	14	3285	1/1	0.95	0.05	77,77,77,77	0
58	MG	13	1723	1/1	0.95	0.08	134,134,134,134	0
58	MG	1H	3058	1/1	0.95	0.07	76,76,76,76	0
58	MG	1H	3080	1/1	0.95	0.09	73,73,73,73	0
58	MG	1G	1677	1/1	0.95	0.06	185,185,185,185	0
58	MG	1H	3345	1/1	0.95	0.11	79,79,79,79	0
58	MG	13	1686	1/1	0.95	0.09	79,79,79,79	0
58	MG	1G	1615	1/1	0.95	0.18	142,142,142,142	0
58	MG	14	3172	1/1	0.95	0.12	75,75,75,75	0
58	MG	1H	3025	1/1	0.95	0.19	55,55,55,55	0
58	MG	13	1622	1/1	0.95	0.11	99,99,99,99	0
58	MG	14	3100	1/1	0.95	0.07	107,107,107,107	0
58	MG	16	206	1/1	0.95	0.07	89,89,89,89	0
58	MG	1H	3195	1/1	0.95	0.31	96,96,96,96	0
58	MG	1H	3245	1/1	0.95	0.05	100,100,100,100	0
58	MG	1H	3084	1/1	0.95	0.28	57,57,57,57	0
58	MG	14	3142	1/1	0.95	0.05	99,99,99,99	0
58	MG	14	3071	1/1	0.95	0.10	69,69,69,69	0
58	MG	13	1636	1/1	0.95	0.08	123,123,123,123	0
58	MG	14	3414	1/1	0.95	0.10	108,108,108,108	0
58	MG	14	3415	1/1	0.95	0.04	126,126,126,126	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	14	3417	1/1	0.95	0.07	140,140,140,140	0
58	MG	14	3145	1/1	0.95	0.12	76,76,76,76	0
58	MG	1H	3265	1/1	0.95	0.30	100,100,100,100	0
58	MG	14	3306	1/1	0.95	0.09	129,129,129,129	0
58	MG	14	3307	1/1	0.95	0.05	80,80,80,80	0
58	MG	13	1615	1/1	0.95	0.12	90,90,90,90	0
58	MG	1H	3113	1/1	0.95	0.05	59,59,59,59	0
58	MG	1H	3411	1/1	0.95	0.07	94,94,94,94	0
58	MG	1H	3423	1/1	0.95	0.13	92,92,92,92	0
58	MG	1H	3438	1/1	0.95	0.13	110,110,110,110	0
58	MG	13	1601	1/1	0.95	0.12	86,86,86,86	0
58	MG	1H	3465	1/1	0.95	0.07	112,112,112,112	0
58	MG	1H	3479	1/1	0.95	0.07	91,91,91,91	0
58	MG	1H	3101	1/1	0.95	0.13	59,59,59,59	0
58	MG	1H	3483	1/1	0.95	0.05	119,119,119,119	0
58	MG	14	3118	1/1	0.95	0.12	73,73,73,73	0
58	MG	1H	3484	1/1	0.95	0.10	81,81,81,81	0
58	MG	14	3198	1/1	0.95	0.06	109,109,109,109	0
58	MG	14	3121	1/1	0.95	0.24	69,69,69,69	0
58	MG	1H	3485	1/1	0.95	0.08	83,83,83,83	0
58	MG	1H	3022	1/1	0.95	0.15	69,69,69,69	0
58	MG	14	3139	1/1	0.96	0.09	75,75,75,75	0
58	MG	1G	1617	1/1	0.96	0.06	159,159,159,159	0
58	MG	1H	3241	1/1	0.96	0.07	100,100,100,100	0
58	MG	14	3386	1/1	0.96	0.06	83,83,83,83	0
58	MG	14	3396	1/1	0.96	0.14	96,96,96,96	0
58	MG	13	1738	1/1	0.96	0.10	106,106,106,106	0
58	MG	1H	3015	1/1	0.96	0.53	77,77,77,77	0
58	MG	1H	3399	1/1	0.96	0.08	75,75,75,75	0
58	MG	1H	3061	1/1	0.96	0.35	79,79,79,79	0
58	MG	14	3012	1/1	0.96	0.22	67,67,67,67	0
58	MG	14	3038	1/1	0.96	0.16	67,67,67,67	0
58	MG	14	3092	1/1	0.96	0.10	91,91,91,91	0
58	MG	1H	3216	1/1	0.96	0.12	65,65,65,65	0
58	MG	1H	3040	1/1	0.96	0.21	71,71,71,71	0
58	MG	13	1736	1/1	0.96	0.07	126,126,126,126	0
58	MG	14	3180	1/1	0.96	0.20	81,81,81,81	0
58	MG	1H	3450	1/1	0.96	0.05	75,75,75,75	0
58	MG	1H	3451	1/1	0.96	0.10	85,85,85,85	0
58	MG	1H	3452	1/1	0.96	0.06	102,102,102,102	0
58	MG	1H	3459	1/1	0.96	0.15	102,102,102,102	0
58	MG	1G	1608	1/1	0.96	0.06	119,119,119,119	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	14	3047	1/1	0.96	0.09	102,102,102,102	0
58	MG	1H	3463	1/1	0.96	0.13	103,103,103,103	0
58	MG	1H	3088	1/1	0.96	0.07	81,81,81,81	0
58	MG	14	3050	1/1	0.96	0.05	87,87,87,87	0
58	MG	45	203	1/1	0.96	0.47	104,104,104,104	0
58	MG	1H	3470	1/1	0.96	0.05	85,85,85,85	0
58	MG	16	212	1/1	0.96	0.04	104,104,104,104	0
58	MG	1H	3472	1/1	0.96	0.07	108,108,108,108	0
58	MG	1H	3249	1/1	0.96	0.05	83,83,83,83	0
58	MG	1H	3138	1/1	0.96	0.05	67,67,67,67	0
58	MG	1H	3004	1/1	0.96	0.12	60,60,60,60	0
60	ZN	C5	202	1/1	0.96	0.11	183,183,183,183	0
58	MG	13	1608	1/1	0.97	0.06	90,90,90,90	0
58	MG	14	3036	1/1	0.97	0.09	70,70,70,70	0
58	MG	13	1616	1/1	0.97	0.07	121,121,121,121	0
58	MG	14	3407	1/1	0.97	0.04	121,121,121,121	0
58	MG	1H	3306	1/1	0.97	0.09	77,77,77,77	0
58	MG	13	1665	1/1	0.97	0.05	105,105,105,105	0
58	MG	1H	3462	1/1	0.97	0.05	90,90,90,90	0
58	MG	1H	3401	1/1	0.97	0.04	71,71,71,71	0
58	MG	1H	3403	1/1	0.97	0.04	81,81,81,81	0
58	MG	1H	3055	1/1	0.97	0.05	74,74,74,74	0
58	MG	1H	3412	1/1	0.97	0.09	84,84,84,84	0
58	MG	1H	3201	1/1	0.97	0.46	97,97,97,97	0
58	MG	1H	3426	1/1	0.97	0.14	109,109,109,109	0
58	MG	1H	3433	1/1	0.97	0.15	113,113,113,113	0
58	MG	1H	3437	1/1	0.97	0.05	85,85,85,85	0
58	MG	13	1614	1/1	0.97	0.05	97,97,97,97	0
58	MG	1H	3233	1/1	0.97	0.04	93,93,93,93	0
58	MG	1H	3448	1/1	0.97	0.07	88,88,88,88	0
58	MG	1H	3449	1/1	0.97	0.07	89,89,89,89	0
58	MG	88	202	1/1	0.97	0.06	91,91,91,91	0
58	MG	14	3349	1/1	0.97	0.07	95,95,95,95	0
58	MG	14	3354	1/1	0.97	0.05	87,87,87,87	0
58	MG	1G	1670	1/1	0.97	0.05	112,112,112,112	0
58	MG	14	3366	1/1	0.97	0.04	114,114,114,114	0
58	MG	14	3368	1/1	0.97	0.05	87,87,87,87	0
58	MG	14	3372	1/1	0.97	0.07	134,134,134,134	0
58	MG	14	3381	1/1	0.97	0.09	116,116,116,116	0
58	MG	1G	1673	1/1	0.97	0.17	145,145,145,145	0
58	MG	1G	1674	1/1	0.97	0.04	124,124,124,124	0
58	MG	13	1726	1/1	0.98	0.05	91,91,91,91	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	1H	3365	1/1	0.98	0.04	64,64,64,64	0
58	MG	1H	3443	1/1	0.98	0.11	80,80,80,80	0
58	MG	14	3364	1/1	0.98	0.10	105,105,105,105	0
58	MG	1H	3445	1/1	0.98	0.06	71,71,71,71	0
58	MG	14	3119	1/1	0.98	0.06	83,83,83,83	0
58	MG	14	3369	1/1	0.98	0.06	105,105,105,105	0
58	MG	1H	3447	1/1	0.98	0.04	115,115,115,115	0
58	MG	14	3374	1/1	0.98	0.10	107,107,107,107	0
58	MG	14	3375	1/1	0.98	0.10	117,117,117,117	0
58	MG	14	3376	1/1	0.98	0.04	124,124,124,124	0
58	MG	1H	3369	1/1	0.98	0.07	90,90,90,90	0
58	MG	14	3382	1/1	0.98	0.10	112,112,112,112	0
58	MG	1H	3375	1/1	0.98	0.04	81,81,81,81	0
58	MG	14	3388	1/1	0.98	0.06	88,88,88,88	0
58	MG	1H	3380	1/1	0.98	0.04	89,89,89,89	0
58	MG	14	3398	1/1	0.98	0.06	111,111,111,111	0
58	MG	1H	3384	1/1	0.98	0.12	87,87,87,87	0
58	MG	1H	3396	1/1	0.98	0.03	99,99,99,99	0
58	MG	14	3405	1/1	0.98	0.05	89,89,89,89	0
58	MG	1H	3454	1/1	0.98	0.11	96,96,96,96	0
58	MG	1H	3457	1/1	0.98	0.09	89,89,89,89	0
58	MG	14	3409	1/1	0.98	0.14	85,85,85,85	0
58	MG	14	3411	1/1	0.98	0.03	134,134,134,134	0
58	MG	13	1727	1/1	0.98	0.07	87,87,87,87	0
58	MG	1H	3461	1/1	0.98	0.09	97,97,97,97	0
58	MG	13	1731	1/1	0.98	0.03	108,108,108,108	0
58	MG	13	1734	1/1	0.98	0.05	131,131,131,131	0
58	MG	1H	3407	1/1	0.98	0.04	83,83,83,83	0
58	MG	1H	3467	1/1	0.98	0.03	115,115,115,115	0
58	MG	1H	3468	1/1	0.98	0.09	122,122,122,122	0
58	MG	P8	101	1/1	0.98	0.06	101,101,101,101	0
58	MG	13	1664	1/1	0.98	0.06	105,105,105,105	0
58	MG	1H	3471	1/1	0.98	0.05	128,128,128,128	0
58	MG	13	1737	1/1	0.98	0.08	116,116,116,116	0
58	MG	1H	3475	1/1	0.98	0.11	89,89,89,89	0
58	MG	1H	3417	1/1	0.98	0.04	77,77,77,77	0
58	MG	1H	3480	1/1	0.98	0.08	114,114,114,114	0
58	MG	1H	3418	1/1	0.98	0.06	86,86,86,86	0
58	MG	1H	3482	1/1	0.98	0.05	119,119,119,119	0
58	MG	1H	3420	1/1	0.98	0.03	81,81,81,81	0
58	MG	13	1656	1/1	0.98	0.05	105,105,105,105	0
58	MG	13	1717	1/1	0.98	0.07	123,123,123,123	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	1H	3431	1/1	0.98	0.03	111,111,111,111	0
58	MG	14	3073	1/1	0.98	0.05	67,67,67,67	0
58	MG	14	3037	1/1	0.98	0.05	80,80,80,80	0
58	MG	13	1632	1/1	0.98	0.06	83,83,83,83	0
58	MG	1H	3434	1/1	0.98	0.07	82,82,82,82	0
60	ZN	5A	101	1/1	0.98	0.04	164,164,164,164	0
58	MG	13	1725	1/1	0.98	0.05	101,101,101,101	0
58	MG	1H	3430	1/1	0.99	0.05	81,81,81,81	0
58	MG	13	1718	1/1	0.99	0.06	110,110,110,110	0
58	MG	1H	3432	1/1	0.99	0.02	111,111,111,111	0
58	MG	13	1719	1/1	0.99	0.04	94,94,94,94	0
58	MG	13	1720	1/1	0.99	0.03	126,126,126,126	0
58	MG	1H	3435	1/1	0.99	0.07	85,85,85,85	0
58	MG	1H	3436	1/1	0.99	0.05	96,96,96,96	0
58	MG	1H	3358	1/1	0.99	0.02	70,70,70,70	0
58	MG	1H	3360	1/1	0.99	0.03	86,86,86,86	0
58	MG	1H	3439	1/1	0.99	0.03	72,72,72,72	0
58	MG	1H	3441	1/1	0.99	0.05	92,92,92,92	0
58	MG	1H	3362	1/1	0.99	0.04	71,71,71,71	0
58	MG	1H	3363	1/1	0.99	0.04	81,81,81,81	0
58	MG	1H	3364	1/1	0.99	0.08	74,74,74,74	0
58	MG	1H	3446	1/1	0.99	0.06	94,94,94,94	0
58	MG	13	1721	1/1	0.99	0.03	100,100,100,100	0
58	MG	1H	3366	1/1	0.99	0.03	73,73,73,73	0
58	MG	13	1722	1/1	0.99	0.03	99,99,99,99	0
58	MG	1H	3370	1/1	0.99	0.04	68,68,68,68	0
58	MG	1H	3371	1/1	0.99	0.03	77,77,77,77	0
58	MG	1H	3372	1/1	0.99	0.10	73,73,73,73	0
58	MG	1H	3453	1/1	0.99	0.05	93,93,93,93	0
58	MG	1H	3374	1/1	0.99	0.03	77,77,77,77	0
58	MG	1H	3455	1/1	0.99	0.05	87,87,87,87	0
58	MG	13	1711	1/1	0.99	0.08	85,85,85,85	0
58	MG	1H	3458	1/1	0.99	0.03	88,88,88,88	0
58	MG	1H	3376	1/1	0.99	0.02	106,106,106,106	0
58	MG	1H	3377	1/1	0.99	0.02	119,119,119,119	0
58	MG	1H	3378	1/1	0.99	0.04	90,90,90,90	0
58	MG	14	3344	1/1	0.99	0.09	91,91,91,91	0
58	MG	14	3345	1/1	0.99	0.04	80,80,80,80	0
58	MG	14	3346	1/1	0.99	0.04	81,81,81,81	0
58	MG	14	3347	1/1	0.99	0.04	87,87,87,87	0
58	MG	14	3348	1/1	0.99	0.03	86,86,86,86	0
58	MG	1H	3379	1/1	0.99	0.05	103,103,103,103	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	14	3351	1/1	0.99	0.05	80,80,80,80	0
58	MG	14	3352	1/1	0.99	0.07	84,84,84,84	0
58	MG	14	3353	1/1	0.99	0.02	73,73,73,73	0
58	MG	1H	3464	1/1	0.99	0.07	95,95,95,95	0
58	MG	14	3355	1/1	0.99	0.03	92,92,92,92	0
58	MG	14	3356	1/1	0.99	0.03	85,85,85,85	0
58	MG	13	1724	1/1	0.99	0.04	99,99,99,99	0
58	MG	14	3359	1/1	0.99	0.02	94,94,94,94	0
58	MG	14	3360	1/1	0.99	0.04	78,78,78,78	0
58	MG	14	3361	1/1	0.99	0.02	79,79,79,79	0
58	MG	14	3362	1/1	0.99	0.03	86,86,86,86	0
58	MG	14	3363	1/1	0.99	0.10	80,80,80,80	0
58	MG	1H	3466	1/1	0.99	0.05	94,94,94,94	0
58	MG	14	3365	1/1	0.99	0.03	96,96,96,96	0
58	MG	1H	3381	1/1	0.99	0.06	80,80,80,80	0
58	MG	1H	3383	1/1	0.99	0.02	75,75,75,75	0
58	MG	1H	3469	1/1	0.99	0.13	124,124,124,124	0
58	MG	14	3370	1/1	0.99	0.03	94,94,94,94	0
58	MG	14	3371	1/1	0.99	0.04	95,95,95,95	0
58	MG	13	1712	1/1	0.99	0.03	98,98,98,98	0
58	MG	14	3373	1/1	0.99	0.02	86,86,86,86	0
58	MG	1H	3385	1/1	0.99	0.02	91,91,91,91	0
58	MG	1H	3386	1/1	0.99	0.03	109,109,109,109	0
58	MG	1H	3473	1/1	0.99	0.02	89,89,89,89	0
58	MG	14	3377	1/1	0.99	0.02	106,106,106,106	0
58	MG	14	3378	1/1	0.99	0.04	83,83,83,83	0
58	MG	14	3379	1/1	0.99	0.07	110,110,110,110	0
58	MG	14	3380	1/1	0.99	0.04	94,94,94,94	0
58	MG	1H	3474	1/1	0.99	0.03	110,110,110,110	0
58	MG	1H	3387	1/1	0.99	0.03	60,60,60,60	0
58	MG	14	3383	1/1	0.99	0.11	137,137,137,137	0
58	MG	14	3384	1/1	0.99	0.05	96,96,96,96	0
58	MG	14	3385	1/1	0.99	0.04	92,92,92,92	0
58	MG	1H	3476	1/1	0.99	0.04	122,122,122,122	0
58	MG	14	3387	1/1	0.99	0.03	88,88,88,88	0
58	MG	1H	3477	1/1	0.99	0.04	114,114,114,114	0
58	MG	14	3389	1/1	0.99	0.06	92,92,92,92	0
58	MG	14	3390	1/1	0.99	0.07	114,114,114,114	0
58	MG	14	3391	1/1	0.99	0.04	87,87,87,87	0
58	MG	14	3392	1/1	0.99	0.08	89,89,89,89	0
58	MG	14	3394	1/1	0.99	0.07	88,88,88,88	0
58	MG	14	3395	1/1	0.99	0.04	85,85,85,85	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
58	MG	1H	3478	1/1	0.99	0.02	95,95,95,95	0
58	MG	14	3397	1/1	0.99	0.06	103,103,103,103	0
58	MG	1H	3388	1/1	0.99	0.03	78,78,78,78	0
58	MG	14	3399	1/1	0.99	0.08	116,116,116,116	0
58	MG	14	3400	1/1	0.99	0.03	113,113,113,113	0
58	MG	1H	3390	1/1	0.99	0.03	74,74,74,74	0
58	MG	14	3402	1/1	0.99	0.03	83,83,83,83	0
58	MG	14	3403	1/1	0.99	0.08	114,114,114,114	0
58	MG	1H	3391	1/1	0.99	0.05	79,79,79,79	0
58	MG	1H	3392	1/1	0.99	0.04	81,81,81,81	0
58	MG	1H	3394	1/1	0.99	0.03	89,89,89,89	0
58	MG	1H	3395	1/1	0.99	0.07	103,103,103,103	0
58	MG	14	3408	1/1	0.99	0.02	130,130,130,130	0
58	MG	13	1713	1/1	0.99	0.08	117,117,117,117	0
58	MG	14	3410	1/1	0.99	0.03	91,91,91,91	0
58	MG	1H	3397	1/1	0.99	0.04	82,82,82,82	0
58	MG	14	3412	1/1	0.99	0.12	128,128,128,128	0
58	MG	14	3413	1/1	0.99	0.03	92,92,92,92	0
58	MG	1H	3398	1/1	0.99	0.08	76,76,76,76	0
58	MG	13	1714	1/1	0.99	0.03	98,98,98,98	0
58	MG	14	3416	1/1	0.99	0.04	124,124,124,124	0
58	MG	1H	3400	1/1	0.99	0.05	86,86,86,86	0
58	MG	14	3418	1/1	0.99	0.02	88,88,88,88	0
58	MG	13	1728	1/1	0.99	0.02	105,105,105,105	0
58	MG	1H	3402	1/1	0.99	0.03	76,76,76,76	0
58	MG	13	1729	1/1	0.99	0.03	96,96,96,96	0
58	MG	1H	3406	1/1	0.99	0.07	82,82,82,82	0
58	MG	13	1730	1/1	0.99	0.08	108,108,108,108	0
58	MG	1H	3410	1/1	0.99	0.03	97,97,97,97	0
58	MG	13	1715	1/1	0.99	0.05	113,113,113,113	0
58	MG	29	301	1/1	0.99	0.03	90,90,90,90	0
58	MG	13	1732	1/1	0.99	0.11	127,127,127,127	0
58	MG	1H	3416	1/1	0.99	0.04	83,83,83,83	0
58	MG	16	210	1/1	0.99	0.03	87,87,87,87	0
58	MG	16	211	1/1	0.99	0.02	92,92,92,92	0
58	MG	1H	3308	1/1	0.99	0.07	81,81,81,81	0
58	MG	13	1733	1/1	0.99	0.06	102,102,102,102	0
58	MG	13	1716	1/1	0.99	0.05	108,108,108,108	0
58	MG	1H	3421	1/1	0.99	0.03	129,129,129,129	0
58	MG	1G	1671	1/1	0.99	0.07	121,121,121,121	0
58	MG	1H	3422	1/1	0.99	0.06	102,102,102,102	0
58	MG	13	1735	1/1	0.99	0.13	146,146,146,146	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	1H	3424	1/1	0.99	0.02	81,81,81,81	0
58	MG	13	1613	1/1	0.99	0.02	109,109,109,109	0
59	SF4	3E	301	8/8	0.99	0.03	95,111,117,118	0
59	SF4	32	302	8/8	0.99	0.02	127,146,153,155	0
58	MG	1H	3427	1/1	0.99	0.02	106,106,106,106	0
58	MG	1H	3428	1/1	0.99	0.09	89,89,89,89	0
58	MG	1H	3429	1/1	0.99	0.03	82,82,82,82	0
58	MG	1H	3382	1/1	1.00	0.09	71,71,71,71	0
58	MG	14	3357	1/1	1.00	0.03	76,76,76,76	0
58	MG	1H	3460	1/1	1.00	0.06	86,86,86,86	0
58	MG	1H	3419	1/1	1.00	0.04	76,76,76,76	0
58	MG	1H	3368	1/1	1.00	0.04	76,76,76,76	0
58	MG	1H	3440	1/1	1.00	0.04	70,70,70,70	0
58	MG	1H	3393	1/1	1.00	0.01	95,95,95,95	0
58	MG	1H	3404	1/1	1.00	0.02	84,84,84,84	0
58	MG	14	3393	1/1	1.00	0.03	89,89,89,89	0
58	MG	1H	3405	1/1	1.00	0.03	75,75,75,75	0
58	MG	1H	3444	1/1	1.00	0.04	85,85,85,85	0
58	MG	1H	3359	1/1	1.00	0.02	71,71,71,71	0
58	MG	14	3367	1/1	1.00	0.02	86,86,86,86	0
58	MG	1G	1672	1/1	1.00	0.02	115,115,115,115	0
58	MG	1H	3425	1/1	1.00	0.02	77,77,77,77	0
58	MG	1H	3357	1/1	1.00	0.02	79,79,79,79	0
58	MG	1H	3408	1/1	1.00	0.05	72,72,72,72	0
58	MG	14	3343	1/1	1.00	0.06	87,87,87,87	0
58	MG	1H	3409	1/1	1.00	0.04	85,85,85,85	0
58	MG	1H	3361	1/1	1.00	0.01	72,72,72,72	0
58	MG	1H	3356	1/1	1.00	0.02	67,67,67,67	0
58	MG	1H	3373	1/1	1.00	0.02	86,86,86,86	0
58	MG	1H	3413	1/1	1.00	0.01	90,90,90,90	0
58	MG	1H	3414	1/1	1.00	0.06	79,79,79,79	0
58	MG	14	3350	1/1	1.00	0.01	116,116,116,116	0
58	MG	1H	3415	1/1	1.00	0.02	90,90,90,90	0
58	MG	1H	3456	1/1	1.00	0.02	68,68,68,68	0
60	ZN	5I	102	1/1	1.00	0.02	114,114,114,114	0
58	MG	1H	3389	1/1	1.00	0.02	71,71,71,71	0
58	MG	14	3002	1/1	1.00	0.01	65,65,65,65	0
58	MG	1H	3367	1/1	1.00	0.04	84,84,84,84	0

5.5 Other polymers ⓘ

There are no such residues in this entry.