



# wwPDB X-ray Structure Validation Summary Report

Mar 30, 2026 – 12:15 PM UTC

PDB ID : 4WT1 / pdb\_00004wt1  
Title : Complex of 70S ribosome with tRNA-Phe and mRNA with A-A mismatch in the second position in the A-site  
Authors : Rozov, A.; Demeshkina, N.; Yusupov, M.; Yusupova, G.  
Deposited on : 2014-10-29  
Resolution : 3.05 Å (reported)

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

We welcome your comments at [validation@mail.wwpdb.org](mailto: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>.

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

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

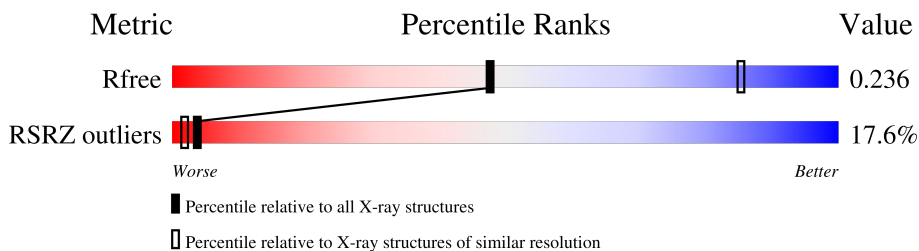
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.05 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	2469 (3.10-3.02)
RSRZ outliers	180081	2469 (3.10-3.02)

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
56	MG	13	1620	-	-	-	X
56	MG	13	1621	-	-	-	X
56	MG	13	1629	-	-	-	X
56	MG	13	1637	-	-	-	X
56	MG	13	1669	-	-	-	X
56	MG	13	1682	-	-	-	X
56	MG	13	1691	-	-	-	X
56	MG	13	1697	-	-	-	X
56	MG	13	1698	-	-	-	X
56	MG	13	1704	-	-	-	X
56	MG	13	1711	-	-	-	X
56	MG	13	1715	-	-	-	X
56	MG	14	3007	-	-	-	X
56	MG	14	3022	-	-	-	X
56	MG	14	3029	-	-	-	X
56	MG	14	3044	-	-	-	X
56	MG	14	3064	-	-	-	X
56	MG	14	3066	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
56	MG	14	3091	-	-	-	X
56	MG	14	3093	-	-	-	X
56	MG	14	3109	-	-	-	X
56	MG	14	3120	-	-	-	X
56	MG	14	3137	-	-	-	X
56	MG	14	3142	-	-	-	X
56	MG	14	3143	-	-	-	X
56	MG	14	3158	-	-	-	X
56	MG	14	3169	-	-	-	X
56	MG	14	3183	-	-	-	X
56	MG	14	3185	-	-	-	X
56	MG	14	3188	-	-	-	X
56	MG	14	3194	-	-	-	X
56	MG	14	3197	-	-	-	X
56	MG	14	3199	-	-	-	X
56	MG	14	3201	-	-	-	X
56	MG	14	3202	-	-	-	X
56	MG	14	3216	-	-	-	X
56	MG	14	3227	-	-	-	X
56	MG	14	3232	-	-	-	X
56	MG	14	3235	-	-	-	X
56	MG	14	3258	-	-	-	X
56	MG	14	3267	-	-	-	X
56	MG	14	3272	-	-	-	X
56	MG	14	3274	-	-	-	X
56	MG	14	3288	-	-	-	X
56	MG	14	3293	-	-	-	X
56	MG	14	3307	-	-	-	X
56	MG	14	3314	-	-	-	X
56	MG	14	3329	-	-	-	X
56	MG	1G	1615	-	-	-	X
56	MG	1G	1626	-	-	-	X
56	MG	1G	1634	-	-	-	X
56	MG	1G	1654	-	-	-	X
56	MG	1G	1670	-	-	-	X
56	MG	1H	3011	-	-	-	X
56	MG	1H	3013	-	-	-	X
56	MG	1H	3026	-	-	-	X
56	MG	1H	3027	-	-	-	X
56	MG	1H	3028	-	-	-	X
56	MG	1H	3033	-	-	-	X
56	MG	1H	3061	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
56	MG	1H	3111	-	-	-	X
56	MG	1H	3119	-	-	-	X
56	MG	1H	3138	-	-	-	X
56	MG	1H	3143	-	-	-	X
56	MG	1H	3158	-	-	-	X
56	MG	1H	3160	-	-	-	X
56	MG	1H	3164	-	-	-	X
56	MG	1H	3204	-	-	-	X
56	MG	1H	3213	-	-	-	X
56	MG	1H	3234	-	-	-	X
56	MG	1H	3242	-	-	-	X
56	MG	1H	3255	-	-	-	X
56	MG	1H	3270	-	-	-	X
56	MG	1H	3272	-	-	-	X
56	MG	1H	3275	-	-	-	X
56	MG	1H	3277	-	-	-	X
56	MG	1H	3288	-	-	-	X
56	MG	1H	3304	-	-	-	X
56	MG	1H	3310	-	-	-	X
56	MG	1H	3320	-	-	-	X
56	MG	1H	3326	-	-	-	X
56	MG	1H	3336	-	-	-	X
56	MG	1H	3340	-	-	-	X
56	MG	1H	3344	-	-	-	X
56	MG	1J	203	-	-	-	X
56	MG	25	202	-	-	-	X
56	MG	2K	105	-	-	-	X
56	MG	2K	106	-	-	-	X
56	MG	2K	107	-	-	-	X
56	MG	88	201	-	-	-	X

## 2 Entry composition

There are 58 unique types of molecules in this entry. The entry contains 299951 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
			Total	C	N	O	P			
1	13	1498	Total 32207	C 14334	N 5973	O 10402	P 1498	0	0	0
1	1G	1497	Total 32182	C 14324	N 5968	O 10394	P 1496	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	1E	237	Total 1924	C 1228	N 344	O 347	S 5	0	0	0
2	12	237	Total 1924	C 1228	N 344	O 347	S 5	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	2E	205	Total 1605	C 1011	N 313	O 280	S 1	0	0	0
3	22	206	Total 1612	C 1016	N 314	O 281	S 1	0	0	0

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	4E	151	Total	C	N	O	S	0	0	0
			1155	729	218	204	4			
5	42	151	Total	C	N	O	S	0	0	0
			1155	729	218	204	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	5E	101	Total	C	N	O	S	0	0	0
			842	531	155	153	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	155	Total	C	N	O	S	0	0	0
			1256	781	252	217	6			
7	62	155	Total	C	N	O	S	0	0	0
			1256	781	252	217	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	138	Total	C	N	O	S	0	0	0
			1115	705	215	192	3			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
9	8E	127	Total	C	N	O	0	0	0
			1009	639	197	173			
9	82	127	Total	C	N	O	0	0	0
			1009	639	197	173			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	1I	99	Total	C	N	O	S	0	0	0
			801	504	157	139	1			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
10	1A	99	801	504	157	139	1	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
11	2I	116	864	537	164	160	3	0	0	0
11	2A	116	864	537	164	160	3	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
12	3I	125	975	614	196	164	1	0	0	0
12	3A	125	975	614	196	164	1	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
13	4I	118	938	580	193	163	2	0	0	0
13	4A	117	933	577	192	162	2	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
4I	119	ALA	GLY	conflict	UNP P80377
4A	119	ALA	GLY	conflict	UNP P80377

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
14	5I	60	491	312	104	71	4	0	0	0
14	5A	58	475	303	99	69	4	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	6I	88	Total	C	N	O	S	0	0	0
			733	459	147	125	2			
15	6A	88	Total	C	N	O	S	0	0	0
			733	459	147	125	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	7I	84	Total	C	N	O	S	0	0	0
			705	446	140	118	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	100	Total	C	N	O	S	0	0	0
			834	534	155	143	2			

- Molecule 18 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
18	9I	72	Total	C	N	O	0	0	0
			590	376	117	97			
18	9A	72	Total	C	N	O	0	0	0
			590	376	117	97			

- 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
			647	413	119	113	2			
19	AA	78	Total	C	N	O	S	0	0	0
			624	398	115	109	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	BI	99	Total	C	N	O	S	0	0	0
			762	470	162	128	2			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
20	BA	99	762	470	162	128	2	0	0	0

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
21	1F	25	217	134	52	31	0	0	0
21	1B	25	217	134	52	31	0	0	0

- Molecule 22 is a RNA chain called tRNA-Phe.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace	
			Total	C	N	O	P				S
22	1K	76	1628	731	290	530	75	2	0	0	0

- Molecule 23 is a RNA chain called tRNA-fMet.

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

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
2K	18	C	U	conflict	GB 675818144
2L	18	C	U	conflict	GB 675818144

- Molecule 24 is a RNA chain called tRNA-Phe.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
24	3K	76	1619	723	290	531	75	0	0	0
24	1L	76	1619	723	290	531	75	0	0	0
24	3L	76	1619	723	290	531	75	0	0	0

- Molecule 25 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
25	4K	13	Total	C	N	O	P	0	0	0
			281	127	57	84	13			
25	4L	9	Total	C	N	O	P	0	0	0
			193	87	37	60	9			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	1H	2912	Total	C	N	O	P	0	0	0
			62707	27911	11722	20163	2911			
26	14	2909	Total	C	N	O	P	0	0	0
			62647	27884	11716	20139	2908			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
1H	161	U	-	insertion	GB 48268
1H	493	G	-	insertion	GB 48268
1H	1228	G	-	insertion	GB 48268
14	161	U	-	insertion	GB 48268
14	493	G	-	insertion	GB 48268
14	1228	G	-	insertion	GB 48268

- 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 L2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
28	11	272	Total	C	N	O	S	0	0	0
			2115	1335	420	357	3			
28	19	273	Total	C	N	O	S	0	0	0
			2120	1338	421	358	3			

- Molecule 29 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
29	21	205	Total	C	N	O	S	0	0	0
			1568	991	300	271	6			
29	29	205	Total	C	N	O	S	0	0	0
			1568	991	300	271	6			

- Molecule 30 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
30	31	202	Total	C	N	O	S	0	0	0
			1585	1011	297	275	2			
30	39	208	Total	C	N	O	S	0	0	0
			1627	1037	304	283	3			

- Molecule 31 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
31	41	181	Total	C	N	O	S	0	0	0
			1473	942	268	259	4			
31	49	181	Total	C	N	O	S	0	0	0
			1473	942	268	259	4			

- Molecule 32 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
32	51	174	Total	C	N	O	S	0	0	0
			1336	848	251	236	1			
32	59	169	Total	C	N	O	S	0	0	0
			1299	823	244	231	1			

- Molecule 33 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
33	61	146	Total	C	N	O	S	0	0	0
			1136	726	201	208	1			
33	69	146	Total	C	N	O	S	0	0	0
			1136	726	201	208	1			

- Molecule 34 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
34	58	138	Total	C	N	O	S	0	0	0
			1104	712	206	182	4			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
34	15	138	1104	712	206	182	4	0	0	0

- Molecule 35 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
35	68	122	932	588	171	169	4	0	0	0
35	25	122	932	588	171	169	4	0	0	0

- Molecule 36 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
36	78	150	1144	712	232	197	3	0	0	0
36	35	150	1144	712	232	197	3	0	0	0

- Molecule 37 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
37	88	138	1086	693	208	179	6	0	0	0
37	45	141	1121	715	212	187	7	0	0	0

- Molecule 38 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
38	98	118	967	604	203	159	1	0	0	0
38	55	117	959	599	202	158		0	0	0

- Molecule 39 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
39	A8	111	881	556	176	149	0	0	0
39	65	111	881	556	176	149	0	0	0

- Molecule 40 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
40	B8	137	Total	C	N	O	S	0	0	0
			1141	710	234	196	1			
40	75	137	Total	C	N	O	S	0	0	0
			1141	710	234	196	1			

- Molecule 41 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
41	C8	117	Total	C	N	O	S	0	0	0
			963	610	202	150	1			
41	85	117	Total	C	N	O	S	0	0	0
			963	610	202	150	1			

- Molecule 42 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
42	D8	101	Total	C	N	O	S	0	0	0
			778	501	142	134	1			
42	95	101	Total	C	N	O	S	0	0	0
			778	501	142	134	1			

- Molecule 43 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
43	E8	113	Total	C	N	O	S	0	0	0
			899	566	177	154	2			
43	A5	113	Total	C	N	O	S	0	0	0
			899	566	177	154	2			

- Molecule 44 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
44	F8	94	Total	C	N	O	S	0	0	0
			742	482	134	125	1			
44	B5	92	Total	C	N	O		0	0	0
			725	471	131	123				

- Molecule 45 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
45	G8	104	Total	C	N	O	S	0	0	0
			791	510	149	127	5			
45	C5	104	Total	C	N	O	S	0	0	0
			794	510	152	127	5			

- Molecule 46 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
46	H8	175	Total	C	N	O	S	0	0	0
			1397	892	251	251	3			
46	D5	179	Total	C	N	O	S	0	0	0
			1428	911	255	259	3			

- Molecule 47 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
47	I8	80	Total	C	N	O	S	0	0	0
			626	388	132	105	1			
47	E5	76	Total	C	N	O	S	0	0	0
			606	376	128	101	1			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
I8	6	ALA	GLY	conflict	UNP P60493
I8	8	ALA	GLY	conflict	UNP P60493
E5	6	ALA	GLY	conflict	UNP P60493
E5	8	ALA	GLY	conflict	UNP P60493

- Molecule 48 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
48	J8	97	Total	C	N	O	S	0	0	0
			762	481	150	130	1			
48	F5	97	Total	C	N	O	S	0	0	0
			762	481	150	130	1			

- Molecule 49 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
49	K8	67	Total	C	N	O	S	0	0	0
			563	349	114	99	1			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
49	G5	66	558	346	113	98	1	0	0	0

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
50	L8	57	452	288	88	76	0	0	0
50	H5	59	468	298	90	80	0	0	0

- Molecule 51 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
51	M8	66	533	335	96	97	5	0	0	0
51	I5	63	515	326	93	91	5	0	0	0

- Molecule 52 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
52	N8	58	453	285	89	74	5	0	0	0
52	J5	56	434	272	87	70	5	0	0	0

- Molecule 53 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
53	O8	45	389	241	79	65	4	0	0	0
53	K5	45	389	241	79	65	4	0	0	0

- Molecule 54 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
54	P8	45	391	240	97	52	2	0	0	0
54	L5	46	398	245	98	53	2	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
55	Q8	61	Total 485	C 309	N 99	O 75	S 2	0	0	0
55	M5	60	Total 477	C 303	N 98	O 74	S 2	0	0	0

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	13	152	Total 152	Mg 152	0	0
56	5E	1	Total 1	Mg 1	0	0
56	3I	2	Total 2	Mg 2	0	0
56	2K	7	Total 7	Mg 7	0	0
56	4K	1	Total 1	Mg 1	0	0
56	1H	506	Total 506	Mg 506	0	0
56	16	15	Total 15	Mg 15	0	0
56	11	2	Total 2	Mg 2	0	0
56	21	2	Total 2	Mg 2	0	0
56	31	1	Total 1	Mg 1	0	0
56	41	2	Total 2	Mg 2	0	0
56	78	2	Total 2	Mg 2	0	0
56	88	2	Total 2	Mg 2	0	0
56	G8	1	Total 1	Mg 1	0	0
56	I8	2	Total 2	Mg 2	0	0
56	J8	1	Total 1	Mg 1	0	0
56	L8	1	Total 1	Mg 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
56	P8	1	Total Mg 1 1	0	0
56	1G	88	Total Mg 88 88	0	0
56	32	1	Total Mg 1 1	0	0
56	52	1	Total Mg 1 1	0	0
56	6A	1	Total Mg 1 1	0	0
56	2L	3	Total Mg 3 3	0	0
56	14	426	Total Mg 426 426	0	0
56	1J	10	Total Mg 10 10	0	0
56	29	2	Total Mg 2 2	0	0
56	39	3	Total Mg 3 3	0	0
56	49	1	Total Mg 1 1	0	0
56	15	1	Total Mg 1 1	0	0
56	25	2	Total Mg 2 2	0	0
56	35	1	Total Mg 1 1	0	0
56	45	2	Total Mg 2 2	0	0
56	85	1	Total Mg 1 1	0	0
56	C5	1	Total Mg 1 1	0	0
56	E5	1	Total Mg 1 1	0	0
56	M5	1	Total Mg 1 1	0	0

- Molecule 57 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	3E	1	Total 1	Zn 1	0	0
57	5I	1	Total 1	Zn 1	0	0
57	G8	1	Total 1	Zn 1	0	0
57	32	1	Total 1	Zn 1	0	0
57	5A	1	Total 1	Zn 1	0	0
57	C5	1	Total 1	Zn 1	0	0

- Molecule 58 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
58	13	164	Total 164	O 164	0	0
58	3E	1	Total 1	O 1	0	0
58	4E	1	Total 1	O 1	0	0
58	1I	1	Total 1	O 1	0	0
58	3I	1	Total 1	O 1	0	0
58	5I	1	Total 1	O 1	0	0
58	6I	1	Total 1	O 1	0	0
58	7I	1	Total 1	O 1	0	0
58	4K	1	Total 1	O 1	0	0
58	1H	920	Total 920	O 920	0	0
58	16	6	Total 6	O 6	0	0
58	11	9	Total 9	O 9	0	0
58	21	5	Total 5	O 5	0	0
58	31	7	Total 7	O 7	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
58	78	6	Total O 6 6	0	0
58	B8	1	Total O 1 1	0	0
58	C8	2	Total O 2 2	0	0
58	E8	1	Total O 1 1	0	0
58	F8	1	Total O 1 1	0	0
58	G8	3	Total O 3 3	0	0
58	J8	1	Total O 1 1	0	0
58	L8	3	Total O 3 3	0	0
58	P8	1	Total O 1 1	0	0
58	Q8	2	Total O 2 2	0	0
58	1G	64	Total O 64 64	0	0
58	32	1	Total O 1 1	0	0
58	7A	1	Total O 1 1	0	0
58	14	543	Total O 543 543	0	0
58	1J	18	Total O 18 18	0	0
58	19	3	Total O 3 3	0	0
58	29	3	Total O 3 3	0	0
58	39	8	Total O 8 8	0	0
58	15	1	Total O 1 1	0	0
58	35	1	Total O 1 1	0	0
58	85	1	Total O 1 1	0	0

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<b>Mol</b>	<b>Chain</b>	<b>Residues</b>	<b>Atoms</b>		<b>ZeroOcc</b>	<b>AltConf</b>
58	L5	2	Total	O	0	0
			2	2		

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

### 3 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	209.90Å 447.90Å 621.50Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	188.03 – 3.05 188.03 – 3.05	Depositor EDS
% Data completeness (in resolution range)	99.8 (188.03-3.05) 91.4 (188.03-3.05)	Depositor EDS
$R_{merge}$	0.28	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	0.71 (at 3.07Å)	Xtrriage
Refinement program	PHENIX	Depositor
R, $R_{free}$	0.199 , (Not available) 0.201 , 0.236	Depositor DCC
$R_{free}$ test set	1998 reflections (0.18%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	95.1	Xtrriage
Anisotropy	0.265	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 220.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.45$ , $\langle L^2 \rangle = 0.27$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.90	EDS
Total number of atoms	299951	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	128.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.50% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

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

## 4 Model quality [i](#)

### 4.1 Standard geometry [i](#)

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

### 4.2 Too-close contacts [i](#)

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

### 4.3 Torsion angles [i](#)

#### 4.3.1 Protein backbone [i](#)

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

#### 4.3.2 Protein sidechains [i](#)

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

#### 4.3.3 RNA [i](#)

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

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
23	7MG	2L	47	23	23,26,27	3.10	7 (30%)	27,39,42	2.83	9 (33%)
22	7MG	1K	46	22	23,26,27	3.05	7 (30%)	27,39,42	2.88	8 (29%)
23	4SU	2L	8	23	18,21,22	2.05	5 (27%)	25,30,33	2.45	6 (24%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
22	PSU	1K	55	22	18,21,22	1.43	1 (5%)	21,30,33	1.60	4 (19%)
23	OMC	2K	33	23	19,22,23	1.80	3 (15%)	25,31,34	1.04	1 (4%)
22	4SU	1K	8	22	18,21,22	1.97	5 (27%)	25,30,33	2.35	5 (20%)
23	4SU	2K	8	23	18,21,22	2.00	3 (16%)	25,30,33	3.34	10 (40%)
23	PSU	2L	56	23	18,21,22	1.35	2 (11%)	21,30,33	1.80	2 (9%)
23	OMC	2L	33	23	19,22,23	1.82	3 (15%)	25,31,34	1.33	3 (12%)
23	5MU	2L	55	23	19,22,23	3.95	5 (26%)	27,32,35	3.40	9 (33%)
22	5MU	1K	54	22	19,22,23	4.01	5 (26%)	27,32,35	3.12	8 (29%)
22	PSU	1K	32	22	18,21,22	1.31	2 (11%)	21,30,33	1.49	3 (14%)
23	PSU	2K	56	23	18,21,22	1.09	2 (11%)	21,30,33	1.87	4 (19%)
23	7MG	2K	47	23	23,26,27	3.18	6 (26%)	27,39,42	2.72	10 (37%)
22	PSU	1K	39	22	18,21,22	1.10	2 (11%)	21,30,33	1.68	5 (23%)
23	5MU	2K	55	23	19,22,23	3.96	5 (26%)	27,32,35	3.38	8 (29%)
22	MIA	1K	37	22	28,31,32	2.47	4 (14%)	38,44,47	2.55	11 (28%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	7MG	2L	47	23	-	1/7/37/38	0/3/3/3
22	7MG	1K	46	22	-	1/7/37/38	0/3/3/3
23	4SU	2L	8	23	-	2/7/25/26	0/2/2/2
22	PSU	1K	55	22	-	2/7/25/26	0/2/2/2
23	OMC	2K	33	23	-	0/9/27/28	0/2/2/2
22	4SU	1K	8	22	-	0/7/25/26	0/2/2/2
23	4SU	2K	8	23	-	3/7/25/26	0/2/2/2
23	PSU	2L	56	23	-	1/7/25/26	0/2/2/2
23	OMC	2L	33	23	-	2/9/27/28	0/2/2/2
23	5MU	2L	55	23	-	0/7/25/26	0/2/2/2
22	5MU	1K	54	22	-	0/7/25/26	0/2/2/2
22	PSU	1K	32	22	-	0/7/25/26	0/2/2/2
23	PSU	2K	56	23	-	0/7/25/26	0/2/2/2
23	7MG	2K	47	23	-	1/7/37/38	0/3/3/3
22	PSU	1K	39	22	-	1/7/25/26	0/2/2/2
23	5MU	2K	55	23	-	0/7/25/26	0/2/2/2
22	MIA	1K	37	22	-	5/15/33/34	0/3/3/3

The worst 5 of 67 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	2L	55	5MU	C2-N1	12.98	1.58	1.38
22	1K	54	5MU	C2-N1	12.93	1.58	1.38
23	2K	55	5MU	C2-N1	12.77	1.58	1.38
22	1K	37	MIA	C13-C14	9.12	1.59	1.32
23	2K	47	7MG	C4-N9	-8.41	1.27	1.37

The worst 5 of 106 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	2K	55	5MU	C5-C4-N3	11.30	125.15	115.32
23	2L	55	5MU	C5-C4-N3	10.89	124.79	115.32
23	2K	8	4SU	C4-N3-C2	-10.86	116.91	127.31
22	1K	54	5MU	C5-C4-N3	10.56	124.50	115.32
22	1K	46	7MG	C4-C5-N7	8.50	115.42	105.38

There are no chirality outliers.

5 of 19 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
23	2K	8	4SU	O4'-C4'-C5'-O5'
22	1K	37	MIA	N1-C2-S10-C11
22	1K	37	MIA	N3-C2-S10-C11
22	1K	37	MIA	C12-C13-C14-C15
22	1K	37	MIA	C12-C13-C14-C16

There are no ring outliers.

No monomer is involved in short contacts.

## 4.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 4.6 Ligand geometry [i](#)

Of 1253 ligands modelled in this entry, 1253 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

#### 4.7 Other polymers [i](#)

There are no such residues in this entry.

#### 4.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 5 Fit of model and data [i](#)

### 5.1 Protein, DNA and RNA chains [i](#)

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	13	1498/1522 (98%)	0.89	255 (17%) 4 2	73, 122, 204, 309	0
1	1G	1497/1522 (98%)	1.10	289 (19%) 3 1	92, 145, 218, 318	0
2	12	237/256 (92%)	1.50	60 (25%) 1 1	168, 199, 220, 228	0
2	1E	237/256 (92%)	0.83	33 (13%) 6 4	132, 167, 193, 205	0
3	22	206/239 (86%)	2.57	103 (50%) 0 0	161, 182, 205, 218	0
3	2E	205/239 (85%)	0.80	22 (10%) 11 6	103, 128, 161, 170	0
4	32	208/209 (99%)	1.04	36 (17%) 4 2	122, 144, 165, 174	0
4	3E	208/209 (99%)	0.95	30 (14%) 6 3	102, 129, 151, 165	0
5	42	151/162 (93%)	1.67	41 (27%) 1 1	136, 154, 171, 203	0
5	4E	151/162 (93%)	0.84	23 (15%) 5 3	97, 120, 143, 176	0
6	52	101/101 (100%)	0.31	4 (3%) 42 23	106, 127, 147, 161	0
6	5E	101/101 (100%)	1.00	14 (13%) 6 4	101, 123, 148, 161	0
7	62	155/156 (99%)	1.74	42 (27%) 1 1	136, 154, 182, 207	0
7	6E	155/156 (99%)	1.18	23 (14%) 5 3	124, 139, 168, 193	0
8	72	138/138 (100%)	1.73	32 (23%) 2 1	130, 158, 174, 179	0
8	7E	138/138 (100%)	0.96	23 (16%) 4 2	105, 129, 141, 149	0
9	82	127/128 (99%)	1.79	41 (32%) 1 0	141, 183, 204, 208	0
9	8E	127/128 (99%)	1.39	27 (21%) 2 1	107, 156, 179, 193	0
10	1A	99/105 (94%)	1.82	28 (28%) 1 1	153, 184, 203, 210	0
10	1I	99/105 (94%)	1.84	41 (41%) 0 0	102, 155, 187, 192	0
11	2A	116/129 (89%)	1.82	28 (24%) 2 1	111, 137, 158, 182	0
11	2I	116/129 (89%)	1.23	20 (17%) 4 2	90, 127, 153, 180	0
12	3A	125/132 (94%)	1.47	29 (23%) 2 1	109, 134, 160, 185	0
12	3I	125/132 (94%)	1.04	22 (17%) 4 2	83, 96, 131, 179	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
13	4A	117/126 (92%)	1.29	23 (19%) 3 1	140, 184, 206, 216	0
13	4I	118/126 (93%)	0.92	20 (16%) 4 2	101, 139, 159, 170	0
14	5A	58/61 (95%)	1.37	13 (22%) 2 1	164, 179, 194, 201	0
14	5I	60/61 (98%)	0.62	7 (11%) 9 5	106, 118, 137, 147	0
15	6A	88/89 (98%)	0.37	5 (5%) 29 15	118, 139, 155, 159	0
15	6I	88/89 (98%)	0.53	9 (10%) 12 6	98, 125, 142, 154	0
16	7A	84/88 (95%)	0.93	11 (13%) 7 4	113, 132, 150, 174	0
16	7I	84/88 (95%)	1.49	23 (27%) 1 1	122, 135, 169, 187	0
17	8A	100/105 (95%)	0.88	14 (14%) 6 3	118, 138, 153, 176	0
17	8I	100/105 (95%)	1.31	21 (21%) 2 1	108, 127, 140, 145	0
18	9A	72/88 (81%)	0.75	9 (12%) 8 4	116, 142, 178, 198	0
18	9I	72/88 (81%)	0.83	11 (15%) 5 3	109, 127, 162, 187	0
19	AA	78/93 (83%)	1.08	16 (20%) 2 1	172, 203, 216, 222	0
19	AI	81/93 (87%)	0.99	11 (13%) 7 4	109, 135, 160, 166	0
20	BA	99/106 (93%)	1.86	42 (42%) 0 0	108, 130, 158, 173	0
20	BI	99/106 (93%)	1.89	43 (43%) 0 0	129, 144, 177, 183	0
21	1B	25/27 (92%)	1.03	2 (8%) 18 9	147, 163, 179, 196	0
21	1F	25/27 (92%)	1.27	5 (20%) 3 1	114, 126, 139, 164	0
22	1K	69/76 (90%)	2.66	25 (36%) 1 0	101, 222, 265, 271	0
23	2K	72/77 (93%)	1.26	15 (20%) 2 1	84, 108, 137, 146	0
23	2L	72/77 (93%)	1.13	10 (13%) 6 4	96, 136, 166, 170	0
24	1L	76/76 (100%)	2.81	32 (42%) 0 0	147, 264, 289, 295	0
24	3K	76/76 (100%)	2.20	27 (35%) 1 0	92, 255, 286, 289	0
24	3L	76/76 (100%)	2.28	33 (43%) 0 0	104, 264, 294, 299	0
25	4K	13/27 (48%)	0.20	0 100 100	88, 101, 151, 157	0
25	4L	9/27 (33%)	0.66	0 100 100	121, 154, 165, 175	0
26	14	2909/2917 (99%)	0.65	383 (13%) 7 4	67, 105, 270, 378	0
26	1H	2912/2917 (99%)	0.50	339 (11%) 9 5	56, 91, 253, 353	0
27	16	122/122 (100%)	0.22	3 (2%) 58 35	83, 111, 133, 217	0
27	1J	122/122 (100%)	1.14	21 (17%) 4 2	106, 152, 174, 226	0
28	11	272/276 (98%)	0.49	24 (8%) 15 8	57, 82, 100, 110	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
28	19	273/276 (98%)	0.59	29 (10%) 11 6	67, 94, 110, 125	0
29	21	205/206 (99%)	0.81	24 (11%) 9 5	66, 109, 151, 165	0
29	29	205/206 (99%)	1.34	50 (24%) 2 1	76, 113, 158, 183	0
30	31	202/210 (96%)	0.63	22 (10%) 10 5	60, 94, 130, 150	0
30	39	208/210 (99%)	1.17	46 (22%) 2 1	76, 123, 179, 199	0
31	41	181/182 (99%)	1.24	43 (23%) 2 1	100, 121, 159, 172	0
31	49	181/182 (99%)	1.05	29 (16%) 5 2	148, 169, 198, 209	0
32	51	174/180 (96%)	1.22	35 (20%) 3 1	99, 122, 139, 150	0
32	59	169/180 (93%)	2.62	84 (49%) 0 0	169, 218, 243, 258	0
33	61	146/148 (98%)	1.39	37 (25%) 1 1	98, 154, 170, 175	0
33	69	146/148 (98%)	2.32	57 (39%) 1 0	102, 146, 170, 175	0
34	15	138/140 (98%)	1.93	37 (26%) 1 1	98, 129, 161, 185	0
34	58	138/140 (98%)	1.14	27 (19%) 3 1	81, 109, 148, 163	0
35	25	122/122 (100%)	0.58	8 (6%) 24 12	85, 107, 125, 135	0
35	68	122/122 (100%)	0.51	14 (11%) 9 5	75, 92, 111, 124	0
36	35	150/150 (100%)	0.96	25 (16%) 4 2	77, 128, 162, 198	0
36	78	150/150 (100%)	0.74	17 (11%) 10 5	64, 98, 124, 176	0
37	45	141/141 (100%)	1.12	29 (20%) 2 1	97, 129, 154, 167	0
37	88	138/141 (97%)	0.51	13 (9%) 14 7	70, 95, 115, 147	0
38	55	117/118 (99%)	0.76	20 (17%) 4 2	77, 97, 113, 133	0
38	98	118/118 (100%)	1.09	23 (19%) 3 1	79, 102, 125, 139	0
39	65	111/112 (99%)	1.46	32 (28%) 1 1	118, 145, 162, 172	0
39	A8	111/112 (99%)	0.54	8 (7%) 21 11	92, 107, 130, 144	0
40	75	137/146 (93%)	1.06	24 (17%) 4 2	96, 115, 173, 208	0
40	B8	137/146 (93%)	1.54	37 (27%) 1 1	86, 111, 170, 202	0
41	85	117/118 (99%)	1.46	29 (24%) 2 1	86, 115, 155, 180	0
41	C8	117/118 (99%)	0.93	17 (14%) 6 3	71, 98, 136, 147	0
42	95	101/101 (100%)	2.16	36 (35%) 1 0	86, 143, 161, 177	0
42	D8	101/101 (100%)	1.85	22 (21%) 2 1	73, 123, 149, 162	0
43	A5	113/113 (100%)	1.17	21 (18%) 3 2	77, 94, 124, 183	0
43	E8	113/113 (100%)	0.50	5 (4%) 39 20	75, 91, 125, 164	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
44	B5	92/96 (95%)	0.86	15 (16%) 4 2	85, 102, 129, 133	0
44	F8	94/96 (97%)	0.46	10 (10%) 11 6	69, 88, 113, 128	0
45	C5	104/110 (94%)	1.48	24 (23%) 2 1	107, 137, 167, 175	0
45	G8	104/110 (94%)	0.94	18 (17%) 4 2	87, 113, 147, 166	0
46	D5	179/206 (86%)	1.32	40 (22%) 2 1	139, 176, 263, 269	0
46	H8	175/206 (84%)	0.88	22 (12%) 8 4	97, 139, 228, 236	0
47	E5	76/85 (89%)	1.16	15 (19%) 3 1	85, 111, 130, 169	0
47	I8	80/85 (94%)	1.50	19 (23%) 2 1	71, 90, 122, 131	0
48	F5	97/98 (98%)	0.85	18 (18%) 3 2	79, 102, 146, 163	0
48	J8	97/98 (98%)	0.73	16 (16%) 4 2	69, 91, 145, 176	0
49	G5	66/72 (91%)	0.90	11 (16%) 4 2	101, 121, 141, 167	0
49	K8	67/72 (93%)	0.74	8 (11%) 9 5	76, 96, 119, 154	0
50	H5	59/60 (98%)	1.33	12 (20%) 3 1	97, 126, 167, 182	0
50	L8	57/60 (95%)	0.37	3 (5%) 32 16	77, 98, 120, 133	0
51	I5	63/71 (88%)	0.70	2 (3%) 50 28	179, 219, 236, 243	0
51	M8	66/71 (92%)	1.33	15 (22%) 2 1	128, 174, 203, 214	0
52	J5	56/60 (93%)	1.47	18 (32%) 1 0	77, 103, 150, 162	0
52	N8	58/60 (96%)	1.22	12 (20%) 2 1	68, 115, 186, 191	0
53	K5	45/54 (83%)	2.05	22 (48%) 0 0	153, 180, 196, 202	0
53	O8	45/54 (83%)	1.24	8 (17%) 4 2	131, 159, 177, 183	0
54	L5	46/49 (93%)	0.27	3 (6%) 25 12	64, 76, 89, 102	0
54	P8	45/49 (91%)	0.43	4 (8%) 15 8	59, 64, 78, 92	0
55	M5	60/65 (92%)	0.89	7 (11%) 9 5	89, 101, 125, 147	0
55	Q8	61/65 (93%)	1.08	9 (14%) 5 3	74, 91, 117, 128	0
All	All	21042/21688 (97%)	0.99	3694 (17%) 4 2	56, 122, 214, 378	0

The worst 5 of 3694 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
22	1K	73	A	25.1
11	2A	125	PHE	15.6
24	1L	76	A	15.1
42	95	93	GLU	15.0
34	15	84	LYS	14.8

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
22	PSU	1K	55	20/21	0.56	0.16	153,172,191,191	0
22	7MG	1K	46	24/25	0.66	0.16	175,197,203,209	0
22	4SU	1K	8	20/21	0.69	0.15	184,192,200,205	0
23	5MU	2L	55	21/22	0.75	0.13	138,142,147,151	0
22	5MU	1K	54	21/22	0.76	0.15	142,157,168,172	0
23	PSU	2L	56	20/21	0.78	0.10	128,135,142,148	0
23	5MU	2K	55	21/22	0.79	0.16	99,116,125,136	0
23	PSU	2K	56	20/21	0.79	0.15	109,113,120,127	0
22	PSU	1K	32	20/21	0.82	0.57	113,119,123,123	0
23	7MG	2K	47	24/25	0.86	0.14	110,120,128,137	0
23	4SU	2K	8	20/21	0.87	0.18	100,108,123,123	0
23	7MG	2L	47	24/25	0.87	0.14	140,151,156,161	0
23	4SU	2L	8	20/21	0.88	0.15	128,140,143,147	0
22	PSU	1K	39	20/21	0.89	0.28	96,108,116,119	0
23	OMC	2K	33	21/22	0.94	0.24	88,94,101,106	0
22	MIA	1K	37	29/30	0.95	0.31	89,100,118,123	0
23	OMC	2L	33	21/22	0.96	0.10	124,127,132,137	0

## 5.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
56	MG	14	3274	1/1	0.18	0.43	122,122,122,122	0
56	MG	14	3329	1/1	0.22	0.61	120,120,120,120	0
56	MG	1J	207	1/1	0.24	0.36	147,147,147,147	0
56	MG	14	3199	1/1	0.26	0.49	126,126,126,126	0
56	MG	1J	203	1/1	0.29	0.48	114,114,114,114	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
56	MG	1G	1604	1/1	0.30	0.32	142,142,142,142	0
56	MG	1G	1670	1/1	0.31	0.50	138,138,138,138	0
56	MG	14	3267	1/1	0.31	0.42	110,110,110,110	0
56	MG	1H	3158	1/1	0.33	0.58	104,104,104,104	0
56	MG	14	3197	1/1	0.34	0.48	119,119,119,119	0
56	MG	14	3260	1/1	0.36	0.34	119,119,119,119	0
56	MG	2K	106	1/1	0.36	0.46	115,115,115,115	0
56	MG	1G	1671	1/1	0.40	0.34	120,120,120,120	0
56	MG	1H	3119	1/1	0.42	0.48	101,101,101,101	0
56	MG	1G	1634	1/1	0.43	0.43	120,120,120,120	0
56	MG	1H	3304	1/1	0.44	0.56	114,114,114,114	0
56	MG	13	1621	1/1	0.45	0.42	115,115,115,115	0
56	MG	1H	3213	1/1	0.46	0.40	113,113,113,113	0
56	MG	14	3239	1/1	0.46	0.28	166,166,166,166	0
56	MG	14	3233	1/1	0.48	0.33	118,118,118,118	0
56	MG	2K	105	1/1	0.48	0.45	107,107,107,107	0
56	MG	14	3307	1/1	0.49	0.52	87,87,87,87	0
56	MG	13	1682	1/1	0.49	0.47	116,116,116,116	0
56	MG	14	3258	1/1	0.50	0.47	104,104,104,104	0
56	MG	1H	3062	1/1	0.50	0.38	101,101,101,101	0
56	MG	13	1651	1/1	0.51	0.35	100,100,100,100	0
56	MG	1J	204	1/1	0.51	0.33	113,113,113,113	0
56	MG	14	3066	1/1	0.51	0.49	96,96,96,96	0
56	MG	13	1711	1/1	0.52	0.48	126,126,126,126	0
56	MG	14	3204	1/1	0.53	0.35	80,80,80,80	0
56	MG	1H	3268	1/1	0.53	0.30	125,125,125,125	0
56	MG	14	3146	1/1	0.53	0.28	128,128,128,128	0
56	MG	25	202	1/1	0.54	0.43	125,125,125,125	0
56	MG	14	3236	1/1	0.55	0.36	99,99,99,99	0
56	MG	14	3093	1/1	0.55	0.48	103,103,103,103	0
56	MG	1H	3011	1/1	0.55	0.47	91,91,91,91	0
56	MG	1H	3251	1/1	0.56	0.25	93,93,93,93	0
56	MG	13	1680	1/1	0.57	0.29	124,124,124,124	0
56	MG	14	3304	1/1	0.57	0.27	121,121,121,121	0
56	MG	1H	3340	1/1	0.57	0.47	93,93,93,93	0
56	MG	14	3017	1/1	0.57	0.38	91,91,91,91	0
56	MG	1H	3286	1/1	0.58	0.18	85,85,85,85	0
56	MG	1J	202	1/1	0.59	0.16	157,157,157,157	0
56	MG	1H	3326	1/1	0.59	0.48	117,117,117,117	0
56	MG	14	3216	1/1	0.59	0.43	111,111,111,111	0
56	MG	1H	3164	1/1	0.59	0.47	102,102,102,102	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
56	MG	1H	3277	1/1	0.59	0.57	109,109,109,109	0
56	MG	13	1658	1/1	0.60	0.30	117,117,117,117	0
56	MG	1H	3255	1/1	0.60	0.54	117,117,117,117	0
56	MG	14	3183	1/1	0.60	0.51	110,110,110,110	0
56	MG	1G	1651	1/1	0.60	0.21	138,138,138,138	0
56	MG	1G	1664	1/1	0.60	0.40	116,116,116,116	0
56	MG	1H	3242	1/1	0.60	0.41	105,105,105,105	0
56	MG	1H	3309	1/1	0.60	0.27	96,96,96,96	0
56	MG	2L	103	1/1	0.60	0.39	115,115,115,115	0
56	MG	1H	3270	1/1	0.60	0.41	98,98,98,98	0
56	MG	14	3064	1/1	0.60	0.49	97,97,97,97	0
56	MG	1H	3275	1/1	0.60	0.42	97,97,97,97	0
56	MG	16	206	1/1	0.61	0.16	102,102,102,102	0
56	MG	1H	3227	1/1	0.61	0.26	123,123,123,123	0
56	MG	14	3268	1/1	0.61	0.33	100,100,100,100	0
56	MG	14	3286	1/1	0.62	0.38	92,92,92,92	0
56	MG	1H	3111	1/1	0.62	0.41	91,91,91,91	0
56	MG	13	1685	1/1	0.62	0.26	112,112,112,112	0
56	MG	C5	201	1/1	0.62	0.26	123,123,123,123	0
56	MG	1G	1645	1/1	0.63	0.39	113,113,113,113	0
56	MG	14	3042	1/1	0.63	0.34	87,87,87,87	0
56	MG	1H	3196	1/1	0.63	0.33	110,110,110,110	0
56	MG	14	3293	1/1	0.63	0.43	95,95,95,95	0
56	MG	14	3227	1/1	0.63	0.44	97,97,97,97	0
56	MG	1H	3149	1/1	0.63	0.37	99,99,99,99	0
56	MG	14	3308	1/1	0.63	0.36	106,106,106,106	0
56	MG	14	3202	1/1	0.64	0.56	100,100,100,100	0
56	MG	14	3022	1/1	0.65	0.40	107,107,107,107	0
56	MG	1G	1632	1/1	0.65	0.30	116,116,116,116	0
56	MG	14	3326	1/1	0.65	0.32	117,117,117,117	0
56	MG	13	1672	1/1	0.65	0.30	100,100,100,100	0
56	MG	1H	3344	1/1	0.65	0.43	95,95,95,95	0
56	MG	1G	1630	1/1	0.66	0.33	116,116,116,116	0
56	MG	1H	3028	1/1	0.66	0.46	115,115,115,115	0
56	MG	1H	3135	1/1	0.66	0.32	111,111,111,111	0
56	MG	1H	3235	1/1	0.66	0.33	75,75,75,75	0
56	MG	14	3235	1/1	0.66	0.47	83,83,83,83	0
56	MG	13	1713	1/1	0.67	0.35	119,119,119,119	0
56	MG	14	3142	1/1	0.67	0.59	100,100,100,100	0
56	MG	88	201	1/1	0.67	0.45	95,95,95,95	0
56	MG	1H	3029	1/1	0.67	0.28	110,110,110,110	0
56	MG	14	3029	1/1	0.67	0.50	97,97,97,97	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1G	1617	1/1	0.67	0.38	110,110,110,110	0
56	MG	13	1704	1/1	0.67	0.49	118,118,118,118	0
56	MG	1H	3143	1/1	0.67	0.41	99,99,99,99	0
56	MG	13	1629	1/1	0.68	0.42	106,106,106,106	0
56	MG	1H	3157	1/1	0.68	0.31	104,104,104,104	0
56	MG	1H	3272	1/1	0.68	0.41	96,96,96,96	0
56	MG	13	1606	1/1	0.68	0.38	115,115,115,115	0
56	MG	14	3330	1/1	0.68	0.38	105,105,105,105	0
56	MG	14	3058	1/1	0.68	0.36	128,128,128,128	0
56	MG	1H	3240	1/1	0.68	0.36	94,94,94,94	0
56	MG	13	1708	1/1	0.68	0.28	119,119,119,119	0
56	MG	14	3091	1/1	0.68	0.44	87,87,87,87	0
56	MG	1H	3146	1/1	0.68	0.37	83,83,83,83	0
56	MG	1H	3200	1/1	0.68	0.35	104,104,104,104	0
56	MG	1G	1661	1/1	0.69	0.36	105,105,105,105	0
56	MG	1H	3033	1/1	0.69	0.40	100,100,100,100	0
56	MG	1G	1669	1/1	0.69	0.31	112,112,112,112	0
56	MG	14	3169	1/1	0.69	0.41	93,93,93,93	0
56	MG	13	1686	1/1	0.69	0.28	134,134,134,134	0
56	MG	13	1693	1/1	0.69	0.33	103,103,103,103	0
56	MG	13	1702	1/1	0.69	0.33	109,109,109,109	0
56	MG	14	3254	1/1	0.69	0.26	87,87,87,87	0
56	MG	13	1639	1/1	0.69	0.29	109,109,109,109	0
56	MG	1G	1628	1/1	0.70	0.33	118,118,118,118	0
56	MG	13	1654	1/1	0.70	0.24	123,123,123,123	0
56	MG	13	1717	1/1	0.70	0.31	114,114,114,114	0
56	MG	1H	3204	1/1	0.70	0.46	104,104,104,104	0
56	MG	1G	1672	1/1	0.70	0.22	126,126,126,126	0
56	MG	1H	3311	1/1	0.70	0.35	109,109,109,109	0
56	MG	1H	3322	1/1	0.70	0.24	96,96,96,96	0
56	MG	1H	3282	1/1	0.70	0.26	107,107,107,107	0
56	MG	14	3312	1/1	0.70	0.39	93,93,93,93	0
56	MG	14	3025	1/1	0.71	0.21	116,116,116,116	0
56	MG	1G	1644	1/1	0.71	0.16	115,115,115,115	0
56	MG	13	1646	1/1	0.71	0.34	104,104,104,104	0
56	MG	14	3311	1/1	0.71	0.32	89,89,89,89	0
56	MG	1H	3331	1/1	0.71	0.19	106,106,106,106	0
56	MG	14	3314	1/1	0.71	0.47	102,102,102,102	0
56	MG	1H	3310	1/1	0.71	0.56	96,96,96,96	0
56	MG	14	3327	1/1	0.71	0.35	117,117,117,117	0
56	MG	1H	3138	1/1	0.72	0.41	94,94,94,94	0
56	MG	1H	3186	1/1	0.72	0.28	93,93,93,93	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
56	MG	14	3238	1/1	0.72	0.22	110,110,110,110	0
56	MG	14	3181	1/1	0.72	0.26	100,100,100,100	0
56	MG	14	3251	1/1	0.72	0.34	105,105,105,105	0
56	MG	13	1683	1/1	0.72	0.17	106,106,106,106	0
56	MG	14	3256	1/1	0.72	0.25	97,97,97,97	0
56	MG	13	1687	1/1	0.72	0.30	109,109,109,109	0
56	MG	14	3007	1/1	0.72	0.47	94,94,94,94	0
56	MG	14	3076	1/1	0.72	0.30	93,93,93,93	0
56	MG	1H	3026	1/1	0.72	0.43	94,94,94,94	0
56	MG	14	3270	1/1	0.72	0.31	107,107,107,107	0
56	MG	13	1707	1/1	0.72	0.38	104,104,104,104	0
56	MG	14	3284	1/1	0.72	0.39	100,100,100,100	0
56	MG	14	3120	1/1	0.72	0.48	80,80,80,80	0
56	MG	13	1602	1/1	0.72	0.36	87,87,87,87	0
56	MG	14	3090	1/1	0.73	0.36	89,89,89,89	0
56	MG	14	3163	1/1	0.73	0.20	105,105,105,105	0
56	MG	14	3164	1/1	0.73	0.29	91,91,91,91	0
56	MG	14	3226	1/1	0.73	0.32	123,123,123,123	0
56	MG	1G	1673	1/1	0.73	0.26	108,108,108,108	0
56	MG	14	3232	1/1	0.73	0.41	103,103,103,103	0
56	MG	14	3175	1/1	0.73	0.40	99,99,99,99	0
56	MG	14	3178	1/1	0.73	0.33	95,95,95,95	0
56	MG	2K	107	1/1	0.73	0.46	106,106,106,106	0
56	MG	13	1669	1/1	0.73	0.42	110,110,110,110	0
56	MG	14	3194	1/1	0.73	0.42	97,97,97,97	0
56	MG	14	3121	1/1	0.73	0.34	84,84,84,84	0
56	MG	1H	3162	1/1	0.73	0.29	74,74,74,74	0
56	MG	1H	3034	1/1	0.74	0.18	96,96,96,96	0
56	MG	13	1697	1/1	0.74	0.46	97,97,97,97	0
56	MG	1H	3027	1/1	0.74	0.43	96,96,96,96	0
56	MG	14	3126	1/1	0.74	0.35	103,103,103,103	0
56	MG	1H	3246	1/1	0.74	0.38	78,78,78,78	0
56	MG	1H	3154	1/1	0.74	0.26	91,91,91,91	0
56	MG	13	1690	1/1	0.74	0.34	108,108,108,108	0
56	MG	1H	3003	1/1	0.74	0.28	75,75,75,75	0
56	MG	13	1655	1/1	0.74	0.34	89,89,89,89	0
56	MG	1G	1601	1/1	0.74	0.27	109,109,109,109	0
56	MG	1G	1654	1/1	0.74	0.41	94,94,94,94	0
56	MG	E5	101	1/1	0.74	0.25	98,98,98,98	0
56	MG	13	1696	1/1	0.75	0.31	108,108,108,108	0
56	MG	1H	3013	1/1	0.75	0.51	104,104,104,104	0
56	MG	14	3243	1/1	0.75	0.30	91,91,91,91	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	16	214	1/1	0.75	0.28	109,109,109,109	0
56	MG	13	1607	1/1	0.75	0.25	78,78,78,78	0
56	MG	13	1620	1/1	0.75	0.43	119,119,119,119	0
56	MG	14	3125	1/1	0.75	0.38	101,101,101,101	0
56	MG	1H	3259	1/1	0.75	0.33	105,105,105,105	0
56	MG	1H	3153	1/1	0.75	0.35	98,98,98,98	0
56	MG	14	3052	1/1	0.75	0.35	110,110,110,110	0
56	MG	14	3158	1/1	0.75	0.41	93,93,93,93	0
56	MG	1H	3115	1/1	0.75	0.40	95,95,95,95	0
56	MG	2K	102	1/1	0.75	0.20	97,97,97,97	0
56	MG	1H	3128	1/1	0.75	0.29	88,88,88,88	0
56	MG	14	3172	1/1	0.75	0.24	107,107,107,107	0
56	MG	1H	3007	1/1	0.75	0.34	97,97,97,97	0
56	MG	13	1698	1/1	0.76	0.42	95,95,95,95	0
56	MG	14	3109	1/1	0.76	0.53	89,89,89,89	0
56	MG	14	3276	1/1	0.76	0.40	103,103,103,103	0
56	MG	1G	1615	1/1	0.76	0.45	115,115,115,115	0
56	MG	1H	3150	1/1	0.76	0.33	86,86,86,86	0
56	MG	14	3288	1/1	0.76	0.40	107,107,107,107	0
56	MG	14	3291	1/1	0.76	0.18	115,115,115,115	0
56	MG	1G	1620	1/1	0.76	0.32	107,107,107,107	0
56	MG	13	1691	1/1	0.76	0.54	95,95,95,95	0
56	MG	14	3137	1/1	0.76	0.49	80,80,80,80	0
56	MG	13	1715	1/1	0.76	0.51	108,108,108,108	0
56	MG	14	3234	1/1	0.76	0.23	98,98,98,98	0
56	MG	13	1674	1/1	0.76	0.24	118,118,118,118	0
56	MG	1H	3338	1/1	0.76	0.25	110,110,110,110	0
56	MG	14	3027	1/1	0.76	0.40	84,84,84,84	0
56	MG	13	1721	1/1	0.76	0.21	101,101,101,101	0
56	MG	13	1677	1/1	0.76	0.30	98,98,98,98	0
56	MG	16	203	1/1	0.76	0.18	107,107,107,107	0
56	MG	14	3252	1/1	0.76	0.25	105,105,105,105	0
56	MG	13	1664	1/1	0.76	0.13	103,103,103,103	0
56	MG	16	211	1/1	0.76	0.39	79,79,79,79	0
56	MG	1J	206	1/1	0.76	0.11	123,123,123,123	0
56	MG	1G	1662	1/1	0.76	0.22	155,155,155,155	0
56	MG	39	302	1/1	0.76	0.14	118,118,118,118	0
56	MG	1H	3169	1/1	0.76	0.31	85,85,85,85	0
56	MG	1H	3170	1/1	0.76	0.23	100,100,100,100	0
56	MG	1H	3177	1/1	0.76	0.34	98,98,98,98	0
56	MG	1H	3094	1/1	0.77	0.28	79,79,79,79	0
56	MG	14	3047	1/1	0.77	0.13	66,66,66,66	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1H	3234	1/1	0.77	0.45	91,91,91,91	0
56	MG	13	1709	1/1	0.77	0.26	141,141,141,141	0
56	MG	1H	3237	1/1	0.77	0.30	70,70,70,70	0
56	MG	1H	3327	1/1	0.77	0.39	91,91,91,91	0
56	MG	14	3074	1/1	0.77	0.33	79,79,79,79	0
56	MG	1H	3273	1/1	0.77	0.34	84,84,84,84	0
56	MG	1H	3336	1/1	0.77	0.52	102,102,102,102	0
56	MG	13	1604	1/1	0.77	0.38	108,108,108,108	0
56	MG	14	3092	1/1	0.77	0.21	109,109,109,109	0
56	MG	14	3196	1/1	0.77	0.33	99,99,99,99	0
56	MG	6A	101	1/1	0.77	0.17	138,138,138,138	0
56	MG	13	1750	1/1	0.77	0.29	131,131,131,131	0
56	MG	14	3201	1/1	0.77	0.48	111,111,111,111	0
56	MG	1H	3211	1/1	0.77	0.23	76,76,76,76	0
56	MG	1G	1640	1/1	0.77	0.37	106,106,106,106	0
56	MG	1H	3250	1/1	0.77	0.30	104,104,104,104	0
56	MG	1H	3288	1/1	0.77	0.60	87,87,87,87	0
56	MG	1H	3180	1/1	0.77	0.21	84,84,84,84	0
56	MG	1H	3221	1/1	0.77	0.31	99,99,99,99	0
56	MG	M5	101	1/1	0.77	0.15	94,94,94,94	0
56	MG	1G	1631	1/1	0.78	0.22	113,113,113,113	0
56	MG	13	1675	1/1	0.78	0.20	121,121,121,121	0
56	MG	1H	3230	1/1	0.78	0.31	91,91,91,91	0
56	MG	14	3319	1/1	0.78	0.22	118,118,118,118	0
56	MG	14	3324	1/1	0.78	0.19	96,96,96,96	0
56	MG	14	3210	1/1	0.78	0.35	98,98,98,98	0
56	MG	14	3167	1/1	0.78	0.32	110,110,110,110	0
56	MG	14	3095	1/1	0.78	0.32	78,78,78,78	0
56	MG	1H	3031	1/1	0.78	0.24	89,89,89,89	0
56	MG	1H	3139	1/1	0.78	0.31	79,79,79,79	0
56	MG	1G	1606	1/1	0.78	0.19	129,129,129,129	0
56	MG	1H	3140	1/1	0.78	0.40	101,101,101,101	0
56	MG	1H	3061	1/1	0.78	0.49	85,85,85,85	0
56	MG	14	3188	1/1	0.78	0.41	91,91,91,91	0
56	MG	14	3190	1/1	0.78	0.31	124,124,124,124	0
56	MG	1H	3320	1/1	0.78	0.45	106,106,106,106	0
56	MG	1H	3281	1/1	0.78	0.33	85,85,85,85	0
56	MG	14	3143	1/1	0.78	0.44	100,100,100,100	0
56	MG	1H	3263	1/1	0.78	0.25	106,106,106,106	0
56	MG	14	3051	1/1	0.79	0.39	100,100,100,100	0
56	MG	16	209	1/1	0.79	0.28	88,88,88,88	0
56	MG	1H	3117	1/1	0.79	0.24	87,87,87,87	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
56	MG	1G	1626	1/1	0.79	0.54	102,102,102,102	0
56	MG	14	3065	1/1	0.79	0.18	87,87,87,87	0
56	MG	14	3318	1/1	0.79	0.22	99,99,99,99	0
56	MG	1G	1657	1/1	0.79	0.23	106,106,106,106	0
56	MG	1H	3008	1/1	0.79	0.33	79,79,79,79	0
56	MG	14	3018	1/1	0.79	0.30	70,70,70,70	0
56	MG	41	202	1/1	0.79	0.22	96,96,96,96	0
56	MG	1H	3178	1/1	0.79	0.28	76,76,76,76	0
56	MG	14	3269	1/1	0.79	0.38	102,102,102,102	0
56	MG	13	1635	1/1	0.79	0.30	88,88,88,88	0
56	MG	13	1689	1/1	0.79	0.33	98,98,98,98	0
56	MG	14	3094	1/1	0.79	0.33	83,83,83,83	0
56	MG	13	1630	1/1	0.79	0.15	74,74,74,74	0
56	MG	14	3044	1/1	0.79	0.40	78,78,78,78	0
56	MG	14	3287	1/1	0.79	0.22	95,95,95,95	0
56	MG	14	3114	1/1	0.79	0.32	97,97,97,97	0
56	MG	13	1703	1/1	0.79	0.27	96,96,96,96	0
56	MG	14	3185	1/1	0.79	0.43	90,90,90,90	0
56	MG	14	3186	1/1	0.79	0.29	86,86,86,86	0
56	MG	14	3296	1/1	0.80	0.48	107,107,107,107	0
56	MG	1H	3004	1/1	0.80	0.33	68,68,68,68	0
56	MG	1H	3492	1/1	0.80	0.13	120,120,120,120	0
56	MG	1H	3321	1/1	0.80	0.18	99,99,99,99	0
56	MG	1H	3160	1/1	0.80	0.40	84,84,84,84	0
56	MG	14	3014	1/1	0.80	0.35	73,73,73,73	0
56	MG	1H	3323	1/1	0.80	0.31	110,110,110,110	0
56	MG	1H	3151	1/1	0.80	0.28	110,110,110,110	0
56	MG	1H	3243	1/1	0.80	0.19	93,93,93,93	0
56	MG	14	3151	1/1	0.80	0.34	91,91,91,91	0
56	MG	1H	3006	1/1	0.80	0.35	91,91,91,91	0
56	MG	14	3161	1/1	0.80	0.22	104,104,104,104	0
56	MG	1G	1668	1/1	0.80	0.19	111,111,111,111	0
56	MG	14	3208	1/1	0.80	0.25	84,84,84,84	0
56	MG	13	1657	1/1	0.80	0.17	104,104,104,104	0
56	MG	14	3272	1/1	0.80	0.46	95,95,95,95	0
56	MG	14	3039	1/1	0.80	0.34	68,68,68,68	0
56	MG	1J	205	1/1	0.80	0.17	101,101,101,101	0
56	MG	14	3220	1/1	0.80	0.34	94,94,94,94	0
56	MG	14	3040	1/1	0.80	0.25	79,79,79,79	0
56	MG	14	3171	1/1	0.80	0.25	73,73,73,73	0
56	MG	13	1637	1/1	0.80	0.41	96,96,96,96	0
56	MG	1G	1635	1/1	0.80	0.16	118,118,118,118	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	14	3113	1/1	0.80	0.48	80,80,80,80	0
56	MG	1H	3175	1/1	0.80	0.22	93,93,93,93	0
56	MG	14	3012	1/1	0.81	0.38	94,94,94,94	0
56	MG	1H	3300	1/1	0.81	0.33	87,87,87,87	0
56	MG	16	204	1/1	0.81	0.13	99,99,99,99	0
56	MG	14	3313	1/1	0.81	0.26	124,124,124,124	0
56	MG	13	1699	1/1	0.81	0.23	102,102,102,102	0
56	MG	1H	3305	1/1	0.81	0.33	104,104,104,104	0
56	MG	1H	3106	1/1	0.81	0.19	95,95,95,95	0
56	MG	16	213	1/1	0.81	0.37	85,85,85,85	0
56	MG	1H	3059	1/1	0.81	0.25	92,92,92,92	0
56	MG	11	302	1/1	0.81	0.17	66,66,66,66	0
56	MG	13	1601	1/1	0.81	0.27	74,74,74,74	0
56	MG	14	3218	1/1	0.81	0.42	75,75,75,75	0
56	MG	1H	3315	1/1	0.81	0.21	105,105,105,105	0
56	MG	1H	3316	1/1	0.81	0.35	94,94,94,94	0
56	MG	13	1628	1/1	0.81	0.29	102,102,102,102	0
56	MG	14	3177	1/1	0.81	0.28	111,111,111,111	0
56	MG	1H	3087	1/1	0.81	0.11	69,69,69,69	0
56	MG	14	3002	1/1	0.81	0.34	70,70,70,70	0
56	MG	14	3054	1/1	0.81	0.29	93,93,93,93	0
56	MG	25	201	1/1	0.81	0.45	111,111,111,111	0
56	MG	1G	1614	1/1	0.81	0.22	140,140,140,140	0
56	MG	14	3060	1/1	0.81	0.35	83,83,83,83	0
56	MG	14	3136	1/1	0.81	0.22	112,112,112,112	0
56	MG	14	3063	1/1	0.81	0.16	104,104,104,104	0
56	MG	1G	1618	1/1	0.82	0.18	104,104,104,104	0
56	MG	14	3189	1/1	0.82	0.57	83,83,83,83	0
56	MG	1H	3228	1/1	0.82	0.34	94,94,94,94	0
56	MG	14	3249	1/1	0.82	0.51	97,97,97,97	0
56	MG	14	3020	1/1	0.82	0.39	92,92,92,92	0
56	MG	14	3067	1/1	0.82	0.23	73,73,73,73	0
56	MG	1H	3079	1/1	0.82	0.18	83,83,83,83	0
56	MG	1G	1627	1/1	0.82	0.27	116,116,116,116	0
56	MG	1H	3201	1/1	0.82	0.22	121,121,121,121	0
56	MG	1H	3337	1/1	0.82	0.23	106,106,106,106	0
56	MG	14	3261	1/1	0.82	0.42	83,83,83,83	0
56	MG	13	1634	1/1	0.82	0.45	85,85,85,85	0
56	MG	1H	3021	1/1	0.82	0.14	79,79,79,79	0
56	MG	1H	3173	1/1	0.82	0.23	98,98,98,98	0
56	MG	14	3213	1/1	0.82	0.29	113,113,113,113	0
56	MG	1H	3266	1/1	0.82	0.52	95,95,95,95	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	14	3106	1/1	0.82	0.26	89,89,89,89	0
56	MG	1H	3502	1/1	0.82	0.12	118,118,118,118	0
56	MG	14	3277	1/1	0.82	0.24	90,90,90,90	0
56	MG	2L	102	1/1	0.82	0.36	89,89,89,89	0
56	MG	13	1663	1/1	0.82	0.14	87,87,87,87	0
56	MG	1H	3199	1/1	0.82	0.31	99,99,99,99	0
56	MG	1G	1649	1/1	0.82	0.20	105,105,105,105	0
56	MG	16	205	1/1	0.82	0.18	91,91,91,91	0
56	MG	1H	3245	1/1	0.82	0.40	96,96,96,96	0
56	MG	14	3132	1/1	0.82	0.22	94,94,94,94	0
56	MG	1G	1655	1/1	0.83	0.19	111,111,111,111	0
56	MG	1G	1656	1/1	0.83	0.30	103,103,103,103	0
56	MG	14	3019	1/1	0.83	0.38	96,96,96,96	0
56	MG	16	202	1/1	0.83	0.28	73,73,73,73	0
56	MG	14	3166	1/1	0.83	0.21	106,106,106,106	0
56	MG	1H	3193	1/1	0.83	0.32	95,95,95,95	0
56	MG	14	3299	1/1	0.83	0.23	84,84,84,84	0
56	MG	13	1684	1/1	0.83	0.21	106,106,106,106	0
56	MG	1H	3197	1/1	0.83	0.32	89,89,89,89	0
56	MG	1H	3241	1/1	0.83	0.26	80,80,80,80	0
56	MG	1H	3023	1/1	0.83	0.39	100,100,100,100	0
56	MG	14	3103	1/1	0.83	0.25	90,90,90,90	0
56	MG	13	1673	1/1	0.83	0.44	91,91,91,91	0
56	MG	13	1712	1/1	0.83	0.34	99,99,99,99	0
56	MG	14	3246	1/1	0.83	0.37	75,75,75,75	0
56	MG	14	3043	1/1	0.83	0.30	101,101,101,101	0
56	MG	1H	3125	1/1	0.83	0.32	68,68,68,68	0
56	MG	14	3118	1/1	0.83	0.44	71,71,71,71	0
56	MG	2K	103	1/1	0.83	0.29	98,98,98,98	0
56	MG	1G	1675	1/1	0.83	0.10	99,99,99,99	0
56	MG	14	3124	1/1	0.83	0.32	85,85,85,85	0
56	MG	1J	201	1/1	0.83	0.18	123,123,123,123	0
56	MG	1H	3296	1/1	0.83	0.48	86,86,86,86	0
56	MG	1H	3176	1/1	0.83	0.32	91,91,91,91	0
56	MG	13	1667	1/1	0.83	0.42	147,147,147,147	0
56	MG	14	3059	1/1	0.83	0.30	74,74,74,74	0
56	MG	1H	3091	1/1	0.83	0.33	70,70,70,70	0
56	MG	14	3003	1/1	0.83	0.36	73,73,73,73	0
56	MG	13	1679	1/1	0.83	0.16	98,98,98,98	0
56	MG	14	3207	1/1	0.83	0.20	68,68,68,68	0
56	MG	14	3144	1/1	0.83	0.45	93,93,93,93	0
56	MG	1H	3185	1/1	0.83	0.38	88,88,88,88	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	14	3280	1/1	0.83	0.20	95,95,95,95	0
56	MG	13	1701	1/1	0.83	0.32	103,103,103,103	0
57	ZN	G8	202	1/1	0.83	0.18	192,192,192,192	0
56	MG	13	1626	1/1	0.84	0.23	109,109,109,109	0
56	MG	14	3281	1/1	0.84	0.23	105,105,105,105	0
56	MG	14	3053	1/1	0.84	0.26	98,98,98,98	0
56	MG	1H	3265	1/1	0.84	0.38	96,96,96,96	0
56	MG	1G	1674	1/1	0.84	0.22	111,111,111,111	0
56	MG	13	1605	1/1	0.84	0.34	93,93,93,93	0
56	MG	13	1640	1/1	0.84	0.45	94,94,94,94	0
56	MG	1H	3165	1/1	0.84	0.35	95,95,95,95	0
56	MG	14	3225	1/1	0.84	0.20	65,65,65,65	0
56	MG	1G	1633	1/1	0.84	0.26	93,93,93,93	0
56	MG	14	3159	1/1	0.84	0.35	112,112,112,112	0
56	MG	13	1714	1/1	0.84	0.30	101,101,101,101	0
56	MG	13	1676	1/1	0.84	0.27	111,111,111,111	0
56	MG	1H	3070	1/1	0.84	0.15	125,125,125,125	0
56	MG	14	3009	1/1	0.84	0.39	65,65,65,65	0
56	MG	1H	3152	1/1	0.84	0.36	93,93,93,93	0
56	MG	21	301	1/1	0.84	0.23	75,75,75,75	0
56	MG	1H	3278	1/1	0.84	0.22	101,101,101,101	0
56	MG	1G	1650	1/1	0.84	0.22	101,101,101,101	0
56	MG	14	3323	1/1	0.84	0.33	101,101,101,101	0
56	MG	14	3244	1/1	0.84	0.20	99,99,99,99	0
56	MG	13	1668	1/1	0.84	0.19	94,94,94,94	0
56	MG	13	1636	1/1	0.84	0.25	100,100,100,100	0
56	MG	13	1647	1/1	0.84	0.31	93,93,93,93	0
56	MG	1H	3248	1/1	0.84	0.29	76,76,76,76	0
56	MG	14	3253	1/1	0.84	0.20	82,82,82,82	0
56	MG	1G	1613	1/1	0.84	0.22	117,117,117,117	0
56	MG	14	3108	1/1	0.84	0.26	92,92,92,92	0
56	MG	1G	1659	1/1	0.84	0.28	102,102,102,102	0
56	MG	14	3038	1/1	0.84	0.31	72,72,72,72	0
56	MG	1H	3290	1/1	0.84	0.19	92,92,92,92	0
56	MG	13	1710	1/1	0.84	0.21	98,98,98,98	0
56	MG	14	3041	1/1	0.84	0.26	80,80,80,80	0
56	MG	1G	1616	1/1	0.84	0.15	149,149,149,149	0
56	MG	1H	3298	1/1	0.84	0.43	92,92,92,92	0
56	MG	1H	3222	1/1	0.84	0.34	79,79,79,79	0
56	MG	1H	3225	1/1	0.84	0.27	69,69,69,69	0
56	MG	1H	3182	1/1	0.84	0.11	74,74,74,74	0
56	MG	14	3135	1/1	0.84	0.30	101,101,101,101	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1H	3055	1/1	0.85	0.19	82,82,82,82	0
56	MG	14	3021	1/1	0.85	0.45	79,79,79,79	0
56	MG	1H	3206	1/1	0.85	0.17	53,53,53,53	0
56	MG	1H	3208	1/1	0.85	0.30	63,63,63,63	0
56	MG	1H	3210	1/1	0.85	0.17	69,69,69,69	0
56	MG	14	3112	1/1	0.85	0.19	98,98,98,98	0
56	MG	13	1662	1/1	0.85	0.26	94,94,94,94	0
56	MG	14	3037	1/1	0.85	0.28	79,79,79,79	0
56	MG	13	1716	1/1	0.85	0.13	111,111,111,111	0
56	MG	14	3282	1/1	0.85	0.37	90,90,90,90	0
56	MG	14	3283	1/1	0.85	0.24	98,98,98,98	0
56	MG	1H	3017	1/1	0.85	0.22	79,79,79,79	0
56	MG	1H	3269	1/1	0.85	0.31	90,90,90,90	0
56	MG	2K	104	1/1	0.85	0.39	90,90,90,90	0
56	MG	1G	1607	1/1	0.85	0.23	98,98,98,98	0
56	MG	1G	1663	1/1	0.85	0.40	92,92,92,92	0
56	MG	13	1612	1/1	0.85	0.26	89,89,89,89	0
56	MG	14	3295	1/1	0.85	0.30	95,95,95,95	0
56	MG	1H	3024	1/1	0.85	0.31	102,102,102,102	0
56	MG	14	3049	1/1	0.85	0.31	87,87,87,87	0
56	MG	13	1720	1/1	0.85	0.23	104,104,104,104	0
56	MG	13	1652	1/1	0.85	0.48	98,98,98,98	0
56	MG	1H	3095	1/1	0.85	0.43	74,74,74,74	0
56	MG	1H	3097	1/1	0.85	0.37	89,89,89,89	0
56	MG	13	1739	1/1	0.85	0.22	120,120,120,120	0
56	MG	14	3148	1/1	0.85	0.22	117,117,117,117	0
56	MG	1G	1622	1/1	0.85	0.15	89,89,89,89	0
56	MG	1H	3187	1/1	0.85	0.19	89,89,89,89	0
56	MG	13	1748	1/1	0.85	0.12	140,140,140,140	0
56	MG	1H	3494	1/1	0.85	0.21	121,121,121,121	0
56	MG	14	3162	1/1	0.85	0.30	88,88,88,88	0
56	MG	13	1631	1/1	0.85	0.12	102,102,102,102	0
56	MG	1H	3294	1/1	0.85	0.13	100,100,100,100	0
56	MG	14	3165	1/1	0.85	0.42	70,70,70,70	0
56	MG	1H	3116	1/1	0.85	0.41	70,70,70,70	0
56	MG	14	3416	1/1	0.85	0.21	126,126,126,126	0
56	MG	14	3247	1/1	0.85	0.31	75,75,75,75	0
56	MG	1H	3198	1/1	0.85	0.38	90,90,90,90	0
56	MG	13	1752	1/1	0.85	0.13	92,92,92,92	0
56	MG	14	3083	1/1	0.85	0.34	81,81,81,81	0
56	MG	14	3089	1/1	0.85	0.24	85,85,85,85	0
56	MG	5E	201	1/1	0.85	0.17	104,104,104,104	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
56	MG	14	3255	1/1	0.85	0.28	99,99,99,99	0
56	MG	14	3176	1/1	0.85	0.56	101,101,101,101	0
56	MG	1H	3052	1/1	0.85	0.32	80,80,80,80	0
56	MG	16	210	1/1	0.85	0.23	107,107,107,107	0
56	MG	1H	3307	1/1	0.85	0.19	99,99,99,99	0
56	MG	14	3263	1/1	0.85	0.49	88,88,88,88	0
56	MG	14	3264	1/1	0.85	0.17	89,89,89,89	0
56	MG	1G	1647	1/1	0.85	0.39	86,86,86,86	0
56	MG	1H	3141	1/1	0.86	0.24	89,89,89,89	0
56	MG	1H	3498	1/1	0.86	0.12	119,119,119,119	0
56	MG	1H	3047	1/1	0.86	0.23	65,65,65,65	0
56	MG	1H	3080	1/1	0.86	0.22	86,86,86,86	0
56	MG	14	3030	1/1	0.86	0.22	115,115,115,115	0
56	MG	1H	3086	1/1	0.86	0.16	72,72,72,72	0
56	MG	1G	1666	1/1	0.86	0.26	89,89,89,89	0
56	MG	13	1700	1/1	0.86	0.25	109,109,109,109	0
56	MG	14	3105	1/1	0.86	0.35	74,74,74,74	0
56	MG	1H	3122	1/1	0.86	0.14	94,94,94,94	0
56	MG	1H	3054	1/1	0.86	0.26	71,71,71,71	0
56	MG	1H	3127	1/1	0.86	0.28	92,92,92,92	0
56	MG	14	3245	1/1	0.86	0.33	71,71,71,71	0
56	MG	14	3110	1/1	0.86	0.26	61,61,61,61	0
56	MG	13	1744	1/1	0.86	0.19	132,132,132,132	0
56	MG	1H	3324	1/1	0.86	0.28	107,107,107,107	0
56	MG	14	3315	1/1	0.86	0.22	92,92,92,92	0
56	MG	14	3316	1/1	0.86	0.42	103,103,103,103	0
56	MG	1H	3132	1/1	0.86	0.48	74,74,74,74	0
56	MG	14	3115	1/1	0.86	0.21	100,100,100,100	0
56	MG	14	3322	1/1	0.86	0.24	90,90,90,90	0
56	MG	14	3117	1/1	0.86	0.27	98,98,98,98	0
56	MG	1H	3216	1/1	0.86	0.24	77,77,77,77	0
56	MG	1H	3328	1/1	0.86	0.24	87,87,87,87	0
56	MG	1G	1636	1/1	0.86	0.10	115,115,115,115	0
56	MG	13	1615	1/1	0.86	0.27	100,100,100,100	0
56	MG	1H	3137	1/1	0.86	0.40	87,87,87,87	0
56	MG	14	3405	1/1	0.86	0.26	102,102,102,102	0
56	MG	14	3191	1/1	0.86	0.30	92,92,92,92	0
56	MG	1H	3192	1/1	0.86	0.19	78,78,78,78	0
56	MG	14	3127	1/1	0.86	0.14	87,87,87,87	0
56	MG	14	3130	1/1	0.86	0.21	71,71,71,71	0
56	MG	14	3005	1/1	0.86	0.24	66,66,66,66	0
56	MG	1H	3012	1/1	0.86	0.25	93,93,93,93	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
56	MG	1G	1602	1/1	0.86	0.21	118,118,118,118	0
56	MG	1H	3194	1/1	0.86	0.17	104,104,104,104	0
56	MG	1H	3038	1/1	0.86	0.14	58,58,58,58	0
56	MG	1H	3346	1/1	0.86	0.48	106,106,106,106	0
56	MG	1H	3395	1/1	0.86	0.14	118,118,118,118	0
56	MG	85	201	1/1	0.86	0.54	93,93,93,93	0
56	MG	1H	3473	1/1	0.86	0.24	127,127,127,127	0
56	MG	1H	3041	1/1	0.86	0.30	67,67,67,67	0
56	MG	1G	1658	1/1	0.86	0.28	110,110,110,110	0
56	MG	14	3152	1/1	0.86	0.29	80,80,80,80	0
56	MG	13	1650	1/1	0.87	0.22	87,87,87,87	0
56	MG	1H	3313	1/1	0.87	0.30	93,93,93,93	0
56	MG	14	3278	1/1	0.87	0.39	85,85,85,85	0
56	MG	1H	3098	1/1	0.87	0.35	72,72,72,72	0
56	MG	1H	3102	1/1	0.87	0.32	67,67,67,67	0
56	MG	14	3128	1/1	0.87	0.18	97,97,97,97	0
56	MG	14	3203	1/1	0.87	0.25	81,81,81,81	0
56	MG	14	3129	1/1	0.87	0.27	78,78,78,78	0
56	MG	1H	3010	1/1	0.87	0.33	83,83,83,83	0
56	MG	14	3055	1/1	0.87	0.20	85,85,85,85	0
56	MG	2L	101	1/1	0.87	0.25	98,98,98,98	0
56	MG	1H	3276	1/1	0.87	0.26	99,99,99,99	0
56	MG	1H	3172	1/1	0.87	0.25	98,98,98,98	0
56	MG	13	1694	1/1	0.87	0.23	121,121,121,121	0
56	MG	1H	3280	1/1	0.87	0.30	100,100,100,100	0
56	MG	14	3221	1/1	0.87	0.31	87,87,87,87	0
56	MG	16	212	1/1	0.87	0.08	99,99,99,99	0
56	MG	14	3305	1/1	0.87	0.24	79,79,79,79	0
56	MG	1H	3114	1/1	0.87	0.27	82,82,82,82	0
56	MG	1H	3063	1/1	0.87	0.24	83,83,83,83	0
56	MG	14	3010	1/1	0.87	0.27	65,65,65,65	0
56	MG	13	1659	1/1	0.87	0.25	109,109,109,109	0
56	MG	14	3156	1/1	0.87	0.38	99,99,99,99	0
56	MG	14	3080	1/1	0.87	0.39	88,88,88,88	0
56	MG	1H	3329	1/1	0.87	0.28	99,99,99,99	0
56	MG	13	1613	1/1	0.87	0.12	96,96,96,96	0
56	MG	1H	3333	1/1	0.87	0.34	91,91,91,91	0
56	MG	1G	1652	1/1	0.87	0.28	103,103,103,103	0
56	MG	1H	3334	1/1	0.87	0.26	99,99,99,99	0
56	MG	1H	3335	1/1	0.87	0.26	85,85,85,85	0
56	MG	13	1614	1/1	0.87	0.12	98,98,98,98	0
56	MG	14	3023	1/1	0.87	0.17	86,86,86,86	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	14	3102	1/1	0.87	0.34	93,93,93,93	0
56	MG	14	3250	1/1	0.87	0.20	86,86,86,86	0
56	MG	1G	1605	1/1	0.87	0.17	98,98,98,98	0
56	MG	1H	3293	1/1	0.87	0.19	85,85,85,85	0
56	MG	14	3413	1/1	0.87	0.20	110,110,110,110	0
56	MG	1H	3081	1/1	0.87	0.24	77,77,77,77	0
56	MG	14	3425	1/1	0.87	0.40	92,92,92,92	0
56	MG	13	1653	1/1	0.87	0.14	78,78,78,78	0
56	MG	14	3031	1/1	0.87	0.24	76,76,76,76	0
56	MG	13	1642	1/1	0.87	0.21	98,98,98,98	0
56	MG	1H	3262	1/1	0.87	0.23	89,89,89,89	0
56	MG	13	1603	1/1	0.87	0.50	97,97,97,97	0
56	MG	1G	1665	1/1	0.87	0.16	110,110,110,110	0
56	MG	1H	3188	1/1	0.87	0.28	100,100,100,100	0
56	MG	14	3187	1/1	0.87	0.35	100,100,100,100	0
56	MG	49	201	1/1	0.87	0.10	143,143,143,143	0
56	MG	13	1627	1/1	0.87	0.32	101,101,101,101	0
56	MG	1H	3133	1/1	0.87	0.14	84,84,84,84	0
56	MG	13	1681	1/1	0.87	0.12	107,107,107,107	0
56	MG	1H	3500	1/1	0.87	0.12	122,122,122,122	0
56	MG	14	3271	1/1	0.87	0.15	87,87,87,87	0
56	MG	14	3123	1/1	0.87	0.29	75,75,75,75	0
56	MG	14	3195	1/1	0.87	0.34	100,100,100,100	0
56	MG	1G	1642	1/1	0.88	0.39	102,102,102,102	0
56	MG	14	3180	1/1	0.88	0.44	83,83,83,83	0
56	MG	1H	3183	1/1	0.88	0.22	83,83,83,83	0
56	MG	14	3182	1/1	0.88	0.18	98,98,98,98	0
56	MG	14	3300	1/1	0.88	0.24	98,98,98,98	0
56	MG	14	3303	1/1	0.88	0.21	100,100,100,100	0
56	MG	14	3078	1/1	0.88	0.38	97,97,97,97	0
56	MG	1H	3009	1/1	0.88	0.28	69,69,69,69	0
56	MG	14	3306	1/1	0.88	0.47	93,93,93,93	0
56	MG	14	3081	1/1	0.88	0.41	90,90,90,90	0
56	MG	14	3035	1/1	0.88	0.30	79,79,79,79	0
56	MG	14	3133	1/1	0.88	0.22	97,97,97,97	0
56	MG	1G	1611	1/1	0.88	0.28	105,105,105,105	0
56	MG	1H	3267	1/1	0.88	0.34	84,84,84,84	0
56	MG	1H	3142	1/1	0.88	0.20	88,88,88,88	0
56	MG	13	1666	1/1	0.88	0.18	105,105,105,105	0
56	MG	13	1745	1/1	0.88	0.34	121,121,121,121	0
56	MG	1H	3129	1/1	0.88	0.25	90,90,90,90	0
56	MG	14	3145	1/1	0.88	0.21	105,105,105,105	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
56	MG	14	3259	1/1	0.88	0.28	100,100,100,100	0
56	MG	13	1688	1/1	0.88	0.31	93,93,93,93	0
56	MG	14	3004	1/1	0.88	0.34	64,64,64,64	0
56	MG	1H	3274	1/1	0.88	0.35	100,100,100,100	0
56	MG	1H	3219	1/1	0.88	0.35	65,65,65,65	0
56	MG	13	1622	1/1	0.88	0.20	102,102,102,102	0
56	MG	1H	3134	1/1	0.88	0.21	57,57,57,57	0
56	MG	1H	3343	1/1	0.88	0.27	92,92,92,92	0
56	MG	1G	1629	1/1	0.88	0.11	124,124,124,124	0
56	MG	1H	3090	1/1	0.88	0.51	91,91,91,91	0
56	MG	14	3423	1/1	0.88	0.16	133,133,133,133	0
56	MG	14	3215	1/1	0.88	0.23	104,104,104,104	0
56	MG	14	3057	1/1	0.88	0.27	91,91,91,91	0
56	MG	14	3275	1/1	0.88	0.14	105,105,105,105	0
56	MG	1H	3015	1/1	0.88	0.36	71,71,71,71	0
56	MG	1H	3064	1/1	0.88	0.17	76,76,76,76	0
56	MG	1H	3444	1/1	0.88	0.16	102,102,102,102	0
56	MG	14	3279	1/1	0.88	0.25	87,87,87,87	0
56	MG	14	3224	1/1	0.88	0.26	80,80,80,80	0
56	MG	29	302	1/1	0.88	0.36	108,108,108,108	0
56	MG	1G	1667	1/1	0.88	0.17	119,119,119,119	0
56	MG	14	3119	1/1	0.88	0.46	66,66,66,66	0
56	MG	1H	3261	1/1	0.88	0.34	99,99,99,99	0
56	MG	1H	3068	1/1	0.88	0.18	98,98,98,98	0
56	MG	14	3174	1/1	0.88	0.23	93,93,93,93	0
56	MG	1H	3002	1/1	0.88	0.28	76,76,76,76	0
56	MG	1H	3264	1/1	0.88	0.23	96,96,96,96	0
56	MG	14	3289	1/1	0.88	0.21	86,86,86,86	0
56	MG	14	3068	1/1	0.88	0.40	86,86,86,86	0
56	MG	14	3302	1/1	0.89	0.31	92,92,92,92	0
56	MG	1H	3491	1/1	0.89	0.22	93,93,93,93	0
56	MG	1H	3058	1/1	0.89	0.24	107,107,107,107	0
56	MG	I8	101	1/1	0.89	0.30	84,84,84,84	0
56	MG	14	3016	1/1	0.89	0.51	71,71,71,71	0
56	MG	14	3155	1/1	0.89	0.26	76,76,76,76	0
56	MG	14	3056	1/1	0.89	0.21	92,92,92,92	0
56	MG	14	3157	1/1	0.89	0.31	76,76,76,76	0
56	MG	1H	3493	1/1	0.89	0.09	130,130,130,130	0
56	MG	13	1749	1/1	0.89	0.22	121,121,121,121	0
56	MG	13	1678	1/1	0.89	0.07	111,111,111,111	0
56	MG	1H	3332	1/1	0.89	0.39	90,90,90,90	0
56	MG	14	3262	1/1	0.89	0.09	81,81,81,81	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	14	3317	1/1	0.89	0.28	98,98,98,98	0
56	MG	14	3061	1/1	0.89	0.25	79,79,79,79	0
56	MG	14	3209	1/1	0.89	0.13	71,71,71,71	0
56	MG	14	3320	1/1	0.89	0.37	96,96,96,96	0
56	MG	14	3062	1/1	0.89	0.17	85,85,85,85	0
56	MG	1H	3217	1/1	0.89	0.13	91,91,91,91	0
56	MG	1G	1638	1/1	0.89	0.45	95,95,95,95	0
56	MG	1H	3074	1/1	0.89	0.31	80,80,80,80	0
56	MG	14	3168	1/1	0.89	0.44	67,67,67,67	0
56	MG	1H	3105	1/1	0.89	0.10	76,76,76,76	0
56	MG	1G	1643	1/1	0.89	0.56	104,104,104,104	0
56	MG	14	3331	1/1	0.89	0.23	112,112,112,112	0
56	MG	14	3340	1/1	0.89	0.11	91,91,91,91	0
56	MG	1H	3314	1/1	0.89	0.17	76,76,76,76	0
56	MG	1H	3155	1/1	0.89	0.25	78,78,78,78	0
56	MG	1H	3203	1/1	0.89	0.20	73,73,73,73	0
56	MG	14	3420	1/1	0.89	0.08	130,130,130,130	0
56	MG	1G	1680	1/1	0.89	0.11	140,140,140,140	0
56	MG	14	3229	1/1	0.89	0.26	83,83,83,83	0
56	MG	14	3231	1/1	0.89	0.22	93,93,93,93	0
56	MG	14	3079	1/1	0.89	0.22	84,84,84,84	0
56	MG	32	301	1/1	0.89	0.22	120,120,120,120	0
56	MG	14	3179	1/1	0.89	0.51	96,96,96,96	0
56	MG	1H	3247	1/1	0.89	0.15	81,81,81,81	0
56	MG	13	1751	1/1	0.89	0.26	94,94,94,94	0
56	MG	1H	3271	1/1	0.89	0.33	93,93,93,93	0
56	MG	1H	3124	1/1	0.89	0.18	72,72,72,72	0
56	MG	14	3240	1/1	0.89	0.36	76,76,76,76	0
56	MG	1H	3147	1/1	0.89	0.40	94,94,94,94	0
56	MG	1G	1623	1/1	0.89	0.14	122,122,122,122	0
56	MG	14	3294	1/1	0.89	0.21	91,91,91,91	0
56	MG	1G	1624	1/1	0.89	0.29	93,93,93,93	0
56	MG	1H	3232	1/1	0.89	0.22	80,80,80,80	0
56	MG	14	3298	1/1	0.89	0.25	115,115,115,115	0
56	MG	1H	3447	1/1	0.89	0.11	105,105,105,105	0
56	MG	13	1649	1/1	0.89	0.19	85,85,85,85	0
56	MG	1G	1641	1/1	0.90	0.10	90,90,90,90	0
56	MG	14	3193	1/1	0.90	0.29	89,89,89,89	0
56	MG	52	201	1/1	0.90	0.11	107,107,107,107	0
56	MG	1H	3037	1/1	0.90	0.27	76,76,76,76	0
56	MG	14	3147	1/1	0.90	0.24	97,97,97,97	0
56	MG	1H	3490	1/1	0.90	0.10	125,125,125,125	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	14	3150	1/1	0.90	0.30	80,80,80,80	0
56	MG	14	3097	1/1	0.90	0.20	69,69,69,69	0
56	MG	1H	3256	1/1	0.90	0.14	88,88,88,88	0
56	MG	14	3153	1/1	0.90	0.45	70,70,70,70	0
56	MG	1H	3089	1/1	0.90	0.18	58,58,58,58	0
56	MG	13	1624	1/1	0.90	0.21	95,95,95,95	0
56	MG	1G	1608	1/1	0.90	0.21	98,98,98,98	0
56	MG	14	3107	1/1	0.90	0.38	80,80,80,80	0
56	MG	13	1648	1/1	0.90	0.23	76,76,76,76	0
56	MG	1G	1612	1/1	0.90	0.16	110,110,110,110	0
56	MG	1H	3495	1/1	0.90	0.22	91,91,91,91	0
56	MG	1H	3093	1/1	0.90	0.26	81,81,81,81	0
56	MG	13	1638	1/1	0.90	0.16	115,115,115,115	0
56	MG	14	3328	1/1	0.90	0.38	111,111,111,111	0
56	MG	1H	3066	1/1	0.90	0.30	71,71,71,71	0
56	MG	16	201	1/1	0.90	0.12	79,79,79,79	0
56	MG	1H	3295	1/1	0.90	0.35	92,92,92,92	0
56	MG	1H	3330	1/1	0.90	0.14	104,104,104,104	0
56	MG	14	3356	1/1	0.90	0.13	118,118,118,118	0
56	MG	14	3398	1/1	0.90	0.13	127,127,127,127	0
56	MG	1H	3048	1/1	0.90	0.14	65,65,65,65	0
56	MG	1H	3049	1/1	0.90	0.27	60,60,60,60	0
56	MG	13	1619	1/1	0.90	0.17	103,103,103,103	0
56	MG	14	3173	1/1	0.90	0.34	87,87,87,87	0
56	MG	1H	3301	1/1	0.90	0.13	79,79,79,79	0
56	MG	14	3424	1/1	0.90	0.15	116,116,116,116	0
56	MG	1H	3181	1/1	0.90	0.35	74,74,74,74	0
56	MG	14	3285	1/1	0.90	0.38	91,91,91,91	0
56	MG	1H	3103	1/1	0.90	0.31	60,60,60,60	0
56	MG	1H	3306	1/1	0.90	0.17	81,81,81,81	0
56	MG	13	1695	1/1	0.90	0.17	112,112,112,112	0
56	MG	1H	3020	1/1	0.90	0.12	90,90,90,90	0
56	MG	14	3290	1/1	0.90	0.16	113,113,113,113	0
56	MG	1H	3108	1/1	0.90	0.23	86,86,86,86	0
56	MG	13	1660	1/1	0.90	0.09	94,94,94,94	0
56	MG	14	3241	1/1	0.90	0.20	92,92,92,92	0
56	MG	14	3033	1/1	0.90	0.28	66,66,66,66	0
56	MG	15	201	1/1	0.90	0.24	102,102,102,102	0
56	MG	1H	3084	1/1	0.90	0.20	61,61,61,61	0
56	MG	1H	3191	1/1	0.90	0.50	87,87,87,87	0
56	MG	45	201	1/1	0.90	0.27	113,113,113,113	0
56	MG	14	3086	1/1	0.90	0.22	84,84,84,84	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	2K	101	1/1	0.90	0.20	76,76,76,76	0
56	MG	14	3140	1/1	0.90	0.28	93,93,93,93	0
56	MG	P8	101	1/1	0.90	0.30	84,84,84,84	0
56	MG	1H	3253	1/1	0.90	0.30	91,91,91,91	0
57	ZN	C5	202	1/1	0.90	0.11	189,189,189,189	0
56	MG	14	3026	1/1	0.91	0.20	92,92,92,92	0
56	MG	1H	3428	1/1	0.91	0.08	123,123,123,123	0
56	MG	14	3301	1/1	0.91	0.12	83,83,83,83	0
56	MG	1H	3258	1/1	0.91	0.51	93,93,93,93	0
56	MG	1H	3303	1/1	0.91	0.21	76,76,76,76	0
56	MG	1H	3218	1/1	0.91	0.18	78,78,78,78	0
56	MG	1H	3260	1/1	0.91	0.23	76,76,76,76	0
56	MG	14	3034	1/1	0.91	0.22	69,69,69,69	0
56	MG	13	1645	1/1	0.91	0.28	86,86,86,86	0
56	MG	14	3036	1/1	0.91	0.22	67,67,67,67	0
56	MG	14	3309	1/1	0.91	0.12	87,87,87,87	0
56	MG	14	3310	1/1	0.91	0.44	96,96,96,96	0
56	MG	1H	3030	1/1	0.91	0.23	79,79,79,79	0
56	MG	4K	101	1/1	0.91	0.19	90,90,90,90	0
56	MG	1H	3223	1/1	0.91	0.15	82,82,82,82	0
56	MG	1H	3109	1/1	0.91	0.32	84,84,84,84	0
56	MG	1H	3312	1/1	0.91	0.33	79,79,79,79	0
56	MG	1H	3226	1/1	0.91	0.32	88,88,88,88	0
56	MG	1G	1625	1/1	0.91	0.08	131,131,131,131	0
56	MG	1H	3136	1/1	0.91	0.14	71,71,71,71	0
56	MG	14	3045	1/1	0.91	0.31	70,70,70,70	0
56	MG	13	1623	1/1	0.91	0.10	84,84,84,84	0
56	MG	1H	3229	1/1	0.91	0.30	83,83,83,83	0
56	MG	14	3184	1/1	0.91	0.31	94,94,94,94	0
56	MG	14	3050	1/1	0.91	0.26	60,60,60,60	0
56	MG	13	1728	1/1	0.91	0.10	131,131,131,131	0
56	MG	1G	1686	1/1	0.91	0.08	129,129,129,129	0
56	MG	1G	1688	1/1	0.91	0.23	117,117,117,117	0
56	MG	1H	3231	1/1	0.91	0.39	90,90,90,90	0
56	MG	1H	3036	1/1	0.91	0.39	61,61,61,61	0
56	MG	1H	3167	1/1	0.91	0.11	92,92,92,92	0
56	MG	16	208	1/1	0.91	0.44	94,94,94,94	0
56	MG	14	3355	1/1	0.91	0.09	102,102,102,102	0
56	MG	1H	3168	1/1	0.91	0.41	83,83,83,83	0
56	MG	14	3370	1/1	0.91	0.15	110,110,110,110	0
56	MG	3I	201	1/1	0.91	0.23	81,81,81,81	0
56	MG	14	3403	1/1	0.91	0.08	122,122,122,122	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1H	3238	1/1	0.91	0.23	84,84,84,84	0
56	MG	13	1670	1/1	0.91	0.38	88,88,88,88	0
56	MG	13	1610	1/1	0.91	0.17	79,79,79,79	0
56	MG	1H	3121	1/1	0.91	0.25	80,80,80,80	0
56	MG	14	3422	1/1	0.91	0.08	132,132,132,132	0
56	MG	14	3006	1/1	0.91	0.22	99,99,99,99	0
56	MG	16	215	1/1	0.91	0.10	113,113,113,113	0
56	MG	1H	3145	1/1	0.91	0.27	57,57,57,57	0
56	MG	1H	3244	1/1	0.91	0.10	90,90,90,90	0
56	MG	13	1706	1/1	0.91	0.26	103,103,103,103	0
56	MG	14	3072	1/1	0.91	0.33	90,90,90,90	0
56	MG	14	3073	1/1	0.91	0.25	74,74,74,74	0
56	MG	14	3013	1/1	0.91	0.13	88,88,88,88	0
56	MG	14	3075	1/1	0.91	0.27	81,81,81,81	0
56	MG	1H	3287	1/1	0.91	0.24	92,92,92,92	0
56	MG	1J	208	1/1	0.91	0.07	121,121,121,121	0
56	MG	1H	3069	1/1	0.91	0.27	89,89,89,89	0
56	MG	14	3219	1/1	0.91	0.16	102,102,102,102	0
56	MG	1H	3289	1/1	0.91	0.34	93,93,93,93	0
56	MG	13	1618	1/1	0.91	0.21	86,86,86,86	0
56	MG	14	3222	1/1	0.91	0.14	99,99,99,99	0
56	MG	1H	3209	1/1	0.91	0.12	82,82,82,82	0
56	MG	1H	3179	1/1	0.91	0.22	96,96,96,96	0
56	MG	14	3292	1/1	0.91	0.32	90,90,90,90	0
56	MG	14	3085	1/1	0.91	0.10	81,81,81,81	0
56	MG	13	1692	1/1	0.91	0.28	102,102,102,102	0
56	MG	1H	3077	1/1	0.91	0.22	67,67,67,67	0
56	MG	13	1609	1/1	0.91	0.18	83,83,83,83	0
56	MG	1H	3130	1/1	0.91	0.27	78,78,78,78	0
56	MG	1H	3072	1/1	0.92	0.27	80,80,80,80	0
56	MG	13	1661	1/1	0.92	0.08	91,91,91,91	0
56	MG	1H	3076	1/1	0.92	0.20	73,73,73,73	0
56	MG	1G	1676	1/1	0.92	0.14	121,121,121,121	0
56	MG	1H	3195	1/1	0.92	0.11	94,94,94,94	0
56	MG	1H	3166	1/1	0.92	0.18	73,73,73,73	0
56	MG	14	3206	1/1	0.92	0.23	83,83,83,83	0
56	MG	1H	3022	1/1	0.92	0.22	64,64,64,64	0
56	MG	1H	3118	1/1	0.92	0.26	76,76,76,76	0
56	MG	14	3154	1/1	0.92	0.26	86,86,86,86	0
56	MG	13	1608	1/1	0.92	0.20	91,91,91,91	0
56	MG	14	3273	1/1	0.92	0.17	87,87,87,87	0
56	MG	1H	3120	1/1	0.92	0.27	80,80,80,80	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1H	3236	1/1	0.92	0.19	77,77,77,77	0
56	MG	14	3046	1/1	0.92	0.17	88,88,88,88	0
56	MG	14	3217	1/1	0.92	0.48	82,82,82,82	0
56	MG	14	3104	1/1	0.92	0.33	81,81,81,81	0
56	MG	14	3343	1/1	0.92	0.11	89,89,89,89	0
56	MG	1H	3171	1/1	0.92	0.35	75,75,75,75	0
56	MG	14	3048	1/1	0.92	0.23	73,73,73,73	0
56	MG	13	1656	1/1	0.92	0.21	103,103,103,103	0
56	MG	14	3391	1/1	0.92	0.07	124,124,124,124	0
56	MG	1H	3239	1/1	0.92	0.17	88,88,88,88	0
56	MG	1H	3431	1/1	0.92	0.13	163,163,163,163	0
56	MG	1H	3439	1/1	0.92	0.08	92,92,92,92	0
56	MG	1G	1646	1/1	0.92	0.08	102,102,102,102	0
56	MG	1H	3441	1/1	0.92	0.07	122,122,122,122	0
56	MG	1G	1603	1/1	0.92	0.10	118,118,118,118	0
56	MG	14	3008	1/1	0.92	0.33	78,78,78,78	0
56	MG	1H	3099	1/1	0.92	0.24	69,69,69,69	0
56	MG	1H	3100	1/1	0.92	0.24	86,86,86,86	0
56	MG	14	3011	1/1	0.92	0.32	61,61,61,61	0
56	MG	1H	3148	1/1	0.92	0.08	79,79,79,79	0
56	MG	1H	3478	1/1	0.92	0.10	118,118,118,118	0
56	MG	14	3122	1/1	0.92	0.19	68,68,68,68	0
56	MG	1H	3485	1/1	0.92	0.12	121,121,121,121	0
56	MG	1H	3065	1/1	0.92	0.30	71,71,71,71	0
56	MG	1H	3082	1/1	0.92	0.19	77,77,77,77	0
56	MG	1H	3104	1/1	0.92	0.27	78,78,78,78	0
56	MG	1H	3319	1/1	0.92	0.24	90,90,90,90	0
56	MG	29	301	1/1	0.92	0.33	101,101,101,101	0
56	MG	13	1705	1/1	0.92	0.12	98,98,98,98	0
56	MG	39	301	1/1	0.92	0.16	111,111,111,111	0
56	MG	1H	3016	1/1	0.92	0.24	66,66,66,66	0
56	MG	39	303	1/1	0.92	0.41	87,87,87,87	0
56	MG	13	1740	1/1	0.92	0.15	106,106,106,106	0
56	MG	13	1718	1/1	0.92	0.12	96,96,96,96	0
56	MG	1H	3283	1/1	0.92	0.13	112,112,112,112	0
56	MG	1H	3504	1/1	0.92	0.06	138,138,138,138	0
56	MG	35	201	1/1	0.92	0.19	91,91,91,91	0
56	MG	1H	3156	1/1	0.92	0.20	110,110,110,110	0
56	MG	1H	3110	1/1	0.92	0.22	67,67,67,67	0
56	MG	14	3139	1/1	0.92	0.17	67,67,67,67	0
56	MG	1H	3071	1/1	0.92	0.05	94,94,94,94	0
56	MG	1H	3113	1/1	0.92	0.15	64,64,64,64	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1H	3257	1/1	0.92	0.17	80,80,80,80	0
56	MG	1H	3161	1/1	0.92	0.35	82,82,82,82	0
56	MG	3I	202	1/1	0.93	0.38	101,101,101,101	0
56	MG	1H	3302	1/1	0.93	0.09	90,90,90,90	0
56	MG	14	3116	1/1	0.93	0.18	73,73,73,73	0
56	MG	14	3325	1/1	0.93	0.19	89,89,89,89	0
56	MG	3I	301	1/1	0.93	0.11	92,92,92,92	0
56	MG	1H	3457	1/1	0.93	0.09	113,113,113,113	0
56	MG	1H	3144	1/1	0.93	0.16	80,80,80,80	0
56	MG	1H	3046	1/1	0.93	0.29	72,72,72,72	0
56	MG	J8	101	1/1	0.93	0.30	78,78,78,78	0
56	MG	14	3070	1/1	0.93	0.34	66,66,66,66	0
56	MG	14	3071	1/1	0.93	0.44	94,94,94,94	0
56	MG	1H	3482	1/1	0.93	0.18	119,119,119,119	0
56	MG	14	3346	1/1	0.93	0.10	92,92,92,92	0
56	MG	14	3354	1/1	0.93	0.07	126,126,126,126	0
56	MG	13	1665	1/1	0.93	0.13	91,91,91,91	0
56	MG	1H	3018	1/1	0.93	0.38	79,79,79,79	0
56	MG	14	3368	1/1	0.93	0.10	117,117,117,117	0
56	MG	1H	3019	1/1	0.93	0.27	54,54,54,54	0
56	MG	1G	1687	1/1	0.93	0.14	135,135,135,135	0
56	MG	14	3077	1/1	0.93	0.22	80,80,80,80	0
56	MG	14	3400	1/1	0.93	0.12	95,95,95,95	0
56	MG	1H	3083	1/1	0.93	0.26	92,92,92,92	0
56	MG	1H	3284	1/1	0.93	0.10	70,70,70,70	0
56	MG	13	1632	1/1	0.93	0.12	64,64,64,64	0
56	MG	1H	3202	1/1	0.93	0.25	93,93,93,93	0
56	MG	1H	3184	1/1	0.93	0.06	107,107,107,107	0
56	MG	1G	1648	1/1	0.93	0.12	100,100,100,100	0
56	MG	14	3138	1/1	0.93	0.20	73,73,73,73	0
56	MG	13	1641	1/1	0.93	0.50	88,88,88,88	0
56	MG	13	1719	1/1	0.93	0.26	95,95,95,95	0
56	MG	14	3426	1/1	0.93	0.18	67,67,67,67	0
56	MG	1H	3341	1/1	0.93	0.11	100,100,100,100	0
56	MG	14	3297	1/1	0.93	0.20	96,96,96,96	0
56	MG	1H	3342	1/1	0.93	0.11	92,92,92,92	0
56	MG	1G	1653	1/1	0.93	0.12	106,106,106,106	0
56	MG	14	3248	1/1	0.93	0.10	85,85,85,85	0
56	MG	14	3192	1/1	0.93	0.14	84,84,84,84	0
56	MG	1H	3056	1/1	0.93	0.19	72,72,72,72	0
56	MG	1H	3317	1/1	0.93	0.32	85,85,85,85	0
56	MG	1H	3345	1/1	0.93	0.14	100,100,100,100	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	13	1633	1/1	0.93	0.15	75,75,75,75	0
56	MG	14	3101	1/1	0.93	0.20	80,80,80,80	0
56	MG	1H	3367	1/1	0.93	0.12	82,82,82,82	0
56	MG	1H	3386	1/1	0.93	0.09	82,82,82,82	0
56	MG	1G	1660	1/1	0.93	0.15	97,97,97,97	0
56	MG	1H	3014	1/1	0.93	0.25	57,57,57,57	0
56	MG	1H	3407	1/1	0.93	0.08	115,115,115,115	0
56	MG	14	3015	1/1	0.93	0.13	81,81,81,81	0
56	MG	1H	3092	1/1	0.93	0.33	70,70,70,70	0
56	MG	1H	3430	1/1	0.93	0.07	116,116,116,116	0
56	MG	45	202	1/1	0.93	0.17	82,82,82,82	0
56	MG	13	1644	1/1	0.93	0.10	96,96,96,96	0
56	MG	14	3265	1/1	0.93	0.23	88,88,88,88	0
56	MG	1H	3299	1/1	0.93	0.15	71,71,71,71	0
56	MG	14	3212	1/1	0.93	0.15	104,104,104,104	0
56	MG	1H	3215	1/1	0.93	0.24	81,81,81,81	0
56	MG	14	3214	1/1	0.93	0.17	70,70,70,70	0
56	MG	16	207	1/1	0.94	0.20	84,84,84,84	0
56	MG	1H	3045	1/1	0.94	0.25	63,63,63,63	0
56	MG	14	3082	1/1	0.94	0.20	71,71,71,71	0
56	MG	1H	3214	1/1	0.94	0.11	103,103,103,103	0
56	MG	14	3084	1/1	0.94	0.21	78,78,78,78	0
56	MG	14	3352	1/1	0.94	0.08	74,74,74,74	0
56	MG	1H	3292	1/1	0.94	0.15	72,72,72,72	0
56	MG	1G	1621	1/1	0.94	0.13	88,88,88,88	0
56	MG	1H	3456	1/1	0.94	0.10	79,79,79,79	0
56	MG	14	3361	1/1	0.94	0.11	86,86,86,86	0
56	MG	14	3362	1/1	0.94	0.10	101,101,101,101	0
56	MG	1H	3163	1/1	0.94	0.40	88,88,88,88	0
56	MG	14	3237	1/1	0.94	0.14	95,95,95,95	0
56	MG	14	3372	1/1	0.94	0.09	134,134,134,134	0
56	MG	1H	3460	1/1	0.94	0.07	110,110,110,110	0
56	MG	1H	3464	1/1	0.94	0.09	133,133,133,133	0
56	MG	1H	3471	1/1	0.94	0.11	128,128,128,128	0
56	MG	14	3401	1/1	0.94	0.11	120,120,120,120	0
56	MG	13	1625	1/1	0.94	0.34	77,77,77,77	0
56	MG	14	3141	1/1	0.94	0.17	80,80,80,80	0
56	MG	14	3409	1/1	0.94	0.13	114,114,114,114	0
56	MG	1H	3475	1/1	0.94	0.19	76,76,76,76	0
56	MG	21	302	1/1	0.94	0.15	82,82,82,82	0
56	MG	14	3419	1/1	0.94	0.08	112,112,112,112	0
56	MG	14	3098	1/1	0.94	0.45	74,74,74,74	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
56	MG	14	3099	1/1	0.94	0.12	106,106,106,106	0
56	MG	14	3100	1/1	0.94	0.20	87,87,87,87	0
56	MG	13	1617	1/1	0.94	0.09	106,106,106,106	0
56	MG	13	1727	1/1	0.94	0.14	121,121,121,121	0
56	MG	78	202	1/1	0.94	0.21	97,97,97,97	0
56	MG	1H	3318	1/1	0.94	0.12	87,87,87,87	0
56	MG	14	3198	1/1	0.94	0.28	88,88,88,88	0
56	MG	13	1611	1/1	0.94	0.18	95,95,95,95	0
56	MG	1H	3005	1/1	0.94	0.18	70,70,70,70	0
56	MG	1H	3112	1/1	0.94	0.12	55,55,55,55	0
56	MG	1G	1637	1/1	0.94	0.11	104,104,104,104	0
56	MG	1H	3053	1/1	0.94	0.09	92,92,92,92	0
56	MG	1G	1639	1/1	0.94	0.17	89,89,89,89	0
56	MG	14	3111	1/1	0.94	0.25	72,72,72,72	0
56	MG	1H	3039	1/1	0.94	0.22	55,55,55,55	0
56	MG	14	3160	1/1	0.94	0.35	85,85,85,85	0
56	MG	1H	3040	1/1	0.94	0.20	78,78,78,78	0
56	MG	14	3211	1/1	0.94	0.12	93,93,93,93	0
56	MG	1H	3385	1/1	0.94	0.15	75,75,75,75	0
56	MG	1G	1682	1/1	0.94	0.14	141,141,141,141	0
56	MG	1G	1683	1/1	0.94	0.16	129,129,129,129	0
56	MG	13	1747	1/1	0.94	0.19	103,103,103,103	0
56	MG	1H	3159	1/1	0.94	0.15	77,77,77,77	0
56	MG	1H	3285	1/1	0.94	0.18	88,88,88,88	0
56	MG	1H	3417	1/1	0.94	0.08	90,90,90,90	0
56	MG	1H	3424	1/1	0.94	0.06	119,119,119,119	0
56	MG	14	3170	1/1	0.94	0.20	77,77,77,77	0
56	MG	1H	3042	1/1	0.94	0.12	53,53,53,53	0
56	MG	1H	3308	1/1	0.94	0.23	90,90,90,90	0
56	MG	1H	3043	1/1	0.94	0.12	72,72,72,72	0
56	MG	1H	3212	1/1	0.94	0.19	61,61,61,61	0
56	MG	14	3149	1/1	0.95	0.14	79,79,79,79	0
56	MG	1H	3189	1/1	0.95	0.38	81,81,81,81	0
56	MG	11	301	1/1	0.95	0.30	62,62,62,62	0
56	MG	1H	3190	1/1	0.95	0.07	77,77,77,77	0
56	MG	1H	3174	1/1	0.95	0.37	78,78,78,78	0
56	MG	1H	3476	1/1	0.95	0.17	93,93,93,93	0
56	MG	14	3374	1/1	0.95	0.06	113,113,113,113	0
56	MG	1H	3254	1/1	0.95	0.28	80,80,80,80	0
56	MG	13	1643	1/1	0.95	0.20	78,78,78,78	0
56	MG	14	3024	1/1	0.95	0.27	73,73,73,73	0
56	MG	1H	3348	1/1	0.95	0.10	84,84,84,84	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
56	MG	1H	3487	1/1	0.95	0.17	126,126,126,126	0
56	MG	14	3205	1/1	0.95	0.07	72,72,72,72	0
56	MG	14	3406	1/1	0.95	0.07	99,99,99,99	0
56	MG	14	3407	1/1	0.95	0.06	116,116,116,116	0
56	MG	14	3069	1/1	0.95	0.17	63,63,63,63	0
56	MG	14	3411	1/1	0.95	0.07	104,104,104,104	0
56	MG	1H	3359	1/1	0.95	0.15	83,83,83,83	0
56	MG	14	3415	1/1	0.95	0.07	107,107,107,107	0
56	MG	14	3028	1/1	0.95	0.14	98,98,98,98	0
56	MG	1H	3025	1/1	0.95	0.47	78,78,78,78	0
56	MG	1H	3001	1/1	0.95	0.20	64,64,64,64	0
56	MG	1H	3279	1/1	0.95	0.15	80,80,80,80	0
56	MG	13	1722	1/1	0.95	0.07	85,85,85,85	0
56	MG	1G	1684	1/1	0.95	0.08	124,124,124,124	0
56	MG	1H	3107	1/1	0.95	0.35	85,85,85,85	0
56	MG	1H	3073	1/1	0.95	0.13	88,88,88,88	0
56	MG	1H	3096	1/1	0.95	0.14	57,57,57,57	0
56	MG	1H	3501	1/1	0.95	0.22	107,107,107,107	0
56	MG	1H	3426	1/1	0.95	0.14	92,92,92,92	0
56	MG	1H	3503	1/1	0.95	0.06	116,116,116,116	0
56	MG	1G	1609	1/1	0.95	0.09	97,97,97,97	0
56	MG	1H	3085	1/1	0.95	0.14	62,62,62,62	0
56	MG	1H	3506	1/1	0.95	0.30	57,57,57,57	0
56	MG	1H	3032	1/1	0.95	0.33	78,78,78,78	0
56	MG	14	3321	1/1	0.95	0.34	99,99,99,99	0
56	MG	14	3087	1/1	0.95	0.12	82,82,82,82	0
56	MG	1H	3220	1/1	0.95	0.13	124,124,124,124	0
56	MG	1H	3434	1/1	0.95	0.13	130,130,130,130	0
56	MG	14	3228	1/1	0.95	0.38	86,86,86,86	0
56	MG	1H	3126	1/1	0.95	0.14	79,79,79,79	0
56	MG	1H	3050	1/1	0.95	0.17	80,80,80,80	0
56	MG	1H	3067	1/1	0.95	0.16	84,84,84,84	0
56	MG	1G	1619	1/1	0.95	0.20	72,72,72,72	0
56	MG	1H	3224	1/1	0.95	0.14	82,82,82,82	0
56	MG	1H	3448	1/1	0.95	0.23	97,97,97,97	0
56	MG	14	3337	1/1	0.95	0.11	76,76,76,76	0
56	MG	1H	3101	1/1	0.95	0.17	49,49,49,49	0
56	MG	1H	3339	1/1	0.95	0.07	90,90,90,90	0
56	MG	1H	3051	1/1	0.95	0.23	53,53,53,53	0
56	MG	1H	3207	1/1	0.95	0.31	60,60,60,60	0
56	MG	1H	3467	1/1	0.95	0.06	106,106,106,106	0
56	MG	1H	3469	1/1	0.95	0.11	106,106,106,106	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1H	3057	1/1	0.96	0.15	72,72,72,72	0
56	MG	1H	3409	1/1	0.96	0.09	76,76,76,76	0
56	MG	1H	3470	1/1	0.96	0.05	99,99,99,99	0
56	MG	1H	3415	1/1	0.96	0.06	99,99,99,99	0
56	MG	14	3131	1/1	0.96	0.17	56,56,56,56	0
56	MG	14	3200	1/1	0.96	0.36	85,85,85,85	0
56	MG	1H	3249	1/1	0.96	0.60	97,97,97,97	0
56	MG	1H	3419	1/1	0.96	0.10	94,94,94,94	0
56	MG	14	3134	1/1	0.96	0.05	103,103,103,103	0
56	MG	1H	3297	1/1	0.96	0.09	86,86,86,86	0
56	MG	14	3242	1/1	0.96	0.09	94,94,94,94	0
56	MG	13	1741	1/1	0.96	0.07	118,118,118,118	0
56	MG	14	3418	1/1	0.96	0.12	130,130,130,130	0
56	MG	13	1743	1/1	0.96	0.14	108,108,108,108	0
56	MG	1H	3088	1/1	0.96	0.28	52,52,52,52	0
56	MG	1H	3347	1/1	0.96	0.10	57,57,57,57	0
56	MG	1H	3488	1/1	0.96	0.15	114,114,114,114	0
56	MG	1H	3060	1/1	0.96	0.18	74,74,74,74	0
56	MG	1H	3349	1/1	0.96	0.10	69,69,69,69	0
56	MG	1H	3351	1/1	0.96	0.08	65,65,65,65	0
56	MG	1H	3291	1/1	0.96	0.35	77,77,77,77	0
56	MG	1H	3325	1/1	0.96	0.15	86,86,86,86	0
56	MG	1H	3374	1/1	0.96	0.07	71,71,71,71	0
56	MG	1G	1678	1/1	0.96	0.13	108,108,108,108	0
56	MG	1H	3497	1/1	0.96	0.05	119,119,119,119	0
56	MG	1G	1681	1/1	0.96	0.13	133,133,133,133	0
56	MG	1H	3453	1/1	0.96	0.07	70,70,70,70	0
56	MG	1H	3455	1/1	0.96	0.12	99,99,99,99	0
56	MG	13	1734	1/1	0.96	0.13	133,133,133,133	0
56	MG	1G	1685	1/1	0.96	0.06	112,112,112,112	0
56	MG	14	3223	1/1	0.96	0.08	81,81,81,81	0
56	MG	1H	3205	1/1	0.96	0.10	64,64,64,64	0
56	MG	14	3088	1/1	0.96	0.19	66,66,66,66	0
56	MG	1H	3458	1/1	0.96	0.06	93,93,93,93	0
56	MG	14	3266	1/1	0.96	0.14	80,80,80,80	0
56	MG	1H	3391	1/1	0.96	0.06	96,96,96,96	0
56	MG	14	3371	1/1	0.96	0.06	101,101,101,101	0
56	MG	L8	101	1/1	0.96	0.15	85,85,85,85	0
56	MG	1H	3505	1/1	0.96	0.06	112,112,112,112	0
56	MG	14	3378	1/1	0.96	0.07	101,101,101,101	0
56	MG	14	3383	1/1	0.96	0.11	98,98,98,98	0
56	MG	14	3386	1/1	0.96	0.10	105,105,105,105	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	14	3390	1/1	0.96	0.11	94,94,94,94	0
56	MG	1H	3078	1/1	0.96	0.07	70,70,70,70	0
56	MG	14	3393	1/1	0.96	0.08	80,80,80,80	0
56	MG	14	3397	1/1	0.96	0.09	101,101,101,101	0
56	MG	14	3396	1/1	0.97	0.09	119,119,119,119	0
56	MG	1H	3390	1/1	0.97	0.10	83,83,83,83	0
56	MG	1H	3449	1/1	0.97	0.06	78,78,78,78	0
56	MG	41	201	1/1	0.97	0.09	89,89,89,89	0
56	MG	1H	3496	1/1	0.97	0.06	131,131,131,131	0
56	MG	78	201	1/1	0.97	0.06	67,67,67,67	0
56	MG	14	3404	1/1	0.97	0.04	97,97,97,97	0
56	MG	1H	3233	1/1	0.97	0.12	65,65,65,65	0
56	MG	1H	3350	1/1	0.97	0.06	64,64,64,64	0
56	MG	1H	3499	1/1	0.97	0.08	110,110,110,110	0
56	MG	I8	102	1/1	0.97	0.24	64,64,64,64	0
56	MG	14	3410	1/1	0.97	0.20	96,96,96,96	0
56	MG	1H	3399	1/1	0.97	0.07	59,59,59,59	0
56	MG	1H	3405	1/1	0.97	0.07	86,86,86,86	0
56	MG	1H	3252	1/1	0.97	0.05	69,69,69,69	0
56	MG	1H	3408	1/1	0.97	0.05	87,87,87,87	0
56	MG	14	3417	1/1	0.97	0.14	148,148,148,148	0
56	MG	1H	3463	1/1	0.97	0.12	113,113,113,113	0
56	MG	1H	3353	1/1	0.97	0.10	77,77,77,77	0
56	MG	1H	3466	1/1	0.97	0.14	94,94,94,94	0
56	MG	14	3421	1/1	0.97	0.12	130,130,130,130	0
56	MG	1H	3354	1/1	0.97	0.07	64,64,64,64	0
56	MG	1H	3358	1/1	0.97	0.06	76,76,76,76	0
56	MG	1H	3418	1/1	0.97	0.14	134,134,134,134	0
56	MG	1G	1679	1/1	0.97	0.05	108,108,108,108	0
56	MG	1H	3075	1/1	0.97	0.06	59,59,59,59	0
56	MG	1H	3363	1/1	0.97	0.06	71,71,71,71	0
56	MG	14	3344	1/1	0.97	0.06	82,82,82,82	0
56	MG	1G	1610	1/1	0.97	0.08	115,115,115,115	0
56	MG	14	3350	1/1	0.97	0.06	80,80,80,80	0
56	MG	13	1725	1/1	0.97	0.05	102,102,102,102	0
56	MG	14	3257	1/1	0.97	0.10	84,84,84,84	0
56	MG	1H	3369	1/1	0.97	0.06	92,92,92,92	0
56	MG	1H	3372	1/1	0.97	0.05	79,79,79,79	0
56	MG	1J	209	1/1	0.97	0.07	125,125,125,125	0
56	MG	1H	3479	1/1	0.97	0.04	126,126,126,126	0
56	MG	1H	3480	1/1	0.97	0.04	109,109,109,109	0
56	MG	14	3363	1/1	0.97	0.11	117,117,117,117	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1H	3035	1/1	0.97	0.23	55,55,55,55	0
56	MG	14	3032	1/1	0.97	0.14	52,52,52,52	0
56	MG	1H	3432	1/1	0.97	0.06	113,113,113,113	0
56	MG	1H	3376	1/1	0.97	0.15	96,96,96,96	0
56	MG	1H	3381	1/1	0.97	0.06	89,89,89,89	0
56	MG	14	3376	1/1	0.97	0.05	119,119,119,119	0
56	MG	1H	3131	1/1	0.97	0.05	56,56,56,56	0
56	MG	1H	3442	1/1	0.97	0.12	57,57,57,57	0
56	MG	1H	3123	1/1	0.97	0.11	68,68,68,68	0
56	MG	14	3388	1/1	0.97	0.06	85,85,85,85	0
56	MG	14	3389	1/1	0.97	0.06	72,72,72,72	0
56	MG	14	3230	1/1	0.97	0.06	86,86,86,86	0
56	MG	14	3001	1/1	0.97	0.05	66,66,66,66	0
56	MG	1H	3387	1/1	0.97	0.06	70,70,70,70	0
57	ZN	5A	101	1/1	0.97	0.05	172,172,172,172	0
56	MG	14	3394	1/1	0.97	0.09	93,93,93,93	0
56	MG	14	3387	1/1	0.98	0.06	76,76,76,76	0
56	MG	13	1671	1/1	0.98	0.04	102,102,102,102	0
56	MG	1H	3468	1/1	0.98	0.04	95,95,95,95	0
56	MG	1H	3375	1/1	0.98	0.06	76,76,76,76	0
56	MG	13	1729	1/1	0.98	0.05	109,109,109,109	0
56	MG	1H	3420	1/1	0.98	0.04	84,84,84,84	0
56	MG	1H	3472	1/1	0.98	0.10	98,98,98,98	0
56	MG	14	3395	1/1	0.98	0.06	96,96,96,96	0
56	MG	1H	3423	1/1	0.98	0.04	102,102,102,102	0
56	MG	1H	3474	1/1	0.98	0.14	124,124,124,124	0
56	MG	1H	3377	1/1	0.98	0.13	97,97,97,97	0
56	MG	1H	3378	1/1	0.98	0.06	94,94,94,94	0
56	MG	1H	3477	1/1	0.98	0.04	108,108,108,108	0
56	MG	13	1730	1/1	0.98	0.07	113,113,113,113	0
56	MG	1H	3429	1/1	0.98	0.11	102,102,102,102	0
56	MG	1H	3382	1/1	0.98	0.13	58,58,58,58	0
56	MG	13	1731	1/1	0.98	0.05	91,91,91,91	0
56	MG	1H	3483	1/1	0.98	0.04	110,110,110,110	0
56	MG	1H	3355	1/1	0.98	0.06	64,64,64,64	0
56	MG	1H	3486	1/1	0.98	0.08	98,98,98,98	0
56	MG	88	202	1/1	0.98	0.07	77,77,77,77	0
56	MG	14	3412	1/1	0.98	0.04	108,108,108,108	0
56	MG	G8	201	1/1	0.98	0.06	83,83,83,83	0
56	MG	14	3414	1/1	0.98	0.07	93,93,93,93	0
56	MG	1H	3433	1/1	0.98	0.06	76,76,76,76	0
56	MG	1H	3044	1/1	0.98	0.13	68,68,68,68	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1H	3489	1/1	0.98	0.04	69,69,69,69	0
56	MG	1H	3436	1/1	0.98	0.05	79,79,79,79	0
56	MG	1H	3437	1/1	0.98	0.05	109,109,109,109	0
56	MG	14	3336	1/1	0.98	0.04	88,88,88,88	0
56	MG	13	1616	1/1	0.98	0.08	82,82,82,82	0
56	MG	14	3339	1/1	0.98	0.05	74,74,74,74	0
56	MG	13	1735	1/1	0.98	0.05	96,96,96,96	0
56	MG	1H	3364	1/1	0.98	0.10	80,80,80,80	0
56	MG	1H	3443	1/1	0.98	0.05	76,76,76,76	0
56	MG	14	3345	1/1	0.98	0.05	84,84,84,84	0
56	MG	1H	3397	1/1	0.98	0.06	77,77,77,77	0
56	MG	1H	3445	1/1	0.98	0.05	83,83,83,83	0
56	MG	1H	3398	1/1	0.98	0.08	92,92,92,92	0
56	MG	1H	3365	1/1	0.98	0.07	69,69,69,69	0
56	MG	1H	3400	1/1	0.98	0.06	61,61,61,61	0
56	MG	1H	3451	1/1	0.98	0.05	87,87,87,87	0
56	MG	14	3359	1/1	0.98	0.09	114,114,114,114	0
56	MG	14	3360	1/1	0.98	0.08	92,92,92,92	0
56	MG	1H	3401	1/1	0.98	0.06	87,87,87,87	0
56	MG	1J	210	1/1	0.98	0.04	109,109,109,109	0
56	MG	1H	3454	1/1	0.98	0.06	85,85,85,85	0
56	MG	1H	3404	1/1	0.98	0.05	62,62,62,62	0
56	MG	14	3364	1/1	0.98	0.04	87,87,87,87	0
56	MG	14	3366	1/1	0.98	0.14	88,88,88,88	0
56	MG	14	3367	1/1	0.98	0.11	111,111,111,111	0
56	MG	1H	3366	1/1	0.98	0.07	60,60,60,60	0
56	MG	14	3369	1/1	0.98	0.05	105,105,105,105	0
56	MG	13	1746	1/1	0.98	0.05	110,110,110,110	0
56	MG	13	1736	1/1	0.98	0.09	102,102,102,102	0
56	MG	1H	3370	1/1	0.98	0.10	84,84,84,84	0
56	MG	1H	3461	1/1	0.98	0.06	110,110,110,110	0
56	MG	14	3375	1/1	0.98	0.05	102,102,102,102	0
56	MG	1H	3462	1/1	0.98	0.05	75,75,75,75	0
56	MG	1H	3412	1/1	0.98	0.04	64,64,64,64	0
56	MG	14	3379	1/1	0.98	0.05	77,77,77,77	0
56	MG	14	3380	1/1	0.98	0.08	97,97,97,97	0
57	ZN	3E	301	1/1	0.98	0.30	115,115,115,115	0
56	MG	14	3382	1/1	0.98	0.15	86,86,86,86	0
56	MG	1H	3413	1/1	0.98	0.06	77,77,77,77	0
56	MG	13	1737	1/1	0.98	0.12	72,72,72,72	0
56	MG	1H	3383	1/1	0.99	0.04	67,67,67,67	0
56	MG	14	3332	1/1	0.99	0.10	72,72,72,72	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	14	3333	1/1	0.99	0.05	73,73,73,73	0
56	MG	14	3334	1/1	0.99	0.05	91,91,91,91	0
56	MG	14	3335	1/1	0.99	0.03	73,73,73,73	0
56	MG	1H	3481	1/1	0.99	0.03	70,70,70,70	0
56	MG	14	3399	1/1	0.99	0.04	78,78,78,78	0
56	MG	1H	3410	1/1	0.99	0.04	73,73,73,73	0
56	MG	14	3338	1/1	0.99	0.04	68,68,68,68	0
56	MG	14	3402	1/1	0.99	0.06	99,99,99,99	0
56	MG	1H	3384	1/1	0.99	0.08	59,59,59,59	0
56	MG	1H	3484	1/1	0.99	0.09	79,79,79,79	0
56	MG	14	3341	1/1	0.99	0.03	78,78,78,78	0
56	MG	14	3342	1/1	0.99	0.06	80,80,80,80	0
56	MG	1H	3446	1/1	0.99	0.04	74,74,74,74	0
56	MG	14	3408	1/1	0.99	0.06	79,79,79,79	0
56	MG	13	1726	1/1	0.99	0.10	90,90,90,90	0
56	MG	1H	3414	1/1	0.99	0.05	65,65,65,65	0
56	MG	1H	3368	1/1	0.99	0.09	79,79,79,79	0
56	MG	14	3347	1/1	0.99	0.04	85,85,85,85	0
56	MG	14	3348	1/1	0.99	0.08	71,71,71,71	0
56	MG	14	3349	1/1	0.99	0.08	71,71,71,71	0
56	MG	1H	3450	1/1	0.99	0.05	66,66,66,66	0
56	MG	14	3351	1/1	0.99	0.12	60,60,60,60	0
56	MG	1H	3416	1/1	0.99	0.05	78,78,78,78	0
56	MG	14	3353	1/1	0.99	0.18	91,91,91,91	0
56	MG	14	3096	1/1	0.99	0.04	77,77,77,77	0
56	MG	1H	3452	1/1	0.99	0.12	65,65,65,65	0
56	MG	1H	3356	1/1	0.99	0.05	58,58,58,58	0
56	MG	14	3357	1/1	0.99	0.06	80,80,80,80	0
56	MG	14	3358	1/1	0.99	0.04	85,85,85,85	0
56	MG	1H	3389	1/1	0.99	0.07	69,69,69,69	0
56	MG	1H	3357	1/1	0.99	0.04	57,57,57,57	0
56	MG	1H	3371	1/1	0.99	0.03	91,91,91,91	0
56	MG	1H	3421	1/1	0.99	0.04	62,62,62,62	0
56	MG	1H	3422	1/1	0.99	0.09	91,91,91,91	0
56	MG	1G	1677	1/1	0.99	0.07	91,91,91,91	0
56	MG	14	3365	1/1	0.99	0.04	80,80,80,80	0
56	MG	1H	3459	1/1	0.99	0.03	81,81,81,81	0
56	MG	1H	3392	1/1	0.99	0.08	65,65,65,65	0
56	MG	1H	3393	1/1	0.99	0.06	60,60,60,60	0
56	MG	1H	3425	1/1	0.99	0.09	95,95,95,95	0
56	MG	13	1724	1/1	0.99	0.05	102,102,102,102	0
56	MG	1H	3396	1/1	0.99	0.12	87,87,87,87	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1H	3465	1/1	0.99	0.04	83,83,83,83	0
56	MG	14	3373	1/1	0.99	0.04	81,81,81,81	0
56	MG	1H	3373	1/1	0.99	0.04	63,63,63,63	0
56	MG	13	1723	1/1	0.99	0.07	105,105,105,105	0
56	MG	1H	3360	1/1	0.99	0.07	58,58,58,58	0
56	MG	14	3377	1/1	0.99	0.05	82,82,82,82	0
56	MG	1H	3362	1/1	0.99	0.03	61,61,61,61	0
56	MG	13	1742	1/1	0.99	0.08	82,82,82,82	0
56	MG	1H	3402	1/1	0.99	0.05	81,81,81,81	0
56	MG	14	3381	1/1	0.99	0.13	101,101,101,101	0
56	MG	1H	3435	1/1	0.99	0.06	72,72,72,72	0
56	MG	1H	3352	1/1	0.99	0.07	61,61,61,61	0
56	MG	14	3384	1/1	0.99	0.06	60,60,60,60	0
56	MG	14	3385	1/1	0.99	0.06	73,73,73,73	0
56	MG	1H	3379	1/1	0.99	0.07	74,74,74,74	0
56	MG	1H	3438	1/1	0.99	0.05	82,82,82,82	0
56	MG	1H	3406	1/1	0.99	0.10	77,77,77,77	0
57	ZN	5I	101	1/1	0.99	0.04	114,114,114,114	0
56	MG	1H	3440	1/1	0.99	0.04	83,83,83,83	0
57	ZN	32	302	1/1	0.99	0.24	131,131,131,131	0
56	MG	13	1733	1/1	0.99	0.06	102,102,102,102	0
56	MG	13	1738	1/1	0.99	0.05	77,77,77,77	0
56	MG	1H	3427	1/1	1.00	0.04	75,75,75,75	0
56	MG	1H	3380	1/1	1.00	0.06	61,61,61,61	0
56	MG	13	1732	1/1	1.00	0.03	81,81,81,81	0
56	MG	1H	3388	1/1	1.00	0.03	65,65,65,65	0
56	MG	1H	3403	1/1	1.00	0.02	73,73,73,73	0
56	MG	14	3392	1/1	1.00	0.02	70,70,70,70	0
56	MG	1H	3361	1/1	1.00	0.06	56,56,56,56	0
56	MG	1H	3411	1/1	1.00	0.07	80,80,80,80	0
56	MG	1H	3394	1/1	1.00	0.02	62,62,62,62	0

## 5.5 Other polymers [\(i\)](#)

There are no such residues in this entry.