



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 30, 2026 – 04:49 PM UTC

PDB ID : 4WQ1 / pdb_00004wq1
Title : Complex of 70S ribosome with tRNA-Tyr and mRNA with C-A mismatch in the first position in the A-site.
Authors : Rozov, A.; Demeshkina, N.; Yusupov, M.; Yusupova, G.
Deposited on : 2014-10-21
Resolution : 3.10 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	FAILED
Mogul	:	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

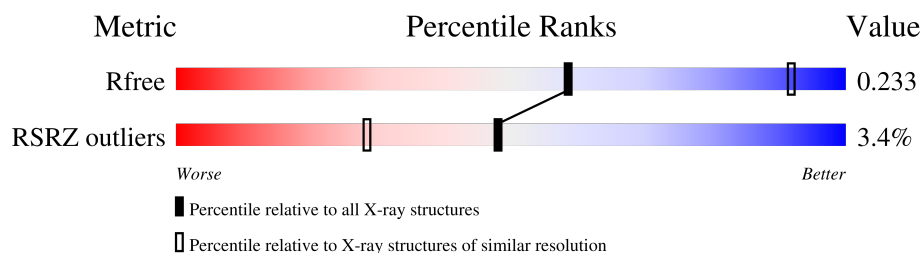
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.10 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	1456 (3.10-3.10)
RSRZ outliers	180081	1456 (3.10-3.10)

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
60	MG	13	1616	-	-	-	X
60	MG	13	1655	-	-	-	X
60	MG	14	3170	-	-	-	X
60	MG	14	3261	-	-	-	X
60	MG	14	3290	-	-	-	X
60	MG	1G	1689	-	-	-	X
60	MG	1H	3107	-	-	-	X
60	MG	1J	204	-	-	-	X

2 Entry composition

There are 62 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
1	13	1498	Total	C	N	O	P	0	0	0
			32207	14334	5973	10402	1498			

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	2I	119	Total	C	N	O	S	0	0	0
			884	549	168	164	3			
11	2A	119	Total	C	N	O	S	0	0	0
			884	549	168	164	3			

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	4I	116	Total	C	N	O	S	0	0	0
			928	574	191	161	2			
13	4A	117	Total	C	N	O	S	0	0	0
			933	577	192	162	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	5I	61	Total	C	N	O	S	0	0	0
			498	316	105	72	5			
14	5A	58	Total	C	N	O	S	0	0	0
			475	303	99	69	4			

- 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	83	Total	C	N	O	S	0	0	0
			665	424	124	115	2			
19	AA	82	Total	C	N	O	S	0	0	0
			640	407	118	113	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			
20	BA	99	Total	C	N	O	S	0	0	0
			762	470	162	128	2			

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

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

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

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

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
22	1K	85	Total	C	N	O	P	S	0	0	0
			1825	822	323	593	85	2			
22	3K	74	Total	C	N	O	P	S	0	0	0
			1595	719	286	514	74	2			
22	1L	74	Total	C	N	O	P	S	0	0	0
			1595	719	286	514	74	2			
22	3L	75	Total	C	N	O	P	S	0	0	0
			1615	728	288	522	75	2			

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

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
23	2K	77	Total	C	N	O	P	S	0	0	0
			1645	734	298	535	77	1			
23	2L	77	Total	C	N	O	P	S	0	0	0
			1645	734	298	535	77	1			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
2K	18	C	U	conflict	GB 675817920
2L	18	C	U	conflict	GB 675817920

- Molecule 24 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	4K	15	Total	C	N	O	P	0	0	0
			325	147	68	95	15			
24	4L	16	Total	C	N	O	P	0	0	0
			347	157	73	101	16			

- Molecule 25 is a RNA chain called 23S ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
25	1H	2912	Total	C	N	O	P	0	0	0
			62707	27911	11722	20163	2911			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
25	14	2907	Total	C	N	O	P	0	0	0
			62605	27865	11708	20126	2906			

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 26 is a RNA chain called 5S ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	16	122	Total	C	N	O	P	0	0	0
			2617	1166	486	844	121			
26	1J	122	Total	C	N	O	P	0	0	0
			2617	1166	486	844	121			

- Molecule 27 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
27	11	272	Total	C	N	O	S	0	0	0
			2115	1335	420	357	3			

- Molecule 28 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
28	21	205	Total	C	N	O	S	0	0	0
			1568	991	300	271	6			
28	29	205	Total	C	N	O	S	0	0	0
			1568	991	300	271	6			

- Molecule 29 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
29	31	202	Total	C	N	O	S	0	0	0
			1585	1011	297	275	2			

- Molecule 30 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
30	41	181	Total	C	N	O	S	0	0	0
			1473	942	268	259	4			
30	49	181	Total	C	N	O	S	0	0	0
			1473	942	268	259	4			

- Molecule 31 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
31	51	174	Total	C	N	O	S	0	0	0
			1336	848	251	236	1			
31	59	171	Total	C	N	O	S	0	0	0
			1316	835	247	233	1			

- Molecule 32 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
32	61	146	Total	C	N	O	S	0	0	0
			1136	726	201	208	1			
32	69	146	Total	C	N	O	S	0	0	0
			1136	726	201	208	1			

- Molecule 33 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
33	58	138	Total	C	N	O	S	0	0	0
			1104	712	206	182	4			
33	15	138	Total	C	N	O	S	0	0	0
			1104	712	206	182	4			

- Molecule 34 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
34	68	122	Total	C	N	O	S	0	0	0
			932	588	171	169	4			
34	25	122	Total	C	N	O	S	0	0	0
			932	588	171	169	4			

- Molecule 35 is a protein called 50S ribosomal protein L15.

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

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

- Molecule 36 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
36	88	141	Total	C	N	O	S	0	0	0
			1121	715	212	187	7			
36	45	141	Total	C	N	O	S	0	0	0
			1121	715	212	187	7			

- Molecule 37 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
37	98	118	Total	C	N	O	S	0	0	0
			967	604	203	159	1			
37	55	117	Total	C	N	O		0	0	0
			959	599	202	158				

- Molecule 38 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
38	A8	111	Total	C	N	O	0	0	0
			881	556	176	149			
38	65	111	Total	C	N	O	0	0	0
			881	556	176	149			

- Molecule 39 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
39	B8	136	Total	C	N	O	0	0	0
			1133	705	233	195			
39	75	137	Total	C	N	O	S	0	0
			1141	710	234	196	1		

- Molecule 40 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
40	C8	117	Total 963	C 610	N 202	O 150	S 1	0	0	0
40	85	117	Total 963	C 610	N 202	O 150	S 1	0	0	0

- Molecule 41 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
41	D8	101	Total	C	N	O	S	0	0	0
			778	501	142	134	1			
41	95	101	Total	C	N	O	S	0	0	0
			778	501	142	134	1			

- Molecule 42 is a protein called 50S ribosomal protein L22.

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

- Molecule 43 is a protein called 50S ribosomal protein L23.

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

- Molecule 44 is a protein called 50S ribosomal protein L24.

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

- Molecule 45 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
45	H8	175	Total	C	N	O	S	0	0	0
			1397	892	251	251	3			

- Molecule 46 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
46	I8	77	Total	C	N	O	S	0	0	0
			612	379	129	103	1			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
46	E5	77	Total	C	N	O	S	0	0	0
			612	379	129	103	1			

- Molecule 47 is a protein called 50S ribosomal protein L28.

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

- Molecule 48 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
48	K8	66	Total	C	N	O	S	0	0	0
			558	346	113	98	1			
48	G5	66	Total	C	N	O	S	0	0	0
			558	346	113	98	1			

- Molecule 49 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
49	L8	59	Total	C	N	O	S	0	0	0
			468	298	90	80				
49	H5	59	Total	C	N	O	S	0	0	0
			468	298	90	80				

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

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

- Molecule 51 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
51	N8	59	Total	C	N	O	S	0	0	0
			458	288	90	75	5			
51	J5	58	Total	C	N	O	S	0	0	0
			453	285	89	74	5			

- Molecule 52 is a protein called 50S ribosomal protein L33.

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

- Molecule 53 is a protein called 50S ribosomal protein L34.

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

- Molecule 54 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
54	Q8	62	Total	C	N	O	S	0	0	0
			442	281	83	76	2			

- Molecule 55 is a RNA chain called 16S ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
55	1G	1498	Total	C	N	O	P	0	0	0
			32204	14334	5973	10400	1497			

- Molecule 56 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
56	19	273	Total	C	N	O	S	0	0	0
			2120	1338	421	358	3			

- Molecule 57 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
57	39	208	Total	C	N	O	S	0	0	0
			1627	1037	304	283	3			

- Molecule 58 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
58	D5	179	Total	C	N	O	S	0	0	0
			1428	911	255	259	3			

- Molecule 59 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
59	M5	60	Total	C	N	O	S	0	0	0
			480	306	98	74	2			

- Molecule 60 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
60	13	140	Total	Mg	0	0
			140	140		
60	3I	1	Total	Mg	0	0
			1	1		
60	4I	1	Total	Mg	0	0
			1	1		
60	5I	1	Total	Mg	0	0
			1	1		
60	1K	1	Total	Mg	0	0
			1	1		
60	2K	4	Total	Mg	0	0
			4	4		
60	3K	1	Total	Mg	0	0
			1	1		
60	1H	438	Total	Mg	0	0
			438	438		
60	16	12	Total	Mg	0	0
			12	12		
60	11	2	Total	Mg	0	0
			2	2		
60	21	2	Total	Mg	0	0
			2	2		
60	41	1	Total	Mg	0	0
			1	1		
60	68	1	Total	Mg	0	0
			1	1		
60	78	3	Total	Mg	0	0
			3	3		
60	88	2	Total	Mg	0	0
			2	2		
60	98	2	Total	Mg	0	0
			2	2		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
60	B8	1	Total 1	Mg 1	0	0
60	C8	1	Total 1	Mg 1	0	0
60	I8	2	Total 2	Mg 2	0	0
60	K8	1	Total 1	Mg 1	0	0
60	P8	1	Total 1	Mg 1	0	0
60	1G	104	Total 104	Mg 104	0	0
60	52	1	Total 1	Mg 1	0	0
60	2L	3	Total 3	Mg 3	0	0
60	14	386	Total 386	Mg 386	0	0
60	1J	7	Total 7	Mg 7	0	0
60	19	1	Total 1	Mg 1	0	0
60	29	2	Total 2	Mg 2	0	0
60	39	1	Total 1	Mg 1	0	0
60	49	1	Total 1	Mg 1	0	0
60	25	1	Total 1	Mg 1	0	0
60	45	3	Total 3	Mg 3	0	0
60	85	1	Total 1	Mg 1	0	0
60	C5	1	Total 1	Mg 1	0	0
60	E5	1	Total 1	Mg 1	0	0

- Molecule 61 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
61	3E	1	Total 1	Zn 1	0	0
61	5I	1	Total 1	Zn 1	0	0
61	G8	1	Total 1	Zn 1	0	0
61	32	1	Total 1	Zn 1	0	0
61	5A	1	Total 1	Zn 1	0	0
61	C5	1	Total 1	Zn 1	0	0

- Molecule 62 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
62	13	125	Total 125	O 125	0	0
62	3E	4	Total 4	O 4	0	0
62	3I	1	Total 1	O 1	0	0
62	5I	2	Total 2	O 2	0	0
62	7I	1	Total 1	O 1	0	0
62	1K	4	Total 4	O 4	0	0
62	3K	1	Total 1	O 1	0	0
62	4K	1	Total 1	O 1	0	0
62	1H	738	Total 738	O 738	0	0
62	16	15	Total 15	O 15	0	0
62	11	10	Total 10	O 10	0	0
62	21	4	Total 4	O 4	0	0
62	31	5	Total 5	O 5	0	0
62	78	3	Total 3	O 3	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
62	98	3	Total O 3 3	0	0
62	B8	1	Total O 1 1	0	0
62	C8	2	Total O 2 2	0	0
62	D8	2	Total O 2 2	0	0
62	G8	2	Total O 2 2	0	0
62	L8	3	Total O 3 3	0	0
62	Q8	1	Total O 1 1	0	0
62	1G	74	Total O 74 74	0	0
62	82	1	Total O 1 1	0	0
62	BA	2	Total O 2 2	0	0
62	4L	1	Total O 1 1	0	0
62	14	446	Total O 446 446	0	0
62	1J	12	Total O 12 12	0	0
62	19	8	Total O 8 8	0	0
62	39	1	Total O 1 1	0	0
62	25	6	Total O 6 6	0	0
62	85	2	Total O 2 2	0	0
62	A5	1	Total O 1 1	0	0
62	E5	1	Total O 1 1	0	0
62	L5	1	Total O 1 1	0	0
62	M5	2	Total O 2 2	0	0

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

3 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	209.90Å 448.70Å 618.50Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	151.80 – 3.10 151.80 – 3.10	Depositor EDS
% Data completeness (in resolution range)	99.9 (151.80-3.10) 94.5 (151.80-3.10)	Depositor EDS
R_{merge}	0.41	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.08 (at 3.07Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.188 , 0.235 0.190 , 0.233	Depositor DCC
R_{free} test set	2000 reflections (0.19%)	wwPDB-VP
Wilson B-factor (Å ²)	78.6	Xtriage
Anisotropy	0.285	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 70.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	299951	wwPDB-VP
Average B, all atoms (Å ²)	105.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.43% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

4 Model quality [i](#)

4.1 Standard geometry [i](#)

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

4.2 Too-close contacts [i](#)

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

4.3 Torsion angles [i](#)

4.3.1 Protein backbone [i](#)

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4.3.2 Protein sidechains [i](#)

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

4.3.3 RNA [i](#)

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

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
22	OMG	1K	17	22	23,26,27	4.93	10 (43%)	32,38,41	4.59	17 (53%)
22	MIA	1K	38	22	28,31,32	2.24	4 (14%)	38,44,47	3.19	14 (36%)
22	PSU	3K	40	22	18,21,22	1.04	1 (5%)	21,30,33	1.59	2 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
22	QUO	3K	35	22	32,35,36	4.93	13 (40%)	36,52,55	4.58	11 (30%)
22	PSU	3L	64	22	18,21,22	1.17	1 (5%)	21,30,33	1.94	4 (19%)
22	PSU	3L	40	22	18,21,22	1.15	1 (5%)	21,30,33	1.57	2 (9%)
22	4SU	1K	8	22	18,21,22	1.90	4 (22%)	25,30,33	2.30	5 (20%)
22	5MU	3L	63	22	19,22,23	3.93	5 (26%)	27,32,35	3.23	9 (33%)
22	5MU	3K	63	22	19,22,23	3.84	5 (26%)	27,32,35	3.36	8 (29%)
22	OMG	3K	17	22	23,26,27	5.18	11 (47%)	32,38,41	4.76	17 (53%)
22	QUO	1K	35	22,24	32,35,36	4.80	14 (43%)	36,52,55	4.45	11 (30%)
23	4SU	2L	8	23	18,21,22	1.98	3 (16%)	25,30,33	2.78	4 (16%)
22	4SU	3K	8	22	18,21,22	1.87	3 (16%)	25,30,33	2.52	6 (24%)
23	OMC	2L	33	23	19,22,23	1.75	3 (15%)	25,31,34	0.90	0
22	PSU	1K	64	22	18,21,22	1.27	3 (16%)	21,30,33	1.90	4 (19%)
23	PSU	2L	56	23	18,21,22	1.28	2 (11%)	21,30,33	1.70	2 (9%)
22	PSU	1K	40	22	18,21,22	1.02	1 (5%)	21,30,33	1.81	4 (19%)
22	MIA	3K	38	22	28,31,32	2.34	4 (14%)	38,44,47	3.00	14 (36%)
22	QUO	3L	35	22	32,35,36	4.93	13 (40%)	36,52,55	4.90	13 (36%)
23	4SU	2K	8	23	18,21,22	2.02	3 (16%)	25,30,33	2.67	7 (28%)
22	PSU	1L	64	22	18,21,22	0.96	1 (5%)	21,30,33	1.70	4 (19%)
22	PSU	1L	40	22	18,21,22	1.16	1 (5%)	21,30,33	1.59	4 (19%)
23	5MU	2K	55	23,60	19,22,23	3.87	5 (26%)	27,32,35	3.29	8 (29%)
22	PSU	3K	64	22	18,21,22	1.25	3 (16%)	21,30,33	1.95	5 (23%)
23	OMC	2K	33	23	19,22,23	1.78	3 (15%)	25,31,34	0.83	1 (4%)
22	5MU	1L	63	22	19,22,23	3.86	5 (26%)	27,32,35	3.25	10 (37%)
23	5MU	2L	55	23	19,22,23	3.89	5 (26%)	27,32,35	3.60	9 (33%)
22	MIA	1L	38	22	28,31,32	2.28	4 (14%)	38,44,47	3.41	12 (31%)
22	MIA	3L	38	22	28,31,32	2.24	5 (17%)	38,44,47	2.76	13 (34%)
22	4SU	1L	8	22	18,21,22	1.83	3 (16%)	25,30,33	2.24	5 (20%)
22	OMG	1L	17	22	23,26,27	5.08	11 (47%)	32,38,41	4.70	17 (53%)
22	OMG	3L	17	22	23,26,27	5.18	11 (47%)	32,38,41	4.79	18 (56%)
23	H2U	2L	21	23	18,21,22	2.24	4 (22%)	19,30,33	1.54	3 (15%)
23	H2U	2K	21	23	18,21,22	2.08	4 (22%)	19,30,33	1.66	4 (21%)
23	PSU	2K	56	23	18,21,22	1.24	2 (11%)	21,30,33	2.04	5 (23%)
22	QUO	1L	35	22,24	32,35,36	4.92	13 (40%)	36,52,55	4.84	11 (30%)
22	5MU	1K	63	22	19,22,23	3.81	5 (26%)	27,32,35	3.17	9 (33%)
22	4SU	3L	8	22	18,21,22	2.03	5 (27%)	25,30,33	2.33	5 (20%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	OMG	1K	17	22	-	1/9/27/28	0/3/3/3
22	MIA	1K	38	22	-	6/15/33/34	0/3/3/3
22	PSU	3K	40	22	-	0/7/25/26	0/2/2/2
22	QUO	3K	35	22	-	4/12/43/44	0/4/4/4
22	PSU	3L	64	22	-	0/7/25/26	0/2/2/2
22	PSU	3L	40	22	-	0/7/25/26	0/2/2/2
22	4SU	1K	8	22	-	2/7/25/26	0/2/2/2
22	5MU	3L	63	22	-	0/7/25/26	0/2/2/2
22	5MU	3K	63	22	-	2/7/25/26	0/2/2/2
22	OMG	3K	17	22	-	1/9/27/28	0/3/3/3
22	QUO	1K	35	22,24	-	4/12/43/44	0/4/4/4
23	4SU	2L	8	23	-	0/7/25/26	0/2/2/2
22	4SU	3K	8	22	-	0/7/25/26	0/2/2/2
23	OMC	2L	33	23	-	0/9/27/28	0/2/2/2
22	PSU	1K	64	22	-	0/7/25/26	0/2/2/2
23	PSU	2L	56	23	-	0/7/25/26	0/2/2/2
22	PSU	1K	40	22	-	0/7/25/26	0/2/2/2
22	MIA	3K	38	22	-	6/15/33/34	0/3/3/3
22	QUO	3L	35	22	-	2/12/43/44	0/4/4/4
23	4SU	2K	8	23	-	0/7/25/26	0/2/2/2
22	PSU	1L	64	22	-	1/7/25/26	0/2/2/2
22	PSU	1L	40	22	-	0/7/25/26	0/2/2/2
23	5MU	2K	55	23,60	-	0/7/25/26	0/2/2/2
22	PSU	3K	64	22	-	3/7/25/26	0/2/2/2
23	OMC	2K	33	23	-	1/9/27/28	0/2/2/2
22	5MU	1L	63	22	-	0/7/25/26	0/2/2/2
23	5MU	2L	55	23	-	0/7/25/26	0/2/2/2
22	MIA	1L	38	22	-	7/15/33/34	0/3/3/3
22	MIA	3L	38	22	-	8/15/33/34	0/3/3/3
22	4SU	1L	8	22	-	1/7/25/26	0/2/2/2
22	OMG	1L	17	22	-	3/9/27/28	0/3/3/3
22	OMG	3L	17	22	-	2/9/27/28	0/3/3/3
23	H2U	2L	21	23	-	6/7/38/39	0/2/2/2
23	H2U	2K	21	23	-	3/7/38/39	0/2/2/2
23	PSU	2K	56	23	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	QUO	1L	35	22,24	-	3/12/43/44	0/4/4/4
22	5MU	1K	63	22	-	1/7/25/26	0/2/2/2
22	4SU	3L	8	22	-	0/7/25/26	0/2/2/2

All (194) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	3L	35	QUO	C4-N3	16.56	1.72	1.34
22	1L	35	QUO	C4-N3	16.32	1.71	1.34
22	3K	35	QUO	C4-N3	16.28	1.71	1.34
22	1K	35	QUO	C4-N3	15.22	1.69	1.34
22	1L	35	QUO	C6-N1	-13.11	1.14	1.38
22	1K	35	QUO	C6-N1	-12.80	1.14	1.38
22	3L	63	5MU	C2-N1	12.79	1.58	1.38
23	2L	55	5MU	C2-N1	12.71	1.58	1.38
22	3L	35	QUO	C6-N1	-12.61	1.15	1.38
22	3K	63	5MU	C2-N1	12.51	1.58	1.38
22	1K	63	5MU	C2-N1	12.44	1.57	1.38
23	2K	55	5MU	C2-N1	12.42	1.57	1.38
22	3K	35	QUO	C6-N1	-12.28	1.15	1.38
22	1L	63	5MU	C2-N1	12.22	1.57	1.38
22	3L	17	OMG	C4-N3	12.07	1.61	1.34
22	3K	17	OMG	C4-N3	11.88	1.61	1.34
22	3K	17	OMG	C5-N7	-11.73	1.15	1.39
22	1L	17	OMG	C4-N3	11.71	1.61	1.34
22	1L	17	OMG	C5-N7	-11.60	1.15	1.39
22	3L	17	OMG	C5-N7	-11.53	1.15	1.39
22	1K	17	OMG	C5-N7	-11.35	1.16	1.39
22	1K	17	OMG	C4-N3	11.25	1.60	1.34
22	3L	17	OMG	C4-N9	9.03	1.61	1.38
22	3K	17	OMG	C4-N9	9.01	1.61	1.38
22	1L	17	OMG	C4-N9	8.87	1.60	1.38
22	3L	17	OMG	C8-N7	-8.62	1.08	1.32
22	3K	17	OMG	C8-N7	-8.57	1.08	1.32
22	3K	35	QUO	C8-N9	-8.55	1.23	1.38
22	1K	17	OMG	C8-N7	-8.48	1.08	1.32
22	1L	17	OMG	C8-N7	-8.38	1.09	1.32
22	3L	35	QUO	C8-N9	-8.37	1.23	1.38
22	3L	38	MIA	C13-C14	8.32	1.57	1.32
22	1K	38	MIA	C13-C14	8.30	1.57	1.32
22	3K	17	OMG	C5-C4	8.25	1.61	1.38
22	3L	17	OMG	C5-C4	8.24	1.61	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	1L	17	OMG	C5-C4	8.21	1.61	1.38
22	1L	38	MIA	C13-C14	8.17	1.56	1.32
22	1L	35	QUO	C8-N9	-8.11	1.23	1.38
22	1K	17	OMG	C5-C4	8.10	1.61	1.38
22	1K	35	QUO	C8-N9	-8.07	1.24	1.38
22	1K	17	OMG	C4-N9	8.06	1.58	1.38
22	3L	35	QUO	C2-N3	8.02	1.52	1.33
22	3K	38	MIA	C13-C14	7.94	1.56	1.32
22	3K	35	QUO	C2-N3	7.77	1.52	1.33
22	3K	17	OMG	C6-N1	-7.72	1.24	1.38
22	1K	35	QUO	C4-N9	-7.61	1.18	1.38
22	3L	17	OMG	C6-N1	-7.60	1.24	1.38
22	1L	35	QUO	C2-N3	7.50	1.51	1.33
22	1L	17	OMG	C6-N1	-7.27	1.25	1.38
22	1K	17	OMG	C6-N1	-7.27	1.25	1.38
22	1K	35	QUO	C2-N3	7.13	1.50	1.33
22	3K	35	QUO	C4-N9	-7.01	1.20	1.38
23	2L	21	H2U	C2-N1	6.93	1.45	1.35
22	3K	35	QUO	C5-C6	-6.92	1.29	1.44
22	3L	35	QUO	C5-C6	-6.91	1.29	1.44
22	1K	35	QUO	C5-C6	-6.88	1.29	1.44
22	3K	38	MIA	C6-N6	6.80	1.45	1.34
22	1L	35	QUO	C8-C7	6.70	1.50	1.37
22	1L	38	MIA	C6-N6	6.62	1.44	1.34
22	1K	35	QUO	C8-C7	6.61	1.50	1.37
22	1K	38	MIA	C6-N6	6.61	1.44	1.34
22	1L	35	QUO	C5-C6	-6.56	1.30	1.44
22	3L	38	MIA	C6-N6	6.48	1.44	1.34
22	1L	63	5MU	C4-N3	-6.47	1.26	1.38
22	3K	35	QUO	C8-C7	6.43	1.49	1.37
22	3L	35	QUO	C4-N9	-6.41	1.21	1.38
22	1L	35	QUO	C4-N9	-6.40	1.21	1.38
23	2L	8	4SU	C5-C4	6.32	1.50	1.42
23	2K	8	4SU	C5-C4	6.32	1.50	1.42
22	3K	63	5MU	C4-N3	-6.32	1.27	1.38
23	2K	21	H2U	C2-N1	6.26	1.44	1.35
23	2L	55	5MU	C4-N3	-6.26	1.27	1.38
22	3L	63	5MU	C4-N3	-6.22	1.27	1.38
22	3L	8	4SU	C5-C4	6.20	1.50	1.42
22	1K	63	5MU	C4-N3	-6.19	1.27	1.38
22	3L	35	QUO	C8-C7	6.13	1.49	1.37
22	1L	8	4SU	C5-C4	5.95	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	2K	55	5MU	C2-N3	5.81	1.48	1.38
22	1K	8	4SU	C5-C4	5.78	1.49	1.42
23	2K	55	5MU	C4-N3	-5.78	1.28	1.38
22	3L	63	5MU	C2-N3	5.76	1.48	1.38
22	3K	8	4SU	C5-C4	5.72	1.49	1.42
22	1L	63	5MU	C2-N3	5.65	1.47	1.38
22	3K	63	5MU	C2-N3	5.58	1.47	1.38
22	3K	35	QUO	C13-C12	-5.58	1.47	1.53
23	2K	55	5MU	C6-N1	5.55	1.47	1.38
22	3L	63	5MU	C6-N1	5.54	1.47	1.38
22	1K	63	5MU	C2-N3	5.54	1.47	1.38
23	2L	55	5MU	C2-N3	5.53	1.47	1.38
22	1L	63	5MU	C6-N1	5.46	1.47	1.38
23	2K	55	5MU	C4-C5	5.41	1.53	1.44
22	1K	63	5MU	C6-N1	5.36	1.47	1.38
22	3K	63	5MU	C6-N1	5.36	1.47	1.38
22	3K	38	MIA	C2-S10	5.25	1.80	1.75
23	2L	55	5MU	C4-C5	5.22	1.53	1.44
22	1L	35	QUO	C13-C12	-5.12	1.48	1.53
22	1L	63	5MU	C4-C5	5.12	1.53	1.44
23	2L	55	5MU	C6-N1	5.11	1.46	1.38
22	3L	35	QUO	C13-C12	-4.81	1.48	1.53
22	3L	63	5MU	C4-C5	4.78	1.52	1.44
22	1K	35	QUO	C13-C12	-4.75	1.48	1.53
23	2K	33	OMC	C2-N3	4.65	1.45	1.36
22	3L	17	OMG	C8-N9	-4.61	1.27	1.37
22	1K	17	OMG	C8-N9	-4.57	1.27	1.37
22	3K	17	OMG	C8-N9	-4.54	1.27	1.37
23	2K	33	OMC	C4-N4	4.52	1.44	1.33
22	1K	63	5MU	C4-C5	4.45	1.52	1.44
22	3K	63	5MU	C4-C5	4.44	1.52	1.44
22	1L	17	OMG	C8-N9	-4.40	1.27	1.37
23	2L	33	OMC	C4-N4	4.39	1.44	1.33
22	3L	35	QUO	C2-N2	4.36	1.44	1.34
22	3K	35	QUO	C2-N2	4.31	1.44	1.34
23	2L	33	OMC	C2-N3	4.31	1.44	1.36
23	2L	21	H2U	C2-N3	4.25	1.45	1.38
23	2L	56	PSU	C6-C5	4.17	1.39	1.35
22	3L	8	4SU	C2-N1	4.13	1.44	1.38
22	3K	64	PSU	C6-C5	4.11	1.39	1.35
22	1L	38	MIA	C2-S10	4.08	1.79	1.75
22	3L	64	PSU	C6-C5	4.04	1.39	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	2K	21	H2U	C2-N3	4.03	1.45	1.38
22	1K	35	QUO	C2-N2	3.92	1.43	1.34
23	2K	8	4SU	C2-N1	3.89	1.44	1.38
22	1L	40	PSU	C6-C5	3.85	1.39	1.35
23	2L	8	4SU	C2-N1	3.82	1.44	1.38
22	3K	8	4SU	C2-N1	3.81	1.44	1.38
23	2K	56	PSU	C6-C5	3.79	1.39	1.35
23	2L	21	H2U	C4-N3	3.77	1.43	1.37
22	1L	35	QUO	C2-N2	3.69	1.42	1.34
23	2L	33	OMC	C5-C4	3.68	1.51	1.42
22	1K	8	4SU	C2-N1	3.60	1.44	1.38
22	1K	64	PSU	C6-C5	3.45	1.39	1.35
23	2K	33	OMC	C5-C4	3.45	1.50	1.42
22	3K	40	PSU	C6-C5	3.40	1.39	1.35
23	2K	21	H2U	C4-N3	3.39	1.43	1.37
22	3L	40	PSU	C6-C5	3.37	1.39	1.35
22	1L	8	4SU	C2-N1	3.29	1.43	1.38
22	3L	35	QUO	C14-C13	-3.21	1.48	1.53
22	1L	64	PSU	C6-C5	3.07	1.38	1.35
22	1L	17	OMG	C2-N2	3.07	1.41	1.34
22	3L	17	OMG	C2-N3	3.06	1.40	1.33
22	1L	35	QUO	C14-C13	-3.06	1.48	1.53
22	1K	40	PSU	C6-C5	3.06	1.38	1.35
22	3K	17	OMG	C2-N3	3.05	1.40	1.33
23	2K	8	4SU	C6-N1	3.05	1.45	1.38
22	3K	17	OMG	C2-N2	2.96	1.41	1.34
22	3L	8	4SU	C6-N1	2.93	1.45	1.38
22	3K	17	OMG	O6-C6	-2.92	1.18	1.23
22	3L	17	OMG	C2-N2	2.88	1.40	1.34
22	3L	17	OMG	O6-C6	-2.87	1.18	1.23
22	1K	17	OMG	C2-N2	2.85	1.40	1.34
22	1L	17	OMG	O6-C6	-2.84	1.18	1.23
23	2L	8	4SU	C6-N1	2.83	1.44	1.38
22	1L	35	QUO	C5-C7	2.83	1.57	1.43
22	1L	17	OMG	C2-N3	2.80	1.40	1.33
22	1K	8	4SU	C6-N1	2.77	1.44	1.38
22	3L	38	MIA	C2-S10	2.77	1.78	1.75
22	3K	35	QUO	C14-C13	-2.76	1.49	1.53
22	1L	35	QUO	C2-N1	-2.75	1.30	1.37
22	3L	35	QUO	C5-C7	2.66	1.56	1.43
22	1K	35	QUO	C16-C15	2.65	1.61	1.54
22	3K	35	QUO	C5-C7	2.63	1.56	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	1L	8	4SU	C6-N1	2.63	1.44	1.38
22	3K	8	4SU	C6-N1	2.62	1.44	1.38
22	1K	35	QUO	C5-C7	2.61	1.56	1.43
22	3L	35	QUO	C16-C15	2.57	1.61	1.54
22	3K	35	QUO	C16-C15	2.54	1.60	1.54
22	3L	38	MIA	C5-N7	-2.52	1.34	1.39
22	1K	17	OMG	O6-C6	-2.51	1.18	1.23
22	1K	35	QUO	C14-C13	-2.51	1.49	1.53
22	1K	17	OMG	C2-N3	2.51	1.39	1.33
22	1K	38	MIA	C5-N7	-2.51	1.34	1.39
23	2K	21	H2U	C6-N1	-2.49	1.42	1.47
23	2L	56	PSU	C2-N1	2.47	1.39	1.36
22	3L	17	OMG	C2-N1	-2.40	1.31	1.37
22	1K	38	MIA	C2-S10	2.38	1.77	1.75
23	2L	21	H2U	C6-N1	-2.36	1.43	1.47
22	3K	17	OMG	C2-N1	-2.31	1.32	1.37
22	1K	64	PSU	C2-N1	2.31	1.39	1.36
22	3L	35	QUO	C2-N1	-2.29	1.32	1.37
22	1K	64	PSU	C4-C5	-2.27	1.38	1.44
22	3K	35	QUO	C2-N1	-2.24	1.32	1.37
22	1L	35	QUO	C16-C15	2.21	1.60	1.54
22	1L	38	MIA	C5-N7	-2.18	1.35	1.39
22	3K	64	PSU	C4-C5	-2.09	1.38	1.44
23	2K	56	PSU	C4-C5	-2.06	1.38	1.44
22	1L	17	OMG	C2-N1	-2.04	1.32	1.37
22	3L	38	MIA	C5-C4	2.04	1.42	1.39
22	3L	8	4SU	C2-N3	2.03	1.41	1.38
22	3K	38	MIA	C5-N7	-2.03	1.35	1.39
22	3L	8	4SU	C4-N3	2.03	1.39	1.37
22	3K	64	PSU	O4'-C1'	-2.02	1.41	1.43
22	1K	35	QUO	C5-C4	-2.02	1.37	1.44
22	1K	35	QUO	C2-N1	-2.01	1.32	1.37
22	1K	8	4SU	C2-N3	2.01	1.41	1.38

All (297) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	1L	35	QUO	C5-C4-N3	-19.13	105.57	127.53
22	3L	35	QUO	C5-C4-N3	-18.92	105.81	127.53
22	3K	35	QUO	C5-C4-N3	-17.87	107.01	127.53
22	1K	35	QUO	C5-C4-N3	-17.25	107.72	127.53
22	1L	38	MIA	C11-S10-C2	12.53	111.65	102.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	3L	35	QUO	N9-C4-N3	12.01	149.97	125.95
22	1K	17	OMG	C6-C5-N7	11.77	151.71	130.29
22	1L	35	QUO	N9-C4-N3	11.70	149.35	125.95
23	2L	55	5MU	C5-C4-N3	11.55	125.36	115.32
22	3K	35	QUO	N9-C4-N3	11.32	148.59	125.95
22	1L	17	OMG	C6-C5-N7	11.19	150.66	130.29
22	3L	35	QUO	C1'-N9-C8	-11.16	113.07	125.72
22	3K	63	5MU	C5-C4-N3	11.14	125.00	115.32
22	1K	35	QUO	C7-C8-N9	-10.88	100.92	111.08
22	3K	17	OMG	C6-C5-N7	10.87	150.07	130.29
22	3L	17	OMG	C6-C5-N7	10.85	150.03	130.29
22	1L	35	QUO	C1'-N9-C8	-10.52	113.80	125.72
23	2K	55	5MU	C5-C4-N3	10.48	124.43	115.32
22	3L	63	5MU	C5-C4-N3	10.41	124.37	115.32
22	3L	17	OMG	N9-C4-N3	10.39	146.72	125.95
22	1K	38	MIA	C12-C13-C14	-10.32	108.49	127.01
22	1K	63	5MU	C5-C4-N3	10.22	124.21	115.32
22	1K	35	QUO	N9-C4-N3	10.22	146.39	125.95
22	1K	38	MIA	C11-S10-C2	10.18	109.89	102.25
22	3K	17	OMG	N9-C4-N3	10.12	146.19	125.95
22	1K	17	OMG	C8-N7-C5	10.09	122.23	104.26
22	1L	63	5MU	C5-C4-N3	10.08	124.08	115.32
22	1L	17	OMG	C8-N7-C5	10.03	122.12	104.26
22	3L	17	OMG	C8-N7-C5	9.95	121.98	104.26
22	3K	17	OMG	C8-N7-C5	9.95	121.98	104.26
22	1L	35	QUO	C7-C8-N9	-9.92	101.82	111.08
22	3K	38	MIA	C12-C13-C14	-9.89	109.26	127.01
22	3L	35	QUO	C7-C8-N9	-9.76	101.96	111.08
22	3K	35	QUO	C7-C8-N9	-9.73	102.00	111.08
22	1L	17	OMG	N9-C4-N3	9.61	145.16	125.95
23	2L	8	4SU	C4-N3-C2	-9.20	118.49	127.31
22	1L	38	MIA	C12-C13-C14	-9.08	110.72	127.01
22	3K	35	QUO	C1'-N9-C8	-8.78	115.77	125.72
22	1K	17	OMG	N9-C4-N3	8.71	143.37	125.95
23	2K	8	4SU	C4-N3-C2	-8.53	119.14	127.31
22	3K	17	OMG	C1'-N9-C4	8.44	151.42	126.49
22	3K	38	MIA	C5-C4-N3	-8.39	118.34	127.18
22	3L	17	OMG	C1'-N9-C4	8.22	150.78	126.49
22	3L	38	MIA	C12-C13-C14	-8.13	112.42	127.01
22	1K	17	OMG	C6-C5-C4	-8.09	106.66	118.83
22	3L	38	MIA	C5-C4-N3	-8.05	118.70	127.18
22	3K	8	4SU	C4-N3-C2	-8.03	119.62	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	1L	17	OMG	C1'-N9-C4	7.87	149.72	126.49
23	2L	8	4SU	C5-C4-N3	7.82	122.03	114.75
22	3L	17	OMG	C6-C5-C4	-7.74	107.18	118.83
22	3L	8	4SU	C4-N3-C2	-7.69	119.94	127.31
22	1L	17	OMG	C6-C5-C4	-7.67	107.30	118.83
22	1L	8	4SU	C4-N3-C2	-7.61	120.02	127.31
22	1L	38	MIA	C5-C4-N3	-7.60	119.18	127.18
22	3K	17	OMG	C6-C5-C4	-7.45	107.62	118.83
22	1K	8	4SU	C4-N3-C2	-7.35	120.27	127.31
22	1K	35	QUO	C7-C5-C4	-7.29	104.32	112.68
23	2L	55	5MU	C5-C6-N1	-7.28	115.41	123.31
23	2K	8	4SU	C5-C4-N3	7.23	121.48	114.75
22	1K	35	QUO	C1'-N9-C8	-7.17	117.59	125.72
22	1K	17	OMG	C1'-N9-C4	7.10	147.45	126.49
23	2L	55	5MU	C4-N3-C2	-7.09	118.05	127.34
22	1L	35	QUO	C7-C5-C4	-6.95	104.72	112.68
22	3L	17	OMG	C5-C6-N1	6.71	130.33	113.25
22	3K	17	OMG	C5-C6-N1	6.58	130.00	113.25
22	1L	17	OMG	C5-C6-N1	6.50	129.81	113.25
23	2K	55	5MU	C5-C6-N1	-6.48	116.27	123.31
22	3K	63	5MU	C4-N3-C2	-6.46	118.86	127.34
22	3L	35	QUO	C7-C5-C4	-6.42	105.32	112.68
22	1L	63	5MU	C4-N3-C2	-6.38	118.98	127.34
22	3K	17	OMG	C5-C4-N3	-6.32	118.33	128.39
22	1K	38	MIA	C5-C4-N3	-6.32	120.53	127.18
22	3K	35	QUO	C7-C5-C4	-6.29	105.47	112.68
23	2L	55	5MU	C6-C5-C4	6.21	123.14	118.02
22	1K	17	OMG	C5-C6-N1	6.19	129.02	113.25
22	3L	17	OMG	C5-C4-N3	-6.19	118.54	128.39
22	3L	63	5MU	C4-N3-C2	-6.16	119.26	127.34
22	3L	38	MIA	N3-C4-N9	6.12	134.76	126.99
22	3L	17	OMG	C5-C4-N9	-6.10	94.74	105.66
22	3K	63	5MU	C5-C6-N1	-5.99	116.81	123.31
22	3K	38	MIA	N3-C4-N9	5.99	134.59	126.99
22	1L	17	OMG	C5-C4-N3	-5.94	118.94	128.39
23	2K	55	5MU	C4-N3-C2	-5.90	119.61	127.34
22	1K	63	5MU	C4-N3-C2	-5.86	119.66	127.34
22	3K	63	5MU	O4-C4-C5	-5.80	118.28	124.92
22	1L	63	5MU	C6-C5-C4	5.77	122.78	118.02
22	1L	38	MIA	N3-C4-N9	5.75	134.28	126.99
22	1K	17	OMG	C4-C5-N7	-5.71	101.63	110.67
22	3K	17	OMG	C5-C4-N9	-5.69	95.47	105.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	1K	8	4SU	C5-C4-N3	5.65	120.01	114.75
22	3K	8	4SU	C5-C4-N3	5.62	119.98	114.75
22	1L	63	5MU	C5-C6-N1	-5.61	117.22	123.31
22	3L	17	OMG	C1'-N9-C8	-5.57	110.92	126.73
22	3L	63	5MU	C6-C5-C4	5.53	122.57	118.02
22	3L	8	4SU	C5-C4-N3	5.52	119.88	114.75
22	3K	63	5MU	C6-C5-C4	5.50	122.55	118.02
23	2K	55	5MU	C6-C5-C4	5.48	122.54	118.02
22	1K	63	5MU	C5-C6-N1	-5.47	117.37	123.31
22	1K	63	5MU	C6-C5-C4	5.46	122.52	118.02
22	3K	17	OMG	C1'-N9-C8	-5.46	111.23	126.73
22	1L	17	OMG	C4-C5-N7	-5.45	102.04	110.67
22	1L	17	OMG	C5-C4-N9	-5.44	95.91	105.66
22	3L	63	5MU	C5-C6-N1	-5.41	117.44	123.31
22	1L	8	4SU	C5-C4-N3	5.38	119.75	114.75
23	2K	55	5MU	C5M-C5-C6	-5.36	115.59	122.85
22	1K	63	5MU	O4-C4-C5	-5.35	118.80	124.92
22	1K	17	OMG	C5-C4-N9	-5.35	96.08	105.66
22	1K	64	PSU	C4-N3-C2	-5.34	119.01	126.37
22	3L	63	5MU	O4-C4-C5	-5.29	118.86	124.92
22	3K	17	OMG	C4-C5-N7	-5.28	102.31	110.67
23	2L	55	5MU	C5M-C5-C6	-5.15	115.87	122.85
22	3K	17	OMG	N9-C8-N7	5.15	122.96	113.40
22	3L	35	QUO	C5-C6-N1	5.15	129.28	115.10
22	3K	35	QUO	C5-C6-N1	4.99	128.86	115.10
22	3L	17	OMG	C4-C5-N7	-4.98	102.78	110.67
22	1L	17	OMG	N9-C8-N7	4.97	122.61	113.40
22	3L	64	PSU	N1-C2-N3	4.97	120.41	115.17
22	1L	35	QUO	C5-C6-N1	4.93	128.69	115.10
22	1K	17	OMG	C5-C4-N3	-4.93	120.54	128.39
23	2L	56	PSU	C4-N3-C2	-4.86	119.68	126.37
22	1L	17	OMG	C1'-N9-C8	-4.85	112.97	126.73
23	2K	56	PSU	N1-C2-N3	4.84	120.28	115.17
22	3K	8	4SU	C5-C4-S4	-4.82	118.80	124.31
22	3L	64	PSU	C4-N3-C2	-4.76	119.81	126.37
22	3L	17	OMG	N9-C8-N7	4.76	122.23	113.40
23	2L	55	5MU	O4-C4-C5	-4.75	119.48	124.92
22	1K	38	MIA	C15-C14-C13	-4.72	108.49	122.66
22	3K	64	PSU	N1-C2-N3	4.71	120.14	115.17
22	1K	38	MIA	N3-C4-N9	4.68	132.93	126.99
22	3K	17	OMG	C8-N9-C4	-4.66	97.29	106.03
22	1K	40	PSU	N1-C2-N3	4.65	120.08	115.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	1L	17	OMG	C8-N9-C4	-4.65	97.31	106.03
23	2K	55	5MU	O4-C4-C5	-4.64	119.61	124.92
22	3K	38	MIA	C16-C14-C13	-4.61	108.83	122.66
23	2K	56	PSU	C4-N3-C2	-4.60	120.03	126.37
22	1K	17	OMG	N9-C8-N7	4.57	121.87	113.40
22	1L	17	OMG	O6-C6-C5	-4.55	114.53	126.53
22	3K	38	MIA	C15-C14-C13	-4.53	109.07	122.66
22	1L	63	5MU	C5M-C5-C6	-4.53	116.72	122.85
22	3L	40	PSU	C4-N3-C2	-4.52	120.14	126.37
22	3L	17	OMG	O6-C6-C5	-4.52	114.59	126.53
22	3L	38	MIA	C15-C14-C13	-4.52	109.10	122.66
23	2K	8	4SU	N3-C2-N1	4.51	120.76	114.89
22	1K	40	PSU	C4-N3-C2	-4.48	120.20	126.37
22	3K	8	4SU	N3-C2-N1	4.46	120.69	114.89
22	1K	35	QUO	C5-C6-N1	4.43	127.32	115.10
22	3K	17	OMG	O6-C6-C5	-4.38	114.96	126.53
22	1K	17	OMG	C1'-N9-C8	-4.35	114.36	126.73
22	3K	35	QUO	N1-C2-N3	-4.35	115.37	123.32
22	3L	8	4SU	N3-C2-N1	4.32	120.52	114.89
22	1K	8	4SU	C5-C4-S4	-4.32	119.37	124.31
22	1K	35	QUO	C1'-N9-C4	-4.29	113.80	126.49
22	3L	35	QUO	N1-C2-N3	-4.29	115.47	123.32
22	3L	38	MIA	C16-C14-C13	-4.23	109.97	122.66
22	1L	40	PSU	C4-N3-C2	-4.20	120.59	126.37
22	3K	64	PSU	C4-N3-C2	-4.19	120.61	126.37
22	1K	17	OMG	C8-N9-C4	-4.18	98.19	106.03
22	3L	17	OMG	C8-N9-C4	-4.14	98.26	106.03
23	2K	21	H2U	C5-C4-N3	4.13	121.08	116.69
22	1L	8	4SU	N3-C2-N1	4.12	120.25	114.89
22	3L	63	5MU	C5M-C5-C6	-4.07	117.34	122.85
22	1L	63	5MU	O4-C4-C5	-4.07	120.26	124.92
22	1L	64	PSU	N1-C2-N3	4.03	119.42	115.17
22	1L	38	MIA	C15-C14-C13	-4.02	110.58	122.66
22	1L	64	PSU	C4-N3-C2	-4.02	120.83	126.37
22	1K	63	5MU	C5M-C5-C6	-4.02	117.41	122.85
23	2L	8	4SU	C5-C4-S4	-4.02	119.72	124.31
22	1K	64	PSU	N1-C2-N3	4.01	119.39	115.17
22	3K	63	5MU	C5M-C5-C6	-3.99	117.45	122.85
22	1L	38	MIA	C16-C14-C13	-3.92	110.90	122.66
22	1K	17	OMG	O6-C6-C5	-3.87	116.31	126.53
22	1L	38	MIA	C5-N7-C8	3.85	109.50	103.45
22	3K	40	PSU	C4-N3-C2	-3.84	121.08	126.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	3L	8	4SU	C5-C4-S4	-3.84	119.92	124.31
22	3K	38	MIA	C5-N7-C8	3.83	109.47	103.45
23	2L	8	4SU	N3-C2-N1	3.73	119.74	114.89
23	2L	56	PSU	N1-C2-N3	3.71	119.08	115.17
23	2L	21	H2U	C5-C6-N1	3.70	122.72	111.52
22	1K	38	MIA	C16-C14-C13	-3.69	111.58	122.66
22	1K	8	4SU	N3-C2-N1	3.67	119.67	114.89
22	1L	35	QUO	N1-C2-N3	-3.63	116.67	123.32
22	3K	64	PSU	O2-C2-N1	-3.63	119.05	122.79
22	3L	38	MIA	C5-N7-C8	3.63	109.15	103.45
22	3K	35	QUO	C1'-N9-C4	-3.63	115.77	126.49
22	1K	38	MIA	C5-N7-C8	3.62	109.14	103.45
23	2K	21	H2U	N3-C2-N1	3.62	120.28	116.65
22	1L	40	PSU	N1-C2-N3	3.60	118.96	115.17
22	1L	35	QUO	O6-C6-N1	-3.58	113.38	120.11
23	2L	21	H2U	C5-C4-N3	3.57	120.49	116.69
22	3K	38	MIA	C4-C5-N7	-3.48	106.61	110.58
23	2K	56	PSU	C6-N1-C2	-3.45	119.49	122.69
22	1K	35	QUO	N2-C2-N1	3.45	124.04	116.76
22	1L	38	MIA	C4-C5-N7	-3.42	106.67	110.58
22	1L	63	5MU	C6-N1-C2	-3.41	117.91	121.30
22	3K	40	PSU	N1-C2-N3	3.39	118.74	115.17
22	3K	38	MIA	C2-N3-C4	3.38	121.15	112.29
22	3K	64	PSU	C6-N1-C2	-3.37	119.56	122.69
22	1K	17	OMG	N2-C2-N1	3.37	123.87	116.76
22	1K	38	MIA	N9-C8-N7	-3.29	109.26	113.94
22	1L	8	4SU	C5-C4-S4	-3.28	120.55	124.31
22	1L	38	MIA	C2-N3-C4	3.28	120.88	112.29
22	1L	17	OMG	N2-C2-N1	3.28	123.68	116.76
22	1K	35	QUO	N1-C2-N3	-3.21	117.45	123.32
22	3L	63	5MU	C6-N1-C2	-3.19	118.13	121.30
22	1L	63	5MU	N3-C2-N1	3.17	119.02	114.89
22	3L	35	QUO	O6-C6-C5	-3.14	116.27	125.69
22	3L	38	MIA	C4-C5-N7	-3.13	107.00	110.58
22	3L	38	MIA	C11-S10-C2	3.09	104.57	102.25
22	3K	35	QUO	O6-C6-C5	-3.09	116.42	125.69
23	2K	56	PSU	C6-C5-C4	3.06	120.24	118.17
22	3L	38	MIA	C2-N3-C4	3.02	120.19	112.29
22	3L	35	QUO	O6-C6-N1	-3.01	114.45	120.11
22	3L	40	PSU	N1-C2-N3	3.00	118.33	115.17
22	1K	38	MIA	N6-C6-N1	2.99	122.35	118.33
22	1K	38	MIA	C4-C5-N7	-2.99	107.16	110.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	2K	21	H2U	C5-C6-N1	2.99	120.57	111.52
23	2K	8	4SU	C5-C4-S4	-2.94	120.94	124.31
23	2K	56	PSU	O2-C2-N1	-2.93	119.76	122.79
22	1K	17	OMG	O6-C6-N1	-2.89	114.68	120.11
23	2K	55	5MU	C5M-C5-C4	2.89	121.87	118.78
22	3K	35	QUO	O6-C6-N1	-2.87	114.72	120.11
22	1K	17	OMG	C2-N1-C6	2.83	130.25	125.11
22	1L	38	MIA	C6-C5-N7	2.83	135.51	132.43
22	3L	17	OMG	C2-N1-C6	2.82	130.23	125.11
22	1K	38	MIA	C2-N3-C4	2.82	119.67	112.29
22	1L	64	PSU	C6-N1-C2	-2.80	120.10	122.69
22	3K	17	OMG	C2-N1-C6	2.78	130.15	125.11
22	3K	38	MIA	O3'-C3'-C2'	2.77	120.71	111.82
22	1L	35	QUO	C1'-N9-C4	-2.77	118.30	126.49
22	1L	38	MIA	N9-C8-N7	-2.77	110.01	113.94
22	1K	35	QUO	O6-C6-N1	-2.76	114.92	120.11
22	1L	17	OMG	C2-N1-C6	2.76	130.12	125.11
22	1K	63	5MU	C6-N1-C2	-2.76	118.56	121.30
22	3L	17	OMG	N1-C2-N3	-2.71	118.35	123.32
22	3K	17	OMG	O6-C6-N1	-2.70	115.04	120.11
22	1L	17	OMG	N1-C2-N3	-2.69	118.39	123.32
23	2L	21	H2U	N3-C2-N1	2.69	119.36	116.65
22	3L	64	PSU	C6-N1-C2	-2.69	120.20	122.69
22	3L	17	OMG	O6-C6-N1	-2.68	115.08	120.11
22	1L	38	MIA	N3-C2-N1	-2.65	122.17	127.00
23	2K	21	H2U	O2-C2-N1	-2.65	119.92	123.10
23	2L	55	5MU	O4-C4-N3	-2.64	115.15	120.11
22	1K	35	QUO	O6-C6-C5	-2.64	117.77	125.69
22	3L	35	QUO	C1'-N9-C4	-2.63	118.72	126.49
22	3K	17	OMG	N1-C2-N3	-2.61	118.55	123.32
22	1L	35	QUO	O6-C6-C5	-2.59	117.93	125.69
22	3L	64	PSU	O2-C2-N1	-2.57	120.14	122.79
22	3L	63	5MU	N3-C2-N1	2.56	118.23	114.89
22	1L	63	5MU	O2-C2-N1	-2.55	119.47	122.80
22	1K	40	PSU	C6-N1-C2	-2.55	120.32	122.69
22	3L	38	MIA	C4-C5-C6	2.54	118.89	116.78
22	3L	38	MIA	N6-C6-N1	2.53	121.72	118.33
23	2K	8	4SU	S4-C4-N3	-2.52	117.57	120.20
22	3K	35	QUO	N2-C2-N1	2.51	122.05	116.76
22	1L	8	4SU	O2-C2-N1	-2.50	119.55	122.80
22	3K	38	MIA	N9-C8-N7	-2.48	110.42	113.94
22	3K	8	4SU	C1'-N1-C2	2.46	122.01	117.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	1K	40	PSU	O2-C2-N1	-2.45	120.27	122.79
22	3K	17	OMG	N2-C2-N1	2.38	121.79	116.76
22	1L	63	5MU	O4-C4-N3	-2.37	115.65	120.11
22	1L	17	OMG	O6-C6-N1	-2.37	115.66	120.11
22	3L	38	MIA	N9-C8-N7	-2.34	110.61	113.94
22	3K	38	MIA	N3-C2-N1	-2.34	122.73	127.00
22	3K	63	5MU	C6-N1-C2	-2.33	118.98	121.30
22	1L	40	PSU	O2-C2-N1	-2.32	120.39	122.79
22	1K	64	PSU	C5-C4-N3	2.28	121.57	116.55
22	3L	38	MIA	C16-C14-C15	-2.28	109.34	114.59
22	1K	63	5MU	C1'-N1-C2	2.25	121.64	117.59
22	3K	8	4SU	O2-C2-N1	-2.23	119.89	122.80
23	2K	8	4SU	C1'-N1-C2	2.23	121.60	117.59
22	3K	38	MIA	C6-C5-N7	2.23	134.86	132.43
22	3K	63	5MU	N3-C2-N1	2.23	117.79	114.89
22	1K	17	OMG	N1-C2-N3	-2.21	119.27	123.32
23	2K	55	5MU	O4-C4-N3	-2.21	115.95	120.11
23	2K	8	4SU	O2-C2-N3	-2.20	117.42	121.49
22	1K	64	PSU	O4-C4-C5	-2.19	118.57	124.01
22	3K	38	MIA	C16-C14-C15	-2.19	109.56	114.59
22	3L	35	QUO	C10-N11-C12	-2.16	110.43	114.83
22	3L	35	QUO	N2-C2-N1	2.16	121.31	116.76
22	3L	35	QUO	O13-C13-C14	-2.15	106.87	111.97
22	3L	17	OMG	N2-C2-N1	2.15	121.30	116.76
22	1K	63	5MU	N3-C2-N1	2.14	117.68	114.89
23	2L	55	5MU	N3-C2-N1	2.13	117.67	114.89
22	1L	64	PSU	O2-C2-N1	-2.13	120.59	122.79
22	3K	64	PSU	C6-C5-C4	2.13	119.61	118.17
22	1K	38	MIA	C6-C5-N7	2.12	134.74	132.43
22	1K	38	MIA	N3-C2-N1	-2.11	123.15	127.00
22	3K	38	MIA	C4-C5-C6	2.11	118.53	116.78
22	3L	63	5MU	C1'-N1-C2	2.10	121.37	117.59
22	3L	17	OMG	C3'-C2'-C1'	-2.07	98.84	102.81
22	1L	35	QUO	N2-C2-N1	2.07	121.14	116.76
22	1L	40	PSU	C6-N1-C2	-2.07	120.77	122.69
22	1K	8	4SU	C1'-N1-C2	2.07	121.31	117.59
23	2L	55	5MU	C5M-C5-C4	2.07	120.99	118.78
22	1K	38	MIA	C4-N9-C8	2.05	107.89	105.74
23	2K	33	OMC	N4-C4-N3	2.03	121.53	117.91
22	3L	8	4SU	O2-C2-N1	-2.02	120.17	122.80

There are no chirality outliers.

All (67) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
22	1K	35	QUO	C13-C12-N11-C10
22	1K	38	MIA	N1-C2-S10-C11
22	1K	38	MIA	N3-C2-S10-C11
22	1K	38	MIA	C12-C13-C14-C15
22	1K	38	MIA	C12-C13-C14-C16
23	2K	33	OMC	C1'-C2'-O2'-CM2
22	3K	35	QUO	C13-C12-N11-C10
22	3K	35	QUO	C16-C12-N11-C10
22	3K	38	MIA	O4'-C4'-C5'-O5'
22	3K	38	MIA	C3'-C4'-C5'-O5'
22	3K	38	MIA	C5-C6-N6-C12
22	3K	38	MIA	C12-C13-C14-C15
22	3K	38	MIA	C12-C13-C14-C16
22	3K	63	5MU	O4'-C4'-C5'-O5'
22	1L	35	QUO	O4'-C4'-C5'-O5'
22	1L	38	MIA	O4'-C4'-C5'-O5'
22	1L	38	MIA	N1-C2-S10-C11
22	1L	38	MIA	N3-C2-S10-C11
22	1L	38	MIA	N6-C12-C13-C14
22	1L	38	MIA	C12-C13-C14-C15
22	1L	38	MIA	C12-C13-C14-C16
23	2L	21	H2U	O4'-C1'-N1-C6
22	3L	38	MIA	C5-C6-N6-C12
22	3L	38	MIA	N1-C6-N6-C12
22	3L	38	MIA	N6-C12-C13-C14
22	3L	38	MIA	C12-C13-C14-C15
22	3L	38	MIA	C12-C13-C14-C16
23	2K	21	H2U	O4'-C4'-C5'-O5'
22	3K	63	5MU	C3'-C4'-C5'-O5'
22	1L	35	QUO	C3'-C4'-C5'-O5'
22	1L	38	MIA	C3'-C4'-C5'-O5'
22	3K	64	PSU	C4'-C5'-O5'-P
22	1L	17	OMG	C4'-C5'-O5'-P
22	1K	35	QUO	C7-C10-N11-C12
22	3K	35	QUO	C7-C10-N11-C12
22	3K	64	PSU	C3'-C4'-C5'-O5'
22	3K	64	PSU	O4'-C4'-C5'-O5'
22	3L	35	QUO	C7-C10-N11-C12
23	2K	21	H2U	C3'-C4'-C5'-O5'
22	1K	8	4SU	O4'-C4'-C5'-O5'
22	1L	17	OMG	C3'-C4'-C5'-O5'
22	3K	38	MIA	N1-C6-N6-C12

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Mol	Chain	Res	Type	Atoms
22	1L	35	QUO	C7-C10-N11-C12
22	1K	35	QUO	O4'-C4'-C5'-O5'
22	3K	35	QUO	N11-C10-C7-C8
22	1L	8	4SU	O4'-C4'-C5'-O5'
23	2L	21	H2U	C3'-C4'-C5'-O5'
23	2L	21	H2U	C2'-C1'-N1-C2
22	3L	38	MIA	C3'-C4'-C5'-O5'
23	2L	21	H2U	C2'-C1'-N1-C6
23	2K	21	H2U	C4'-C5'-O5'-P
22	3L	38	MIA	C4'-C5'-O5'-P
23	2L	21	H2U	O4'-C4'-C5'-O5'
22	3K	17	OMG	C3'-C2'-O2'-CM2
23	2L	21	H2U	O4'-C1'-N1-C2
22	1K	8	4SU	C3'-C4'-C5'-O5'
22	1K	38	MIA	C5-C6-N6-C12
22	3L	35	QUO	O4'-C4'-C5'-O5'
22	1L	64	PSU	O4'-C1'-C5-C6
22	3L	17	OMG	C3'-C2'-O2'-CM2
22	1K	17	OMG	C4'-C5'-O5'-P
22	3L	17	OMG	C3'-C4'-C5'-O5'
22	3L	38	MIA	O4'-C4'-C5'-O5'
22	1K	63	5MU	C3'-C4'-C5'-O5'
22	1K	38	MIA	N1-C6-N6-C12
22	1L	17	OMG	O4'-C4'-C5'-O5'
22	1K	35	QUO	C3'-C4'-C5'-O5'

There are no ring outliers.

No monomer is involved in short contacts.

4.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

4.6 Ligand geometry [i](#)

Of 1137 ligands modelled in this entry, 1137 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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
55	1G	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	1G	1530:G	O3'	1531:A	P	3.01

5 Fit of model and data ⓘ

5.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	13	1498/1522 (98%)	-0.29	11 (0%) 84 68	52, 95, 191, 430	0
2	12	237/256 (92%)	0.57	21 (8%) 15 8	115, 168, 226, 251	0
2	1E	237/256 (92%)	0.32	9 (3%) 44 25	104, 142, 195, 252	0
3	22	206/239 (86%)	0.40	9 (4%) 39 21	124, 151, 185, 240	0
3	2E	205/239 (85%)	0.11	1 (0%) 87 73	83, 109, 154, 191	0
4	32	208/208 (100%)	0.69	19 (9%) 15 8	90, 116, 161, 199	0
4	3E	208/208 (100%)	0.41	11 (5%) 32 17	75, 106, 145, 171	0
5	42	151/162 (93%)	0.36	2 (1%) 75 56	98, 124, 157, 188	0
5	4E	151/162 (93%)	0.11	2 (1%) 75 56	73, 98, 129, 175	0
6	52	101/101 (100%)	-0.26	0 100 100	78, 101, 133, 177	0
6	5E	101/101 (100%)	-0.12	0 100 100	75, 102, 131, 171	0
7	62	155/156 (99%)	0.27	6 (3%) 43 24	101, 128, 163, 204	0
7	6E	155/156 (99%)	0.24	6 (3%) 43 24	95, 117, 154, 199	0
8	72	138/138 (100%)	0.43	9 (6%) 25 13	93, 127, 152, 171	0
8	7E	138/138 (100%)	0.17	4 (2%) 53 32	81, 106, 133, 157	0
9	82	127/128 (99%)	0.86	17 (13%) 7 4	110, 159, 203, 214	0
9	8E	127/128 (99%)	0.47	5 (3%) 43 24	86, 139, 183, 217	0
10	1A	99/105 (94%)	0.72	10 (10%) 12 6	120, 162, 202, 221	0
10	1I	99/105 (94%)	0.52	3 (3%) 52 31	84, 134, 180, 197	0
11	2A	119/129 (92%)	0.33	7 (5%) 28 15	85, 111, 149, 259	0
11	2I	119/129 (92%)	0.49	8 (6%) 24 13	68, 101, 158, 186	0
12	3A	125/132 (94%)	0.34	10 (8%) 18 10	78, 103, 165, 208	0
12	3I	125/132 (94%)	-0.09	4 (3%) 50 30	60, 72, 138, 239	0
13	4A	117/126 (92%)	0.49	13 (11%) 10 5	107, 146, 182, 217	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	4I	116/126 (92%)	0.34	7 (6%) 27 15	85, 122, 159, 196	0
14	5A	58/61 (95%)	1.24	10 (17%) 4 2	120, 150, 175, 199	0
14	5I	61/61 (100%)	0.57	6 (9%) 13 7	83, 100, 131, 187	0
15	6A	88/89 (98%)	0.10	2 (2%) 61 39	78, 110, 141, 162	0
15	6I	88/89 (98%)	0.25	4 (4%) 38 20	75, 99, 133, 167	0
16	7A	84/88 (95%)	0.35	1 (1%) 76 58	87, 101, 148, 183	0
16	7I	84/88 (95%)	1.04	16 (19%) 3 1	95, 115, 160, 193	0
17	8A	100/105 (95%)	0.45	8 (8%) 18 10	88, 111, 142, 212	0
17	8I	100/105 (95%)	0.44	9 (9%) 15 8	85, 108, 137, 174	0
18	9A	72/88 (81%)	-0.14	0 100 100	90, 117, 165, 216	0
18	9I	72/88 (81%)	-0.23	0 100 100	81, 106, 165, 192	0
19	AA	82/93 (88%)	0.40	4 (4%) 35 18	120, 163, 207, 254	0
19	AI	83/93 (89%)	0.68	6 (7%) 21 11	91, 122, 184, 229	0
20	BA	99/106 (93%)	0.34	2 (2%) 65 44	85, 110, 159, 210	0
20	BI	99/106 (93%)	0.59	6 (6%) 27 15	101, 123, 179, 208	0
21	1B	25/27 (92%)	1.54	9 (36%) 1 0	109, 131, 161, 194	0
21	1F	25/27 (92%)	0.89	5 (20%) 3 1	88, 106, 144, 196	0
22	1K	78/85 (91%)	0.04	3 (3%) 44 25	78, 184, 302, 353	0
22	1L	67/85 (78%)	0.37	3 (4%) 38 20	118, 208, 263, 287	0
22	3K	67/85 (78%)	-0.28	1 (1%) 72 52	64, 176, 247, 292	0
22	3L	68/85 (80%)	-0.02	2 (2%) 53 32	72, 188, 243, 285	0
23	2K	72/77 (93%)	-0.45	0 100 100	60, 89, 126, 155	0
23	2L	72/77 (93%)	-0.31	0 100 100	72, 104, 146, 163	0
24	4K	15/30 (50%)	0.37	2 (13%) 7 4	64, 95, 185, 192	0
24	4L	16/30 (53%)	0.92	2 (12%) 8 5	84, 129, 213, 234	0
25	14	2907/2912 (99%)	-0.52	15 (0%) 87 73	48, 80, 246, 500	0
25	1H	2912/2912 (100%)	-0.66	9 (0%) 90 80	37, 68, 231, 416	0
26	16	122/122 (100%)	-0.63	0 100 100	65, 88, 112, 273	0
26	1J	122/122 (100%)	-0.13	2 (1%) 70 49	79, 111, 139, 235	0
27	11	272/272 (100%)	-0.18	5 (1%) 67 47	39, 60, 90, 171	0
28	21	205/205 (100%)	0.29	13 (6%) 26 14	47, 86, 159, 216	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
28	29	205/205 (100%)	0.54	22 (10%) 11 6	55, 92, 186, 254	0
29	31	202/202 (100%)	-0.07	2 (0%) 79 61	44, 75, 130, 195	0
30	41	181/181 (100%)	0.24	5 (2%) 55 34	80, 104, 154, 203	0
30	49	181/181 (100%)	0.38	9 (4%) 34 18	99, 133, 183, 213	0
31	51	174/180 (96%)	0.23	6 (3%) 48 28	74, 108, 142, 187	0
31	59	171/180 (95%)	0.68	18 (10%) 11 6	129, 194, 264, 306	0
32	61	146/146 (100%)	0.22	4 (2%) 56 35	71, 128, 164, 189	0
32	69	146/146 (100%)	0.47	7 (4%) 35 19	78, 126, 180, 217	0
33	15	138/138 (100%)	0.41	4 (2%) 53 32	73, 104, 157, 174	0
33	58	138/138 (100%)	0.44	8 (5%) 29 16	60, 90, 143, 192	0
34	25	122/122 (100%)	-0.04	0 100 100	64, 84, 113, 129	0
34	68	122/122 (100%)	-0.28	0 100 100	54, 72, 94, 105	0
35	35	150/150 (100%)	0.61	14 (9%) 14 8	55, 107, 169, 217	0
35	78	150/150 (100%)	0.16	3 (2%) 65 44	45, 82, 117, 215	0
36	45	141/141 (100%)	0.75	20 (14%) 6 3	73, 107, 152, 190	0
36	88	141/141 (100%)	0.32	10 (7%) 22 12	55, 79, 127, 152	0
37	55	117/118 (99%)	-0.06	1 (0%) 81 63	54, 77, 104, 141	0
37	98	118/118 (100%)	0.09	1 (0%) 82 65	55, 79, 105, 134	0
38	65	111/111 (100%)	0.52	10 (9%) 15 8	87, 113, 162, 234	0
38	A8	111/111 (100%)	0.11	4 (3%) 46 26	72, 90, 136, 206	0
39	75	137/137 (100%)	0.27	7 (5%) 33 18	75, 95, 162, 229	0
39	B8	136/137 (99%)	0.22	5 (3%) 45 25	67, 90, 153, 191	0
40	85	117/117 (100%)	0.21	4 (3%) 48 28	65, 89, 142, 206	0
40	C8	117/117 (100%)	0.35	6 (5%) 33 18	51, 79, 131, 184	0
41	95	101/101 (100%)	0.69	10 (9%) 13 7	61, 129, 158, 199	0
41	D8	101/101 (100%)	0.63	10 (9%) 13 7	53, 105, 180, 251	0
42	A5	113/113 (100%)	-0.03	2 (1%) 67 47	57, 72, 119, 205	0
42	E8	113/113 (100%)	-0.07	0 100 100	54, 69, 115, 197	0
43	B5	92/94 (97%)	-0.02	4 (4%) 40 22	60, 80, 115, 161	0
43	F8	94/94 (100%)	-0.04	1 (1%) 78 59	51, 66, 102, 136	0
44	C5	104/110 (94%)	1.30	25 (24%) 2 1	88, 130, 215, 257	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
44	G8	104/110 (94%)	0.68	12 (11%) 9 5	67, 98, 165, 204	0
45	H8	175/175 (100%)	0.22	2 (1%) 78 59	83, 136, 224, 250	0
46	E5	77/85 (90%)	0.35	1 (1%) 75 56	61, 85, 112, 202	0
46	I8	77/85 (90%)	0.08	0 100 100	52, 69, 99, 223	0
47	F5	97/98 (98%)	0.40	7 (7%) 21 11	55, 80, 162, 236	0
47	J8	97/98 (98%)	0.18	9 (9%) 14 8	46, 69, 184, 208	0
48	G5	66/66 (100%)	0.28	5 (7%) 20 11	77, 102, 150, 231	0
48	K8	66/66 (100%)	-0.10	2 (3%) 52 31	58, 77, 117, 208	0
49	H5	59/59 (100%)	0.18	1 (1%) 69 48	76, 98, 151, 172	0
49	L8	59/59 (100%)	-0.28	0 100 100	59, 77, 114, 147	0
50	I5	63/66 (95%)	0.46	3 (4%) 35 19	165, 220, 260, 276	0
50	M8	66/66 (100%)	0.73	6 (9%) 15 8	114, 177, 241, 262	0
51	J5	58/59 (98%)	0.45	3 (5%) 33 17	56, 81, 192, 229	0
51	N8	59/59 (100%)	0.44	2 (3%) 48 28	46, 82, 212, 227	0
52	K5	45/45 (100%)	2.20	23 (51%) 0 0	136, 199, 245, 278	0
52	O8	45/45 (100%)	0.95	5 (11%) 10 5	111, 162, 201, 227	0
53	L5	45/49 (91%)	-0.27	1 (2%) 62 41	47, 56, 71, 90	0
53	P8	45/49 (91%)	-0.49	1 (2%) 62 41	38, 46, 61, 76	0
54	Q8	62/65 (95%)	1.10	14 (22%) 2 1	56, 72, 111, 166	0
55	1G	1498/1522 (98%)	-0.14	19 (1%) 75 56	65, 110, 185, 415	0
56	19	273/276 (98%)	0.12	12 (4%) 39 21	47, 71, 97, 127	0
57	39	208/210 (99%)	0.15	1 (0%) 87 73	56, 99, 194, 251	0
58	D5	179/206 (86%)	0.52	10 (5%) 30 16	111, 162, 259, 295	0
59	M5	60/61 (98%)	0.69	8 (13%) 7 4	67, 81, 131, 191	0
All	All	21050/21589 (97%)	-0.02	708 (3%) 48 28	37, 98, 201, 500	0

All (708) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
11	2I	129	SER	10.5
19	AI	2	PRO	9.1
11	2A	129	SER	8.0
26	1J	88	C	6.7
14	5A	6	LEU	6.6

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Mol	Chain	Res	Type	RSRZ
20	BI	9	ASN	6.5
7	62	81	GLY	6.4
52	K5	13	CYS	6.3
2	12	163	PHE	6.1
4	32	161	ASN	5.9
28	29	76	ARG	5.9
44	C5	49	VAL	5.6
13	4I	8	GLU	5.5
28	29	73	GLU	5.5
8	72	131	GLY	5.4
44	G8	91	GLU	5.4
54	Q8	62	LEU	5.3
52	K5	42	TRP	5.3
39	75	104	ASN	5.3
31	51	171	LEU	5.3
36	88	80	GLU	5.3
13	4A	100	GLY	5.2
47	F5	96	LYS	5.2
44	C5	90	LEU	5.2
28	29	77	ILE	5.2
19	AI	3	ARG	5.1
31	59	89	ILE	5.1
52	K5	22	ALA	5.0
4	32	23	GLY	5.0
36	45	88	GLY	5.0
4	32	5	ILE	4.9
12	3A	48	PRO	4.9
11	2A	128	ALA	4.8
4	32	160	GLN	4.8
38	65	20	ARG	4.8
38	A8	109	GLY	4.8
13	4A	8	GLU	4.7
52	K5	25	LYS	4.7
39	B8	21	GLU	4.7
38	65	2	ALA	4.7
22	1L	85	A	4.5
4	3E	31	CYS	4.5
28	21	78	LEU	4.4
7	62	4	ARG	4.4
15	6I	65	ARG	4.4
54	Q8	43	GLN	4.4
52	K5	23	THR	4.3

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Mol	Chain	Res	Type	RSRZ
2	12	70	PHE	4.3
30	41	2	PRO	4.3
13	4A	4	ILE	4.2
36	45	91	GLU	4.2
54	Q8	20	GLY	4.2
59	M5	40	GLU	4.2
53	L5	45	ALA	4.2
47	F5	98	LEU	4.2
41	D8	48	GLY	4.1
50	M8	32	TYR	4.1
40	85	91	ASP	4.1
44	G8	92	ASN	4.1
13	4I	100	GLY	4.1
13	4A	6	GLY	4.1
33	58	72	TYR	4.1
41	95	80	GLN	4.1
11	2I	12	ARG	4.1
30	49	2	PRO	4.1
44	C5	92	ASN	4.1
54	Q8	34	TRP	4.1
12	3A	18	VAL	4.1
40	85	90	VAL	4.1
44	C5	87	LYS	4.1
10	1I	64	GLU	4.0
51	J5	59	GLU	4.0
14	5A	38	GLY	4.0
10	1A	58	ASP	4.0
20	BA	10	LEU	4.0
28	29	75	VAL	4.0
44	C5	93	GLY	4.0
3	22	2	GLY	3.9
9	82	115	GLY	3.9
17	8I	36	ILE	3.9
52	K5	39	TYR	3.9
56	19	5	LYS	3.9
14	5A	39	LEU	3.9
41	D8	47	VAL	3.9
54	Q8	63	PRO	3.9
13	4A	7	VAL	3.9
2	1E	26	PRO	3.9
36	45	80	GLU	3.8
50	M8	34	GLU	3.8

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Mol	Chain	Res	Type	RSRZ
59	M5	34	TRP	3.8
2	12	165	VAL	3.8
10	1A	59	SER	3.8
44	C5	47	LYS	3.8
11	2I	128	ALA	3.8
4	3E	12	CYS	3.8
3	22	103	VAL	3.7
21	1B	6	ARG	3.7
28	29	63	LEU	3.7
56	19	55	GLY	3.7
4	32	157	LEU	3.7
8	72	133	LEU	3.7
2	12	164	VAL	3.6
36	88	21	THR	3.6
21	1B	26	LYS	3.6
54	Q8	21	LYS	3.6
31	59	131	VAL	3.6
11	2A	127	LYS	3.6
44	C5	91	GLU	3.6
16	7I	29	ASP	3.6
4	32	158	ILE	3.6
12	3I	19	ARG	3.6
35	35	18	ARG	3.6
44	G8	86	ARG	3.6
36	45	90	VAL	3.6
27	11	236	GLY	3.6
41	D8	46	VAL	3.6
55	1G	974	A	3.5
28	29	187	ALA	3.5
40	C8	95	LEU	3.5
17	8A	7	THR	3.5
28	21	75	VAL	3.5
49	H5	2	PRO	3.5
41	95	93	GLU	3.5
9	8E	126	SER	3.5
4	3E	26	CYS	3.4
36	45	103	MET	3.4
25	14	1537	C	3.4
31	59	126	PRO	3.4
39	75	99	LEU	3.4
7	6E	5	ARG	3.4
21	1B	15	ARG	3.4

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Mol	Chain	Res	Type	RSRZ
39	75	1	MET	3.4
8	72	86	ILE	3.4
59	M5	56	GLU	3.4
28	21	63	LEU	3.4
36	45	83	MET	3.4
52	O8	22	ALA	3.4
28	29	52	LEU	3.4
52	K5	35	GLU	3.4
40	C8	86	ALA	3.4
35	35	36	LYS	3.4
52	K5	53	LYS	3.4
19	AI	9	VAL	3.3
36	88	79	LEU	3.3
25	14	1026	U	3.3
30	49	35	GLU	3.3
43	B5	69	TYR	3.3
52	K5	41	PRO	3.3
14	5I	25	VAL	3.3
35	78	71	VAL	3.3
12	3A	17	LYS	3.3
24	4K	12	A	3.3
47	F5	92	LYS	3.3
9	82	106	ALA	3.3
1	13	63	C	3.3
55	1G	1286	A	3.3
51	N8	26	THR	3.3
2	12	71	VAL	3.3
12	3A	47	LYS	3.3
40	C8	90	VAL	3.3
20	BA	9	ASN	3.3
13	4I	5	ALA	3.3
10	1A	66	ARG	3.3
40	C8	117	GLN	3.3
52	K5	49	HIS	3.3
44	G8	105	ALA	3.3
36	45	100	GLY	3.3
33	58	138	LEU	3.2
16	7I	9	PHE	3.2
13	4A	118	ALA	3.2
30	41	35	GLU	3.2
16	7I	17	TYR	3.2
22	1K	83	C	3.2

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Mol	Chain	Res	Type	RSRZ
5	4E	81	GLU	3.2
12	3I	16	GLU	3.2
14	5A	55	GLY	3.2
44	C5	59	GLY	3.2
55	1G	1032(B)	G	3.2
31	51	9	ILE	3.2
19	AI	75	ALA	3.2
44	C5	19	LYS	3.2
39	75	106	SER	3.2
2	12	44	LEU	3.2
31	59	98	LEU	3.2
35	35	35	HIS	3.2
31	59	96	ALA	3.2
41	D8	74	LYS	3.1
4	32	31	CYS	3.1
39	B8	104	ASN	3.1
22	3L	19	C	3.1
35	35	16	ARG	3.1
7	6E	83	ALA	3.1
41	95	74	LYS	3.1
38	65	5	THR	3.1
7	62	82	GLY	3.1
19	AI	84	GLY	3.1
47	J8	84	GLY	3.1
36	88	91	GLU	3.1
36	88	10	ARG	3.1
25	1H	2476	A	3.1
21	1F	25	LYS	3.1
38	A8	2	ALA	3.1
39	75	105	LEU	3.1
52	O8	23	THR	3.1
9	82	75	ASP	3.1
44	C5	29	GLU	3.1
48	G5	66	GLU	3.1
17	8I	35	VAL	3.1
59	M5	53	PRO	3.1
28	21	193	GLY	3.1
9	8E	105	ASP	3.1
36	88	81	VAL	3.1
33	15	84	LYS	3.1
25	14	91	A	3.1
20	BI	72	LEU	3.0

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Mol	Chain	Res	Type	RSRZ
32	61	35	LEU	3.0
28	21	64	LYS	3.0
20	BI	11	SER	3.0
44	C5	61	ILE	3.0
48	G5	18	PRO	3.0
1	13	59	A	3.0
1	13	1286	A	3.0
4	32	26	CYS	3.0
35	35	13	ASN	3.0
54	Q8	39	LYS	3.0
28	29	51	PHE	3.0
35	35	106	LEU	3.0
16	7A	76	GLN	3.0
32	69	1	MET	3.0
35	35	63	PRO	3.0
9	8E	106	ALA	3.0
44	C5	86	ARG	3.0
4	3E	9	CYS	3.0
31	51	5	GLY	3.0
41	95	71	LEU	3.0
44	G8	106	LEU	3.0
13	4A	102	ARG	3.0
17	8A	101	ARG	3.0
44	C5	33	LYS	3.0
13	4I	6	GLY	3.0
33	15	46	VAL	3.0
58	D5	53	ILE	3.0
15	6A	31	LEU	2.9
36	88	78	PRO	2.9
56	19	2	ALA	2.9
12	3A	64	TYR	2.9
3	22	87	LEU	2.9
14	5A	29	ARG	2.9
31	59	105	LEU	2.9
1	13	933	G	2.9
8	72	31	PHE	2.9
55	1G	331	G	2.9
2	12	185	ILE	2.9
36	45	1	MET	2.9
13	4A	88	ARG	2.9
36	88	5	ARG	2.9
2	12	201	ILE	2.9

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Mol	Chain	Res	Type	RSRZ
21	1F	26	LYS	2.9
1	13	631	G	2.9
2	12	9	GLU	2.9
32	61	7	GLU	2.9
47	J8	77	ALA	2.9
56	19	181	GLU	2.9
55	1G	1492	A	2.9
30	41	80	PHE	2.9
41	95	83	ARG	2.9
28	21	171	GLU	2.9
15	6I	60	VAL	2.9
47	J8	98	LEU	2.9
2	12	72	GLY	2.8
16	7I	30	GLY	2.8
47	F5	28	GLY	2.8
25	1H	2799	A	2.8
25	14	530	G	2.8
38	65	21	THR	2.8
19	AI	78	ARG	2.8
11	2I	11	LYS	2.8
9	82	79	LEU	2.8
28	29	71	GLY	2.8
44	C5	48	ALA	2.8
54	Q8	51	ALA	2.8
32	69	111	PRO	2.8
44	C5	50	ARG	2.8
54	Q8	56	GLU	2.8
24	4L	10	A	2.8
55	1G	353	A	2.8
31	59	71	LEU	2.8
47	F5	97	LEU	2.8
20	BI	74	LYS	2.8
30	49	36	LYS	2.8
56	19	261	LYS	2.8
8	7E	2	LEU	2.8
35	35	30	THR	2.8
43	B5	66	LEU	2.8
54	Q8	61	LEU	2.8
8	7E	4	ASP	2.8
55	1G	1531	A	2.8
33	58	47	ALA	2.8
31	59	169	VAL	2.8

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Mol	Chain	Res	Type	RSRZ
55	1G	1032(A)	G	2.8
30	41	3	LEU	2.8
36	45	2	LEU	2.8
52	K5	9	LEU	2.8
8	7E	1	MET	2.7
44	C5	58	GLY	2.7
48	G5	52	ASP	2.7
52	K5	20	ASN	2.7
35	35	110	TYR	2.7
22	1K	82	A	2.7
22	1K	85	A	2.7
39	B8	106	SER	2.7
9	82	103	THR	2.7
54	Q8	45	GLY	2.7
12	3A	19	ARG	2.7
21	1B	25	LYS	2.7
2	1E	188	ALA	2.7
36	45	140	ALA	2.7
53	P8	45	ALA	2.7
8	72	112	LEU	2.7
47	F5	85	LEU	2.7
39	75	101	PHE	2.7
55	1G	59	A	2.7
7	6E	4	ARG	2.7
28	21	76	ARG	2.7
25	14	2803	C	2.7
13	4I	98	VAL	2.7
28	29	116	VAL	2.7
33	15	116	LEU	2.7
52	K5	11	LEU	2.7
28	29	54	GLN	2.7
2	12	127	ILE	2.7
41	D8	73	SER	2.7
38	65	37	ALA	2.7
41	D8	81	TYR	2.7
2	12	196	LEU	2.7
10	1A	65	LEU	2.7
35	35	62	LEU	2.7
44	C5	89	PHE	2.7
5	4E	122	GLU	2.7
28	29	66	HIS	2.7
25	14	1103	A	2.6

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Mol	Chain	Res	Type	RSRZ
25	14	2799	A	2.6
44	C5	2	ARG	2.6
11	2I	127	LYS	2.6
27	11	28	GLU	2.6
41	D8	70	ILE	2.6
12	3I	20	LYS	2.6
35	35	29	LYS	2.6
25	14	2062	A	2.6
50	M8	16	CYS	2.6
3	22	207	VAL	2.6
9	82	50	LEU	2.6
19	AA	9	VAL	2.6
28	21	52	LEU	2.6
30	49	34	LEU	2.6
1	13	1325	C	2.6
55	1G	1490	C	2.6
7	62	5	ARG	2.6
15	6I	68	ARG	2.6
8	72	1	MET	2.6
17	8A	82	MET	2.6
36	45	104	PHE	2.6
44	G8	89	PHE	2.6
16	7I	68	ASP	2.6
35	35	47	ASP	2.6
14	5A	28	GLY	2.6
17	8I	33	GLY	2.6
16	7I	84	ALA	2.6
5	42	45	PHE	2.6
36	45	138	ASP	2.6
4	32	77	ASN	2.6
4	32	120	LEU	2.6
11	2I	98	LEU	2.6
44	C5	42	VAL	2.6
44	G8	94	LYS	2.6
11	2I	75	TYR	2.6
36	45	7	MET	2.6
26	1J	89	G	2.6
55	1G	1224	G	2.6
58	D5	25	PRO	2.6
36	45	79	LEU	2.6
1	13	754	C	2.6
17	8A	11	VAL	2.6

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Mol	Chain	Res	Type	RSRZ
22	3K	19	C	2.6
44	G8	98	VAL	2.6
12	3A	28	LYS	2.6
44	C5	60	PHE	2.5
44	G8	41	GLY	2.5
45	H8	106	GLY	2.5
12	3A	55	VAL	2.5
17	8I	101	ARG	2.5
28	29	81	ILE	2.5
25	14	2475	C	2.5
52	K5	43	CYS	2.5
2	1E	196	LEU	2.5
21	1F	16	GLY	2.5
32	69	110	ASP	2.5
22	1L	24	G	2.5
10	1A	53	PRO	2.5
28	29	53	PRO	2.5
28	29	151	TYR	2.5
28	29	78	LEU	2.5
21	1B	2	GLY	2.5
2	1E	229	VAL	2.5
4	32	156	GLU	2.5
47	J8	89	GLU	2.5
36	45	89	ASN	2.5
8	72	84	ARG	2.5
9	82	127	LYS	2.5
17	8A	81	ARG	2.5
28	21	19	ARG	2.5
38	65	32	LEU	2.5
59	M5	29	LYS	2.5
29	31	207	GLY	2.5
31	59	40	GLU	2.5
41	D8	43	GLU	2.5
2	1E	21	ARG	2.5
17	8I	100	LYS	2.5
33	58	84	LYS	2.5
38	65	33	LYS	2.5
8	72	101	PRO	2.5
48	G5	44	LEU	2.5
59	M5	61	LEU	2.5
41	95	81	TYR	2.5
43	B5	94	GLY	2.5

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Mol	Chain	Res	Type	RSRZ
35	35	71	VAL	2.5
41	D8	37	VAL	2.5
28	29	70	ALA	2.4
58	D5	172	ALA	2.4
55	1G	994	A	2.4
16	7I	28	ARG	2.4
28	29	79	ARG	2.4
56	19	262	ARG	2.4
12	3A	27	LEU	2.4
38	A8	110	LEU	2.4
16	7I	66	PRO	2.4
50	M8	63	TYR	2.4
2	12	197	VAL	2.4
28	21	59	VAL	2.4
35	78	70	GLN	2.4
35	78	150	ALA	2.4
56	19	270	ILE	2.4
27	11	32	SER	2.4
4	32	79	PHE	2.4
10	1I	55	LYS	2.4
3	22	43	LEU	2.4
50	I5	9	LEU	2.4
58	D5	5	LEU	2.4
1	13	389	A	2.4
25	1H	2170	A	2.4
33	58	40	PRO	2.4
28	29	59	VAL	2.4
42	A5	17	VAL	2.4
55	1G	1181	G	2.4
50	I5	28	LYS	2.4
57	39	93	LYS	2.4
10	1A	63	PHE	2.4
31	59	103	LEU	2.4
14	5I	14	PRO	2.4
30	49	160	VAL	2.4
31	51	57	ASP	2.4
33	58	46	VAL	2.4
37	55	69	ASP	2.4
2	12	214	ILE	2.4
4	32	32	ALA	2.4
37	98	103	ARG	2.4
44	G8	84	ARG	2.4

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Mol	Chain	Res	Type	RSRZ
25	1H	2113	U	2.4
52	K5	10	LEU	2.4
55	1G	354	G	2.4
44	C5	98	VAL	2.4
51	N8	51	TYR	2.4
11	2A	11	LYS	2.4
9	82	9	ARG	2.4
9	82	128	ARG	2.4
16	7I	42	ARG	2.4
59	M5	50	LEU	2.4
24	4K	26	A	2.4
39	B8	11	GLU	2.4
17	8A	99	SER	2.4
17	8I	28	PRO	2.4
36	45	27	VAL	2.4
55	1G	1450	U	2.4
21	1B	4	GLY	2.3
31	59	106	THR	2.3
51	J5	54	GLY	2.3
8	72	88	LYS	2.3
10	1A	55	LYS	2.3
52	K5	38	LYS	2.3
2	1E	96	ARG	2.3
9	82	33	PHE	2.3
10	1A	47	PHE	2.3
14	5A	37	PHE	2.3
32	69	35	LEU	2.3
40	85	89	GLU	2.3
16	7I	12	LYS	2.3
36	88	85	LYS	2.3
7	6E	32	ARG	2.3
31	59	4	ILE	2.3
28	29	159	HIS	2.3
44	G8	102	CYS	2.3
14	5I	1	MET	2.3
16	7I	39	TYR	2.3
1	13	307	C	2.3
25	1H	2145	C	2.3
40	C8	91	ASP	2.3
47	J8	80	LEU	2.3
19	AA	11	VAL	2.3
10	1I	66	ARG	2.3

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Mol	Chain	Res	Type	RSRZ
44	C5	77	PRO	2.3
52	O8	42	TRP	2.3
16	7I	49	LEU	2.3
41	95	94	LEU	2.3
47	F5	95	LEU	2.3
14	5A	4	LYS	2.3
31	51	172	LYS	2.3
41	95	46	VAL	2.3
48	K8	69	ARG	2.3
15	6I	19	PRO	2.3
9	8E	8	GLY	2.3
38	65	18	ILE	2.3
10	1A	62	HIS	2.3
25	14	1087	G	2.3
36	45	26	TYR	2.3
55	1G	966	G	2.3
4	32	9	CYS	2.3
32	69	11	ASN	2.3
13	4I	101	GLN	2.3
2	1E	27	LYS	2.3
9	82	28	VAL	2.3
25	1H	2119	A	2.3
39	B8	109	GLU	2.3
52	K5	24	GLU	2.3
3	22	124	ILE	2.3
13	4A	97	PRO	2.3
31	59	168	PRO	2.3
4	3E	21	LEU	2.3
41	95	20	LEU	2.3
45	H8	104	PHE	2.3
48	G5	45	SER	2.3
51	J5	51	TYR	2.3
38	65	19	LYS	2.3
41	95	79	VAL	2.3
9	8E	12	GLU	2.2
35	35	12	ALA	2.2
25	14	1105	U	2.2
21	1B	14	TRP	2.2
17	8I	27	PHE	2.2
2	12	192	SER	2.2
31	51	86	GLU	2.2
32	69	20	ASP	2.2

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Mol	Chain	Res	Type	RSRZ
21	1B	23	PRO	2.2
2	12	152	PHE	2.2
8	7E	88	LYS	2.2
11	2A	125	PHE	2.2
1	13	630	G	2.2
36	45	22	LYS	2.2
4	32	73	ARG	2.2
44	C5	45	VAL	2.2
1	13	1066	C	2.2
2	12	186	ALA	2.2
50	I5	29	PRO	2.2
59	M5	36	LYS	2.2
10	1A	54	PHE	2.2
38	A8	3	ARG	2.2
46	E5	9	SER	2.2
22	3L	18	G	2.2
25	14	2899	G	2.2
30	49	3	LEU	2.2
30	49	82	LEU	2.2
32	61	140	LEU	2.2
50	M8	3	GLU	2.2
33	15	1	MET	2.2
52	K5	34	LEU	2.2
2	12	188	ALA	2.2
27	11	29	PRO	2.2
31	59	128	PRO	2.2
31	59	172	LYS	2.2
14	5I	26	ARG	2.2
56	19	40	THR	2.2
13	4A	101	GLN	2.2
30	41	135	LEU	2.2
4	3E	32	ALA	2.2
16	7I	10	GLY	2.2
16	7I	41	PRO	2.2
11	2A	126	ARG	2.2
25	14	1177	A	2.2
42	A5	111	HIS	2.2
33	58	73	THR	2.1
44	C5	51	VAL	2.1
56	19	259	THR	2.1
7	6E	120	ILE	2.1
4	32	19	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
7	62	13	GLN	2.1
17	8I	98	LEU	2.1
36	88	76	LYS	2.1
12	3A	68	ALA	2.1
58	D5	152	ALA	2.1
20	BI	8	ARG	2.1
33	58	115	ARG	2.1
5	42	130	ASN	2.1
58	D5	177	PRO	2.1
38	65	112	PHE	2.1
20	BI	64	ASP	2.1
52	O8	13	CYS	2.1
3	22	195	VAL	2.1
43	B5	3	THR	2.1
52	K5	21	TYR	2.1
3	22	101	LEU	2.1
47	J8	97	LEU	2.1
48	K8	15	LYS	2.1
13	4A	99	ARG	2.1
55	1G	1054	C	2.1
30	49	23	PHE	2.1
2	12	93	VAL	2.1
32	69	37	VAL	2.1
52	K5	40	CYS	2.1
54	Q8	49	VAL	2.1
4	32	196	LEU	2.1
54	Q8	41	ILE	2.1
36	45	137	TYR	2.1
56	19	147	LEU	2.1
43	F8	76	ARG	2.1
56	19	274	ARG	2.1
2	1E	13	ALA	2.1
55	1G	1236	A	2.1
4	3E	137	SER	2.1
47	J8	86	SER	2.1
50	M8	59	PHE	2.1
28	29	72	VAL	2.1
25	1H	2804	C	2.1
30	49	39	ILE	2.1
47	J8	95	LEU	2.1
32	61	65	ALA	2.1
39	75	94	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
44	C5	65	ALA	2.1
4	32	119	GLN	2.1
9	82	8	GLY	2.1
27	11	234	GLY	2.1
3	22	161	GLU	2.1
17	8I	99	SER	2.1
58	D5	52	SER	2.1
9	82	26	VAL	2.1
17	8A	100	LYS	2.1
19	AA	7	LYS	2.1
52	K5	17	LYS	2.1
2	12	102	LEU	2.1
4	3E	3	ARG	2.1
4	3E	135	LEU	2.1
14	5A	7	ILE	2.1
14	5A	35	ARG	2.1
15	6A	57	LEU	2.1
16	7I	71	ARG	2.1
19	AA	78	ARG	2.1
21	1B	10	ARG	2.1
2	1E	148	TYR	2.1
11	2A	31	THR	2.1
58	D5	28	MET	2.1
13	4A	87	TYR	2.1
7	62	83	ALA	2.1
13	4A	5	ALA	2.1
28	29	50	GLY	2.1
56	19	216	GLY	2.1
3	2E	166	GLU	2.1
9	82	12	GLU	2.1
52	K5	12	GLU	2.1
52	K5	51	GLU	2.1
58	D5	68	PRO	2.1
4	3E	85	LYS	2.0
25	1H	1026	U	2.0
31	59	113	VAL	2.0
58	D5	116	VAL	2.0
4	32	168	ARG	2.0
14	5I	3	ARG	2.0
21	1F	24	ARG	2.0
40	C8	92	ARG	2.0
41	D8	38	LEU	2.0

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Mol	Chain	Res	Type	RSRZ
54	Q8	33	ASN	2.0
7	6E	103	TRP	2.0
2	12	79	ASP	2.0
9	82	125	TYR	2.0
28	21	204	ALA	2.0
29	31	131	GLY	2.0
40	85	2	PRO	2.0
47	J8	87	PRO	2.0
9	82	110	GLU	2.0
14	5I	8	GLU	2.0
17	8A	24	GLU	2.0
13	4I	117	VAL	2.0
44	G8	42	VAL	2.0
28	21	195	LEU	2.0
31	59	171	LEU	2.0
55	1G	1053	G	2.0
28	21	187	ALA	2.0
11	2I	25	TYR	2.0
31	59	5	GLY	2.0
4	3E	46	LYS	2.0
12	3I	17	LYS	2.0
16	7I	15	PRO	2.0
36	45	87	LYS	2.0
22	1L	21	A	2.0
24	4L	22	A	2.0
25	1H	2062	A	2.0
52	O8	12	GLU	2.0
9	82	42	ARG	2.0
21	1F	15	ARG	2.0
25	14	1049	C	2.0
25	14	2804	C	2.0

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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
22	PSU	3K	64	20/21	0.46	0.12	204,248,266,281	0
22	5MU	3K	63	21/22	0.50	0.11	197,231,241,247	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
23	H2U	2L	21	20/21	0.66	0.11	165,170,178,179	0
22	OMG	1L	17	24/25	0.69	0.10	214,233,260,267	0
22	PSU	3L	64	20/21	0.71	0.11	190,201,215,215	0
23	H2U	2K	21	20/21	0.74	0.13	133,176,266,270	0
22	OMG	3L	17	24/25	0.75	0.13	197,218,241,244	0
22	OMG	3K	17	24/25	0.79	0.11	198,221,226,229	0
22	OMG	1K	17	24/25	0.81	0.10	148,195,234,241	0
22	5MU	3L	63	21/22	0.81	0.12	184,193,204,205	0
22	4SU	3L	8	20/21	0.81	0.09	189,200,212,215	0
22	MIA	3L	38	29/30	0.86	0.12	112,126,138,143	0
22	5MU	1L	63	21/22	0.86	0.08	179,192,198,199	0
22	4SU	3K	8	20/21	0.86	0.07	175,183,197,200	0
22	4SU	1K	8	20/21	0.87	0.08	149,171,199,201	0
22	4SU	1L	8	20/21	0.88	0.08	196,199,202,204	0
22	MIA	3K	38	29/30	0.90	0.12	100,113,136,140	0
23	5MU	2L	55	21/22	0.90	0.09	118,122,133,134	0
22	PSU	3L	40	20/21	0.90	0.09	112,122,127,128	0
23	PSU	2L	56	20/21	0.90	0.07	107,113,120,121	0
22	5MU	1K	63	21/22	0.90	0.09	137,144,151,152	0
22	PSU	1L	64	20/21	0.91	0.07	160,190,212,217	0
22	QUO	3L	35	32/33	0.91	0.15	124,129,153,158	0
22	QUO	3K	35	32/33	0.91	0.10	109,116,133,141	0
22	PSU	1K	64	20/21	0.91	0.07	119,139,152,156	0
22	PSU	3K	40	20/21	0.91	0.08	101,110,114,118	0
23	5MU	2K	55	21/22	0.91	0.10	93,103,114,118	0
23	4SU	2L	8	20/21	0.92	0.07	103,112,116,121	0
23	4SU	2K	8	20/21	0.93	0.08	87,91,98,101	0
22	QUO	1L	35	32/33	0.93	0.20	107,128,151,155	0
23	PSU	2K	56	20/21	0.93	0.07	92,99,106,110	0
22	MIA	1L	38	29/30	0.94	0.13	102,126,149,151	0
22	QUO	1K	35	32/33	0.95	0.11	73,84,105,108	0
23	OMC	2L	33	21/22	0.96	0.08	90,96,100,103	0
22	PSU	1K	40	20/21	0.96	0.07	81,102,111,111	0
23	OMC	2K	33	21/22	0.96	0.09	72,75,81,86	0
22	MIA	1K	38	29/30	0.96	0.10	64,83,97,102	0
22	PSU	1L	40	20/21	0.96	0.07	106,139,158,159	0

5.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
60	MG	1G	1673	1/1	0.12	0.26	186,186,186,186	0
60	MG	14	3261	1/1	0.12	0.41	136,136,136,136	0
60	MG	13	1708	1/1	0.16	0.25	167,167,167,167	0
60	MG	13	1707	1/1	0.42	0.33	114,114,114,114	0
60	MG	1G	1683	1/1	0.44	0.35	109,109,109,109	0
60	MG	16	204	1/1	0.50	0.24	83,83,83,83	0
60	MG	14	3018	1/1	0.51	0.38	103,103,103,103	0
60	MG	1H	3305	1/1	0.53	0.27	99,99,99,99	0
60	MG	1G	1685	1/1	0.53	0.23	136,136,136,136	0
60	MG	1H	3167	1/1	0.55	0.38	83,83,83,83	0
60	MG	1H	3251	1/1	0.57	0.17	73,73,73,73	0
60	MG	1G	1680	1/1	0.57	0.18	162,162,162,162	0
60	MG	1G	1629	1/1	0.58	0.25	99,99,99,99	0
60	MG	14	3180	1/1	0.59	0.35	85,85,85,85	0
60	MG	14	3152	1/1	0.59	0.24	96,96,96,96	0
60	MG	1G	1635	1/1	0.60	0.32	104,104,104,104	0
60	MG	1G	1659	1/1	0.60	0.26	118,118,118,118	0
60	MG	1G	1682	1/1	0.60	0.24	115,115,115,115	0
60	MG	1G	1632	1/1	0.61	0.37	89,89,89,89	0
60	MG	13	1616	1/1	0.61	0.41	100,100,100,100	0
60	MG	14	3296	1/1	0.61	0.26	135,135,135,135	0
60	MG	1G	1657	1/1	0.62	0.35	102,102,102,102	0
60	MG	13	1662	1/1	0.62	0.30	89,89,89,89	0
60	MG	13	1617	1/1	0.63	0.34	99,99,99,99	0
60	MG	14	3195	1/1	0.63	0.34	90,90,90,90	0
60	MG	14	3128	1/1	0.63	0.31	86,86,86,86	0
60	MG	13	1699	1/1	0.63	0.33	89,89,89,89	0
60	MG	14	3212	1/1	0.64	0.32	106,106,106,106	0
60	MG	1G	1641	1/1	0.65	0.25	130,130,130,130	0
60	MG	14	3192	1/1	0.65	0.30	80,80,80,80	0
60	MG	13	1709	1/1	0.66	0.23	81,81,81,81	0
60	MG	13	1667	1/1	0.66	0.31	102,102,102,102	0
60	MG	13	1700	1/1	0.66	0.19	102,102,102,102	0
60	MG	13	1678	1/1	0.66	0.40	163,163,163,163	0
60	MG	13	1696	1/1	0.66	0.32	82,82,82,82	0
60	MG	1J	204	1/1	0.66	0.44	92,92,92,92	0
60	MG	1H	3154	1/1	0.67	0.28	89,89,89,89	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
60	MG	1G	1681	1/1	0.68	0.30	107,107,107,107	0
60	MG	14	3294	1/1	0.68	0.36	91,91,91,91	0
60	MG	14	3189	1/1	0.69	0.27	73,73,73,73	0
60	MG	1G	1688	1/1	0.69	0.36	105,105,105,105	0
60	MG	2L	102	1/1	0.69	0.39	95,95,95,95	0
60	MG	13	1689	1/1	0.69	0.22	83,83,83,83	0
61	ZN	G8	201	1/1	0.69	0.19	209,209,209,209	0
60	MG	14	3266	1/1	0.70	0.28	81,81,81,81	0
60	MG	1G	1655	1/1	0.70	0.31	96,96,96,96	0
60	MG	13	1674	1/1	0.70	0.22	184,184,184,184	0
60	MG	1G	1616	1/1	0.70	0.21	125,125,125,125	0
60	MG	1H	3231	1/1	0.70	0.26	91,91,91,91	0
60	MG	1G	1614	1/1	0.71	0.21	109,109,109,109	0
60	MG	14	3185	1/1	0.71	0.27	76,76,76,76	0
60	MG	13	1710	1/1	0.71	0.23	104,104,104,104	0
60	MG	14	3123	1/1	0.72	0.36	81,81,81,81	0
60	MG	1G	1613	1/1	0.72	0.21	116,116,116,116	0
60	MG	14	3105	1/1	0.72	0.24	82,82,82,82	0
60	MG	14	3211	1/1	0.73	0.36	108,108,108,108	0
60	MG	1H	3213	1/1	0.73	0.30	95,95,95,95	0
60	MG	14	3214	1/1	0.73	0.29	84,84,84,84	0
60	MG	1H	3288	1/1	0.74	0.32	92,92,92,92	0
60	MG	14	3147	1/1	0.74	0.23	99,99,99,99	0
60	MG	14	3276	1/1	0.74	0.16	66,66,66,66	0
60	MG	1H	3219	1/1	0.74	0.19	123,123,123,123	0
60	MG	14	3167	1/1	0.74	0.21	93,93,93,93	0
60	MG	13	1659	1/1	0.74	0.31	79,79,79,79	0
60	MG	13	1695	1/1	0.74	0.32	90,90,90,90	0
60	MG	13	1698	1/1	0.75	0.13	86,86,86,86	0
60	MG	1H	3145	1/1	0.75	0.32	63,63,63,63	0
60	MG	14	3170	1/1	0.75	0.41	81,81,81,81	0
60	MG	14	3232	1/1	0.75	0.31	92,92,92,92	0
60	MG	14	3245	1/1	0.75	0.26	82,82,82,82	0
60	MG	16	203	1/1	0.75	0.19	77,77,77,77	0
60	MG	1G	1666	1/1	0.76	0.27	113,113,113,113	0
60	MG	1H	3031	1/1	0.76	0.18	78,78,78,78	0
60	MG	14	3307	1/1	0.76	0.27	82,82,82,82	0
60	MG	14	3274	1/1	0.76	0.30	79,79,79,79	0
60	MG	13	1655	1/1	0.76	0.42	97,97,97,97	0
60	MG	14	3166	1/1	0.77	0.34	73,73,73,73	0
60	MG	1H	3126	1/1	0.77	0.09	79,79,79,79	0
60	MG	14	3104	1/1	0.77	0.34	70,70,70,70	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
60	MG	1G	1634	1/1	0.77	0.32	112,112,112,112	0
60	MG	13	1668	1/1	0.77	0.33	114,114,114,114	0
60	MG	1G	1672	1/1	0.77	0.29	84,84,84,84	0
60	MG	14	3136	1/1	0.77	0.34	90,90,90,90	0
60	MG	14	3144	1/1	0.77	0.27	80,80,80,80	0
60	MG	1H	3093	1/1	0.77	0.19	64,64,64,64	0
60	MG	1H	3103	1/1	0.77	0.25	88,88,88,88	0
60	MG	14	3163	1/1	0.77	0.18	80,80,80,80	0
60	MG	14	3248	1/1	0.78	0.35	80,80,80,80	0
60	MG	13	1705	1/1	0.78	0.26	83,83,83,83	0
60	MG	13	1711	1/1	0.78	0.33	83,83,83,83	0
60	MG	14	3149	1/1	0.78	0.28	73,73,73,73	0
60	MG	14	3031	1/1	0.78	0.28	75,75,75,75	0
60	MG	1H	3298	1/1	0.78	0.23	56,56,56,56	0
60	MG	1H	3107	1/1	0.78	0.44	63,63,63,63	0
60	MG	1G	1631	1/1	0.78	0.31	83,83,83,83	0
60	MG	4I	201	1/1	0.78	0.19	86,86,86,86	0
60	MG	49	201	1/1	0.78	0.18	93,93,93,93	0
60	MG	13	1656	1/1	0.78	0.16	84,84,84,84	0
60	MG	14	3057	1/1	0.79	0.31	62,62,62,62	0
60	MG	14	3074	1/1	0.79	0.35	53,53,53,53	0
60	MG	1H	3212	1/1	0.79	0.30	89,89,89,89	0
60	MG	1G	1671	1/1	0.79	0.29	77,77,77,77	0
60	MG	14	3118	1/1	0.79	0.29	60,60,60,60	0
60	MG	13	1682	1/1	0.79	0.38	85,85,85,85	0
60	MG	14	3223	1/1	0.79	0.30	67,67,67,67	0
60	MG	13	1615	1/1	0.79	0.38	75,75,75,75	0
60	MG	13	1716	1/1	0.79	0.28	77,77,77,77	0
60	MG	1H	3248	1/1	0.79	0.22	97,97,97,97	0
60	MG	13	1690	1/1	0.79	0.24	86,86,86,86	0
60	MG	13	1618	1/1	0.79	0.28	77,77,77,77	0
60	MG	1H	3047	1/1	0.79	0.21	73,73,73,73	0
60	MG	1H	3056	1/1	0.79	0.18	67,67,67,67	0
60	MG	14	3290	1/1	0.79	0.44	78,78,78,78	0
60	MG	1G	1689	1/1	0.79	0.45	86,86,86,86	0
60	MG	1H	3178	1/1	0.79	0.30	80,80,80,80	0
60	MG	14	3169	1/1	0.79	0.15	46,46,46,46	0
60	MG	1H	3182	1/1	0.79	0.37	91,91,91,91	0
60	MG	11	302	1/1	0.79	0.14	54,54,54,54	0
60	MG	14	3039	1/1	0.79	0.21	75,75,75,75	0
60	MG	1G	1674	1/1	0.80	0.32	84,84,84,84	0
60	MG	2K	101	1/1	0.80	0.16	81,81,81,81	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
60	MG	13	1663	1/1	0.80	0.29	93,93,93,93	0
60	MG	1H	3170	1/1	0.80	0.23	76,76,76,76	0
60	MG	1H	3173	1/1	0.80	0.19	72,72,72,72	0
60	MG	14	3297	1/1	0.80	0.39	100,100,100,100	0
60	MG	1H	3141	1/1	0.80	0.33	70,70,70,70	0
60	MG	14	3081	1/1	0.80	0.32	86,86,86,86	0
60	MG	13	1701	1/1	0.80	0.45	85,85,85,85	0
60	MG	1H	3203	1/1	0.80	0.31	91,91,91,91	0
60	MG	13	1686	1/1	0.81	0.31	76,76,76,76	0
60	MG	1G	1686	1/1	0.81	0.19	115,115,115,115	0
60	MG	1G	1604	1/1	0.81	0.26	78,78,78,78	0
60	MG	1G	1608	1/1	0.81	0.28	95,95,95,95	0
60	MG	13	1713	1/1	0.81	0.30	96,96,96,96	0
60	MG	2L	103	1/1	0.81	0.24	67,67,67,67	0
60	MG	1H	3169	1/1	0.81	0.20	63,63,63,63	0
60	MG	14	3303	1/1	0.81	0.54	93,93,93,93	0
60	MG	14	3029	1/1	0.81	0.21	75,75,75,75	0
60	MG	1H	3295	1/1	0.81	0.31	87,87,87,87	0
60	MG	14	3132	1/1	0.81	0.33	84,84,84,84	0
60	MG	14	3032	1/1	0.81	0.20	103,103,103,103	0
60	MG	1H	3098	1/1	0.82	0.31	69,69,69,69	0
60	MG	14	3082	1/1	0.82	0.26	65,65,65,65	0
60	MG	14	3204	1/1	0.82	0.27	105,105,105,105	0
60	MG	14	3092	1/1	0.82	0.23	62,62,62,62	0
60	MG	1H	3303	1/1	0.82	0.37	90,90,90,90	0
60	MG	1H	3023	1/1	0.82	0.34	58,58,58,58	0
60	MG	16	201	1/1	0.82	0.28	78,78,78,78	0
60	MG	1G	1640	1/1	0.82	0.35	105,105,105,105	0
60	MG	13	1673	1/1	0.82	0.15	69,69,69,69	0
60	MG	1G	1644	1/1	0.82	0.36	85,85,85,85	0
60	MG	14	3256	1/1	0.82	0.18	64,64,64,64	0
60	MG	14	3257	1/1	0.82	0.17	69,69,69,69	0
60	MG	13	1650	1/1	0.82	0.26	77,77,77,77	0
60	MG	14	3264	1/1	0.82	0.33	91,91,91,91	0
60	MG	1H	3172	1/1	0.82	0.27	71,71,71,71	0
60	MG	14	3007	1/1	0.82	0.31	54,54,54,54	0
60	MG	14	3014	1/1	0.82	0.29	79,79,79,79	0
60	MG	88	202	1/1	0.82	0.30	78,78,78,78	0
60	MG	14	3025	1/1	0.82	0.19	81,81,81,81	0
60	MG	1H	3241	1/1	0.82	0.23	61,61,61,61	0
60	MG	13	1606	1/1	0.82	0.29	78,78,78,78	0
60	MG	13	1680	1/1	0.82	0.15	68,68,68,68	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
60	MG	1H	3255	1/1	0.82	0.22	71,71,71,71	0
60	MG	1H	3181	1/1	0.82	0.30	81,81,81,81	0
60	MG	1H	3149	1/1	0.82	0.14	56,56,56,56	0
60	MG	14	3075	1/1	0.82	0.22	49,49,49,49	0
60	MG	14	3227	1/1	0.83	0.21	69,69,69,69	0
60	MG	1H	3046	1/1	0.83	0.17	90,90,90,90	0
60	MG	1H	3114	1/1	0.83	0.30	61,61,61,61	0
60	MG	1H	3116	1/1	0.83	0.21	69,69,69,69	0
60	MG	1G	1633	1/1	0.83	0.38	95,95,95,95	0
60	MG	13	1651	1/1	0.83	0.25	54,54,54,54	0
60	MG	13	1638	1/1	0.83	0.33	80,80,80,80	0
60	MG	13	1669	1/1	0.83	0.27	84,84,84,84	0
60	MG	68	201	1/1	0.83	0.27	83,83,83,83	0
60	MG	14	3173	1/1	0.83	0.31	61,61,61,61	0
60	MG	13	1666	1/1	0.83	0.19	94,94,94,94	0
60	MG	13	1714	1/1	0.83	0.28	89,89,89,89	0
60	MG	1H	3278	1/1	0.83	0.30	64,64,64,64	0
60	MG	14	3107	1/1	0.83	0.31	69,69,69,69	0
60	MG	1G	1658	1/1	0.83	0.33	71,71,71,71	0
60	MG	1H	3184	1/1	0.83	0.24	58,58,58,58	0
60	MG	1G	1665	1/1	0.83	0.37	75,75,75,75	0
60	MG	14	3358	1/1	0.83	0.17	86,86,86,86	0
60	MG	1H	3191	1/1	0.83	0.37	73,73,73,73	0
60	MG	1G	1615	1/1	0.83	0.45	87,87,87,87	0
60	MG	45	201	1/1	0.83	0.33	81,81,81,81	0
60	MG	1H	3159	1/1	0.83	0.29	77,77,77,77	0
60	MG	1G	1676	1/1	0.84	0.32	90,90,90,90	0
60	MG	14	3026	1/1	0.84	0.27	77,77,77,77	0
60	MG	14	3229	1/1	0.84	0.21	84,84,84,84	0
60	MG	14	3141	1/1	0.84	0.33	85,85,85,85	0
60	MG	1G	1677	1/1	0.84	0.29	88,88,88,88	0
60	MG	1G	1643	1/1	0.84	0.25	80,80,80,80	0
60	MG	78	201	1/1	0.84	0.28	66,66,66,66	0
60	MG	1G	1650	1/1	0.84	0.39	88,88,88,88	0
60	MG	14	3055	1/1	0.84	0.22	60,60,60,60	0
60	MG	1G	1626	1/1	0.84	0.17	87,87,87,87	0
60	MG	13	1703	1/1	0.84	0.25	111,111,111,111	0
60	MG	1H	3027	1/1	0.84	0.20	79,79,79,79	0
60	MG	14	3079	1/1	0.84	0.33	68,68,68,68	0
60	MG	13	1653	1/1	0.84	0.31	83,83,83,83	0
60	MG	1G	1610	1/1	0.84	0.18	78,78,78,78	0
60	MG	1G	1612	1/1	0.84	0.32	84,84,84,84	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
60	MG	13	1622	1/1	0.84	0.26	86,86,86,86	0
60	MG	1G	1636	1/1	0.84	0.30	89,89,89,89	0
60	MG	14	3012	1/1	0.84	0.24	59,59,59,59	0
60	MG	13	1614	1/1	0.84	0.34	82,82,82,82	0
60	MG	1J	201	1/1	0.84	0.22	105,105,105,105	0
60	MG	1J	202	1/1	0.84	0.34	85,85,85,85	0
60	MG	1H	3010	1/1	0.84	0.31	50,50,50,50	0
60	MG	14	3127	1/1	0.84	0.31	71,71,71,71	0
60	MG	14	3024	1/1	0.84	0.30	81,81,81,81	0
60	MG	14	3216	1/1	0.84	0.29	80,80,80,80	0
61	ZN	C5	202	1/1	0.84	0.15	197,197,197,197	0
60	MG	1H	3229	1/1	0.85	0.27	56,56,56,56	0
60	MG	13	1661	1/1	0.85	0.38	70,70,70,70	0
60	MG	14	3225	1/1	0.85	0.26	53,53,53,53	0
60	MG	14	3037	1/1	0.85	0.28	79,79,79,79	0
60	MG	14	3228	1/1	0.85	0.27	76,76,76,76	0
60	MG	14	3145	1/1	0.85	0.31	82,82,82,82	0
60	MG	1H	3143	1/1	0.85	0.24	50,50,50,50	0
60	MG	14	3241	1/1	0.85	0.16	65,65,65,65	0
60	MG	1H	3246	1/1	0.85	0.20	73,73,73,73	0
60	MG	14	3150	1/1	0.85	0.23	92,92,92,92	0
60	MG	14	3253	1/1	0.85	0.43	71,71,71,71	0
60	MG	1H	3035	1/1	0.85	0.22	63,63,63,63	0
60	MG	14	3153	1/1	0.85	0.24	61,61,61,61	0
60	MG	14	3258	1/1	0.85	0.21	65,65,65,65	0
60	MG	13	1608	1/1	0.85	0.20	70,70,70,70	0
60	MG	13	1652	1/1	0.85	0.27	61,61,61,61	0
60	MG	1H	3265	1/1	0.85	0.18	75,75,75,75	0
60	MG	14	3273	1/1	0.85	0.10	65,65,65,65	0
60	MG	14	3168	1/1	0.85	0.28	77,77,77,77	0
60	MG	1H	3267	1/1	0.85	0.21	83,83,83,83	0
60	MG	14	3288	1/1	0.85	0.21	61,61,61,61	0
60	MG	13	1635	1/1	0.85	0.30	63,63,63,63	0
60	MG	1H	3194	1/1	0.85	0.26	71,71,71,71	0
60	MG	1G	1663	1/1	0.85	0.30	93,93,93,93	0
60	MG	14	3182	1/1	0.85	0.63	81,81,81,81	0
60	MG	1H	3117	1/1	0.85	0.25	57,57,57,57	0
60	MG	14	3306	1/1	0.85	0.29	67,67,67,67	0
60	MG	1H	3207	1/1	0.85	0.28	63,63,63,63	0
60	MG	1H	3211	1/1	0.85	0.23	84,84,84,84	0
60	MG	1H	3123	1/1	0.85	0.18	65,65,65,65	0
60	MG	14	3198	1/1	0.85	0.16	63,63,63,63	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
60	MG	14	3202	1/1	0.85	0.32	72,72,72,72	0
60	MG	14	3124	1/1	0.85	0.23	82,82,82,82	0
60	MG	1H	3030	1/1	0.85	0.28	70,70,70,70	0
60	MG	E5	101	1/1	0.85	0.23	80,80,80,80	0
60	MG	1H	3218	1/1	0.85	0.30	84,84,84,84	0
60	MG	1H	3140	1/1	0.85	0.21	59,59,59,59	0
60	MG	13	1624	1/1	0.86	0.29	77,77,77,77	0
60	MG	1H	3132	1/1	0.86	0.28	73,73,73,73	0
60	MG	13	1665	1/1	0.86	0.37	91,91,91,91	0
60	MG	14	3148	1/1	0.86	0.38	86,86,86,86	0
60	MG	1H	3064	1/1	0.86	0.21	51,51,51,51	0
60	MG	13	1693	1/1	0.86	0.26	89,89,89,89	0
60	MG	1H	3270	1/1	0.86	0.13	58,58,58,58	0
60	MG	1H	3276	1/1	0.86	0.30	76,76,76,76	0
60	MG	14	3255	1/1	0.86	0.31	75,75,75,75	0
60	MG	1G	1627	1/1	0.86	0.32	66,66,66,66	0
60	MG	14	3165	1/1	0.86	0.31	84,84,84,84	0
60	MG	1H	3196	1/1	0.86	0.33	91,91,91,91	0
60	MG	1H	3197	1/1	0.86	0.26	70,70,70,70	0
60	MG	1H	3293	1/1	0.86	0.40	80,80,80,80	0
60	MG	1H	3020	1/1	0.86	0.22	59,59,59,59	0
60	MG	14	3272	1/1	0.86	0.14	55,55,55,55	0
60	MG	1H	3100	1/1	0.86	0.26	74,74,74,74	0
60	MG	14	3171	1/1	0.86	0.29	78,78,78,78	0
60	MG	1H	3210	1/1	0.86	0.18	72,72,72,72	0
60	MG	14	3280	1/1	0.86	0.09	55,55,55,55	0
60	MG	14	3090	1/1	0.86	0.45	63,63,63,63	0
60	MG	13	1702	1/1	0.86	0.22	80,80,80,80	0
60	MG	14	3183	1/1	0.86	0.34	84,84,84,84	0
60	MG	14	3095	1/1	0.86	0.14	66,66,66,66	0
60	MG	1H	3106	1/1	0.86	0.25	66,66,66,66	0
60	MG	13	1712	1/1	0.86	0.15	112,112,112,112	0
60	MG	1H	3168	1/1	0.86	0.25	72,72,72,72	0
60	MG	1H	3110	1/1	0.86	0.18	43,43,43,43	0
60	MG	14	3121	1/1	0.86	0.36	64,64,64,64	0
60	MG	1H	3227	1/1	0.86	0.23	65,65,65,65	0
60	MG	14	3206	1/1	0.86	0.19	63,63,63,63	0
60	MG	13	1681	1/1	0.86	0.29	88,88,88,88	0
60	MG	13	1607	1/1	0.86	0.12	75,75,75,75	0
60	MG	14	3017	1/1	0.86	0.22	68,68,68,68	0
60	MG	13	1715	1/1	0.86	0.32	82,82,82,82	0
60	MG	14	3023	1/1	0.86	0.34	74,74,74,74	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
60	MG	13	1601	1/1	0.86	0.24	66,66,66,66	0
60	MG	1H	3193	1/1	0.87	0.34	67,67,67,67	0
60	MG	1G	1642	1/1	0.87	0.20	87,87,87,87	0
60	MG	14	3215	1/1	0.87	0.41	69,69,69,69	0
60	MG	13	1697	1/1	0.87	0.08	95,95,95,95	0
60	MG	13	1657	1/1	0.87	0.39	73,73,73,73	0
60	MG	1H	3111	1/1	0.87	0.23	49,49,49,49	0
60	MG	1G	1651	1/1	0.87	0.40	87,87,87,87	0
60	MG	13	1664	1/1	0.87	0.27	68,68,68,68	0
60	MG	1H	3263	1/1	0.87	0.28	72,72,72,72	0
60	MG	14	3143	1/1	0.87	0.36	76,76,76,76	0
60	MG	13	1688	1/1	0.87	0.29	66,66,66,66	0
60	MG	14	3244	1/1	0.87	0.23	75,75,75,75	0
60	MG	1G	1609	1/1	0.87	0.27	74,74,74,74	0
60	MG	14	3246	1/1	0.87	0.26	81,81,81,81	0
60	MG	14	3028	1/1	0.87	0.29	77,77,77,77	0
60	MG	14	3250	1/1	0.87	0.23	65,65,65,65	0
60	MG	1H	3073	1/1	0.87	0.20	53,53,53,53	0
60	MG	1H	3029	1/1	0.87	0.30	65,65,65,65	0
60	MG	5I	101	1/1	0.87	0.21	83,83,83,83	0
60	MG	14	3035	1/1	0.87	0.30	57,57,57,57	0
60	MG	13	1605	1/1	0.87	0.24	71,71,71,71	0
60	MG	14	3162	1/1	0.87	0.17	83,83,83,83	0
60	MG	1H	3281	1/1	0.87	0.12	69,69,69,69	0
60	MG	14	3041	1/1	0.87	0.36	72,72,72,72	0
60	MG	14	3047	1/1	0.87	0.26	72,72,72,72	0
60	MG	1H	3214	1/1	0.87	0.19	62,62,62,62	0
60	MG	1G	1618	1/1	0.87	0.33	86,86,86,86	0
60	MG	14	3070	1/1	0.87	0.22	61,61,61,61	0
60	MG	14	3277	1/1	0.87	0.13	81,81,81,81	0
60	MG	14	3071	1/1	0.87	0.26	68,68,68,68	0
60	MG	14	3281	1/1	0.87	0.08	63,63,63,63	0
60	MG	1H	3292	1/1	0.87	0.23	89,89,89,89	0
60	MG	1H	3136	1/1	0.87	0.23	72,72,72,72	0
60	MG	1H	3101	1/1	0.87	0.38	77,77,77,77	0
60	MG	1H	3222	1/1	0.87	0.29	77,77,77,77	0
60	MG	1H	3002	1/1	0.87	0.24	51,51,51,51	0
60	MG	14	3299	1/1	0.87	0.20	60,60,60,60	0
60	MG	14	3302	1/1	0.87	0.44	87,87,87,87	0
60	MG	1H	3104	1/1	0.87	0.34	63,63,63,63	0
60	MG	14	3187	1/1	0.87	0.32	84,84,84,84	0
60	MG	14	3188	1/1	0.87	0.21	93,93,93,93	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
60	MG	1H	3307	1/1	0.87	0.30	74,74,74,74	0
60	MG	14	3386	1/1	0.87	0.27	57,57,57,57	0
60	MG	1H	3043	1/1	0.87	0.16	70,70,70,70	0
60	MG	16	202	1/1	0.87	0.32	82,82,82,82	0
60	MG	1G	1638	1/1	0.87	0.29	88,88,88,88	0
60	MG	1G	1703	1/1	0.87	0.07	128,128,128,128	0
60	MG	14	3109	1/1	0.87	0.28	82,82,82,82	0
60	MG	45	202	1/1	0.87	0.24	94,94,94,94	0
60	MG	14	3114	1/1	0.87	0.23	91,91,91,91	0
60	MG	14	3210	1/1	0.87	0.30	79,79,79,79	0
60	MG	1H	3239	1/1	0.87	0.18	48,48,48,48	0
60	MG	1H	3273	1/1	0.88	0.19	55,55,55,55	0
60	MG	14	3237	1/1	0.88	0.25	66,66,66,66	0
60	MG	1G	1668	1/1	0.88	0.39	95,95,95,95	0
60	MG	1H	3088	1/1	0.88	0.18	66,66,66,66	0
60	MG	1H	3091	1/1	0.88	0.19	60,60,60,60	0
60	MG	1H	3280	1/1	0.88	0.20	70,70,70,70	0
60	MG	13	1644	1/1	0.88	0.27	55,55,55,55	0
60	MG	1H	3034	1/1	0.88	0.22	38,38,38,38	0
60	MG	14	3058	1/1	0.88	0.26	64,64,64,64	0
60	MG	14	3059	1/1	0.88	0.36	72,72,72,72	0
60	MG	14	3064	1/1	0.88	0.31	70,70,70,70	0
60	MG	1H	3003	1/1	0.88	0.25	45,45,45,45	0
60	MG	1G	1619	1/1	0.88	0.29	82,82,82,82	0
60	MG	14	3260	1/1	0.88	0.17	73,73,73,73	0
60	MG	1H	3175	1/1	0.88	0.28	81,81,81,81	0
60	MG	13	1683	1/1	0.88	0.26	89,89,89,89	0
60	MG	1H	3180	1/1	0.88	0.32	87,87,87,87	0
60	MG	13	1636	1/1	0.88	0.30	66,66,66,66	0
60	MG	13	1654	1/1	0.88	0.25	69,69,69,69	0
60	MG	1H	3306	1/1	0.88	0.24	77,77,77,77	0
60	MG	1H	3232	1/1	0.88	0.22	71,71,71,71	0
60	MG	1H	3339	1/1	0.88	0.20	75,75,75,75	0
60	MG	14	3096	1/1	0.88	0.16	60,60,60,60	0
60	MG	1H	3142	1/1	0.88	0.25	57,57,57,57	0
60	MG	14	3282	1/1	0.88	0.26	73,73,73,73	0
60	MG	1H	3240	1/1	0.88	0.19	109,109,109,109	0
60	MG	13	1634	1/1	0.88	0.36	67,67,67,67	0
60	MG	14	3008	1/1	0.88	0.28	53,53,53,53	0
60	MG	1H	3057	1/1	0.88	0.22	47,47,47,47	0
60	MG	1H	3147	1/1	0.88	0.24	76,76,76,76	0
60	MG	13	1671	1/1	0.88	0.13	64,64,64,64	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
60	MG	14	3301	1/1	0.88	0.32	75,75,75,75	0
60	MG	2K	103	1/1	0.88	0.32	76,76,76,76	0
60	MG	14	3209	1/1	0.88	0.41	77,77,77,77	0
60	MG	14	3305	1/1	0.88	0.26	94,94,94,94	0
60	MG	78	203	1/1	0.88	0.26	87,87,87,87	0
60	MG	1H	3199	1/1	0.88	0.19	74,74,74,74	0
60	MG	1G	1601	1/1	0.88	0.29	59,59,59,59	0
60	MG	1G	1602	1/1	0.88	0.22	69,69,69,69	0
60	MG	14	3133	1/1	0.88	0.33	80,80,80,80	0
60	MG	14	3027	1/1	0.88	0.28	65,65,65,65	0
60	MG	14	3137	1/1	0.88	0.42	69,69,69,69	0
60	MG	1J	205	1/1	0.88	0.12	119,119,119,119	0
60	MG	1H	3087	1/1	0.88	0.37	72,72,72,72	0
60	MG	14	3226	1/1	0.88	0.28	68,68,68,68	0
60	MG	1G	1605	1/1	0.88	0.22	81,81,81,81	0
60	MG	85	201	1/1	0.88	0.53	71,71,71,71	0
60	MG	C5	201	1/1	0.88	0.33	107,107,107,107	0
60	MG	1H	3161	1/1	0.88	0.17	50,50,50,50	0
60	MG	1H	3115	1/1	0.88	0.36	52,52,52,52	0
60	MG	14	3231	1/1	0.88	0.21	79,79,79,79	0
60	MG	1H	3158	1/1	0.89	0.32	65,65,65,65	0
60	MG	1G	1628	1/1	0.89	0.22	78,78,78,78	0
60	MG	13	1675	1/1	0.89	0.31	67,67,67,67	0
60	MG	1H	3254	1/1	0.89	0.21	57,57,57,57	0
60	MG	13	1603	1/1	0.89	0.23	57,57,57,57	0
60	MG	1H	3259	1/1	0.89	0.20	59,59,59,59	0
60	MG	1H	3162	1/1	0.89	0.15	67,67,67,67	0
60	MG	1H	3165	1/1	0.89	0.31	77,77,77,77	0
60	MG	1G	1687	1/1	0.89	0.20	83,83,83,83	0
60	MG	78	202	1/1	0.89	0.11	46,46,46,46	0
60	MG	1H	3166	1/1	0.89	0.39	83,83,83,83	0
60	MG	14	3175	1/1	0.89	0.36	80,80,80,80	0
60	MG	1G	1702	1/1	0.89	0.08	124,124,124,124	0
60	MG	14	3269	1/1	0.89	0.28	60,60,60,60	0
60	MG	1G	1639	1/1	0.89	0.35	82,82,82,82	0
60	MG	13	1629	1/1	0.89	0.30	62,62,62,62	0
60	MG	14	3094	1/1	0.89	0.35	58,58,58,58	0
60	MG	14	3275	1/1	0.89	0.29	76,76,76,76	0
60	MG	1H	3102	1/1	0.89	0.28	61,61,61,61	0
60	MG	14	3005	1/1	0.89	0.24	46,46,46,46	0
60	MG	2K	102	1/1	0.89	0.30	84,84,84,84	0
60	MG	1H	3072	1/1	0.89	0.48	70,70,70,70	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
60	MG	14	3010	1/1	0.89	0.30	54,54,54,54	0
60	MG	14	3286	1/1	0.89	0.15	60,60,60,60	0
60	MG	1H	3105	1/1	0.89	0.16	59,59,59,59	0
60	MG	1G	1647	1/1	0.89	0.33	76,76,76,76	0
60	MG	1G	1607	1/1	0.89	0.20	98,98,98,98	0
60	MG	14	3205	1/1	0.89	0.32	72,72,72,72	0
60	MG	13	1706	1/1	0.89	0.30	85,85,85,85	0
60	MG	14	3207	1/1	0.89	0.35	74,74,74,74	0
60	MG	1G	1653	1/1	0.89	0.33	73,73,73,73	0
60	MG	13	1646	1/1	0.89	0.13	111,111,111,111	0
60	MG	14	3126	1/1	0.89	0.22	82,82,82,82	0
60	MG	1H	3109	1/1	0.89	0.21	50,50,50,50	0
60	MG	1G	1611	1/1	0.89	0.25	103,103,103,103	0
60	MG	13	1647	1/1	0.89	0.34	83,83,83,83	0
60	MG	14	3308	1/1	0.89	0.22	66,66,66,66	0
60	MG	14	3309	1/1	0.89	0.32	72,72,72,72	0
60	MG	13	1630	1/1	0.89	0.20	51,51,51,51	0
60	MG	14	3222	1/1	0.89	0.23	43,43,43,43	0
60	MG	1G	1664	1/1	0.89	0.30	74,74,74,74	0
60	MG	13	1740	1/1	0.89	0.16	54,54,54,54	0
60	MG	1H	3151	1/1	0.89	0.30	77,77,77,77	0
60	MG	1H	3186	1/1	0.89	0.23	79,79,79,79	0
60	MG	1H	3187	1/1	0.89	0.32	60,60,60,60	0
60	MG	1H	3153	1/1	0.89	0.29	59,59,59,59	0
60	MG	14	3040	1/1	0.89	0.14	66,66,66,66	0
60	MG	1G	1625	1/1	0.89	0.22	72,72,72,72	0
60	MG	14	3235	1/1	0.89	0.23	78,78,78,78	0
60	MG	14	3043	1/1	0.89	0.42	64,64,64,64	0
60	MG	14	3046	1/1	0.89	0.47	80,80,80,80	0
60	MG	1H	3096	1/1	0.89	0.23	53,53,53,53	0
60	MG	14	3089	1/1	0.90	0.25	52,52,52,52	0
60	MG	14	3013	1/1	0.90	0.25	61,61,61,61	0
60	MG	13	1602	1/1	0.90	0.17	65,65,65,65	0
60	MG	1H	3195	1/1	0.90	0.28	75,75,75,75	0
60	MG	1H	3144	1/1	0.90	0.17	78,78,78,78	0
60	MG	14	3021	1/1	0.90	0.24	68,68,68,68	0
60	MG	1G	1669	1/1	0.90	0.18	84,84,84,84	0
60	MG	1G	1670	1/1	0.90	0.11	93,93,93,93	0
60	MG	1H	3238	1/1	0.90	0.24	50,50,50,50	0
60	MG	13	1626	1/1	0.90	0.24	50,50,50,50	0
60	MG	14	3110	1/1	0.90	0.27	56,56,56,56	0
60	MG	14	3111	1/1	0.90	0.23	72,72,72,72	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
60	MG	13	1627	1/1	0.90	0.30	50,50,50,50	0
60	MG	1H	3065	1/1	0.90	0.07	39,39,39,39	0
60	MG	14	3200	1/1	0.90	0.40	91,91,91,91	0
60	MG	14	3278	1/1	0.90	0.18	71,71,71,71	0
60	MG	14	3120	1/1	0.90	0.20	53,53,53,53	0
60	MG	1G	1675	1/1	0.90	0.26	86,86,86,86	0
60	MG	1H	3033	1/1	0.90	0.20	61,61,61,61	0
60	MG	14	3283	1/1	0.90	0.33	79,79,79,79	0
60	MG	1H	3209	1/1	0.90	0.28	81,81,81,81	0
60	MG	14	3125	1/1	0.90	0.12	63,63,63,63	0
60	MG	1H	3119	1/1	0.90	0.32	67,67,67,67	0
60	MG	14	3291	1/1	0.90	0.24	80,80,80,80	0
60	MG	13	1621	1/1	0.90	0.40	62,62,62,62	0
60	MG	14	3295	1/1	0.90	0.18	77,77,77,77	0
60	MG	14	3038	1/1	0.90	0.32	60,60,60,60	0
60	MG	1H	3083	1/1	0.90	0.26	44,44,44,44	0
60	MG	1H	3256	1/1	0.90	0.35	93,93,93,93	0
60	MG	1H	3258	1/1	0.90	0.35	64,64,64,64	0
60	MG	1H	3086	1/1	0.90	0.20	53,53,53,53	0
60	MG	14	3218	1/1	0.90	0.33	67,67,67,67	0
60	MG	1G	1648	1/1	0.90	0.30	78,78,78,78	0
60	MG	1H	3022	1/1	0.90	0.12	51,51,51,51	0
60	MG	14	3052	1/1	0.90	0.24	55,55,55,55	0
60	MG	1H	3138	1/1	0.90	0.28	81,81,81,81	0
60	MG	1G	1690	1/1	0.90	0.34	75,75,75,75	0
60	MG	14	3356	1/1	0.90	0.14	66,66,66,66	0
60	MG	13	1676	1/1	0.90	0.33	63,63,63,63	0
60	MG	16	205	1/1	0.90	0.26	79,79,79,79	0
60	MG	14	3062	1/1	0.90	0.41	66,66,66,66	0
60	MG	2L	101	1/1	0.90	0.20	72,72,72,72	0
60	MG	1G	1620	1/1	0.90	0.16	83,83,83,83	0
60	MG	14	3159	1/1	0.90	0.24	64,64,64,64	0
60	MG	14	3240	1/1	0.90	0.15	50,50,50,50	0
60	MG	16	207	1/1	0.90	0.14	62,62,62,62	0
60	MG	13	1613	1/1	0.90	0.25	66,66,66,66	0
60	MG	1G	1660	1/1	0.90	0.35	78,78,78,78	0
60	MG	1G	1662	1/1	0.90	0.32	84,84,84,84	0
60	MG	14	3080	1/1	0.90	0.17	78,78,78,78	0
60	MG	1H	3272	1/1	0.90	0.33	72,72,72,72	0
60	MG	1H	3028	1/1	0.90	0.17	51,51,51,51	0
60	MG	14	3203	1/1	0.91	0.27	66,66,66,66	0
60	MG	14	3270	1/1	0.91	0.22	57,57,57,57	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
60	MG	2K	104	1/1	0.91	0.20	54,54,54,54	0
60	MG	1H	3217	1/1	0.91	0.28	75,75,75,75	0
60	MG	13	1604	1/1	0.91	0.25	74,74,74,74	0
60	MG	14	3020	1/1	0.91	0.18	57,57,57,57	0
60	MG	14	3208	1/1	0.91	0.25	66,66,66,66	0
60	MG	1H	3188	1/1	0.91	0.23	63,63,63,63	0
60	MG	1G	1645	1/1	0.91	0.14	78,78,78,78	0
60	MG	1H	3049	1/1	0.91	0.27	66,66,66,66	0
60	MG	1H	3089	1/1	0.91	0.22	69,69,69,69	0
60	MG	1G	1617	1/1	0.91	0.09	83,83,83,83	0
60	MG	1H	3090	1/1	0.91	0.32	67,67,67,67	0
60	MG	14	3284	1/1	0.91	0.20	75,75,75,75	0
60	MG	1H	3053	1/1	0.91	0.18	51,51,51,51	0
60	MG	14	3091	1/1	0.91	0.22	67,67,67,67	0
60	MG	16	208	1/1	0.91	0.12	84,84,84,84	0
60	MG	1G	1656	1/1	0.91	0.32	86,86,86,86	0
60	MG	13	1631	1/1	0.91	0.28	74,74,74,74	0
60	MG	14	3034	1/1	0.91	0.27	62,62,62,62	0
60	MG	14	3097	1/1	0.91	0.41	54,54,54,54	0
60	MG	14	3098	1/1	0.91	0.33	59,59,59,59	0
60	MG	1H	3095	1/1	0.91	0.20	49,49,49,49	0
60	MG	1H	3025	1/1	0.91	0.23	51,51,51,51	0
60	MG	1G	1701	1/1	0.91	0.09	106,106,106,106	0
60	MG	1H	3026	1/1	0.91	0.20	80,80,80,80	0
60	MG	1H	3006	1/1	0.91	0.21	42,42,42,42	0
60	MG	1H	3208	1/1	0.91	0.15	56,56,56,56	0
60	MG	14	3042	1/1	0.91	0.19	44,44,44,44	0
60	MG	14	3242	1/1	0.91	0.21	53,53,53,53	0
60	MG	1H	3039	1/1	0.91	0.28	46,46,46,46	0
60	MG	14	3318	1/1	0.91	0.09	76,76,76,76	0
60	MG	14	3181	1/1	0.91	0.18	73,73,73,73	0
60	MG	14	3119	1/1	0.91	0.24	65,65,65,65	0
60	MG	13	1640	1/1	0.91	0.27	76,76,76,76	0
60	MG	1H	3296	1/1	0.91	0.08	69,69,69,69	0
60	MG	1H	3297	1/1	0.91	0.16	63,63,63,63	0
60	MG	1J	203	1/1	0.91	0.26	91,91,91,91	0
60	MG	14	3054	1/1	0.91	0.36	64,64,64,64	0
60	MG	1H	3253	1/1	0.91	0.11	56,56,56,56	0
60	MG	29	301	1/1	0.91	0.19	48,48,48,48	0
60	MG	14	3009	1/1	0.91	0.20	50,50,50,50	0
60	MG	14	3193	1/1	0.91	0.41	76,76,76,76	0
60	MG	1H	3045	1/1	0.91	0.33	65,65,65,65	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
60	MG	1H	3130	1/1	0.91	0.26	73,73,73,73	0
60	MG	14	3130	1/1	0.91	0.17	53,53,53,53	0
60	MG	1H	3131	1/1	0.91	0.35	76,76,76,76	0
60	MG	14	3267	1/1	0.91	0.16	71,71,71,71	0
60	MG	14	3268	1/1	0.91	0.20	74,74,74,74	0
60	MG	14	3060	1/1	0.92	0.27	63,63,63,63	0
60	MG	13	1677	1/1	0.92	0.15	67,67,67,67	0
60	MG	1H	3225	1/1	0.92	0.22	38,38,38,38	0
60	MG	14	3065	1/1	0.92	0.28	71,71,71,71	0
60	MG	1H	3127	1/1	0.92	0.16	44,44,44,44	0
60	MG	1H	3074	1/1	0.92	0.27	57,57,57,57	0
60	MG	14	3072	1/1	0.92	0.25	66,66,66,66	0
60	MG	13	1620	1/1	0.92	0.23	64,64,64,64	0
60	MG	B8	201	1/1	0.92	0.11	97,97,97,97	0
60	MG	14	3263	1/1	0.92	0.23	63,63,63,63	0
60	MG	C8	201	1/1	0.92	0.24	89,89,89,89	0
60	MG	1G	1649	1/1	0.92	0.34	76,76,76,76	0
60	MG	1H	3014	1/1	0.92	0.24	52,52,52,52	0
60	MG	1H	3282	1/1	0.92	0.10	56,56,56,56	0
60	MG	14	3174	1/1	0.92	0.29	77,77,77,77	0
60	MG	14	3085	1/1	0.92	0.17	52,52,52,52	0
60	MG	1H	3133	1/1	0.92	0.35	83,83,83,83	0
60	MG	1H	3289	1/1	0.92	0.43	71,71,71,71	0
60	MG	1H	3037	1/1	0.92	0.14	53,53,53,53	0
60	MG	1H	3016	1/1	0.92	0.23	42,42,42,42	0
60	MG	14	3016	1/1	0.92	0.31	52,52,52,52	0
60	MG	1H	3294	1/1	0.92	0.21	66,66,66,66	0
60	MG	1H	3058	1/1	0.92	0.15	57,57,57,57	0
60	MG	14	3279	1/1	0.92	0.15	76,76,76,76	0
60	MG	1H	3245	1/1	0.92	0.07	50,50,50,50	0
60	MG	1H	3060	1/1	0.92	0.32	64,64,64,64	0
60	MG	14	3102	1/1	0.92	0.19	46,46,46,46	0
60	MG	1H	3061	1/1	0.92	0.23	56,56,56,56	0
60	MG	1H	3299	1/1	0.92	0.12	72,72,72,72	0
60	MG	14	3285	1/1	0.92	0.09	62,62,62,62	0
60	MG	3K	101	1/1	0.92	0.21	83,83,83,83	0
60	MG	14	3201	1/1	0.92	0.30	81,81,81,81	0
60	MG	1H	3304	1/1	0.92	0.22	69,69,69,69	0
60	MG	1H	3252	1/1	0.92	0.32	66,66,66,66	0
60	MG	13	1736	1/1	0.92	0.05	141,141,141,141	0
60	MG	14	3112	1/1	0.92	0.17	72,72,72,72	0
60	MG	1H	3174	1/1	0.92	0.24	53,53,53,53	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
60	MG	14	3117	1/1	0.92	0.31	74,74,74,74	0
60	MG	14	3030	1/1	0.92	0.18	71,71,71,71	0
60	MG	14	3300	1/1	0.92	0.34	76,76,76,76	0
60	MG	1H	3067	1/1	0.92	0.16	46,46,46,46	0
60	MG	1G	1621	1/1	0.92	0.15	68,68,68,68	0
60	MG	14	3033	1/1	0.92	0.17	58,58,58,58	0
60	MG	14	3122	1/1	0.92	0.28	66,66,66,66	0
60	MG	1G	1624	1/1	0.92	0.32	70,70,70,70	0
60	MG	1H	3360	1/1	0.92	0.09	99,99,99,99	0
60	MG	1H	3378	1/1	0.92	0.09	67,67,67,67	0
60	MG	14	3217	1/1	0.92	0.33	71,71,71,71	0
60	MG	1H	3421	1/1	0.92	0.10	138,138,138,138	0
60	MG	1H	3437	1/1	0.92	0.20	52,52,52,52	0
60	MG	1G	1678	1/1	0.92	0.26	79,79,79,79	0
60	MG	14	3379	1/1	0.92	0.11	104,104,104,104	0
60	MG	1G	1679	1/1	0.92	0.21	71,71,71,71	0
60	MG	1H	3069	1/1	0.92	0.32	60,60,60,60	0
60	MG	1H	3148	1/1	0.92	0.32	67,67,67,67	0
60	MG	14	3134	1/1	0.92	0.16	84,84,84,84	0
60	MG	14	3135	1/1	0.92	0.37	78,78,78,78	0
60	MG	14	3045	1/1	0.92	0.26	45,45,45,45	0
60	MG	1J	206	1/1	0.92	0.09	125,125,125,125	0
60	MG	1H	3070	1/1	0.92	0.26	45,45,45,45	0
60	MG	1H	3262	1/1	0.92	0.28	80,80,80,80	0
60	MG	1H	3120	1/1	0.92	0.29	63,63,63,63	0
60	MG	1H	3152	1/1	0.92	0.31	76,76,76,76	0
60	MG	13	1643	1/1	0.92	0.13	75,75,75,75	0
60	MG	14	3056	1/1	0.92	0.26	65,65,65,65	0
60	MG	1H	3220	1/1	0.92	0.47	78,78,78,78	0
60	MG	21	301	1/1	0.92	0.28	49,49,49,49	0
60	MG	41	201	1/1	0.92	0.15	75,75,75,75	0
60	MG	1H	3155	1/1	0.93	0.34	60,60,60,60	0
60	MG	1H	3215	1/1	0.93	0.30	80,80,80,80	0
60	MG	1H	3134	1/1	0.93	0.32	64,64,64,64	0
60	MG	1H	3050	1/1	0.93	0.25	54,54,54,54	0
60	MG	1H	3326	1/1	0.93	0.11	57,57,57,57	0
60	MG	1H	3097	1/1	0.93	0.25	60,60,60,60	0
60	MG	1H	3021	1/1	0.93	0.15	59,59,59,59	0
60	MG	14	3050	1/1	0.93	0.24	54,54,54,54	0
60	MG	14	3194	1/1	0.93	0.24	63,63,63,63	0
60	MG	1H	3163	1/1	0.93	0.41	64,64,64,64	0
60	MG	1H	3223	1/1	0.93	0.19	44,44,44,44	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
60	MG	1H	3427	1/1	0.93	0.10	92,92,92,92	0
60	MG	1H	3224	1/1	0.93	0.15	37,37,37,37	0
60	MG	1H	3271	1/1	0.93	0.13	62,62,62,62	0
60	MG	1H	3164	1/1	0.93	0.24	60,60,60,60	0
60	MG	14	3011	1/1	0.93	0.15	58,58,58,58	0
60	MG	1H	3099	1/1	0.93	0.09	49,49,49,49	0
60	MG	1H	3274	1/1	0.93	0.11	71,71,71,71	0
60	MG	14	3129	1/1	0.93	0.19	56,56,56,56	0
60	MG	14	3063	1/1	0.93	0.44	70,70,70,70	0
60	MG	1G	1622	1/1	0.93	0.31	52,52,52,52	0
60	MG	14	3015	1/1	0.93	0.16	50,50,50,50	0
60	MG	13	1739	1/1	0.93	0.16	68,68,68,68	0
60	MG	1H	3118	1/1	0.93	0.17	56,56,56,56	0
60	MG	13	1648	1/1	0.93	0.38	76,76,76,76	0
60	MG	14	3292	1/1	0.93	0.23	77,77,77,77	0
60	MG	13	1632	1/1	0.93	0.16	55,55,55,55	0
60	MG	14	3140	1/1	0.93	0.15	46,46,46,46	0
60	MG	1H	3200	1/1	0.93	0.30	69,69,69,69	0
60	MG	14	3078	1/1	0.93	0.21	59,59,59,59	0
60	MG	14	3221	1/1	0.93	0.26	56,56,56,56	0
60	MG	14	3022	1/1	0.93	0.17	48,48,48,48	0
60	MG	1H	3201	1/1	0.93	0.31	65,65,65,65	0
60	MG	1G	1630	1/1	0.93	0.32	80,80,80,80	0
60	MG	1H	3146	1/1	0.93	0.19	84,84,84,84	0
60	MG	14	3083	1/1	0.93	0.21	56,56,56,56	0
60	MG	1H	3242	1/1	0.93	0.32	74,74,74,74	0
60	MG	14	3087	1/1	0.93	0.20	78,78,78,78	0
60	MG	14	3088	1/1	0.93	0.21	64,64,64,64	0
60	MG	1H	3243	1/1	0.93	0.25	60,60,60,60	0
60	MG	14	3161	1/1	0.93	0.29	69,69,69,69	0
60	MG	13	1637	1/1	0.93	0.29	76,76,76,76	0
60	MG	88	201	1/1	0.93	0.18	81,81,81,81	0
60	MG	14	3164	1/1	0.93	0.36	75,75,75,75	0
60	MG	13	1625	1/1	0.93	0.26	75,75,75,75	0
60	MG	14	3093	1/1	0.93	0.37	70,70,70,70	0
60	MG	13	1691	1/1	0.93	0.21	96,96,96,96	0
60	MG	13	1610	1/1	0.93	0.16	67,67,67,67	0
60	MG	I8	101	1/1	0.93	0.26	70,70,70,70	0
60	MG	I8	102	1/1	0.93	0.20	56,56,56,56	0
60	MG	14	3252	1/1	0.93	0.22	76,76,76,76	0
60	MG	1H	3017	1/1	0.93	0.16	54,54,54,54	0
60	MG	29	302	1/1	0.93	0.34	79,79,79,79	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
60	MG	14	3254	1/1	0.93	0.12	78,78,78,78	0
60	MG	14	3100	1/1	0.93	0.26	49,49,49,49	0
60	MG	14	3036	1/1	0.93	0.35	66,66,66,66	0
60	MG	1H	3048	1/1	0.93	0.20	51,51,51,51	0
60	MG	14	3177	1/1	0.93	0.23	61,61,61,61	0
60	MG	14	3259	1/1	0.93	0.16	76,76,76,76	0
60	MG	1H	3300	1/1	0.93	0.18	52,52,52,52	0
60	MG	13	1684	1/1	0.93	0.31	66,66,66,66	0
60	MG	1H	3291	1/1	0.94	0.23	71,71,71,71	0
60	MG	1H	3036	1/1	0.94	0.27	52,52,52,52	0
60	MG	13	1612	1/1	0.94	0.18	67,67,67,67	0
60	MG	1H	3038	1/1	0.94	0.30	59,59,59,59	0
60	MG	1H	3011	1/1	0.94	0.16	37,37,37,37	0
60	MG	14	3099	1/1	0.94	0.20	58,58,58,58	0
60	MG	1H	3108	1/1	0.94	0.36	77,77,77,77	0
60	MG	14	3101	1/1	0.94	0.37	65,65,65,65	0
60	MG	14	3262	1/1	0.94	0.20	63,63,63,63	0
60	MG	14	3176	1/1	0.94	0.22	67,67,67,67	0
60	MG	1H	3183	1/1	0.94	0.24	61,61,61,61	0
60	MG	13	1619	1/1	0.94	0.22	70,70,70,70	0
60	MG	1H	3092	1/1	0.94	0.15	44,44,44,44	0
60	MG	14	3106	1/1	0.94	0.23	62,62,62,62	0
60	MG	98	201	1/1	0.94	0.21	62,62,62,62	0
60	MG	1G	1637	1/1	0.94	0.31	67,67,67,67	0
60	MG	1G	1684	1/1	0.94	0.13	91,91,91,91	0
60	MG	1H	3137	1/1	0.94	0.31	72,72,72,72	0
60	MG	1H	3302	1/1	0.94	0.27	67,67,67,67	0
60	MG	1H	3015	1/1	0.94	0.14	56,56,56,56	0
60	MG	14	3116	1/1	0.94	0.31	53,53,53,53	0
60	MG	1H	3190	1/1	0.94	0.23	61,61,61,61	0
60	MG	K8	101	1/1	0.94	0.20	69,69,69,69	0
60	MG	14	3196	1/1	0.94	0.26	82,82,82,82	0
60	MG	14	3197	1/1	0.94	0.28	79,79,79,79	0
60	MG	P8	101	1/1	0.94	0.28	70,70,70,70	0
60	MG	14	3199	1/1	0.94	0.35	66,66,66,66	0
60	MG	1G	1700	1/1	0.94	0.10	152,152,152,152	0
60	MG	13	1658	1/1	0.94	0.10	57,57,57,57	0
60	MG	13	1609	1/1	0.94	0.29	64,64,64,64	0
60	MG	1H	3018	1/1	0.94	0.18	53,53,53,53	0
60	MG	52	201	1/1	0.94	0.09	77,77,77,77	0
60	MG	1H	3316	1/1	0.94	0.07	42,42,42,42	0
60	MG	1H	3019	1/1	0.94	0.16	33,33,33,33	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
60	MG	1H	3005	1/1	0.94	0.22	47,47,47,47	0
60	MG	14	3293	1/1	0.94	0.10	85,85,85,85	0
60	MG	14	3002	1/1	0.94	0.20	50,50,50,50	0
60	MG	14	3003	1/1	0.94	0.19	45,45,45,45	0
60	MG	14	3004	1/1	0.94	0.22	53,53,53,53	0
60	MG	13	1639	1/1	0.94	0.16	93,93,93,93	0
60	MG	1G	1652	1/1	0.94	0.36	72,72,72,72	0
60	MG	1H	3365	1/1	0.94	0.11	88,88,88,88	0
60	MG	14	3066	1/1	0.94	0.26	47,47,47,47	0
60	MG	14	3068	1/1	0.94	0.24	53,53,53,53	0
60	MG	1H	3198	1/1	0.94	0.23	64,64,64,64	0
60	MG	14	3304	1/1	0.94	0.24	66,66,66,66	0
60	MG	14	3138	1/1	0.94	0.36	50,50,50,50	0
60	MG	14	3139	1/1	0.94	0.17	53,53,53,53	0
60	MG	1H	3379	1/1	0.94	0.10	75,75,75,75	0
60	MG	1H	3390	1/1	0.94	0.14	74,74,74,74	0
60	MG	14	3224	1/1	0.94	0.24	51,51,51,51	0
60	MG	1H	3080	1/1	0.94	0.18	59,59,59,59	0
60	MG	14	3332	1/1	0.94	0.10	71,71,71,71	0
60	MG	14	3346	1/1	0.94	0.07	108,108,108,108	0
60	MG	1H	3426	1/1	0.94	0.06	112,112,112,112	0
60	MG	1H	3236	1/1	0.94	0.16	55,55,55,55	0
60	MG	14	3378	1/1	0.94	0.09	75,75,75,75	0
60	MG	14	3146	1/1	0.94	0.18	74,74,74,74	0
60	MG	1G	1661	1/1	0.94	0.23	69,69,69,69	0
60	MG	1H	3237	1/1	0.94	0.09	63,63,63,63	0
60	MG	1H	3122	1/1	0.94	0.25	56,56,56,56	0
60	MG	14	3233	1/1	0.94	0.41	69,69,69,69	0
60	MG	1H	3279	1/1	0.94	0.36	71,71,71,71	0
60	MG	14	3151	1/1	0.94	0.18	55,55,55,55	0
60	MG	14	3019	1/1	0.94	0.06	44,44,44,44	0
60	MG	1H	3171	1/1	0.94	0.43	69,69,69,69	0
60	MG	14	3158	1/1	0.94	0.19	54,54,54,54	0
60	MG	14	3243	1/1	0.94	0.31	61,61,61,61	0
60	MG	1H	3054	1/1	0.94	0.29	56,56,56,56	0
60	MG	1G	1667	1/1	0.94	0.27	66,66,66,66	0
60	MG	1H	3204	1/1	0.94	0.33	62,62,62,62	0
60	MG	1G	1623	1/1	0.94	0.42	82,82,82,82	0
60	MG	1H	3008	1/1	0.94	0.20	47,47,47,47	0
60	MG	1H	3150	1/1	0.94	0.29	63,63,63,63	0
60	MG	11	301	1/1	0.94	0.15	42,42,42,42	0
60	MG	1H	3235	1/1	0.95	0.20	59,59,59,59	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
60	MG	1H	3407	1/1	0.95	0.12	76,76,76,76	0
60	MG	1H	3202	1/1	0.95	0.30	43,43,43,43	0
60	MG	1H	3277	1/1	0.95	0.18	59,59,59,59	0
60	MG	1H	3009	1/1	0.95	0.17	48,48,48,48	0
60	MG	14	3077	1/1	0.95	0.15	49,49,49,49	0
60	MG	1H	3432	1/1	0.95	0.06	107,107,107,107	0
60	MG	1H	3051	1/1	0.95	0.32	61,61,61,61	0
60	MG	1H	3438	1/1	0.95	0.12	78,78,78,78	0
60	MG	1H	3205	1/1	0.95	0.36	60,60,60,60	0
60	MG	1H	3135	1/1	0.95	0.15	50,50,50,50	0
60	MG	1H	3156	1/1	0.95	0.24	62,62,62,62	0
60	MG	14	3142	1/1	0.95	0.26	68,68,68,68	0
60	MG	14	3084	1/1	0.95	0.14	60,60,60,60	0
60	MG	1H	3283	1/1	0.95	0.23	64,64,64,64	0
60	MG	1H	3285	1/1	0.95	0.12	61,61,61,61	0
60	MG	16	206	1/1	0.95	0.28	70,70,70,70	0
60	MG	14	3213	1/1	0.95	0.31	69,69,69,69	0
60	MG	1H	3287	1/1	0.95	0.09	54,54,54,54	0
60	MG	13	1641	1/1	0.95	0.38	74,74,74,74	0
60	MG	13	1692	1/1	0.95	0.33	78,78,78,78	0
60	MG	1H	3244	1/1	0.95	0.23	56,56,56,56	0
60	MG	1H	3160	1/1	0.95	0.24	76,76,76,76	0
60	MG	14	3219	1/1	0.95	0.16	48,48,48,48	0
60	MG	14	3220	1/1	0.95	0.10	44,44,44,44	0
60	MG	1H	3185	1/1	0.95	0.23	65,65,65,65	0
60	MG	1H	3247	1/1	0.95	0.18	60,60,60,60	0
60	MG	14	3154	1/1	0.95	0.13	64,64,64,64	0
60	MG	1H	3055	1/1	0.95	0.12	45,45,45,45	0
60	MG	1H	3249	1/1	0.95	0.35	72,72,72,72	0
60	MG	1H	3042	1/1	0.95	0.20	54,54,54,54	0
60	MG	1H	3077	1/1	0.95	0.34	70,70,70,70	0
60	MG	1H	3078	1/1	0.95	0.15	46,46,46,46	0
60	MG	1H	3004	1/1	0.95	0.20	45,45,45,45	0
60	MG	1H	3301	1/1	0.95	0.21	70,70,70,70	0
60	MG	1H	3192	1/1	0.95	0.09	84,84,84,84	0
60	MG	1H	3032	1/1	0.95	0.25	41,41,41,41	0
60	MG	1G	1646	1/1	0.95	0.35	77,77,77,77	0
60	MG	1H	3221	1/1	0.95	0.29	58,58,58,58	0
60	MG	14	3238	1/1	0.95	0.17	56,56,56,56	0
60	MG	14	3312	1/1	0.95	0.10	57,57,57,57	0
60	MG	14	3317	1/1	0.95	0.09	54,54,54,54	0
60	MG	14	3239	1/1	0.95	0.16	83,83,83,83	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
60	MG	14	3108	1/1	0.95	0.29	71,71,71,71	0
60	MG	14	3344	1/1	0.95	0.06	54,54,54,54	0
60	MG	14	3049	1/1	0.95	0.22	53,53,53,53	0
60	MG	1H	3084	1/1	0.95	0.22	43,43,43,43	0
60	MG	14	3051	1/1	0.95	0.19	61,61,61,61	0
60	MG	1H	3085	1/1	0.95	0.21	47,47,47,47	0
60	MG	1H	3124	1/1	0.95	0.36	68,68,68,68	0
60	MG	1H	3264	1/1	0.95	0.27	66,66,66,66	0
60	MG	14	3178	1/1	0.95	0.38	66,66,66,66	0
60	MG	14	3249	1/1	0.95	0.21	61,61,61,61	0
60	MG	14	3179	1/1	0.95	0.16	51,51,51,51	0
60	MG	1H	3322	1/1	0.95	0.09	48,48,48,48	0
60	MG	1H	3059	1/1	0.95	0.26	41,41,41,41	0
60	MG	1H	3332	1/1	0.95	0.10	49,49,49,49	0
60	MG	19	301	1/1	0.95	0.13	87,87,87,87	0
60	MG	13	1649	1/1	0.95	0.19	75,75,75,75	0
60	MG	13	1672	1/1	0.95	0.22	63,63,63,63	0
60	MG	14	3186	1/1	0.95	0.34	62,62,62,62	0
60	MG	14	3061	1/1	0.95	0.31	49,49,49,49	0
60	MG	1H	3007	1/1	0.95	0.18	33,33,33,33	0
60	MG	45	203	1/1	0.95	0.16	66,66,66,66	0
60	MG	1H	3375	1/1	0.95	0.10	48,48,48,48	0
60	MG	1H	3377	1/1	0.95	0.10	60,60,60,60	0
60	MG	13	1734	1/1	0.95	0.07	108,108,108,108	0
60	MG	1H	3233	1/1	0.95	0.38	69,69,69,69	0
60	MG	1H	3384	1/1	0.95	0.06	85,85,85,85	0
60	MG	1H	3024	1/1	0.96	0.06	51,51,51,51	0
60	MG	1H	3275	1/1	0.96	0.16	58,58,58,58	0
60	MG	1H	3052	1/1	0.96	0.08	44,44,44,44	0
60	MG	1H	3071	1/1	0.96	0.30	57,57,57,57	0
60	MG	1H	3013	1/1	0.96	0.22	48,48,48,48	0
60	MG	1H	3364	1/1	0.96	0.08	51,51,51,51	0
60	MG	3I	201	1/1	0.96	0.20	59,59,59,59	0
60	MG	1H	3371	1/1	0.96	0.06	91,91,91,91	0
60	MG	1G	1704	1/1	0.96	0.11	91,91,91,91	0
60	MG	13	1623	1/1	0.96	0.32	76,76,76,76	0
60	MG	1H	3075	1/1	0.96	0.19	41,41,41,41	0
60	MG	14	3160	1/1	0.96	0.21	56,56,56,56	0
60	MG	1H	3041	1/1	0.96	0.33	58,58,58,58	0
60	MG	13	1728	1/1	0.96	0.09	88,88,88,88	0
60	MG	14	3289	1/1	0.96	0.19	65,65,65,65	0
60	MG	1H	3284	1/1	0.96	0.23	66,66,66,66	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
60	MG	1H	3250	1/1	0.96	0.17	68,68,68,68	0
60	MG	14	3053	1/1	0.96	0.45	66,66,66,66	0
60	MG	1H	3396	1/1	0.96	0.09	56,56,56,56	0
60	MG	1H	3286	1/1	0.96	0.20	72,72,72,72	0
60	MG	14	3006	1/1	0.96	0.18	49,49,49,49	0
60	MG	1H	3409	1/1	0.96	0.10	99,99,99,99	0
60	MG	1H	3413	1/1	0.96	0.07	103,103,103,103	0
60	MG	14	3113	1/1	0.96	0.14	58,58,58,58	0
60	MG	14	3172	1/1	0.96	0.09	57,57,57,57	0
60	MG	1H	3415	1/1	0.96	0.09	75,75,75,75	0
60	MG	14	3234	1/1	0.96	0.19	57,57,57,57	0
60	MG	14	3115	1/1	0.96	0.26	39,39,39,39	0
60	MG	13	1730	1/1	0.96	0.06	103,103,103,103	0
60	MG	1H	3125	1/1	0.96	0.15	34,34,34,34	0
60	MG	1H	3081	1/1	0.96	0.18	34,34,34,34	0
60	MG	1H	3290	1/1	0.96	0.14	76,76,76,76	0
60	MG	1H	3433	1/1	0.96	0.08	91,91,91,91	0
60	MG	1H	3082	1/1	0.96	0.22	39,39,39,39	0
60	MG	13	1645	1/1	0.96	0.40	57,57,57,57	0
60	MG	14	3067	1/1	0.96	0.31	48,48,48,48	0
60	MG	13	1628	1/1	0.96	0.40	72,72,72,72	0
60	MG	14	3328	1/1	0.96	0.10	72,72,72,72	0
60	MG	14	3184	1/1	0.96	0.37	75,75,75,75	0
60	MG	14	3247	1/1	0.96	0.31	73,73,73,73	0
60	MG	1H	3228	1/1	0.96	0.13	42,42,42,42	0
60	MG	1H	3176	1/1	0.96	0.14	73,73,73,73	0
60	MG	1H	3260	1/1	0.96	0.14	62,62,62,62	0
60	MG	14	3363	1/1	0.96	0.10	73,73,73,73	0
60	MG	14	3371	1/1	0.96	0.05	106,106,106,106	0
60	MG	14	3073	1/1	0.96	0.25	40,40,40,40	0
60	MG	1H	3261	1/1	0.96	0.16	44,44,44,44	0
60	MG	14	3384	1/1	0.96	0.05	122,122,122,122	0
60	MG	14	3190	1/1	0.96	0.37	68,68,68,68	0
60	MG	14	3191	1/1	0.96	0.24	69,69,69,69	0
60	MG	1H	3177	1/1	0.96	0.24	62,62,62,62	0
60	MG	14	3131	1/1	0.96	0.18	39,39,39,39	0
60	MG	14	3076	1/1	0.96	0.31	44,44,44,44	0
60	MG	13	1738	1/1	0.96	0.09	81,81,81,81	0
60	MG	1H	3179	1/1	0.96	0.25	57,57,57,57	0
60	MG	1H	3062	1/1	0.96	0.14	39,39,39,39	0
60	MG	1H	3266	1/1	0.96	0.12	65,65,65,65	0
60	MG	1H	3206	1/1	0.96	0.17	58,58,58,58	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
60	MG	21	302	1/1	0.96	0.12	64,64,64,64	0
60	MG	14	3265	1/1	0.96	0.19	78,78,78,78	0
60	MG	1H	3268	1/1	0.96	0.20	58,58,58,58	0
60	MG	13	1642	1/1	0.96	0.34	63,63,63,63	0
60	MG	13	1633	1/1	0.96	0.14	46,46,46,46	0
60	MG	1H	3066	1/1	0.96	0.22	36,36,36,36	0
60	MG	1H	3312	1/1	0.96	0.07	45,45,45,45	0
60	MG	1H	3012	1/1	0.96	0.30	49,49,49,49	0
60	MG	1H	3317	1/1	0.96	0.12	74,74,74,74	0
60	MG	1H	3428	1/1	0.97	0.07	102,102,102,102	0
60	MG	1H	3430	1/1	0.97	0.07	95,95,95,95	0
60	MG	13	1694	1/1	0.97	0.05	115,115,115,115	0
60	MG	13	1611	1/1	0.97	0.07	84,84,84,84	0
60	MG	1H	3434	1/1	0.97	0.11	44,44,44,44	0
60	MG	1H	3333	1/1	0.97	0.07	55,55,55,55	0
60	MG	14	3230	1/1	0.97	0.12	51,51,51,51	0
60	MG	1H	3336	1/1	0.97	0.04	88,88,88,88	0
60	MG	1H	3338	1/1	0.97	0.05	83,83,83,83	0
60	MG	1H	3189	1/1	0.97	0.35	62,62,62,62	0
60	MG	1H	3342	1/1	0.97	0.06	59,59,59,59	0
60	MG	1H	3344	1/1	0.97	0.06	47,47,47,47	0
60	MG	14	3236	1/1	0.97	0.23	66,66,66,66	0
60	MG	1H	3350	1/1	0.97	0.09	47,47,47,47	0
60	MG	1H	3352	1/1	0.97	0.06	46,46,46,46	0
60	MG	1H	3355	1/1	0.97	0.09	51,51,51,51	0
60	MG	1H	3357	1/1	0.97	0.08	69,69,69,69	0
60	MG	16	209	1/1	0.97	0.07	81,81,81,81	0
60	MG	1H	3230	1/1	0.97	0.06	39,39,39,39	0
60	MG	1H	3361	1/1	0.97	0.14	78,78,78,78	0
60	MG	1H	3079	1/1	0.97	0.30	39,39,39,39	0
60	MG	13	1726	1/1	0.97	0.06	97,97,97,97	0
60	MG	1H	3121	1/1	0.97	0.12	43,43,43,43	0
60	MG	1H	3139	1/1	0.97	0.15	39,39,39,39	0
60	MG	1H	3157	1/1	0.97	0.17	58,58,58,58	0
60	MG	14	3310	1/1	0.97	0.05	46,46,46,46	0
60	MG	1H	3257	1/1	0.97	0.05	52,52,52,52	0
60	MG	13	1687	1/1	0.97	0.13	73,73,73,73	0
60	MG	14	3251	1/1	0.97	0.28	69,69,69,69	0
60	MG	14	3319	1/1	0.97	0.04	98,98,98,98	0
60	MG	14	3321	1/1	0.97	0.06	78,78,78,78	0
60	MG	14	3325	1/1	0.97	0.07	50,50,50,50	0
60	MG	1H	3094	1/1	0.97	0.12	35,35,35,35	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
60	MG	1H	3387	1/1	0.97	0.05	53,53,53,53	0
60	MG	14	3339	1/1	0.97	0.06	62,62,62,62	0
60	MG	14	3341	1/1	0.97	0.08	66,66,66,66	0
60	MG	13	1660	1/1	0.97	0.36	70,70,70,70	0
60	MG	1H	3393	1/1	0.97	0.09	68,68,68,68	0
60	MG	14	3348	1/1	0.97	0.09	83,83,83,83	0
60	MG	14	3351	1/1	0.97	0.10	93,93,93,93	0
60	MG	1H	3395	1/1	0.97	0.05	69,69,69,69	0
60	MG	14	3357	1/1	0.97	0.04	96,96,96,96	0
60	MG	1H	3001	1/1	0.97	0.17	36,36,36,36	0
60	MG	1H	3401	1/1	0.97	0.09	61,61,61,61	0
60	MG	14	3367	1/1	0.97	0.05	90,90,90,90	0
60	MG	14	3369	1/1	0.97	0.05	79,79,79,79	0
60	MG	14	3370	1/1	0.97	0.06	116,116,116,116	0
60	MG	1H	3403	1/1	0.97	0.08	83,83,83,83	0
60	MG	1G	1694	1/1	0.97	0.08	110,110,110,110	0
60	MG	1G	1695	1/1	0.97	0.06	83,83,83,83	0
60	MG	14	3380	1/1	0.97	0.10	92,92,92,92	0
60	MG	14	3381	1/1	0.97	0.10	79,79,79,79	0
60	MG	14	3382	1/1	0.97	0.06	100,100,100,100	0
60	MG	1G	1696	1/1	0.97	0.05	108,108,108,108	0
60	MG	1G	1698	1/1	0.97	0.07	113,113,113,113	0
60	MG	1G	1699	1/1	0.97	0.11	108,108,108,108	0
60	MG	13	1685	1/1	0.97	0.10	80,80,80,80	0
60	MG	1H	3044	1/1	0.97	0.12	73,73,73,73	0
60	MG	1H	3129	1/1	0.97	0.32	72,72,72,72	0
60	MG	14	3155	1/1	0.97	0.05	63,63,63,63	0
60	MG	14	3156	1/1	0.97	0.11	54,54,54,54	0
60	MG	1J	207	1/1	0.97	0.05	92,92,92,92	0
60	MG	14	3157	1/1	0.97	0.20	69,69,69,69	0
60	MG	14	3048	1/1	0.97	0.24	59,59,59,59	0
60	MG	1G	1603	1/1	0.97	0.10	79,79,79,79	0
60	MG	39	301	1/1	0.97	0.08	86,86,86,86	0
60	MG	1H	3112	1/1	0.97	0.12	62,62,62,62	0
60	MG	25	201	1/1	0.97	0.05	125,125,125,125	0
60	MG	1H	3417	1/1	0.97	0.09	98,98,98,98	0
60	MG	1G	1606	1/1	0.97	0.11	85,85,85,85	0
60	MG	1H	3420	1/1	0.97	0.08	111,111,111,111	0
60	MG	1H	3063	1/1	0.97	0.11	43,43,43,43	0
60	MG	1G	1654	1/1	0.97	0.28	66,66,66,66	0
60	MG	1H	3424	1/1	0.97	0.06	115,115,115,115	0
60	MG	13	1735	1/1	0.97	0.08	153,153,153,153	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
60	MG	1H	3076	1/1	0.97	0.32	44,44,44,44	0
60	MG	1H	3431	1/1	0.98	0.08	73,73,73,73	0
60	MG	1H	3309	1/1	0.98	0.06	56,56,56,56	0
60	MG	14	3320	1/1	0.98	0.05	52,52,52,52	0
60	MG	1H	3310	1/1	0.98	0.06	50,50,50,50	0
60	MG	14	3324	1/1	0.98	0.05	63,63,63,63	0
60	MG	1G	1697	1/1	0.98	0.07	111,111,111,111	0
60	MG	14	3327	1/1	0.98	0.05	58,58,58,58	0
60	MG	1H	3311	1/1	0.98	0.07	42,42,42,42	0
60	MG	14	3329	1/1	0.98	0.06	65,65,65,65	0
60	MG	13	1679	1/1	0.98	0.05	70,70,70,70	0
60	MG	14	3333	1/1	0.98	0.05	55,55,55,55	0
60	MG	14	3334	1/1	0.98	0.05	80,80,80,80	0
60	MG	14	3336	1/1	0.98	0.06	80,80,80,80	0
60	MG	1H	3366	1/1	0.98	0.06	53,53,53,53	0
60	MG	14	3340	1/1	0.98	0.04	50,50,50,50	0
60	MG	1H	3314	1/1	0.98	0.05	38,38,38,38	0
60	MG	1H	3374	1/1	0.98	0.08	86,86,86,86	0
60	MG	1H	3068	1/1	0.98	0.19	52,52,52,52	0
60	MG	14	3347	1/1	0.98	0.07	83,83,83,83	0
60	MG	1H	3216	1/1	0.98	0.29	73,73,73,73	0
60	MG	14	3086	1/1	0.98	0.33	48,48,48,48	0
60	MG	14	3354	1/1	0.98	0.05	74,74,74,74	0
60	MG	14	3355	1/1	0.98	0.07	68,68,68,68	0
60	MG	1H	3319	1/1	0.98	0.06	46,46,46,46	0
60	MG	1H	3113	1/1	0.98	0.31	53,53,53,53	0
60	MG	1H	3380	1/1	0.98	0.05	53,53,53,53	0
60	MG	14	3361	1/1	0.98	0.04	60,60,60,60	0
60	MG	14	3044	1/1	0.98	0.16	39,39,39,39	0
60	MG	14	3364	1/1	0.98	0.06	89,89,89,89	0
60	MG	14	3365	1/1	0.98	0.07	90,90,90,90	0
60	MG	13	1704	1/1	0.98	0.07	71,71,71,71	0
60	MG	14	3368	1/1	0.98	0.04	83,83,83,83	0
60	MG	1H	3329	1/1	0.98	0.05	51,51,51,51	0
60	MG	16	210	1/1	0.98	0.04	64,64,64,64	0
60	MG	16	211	1/1	0.98	0.07	87,87,87,87	0
60	MG	14	3372	1/1	0.98	0.06	79,79,79,79	0
60	MG	14	3376	1/1	0.98	0.05	91,91,91,91	0
60	MG	16	212	1/1	0.98	0.05	71,71,71,71	0
60	MG	1H	3330	1/1	0.98	0.04	51,51,51,51	0
60	MG	1H	3331	1/1	0.98	0.09	44,44,44,44	0
60	MG	13	1717	1/1	0.98	0.05	63,63,63,63	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
60	MG	1H	3128	1/1	0.98	0.26	49,49,49,49	0
60	MG	14	3383	1/1	0.98	0.04	101,101,101,101	0
60	MG	1H	3399	1/1	0.98	0.04	60,60,60,60	0
60	MG	1H	3400	1/1	0.98	0.07	82,82,82,82	0
60	MG	1H	3335	1/1	0.98	0.07	74,74,74,74	0
60	MG	14	3103	1/1	0.98	0.16	55,55,55,55	0
60	MG	1H	3402	1/1	0.98	0.04	109,109,109,109	0
60	MG	1H	3040	1/1	0.98	0.06	58,58,58,58	0
60	MG	1K	101	1/1	0.98	0.04	93,93,93,93	0
60	MG	1H	3269	1/1	0.98	0.06	58,58,58,58	0
60	MG	14	3298	1/1	0.98	0.30	64,64,64,64	0
60	MG	1H	3410	1/1	0.98	0.04	87,87,87,87	0
60	MG	1H	3412	1/1	0.98	0.04	93,93,93,93	0
60	MG	13	1719	1/1	0.98	0.04	74,74,74,74	0
60	MG	13	1720	1/1	0.98	0.05	96,96,96,96	0
60	MG	1H	3345	1/1	0.98	0.04	65,65,65,65	0
60	MG	1H	3349	1/1	0.98	0.13	58,58,58,58	0
60	MG	13	1723	1/1	0.98	0.03	85,85,85,85	0
60	MG	1H	3226	1/1	0.98	0.09	41,41,41,41	0
60	MG	14	3069	1/1	0.98	0.51	78,78,78,78	0
60	MG	13	1670	1/1	0.98	0.08	66,66,66,66	0
60	MG	1H	3356	1/1	0.98	0.06	54,54,54,54	0
60	MG	13	1727	1/1	0.98	0.05	86,86,86,86	0
60	MG	1H	3429	1/1	0.98	0.12	61,61,61,61	0
61	ZN	5A	101	1/1	0.98	0.05	129,129,129,129	0
60	MG	1H	3359	1/1	0.98	0.04	83,83,83,83	0
60	MG	1H	3435	1/1	0.99	0.03	36,36,36,36	0
60	MG	14	3322	1/1	0.99	0.03	42,42,42,42	0
60	MG	14	3323	1/1	0.99	0.05	57,57,57,57	0
60	MG	1H	3436	1/1	0.99	0.08	63,63,63,63	0
60	MG	1H	3324	1/1	0.99	0.03	45,45,45,45	0
60	MG	14	3326	1/1	0.99	0.04	54,54,54,54	0
60	MG	1H	3381	1/1	0.99	0.03	41,41,41,41	0
60	MG	1H	3382	1/1	0.99	0.04	68,68,68,68	0
60	MG	1H	3346	1/1	0.99	0.07	67,67,67,67	0
60	MG	14	3330	1/1	0.99	0.05	58,58,58,58	0
60	MG	14	3331	1/1	0.99	0.04	51,51,51,51	0
60	MG	1H	3385	1/1	0.99	0.02	66,66,66,66	0
60	MG	1H	3386	1/1	0.99	0.03	53,53,53,53	0
60	MG	13	1732	1/1	0.99	0.04	86,86,86,86	0
60	MG	14	3335	1/1	0.99	0.04	60,60,60,60	0
60	MG	1H	3388	1/1	0.99	0.04	57,57,57,57	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
60	MG	14	3338	1/1	0.99	0.04	52,52,52,52	0
60	MG	1H	3389	1/1	0.99	0.05	47,47,47,47	0
60	MG	1H	3327	1/1	0.99	0.08	45,45,45,45	0
60	MG	1H	3391	1/1	0.99	0.05	58,58,58,58	0
60	MG	14	3342	1/1	0.99	0.04	48,48,48,48	0
60	MG	1H	3392	1/1	0.99	0.04	53,53,53,53	0
60	MG	14	3345	1/1	0.99	0.04	69,69,69,69	0
60	MG	1H	3351	1/1	0.99	0.06	68,68,68,68	0
60	MG	14	3271	1/1	0.99	0.07	67,67,67,67	0
60	MG	1H	3328	1/1	0.99	0.04	50,50,50,50	0
60	MG	14	3349	1/1	0.99	0.03	61,61,61,61	0
60	MG	14	3350	1/1	0.99	0.04	65,65,65,65	0
60	MG	1H	3353	1/1	0.99	0.04	51,51,51,51	0
60	MG	14	3353	1/1	0.99	0.06	72,72,72,72	0
60	MG	1G	1691	1/1	0.99	0.05	85,85,85,85	0
60	MG	1G	1692	1/1	0.99	0.07	67,67,67,67	0
60	MG	1G	1693	1/1	0.99	0.04	76,76,76,76	0
60	MG	1H	3397	1/1	0.99	0.06	50,50,50,50	0
60	MG	1H	3398	1/1	0.99	0.06	71,71,71,71	0
60	MG	14	3360	1/1	0.99	0.03	103,103,103,103	0
60	MG	1H	3354	1/1	0.99	0.04	39,39,39,39	0
60	MG	14	3362	1/1	0.99	0.03	74,74,74,74	0
60	MG	13	1733	1/1	0.99	0.07	75,75,75,75	0
60	MG	13	1721	1/1	0.99	0.04	80,80,80,80	0
60	MG	13	1722	1/1	0.99	0.08	82,82,82,82	0
60	MG	14	3366	1/1	0.99	0.05	102,102,102,102	0
60	MG	1H	3358	1/1	0.99	0.03	55,55,55,55	0
60	MG	1H	3404	1/1	0.99	0.08	79,79,79,79	0
60	MG	1H	3405	1/1	0.99	0.05	73,73,73,73	0
60	MG	1H	3406	1/1	0.99	0.03	44,44,44,44	0
60	MG	14	3287	1/1	0.99	0.03	57,57,57,57	0
60	MG	1H	3313	1/1	0.99	0.05	36,36,36,36	0
60	MG	14	3373	1/1	0.99	0.04	65,65,65,65	0
60	MG	14	3374	1/1	0.99	0.02	107,107,107,107	0
60	MG	14	3375	1/1	0.99	0.03	90,90,90,90	0
60	MG	98	202	1/1	0.99	0.14	69,69,69,69	0
60	MG	14	3377	1/1	0.99	0.15	71,71,71,71	0
60	MG	13	1718	1/1	0.99	0.04	54,54,54,54	0
60	MG	1H	3334	1/1	0.99	0.04	59,59,59,59	0
60	MG	1H	3411	1/1	0.99	0.04	68,68,68,68	0
60	MG	14	3001	1/1	0.99	0.03	44,44,44,44	0
60	MG	1H	3362	1/1	0.99	0.07	47,47,47,47	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
60	MG	1H	3363	1/1	0.99	0.04	52,52,52,52	0
60	MG	1H	3414	1/1	0.99	0.04	75,75,75,75	0
60	MG	14	3385	1/1	0.99	0.04	44,44,44,44	0
60	MG	1H	3315	1/1	0.99	0.04	59,59,59,59	0
60	MG	13	1737	1/1	0.99	0.04	91,91,91,91	0
60	MG	1H	3418	1/1	0.99	0.03	81,81,81,81	0
60	MG	1H	3419	1/1	0.99	0.03	99,99,99,99	0
60	MG	1H	3337	1/1	0.99	0.04	66,66,66,66	0
60	MG	1H	3367	1/1	0.99	0.10	56,56,56,56	0
60	MG	1H	3422	1/1	0.99	0.03	87,87,87,87	0
60	MG	1H	3423	1/1	0.99	0.06	60,60,60,60	0
60	MG	1H	3369	1/1	0.99	0.04	46,46,46,46	0
60	MG	1H	3425	1/1	0.99	0.04	60,60,60,60	0
60	MG	1H	3370	1/1	0.99	0.03	45,45,45,45	0
60	MG	1H	3234	1/1	0.99	0.29	53,53,53,53	0
60	MG	1H	3372	1/1	0.99	0.02	61,61,61,61	0
60	MG	13	1725	1/1	0.99	0.04	96,96,96,96	0
60	MG	14	3311	1/1	0.99	0.04	58,58,58,58	0
60	MG	1H	3340	1/1	0.99	0.03	65,65,65,65	0
60	MG	14	3313	1/1	0.99	0.03	53,53,53,53	0
60	MG	14	3314	1/1	0.99	0.04	63,63,63,63	0
60	MG	14	3316	1/1	0.99	0.04	58,58,58,58	0
60	MG	1H	3376	1/1	0.99	0.05	43,43,43,43	0
61	ZN	3E	301	1/1	0.99	0.25	90,90,90,90	0
61	ZN	5I	102	1/1	0.99	0.02	90,90,90,90	0
60	MG	1H	3341	1/1	0.99	0.05	77,77,77,77	0
61	ZN	32	301	1/1	0.99	0.23	108,108,108,108	0
60	MG	1H	3308	1/1	0.99	0.05	39,39,39,39	0
60	MG	1H	3323	1/1	0.99	0.05	58,58,58,58	0
60	MG	1H	3348	1/1	1.00	0.03	82,82,82,82	0
60	MG	1H	3325	1/1	1.00	0.04	41,41,41,41	0
60	MG	14	3315	1/1	1.00	0.03	52,52,52,52	0
60	MG	14	3352	1/1	1.00	0.04	77,77,77,77	0
60	MG	1H	3383	1/1	1.00	0.02	64,64,64,64	0
60	MG	13	1731	1/1	1.00	0.02	63,63,63,63	0
60	MG	1H	3320	1/1	1.00	0.03	41,41,41,41	0
60	MG	1H	3373	1/1	1.00	0.02	70,70,70,70	0
60	MG	14	3337	1/1	1.00	0.06	59,59,59,59	0
60	MG	1H	3416	1/1	1.00	0.03	55,55,55,55	0
60	MG	14	3359	1/1	1.00	0.03	69,69,69,69	0
60	MG	1H	3321	1/1	1.00	0.03	57,57,57,57	0
60	MG	1H	3343	1/1	1.00	0.03	44,44,44,44	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
60	MG	13	1729	1/1	1.00	0.03	76,76,76,76	0
60	MG	13	1724	1/1	1.00	0.02	82,82,82,82	0
60	MG	14	3343	1/1	1.00	0.04	46,46,46,46	0
60	MG	1H	3318	1/1	1.00	0.02	45,45,45,45	0
60	MG	1H	3347	1/1	1.00	0.02	70,70,70,70	0
60	MG	1H	3368	1/1	1.00	0.05	46,46,46,46	0
60	MG	1H	3408	1/1	1.00	0.02	50,50,50,50	0
60	MG	1H	3394	1/1	1.00	0.02	43,43,43,43	0

5.5 Other polymers [i](#)

There are no such residues in this entry.