Full wwPDB X-ray Structure Validation Report (i)

Sep 16, 2026 – 06:10 am BST

PDB ID	:	5IB8 / pdb_00005ib8
Title	:	Structure of T. thermophilus 70S ribosome complex with mRNA, tRNAfMet and near-cognate tRNALys with U-G mismatch in the A-site
Authors	:	Rozov, A.; Demeshkina, N.; Yusupov, M.; Yusupova, G.
Deposited on	:	2016-02-22
Resolution	:	3.13 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 (i) 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 (i)) were used in the production of this report:

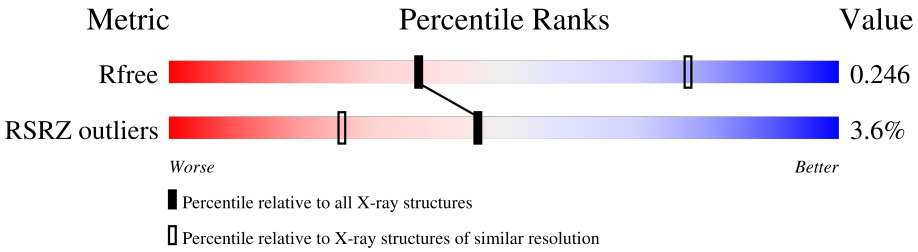
MolProbity	:	FAILED
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.13 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	2351 (3.18-3.10)
RSRZ outliers	180081	2351 (3.18-3.10)

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
57	MG	13	1659	-	-	-	X
57	MG	13	1668	-	-	-	X
57	MG	14	3103	-	-	-	X
57	MG	14	3133	-	-	-	X
57	MG	14	3134	-	-	-	X
57	MG	14	3147	-	-	-	X
57	MG	1G	1621	-	-	-	X
57	MG	1G	1642	-	-	-	X
57	MG	1H	3130	-	-	-	X
57	MG	1H	3159	-	-	-	X
57	MG	1H	3167	-	-	-	X
57	MG	E5	101	-	-	-	X

2 Entry composition (i)

There are 61 unique types of molecules in this entry. The entry contains 296999 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	1500	Total	C	N	O	P	0	0	0
			32246	14352	5978	10416	1500			
1	1G	1509	Total	C	N	O	P	0	0	0
			32437	14437	6010	10481	1509			

There are 2 discrepancies between the modelled and reference sequences:

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	1E	231	Total	C	N	O	S	0	0	0
			1874	1199	334	336	5			
2	12	207	Total	C	N	O	S	0	0	0
			1696	1083	306	303	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	2E	205	Total	C	N	O	S	0	0	0
			1605	1011	313	280	1			
3	22	195	Total	C	N	O	S	0	0	0
			1537	973	297	266	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	3E	207	Total	C	N	O	S	0	0	0
			1698	1064	338	289	7			

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	4E	149	Total	C	N	O	S	0	0	0
			1142	722	216	200	4			
5	42	150	Total	C	N	O	S	0	0	0
			1141	719	217	201	4			

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
9	8E	126	Total	C	N	O	0	0	0
			1000	634	196	170			
9	82	121	Total	C	N	O	0	0	0
			953	605	186	162			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	1I	94	Total	C	N	O	S	0	0	0
			749	468	147	133	1			
10	1A	80	Total	C	N	O		0	0	0
			646	403	129	114				

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	2I	111	Total	C	N	O	S	0	0	0
			823	512	154	154	3			
11	2A	113	Total	C	N	O	S	0	0	0
			835	520	156	156	3			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	3I	122	Total	C	N	O	S	0	0	0
			956	603	193	159	1			
12	3A	121	Total	C	N	O	S	0	0	0
			947	597	191	158	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	4I	117	Total	C	N	O	S	0	0	0
			933	577	192	162	2			
13	4A	109	Total	C	N	O	S	0	0	0
			879	544	181	152	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	5I	59	Total	C	N	O	S	0	0	0
			486	309	103	70	4			
14	5A	59	Total	C	N	O	S	0	0	0
			486	309	103	70	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	6I	87	Total	C	N	O	S	0	0	0
			729	457	146	124	2			
15	6A	87	Total	C	N	O	S	0	0	0
			729	457	146	124	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	7I	83	Total	C	N	O	S	0	0	0
			700	443	139	117	1			
16	7A	84	Total	C	N	O	S	0	0	0
			705	446	140	118	1			

- Molecule 17 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	8I	100	Total	C	N	O	S	0	0	0
			834	534	155	143	2			
17	8A	99	Total	C	N	O	S	0	0	0
			823	528	151	142	2			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
18	9I	68	Total	C	N	O	0	0	0
			549	352	105	92			
18	9A	67	Total	C	N	O	0	0	0
			544	349	104	91			

- Molecule 19 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	AI	82	Total	C	N	O	S	0	0	0
			661	422	123	114	2			
19	AA	65	Total	C	N	O	S	0	0	0
			510	324	92	92	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	BI	97	Total	C	N	O	S	0	0	0
			746	461	157	126	2			

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

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

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

- Molecule 22 is a RNA chain called tRNALys.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
22	1K	72	Total	C	N	O	P	S	0	0	0
			1542	691	269	509	72	1			

- Molecule 23 is a RNA chain called tRNAfMet.

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

- Molecule 24 is a RNA chain called tRNALys.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	3K	70	Total	C	N	O	P	0	0	0
			1483	664	260	490	69			
24	3L	72	Total	C	N	O	P	0	0	0
			1528	684	270	503	71			

- Molecule 25 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
25	4K	20	Total	C	N	O	P	0	0	0
			442	198	94	130	20			
25	4L	19	Total	C	N	O	P	0	0	0
			419	188	89	123	19			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	1H	2831	Total	C	N	O	P	0	0	0
			60991	27142	11416	19602	2831			
26	14	2825	Total	C	N	O	P	0	0	0
			60857	27083	11390	19559	2825			

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
1H	161	U	UNK	conflict	GB 55771382
1H	654A	A	G	conflict	GB 55771382
1H	654E	C	G	conflict	GB 55771382
1H	654P	G	C	conflict	GB 55771382
1H	654T	A	C	conflict	GB 55771382
1H	1058	U	G	conflict	GB 55771382
1H	1080	A	C	conflict	GB 55771382
14	158	U	UNK	conflict	GB 55771382
14	654A	A	G	conflict	GB 55771382
14	654E	C	G	conflict	GB 55771382
14	654P	G	C	conflict	GB 55771382
14	654T	A	C	conflict	GB 55771382
14	1058	U	G	conflict	GB 55771382
14	1080	A	C	conflict	GB 55771382

- Molecule 27 is a RNA chain called 5S ribosomal RNA.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
28	71	132	Total	C	N	O	S	0	0	0
			1027	648	193	185	1			

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

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

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
29	19	274	Total	C	N	O	S	0	0	0
			2125	1341	422	359	3			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
30	21	203	Total	C	N	O	S	0	0	0
			1546	978	295	267	6			
30	29	204	Total	C	N	O	S	0	0	0
			1563	988	299	270	6			

- Molecule 31 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
31	31	202	Total	C	N	O	S	0	0	0
			1585	1011	297	275	2			
31	39	204	Total	C	N	O	S	0	0	0
			1602	1022	299	279	2			

- Molecule 32 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
32	41	179	Total	C	N	O	S	0	0	0
			1457	931	265	257	4			
32	49	180	Total	C	N	O	S	0	0	0
			1459	931	266	258	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
33	51	174	Total	C	N	O	S	0	0	0
			1328	842	249	236	1			
33	59	169	Total	C	N	O	S	0	0	0
			1295	823	241	230	1			

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
35	58	137	Total	C	N	O	S	0	0	0
			1096	706	205	181	4			
35	15	137	Total	C	N	O	S	0	0	0
			1096	707	205	181	3			

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
37	78	147	Total	C	N	O	S	0	0	0
			1122	698	229	192	3			
37	35	147	Total	C	N	O	S	0	0	0
			1122	698	229	192	3			

- Molecule 38 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
38	88	141	Total	C	N	O	S	0	0	0
			1117	712	211	187	7			
38	45	138	Total	C	N	O	S	0	0	0
			1099	702	208	183	6			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
39	98	118	Total	C	N	O	S	0	0	0
			967	604	203	159	1			
39	55	118	Total	C	N	O	S	0	0	0
			967	604	203	159	1			

- Molecule 40 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
40	A8	111	Total 881	C 556	N 176	O 149	0	0	0
40	65	110	Total 876	C 553	N 175	O 148	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
41	B8	135	Total 1119	C 697	N 230	O 191	S 1	0	0	0
41	75	133	Total 1109	C 691	N 228	O 189	S 1	0	0	0

- Molecule 42 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
42	C8	115	Total 950	C 603	N 199	O 147	S 1	0	0	0
42	85	116	Total 959	C 608	N 201	O 149	S 1	0	0	0

- Molecule 43 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
43	D8	100	Total 774	C 499	N 141	O 133	S 1	0	0	0
43	95	100	Total 770	C 496	N 140	O 133	S 1	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
44	E8	110	Total 876	C 552	N 171	O 151	S 2	0	0	0
44	A5	111	Total 886	C 558	N 174	O 152	S 2	0	0	0

- Molecule 45 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
45	F8	95	Total 750	C 488	N 135	O 126	S 1	0	0	0

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
45	B5	94	Total	C	N	O	0	0	0
			735	477	133	125			

- Molecule 46 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
46	G8	103	Total	C	N	O	S	0	0	0
			783	504	148	126	5			
46	C5	104	Total	C	N	O	S	0	0	0
			794	510	152	127	5			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
47	H8	170	Total	C	N	O	S	0	0	0
			1365	870	246	246	3			
47	D5	177	Total	C	N	O	S	0	0	0
			1411	901	253	255	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
48	I8	77	Total	C	N	O	S	0	0	0
			611	378	129	103	1			
48	E5	76	Total	C	N	O	S	0	0	0
			603	372	128	102	1			

- Molecule 49 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
49	J8	96	Total	C	N	O	S	0	0	0
			747	469	148	129	1			
49	F5	94	Total	C	N	O	S	0	0	0
			737	463	146	127	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
50	K8	68	Total	C	N	O	S	0	0	0
			575	358	116	100	1			
50	G5	69	Total	C	N	O	S	0	0	0
			576	358	116	101	1			

- Molecule 51 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
51	L8	58	Total	C	N	O	0	0	0
			459	293	89	77			
51	H5	58	Total	C	N	O	0	0	0
			459	293	89	77			

- Molecule 52 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
52	M8	60	Total	C	N	O	S	0	0	0
			475	300	84	86	5			

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

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

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

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

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

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

- Molecule 56 is a RNA chain called tRNALys.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
56	1L	66	Total	C	N	O	P	0	0	0
			1402	627	244	465	66			

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

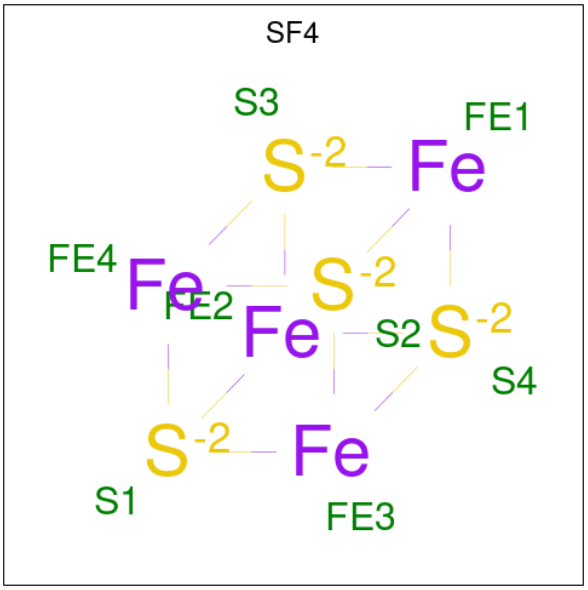
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
57	13	141	Total Mg 141 141	0	0
57	2I	1	Total Mg 1 1	0	0
57	3I	1	Total Mg 1 1	0	0
57	2K	3	Total Mg 3 3	0	0
57	1H	552	Total Mg 552 552	0	0
57	16	12	Total Mg 12 12	0	0
57	21	3	Total Mg 3 3	0	0
57	31	1	Total Mg 1 1	0	0
57	41	1	Total Mg 1 1	0	0
57	88	3	Total Mg 3 3	0	0
57	F8	1	Total Mg 1 1	0	0
57	I8	2	Total Mg 2 2	0	0
57	P8	1	Total Mg 1 1	0	0
57	Q8	1	Total Mg 1 1	0	0
57	1G	125	Total Mg 125 125	0	0
57	32	1	Total Mg 1 1	0	0
57	42	2	Total Mg 2 2	0	0
57	52	1	Total Mg 1 1	0	0
57	7A	1	Total Mg 1 1	0	0
57	2L	2	Total Mg 2 2	0	0
57	4L	1	Total Mg 1 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
57	14	460	Total Mg 460 460	0	0
57	1J	10	Total Mg 10 10	0	0
57	19	1	Total Mg 1 1	0	0
57	29	1	Total Mg 1 1	0	0
57	39	1	Total Mg 1 1	0	0
57	25	1	Total Mg 1 1	0	0
57	35	2	Total Mg 2 2	0	0
57	45	1	Total Mg 1 1	0	0
57	B5	1	Total Mg 1 1	0	0
57	E5	2	Total Mg 2 2	0	0
57	M5	1	Total Mg 1 1	0	0

- Molecule 58 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4).

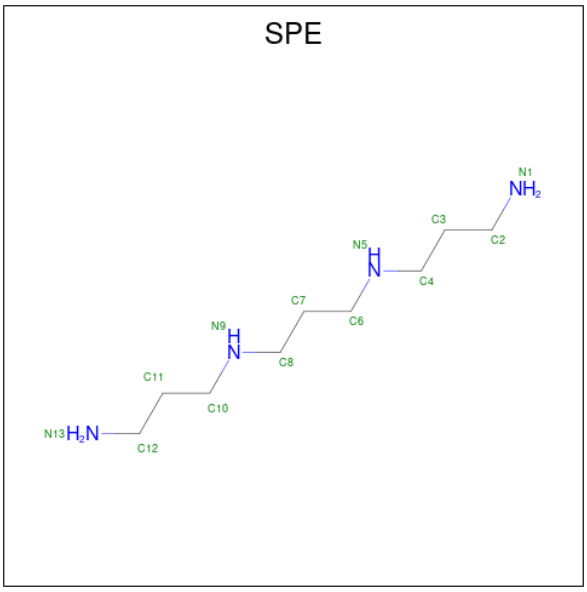


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
58	3E	1	Total Fe S 8 4 4	0	0
58	32	1	Total Fe S 8 4 4	0	0

- Molecule 59 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
59	5I	1	Total Zn 1 1	0	0
59	G8	1	Total Zn 1 1	0	0
59	5A	1	Total Zn 1 1	0	0
59	C5	1	Total Zn 1 1	0	0

- Molecule 60 is THERMINE (CCD ID: SPE) (formula: $C_9H_{24}N_4$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
60	1G	1	Total C N 13 9 4	0	0
60	14	1	Total C N 13 9 4	0	0

- Molecule 61 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
61	13	354	Total O 354 354	0	0
61	3E	2	Total O 2 2	0	0
61	4E	3	Total O 3 3	0	0
61	8E	2	Total O 2 2	0	0
61	1I	2	Total O 2 2	0	0
61	3I	2	Total O 2 2	0	0
61	5I	1	Total O 1 1	0	0
61	7I	2	Total O 2 2	0	0
61	BI	3	Total O 3 3	0	0
61	1K	1	Total O 1 1	0	0
61	2K	8	Total O 8 8	0	0
61	3K	1	Total O 1 1	0	0
61	4K	5	Total O 5 5	0	0
61	1H	1720	Total O 1720 1720	0	0
61	16	12	Total O 12 12	0	0
61	11	10	Total O 10 10	0	0
61	21	6	Total O 6 6	0	0
61	31	6	Total O 6 6	0	0
61	58	2	Total O 2 2	0	0
61	68	2	Total O 2 2	0	0
61	78	13	Total O 13 13	0	0
61	98	1	Total O 1 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
61	B8	1	Total O 1 1	0	0
61	C8	4	Total O 4 4	0	0
61	E8	1	Total O 1 1	0	0
61	F8	3	Total O 3 3	0	0
61	G8	3	Total O 3 3	0	0
61	I8	6	Total O 6 6	0	0
61	J8	5	Total O 5 5	0	0
61	L8	4	Total O 4 4	0	0
61	N8	1	Total O 1 1	0	0
61	Q8	5	Total O 5 5	0	0
61	1G	364	Total O 364 364	0	0
61	32	4	Total O 4 4	0	0
61	42	1	Total O 1 1	0	0
61	52	4	Total O 4 4	0	0
61	1A	2	Total O 2 2	0	0
61	2A	1	Total O 1 1	0	0
61	4A	2	Total O 2 2	0	0
61	6A	3	Total O 3 3	0	0
61	7A	4	Total O 4 4	0	0
61	9A	2	Total O 2 2	0	0
61	BA	3	Total O 3 3	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
61	2L	8	Total O 8 8	0	0
61	4L	3	Total O 3 3	0	0
61	14	1303	Total O 1303 1303	0	0
61	1J	27	Total O 27 27	0	0
61	19	14	Total O 14 14	0	0
61	29	6	Total O 6 6	0	0
61	39	8	Total O 8 8	0	0
61	15	3	Total O 3 3	0	0
61	25	8	Total O 8 8	0	0
61	35	8	Total O 8 8	0	0
61	55	1	Total O 1 1	0	0
61	75	1	Total O 1 1	0	0
61	85	1	Total O 1 1	0	0
61	B5	1	Total O 1 1	0	0
61	C5	3	Total O 3 3	0	0
61	F5	1	Total O 1 1	0	0
61	H5	1	Total O 1 1	0	0
61	L5	1	Total O 1 1	0	0
61	M5	8	Total O 8 8	0	0

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

3 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	209.15Å 448.16Å 617.80Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	154.45 – 3.13 154.45 – 3.13	Depositor EDS
% Data completeness (in resolution range)	100.0 (154.45-3.13) 90.9 (154.45-3.13)	Depositor EDS
R_{merge}	0.42	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	0.81 (at 3.13Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.192 , 0.244 0.195 , 0.246	Depositor DCC
R_{free} test set	2000 reflections (0.20%)	wwPDB-VP
Wilson B-factor (Å^2)	89.4	Xtriage
Anisotropy	0.275	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 74.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	296999	wwPDB-VP
Average B, all atoms (Å^2)	109.0	wwPDB-VP

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

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

4 Model quality

4.1 Standard geometry

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

4.2 Too-close contacts

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

4.3 Torsion angles

4.3.1 Protein backbone

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

4.3.2 Protein sidechains

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

4.3.3 RNA

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

4.4 Non-standard residues in protein, DNA, RNA chains

18 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	$\#\|Z\| > 2$
56	5MU	1L	54	56	19,22,23	3.97	5 (26%)	28,32,35	3.19	9 (32%)
22	PSU	1K	55	22	18,21,22	1.17	1 (5%)	22,30,33	1.72	4 (18%)
22	U8U	1K	34	25,22	19,24,25	2.50	7 (36%)	23,34,37	1.25	3 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
23	OMC	2L	33	23	19,22,23	1.79	3 (15%)	26,31,34	0.82	0
23	5MU	2K	55	23	19,22,23	3.79	5 (26%)	28,32,35	3.27	10 (35%)
22	H2U	1K	17	22	18,21,22	2.07	4 (22%)	21,30,33	2.18	5 (23%)
22	PSU	1K	39	22	18,21,22	1.20	1 (5%)	22,30,33	1.58	3 (13%)
23	4SU	2L	8	23	18,21,22	1.90	3 (16%)	26,30,33	2.45	5 (19%)
23	OMC	2K	33	23	19,22,23	1.72	3 (15%)	26,31,34	0.89	1 (3%)
23	7MG	2K	47	23	22,26,27	3.31	6 (27%)	29,39,42	3.07	12 (41%)
23	7MG	2L	47	23	22,26,27	2.84	6 (27%)	29,39,42	2.98	10 (34%)
23	5MU	2L	55	23	19,22,23	3.96	5 (26%)	28,32,35	3.17	8 (28%)
23	PSU	2L	56	23	18,21,22	1.34	2 (11%)	22,30,33	1.73	3 (13%)
56	PSU	1L	55	56	18,21,22	1.27	1 (5%)	22,30,33	1.62	4 (18%)
22	T6A	1K	37	22	31,34,35	2.23	8 (25%)	44,49,52	2.28	12 (27%)
23	4SU	2K	8	23	18,21,22	1.57	3 (16%)	26,30,33	2.62	5 (19%)
22	5MU	1K	54	22	19,22,23	3.97	5 (26%)	28,32,35	3.00	9 (32%)
23	PSU	2K	56	23	18,21,22	1.19	2 (11%)	22,30,33	1.91	4 (18%)

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
56	5MU	1L	54	56	-	3/7/25/26	0/2/2/2
22	PSU	1K	55	22	-	0/7/25/26	0/2/2/2
22	U8U	1K	34	25,22	-	1/9/28/29	0/2/2/2
23	OMC	2L	33	23	-	0/9/27/28	0/2/2/2
23	5MU	2K	55	23	-	2/7/25/26	0/2/2/2
22	H2U	1K	17	22	-	0/7/38/39	0/2/2/2
22	PSU	1K	39	22	-	0/7/25/26	0/2/2/2
23	4SU	2L	8	23	-	2/7/25/26	0/2/2/2
23	OMC	2K	33	23	-	0/9/27/28	0/2/2/2
23	7MG	2K	47	23	-	3/7/37/38	0/3/3/3
23	7MG	2L	47	23	-	4/7/37/38	0/3/3/3
23	5MU	2L	55	23	-	0/7/25/26	0/2/2/2
23	PSU	2L	56	23	-	0/7/25/26	0/2/2/2
56	PSU	1L	55	56	-	0/7/25/26	0/2/2/2
22	T6A	1K	37	22	-	5/23/41/42	0/3/3/3
23	4SU	2K	8	23	-	3/7/25/26	0/2/2/2

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

All (70) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	1K	54	5MU	C2-N1	13.05	1.59	1.38
56	1L	54	5MU	C2-N1	13.01	1.59	1.38
23	2L	55	5MU	C2-N1	12.77	1.58	1.38
23	2K	55	5MU	C2-N1	12.08	1.57	1.38
23	2K	47	7MG	C5-N7	8.64	1.45	1.35
23	2L	47	7MG	C5-N7	7.44	1.44	1.35
23	2K	47	7MG	C4-N9	-7.14	1.29	1.37
22	1K	37	T6A	C10-N11	6.73	1.50	1.35
23	2L	47	7MG	C4-N9	-6.39	1.30	1.37
23	2K	55	5MU	C4-N3	-6.23	1.27	1.38
22	1K	54	5MU	C2-N3	6.22	1.49	1.38
23	2L	55	5MU	C4-N3	-6.20	1.27	1.38
22	1K	17	H2U	C2-N1	6.13	1.44	1.35
23	2L	47	7MG	C4-N3	6.08	1.48	1.34
56	1L	54	5MU	C2-N3	5.99	1.48	1.38
22	1K	37	T6A	C10-N6	5.98	1.49	1.37
56	1L	54	5MU	C4-N3	-5.98	1.27	1.38
23	2L	55	5MU	C2-N3	5.88	1.48	1.38
22	1K	54	5MU	C6-N1	5.84	1.48	1.38
23	2L	8	4SU	C5-C4	5.75	1.50	1.42
23	2K	55	5MU	C2-N3	5.66	1.48	1.38
23	2K	47	7MG	C4-N3	5.65	1.47	1.34
22	1K	54	5MU	C4-N3	-5.62	1.28	1.38
23	2L	55	5MU	C6-N1	5.54	1.47	1.38
56	1L	54	5MU	C6-N1	5.47	1.47	1.38
22	1K	37	T6A	C6-N6	5.42	1.50	1.39
22	1K	34	U8U	C2-N3	5.35	1.49	1.37
23	2K	47	7MG	C2-N2	5.33	1.46	1.34
23	2K	55	5MU	C6-N1	5.29	1.47	1.38
23	2L	55	5MU	C4-C5	5.02	1.53	1.44
56	1L	54	5MU	C4-C5	5.02	1.53	1.44
23	2K	55	5MU	C4-C5	4.98	1.53	1.44
23	2K	47	7MG	C8-N9	4.97	1.48	1.46
22	1K	34	U8U	C6-C5	4.94	1.48	1.34
23	2K	33	OMC	C2-N3	4.79	1.46	1.36
23	2K	8	4SU	C5-C4	4.59	1.48	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
56	1L	55	PSU	C6-C5	4.54	1.40	1.35
23	2L	33	OMC	C2-N3	4.45	1.45	1.36
22	1K	54	5MU	C4-C5	4.42	1.52	1.44
22	1K	34	U8U	C2-S2	-4.42	1.60	1.67
23	2L	56	PSU	C6-C5	4.35	1.40	1.35
23	2K	47	7MG	C5-C4	-4.30	1.24	1.38
23	2L	33	OMC	C4-N4	4.19	1.43	1.33
23	2L	47	7MG	C5-C4	-4.13	1.24	1.38
23	2K	33	OMC	C4-N4	4.11	1.43	1.33
22	1K	34	U8U	C6-N1	4.11	1.45	1.38
22	1K	39	PSU	C6-C5	4.06	1.40	1.35
22	1K	55	PSU	C6-C5	4.06	1.40	1.35
22	1K	17	H2U	C2-N3	3.93	1.45	1.38
22	1K	34	U8U	C4-N3	3.92	1.46	1.38
23	2K	56	PSU	C6-C5	3.85	1.39	1.35
23	2L	33	OMC	C5-C4	3.73	1.51	1.42
23	2L	8	4SU	C2-N1	3.55	1.44	1.38
22	1K	17	H2U	C4-N3	3.34	1.43	1.37
23	2K	33	OMC	C5-C4	3.20	1.50	1.42
23	2L	47	7MG	C2-N2	3.16	1.41	1.34
23	2K	8	4SU	C2-N1	3.01	1.43	1.38
23	2L	8	4SU	C6-N1	2.97	1.45	1.38
22	1K	37	T6A	C5-C4	-2.83	1.33	1.39
22	1K	17	H2U	C6-N1	-2.72	1.42	1.47
23	2K	8	4SU	C6-N1	2.39	1.43	1.38
23	2L	47	7MG	C8-N9	2.38	1.47	1.46
22	1K	34	U8U	C4-C5	2.34	1.50	1.45
22	1K	37	T6A	C4-N9	-2.33	1.32	1.37
23	2L	56	PSU	C2-N1	2.27	1.39	1.36
22	1K	37	T6A	C5-N7	-2.25	1.34	1.39
22	1K	37	T6A	C6-N1	-2.23	1.31	1.35
22	1K	34	U8U	O4-C4	-2.21	1.19	1.23
22	1K	37	T6A	ODB-C13	-2.18	1.23	1.30
23	2K	56	PSU	C4-C5	-2.05	1.38	1.44

All (107) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
56	1L	54	5MU	C5-C4-N3	10.43	124.21	115.31
23	2K	55	5MU	C5-C4-N3	10.25	124.06	115.31
23	2L	55	5MU	C5-C4-N3	10.10	123.93	115.31
22	1K	54	5MU	C5-C4-N3	9.86	123.72	115.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	2K	8	4SU	C4-N3-C2	-8.30	119.28	127.34
23	2L	8	4SU	C4-N3-C2	-8.10	119.47	127.34
22	1K	37	T6A	C12-N11-C10	7.51	134.45	121.94
23	2L	47	7MG	C4-C5-N7	7.34	115.72	105.53
23	2K	47	7MG	C4-C5-N7	7.17	115.48	105.53
23	2K	8	4SU	C5-C4-N3	6.76	120.96	114.69
22	1K	17	H2U	C4-N3-C2	-6.72	120.22	125.79
23	2L	8	4SU	C5-C4-N3	6.71	120.91	114.69
23	2K	47	7MG	C5-C4-N9	6.61	114.93	106.35
23	2K	55	5MU	C4-N3-C2	-6.39	119.08	127.35
56	1L	54	5MU	C4-N3-C2	-6.29	119.21	127.35
22	1K	54	5MU	O4-C4-C5	-6.27	117.64	124.90
23	2L	55	5MU	C4-N3-C2	-6.17	119.37	127.35
23	2L	47	7MG	C6-C5-N7	-6.09	122.34	131.91
23	2K	55	5MU	C5-C6-N1	-6.02	117.15	123.34
22	1K	37	T6A	N3-C2-N1	-5.90	119.37	128.60
23	2L	55	5MU	C6-C5-C4	5.83	122.91	118.03
23	2K	55	5MU	C6-C5-C4	5.80	122.88	118.03
23	2L	47	7MG	C5-C4-N9	5.77	113.84	106.35
23	2L	55	5MU	C5-C6-N1	-5.67	117.51	123.34
23	2L	47	7MG	CM7-N7-C5	5.55	140.73	126.40
56	1L	54	5MU	C6-C5-C4	5.52	122.64	118.03
23	2K	47	7MG	C2-N3-C4	5.49	122.08	112.30
56	1L	54	5MU	C5-C6-N1	-5.38	117.81	123.34
22	1K	54	5MU	C4-N3-C2	-5.37	120.39	127.35
23	2K	55	5MU	C5M-C5-C6	-5.25	115.83	122.85
23	2K	8	4SU	C5-C4-S4	-5.22	117.74	124.47
23	2K	47	7MG	C5-C6-N1	5.15	120.06	110.99
23	2K	47	7MG	CM7-N7-C5	4.99	139.27	126.40
23	2L	47	7MG	C5-C4-N3	-4.97	118.67	128.13
23	2K	56	PSU	N1-C2-N3	4.88	120.66	115.13
56	1L	54	5MU	O4-C4-C5	-4.84	119.29	124.90
23	2L	47	7MG	C5-C6-N1	4.66	119.20	110.99
23	2L	55	5MU	C5M-C5-C6	-4.65	116.64	122.85
22	1K	37	T6A	C4-C5-C6	4.60	120.37	116.81
23	2K	55	5MU	O4-C4-C5	-4.55	119.63	124.90
23	2K	47	7MG	C6-C5-N7	-4.53	124.80	131.91
22	1K	54	5MU	C6-N1-C2	-4.51	116.73	121.30
23	2L	47	7MG	C2-N3-C4	4.50	120.33	112.30
56	1L	54	5MU	C5M-C5-C6	-4.47	116.88	122.85
22	1K	54	5MU	C6-C5-C4	4.46	121.76	118.03
23	2L	55	5MU	O4-C4-C5	-4.43	119.76	124.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	1K	37	T6A	N9-C8-N7	-4.40	107.90	113.91
22	1K	37	T6A	C5-C4-N3	-4.38	121.04	126.75
23	2L	56	PSU	C4-N3-C2	-4.29	120.15	126.34
22	1K	39	PSU	C4-N3-C2	-4.26	120.19	126.34
23	2K	56	PSU	C4-N3-C2	-4.21	120.27	126.34
22	1K	55	PSU	N1-C2-N3	4.16	119.85	115.13
23	2K	47	7MG	C5-C4-N3	-4.14	120.24	128.13
23	2L	8	4SU	N3-C2-N1	4.06	120.28	114.89
22	1K	17	H2U	N3-C2-N1	3.99	120.87	116.65
56	1L	55	PSU	N1-C2-N3	3.98	119.64	115.13
22	1K	55	PSU	C4-N3-C2	-3.97	120.62	126.34
23	2L	56	PSU	N1-C2-N3	3.93	119.59	115.13
22	1K	39	PSU	N1-C2-N3	3.88	119.53	115.13
23	2L	8	4SU	C5-C4-S4	-3.83	119.53	124.47
23	2K	56	PSU	C6-N1-C2	-3.72	118.88	122.68
23	2K	8	4SU	N3-C2-N1	3.72	119.83	114.89
56	1L	55	PSU	C4-N3-C2	-3.59	121.16	126.34
22	1K	54	5MU	C5M-C5-C6	-3.59	118.06	122.85
22	1K	54	5MU	C5-C6-N1	-3.53	119.71	123.34
23	2K	47	7MG	N1-C2-N3	-3.51	116.77	123.32
23	2K	8	4SU	O2-C2-N1	-3.43	118.23	122.79
22	1K	17	H2U	C5-C4-N3	3.43	120.50	116.65
23	2L	55	5MU	C6-N1-C2	-3.41	117.84	121.30
56	1L	54	5MU	C6-N1-C2	-3.33	117.92	121.30
22	1K	34	U8U	C5-C4-N3	3.31	119.62	114.97
23	2K	47	7MG	N2-C2-N1	3.29	123.72	116.71
23	2L	47	7MG	O6-C6-C5	-3.25	119.56	127.54
23	2K	47	7MG	O6-C6-C5	-3.25	119.57	127.54
22	1K	37	T6A	C2-N3-C4	3.21	119.32	111.75
22	1K	55	PSU	O2-C2-N1	-3.16	119.31	122.79
23	2K	56	PSU	O2-C2-N1	-3.10	119.38	122.79
23	2L	47	7MG	C2-N1-C6	-3.06	119.53	125.10
22	1K	37	T6A	C14-C12-C13	3.05	115.39	110.19
22	1K	37	T6A	C5-N7-C8	3.01	107.79	103.51
56	1L	55	PSU	C6-N1-C2	-2.95	119.67	122.68
56	1L	55	PSU	O2-C2-N1	-2.86	119.64	122.79
23	2K	55	5MU	C6-N1-C2	-2.81	118.45	121.30
22	1K	17	H2U	C5-C6-N1	2.74	120.63	111.61
22	1K	34	U8U	C1'-N1-C6	-2.72	116.60	121.12
23	2L	56	PSU	C6-C5-C4	2.72	120.10	118.20
23	2L	55	5MU	N3-C2-N1	2.68	118.45	114.89
22	1K	55	PSU	C6-N1-C2	-2.64	119.98	122.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	2K	55	5MU	N3-C2-N1	2.61	118.36	114.89
22	1K	34	U8U	O4-C4-C5	-2.55	121.17	124.96
23	2K	47	7MG	N9-C8-N7	-2.51	99.78	103.38
56	1L	54	5MU	N3-C2-N1	2.50	118.20	114.89
22	1K	37	T6A	N3-C4-N9	2.41	131.06	127.08
22	1K	54	5MU	C1'-N1-C2	2.41	121.93	117.57
23	2K	33	OMC	N4-C4-N3	2.37	122.13	117.97
22	1K	37	T6A	O10-C10-N6	-2.32	119.70	123.62
22	1K	17	H2U	O2-C2-N1	-2.30	120.22	123.11
23	2K	55	5MU	C5M-C5-C4	2.29	121.29	118.77
22	1K	37	T6A	C4-N9-C8	2.27	108.18	105.73
23	2K	55	5MU	O2-C2-N1	-2.23	119.82	122.79
23	2K	47	7MG	C2-N1-C6	-2.19	121.11	125.10
23	2L	47	7MG	N9-C8-N7	-2.14	100.32	103.38
22	1K	54	5MU	N3-C2-N1	2.09	117.66	114.89
56	1L	54	5MU	C1'-N1-C2	2.08	121.34	117.57
22	1K	39	PSU	C6-N1-C2	-2.08	120.55	122.68
22	1K	37	T6A	C2-N1-C6	2.05	122.14	115.25
23	2L	8	4SU	O2-C2-N1	-2.02	120.10	122.79

There are no chirality outliers.

All (25) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
22	1K	37	T6A	C14-C12-N11-C10
22	1K	37	T6A	N11-C12-C14-O14
22	1K	37	T6A	N11-C12-C14-C15
22	1K	37	T6A	C13-C12-C14-O14
22	1K	37	T6A	C13-C12-C14-C15
23	2L	8	4SU	O4'-C4'-C5'-O5'
22	1K	54	5MU	C3'-C4'-C5'-O5'
22	1K	54	5MU	O4'-C4'-C5'-O5'
23	2K	8	4SU	O4'-C4'-C5'-O5'
56	1L	54	5MU	C3'-C4'-C5'-O5'
23	2K	8	4SU	C3'-C4'-C5'-O5'
23	2K	55	5MU	C3'-C4'-C5'-O5'
23	2K	55	5MU	O4'-C4'-C5'-O5'
56	1L	54	5MU	O4'-C4'-C5'-O5'
23	2K	47	7MG	C2'-C1'-N9-C8
23	2L	47	7MG	C2'-C1'-N9-C8
23	2K	47	7MG	C4'-C5'-O5'-P
56	1L	54	5MU	C4'-C5'-O5'-P

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Mol	Chain	Res	Type	Atoms
23	2K	47	7MG	O4'-C1'-N9-C8
23	2L	47	7MG	O4'-C1'-N9-C8
23	2K	8	4SU	C4'-C5'-O5'-P
23	2L	8	4SU	C4'-C5'-O5'-P
23	2L	47	7MG	C4'-C5'-O5'-P
23	2L	47	7MG	O4'-C4'-C5'-O5'
22	1K	34	U8U	C4'-C5'-O5'-P

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 1345 ligands modelled in this entry, 1341 are monoatomic - leaving 4 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
60	SPE	14	3458	-	12,12,12	0.45	0	11,11,11	0.76	0
58	SF4	32	302	-	0,12,12	-	-	-		
58	SF4	3E	301	4	0,12,12	-	-	-		
60	SPE	1G	1725	1	12,12,12	0.41	0	11,11,11	0.73	0

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
60	SPE	14	3458	-	-	5/10/10/10	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
58	SF4	3E	301	4	-	-	0/6/5/5
58	SF4	32	302	-	-	-	0/6/5/5
60	SPE	1G	1725	1	-	5/10/10/10	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
60	1G	1725	SPE	C2-C3-C4-N5
60	14	3458	SPE	N9-C10-C11-C12
60	14	3458	SPE	C2-C3-C4-N5
60	14	3458	SPE	C6-C7-C8-N9
60	1G	1725	SPE	C11-C10-N9-C8
60	14	3458	SPE	C11-C10-N9-C8
60	1G	1725	SPE	C7-C6-N5-C4
60	14	3458	SPE	N1-C2-C3-C4
60	1G	1725	SPE	C7-C8-N9-C10
60	1G	1725	SPE	C3-C4-N5-C6

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
56	1L	1
47	D5	1
10	1A	1
34	69	1
4	3E	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	1L	72:C	O3'	73:A	P	3.48
1	D5	94:GLU	C	95:PRO	N	1.78
1	1A	38:ILE	C	39:PRO	N	1.71
1	69	79:ILE	C	80:PRO	N	1.17
1	3E	36:ARG	C	37:PRO	N	1.15

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, 95^{th} 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	1500/1522 (98%)	-0.13	43 (2%) 53 32	67, 111, 176, 243	0
1	1G	1509/1522 (99%)	-0.02	49 (3%) 50 29	76, 123, 193, 253	0
2	12	207/256 (80%)	0.42	8 (3%) 43 23	139, 165, 185, 196	0
2	1E	231/256 (90%)	0.34	6 (2%) 57 35	118, 145, 172, 180	0
3	22	195/239 (81%)	0.26	6 (3%) 51 30	123, 147, 164, 175	0
3	2E	205/239 (85%)	0.21	4 (1%) 65 43	97, 117, 144, 155	0
4	32	208/209 (99%)	0.37	6 (2%) 53 32	104, 123, 142, 149	0
4	3E	207/209 (99%)	0.50	8 (3%) 43 23	93, 118, 137, 144	0
5	42	150/162 (92%)	0.26	3 (2%) 65 43	106, 123, 139, 146	0
5	4E	149/162 (91%)	0.40	3 (2%) 65 43	87, 109, 128, 133	0
6	52	101/101 (100%)	0.17	1 (0%) 79 61	93, 110, 124, 135	0
6	5E	100/101 (99%)	0.20	2 (2%) 65 43	92, 111, 127, 135	0
7	62	138/156 (88%)	0.18	4 (2%) 53 32	122, 135, 145, 151	0
7	6E	154/156 (98%)	0.05	2 (1%) 75 55	111, 127, 155, 174	0
8	72	137/138 (99%)	0.35	4 (2%) 53 32	106, 129, 141, 149	0
8	7E	138/138 (100%)	0.16	1 (0%) 84 68	102, 117, 129, 139	0
9	82	121/128 (94%)	0.39	3 (2%) 58 36	118, 161, 171, 178	0
9	8E	126/128 (98%)	0.20	5 (3%) 42 22	96, 141, 159, 165	0
10	1A	80/105 (76%)	1.14	21 (26%) 1 1	122, 152, 167, 170	0
10	1I	94/105 (89%)	0.25	0 100 100	92, 136, 171, 178	0
11	2A	113/129 (87%)	0.41	4 (3%) 47 26	91, 116, 131, 138	0
11	2I	111/129 (86%)	0.24	2 (1%) 67 46	84, 113, 129, 138	0
12	3A	121/132 (91%)	0.74	17 (14%) 6 3	94, 109, 128, 144	0
12	3I	122/132 (92%)	0.35	11 (9%) 15 7	81, 89, 110, 132	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
13	4A	109/126 (86%)	0.32	7 (6%) 25 13	125, 152, 170, 187	0
13	4I	117/126 (92%)	0.18	7 (5%) 27 14	97, 125, 138, 145	0
14	5A	59/61 (96%)	0.95	10 (16%) 4 2	131, 146, 164, 167	0
14	5I	59/61 (96%)	-0.07	0 100 100	92, 106, 121, 129	0
15	6A	87/89 (97%)	-0.07	1 (1%) 78 59	93, 117, 133, 137	0
15	6I	87/89 (97%)	-0.11	0 100 100	89, 107, 126, 130	0
16	7A	84/88 (95%)	0.41	4 (4%) 35 18	100, 116, 137, 159	0
16	7I	83/88 (94%)	0.59	5 (6%) 27 14	107, 119, 145, 163	0
17	8A	99/105 (94%)	-0.06	0 100 100	100, 112, 125, 131	0
17	8I	100/105 (95%)	0.11	3 (3%) 52 31	95, 114, 124, 128	0
18	9A	67/88 (76%)	0.49	6 (8%) 15 7	101, 117, 135, 140	0
18	9I	68/88 (77%)	0.08	1 (1%) 72 51	97, 113, 133, 138	0
19	AA	65/93 (69%)	0.75	6 (9%) 14 7	130, 162, 174, 180	0
19	AI	82/93 (88%)	0.09	2 (2%) 59 38	108, 126, 146, 153	0
20	BA	99/106 (93%)	0.09	2 (2%) 65 43	94, 119, 140, 153	0
20	BI	97/106 (91%)	0.22	3 (3%) 51 30	113, 127, 150, 157	0
21	1B	22/27 (81%)	0.27	1 (4%) 38 20	122, 139, 143, 150	0
21	1F	23/27 (85%)	-0.40	0 100 100	103, 110, 116, 123	0
22	1K	66/76 (86%)	1.20	12 (18%) 3 1	104, 183, 206, 212	0
23	2K	72/77 (93%)	-0.07	1 (1%) 73 53	75, 100, 133, 145	0
23	2L	72/77 (93%)	0.25	3 (4%) 40 21	85, 120, 153, 162	0
24	3K	70/76 (92%)	0.81	5 (7%) 22 11	82, 225, 245, 249	0
24	3L	72/76 (94%)	1.41	16 (22%) 2 1	87, 206, 223, 228	0
25	4K	20/30 (66%)	0.57	1 (5%) 34 17	81, 145, 215, 216	0
25	4L	19/30 (63%)	1.22	5 (26%) 1 1	101, 162, 218, 218	0
26	14	2825/2917 (96%)	-0.20	89 (3%) 50 29	62, 91, 198, 251	0
26	1H	2831/2917 (97%)	-0.41	44 (1%) 70 49	51, 79, 176, 251	0
27	16	122/122 (100%)	-0.60	3 (2%) 58 36	76, 98, 118, 204	0
27	1J	122/122 (100%)	-0.19	1 (0%) 82 65	94, 133, 152, 210	0
28	71	132/229 (57%)	0.33	4 (3%) 52 31	143, 206, 228, 235	0
29	11	273/276 (98%)	0.08	8 (2%) 53 32	48, 71, 88, 95	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
29	19	274/276 (99%)	0.16	12 (4%) 39 20	56, 80, 94, 111	0
30	21	203/206 (98%)	0.35	9 (4%) 39 20	57, 90, 121, 133	0
30	29	204/206 (99%)	0.32	18 (8%) 15 8	66, 97, 133, 147	0
31	31	202/210 (96%)	-0.22	3 (1%) 72 51	51, 82, 114, 134	0
31	39	204/210 (97%)	0.27	18 (8%) 15 8	64, 105, 148, 175	0
32	41	179/182 (98%)	0.02	7 (3%) 43 23	90, 109, 139, 154	0
32	49	180/182 (98%)	0.28	6 (3%) 49 28	125, 147, 166, 179	0
33	51	174/180 (96%)	0.27	8 (4%) 37 19	82, 105, 123, 133	0
33	59	169/180 (93%)	1.20	35 (20%) 2 1	157, 203, 223, 233	0
34	61	145/148 (97%)	0.21	3 (2%) 63 42	82, 128, 147, 153	0
34	69	145/148 (97%)	0.20	8 (5%) 30 16	91, 129, 149, 154	0
35	15	137/140 (97%)	0.86	16 (11%) 9 4	82, 110, 140, 150	0
35	58	137/140 (97%)	0.13	2 (1%) 72 51	71, 90, 122, 138	0
36	25	122/122 (100%)	-0.18	0 100 100	74, 90, 108, 120	0
36	68	122/122 (100%)	0.17	4 (3%) 49 28	67, 82, 98, 106	0
37	35	147/150 (98%)	0.48	12 (8%) 17 9	64, 106, 141, 158	0
37	78	147/150 (98%)	-0.15	1 (0%) 84 68	58, 84, 106, 114	0
38	45	138/141 (97%)	0.31	4 (2%) 53 32	79, 106, 127, 138	0
38	88	141/141 (100%)	-0.16	0 100 100	62, 83, 104, 133	0
39	55	118/118 (100%)	-0.22	2 (1%) 69 48	68, 85, 100, 113	0
39	98	118/118 (100%)	-0.11	0 100 100	67, 86, 103, 117	0
40	65	110/112 (98%)	0.24	1 (0%) 81 63	99, 124, 141, 145	0
40	A8	111/112 (99%)	-0.15	1 (0%) 81 63	82, 95, 114, 127	0
41	75	133/146 (91%)	-0.07	3 (2%) 61 39	82, 97, 127, 145	0
41	B8	135/146 (92%)	0.48	11 (8%) 18 9	79, 96, 135, 151	0
42	85	116/118 (98%)	0.50	7 (6%) 27 14	72, 101, 129, 136	0
42	C8	115/118 (97%)	0.11	2 (1%) 69 48	60, 82, 108, 115	0
43	95	100/101 (99%)	0.51	3 (3%) 52 31	72, 120, 140, 147	0
43	D8	100/101 (99%)	0.16	4 (4%) 42 22	62, 100, 120, 130	0
44	A5	111/113 (98%)	0.17	3 (2%) 56 34	71, 81, 107, 139	0
44	E8	110/113 (97%)	0.07	5 (4%) 38 20	64, 77, 100, 113	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
45	B5	94/96 (97%)	-0.10	3 (3%) 50 29	78, 90, 111, 121	0
45	F8	95/96 (98%)	-0.11	1 (1%) 78 59	59, 74, 98, 108	0
46	C5	104/110 (94%)	1.10	18 (17%) 4 2	92, 119, 152, 158	0
46	G8	103/110 (93%)	0.61	7 (6%) 23 12	76, 97, 124, 134	0
47	D5	177/206 (85%)	0.09	0 100 100	117, 159, 218, 223	0
47	H8	170/206 (82%)	-0.28	0 100 100	88, 121, 189, 196	0
48	E5	76/85 (89%)	0.15	2 (2%) 57 35	78, 97, 111, 120	0
48	I8	77/85 (90%)	-0.30	1 (1%) 75 55	64, 79, 96, 108	0
49	F5	94/98 (95%)	0.29	3 (3%) 50 29	69, 89, 125, 139	0
49	J8	96/98 (97%)	0.48	6 (6%) 26 13	61, 80, 117, 123	0
50	G5	69/72 (95%)	0.08	3 (4%) 40 21	90, 109, 132, 144	0
50	K8	68/72 (94%)	0.10	1 (1%) 72 51	68, 84, 105, 129	0
51	H5	58/60 (96%)	0.03	0 100 100	81, 101, 126, 136	0
51	L8	58/60 (96%)	-0.36	0 100 100	70, 84, 110, 122	0
52	M8	60/71 (84%)	0.32	1 (1%) 69 48	114, 150, 177, 181	0
53	J5	56/60 (93%)	0.27	2 (3%) 46 26	67, 90, 133, 143	0
53	N8	48/60 (80%)	-0.16	0 100 100	56, 85, 128, 135	0
54	L5	47/49 (95%)	-0.40	1 (2%) 63 42	61, 69, 91, 100	0
54	P8	47/49 (95%)	-0.46	0 100 100	54, 59, 77, 89	0
55	M5	64/65 (98%)	0.49	5 (7%) 19 9	76, 86, 101, 117	0
55	Q8	64/65 (98%)	-0.01	1 (1%) 70 49	61, 75, 88, 101	0
56	1L	64/76 (84%)	1.25	16 (25%) 2 1	140, 201, 221, 227	0
All	All	20656/21744 (94%)	0.04	742 (3%) 46 26	48, 105, 181, 253	0

All (742) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
22	1K	76	A	11.0
20	BA	9	ASN	9.1
43	D8	37	VAL	8.3
41	B8	104	ASN	8.1
26	14	229	A	7.4
12	3A	28	LYS	7.3
18	9A	84	LYS	7.1

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Mol	Chain	Res	Type	RSRZ
41	B8	106	SER	7.1
12	3A	27	LEU	6.9
24	3L	34	U	6.3
1	1G	1202	G	6.2
33	59	89	ILE	5.9
12	3A	26	ALA	5.9
46	G8	104	GLY	5.8
24	3L	35	U	5.8
9	8E	127	LYS	5.7
27	1J	88	C	5.6
22	1K	73	A	5.6
33	59	151	ILE	5.6
1	1G	82	U	5.5
56	1L	69	A	5.3
12	3A	64	TYR	5.3
30	29	116	VAL	5.2
32	41	23	PHE	5.2
33	59	169	VAL	5.2
46	C5	49	VAL	5.1
22	1K	74	C	5.1
24	3L	72	C	5.1
9	82	115	GLY	4.9
12	3A	62	SER	4.9
22	1K	72	C	4.9
22	1K	75	C	4.9
10	1A	47	PHE	4.8
33	59	87	LEU	4.8
56	1L	1	G	4.7
46	C5	105	ALA	4.7
26	1H	790	C	4.6
56	1L	71	C	4.6
31	39	72	ARG	4.6
18	9A	46	GLU	4.6
35	15	92	ALA	4.5
33	51	39	PRO	4.5
46	C5	29	GLU	4.5
35	15	84	LYS	4.5
1	13	1508	G	4.5
5	4E	21	ALA	4.5
13	4A	95	GLY	4.5
12	3I	7	ILE	4.4
34	69	1	MET	4.4

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Mol	Chain	Res	Type	RSRZ
29	19	5	LYS	4.4
33	59	155	SER	4.4
1	13	1509	C	4.4
26	1H	2062	A	4.4
1	13	1516	G	4.3
5	4E	23	GLY	4.3
26	14	1026	U	4.3
33	59	167	GLU	4.3
41	B8	109	GLU	4.3
35	15	138	LEU	4.3
12	3A	21	LYS	4.2
33	59	80	SER	4.2
42	C8	116	ALA	4.2
10	1A	61	GLU	4.2
37	35	47	ASP	4.2
49	F5	91	LYS	4.2
1	1G	88	C	4.1
2	12	163	PHE	4.1
24	3L	6	G	4.1
33	51	9	ILE	4.1
19	AA	53	ASN	4.1
26	14	271(C)	U	4.1
28	71	202	GLU	4.1
40	65	20	ARG	4.1
1	13	1533	C	4.1
24	3L	70	C	4.1
35	15	46	VAL	4.1
12	3I	19	ARG	4.1
13	4A	117	VAL	4.0
33	59	107	VAL	4.0
10	1A	59	SER	4.0
1	13	1513	A	4.0
26	1H	1660	C	4.0
41	75	106	SER	4.0
1	13	1510	U	4.0
12	3I	28	LYS	4.0
14	5A	39	LEU	4.0
33	59	98	LEU	4.0
1	13	1527	C	4.0
46	G8	89	PHE	3.9
1	13	1514	C	3.9
26	14	2797	U	3.9

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Mol	Chain	Res	Type	RSRZ
11	2A	25	TYR	3.9
33	59	165	ALA	3.9
1	13	1531	A	3.9
1	13	1511	G	3.9
23	2L	40	C	3.9
31	31	66	PRO	3.9
33	59	171	LEU	3.8
56	1L	40	C	3.8
26	1H	1272	A	3.8
31	39	64	ILE	3.8
29	19	27	THR	3.8
26	14	205	G	3.8
34	69	21	VAL	3.8
30	29	134	ILE	3.8
10	1A	64	GLU	3.8
32	41	25	TYR	3.8
46	C5	50	ARG	3.8
26	1H	2690	C	3.7
44	E8	92	ARG	3.7
26	14	2611	U	3.7
1	1G	1493	A	3.7
26	1H	2612	C	3.7
31	39	65	TRP	3.7
31	39	56	GLU	3.7
33	59	126	PRO	3.7
33	59	76	VAL	3.7
55	M5	34	TRP	3.7
19	AA	60	VAL	3.7
24	3L	1	G	3.7
40	A8	110	LEU	3.7
46	C5	59	GLY	3.7
26	14	2895	U	3.7
1	1G	912	C	3.7
56	1L	72	C	3.7
31	39	55	GLY	3.7
1	1G	966	G	3.6
24	3L	33	U	3.6
16	7A	76	GLN	3.6
31	39	83	PHE	3.6
56	1L	31	A	3.6
1	13	1403	C	3.6
24	3L	74	C	3.6

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Mol	Chain	Res	Type	RSRZ
37	35	71	VAL	3.6
46	G8	98	VAL	3.6
1	13	1523	G	3.6
26	1H	254	G	3.6
22	1K	69	A	3.6
26	1H	2712(A)	A	3.6
32	41	3	LEU	3.6
6	5E	46	ARG	3.5
12	3I	11	VAL	3.5
10	1A	50	ILE	3.5
26	14	2610	C	3.5
30	29	151	TYR	3.5
24	3L	75	C	3.5
33	59	148	ILE	3.5
2	1E	81	VAL	3.5
32	49	34	LEU	3.5
1	1G	163	C	3.5
22	1K	71	C	3.5
26	14	2581	G	3.5
26	1H	958	U	3.5
1	13	815	A	3.4
26	1H	1536	A	3.4
25	4L	7	G	3.4
26	1H	1055	G	3.4
1	13	1515	C	3.4
26	14	383	U	3.4
29	19	275	LYS	3.4
1	13	769	G	3.4
9	8E	126	SER	3.4
33	59	131	VAL	3.4
29	19	262	ARG	3.4
24	3K	70	C	3.3
26	14	2791	C	3.3
26	14	382	G	3.3
26	14	669	G	3.3
2	1E	29	ALA	3.3
1	1G	1115	C	3.3
34	69	3	VAL	3.3
45	B5	94	GLY	3.3
33	51	175	LYS	3.3
35	15	85	ILE	3.3
30	29	128	SER	3.3

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Mol	Chain	Res	Type	RSRZ
26	14	743	G	3.3
37	35	46	LYS	3.3
46	C5	63	LYS	3.3
3	2E	166	GLU	3.3
41	75	50	ILE	3.3
16	7A	84	ALA	3.2
1	13	1526	G	3.2
1	1G	973	G	3.2
13	4A	102	ARG	3.2
46	C5	55	TYR	3.2
1	13	701	C	3.2
18	9A	85	LEU	3.2
10	1A	49	VAL	3.2
46	C5	51	VAL	3.2
29	19	26	LYS	3.2
24	3L	36	U	3.2
1	1G	1195	C	3.2
34	69	2	LYS	3.2
26	1H	2712	U	3.2
10	1A	60	ARG	3.2
1	1G	1061	G	3.2
26	14	274	G	3.2
49	J8	79	GLY	3.2
2	12	102	LEU	3.2
33	59	168	PRO	3.2
35	15	132	ALA	3.2
26	1H	1659	U	3.1
11	2A	75	TYR	3.1
3	22	177	THR	3.1
26	1H	1273	U	3.1
1	13	1394	A	3.1
1	1G	975	A	3.1
26	14	204	A	3.1
10	1A	62	HIS	3.1
26	14	252	G	3.1
26	14	2609	U	3.1
29	11	2	ALA	3.1
31	39	69	HIS	3.1
25	4K	25	A	3.1
1	1G	155	C	3.1
1	1G	1226	C	3.1
7	62	9	VAL	3.1

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Mol	Chain	Res	Type	RSRZ
13	4I	102	ARG	3.1
26	14	1306	C	3.1
49	J8	21	ARG	3.1
1	13	1529	G	3.1
2	1E	211	ILE	3.1
20	BI	12	ALA	3.1
30	29	135	HIS	3.1
12	3A	29	GLY	3.1
33	59	93	GLY	3.1
31	31	72	ARG	3.1
43	95	73	SER	3.1
37	35	74	GLU	3.1
37	35	110	TYR	3.1
1	13	933	G	3.0
1	1G	1187	G	3.0
12	3A	19	ARG	3.0
46	C5	45	VAL	3.0
12	3I	17	LYS	3.0
12	3A	20	LYS	3.0
42	85	25	TRP	3.0
29	19	36	PRO	3.0
37	35	48	PRO	3.0
14	5A	44	LEU	3.0
23	2L	1	C	3.0
46	C5	58	GLY	3.0
26	14	206	U	3.0
9	8E	117	HIS	3.0
12	3A	23	LYS	3.0
13	4I	115	LYS	3.0
1	13	968	A	3.0
30	21	90	THR	3.0
30	21	195	LEU	3.0
26	14	2506	U	3.0
35	15	73	THR	3.0
14	5A	47	LEU	2.9
26	14	189	G	2.9
26	14	530	G	2.9
34	69	20	ASP	2.9
26	1H	1657	C	2.9
33	59	72	ILE	2.9
26	1H	2611	U	2.9
46	C5	98	VAL	2.9

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Mol	Chain	Res	Type	RSRZ
1	1G	3	G	2.9
37	35	64	LYS	2.9
26	1H	856	C	2.9
26	14	756	C	2.9
10	1A	54	PHE	2.9
10	1A	51	ARG	2.9
38	45	2	LEU	2.9
1	13	1520	G	2.9
1	1G	1117	G	2.9
36	68	45	GLU	2.9
1	13	1384	C	2.9
10	1A	56	HIS	2.9
13	4I	96	LEU	2.9
17	8I	29	HIS	2.9
32	41	26	GLN	2.9
41	75	104	ASN	2.9
23	2L	39	A	2.9
24	3L	69	A	2.9
26	1H	2003	G	2.9
26	14	2712	U	2.8
56	1L	32	C	2.8
56	1L	70	C	2.8
12	3I	16	GLU	2.8
30	21	130	GLY	2.8
50	G5	44	LEU	2.8
26	1H	746	A	2.8
1	1G	156	G	2.8
26	14	2893	G	2.8
42	85	56	ASP	2.8
32	49	133	LEU	2.8
48	E5	8	GLY	2.8
33	59	94	TYR	2.8
35	15	75	TYR	2.8
44	A5	111	HIS	2.8
30	29	149	ARG	2.8
1	1G	89	U	2.8
1	13	3	G	2.8
1	1G	154	C	2.8
2	12	13	ALA	2.8
30	29	131	ALA	2.8
34	69	36	ALA	2.8
50	G5	43	GLN	2.8

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Mol	Chain	Res	Type	RSRZ
10	1A	85	LEU	2.8
41	B8	105	LEU	2.8
55	Q8	56	GLU	2.8
42	85	40	PHE	2.8
1	1G	328	C	2.8
24	3K	71	C	2.8
1	1G	886	G	2.8
1	1G	887	G	2.8
12	3I	5	PRO	2.8
26	14	668	G	2.8
14	5A	6	LEU	2.8
55	M5	40	GLU	2.8
1	1G	915	A	2.7
12	3A	24	VAL	2.7
24	3L	7	U	2.7
26	14	958	U	2.7
31	39	66	PRO	2.7
35	58	129	PRO	2.7
46	C5	77	PRO	2.7
26	1H	756	C	2.7
26	14	277	C	2.7
33	59	106	THR	2.7
16	7I	30	GLY	2.7
31	39	71	GLY	2.7
26	14	1661	G	2.7
20	BI	80	ARG	2.7
2	1E	33	TYR	2.7
14	5A	48	ALA	2.7
38	45	96	VAL	2.7
50	K8	69	ARG	2.7
26	14	755	C	2.7
16	7I	32	TYR	2.7
3	22	6	HIS	2.7
25	4L	9	G	2.7
26	1H	1650	G	2.7
19	AA	62	ILE	2.7
30	21	51	PHE	2.7
33	59	162	ILE	2.7
9	8E	115	GLY	2.7
1	13	768	A	2.7
1	1G	1225	A	2.7
23	2K	1	C	2.7

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Mol	Chain	Res	Type	RSRZ
26	1H	34	C	2.7
10	1A	63	PHE	2.7
41	B8	101	PHE	2.7
30	29	139	GLY	2.7
36	68	66	LYS	2.7
46	C5	46	LYS	2.7
10	1A	48	THR	2.7
24	3K	1	G	2.7
14	5A	53	LEU	2.7
26	14	387	U	2.7
33	59	17	VAL	2.7
20	BA	16	HIS	2.7
29	11	112	GLN	2.6
37	35	68	GLN	2.6
46	G8	94	LYS	2.6
30	29	65	GLY	2.6
45	F8	86	GLY	2.6
1	13	328	C	2.6
4	3E	195	ALA	2.6
42	C8	90	VAL	2.6
1	1G	333	G	2.6
29	11	274	ARG	2.6
56	1L	3	G	2.6
30	29	125	GLY	2.6
1	13	935	A	2.6
11	2I	42	TRP	2.6
22	1K	70	C	2.6
26	14	589	C	2.6
26	14	1660	C	2.6
4	32	207	TYR	2.6
31	39	68	LYS	2.6
1	13	1512	U	2.6
26	14	1659	U	2.6
1	1G	331	G	2.6
26	1H	529	A	2.6
29	19	35	LYS	2.6
35	15	89	LYS	2.6
43	95	81	TYR	2.6
46	C5	53	PRO	2.6
22	1K	40	C	2.6
26	14	790	C	2.6
44	E8	93	ALA	2.6

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Mol	Chain	Res	Type	RSRZ
26	1H	2002	G	2.6
26	14	654(D)	G	2.6
26	14	2024	G	2.6
30	21	139	GLY	2.6
33	51	57	ASP	2.6
37	35	50	ARG	2.6
44	A5	92	ARG	2.6
26	14	767	U	2.5
5	4E	22	GLY	2.5
10	1A	65	LEU	2.5
1	13	1338	G	2.5
1	1G	1186	G	2.5
35	15	74	ARG	2.5
26	1H	951	C	2.5
26	14	888	C	2.5
46	C5	60	PHE	2.5
3	22	184	TYR	2.5
33	51	174	GLY	2.5
13	4I	114	ARG	2.5
30	29	127	ASP	2.5
41	B8	135	ALA	2.5
46	C5	61	ILE	2.5
32	49	178	PHE	2.5
26	14	2712(A)	A	2.5
26	14	2630	G	2.5
45	B5	69	TYR	2.5
4	3E	73	ARG	2.5
5	42	153	LYS	2.5
10	1A	46	ARG	2.5
26	1H	1658	C	2.5
26	14	1657	C	2.5
30	29	64	LYS	2.5
31	39	93	LYS	2.5
26	14	1963	U	2.5
3	22	39	ILE	2.5
31	39	96	ASP	2.5
41	B8	2	ASN	2.5
11	2A	91	ARG	2.5
31	39	62	ARG	2.5
26	14	2801	A	2.5
26	14	245	G	2.5
26	14	2508	G	2.5

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Mol	Chain	Res	Type	RSRZ
18	9A	83	GLU	2.5
13	4A	103	THR	2.5
30	21	203	LYS	2.5
12	3I	29	GLY	2.5
48	I8	8	GLY	2.5
1	13	965	A	2.4
32	41	164	GLU	2.4
41	B8	134	GLU	2.4
12	3A	61	THR	2.4
26	14	591	C	2.4
26	14	832	G	2.4
35	15	86	PRO	2.4
43	D8	36	PRO	2.4
24	3K	36	U	2.4
55	M5	35	GLN	2.4
8	72	22	GLU	2.4
33	59	159	GLU	2.4
30	21	136	ARG	2.4
33	59	90	LYS	2.4
34	61	116	LEU	2.4
1	13	1519	A	2.4
1	1G	101	A	2.4
26	14	257	A	2.4
30	29	150	VAL	2.4
33	59	24	VAL	2.4
1	13	934	C	2.4
24	3K	72	C	2.4
24	3L	71	C	2.4
26	1H	2610	C	2.4
1	13	1405	G	2.4
1	1G	81	G	2.4
2	1E	208	ILE	2.4
42	85	42	ALA	2.4
26	14	799	G	2.4
26	14	2509	G	2.4
54	L5	47	ARG	2.4
10	1A	35	SER	2.4
12	3I	63	GLY	2.4
14	5A	38	GLY	2.4
29	19	216	GLY	2.4
1	1G	162	A	2.4
24	3L	37	A	2.4

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Mol	Chain	Res	Type	RSRZ
26	14	752	A	2.4
26	14	1050	A	2.4
13	4I	111	LYS	2.4
14	5A	37	PHE	2.4
1	13	1404	C	2.4
1	13	1528	U	2.4
9	82	50	LEU	2.4
37	35	45	LEU	2.4
43	D8	38	LEU	2.4
56	1L	48	C	2.4
1	13	773	G	2.4
1	1G	332	G	2.4
26	14	1645	G	2.4
31	39	53	THR	2.4
32	49	160	VAL	2.4
2	12	218	ALA	2.4
38	45	93	TYR	2.4
49	F5	77	ALA	2.4
13	4A	111	LYS	2.4
30	29	133	LYS	2.4
44	E8	90	ARG	2.4
4	3E	150	GLU	2.4
26	1H	2713	A	2.4
26	14	1847	A	2.4
4	32	198	VAL	2.4
33	51	21	PRO	2.4
1	1G	1114	C	2.3
10	1A	67	THR	2.3
19	AI	48	THR	2.3
26	14	766	C	2.3
29	11	100	GLY	2.3
15	6A	87	ILE	2.3
45	B5	79	ALA	2.3
10	1A	58	ASP	2.3
1	13	1497	G	2.3
1	13	1525	G	2.3
7	6E	80	VAL	2.3
19	AA	76	PRO	2.3
26	1H	1847	A	2.3
31	31	65	TRP	2.3
10	1A	74	ILE	2.3
13	4I	116	THR	2.3

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Mol	Chain	Res	Type	RSRZ
36	68	53	LYS	2.3
49	F5	22	GLY	2.3
30	29	60	ASN	2.3
1	1G	334	C	2.3
26	14	1305	C	2.3
3	22	10	PHE	2.3
32	41	80	PHE	2.3
1	1G	890	G	2.3
31	39	12	LEU	2.3
49	J8	80	LEU	2.3
22	1K	31	A	2.3
26	14	1272	A	2.3
56	1L	41	A	2.3
1	1G	1062	U	2.3
26	14	667	U	2.3
29	19	23	GLU	2.3
16	7I	19	ILE	2.3
5	42	12	LEU	2.3
18	9A	44	LEU	2.3
34	69	38	LEU	2.3
42	85	49	HIS	2.3
7	62	37	ASN	2.3
19	AI	56	GLN	2.3
1	1G	87	A	2.3
29	11	205	VAL	2.3
30	29	136	ARG	2.3
42	85	90	VAL	2.3
1	1G	164	U	2.3
13	4A	9	ILE	2.3
1	13	1228	C	2.3
26	14	203	C	2.3
26	14	1663	C	2.3
37	35	51	PHE	2.3
50	G5	45	SER	2.3
26	1H	2358	G	2.2
33	59	92	ILE	2.2
4	32	2	GLY	2.2
4	32	167	GLY	2.2
12	3A	30	ALA	2.2
30	21	187	ALA	2.2
1	1G	323	U	2.2
7	6E	99	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
41	B8	114	LEU	2.2
31	39	90	PHE	2.2
55	M5	12	LYS	2.2
26	14	1658	C	2.2
26	14	2789	C	2.2
46	C5	2	ARG	2.2
13	4I	106	ASN	2.2
14	5A	18	VAL	2.2
33	59	35	VAL	2.2
13	4A	113	PRO	2.2
29	19	2	ALA	2.2
32	49	82	LEU	2.2
39	55	18	LEU	2.2
6	5E	54	LYS	2.2
16	7I	27	LYS	2.2
26	1H	615	G	2.2
26	14	188	G	2.2
26	14	742	G	2.2
27	16	87	G	2.2
53	J5	10	LYS	2.2
26	14	2584	U	2.2
29	11	176	ARG	2.2
9	8E	44	VAL	2.2
52	M8	22	ILE	2.2
1	1G	1437	C	2.2
26	14	47	C	2.2
4	3E	197	PRO	2.2
9	82	47	LEU	2.2
11	2A	36	ASP	2.2
30	29	63	LEU	2.2
43	D8	35	LEU	2.2
44	E8	53	SER	2.2
26	1H	1963	U	2.2
26	14	230	U	2.2
26	14	1396	U	2.2
28	71	193	ILE	2.2
1	13	1340	A	2.2
4	3E	96	LEU	2.2
22	1K	38	A	2.2
25	4L	15	A	2.2
26	1H	2004	G	2.2
26	1H	2659	G	2.2

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Mol	Chain	Res	Type	RSRZ
26	14	6	A	2.2
26	14	213	A	2.2
26	14	654(S)	G	2.2
26	14	1307	A	2.2
26	14	2583	G	2.2
3	22	7	PRO	2.2
37	78	141	ALA	2.2
46	G8	100	ALA	2.2
17	8I	100	LYS	2.2
46	C5	54	LYS	2.2
8	72	91	ARG	2.2
12	3A	85	ILE	2.2
19	AA	56	GLN	2.2
28	71	47	LEU	2.2
34	61	117	GLU	2.2
38	45	91	GLU	2.2
12	3A	25	PRO	2.2
35	15	2	LYS	2.2
29	11	262	ARG	2.2
49	J8	26	ARG	2.2
2	12	70	PHE	2.2
3	2E	128	PHE	2.2
25	4L	8	A	2.2
27	16	1(M)	A	2.2
1	1G	1438	G	2.2
26	14	1678	G	2.2
56	1L	45	G	2.2
18	9A	86	VAL	2.1
24	3L	5	C	2.1
26	14	246	C	2.1
26	14	2579	C	2.1
33	59	156	ALA	2.1
49	J8	93	GLU	2.1
29	19	55	GLY	2.1
32	41	24	GLY	2.1
53	J5	50	GLY	2.1
48	E5	12	ASN	2.1
7	62	141	VAL	2.1
3	2E	193	TYR	2.1
26	1H	835	A	2.1
6	52	45	LEU	2.1
26	14	1992	G	2.1

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Mol	Chain	Res	Type	RSRZ
26	14	2631	G	2.1
8	72	115	SER	2.1
12	3A	88	GLY	2.1
1	1G	811	C	2.1
1	1G	1059	C	2.1
1	1G	1060	C	2.1
1	1G	1535	C	2.1
10	1A	91	PRO	2.1
32	49	177	GLY	2.1
33	51	56	SER	2.1
33	59	21	PRO	2.1
33	59	36	PRO	2.1
46	G8	91	GLU	2.1
4	32	5	ILE	2.1
33	59	163	TYR	2.1
41	B8	9	LEU	2.1
29	11	119	ALA	2.1
1	1G	1188	A	2.1
2	12	129	GLU	2.1
4	3E	24	GLU	2.1
8	72	131	GLY	2.1
25	4L	14	A	2.1
26	1H	1274	A	2.1
26	14	2062	A	2.1
33	59	91	GLY	2.1
33	59	112	PRO	2.1
35	15	81	GLY	2.1
56	1L	14	A	2.1
4	32	79	PHE	2.1
26	1H	1845	G	2.1
34	69	19	VAL	2.1
35	15	9	VAL	2.1
26	14	2510	C	2.1
43	95	74	LYS	2.1
3	2E	196	LEU	2.1
8	7E	10	LEU	2.1
14	5A	42	ILE	2.1
35	15	91	LEU	2.1
19	AA	77	THR	2.1
44	A5	90	ARG	2.1
30	29	123	ALA	2.1
35	15	131	GLN	2.1

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Mol	Chain	Res	Type	RSRZ
33	59	5	GLY	2.1
49	J8	36	GLY	2.1
33	51	86	GLU	2.1
29	19	179	SER	2.1
2	12	164	VAL	2.1
4	3E	88	VAL	2.1
16	7I	20	VAL	2.1
26	1H	789	A	2.1
28	71	49	ILE	2.1
39	55	70	LEU	2.1
30	21	135	HIS	2.1
42	85	91	ASP	2.1
35	58	73	THR	2.1
1	1G	1385	G	2.1
18	9I	20	ALA	2.1
26	1H	893	C	2.1
26	1H	949	C	2.1
26	1H	1678	G	2.1
26	1H	2655	G	2.1
2	1E	14	GLY	2.1
37	35	38	GLN	2.1
31	39	81	PRO	2.1
26	1H	2357	U	2.0
56	1L	39	U	2.0
16	7A	26	ARG	2.0
17	8I	36	ILE	2.0
20	BI	72	LEU	2.0
12	3I	64	TYR	2.0
16	7A	39	TYR	2.0
36	68	80	ASP	2.0
56	1L	73	A	2.0
11	2I	118	GLY	2.0
1	13	1382	C	2.0
22	1K	32	C	2.0
26	14	1625	C	2.0
46	G8	95	LYS	2.0
12	3A	89	ARG	2.0
26	1H	966	G	2.0
26	14	250	G	2.0
26	14	360	G	2.0
26	14	2023	G	2.0
27	16	86	G	2.0

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Mol	Chain	Res	Type	RSRZ
33	59	7	LEU	2.0
41	B8	112	ARG	2.0
56	1L	18	G	2.0
12	3I	62	SER	2.0
44	E8	96	ILE	2.0
5	42	21	ALA	2.0
7	62	2	ALA	2.0
4	3E	110	PHE	2.0
55	M5	9	GLY	2.0
21	1B	23	PRO	2.0
1	13	1503	A	2.0
1	1G	913	A	2.0
1	1G	974	A	2.0
24	3L	38	A	2.0
26	14	256	A	2.0
26	14	1762	A	2.0
26	14	2577	A	2.0
34	61	122	GLU	2.0
2	12	44	LEU	2.0
31	39	9	ILE	2.0
1	13	810	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, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
22	H2U	1K	17	20/21	0.68	0.10	130,139,153,158	0
56	PSU	1L	55	20/21	0.72	0.10	121,135,144,145	0
22	PSU	1K	55	20/21	0.77	0.10	115,126,136,137	0
56	5MU	1L	54	21/22	0.82	0.09	125,136,146,154	0
22	5MU	1K	54	21/22	0.82	0.10	116,121,138,149	0
23	7MG	2K	47	24/25	0.84	0.12	99,108,119,120	0
23	PSU	2L	56	20/21	0.84	0.09	112,122,130,133	0
23	5MU	2L	55	21/22	0.86	0.09	115,126,133,135	0
23	PSU	2K	56	20/21	0.87	0.07	102,108,119,120	0
23	7MG	2L	47	24/25	0.88	0.11	124,131,143,146	0
23	4SU	2L	8	20/21	0.89	0.14	108,116,123,125	0
23	5MU	2K	55	21/22	0.91	0.07	105,112,118,128	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
23	4SU	2K	8	20/21	0.91	0.12	91,99,105,106	0
22	PSU	1K	39	20/21	0.92	0.14	100,119,123,124	0
22	T6A	1K	37	32/33	0.94	0.18	91,108,133,134	0
23	OMC	2K	33	21/22	0.94	0.15	85,89,90,91	0
22	U8U	1K	34	23/24	0.95	0.10	98,105,115,118	0
23	OMC	2L	33	21/22	0.95	0.10	100,107,110,117	0

5.3 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	1G	1638	1/1	0.32	0.30	119,119,119,119	0
57	MG	14	3019	1/1	0.35	0.28	131,131,131,131	0
57	MG	1G	1648	1/1	0.36	0.35	121,121,121,121	0
57	MG	1G	1621	1/1	0.36	0.43	105,105,105,105	0
57	MG	1G	1629	1/1	0.41	0.26	129,129,129,129	0
57	MG	14	3163	1/1	0.49	0.34	104,104,104,104	0
57	MG	13	1669	1/1	0.51	0.31	111,111,111,111	0
57	MG	1J	205	1/1	0.51	0.16	101,101,101,101	0
57	MG	1H	3147	1/1	0.52	0.31	125,125,125,125	0
57	MG	13	1665	1/1	0.52	0.23	128,128,128,128	0
57	MG	16	202	1/1	0.53	0.28	103,103,103,103	0
57	MG	1H	3197	1/1	0.53	0.39	93,93,93,93	0
57	MG	1G	1623	1/1	0.53	0.24	109,109,109,109	0
57	MG	1H	3238	1/1	0.54	0.34	102,102,102,102	0
57	MG	14	3135	1/1	0.55	0.25	112,112,112,112	0
57	MG	13	1647	1/1	0.55	0.35	99,99,99,99	0
57	MG	1H	3117	1/1	0.55	0.35	96,96,96,96	0
57	MG	13	1648	1/1	0.56	0.30	117,117,117,117	0
57	MG	1H	3130	1/1	0.56	0.42	97,97,97,97	0
57	MG	14	3094	1/1	0.56	0.39	100,100,100,100	0
57	MG	13	1659	1/1	0.57	0.42	109,109,109,109	0
57	MG	14	3020	1/1	0.58	0.16	69,69,69,69	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	13	1668	1/1	0.59	0.40	112,112,112,112	0
57	MG	1G	1602	1/1	0.59	0.33	105,105,105,105	0
57	MG	1G	1628	1/1	0.59	0.30	123,123,123,123	0
57	MG	14	3187	1/1	0.59	0.33	106,106,106,106	0
57	MG	1G	1605	1/1	0.59	0.30	109,109,109,109	0
57	MG	13	1656	1/1	0.60	0.28	107,107,107,107	0
57	MG	1H	3156	1/1	0.60	0.33	106,106,106,106	0
57	MG	14	3142	1/1	0.61	0.34	98,98,98,98	0
57	MG	1J	202	1/1	0.61	0.36	106,106,106,106	0
57	MG	13	1662	1/1	0.61	0.29	90,90,90,90	0
57	MG	14	3161	1/1	0.62	0.17	94,94,94,94	0
57	MG	1H	3235	1/1	0.62	0.17	96,96,96,96	0
57	MG	1G	1642	1/1	0.62	0.45	100,100,100,100	0
57	MG	13	1651	1/1	0.62	0.23	118,118,118,118	0
57	MG	1H	3222	1/1	0.62	0.34	86,86,86,86	0
57	MG	13	1645	1/1	0.63	0.38	117,117,117,117	0
57	MG	14	3102	1/1	0.63	0.26	94,94,94,94	0
57	MG	13	1627	1/1	0.63	0.30	94,94,94,94	0
57	MG	14	3175	1/1	0.64	0.37	100,100,100,100	0
57	MG	14	3103	1/1	0.66	0.46	80,80,80,80	0
57	MG	E5	101	1/1	0.66	0.42	99,99,99,99	0
57	MG	13	1638	1/1	0.67	0.29	103,103,103,103	0
57	MG	14	3064	1/1	0.67	0.26	99,99,99,99	0
57	MG	14	3157	1/1	0.68	0.33	96,96,96,96	0
57	MG	1H	3125	1/1	0.68	0.28	79,79,79,79	0
57	MG	1H	3210	1/1	0.68	0.34	87,87,87,87	0
57	MG	13	1602	1/1	0.68	0.23	130,130,130,130	0
57	MG	1H	3176	1/1	0.68	0.34	102,102,102,102	0
57	MG	1H	3182	1/1	0.68	0.22	108,108,108,108	0
57	MG	1H	3530	1/1	0.68	0.26	99,99,99,99	0
57	MG	14	3147	1/1	0.68	0.41	86,86,86,86	0
57	MG	14	3107	1/1	0.69	0.34	94,94,94,94	0
57	MG	1H	3140	1/1	0.69	0.20	90,90,90,90	0
57	MG	14	3078	1/1	0.70	0.23	88,88,88,88	0
57	MG	14	3443	1/1	0.70	0.21	115,115,115,115	0
57	MG	1H	3493	1/1	0.70	0.20	106,106,106,106	0
57	MG	1H	3159	1/1	0.70	0.45	95,95,95,95	0
57	MG	1H	3074	1/1	0.70	0.26	75,75,75,75	0
57	MG	1H	3177	1/1	0.71	0.17	143,143,143,143	0
57	MG	1H	3131	1/1	0.71	0.32	101,101,101,101	0
57	MG	1G	1624	1/1	0.71	0.26	103,103,103,103	0
57	MG	1G	1712	1/1	0.71	0.14	110,110,110,110	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	13	1629	1/1	0.71	0.27	100,100,100,100	0
57	MG	1H	3056	1/1	0.71	0.40	86,86,86,86	0
57	MG	1J	204	1/1	0.72	0.18	102,102,102,102	0
57	MG	1G	1650	1/1	0.72	0.22	111,111,111,111	0
57	MG	1G	1620	1/1	0.72	0.33	93,93,93,93	0
57	MG	13	1661	1/1	0.73	0.25	101,101,101,101	0
57	MG	14	3153	1/1	0.73	0.23	123,123,123,123	0
57	MG	13	1601	1/1	0.73	0.28	97,97,97,97	0
57	MG	14	3133	1/1	0.73	0.47	89,89,89,89	0
57	MG	1H	3124	1/1	0.73	0.24	90,90,90,90	0
57	MG	13	1641	1/1	0.73	0.34	79,79,79,79	0
57	MG	13	1612	1/1	0.74	0.21	111,111,111,111	0
57	MG	13	1666	1/1	0.74	0.31	98,98,98,98	0
57	MG	1H	3060	1/1	0.74	0.33	90,90,90,90	0
57	MG	13	1643	1/1	0.74	0.19	95,95,95,95	0
57	MG	1H	3532	1/1	0.74	0.27	79,79,79,79	0
57	MG	14	3176	1/1	0.74	0.28	90,90,90,90	0
57	MG	14	3109	1/1	0.74	0.35	94,94,94,94	0
57	MG	14	3017	1/1	0.74	0.26	74,74,74,74	0
57	MG	1H	3545	1/1	0.74	0.32	102,102,102,102	0
57	MG	14	3140	1/1	0.74	0.26	89,89,89,89	0
57	MG	1H	3550	1/1	0.74	0.27	111,111,111,111	0
57	MG	39	301	1/1	0.74	0.12	80,80,80,80	0
57	MG	1H	3077	1/1	0.74	0.31	76,76,76,76	0
57	MG	1G	1647	1/1	0.75	0.27	99,99,99,99	0
57	MG	P8	101	1/1	0.75	0.26	76,76,76,76	0
57	MG	14	3180	1/1	0.75	0.31	86,86,86,86	0
57	MG	1H	3184	1/1	0.75	0.31	100,100,100,100	0
57	MG	1H	3143	1/1	0.75	0.22	79,79,79,79	0
57	MG	42	201	1/1	0.75	0.29	107,107,107,107	0
57	MG	1G	1612	1/1	0.75	0.18	103,103,103,103	0
57	MG	13	1673	1/1	0.75	0.19	110,110,110,110	0
57	MG	1H	3167	1/1	0.75	0.43	86,86,86,86	0
57	MG	14	3165	1/1	0.75	0.32	97,97,97,97	0
57	MG	14	3134	1/1	0.76	0.45	99,99,99,99	0
57	MG	1H	3120	1/1	0.76	0.32	69,69,69,69	0
57	MG	1G	1652	1/1	0.76	0.26	105,105,105,105	0
57	MG	1H	3085	1/1	0.76	0.27	79,79,79,79	0
57	MG	1H	3089	1/1	0.76	0.36	88,88,88,88	0
57	MG	14	3149	1/1	0.76	0.31	94,94,94,94	0
57	MG	35	201	1/1	0.76	0.24	81,81,81,81	0
57	MG	1H	3050	1/1	0.76	0.27	85,85,85,85	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	14	3050	1/1	0.77	0.27	87,87,87,87	0
57	MG	13	1667	1/1	0.77	0.23	104,104,104,104	0
57	MG	1H	3497	1/1	0.77	0.24	96,96,96,96	0
57	MG	14	3088	1/1	0.77	0.32	82,82,82,82	0
57	MG	16	206	1/1	0.77	0.13	83,83,83,83	0
57	MG	1H	3227	1/1	0.77	0.21	90,90,90,90	0
57	MG	1H	3122	1/1	0.77	0.25	80,80,80,80	0
57	MG	13	1642	1/1	0.77	0.20	95,95,95,95	0
57	MG	14	3110	1/1	0.78	0.26	85,85,85,85	0
57	MG	1H	3014	1/1	0.78	0.28	86,86,86,86	0
57	MG	14	3030	1/1	0.78	0.20	90,90,90,90	0
57	MG	13	1634	1/1	0.78	0.28	91,91,91,91	0
57	MG	1G	1649	1/1	0.78	0.39	96,96,96,96	0
57	MG	14	3194	1/1	0.78	0.39	84,84,84,84	0
57	MG	1H	3172	1/1	0.78	0.14	64,64,64,64	0
57	MG	1H	3090	1/1	0.78	0.19	82,82,82,82	0
57	MG	13	1637	1/1	0.78	0.18	90,90,90,90	0
57	MG	1G	1637	1/1	0.78	0.30	106,106,106,106	0
57	MG	42	202	1/1	0.78	0.24	115,115,115,115	0
57	MG	1H	3233	1/1	0.78	0.29	94,94,94,94	0
57	MG	1H	3119	1/1	0.78	0.27	79,79,79,79	0
57	MG	1H	3200	1/1	0.79	0.20	82,82,82,82	0
57	MG	14	3179	1/1	0.79	0.12	103,103,103,103	0
57	MG	1H	3010	1/1	0.79	0.34	87,87,87,87	0
57	MG	14	3144	1/1	0.79	0.17	84,84,84,84	0
57	MG	14	3190	1/1	0.79	0.26	89,89,89,89	0
57	MG	1H	3211	1/1	0.79	0.27	69,69,69,69	0
57	MG	13	1692	1/1	0.79	0.13	110,110,110,110	0
57	MG	1H	3135	1/1	0.79	0.14	73,73,73,73	0
57	MG	1H	3139	1/1	0.79	0.33	90,90,90,90	0
57	MG	1H	3166	1/1	0.79	0.18	67,67,67,67	0
57	MG	1H	3096	1/1	0.79	0.34	83,83,83,83	0
57	MG	1H	3404	1/1	0.79	0.32	71,71,71,71	0
57	MG	14	3087	1/1	0.79	0.18	75,75,75,75	0
57	MG	1H	3196	1/1	0.80	0.28	103,103,103,103	0
57	MG	1H	3152	1/1	0.80	0.28	87,87,87,87	0
57	MG	1H	3178	1/1	0.80	0.27	80,80,80,80	0
57	MG	1H	3160	1/1	0.80	0.30	79,79,79,79	0
57	MG	1H	3364	1/1	0.80	0.14	85,85,85,85	0
57	MG	1H	3552	1/1	0.80	0.10	113,113,113,113	0
57	MG	1H	3057	1/1	0.80	0.29	71,71,71,71	0
57	MG	14	3046	1/1	0.80	0.12	77,77,77,77	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	14	3455	1/1	0.80	0.17	115,115,115,115	0
57	MG	1H	3188	1/1	0.80	0.24	88,88,88,88	0
57	MG	14	3158	1/1	0.80	0.19	84,84,84,84	0
57	MG	14	3114	1/1	0.80	0.13	77,77,77,77	0
57	MG	14	3125	1/1	0.80	0.20	92,92,92,92	0
57	MG	21	301	1/1	0.80	0.26	77,77,77,77	0
57	MG	14	3170	1/1	0.80	0.14	76,76,76,76	0
57	MG	16	207	1/1	0.81	0.16	91,91,91,91	0
57	MG	14	3177	1/1	0.81	0.27	81,81,81,81	0
57	MG	13	1614	1/1	0.81	0.30	102,102,102,102	0
57	MG	1G	1645	1/1	0.81	0.12	124,124,124,124	0
57	MG	14	3183	1/1	0.81	0.24	88,88,88,88	0
57	MG	14	3058	1/1	0.81	0.25	83,83,83,83	0
57	MG	14	3151	1/1	0.81	0.24	108,108,108,108	0
57	MG	14	3193	1/1	0.81	0.33	96,96,96,96	0
57	MG	1G	1614	1/1	0.81	0.32	91,91,91,91	0
57	MG	2L	102	1/1	0.81	0.13	126,126,126,126	0
57	MG	14	3079	1/1	0.81	0.17	86,86,86,86	0
57	MG	1J	201	1/1	0.81	0.25	97,97,97,97	0
57	MG	1H	3391	1/1	0.81	0.26	90,90,90,90	0
57	MG	1G	1631	1/1	0.81	0.15	103,103,103,103	0
57	MG	1H	3078	1/1	0.81	0.29	85,85,85,85	0
57	MG	14	3166	1/1	0.81	0.23	95,95,95,95	0
57	MG	14	3138	1/1	0.81	0.27	91,91,91,91	0
57	MG	14	3095	1/1	0.81	0.39	72,72,72,72	0
57	MG	14	3108	1/1	0.82	0.26	103,103,103,103	0
57	MG	1H	3133	1/1	0.82	0.12	72,72,72,72	0
57	MG	1H	3540	1/1	0.82	0.29	110,110,110,110	0
57	MG	14	3152	1/1	0.82	0.23	99,99,99,99	0
57	MG	1H	3062	1/1	0.82	0.17	64,64,64,64	0
57	MG	1H	3411	1/1	0.82	0.12	95,95,95,95	0
57	MG	14	3130	1/1	0.82	0.24	92,92,92,92	0
57	MG	1G	1625	1/1	0.82	0.34	89,89,89,89	0
57	MG	14	3333	1/1	0.82	0.13	97,97,97,97	0
57	MG	1G	1626	1/1	0.82	0.13	119,119,119,119	0
57	MG	1H	3175	1/1	0.82	0.18	73,73,73,73	0
57	MG	14	3099	1/1	0.82	0.26	101,101,101,101	0
57	MG	14	3167	1/1	0.82	0.12	95,95,95,95	0
57	MG	14	3169	1/1	0.82	0.14	88,88,88,88	0
57	MG	1H	3138	1/1	0.82	0.25	98,98,98,98	0
57	MG	14	3173	1/1	0.82	0.16	90,90,90,90	0
57	MG	1H	3026	1/1	0.82	0.17	82,82,82,82	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	1G	1636	1/1	0.82	0.23	87,87,87,87	0
57	MG	1H	3213	1/1	0.83	0.28	83,83,83,83	0
57	MG	1H	3015	1/1	0.83	0.24	77,77,77,77	0
57	MG	14	3141	1/1	0.83	0.20	85,85,85,85	0
57	MG	1H	3086	1/1	0.83	0.17	67,67,67,67	0
57	MG	1H	3229	1/1	0.83	0.16	84,84,84,84	0
57	MG	1H	3087	1/1	0.83	0.27	75,75,75,75	0
57	MG	1H	3151	1/1	0.83	0.24	79,79,79,79	0
57	MG	13	1655	1/1	0.83	0.36	83,83,83,83	0
57	MG	1H	3035	1/1	0.83	0.21	83,83,83,83	0
57	MG	1H	3094	1/1	0.83	0.30	64,64,64,64	0
57	MG	88	201	1/1	0.83	0.21	83,83,83,83	0
57	MG	1H	3013	1/1	0.83	0.25	94,94,94,94	0
57	MG	1H	3113	1/1	0.83	0.20	70,70,70,70	0
57	MG	14	3456	1/1	0.83	0.09	118,118,118,118	0
57	MG	14	3121	1/1	0.83	0.35	92,92,92,92	0
57	MG	1H	3051	1/1	0.83	0.22	74,74,74,74	0
57	MG	1H	3169	1/1	0.83	0.30	91,91,91,91	0
57	MG	14	3132	1/1	0.83	0.19	90,90,90,90	0
57	MG	1H	3509	1/1	0.83	0.20	114,114,114,114	0
57	MG	13	1670	1/1	0.83	0.39	85,85,85,85	0
57	MG	14	3080	1/1	0.83	0.13	71,71,71,71	0
57	MG	14	3155	1/1	0.84	0.15	83,83,83,83	0
57	MG	14	3093	1/1	0.84	0.23	86,86,86,86	0
57	MG	1H	3055	1/1	0.84	0.17	62,62,62,62	0
57	MG	1H	3012	1/1	0.84	0.12	81,81,81,81	0
57	MG	13	1628	1/1	0.84	0.47	90,90,90,90	0
57	MG	13	1623	1/1	0.84	0.21	70,70,70,70	0
57	MG	1H	3109	1/1	0.84	0.36	79,79,79,79	0
57	MG	13	1675	1/1	0.84	0.11	91,91,91,91	0
57	MG	1H	3114	1/1	0.84	0.12	71,71,71,71	0
57	MG	1H	3187	1/1	0.84	0.38	83,83,83,83	0
57	MG	14	3171	1/1	0.84	0.27	86,86,86,86	0
57	MG	14	3172	1/1	0.84	0.29	82,82,82,82	0
57	MG	14	3004	1/1	0.84	0.27	81,81,81,81	0
57	MG	14	3014	1/1	0.84	0.21	72,72,72,72	0
57	MG	14	3120	1/1	0.84	0.14	84,84,84,84	0
57	MG	1H	3063	1/1	0.84	0.25	59,59,59,59	0
57	MG	1H	3069	1/1	0.84	0.24	76,76,76,76	0
57	MG	14	3126	1/1	0.84	0.27	89,89,89,89	0
57	MG	13	1631	1/1	0.84	0.27	106,106,106,106	0
57	MG	14	3027	1/1	0.84	0.18	85,85,85,85	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	1H	3008	1/1	0.84	0.23	81,81,81,81	0
57	MG	1H	3036	1/1	0.84	0.23	73,73,73,73	0
57	MG	1H	3163	1/1	0.84	0.20	86,86,86,86	0
57	MG	1H	3047	1/1	0.84	0.34	64,64,64,64	0
57	MG	14	3341	1/1	0.84	0.29	78,78,78,78	0
57	MG	14	3425	1/1	0.84	0.13	106,106,106,106	0
57	MG	14	3063	1/1	0.84	0.17	93,93,93,93	0
57	MG	1H	3009	1/1	0.84	0.12	82,82,82,82	0
57	MG	14	3072	1/1	0.84	0.23	88,88,88,88	0
57	MG	1H	3225	1/1	0.84	0.36	74,74,74,74	0
57	MG	13	1632	1/1	0.84	0.14	95,95,95,95	0
57	MG	14	3148	1/1	0.84	0.18	113,113,113,113	0
57	MG	1H	3170	1/1	0.84	0.15	80,80,80,80	0
57	MG	16	210	1/1	0.84	0.25	86,86,86,86	0
57	MG	1H	3232	1/1	0.84	0.17	100,100,100,100	0
57	MG	45	201	1/1	0.84	0.27	84,84,84,84	0
57	MG	14	3090	1/1	0.84	0.25	77,77,77,77	0
57	MG	1G	1644	1/1	0.85	0.11	130,130,130,130	0
57	MG	14	3091	1/1	0.85	0.24	92,92,92,92	0
57	MG	1H	3179	1/1	0.85	0.21	74,74,74,74	0
57	MG	1H	3180	1/1	0.85	0.18	81,81,81,81	0
57	MG	1H	3097	1/1	0.85	0.16	43,43,43,43	0
57	MG	1H	3100	1/1	0.85	0.28	77,77,77,77	0
57	MG	1H	3239	1/1	0.85	0.13	97,97,97,97	0
57	MG	1H	3241	1/1	0.85	0.15	82,82,82,82	0
57	MG	1H	3161	1/1	0.85	0.30	77,77,77,77	0
57	MG	1H	3371	1/1	0.85	0.11	88,88,88,88	0
57	MG	1G	1609	1/1	0.85	0.35	96,96,96,96	0
57	MG	1G	1610	1/1	0.85	0.17	84,84,84,84	0
57	MG	13	1736	1/1	0.85	0.09	129,129,129,129	0
57	MG	14	3118	1/1	0.85	0.12	96,96,96,96	0
57	MG	14	3119	1/1	0.85	0.16	69,69,69,69	0
57	MG	14	3178	1/1	0.85	0.11	83,83,83,83	0
57	MG	14	3007	1/1	0.85	0.15	61,61,61,61	0
57	MG	1G	1613	1/1	0.85	0.37	93,93,93,93	0
57	MG	1H	3194	1/1	0.85	0.25	80,80,80,80	0
57	MG	14	3185	1/1	0.85	0.24	93,93,93,93	0
57	MG	1H	3110	1/1	0.85	0.34	86,86,86,86	0
57	MG	1H	3059	1/1	0.85	0.34	72,72,72,72	0
57	MG	13	1646	1/1	0.85	0.34	91,91,91,91	0
57	MG	1H	3207	1/1	0.85	0.36	77,77,77,77	0
57	MG	14	3195	1/1	0.85	0.25	98,98,98,98	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	14	3204	1/1	0.85	0.16	120,120,120,120	0
57	MG	1H	3525	1/1	0.85	0.16	99,99,99,99	0
57	MG	1H	3049	1/1	0.85	0.21	79,79,79,79	0
57	MG	1G	1627	1/1	0.85	0.16	122,122,122,122	0
57	MG	13	1653	1/1	0.85	0.15	95,95,95,95	0
57	MG	14	3452	1/1	0.85	0.13	122,122,122,122	0
57	MG	1H	3173	1/1	0.85	0.12	77,77,77,77	0
57	MG	14	3067	1/1	0.85	0.17	77,77,77,77	0
57	MG	14	3461	1/1	0.85	0.12	108,108,108,108	0
57	MG	1H	3018	1/1	0.85	0.25	63,63,63,63	0
57	MG	14	3074	1/1	0.85	0.22	95,95,95,95	0
57	MG	1H	3548	1/1	0.85	0.23	98,98,98,98	0
57	MG	1H	3093	1/1	0.85	0.29	73,73,73,73	0
57	MG	13	1605	1/1	0.85	0.17	88,88,88,88	0
57	MG	14	3082	1/1	0.85	0.20	80,80,80,80	0
57	MG	1G	1641	1/1	0.85	0.19	115,115,115,115	0
57	MG	13	1639	1/1	0.85	0.34	80,80,80,80	0
57	MG	16	209	1/1	0.86	0.12	86,86,86,86	0
57	MG	14	3113	1/1	0.86	0.27	74,74,74,74	0
57	MG	1H	3181	1/1	0.86	0.28	98,98,98,98	0
57	MG	14	3028	1/1	0.86	0.18	67,67,67,67	0
57	MG	1G	1634	1/1	0.86	0.11	98,98,98,98	0
57	MG	1G	1635	1/1	0.86	0.23	94,94,94,94	0
57	MG	1H	3155	1/1	0.86	0.26	106,106,106,106	0
57	MG	1H	3219	1/1	0.86	0.20	83,83,83,83	0
57	MG	14	3062	1/1	0.86	0.23	97,97,97,97	0
57	MG	14	3128	1/1	0.86	0.22	88,88,88,88	0
57	MG	1H	3081	1/1	0.86	0.13	77,77,77,77	0
57	MG	1G	1640	1/1	0.86	0.30	80,80,80,80	0
57	MG	1H	3111	1/1	0.86	0.21	94,94,94,94	0
57	MG	1G	1604	1/1	0.86	0.14	132,132,132,132	0
57	MG	1H	3071	1/1	0.86	0.16	101,101,101,101	0
57	MG	1G	1607	1/1	0.86	0.16	107,107,107,107	0
57	MG	1H	3191	1/1	0.86	0.19	79,79,79,79	0
57	MG	1H	3192	1/1	0.86	0.27	83,83,83,83	0
57	MG	1H	3535	1/1	0.86	0.17	110,110,110,110	0
57	MG	14	3143	1/1	0.86	0.23	93,93,93,93	0
57	MG	14	3083	1/1	0.86	0.23	58,58,58,58	0
57	MG	1H	3193	1/1	0.86	0.44	89,89,89,89	0
57	MG	14	3355	1/1	0.86	0.13	99,99,99,99	0
57	MG	13	1611	1/1	0.86	0.17	78,78,78,78	0
57	MG	1G	1617	1/1	0.86	0.12	89,89,89,89	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	14	3150	1/1	0.86	0.16	75,75,75,75	0
57	MG	1H	3162	1/1	0.86	0.33	92,92,92,92	0
57	MG	1H	3075	1/1	0.86	0.25	75,75,75,75	0
57	MG	1H	3164	1/1	0.86	0.23	85,85,85,85	0
57	MG	14	3002	1/1	0.86	0.18	63,63,63,63	0
57	MG	14	3156	1/1	0.86	0.22	81,81,81,81	0
57	MG	1H	3064	1/1	0.86	0.33	82,82,82,82	0
57	MG	16	203	1/1	0.86	0.19	84,84,84,84	0
57	MG	14	3012	1/1	0.86	0.20	69,69,69,69	0
57	MG	16	204	1/1	0.86	0.16	89,89,89,89	0
57	MG	1H	3209	1/1	0.86	0.38	92,92,92,92	0
57	MG	13	1610	1/1	0.86	0.42	81,81,81,81	0
57	MG	1H	3154	1/1	0.87	0.24	67,67,67,67	0
57	MG	13	1616	1/1	0.87	0.22	101,101,101,101	0
57	MG	14	3005	1/1	0.87	0.32	83,83,83,83	0
57	MG	1H	3076	1/1	0.87	0.22	75,75,75,75	0
57	MG	14	3010	1/1	0.87	0.32	84,84,84,84	0
57	MG	14	3105	1/1	0.87	0.18	92,92,92,92	0
57	MG	1H	3158	1/1	0.87	0.21	71,71,71,71	0
57	MG	1H	3226	1/1	0.87	0.24	92,92,92,92	0
57	MG	13	1652	1/1	0.87	0.20	82,82,82,82	0
57	MG	16	201	1/1	0.87	0.23	73,73,73,73	0
57	MG	14	3112	1/1	0.87	0.23	68,68,68,68	0
57	MG	13	1624	1/1	0.87	0.25	83,83,83,83	0
57	MG	14	3025	1/1	0.87	0.15	78,78,78,78	0
57	MG	1H	3185	1/1	0.87	0.25	76,76,76,76	0
57	MG	1H	3040	1/1	0.87	0.17	76,76,76,76	0
57	MG	1H	3042	1/1	0.87	0.15	67,67,67,67	0
57	MG	14	3038	1/1	0.87	0.22	68,68,68,68	0
57	MG	14	3123	1/1	0.87	0.12	75,75,75,75	0
57	MG	1H	3112	1/1	0.87	0.28	79,79,79,79	0
57	MG	14	3047	1/1	0.87	0.16	87,87,87,87	0
57	MG	13	1621	1/1	0.87	0.27	94,94,94,94	0
57	MG	14	3057	1/1	0.87	0.12	93,93,93,93	0
57	MG	14	3191	1/1	0.87	0.21	76,76,76,76	0
57	MG	14	3131	1/1	0.87	0.14	84,84,84,84	0
57	MG	13	1704	1/1	0.87	0.21	111,111,111,111	0
57	MG	1H	3141	1/1	0.87	0.12	75,75,75,75	0
57	MG	31	301	1/1	0.87	0.08	70,70,70,70	0
57	MG	1H	3142	1/1	0.87	0.24	87,87,87,87	0
57	MG	14	3137	1/1	0.87	0.16	76,76,76,76	0
57	MG	13	1664	1/1	0.87	0.31	91,91,91,91	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	14	3068	1/1	0.87	0.21	78,78,78,78	0
57	MG	14	3431	1/1	0.87	0.09	107,107,107,107	0
57	MG	1H	3146	1/1	0.87	0.35	85,85,85,85	0
57	MG	1H	3204	1/1	0.87	0.26	80,80,80,80	0
57	MG	1H	3421	1/1	0.87	0.26	93,93,93,93	0
57	MG	1H	3432	1/1	0.87	0.09	116,116,116,116	0
57	MG	1H	3205	1/1	0.87	0.29	71,71,71,71	0
57	MG	1H	3206	1/1	0.87	0.28	55,55,55,55	0
57	MG	1G	1611	1/1	0.87	0.35	84,84,84,84	0
57	MG	14	3086	1/1	0.87	0.23	73,73,73,73	0
57	MG	13	1741	1/1	0.87	0.14	95,95,95,95	0
57	MG	1G	1723	1/1	0.87	0.10	127,127,127,127	0
57	MG	1H	3150	1/1	0.87	0.23	81,81,81,81	0
57	MG	1H	3073	1/1	0.87	0.26	84,84,84,84	0
57	MG	1H	3004	1/1	0.87	0.19	64,64,64,64	0
57	MG	14	3056	1/1	0.88	0.19	74,74,74,74	0
57	MG	1H	3402	1/1	0.88	0.17	71,71,71,71	0
57	MG	13	1636	1/1	0.88	0.22	81,81,81,81	0
57	MG	1H	3101	1/1	0.88	0.10	72,72,72,72	0
57	MG	1H	3116	1/1	0.88	0.17	82,82,82,82	0
57	MG	1H	3215	1/1	0.88	0.38	94,94,94,94	0
57	MG	1H	3217	1/1	0.88	0.35	79,79,79,79	0
57	MG	14	3372	1/1	0.88	0.09	112,112,112,112	0
57	MG	1H	3190	1/1	0.88	0.15	73,73,73,73	0
57	MG	14	3070	1/1	0.88	0.30	66,66,66,66	0
57	MG	13	1657	1/1	0.88	0.30	75,75,75,75	0
57	MG	14	3444	1/1	0.88	0.26	102,102,102,102	0
57	MG	1H	3512	1/1	0.88	0.20	100,100,100,100	0
57	MG	14	3453	1/1	0.88	0.11	118,118,118,118	0
57	MG	13	1649	1/1	0.88	0.17	83,83,83,83	0
57	MG	1G	1653	1/1	0.88	0.10	125,125,125,125	0
57	MG	1G	1633	1/1	0.88	0.08	102,102,102,102	0
57	MG	13	1615	1/1	0.88	0.27	75,75,75,75	0
57	MG	14	3035	1/1	0.88	0.15	69,69,69,69	0
57	MG	1J	203	1/1	0.88	0.18	92,92,92,92	0
57	MG	1H	3383	1/1	0.88	0.17	74,74,74,74	0
57	MG	14	3040	1/1	0.88	0.26	80,80,80,80	0
57	MG	14	3043	1/1	0.88	0.27	96,96,96,96	0
57	MG	1H	3533	1/1	0.88	0.24	99,99,99,99	0
57	MG	1H	3044	1/1	0.88	0.28	80,80,80,80	0
57	MG	1G	1619	1/1	0.88	0.10	118,118,118,118	0
57	MG	1H	3168	1/1	0.89	0.18	89,89,89,89	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	1H	3223	1/1	0.89	0.24	79,79,79,79	0
57	MG	14	3039	1/1	0.89	0.20	85,85,85,85	0
57	MG	1G	1659	1/1	0.89	0.07	120,120,120,120	0
57	MG	1G	1667	1/1	0.89	0.09	111,111,111,111	0
57	MG	2K	103	1/1	0.89	0.17	88,88,88,88	0
57	MG	14	3145	1/1	0.89	0.16	71,71,71,71	0
57	MG	1G	1720	1/1	0.89	0.09	135,135,135,135	0
57	MG	13	1699	1/1	0.89	0.10	114,114,114,114	0
57	MG	14	3054	1/1	0.89	0.21	67,67,67,67	0
57	MG	14	3202	1/1	0.89	0.12	106,106,106,106	0
57	MG	1G	1726	1/1	0.89	0.22	94,94,94,94	0
57	MG	14	3205	1/1	0.89	0.06	102,102,102,102	0
57	MG	14	3207	1/1	0.89	0.12	70,70,70,70	0
57	MG	14	3270	1/1	0.89	0.10	74,74,74,74	0
57	MG	13	1650	1/1	0.89	0.27	85,85,85,85	0
57	MG	1H	3228	1/1	0.89	0.08	81,81,81,81	0
57	MG	1G	1608	1/1	0.89	0.17	100,100,100,100	0
57	MG	1H	3145	1/1	0.89	0.18	74,74,74,74	0
57	MG	1H	3413	1/1	0.89	0.22	93,93,93,93	0
57	MG	14	3430	1/1	0.89	0.16	102,102,102,102	0
57	MG	14	3065	1/1	0.89	0.23	70,70,70,70	0
57	MG	1H	3174	1/1	0.89	0.17	73,73,73,73	0
57	MG	14	3160	1/1	0.89	0.11	85,85,85,85	0
57	MG	14	3006	1/1	0.89	0.10	78,78,78,78	0
57	MG	1H	3031	1/1	0.89	0.20	90,90,90,90	0
57	MG	14	3122	1/1	0.89	0.20	90,90,90,90	0
57	MG	1H	3445	1/1	0.89	0.17	87,87,87,87	0
57	MG	1H	3126	1/1	0.89	0.14	71,71,71,71	0
57	MG	1H	3237	1/1	0.89	0.31	85,85,85,85	0
57	MG	14	3015	1/1	0.89	0.13	65,65,65,65	0
57	MG	1H	3201	1/1	0.89	0.23	80,80,80,80	0
57	MG	16	208	1/1	0.89	0.17	86,86,86,86	0
57	MG	1H	3218	1/1	0.89	0.33	70,70,70,70	0
57	MG	1H	3514	1/1	0.89	0.12	112,112,112,112	0
57	MG	3I	201	1/1	0.89	0.19	75,75,75,75	0
57	MG	1H	3264	1/1	0.89	0.10	55,55,55,55	0
57	MG	1G	1651	1/1	0.89	0.29	97,97,97,97	0
57	MG	1H	3023	1/1	0.90	0.15	71,71,71,71	0
57	MG	1H	3025	1/1	0.90	0.18	52,52,52,52	0
57	MG	1H	3401	1/1	0.90	0.14	99,99,99,99	0
57	MG	14	3101	1/1	0.90	0.14	87,87,87,87	0
57	MG	14	3051	1/1	0.90	0.20	70,70,70,70	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	1H	3123	1/1	0.90	0.18	68,68,68,68	0
57	MG	13	1608	1/1	0.90	0.09	93,93,93,93	0
57	MG	14	3199	1/1	0.90	0.33	99,99,99,99	0
57	MG	1H	3536	1/1	0.90	0.15	104,104,104,104	0
57	MG	14	3203	1/1	0.90	0.15	95,95,95,95	0
57	MG	14	3009	1/1	0.90	0.09	77,77,77,77	0
57	MG	14	3061	1/1	0.90	0.17	60,60,60,60	0
57	MG	88	203	1/1	0.90	0.16	83,83,83,83	0
57	MG	14	3259	1/1	0.90	0.08	97,97,97,97	0
57	MG	14	3111	1/1	0.90	0.13	83,83,83,83	0
57	MG	14	3011	1/1	0.90	0.23	76,76,76,76	0
57	MG	1H	3030	1/1	0.90	0.18	89,89,89,89	0
57	MG	1H	3543	1/1	0.90	0.10	166,166,166,166	0
57	MG	14	3359	1/1	0.90	0.08	122,122,122,122	0
57	MG	14	3115	1/1	0.90	0.26	78,78,78,78	0
57	MG	14	3388	1/1	0.90	0.17	72,72,72,72	0
57	MG	14	3406	1/1	0.90	0.08	121,121,121,121	0
57	MG	14	3420	1/1	0.90	0.07	119,119,119,119	0
57	MG	14	3117	1/1	0.90	0.10	69,69,69,69	0
57	MG	1H	3199	1/1	0.90	0.14	81,81,81,81	0
57	MG	13	1635	1/1	0.90	0.22	83,83,83,83	0
57	MG	1H	3422	1/1	0.90	0.08	114,114,114,114	0
57	MG	14	3071	1/1	0.90	0.14	82,82,82,82	0
57	MG	14	3450	1/1	0.90	0.23	116,116,116,116	0
57	MG	1H	3011	1/1	0.90	0.24	79,79,79,79	0
57	MG	14	3022	1/1	0.90	0.14	77,77,77,77	0
57	MG	14	3023	1/1	0.90	0.20	58,58,58,58	0
57	MG	14	3024	1/1	0.90	0.12	88,88,88,88	0
57	MG	1G	1686	1/1	0.90	0.07	113,113,113,113	0
57	MG	1G	1704	1/1	0.90	0.12	127,127,127,127	0
57	MG	1G	1711	1/1	0.90	0.08	156,156,156,156	0
57	MG	1H	3221	1/1	0.90	0.25	81,81,81,81	0
57	MG	1H	3065	1/1	0.90	0.18	72,72,72,72	0
57	MG	1H	3017	1/1	0.90	0.19	56,56,56,56	0
57	MG	1H	3134	1/1	0.90	0.30	77,77,77,77	0
57	MG	1H	3369	1/1	0.90	0.14	90,90,90,90	0
57	MG	13	1630	1/1	0.90	0.20	86,86,86,86	0
57	MG	14	3139	1/1	0.90	0.38	88,88,88,88	0
57	MG	1H	3107	1/1	0.91	0.22	62,62,62,62	0
57	MG	32	301	1/1	0.91	0.12	137,137,137,137	0
57	MG	13	1663	1/1	0.91	0.10	77,77,77,77	0
57	MG	14	3096	1/1	0.91	0.16	84,84,84,84	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	13	1622	1/1	0.91	0.17	111,111,111,111	0
57	MG	14	3100	1/1	0.91	0.15	77,77,77,77	0
57	MG	14	3196	1/1	0.91	0.10	85,85,85,85	0
57	MG	14	3197	1/1	0.91	0.23	92,92,92,92	0
57	MG	13	1660	1/1	0.91	0.22	91,91,91,91	0
57	MG	1H	3165	1/1	0.91	0.13	85,85,85,85	0
57	MG	1H	3459	1/1	0.91	0.13	88,88,88,88	0
57	MG	14	3052	1/1	0.91	0.26	59,59,59,59	0
57	MG	14	3053	1/1	0.91	0.39	82,82,82,82	0
57	MG	1H	3484	1/1	0.91	0.20	97,97,97,97	0
57	MG	1H	3492	1/1	0.91	0.07	107,107,107,107	0
57	MG	14	3263	1/1	0.91	0.09	86,86,86,86	0
57	MG	16	205	1/1	0.91	0.10	84,84,84,84	0
57	MG	14	3284	1/1	0.91	0.14	107,107,107,107	0
57	MG	14	3314	1/1	0.91	0.10	78,78,78,78	0
57	MG	1G	1618	1/1	0.91	0.20	91,91,91,91	0
57	MG	13	1603	1/1	0.91	0.18	92,92,92,92	0
57	MG	14	3347	1/1	0.91	0.09	97,97,97,97	0
57	MG	14	3349	1/1	0.91	0.08	99,99,99,99	0
57	MG	1H	3347	1/1	0.91	0.07	113,113,113,113	0
57	MG	14	3356	1/1	0.91	0.20	78,78,78,78	0
57	MG	1H	3362	1/1	0.91	0.09	78,78,78,78	0
57	MG	1H	3092	1/1	0.91	0.13	67,67,67,67	0
57	MG	1H	3203	1/1	0.91	0.26	78,78,78,78	0
57	MG	14	3395	1/1	0.91	0.18	98,98,98,98	0
57	MG	13	1674	1/1	0.91	0.16	105,105,105,105	0
57	MG	14	3415	1/1	0.91	0.21	93,93,93,93	0
57	MG	14	3162	1/1	0.91	0.17	91,91,91,91	0
57	MG	14	3018	1/1	0.91	0.15	82,82,82,82	0
57	MG	14	3429	1/1	0.91	0.21	109,109,109,109	0
57	MG	1H	3380	1/1	0.91	0.15	76,76,76,76	0
57	MG	13	1613	1/1	0.91	0.19	94,94,94,94	0
57	MG	14	3434	1/1	0.91	0.20	110,110,110,110	0
57	MG	14	3438	1/1	0.91	0.12	111,111,111,111	0
57	MG	13	1678	1/1	0.91	0.08	114,114,114,114	0
57	MG	1G	1687	1/1	0.91	0.08	111,111,111,111	0
57	MG	14	3445	1/1	0.91	0.07	119,119,119,119	0
57	MG	14	3124	1/1	0.91	0.25	64,64,64,64	0
57	MG	1G	1702	1/1	0.91	0.07	117,117,117,117	0
57	MG	1H	3082	1/1	0.91	0.19	69,69,69,69	0
57	MG	1G	1630	1/1	0.91	0.14	132,132,132,132	0
57	MG	1H	3099	1/1	0.91	0.17	53,53,53,53	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	14	3029	1/1	0.91	0.21	80,80,80,80	0
57	MG	1G	1713	1/1	0.91	0.09	120,120,120,120	0
57	MG	14	3033	1/1	0.91	0.20	57,57,57,57	0
57	MG	14	3034	1/1	0.91	0.20	75,75,75,75	0
57	MG	1H	3084	1/1	0.91	0.20	77,77,77,77	0
57	MG	14	3181	1/1	0.91	0.17	91,91,91,91	0
57	MG	1J	208	1/1	0.91	0.07	124,124,124,124	0
57	MG	14	3136	1/1	0.91	0.26	95,95,95,95	0
57	MG	14	3184	1/1	0.91	0.16	78,78,78,78	0
57	MG	35	202	1/1	0.91	0.09	80,80,80,80	0
57	MG	1H	3058	1/1	0.91	0.24	68,68,68,68	0
57	MG	14	3186	1/1	0.91	0.13	95,95,95,95	0
57	MG	E5	102	1/1	0.91	0.18	68,68,68,68	0
60	SPE	1G	1725	13/13	0.91	0.12	110,113,117,118	0
57	MG	13	1625	1/1	0.92	0.15	68,68,68,68	0
57	MG	1H	3079	1/1	0.92	0.20	85,85,85,85	0
57	MG	1H	3386	1/1	0.92	0.10	72,72,72,72	0
57	MG	1H	3080	1/1	0.92	0.15	75,75,75,75	0
57	MG	1H	3392	1/1	0.92	0.09	74,74,74,74	0
57	MG	1G	1663	1/1	0.92	0.09	112,112,112,112	0
57	MG	14	3206	1/1	0.92	0.06	97,97,97,97	0
57	MG	1H	3048	1/1	0.92	0.11	68,68,68,68	0
57	MG	1G	1678	1/1	0.92	0.07	98,98,98,98	0
57	MG	13	1633	1/1	0.92	0.09	82,82,82,82	0
57	MG	13	1715	1/1	0.92	0.11	119,119,119,119	0
57	MG	14	3275	1/1	0.92	0.09	85,85,85,85	0
57	MG	14	3098	1/1	0.92	0.20	63,63,63,63	0
57	MG	14	3289	1/1	0.92	0.07	89,89,89,89	0
57	MG	14	3291	1/1	0.92	0.11	71,71,71,71	0
57	MG	1G	1688	1/1	0.92	0.09	123,123,123,123	0
57	MG	1H	3102	1/1	0.92	0.09	52,52,52,52	0
57	MG	1H	3234	1/1	0.92	0.26	84,84,84,84	0
57	MG	1H	3418	1/1	0.92	0.09	122,122,122,122	0
57	MG	14	3154	1/1	0.92	0.21	78,78,78,78	0
57	MG	1H	3420	1/1	0.92	0.17	94,94,94,94	0
57	MG	14	3104	1/1	0.92	0.15	89,89,89,89	0
57	MG	1H	3103	1/1	0.92	0.15	64,64,64,64	0
57	MG	14	3106	1/1	0.92	0.20	79,79,79,79	0
57	MG	14	3379	1/1	0.92	0.07	107,107,107,107	0
57	MG	14	3159	1/1	0.92	0.11	80,80,80,80	0
57	MG	1H	3149	1/1	0.92	0.27	81,81,81,81	0
57	MG	14	3400	1/1	0.92	0.07	135,135,135,135	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	1H	3427	1/1	0.92	0.12	102,102,102,102	0
57	MG	1H	3189	1/1	0.92	0.18	83,83,83,83	0
57	MG	1H	3444	1/1	0.92	0.21	72,72,72,72	0
57	MG	14	3423	1/1	0.92	0.11	118,118,118,118	0
57	MG	1H	3006	1/1	0.92	0.23	77,77,77,77	0
57	MG	1H	3454	1/1	0.92	0.15	104,104,104,104	0
57	MG	14	3055	1/1	0.92	0.14	64,64,64,64	0
57	MG	2L	101	1/1	0.92	0.24	83,83,83,83	0
57	MG	1G	1632	1/1	0.92	0.10	108,108,108,108	0
57	MG	4L	101	1/1	0.92	0.12	102,102,102,102	0
57	MG	14	3439	1/1	0.92	0.20	100,100,100,100	0
57	MG	1H	3007	1/1	0.92	0.17	57,57,57,57	0
57	MG	13	1672	1/1	0.92	0.09	92,92,92,92	0
57	MG	14	3174	1/1	0.92	0.13	78,78,78,78	0
57	MG	14	3447	1/1	0.92	0.06	107,107,107,107	0
57	MG	1H	3486	1/1	0.92	0.20	99,99,99,99	0
57	MG	21	302	1/1	0.92	0.21	85,85,85,85	0
57	MG	1H	3489	1/1	0.92	0.12	107,107,107,107	0
57	MG	1H	3286	1/1	0.92	0.13	65,65,65,65	0
57	MG	13	1609	1/1	0.92	0.15	88,88,88,88	0
57	MG	14	3460	1/1	0.92	0.19	92,92,92,92	0
57	MG	1H	3360	1/1	0.92	0.10	102,102,102,102	0
57	MG	1H	3504	1/1	0.92	0.12	104,104,104,104	0
57	MG	14	3182	1/1	0.92	0.15	66,66,66,66	0
57	MG	14	3127	1/1	0.92	0.11	70,70,70,70	0
57	MG	1G	1643	1/1	0.92	0.10	100,100,100,100	0
57	MG	14	3129	1/1	0.92	0.25	90,90,90,90	0
57	MG	14	3073	1/1	0.92	0.20	61,61,61,61	0
57	MG	1H	3506	1/1	0.92	0.13	103,103,103,103	0
57	MG	14	3075	1/1	0.92	0.16	65,65,65,65	0
57	MG	1H	3020	1/1	0.92	0.15	60,60,60,60	0
57	MG	1H	3043	1/1	0.92	0.11	64,64,64,64	0
57	MG	1H	3136	1/1	0.92	0.12	63,63,63,63	0
57	MG	14	3081	1/1	0.92	0.15	79,79,79,79	0
59	ZN	C5	201	1/1	0.92	0.06	167,167,167,167	0
57	MG	2I	201	1/1	0.92	0.11	97,97,97,97	0
57	MG	88	202	1/1	0.93	0.12	71,71,71,71	0
57	MG	1H	3499	1/1	0.93	0.19	89,89,89,89	0
57	MG	14	3225	1/1	0.93	0.10	79,79,79,79	0
57	MG	14	3257	1/1	0.93	0.09	118,118,118,118	0
57	MG	14	3084	1/1	0.93	0.18	67,67,67,67	0
57	MG	14	3085	1/1	0.93	0.15	52,52,52,52	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	1H	3061	1/1	0.93	0.17	62,62,62,62	0
57	MG	1H	3379	1/1	0.93	0.11	87,87,87,87	0
57	MG	1G	1603	1/1	0.93	0.12	91,91,91,91	0
57	MG	14	3089	1/1	0.93	0.06	73,73,73,73	0
57	MG	1H	3095	1/1	0.93	0.09	76,76,76,76	0
57	MG	14	3302	1/1	0.93	0.16	94,94,94,94	0
57	MG	1H	3041	1/1	0.93	0.12	57,57,57,57	0
57	MG	1H	3513	1/1	0.93	0.14	104,104,104,104	0
57	MG	14	3338	1/1	0.93	0.09	112,112,112,112	0
57	MG	1H	3121	1/1	0.93	0.10	89,89,89,89	0
57	MG	1H	3523	1/1	0.93	0.09	102,102,102,102	0
57	MG	1H	3171	1/1	0.93	0.18	88,88,88,88	0
57	MG	14	3351	1/1	0.93	0.08	101,101,101,101	0
57	MG	14	3097	1/1	0.93	0.11	84,84,84,84	0
57	MG	13	1644	1/1	0.93	0.14	99,99,99,99	0
57	MG	1H	3396	1/1	0.93	0.09	81,81,81,81	0
57	MG	14	3360	1/1	0.93	0.10	107,107,107,107	0
57	MG	14	3368	1/1	0.93	0.14	92,92,92,92	0
57	MG	1G	1670	1/1	0.93	0.20	109,109,109,109	0
57	MG	14	3378	1/1	0.93	0.08	101,101,101,101	0
57	MG	14	3032	1/1	0.93	0.26	72,72,72,72	0
57	MG	1H	3098	1/1	0.93	0.17	59,59,59,59	0
57	MG	14	3391	1/1	0.93	0.11	87,87,87,87	0
57	MG	14	3392	1/1	0.93	0.06	98,98,98,98	0
57	MG	14	3394	1/1	0.93	0.16	91,91,91,91	0
57	MG	1G	1684	1/1	0.93	0.07	109,109,109,109	0
57	MG	1H	3052	1/1	0.93	0.18	58,58,58,58	0
57	MG	14	3405	1/1	0.93	0.07	118,118,118,118	0
57	MG	1G	1616	1/1	0.93	0.17	84,84,84,84	0
57	MG	14	3414	1/1	0.93	0.13	99,99,99,99	0
57	MG	1H	3053	1/1	0.93	0.10	47,47,47,47	0
57	MG	14	3419	1/1	0.93	0.16	119,119,119,119	0
57	MG	1H	3537	1/1	0.93	0.10	112,112,112,112	0
57	MG	14	3042	1/1	0.93	0.16	54,54,54,54	0
57	MG	14	3424	1/1	0.93	0.07	117,117,117,117	0
57	MG	14	3168	1/1	0.93	0.11	70,70,70,70	0
57	MG	1G	1703	1/1	0.93	0.06	107,107,107,107	0
57	MG	1H	3066	1/1	0.93	0.19	65,65,65,65	0
57	MG	1G	1707	1/1	0.93	0.09	115,115,115,115	0
57	MG	1H	3541	1/1	0.93	0.09	109,109,109,109	0
57	MG	1H	3202	1/1	0.93	0.19	80,80,80,80	0
57	MG	1H	3083	1/1	0.93	0.19	80,80,80,80	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	1G	1714	1/1	0.93	0.07	126,126,126,126	0
57	MG	14	3116	1/1	0.93	0.11	77,77,77,77	0
57	MG	13	1654	1/1	0.93	0.25	85,85,85,85	0
57	MG	1G	1721	1/1	0.93	0.05	128,128,128,128	0
57	MG	1G	1722	1/1	0.93	0.13	116,116,116,116	0
57	MG	1H	3070	1/1	0.93	0.11	51,51,51,51	0
57	MG	1H	3551	1/1	0.93	0.07	86,86,86,86	0
57	MG	13	1719	1/1	0.93	0.06	118,118,118,118	0
57	MG	1H	3072	1/1	0.93	0.10	60,60,60,60	0
57	MG	14	3457	1/1	0.93	0.05	134,134,134,134	0
57	MG	1H	3240	1/1	0.93	0.17	86,86,86,86	0
57	MG	1H	3088	1/1	0.93	0.10	87,87,87,87	0
57	MG	1H	3183	1/1	0.93	0.19	75,75,75,75	0
57	MG	1H	3045	1/1	0.93	0.27	63,63,63,63	0
57	MG	1H	3341	1/1	0.93	0.07	113,113,113,113	0
57	MG	14	3003	1/1	0.93	0.13	68,68,68,68	0
57	MG	1H	3460	1/1	0.93	0.23	85,85,85,85	0
57	MG	1J	207	1/1	0.93	0.11	119,119,119,119	0
57	MG	1H	3212	1/1	0.93	0.09	87,87,87,87	0
57	MG	1J	210	1/1	0.93	0.04	135,135,135,135	0
57	MG	19	301	1/1	0.93	0.20	61,61,61,61	0
57	MG	1H	3354	1/1	0.93	0.09	78,78,78,78	0
57	MG	1H	3021	1/1	0.93	0.17	60,60,60,60	0
57	MG	14	3008	1/1	0.93	0.12	73,73,73,73	0
57	MG	14	3076	1/1	0.93	0.10	80,80,80,80	0
57	MG	1H	3491	1/1	0.93	0.11	100,100,100,100	0
57	MG	13	1701	1/1	0.93	0.06	124,124,124,124	0
57	MG	1H	3115	1/1	0.93	0.13	64,64,64,64	0
57	MG	13	1740	1/1	0.93	0.05	162,162,162,162	0
57	MG	1H	3326	1/1	0.94	0.10	109,109,109,109	0
57	MG	1H	3338	1/1	0.94	0.07	99,99,99,99	0
57	MG	1H	3500	1/1	0.94	0.08	90,90,90,90	0
57	MG	13	1671	1/1	0.94	0.10	108,108,108,108	0
57	MG	1H	3001	1/1	0.94	0.21	49,49,49,49	0
57	MG	1G	1716	1/1	0.94	0.10	110,110,110,110	0
57	MG	1G	1719	1/1	0.94	0.08	115,115,115,115	0
57	MG	14	3069	1/1	0.94	0.07	56,56,56,56	0
57	MG	14	3295	1/1	0.94	0.12	88,88,88,88	0
57	MG	1H	3353	1/1	0.94	0.08	62,62,62,62	0
57	MG	14	3306	1/1	0.94	0.15	93,93,93,93	0
57	MG	1G	1615	1/1	0.94	0.12	89,89,89,89	0
57	MG	14	3324	1/1	0.94	0.06	90,90,90,90	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	1H	3510	1/1	0.94	0.07	104,104,104,104	0
57	MG	1H	3153	1/1	0.94	0.24	71,71,71,71	0
57	MG	1H	3028	1/1	0.94	0.21	62,62,62,62	0
57	MG	13	1626	1/1	0.94	0.08	96,96,96,96	0
57	MG	1H	3129	1/1	0.94	0.15	85,85,85,85	0
57	MG	1H	3216	1/1	0.94	0.45	79,79,79,79	0
57	MG	1G	1622	1/1	0.94	0.11	104,104,104,104	0
57	MG	1H	3157	1/1	0.94	0.26	89,89,89,89	0
57	MG	1H	3377	1/1	0.94	0.09	94,94,94,94	0
57	MG	13	1618	1/1	0.94	0.09	72,72,72,72	0
57	MG	14	3362	1/1	0.94	0.07	99,99,99,99	0
57	MG	13	1640	1/1	0.94	0.05	97,97,97,97	0
57	MG	14	3371	1/1	0.94	0.07	108,108,108,108	0
57	MG	1H	3105	1/1	0.94	0.08	78,78,78,78	0
57	MG	14	3373	1/1	0.94	0.08	94,94,94,94	0
57	MG	13	1718	1/1	0.94	0.06	130,130,130,130	0
57	MG	1H	3539	1/1	0.94	0.16	95,95,95,95	0
57	MG	14	3381	1/1	0.94	0.08	136,136,136,136	0
57	MG	14	3384	1/1	0.94	0.06	88,88,88,88	0
57	MG	13	1607	1/1	0.94	0.16	83,83,83,83	0
57	MG	1H	3224	1/1	0.94	0.06	72,72,72,72	0
57	MG	13	1722	1/1	0.94	0.13	99,99,99,99	0
57	MG	1H	3399	1/1	0.94	0.06	109,109,109,109	0
57	MG	1H	3137	1/1	0.94	0.18	67,67,67,67	0
57	MG	14	3397	1/1	0.94	0.10	162,162,162,162	0
57	MG	14	3092	1/1	0.94	0.11	67,67,67,67	0
57	MG	1H	3549	1/1	0.94	0.10	94,94,94,94	0
57	MG	13	1723	1/1	0.94	0.09	118,118,118,118	0
57	MG	14	3412	1/1	0.94	0.10	106,106,106,106	0
57	MG	14	3413	1/1	0.94	0.08	125,125,125,125	0
57	MG	13	1727	1/1	0.94	0.06	124,124,124,124	0
57	MG	14	3016	1/1	0.94	0.13	69,69,69,69	0
57	MG	14	3417	1/1	0.94	0.05	117,117,117,117	0
57	MG	1H	3195	1/1	0.94	0.10	85,85,85,85	0
57	MG	1G	1639	1/1	0.94	0.32	90,90,90,90	0
57	MG	14	3422	1/1	0.94	0.10	104,104,104,104	0
57	MG	13	1728	1/1	0.94	0.06	117,117,117,117	0
57	MG	1H	3415	1/1	0.94	0.11	95,95,95,95	0
57	MG	14	3021	1/1	0.94	0.22	63,63,63,63	0
57	MG	14	3427	1/1	0.94	0.06	121,121,121,121	0
57	MG	13	1731	1/1	0.94	0.11	109,109,109,109	0
57	MG	13	1735	1/1	0.94	0.08	105,105,105,105	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	13	1617	1/1	0.94	0.18	69,69,69,69	0
57	MG	1H	3236	1/1	0.94	0.11	93,93,93,93	0
57	MG	1G	1646	1/1	0.94	0.23	78,78,78,78	0
57	MG	1H	3144	1/1	0.94	0.09	71,71,71,71	0
57	MG	13	1683	1/1	0.94	0.10	119,119,119,119	0
57	MG	1H	3434	1/1	0.94	0.08	96,96,96,96	0
57	MG	13	1689	1/1	0.94	0.11	98,98,98,98	0
57	MG	13	1691	1/1	0.94	0.08	107,107,107,107	0
57	MG	1H	3452	1/1	0.94	0.06	115,115,115,115	0
57	MG	1H	3148	1/1	0.94	0.12	88,88,88,88	0
57	MG	14	3036	1/1	0.94	0.23	85,85,85,85	0
57	MG	1H	3246	1/1	0.94	0.08	54,54,54,54	0
57	MG	13	1658	1/1	0.94	0.44	83,83,83,83	0
57	MG	1G	1666	1/1	0.94	0.08	110,110,110,110	0
57	MG	1H	3466	1/1	0.94	0.10	103,103,103,103	0
57	MG	1H	3481	1/1	0.94	0.09	92,92,92,92	0
57	MG	14	3045	1/1	0.94	0.16	72,72,72,72	0
57	MG	1G	1674	1/1	0.94	0.08	106,106,106,106	0
57	MG	Q8	101	1/1	0.94	0.20	82,82,82,82	0
57	MG	1H	3268	1/1	0.94	0.11	70,70,70,70	0
57	MG	1H	3270	1/1	0.94	0.14	78,78,78,78	0
57	MG	14	3200	1/1	0.94	0.10	86,86,86,86	0
57	MG	14	3201	1/1	0.94	0.10	82,82,82,82	0
57	MG	1H	3281	1/1	0.94	0.07	85,85,85,85	0
57	MG	1H	3024	1/1	0.94	0.17	64,64,64,64	0
57	MG	29	301	1/1	0.94	0.13	65,65,65,65	0
57	MG	1G	1693	1/1	0.94	0.07	121,121,121,121	0
57	MG	1G	1606	1/1	0.94	0.12	87,87,87,87	0
57	MG	1H	3301	1/1	0.94	0.07	86,86,86,86	0
57	MG	1H	3304	1/1	0.94	0.07	64,64,64,64	0
57	MG	14	3222	1/1	0.94	0.09	73,73,73,73	0
57	MG	1G	1706	1/1	0.94	0.06	138,138,138,138	0
57	MG	14	3245	1/1	0.94	0.09	74,74,74,74	0
57	MG	14	3255	1/1	0.94	0.08	110,110,110,110	0
60	SPE	14	3458	13/13	0.94	0.16	92,101,106,108	0
57	MG	1H	3528	1/1	0.95	0.06	117,117,117,117	0
57	MG	14	3328	1/1	0.95	0.09	95,95,95,95	0
57	MG	1H	3214	1/1	0.95	0.20	77,77,77,77	0
57	MG	14	3334	1/1	0.95	0.08	83,83,83,83	0
57	MG	14	3336	1/1	0.95	0.09	109,109,109,109	0
57	MG	1H	3424	1/1	0.95	0.12	84,84,84,84	0
57	MG	13	1606	1/1	0.95	0.13	88,88,88,88	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	1G	1680	1/1	0.95	0.10	103,103,103,103	0
57	MG	14	3348	1/1	0.95	0.06	102,102,102,102	0
57	MG	1G	1681	1/1	0.95	0.04	131,131,131,131	0
57	MG	1H	3534	1/1	0.95	0.06	113,113,113,113	0
57	MG	1H	3358	1/1	0.95	0.06	100,100,100,100	0
57	MG	13	1703	1/1	0.95	0.08	71,71,71,71	0
57	MG	1H	3435	1/1	0.95	0.16	100,100,100,100	0
57	MG	1G	1692	1/1	0.95	0.09	103,103,103,103	0
57	MG	1H	3436	1/1	0.95	0.08	87,87,87,87	0
57	MG	1G	1696	1/1	0.95	0.09	109,109,109,109	0
57	MG	14	3370	1/1	0.95	0.08	90,90,90,90	0
57	MG	14	3037	1/1	0.95	0.23	54,54,54,54	0
57	MG	1G	1698	1/1	0.95	0.07	138,138,138,138	0
57	MG	1G	1699	1/1	0.95	0.06	113,113,113,113	0
57	MG	14	3375	1/1	0.95	0.15	116,116,116,116	0
57	MG	1G	1700	1/1	0.95	0.12	107,107,107,107	0
57	MG	1H	3002	1/1	0.95	0.09	51,51,51,51	0
57	MG	13	1696	1/1	0.95	0.13	114,114,114,114	0
57	MG	14	3044	1/1	0.95	0.10	71,71,71,71	0
57	MG	1H	3027	1/1	0.95	0.11	60,60,60,60	0
57	MG	1H	3370	1/1	0.95	0.14	80,80,80,80	0
57	MG	1H	3547	1/1	0.95	0.06	131,131,131,131	0
57	MG	14	3048	1/1	0.95	0.15	72,72,72,72	0
57	MG	1G	1709	1/1	0.95	0.08	119,119,119,119	0
57	MG	1H	3455	1/1	0.95	0.09	120,120,120,120	0
57	MG	14	3399	1/1	0.95	0.05	122,122,122,122	0
57	MG	13	1739	1/1	0.95	0.08	119,119,119,119	0
57	MG	1H	3029	1/1	0.95	0.11	59,59,59,59	0
57	MG	1H	3463	1/1	0.95	0.15	70,70,70,70	0
57	MG	14	3410	1/1	0.95	0.09	107,107,107,107	0
57	MG	1H	3249	1/1	0.95	0.07	61,61,61,61	0
57	MG	1H	3261	1/1	0.95	0.14	61,61,61,61	0
57	MG	14	3188	1/1	0.95	0.14	69,69,69,69	0
57	MG	1H	3016	1/1	0.95	0.32	52,52,52,52	0
57	MG	1H	3485	1/1	0.95	0.12	102,102,102,102	0
57	MG	14	3059	1/1	0.95	0.11	58,58,58,58	0
57	MG	1H	3384	1/1	0.95	0.09	59,59,59,59	0
57	MG	14	3421	1/1	0.95	0.12	96,96,96,96	0
57	MG	1H	3488	1/1	0.95	0.09	84,84,84,84	0
57	MG	13	1706	1/1	0.95	0.10	88,88,88,88	0
57	MG	13	1724	1/1	0.95	0.07	116,116,116,116	0
57	MG	14	3198	1/1	0.95	0.32	88,88,88,88	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	1H	3279	1/1	0.95	0.13	68,68,68,68	0
57	MG	1H	3054	1/1	0.95	0.12	63,63,63,63	0
57	MG	52	300	1/1	0.95	0.05	133,133,133,133	0
57	MG	1H	3494	1/1	0.95	0.16	87,87,87,87	0
57	MG	1H	3285	1/1	0.95	0.07	69,69,69,69	0
57	MG	1H	3208	1/1	0.95	0.06	69,69,69,69	0
57	MG	21	303	1/1	0.95	0.10	61,61,61,61	0
57	MG	1H	3019	1/1	0.95	0.17	53,53,53,53	0
57	MG	1H	3502	1/1	0.95	0.08	90,90,90,90	0
57	MG	14	3214	1/1	0.95	0.07	83,83,83,83	0
57	MG	14	3215	1/1	0.95	0.06	98,98,98,98	0
57	MG	14	3448	1/1	0.95	0.08	120,120,120,120	0
57	MG	13	1712	1/1	0.95	0.08	106,106,106,106	0
57	MG	14	3451	1/1	0.95	0.21	110,110,110,110	0
57	MG	1H	3505	1/1	0.95	0.07	112,112,112,112	0
57	MG	14	3228	1/1	0.95	0.09	64,64,64,64	0
57	MG	14	3454	1/1	0.95	0.08	108,108,108,108	0
57	MG	14	3243	1/1	0.95	0.15	93,93,93,93	0
57	MG	1H	3410	1/1	0.95	0.08	108,108,108,108	0
57	MG	1H	3313	1/1	0.95	0.06	62,62,62,62	0
57	MG	14	3459	1/1	0.95	0.09	68,68,68,68	0
57	MG	1G	1601	1/1	0.95	0.13	92,92,92,92	0
57	MG	1H	3230	1/1	0.95	0.12	90,90,90,90	0
57	MG	14	3262	1/1	0.95	0.07	104,104,104,104	0
57	MG	1H	3334	1/1	0.95	0.10	103,103,103,103	0
57	MG	14	3265	1/1	0.95	0.07	100,100,100,100	0
57	MG	13	1684	1/1	0.95	0.09	105,105,105,105	0
57	MG	14	3272	1/1	0.95	0.08	71,71,71,71	0
57	MG	14	3273	1/1	0.95	0.07	61,61,61,61	0
57	MG	1H	3419	1/1	0.95	0.24	73,73,73,73	0
57	MG	1J	209	1/1	0.95	0.05	131,131,131,131	0
57	MG	14	3276	1/1	0.95	0.10	85,85,85,85	0
57	MG	1H	3519	1/1	0.95	0.10	104,104,104,104	0
57	MG	1G	1654	1/1	0.95	0.12	102,102,102,102	0
57	MG	1G	1655	1/1	0.95	0.08	90,90,90,90	0
57	MG	1G	1656	1/1	0.95	0.07	89,89,89,89	0
57	MG	14	3300	1/1	0.95	0.09	86,86,86,86	0
57	MG	14	3301	1/1	0.95	0.14	89,89,89,89	0
57	MG	B5	101	1/1	0.95	0.09	99,99,99,99	0
57	MG	1H	3022	1/1	0.95	0.13	56,56,56,56	0
57	MG	1H	3524	1/1	0.95	0.09	61,61,61,61	0
57	MG	14	3311	1/1	0.95	0.07	84,84,84,84	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	14	3312	1/1	0.95	0.06	109,109,109,109	0
57	MG	1H	3091	1/1	0.95	0.42	77,77,77,77	0
57	MG	14	3365	1/1	0.96	0.10	93,93,93,93	0
57	MG	1H	3299	1/1	0.96	0.10	105,105,105,105	0
57	MG	1H	3034	1/1	0.96	0.13	74,74,74,74	0
57	MG	1H	3472	1/1	0.96	0.12	63,63,63,63	0
57	MG	1H	3474	1/1	0.96	0.09	83,83,83,83	0
57	MG	1H	3480	1/1	0.96	0.23	90,90,90,90	0
57	MG	14	3374	1/1	0.96	0.05	94,94,94,94	0
57	MG	13	1705	1/1	0.96	0.05	108,108,108,108	0
57	MG	14	3377	1/1	0.96	0.13	72,72,72,72	0
57	MG	1G	1694	1/1	0.96	0.06	105,105,105,105	0
57	MG	1H	3387	1/1	0.96	0.07	87,87,87,87	0
57	MG	1G	1697	1/1	0.96	0.06	125,125,125,125	0
57	MG	14	3382	1/1	0.96	0.05	116,116,116,116	0
57	MG	14	3383	1/1	0.96	0.06	91,91,91,91	0
57	MG	1H	3306	1/1	0.96	0.07	79,79,79,79	0
57	MG	14	3385	1/1	0.96	0.19	82,82,82,82	0
57	MG	1H	3307	1/1	0.96	0.07	56,56,56,56	0
57	MG	14	3389	1/1	0.96	0.21	72,72,72,72	0
57	MG	14	3390	1/1	0.96	0.14	73,73,73,73	0
57	MG	1H	3394	1/1	0.96	0.12	83,83,83,83	0
57	MG	1G	1701	1/1	0.96	0.06	115,115,115,115	0
57	MG	1H	3311	1/1	0.96	0.09	91,91,91,91	0
57	MG	14	3221	1/1	0.96	0.06	65,65,65,65	0
57	MG	1H	3397	1/1	0.96	0.07	87,87,87,87	0
57	MG	14	3398	1/1	0.96	0.07	86,86,86,86	0
57	MG	1H	3312	1/1	0.96	0.10	69,69,69,69	0
57	MG	1H	3400	1/1	0.96	0.06	79,79,79,79	0
57	MG	14	3404	1/1	0.96	0.07	121,121,121,121	0
57	MG	13	1732	1/1	0.96	0.07	108,108,108,108	0
57	MG	1G	1708	1/1	0.96	0.11	127,127,127,127	0
57	MG	14	3248	1/1	0.96	0.07	76,76,76,76	0
57	MG	14	3250	1/1	0.96	0.12	84,84,84,84	0
57	MG	14	3254	1/1	0.96	0.11	87,87,87,87	0
57	MG	1H	3220	1/1	0.96	0.11	71,71,71,71	0
57	MG	1H	3333	1/1	0.96	0.06	98,98,98,98	0
57	MG	13	1734	1/1	0.96	0.10	143,143,143,143	0
57	MG	1H	3335	1/1	0.96	0.06	83,83,83,83	0
57	MG	1H	3337	1/1	0.96	0.06	98,98,98,98	0
57	MG	13	1686	1/1	0.96	0.08	107,107,107,107	0
57	MG	14	3267	1/1	0.96	0.09	119,119,119,119	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	41	201	1/1	0.96	0.10	81,81,81,81	0
57	MG	1H	3108	1/1	0.96	0.17	68,68,68,68	0
57	MG	14	3049	1/1	0.96	0.16	69,69,69,69	0
57	MG	1H	3346	1/1	0.96	0.05	75,75,75,75	0
57	MG	2K	101	1/1	0.96	0.06	80,80,80,80	0
57	MG	14	3280	1/1	0.96	0.08	76,76,76,76	0
57	MG	1H	3511	1/1	0.96	0.04	113,113,113,113	0
57	MG	14	3433	1/1	0.96	0.13	90,90,90,90	0
57	MG	14	3287	1/1	0.96	0.06	74,74,74,74	0
57	MG	14	3436	1/1	0.96	0.06	136,136,136,136	0
57	MG	1H	3068	1/1	0.96	0.27	66,66,66,66	0
57	MG	14	3290	1/1	0.96	0.12	71,71,71,71	0
57	MG	14	3442	1/1	0.96	0.08	83,83,83,83	0
57	MG	1H	3255	1/1	0.96	0.07	72,72,72,72	0
57	MG	14	3293	1/1	0.96	0.06	70,70,70,70	0
57	MG	14	3294	1/1	0.96	0.06	66,66,66,66	0
57	MG	1H	3423	1/1	0.96	0.04	115,115,115,115	0
57	MG	1H	3356	1/1	0.96	0.07	79,79,79,79	0
57	MG	13	1709	1/1	0.96	0.06	128,128,128,128	0
57	MG	1H	3127	1/1	0.96	0.21	69,69,69,69	0
57	MG	1H	3128	1/1	0.96	0.06	66,66,66,66	0
57	MG	14	3307	1/1	0.96	0.09	80,80,80,80	0
57	MG	1H	3526	1/1	0.96	0.16	96,96,96,96	0
57	MG	1H	3363	1/1	0.96	0.06	73,73,73,73	0
57	MG	13	1737	1/1	0.96	0.14	107,107,107,107	0
57	MG	14	3315	1/1	0.96	0.07	83,83,83,83	0
57	MG	14	3318	1/1	0.96	0.07	65,65,65,65	0
57	MG	14	3323	1/1	0.96	0.06	84,84,84,84	0
57	MG	1H	3365	1/1	0.96	0.10	82,82,82,82	0
57	MG	1G	1657	1/1	0.96	0.05	114,114,114,114	0
57	MG	14	3066	1/1	0.96	0.12	63,63,63,63	0
57	MG	1H	3276	1/1	0.96	0.11	80,80,80,80	0
57	MG	14	3335	1/1	0.96	0.06	94,94,94,94	0
57	MG	1G	1660	1/1	0.96	0.09	128,128,128,128	0
57	MG	1H	3448	1/1	0.96	0.23	76,76,76,76	0
57	MG	14	3339	1/1	0.96	0.04	106,106,106,106	0
57	MG	13	1697	1/1	0.96	0.08	110,110,110,110	0
57	MG	14	3343	1/1	0.96	0.10	84,84,84,84	0
57	MG	14	3345	1/1	0.96	0.10	100,100,100,100	0
57	MG	1H	3453	1/1	0.96	0.09	82,82,82,82	0
57	MG	1G	1669	1/1	0.96	0.07	114,114,114,114	0
57	MG	25	301	1/1	0.96	0.11	120,120,120,120	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	1H	3046	1/1	0.96	0.09	43,43,43,43	0
57	MG	14	3189	1/1	0.96	0.22	81,81,81,81	0
57	MG	14	3352	1/1	0.96	0.06	95,95,95,95	0
57	MG	1H	3003	1/1	0.96	0.14	67,67,67,67	0
57	MG	1H	3456	1/1	0.96	0.09	92,92,92,92	0
57	MG	14	3357	1/1	0.96	0.10	116,116,116,116	0
59	ZN	G8	201	1/1	0.96	0.12	150,150,150,150	0
57	MG	1H	3032	1/1	0.96	0.18	68,68,68,68	0
57	MG	1H	3287	1/1	0.96	0.06	76,76,76,76	0
57	MG	1G	1683	1/1	0.96	0.10	132,132,132,132	0
57	MG	1H	3471	1/1	0.97	0.13	83,83,83,83	0
57	MG	14	3344	1/1	0.97	0.05	104,104,104,104	0
57	MG	1H	3382	1/1	0.97	0.07	43,43,43,43	0
57	MG	14	3346	1/1	0.97	0.05	98,98,98,98	0
57	MG	1H	3473	1/1	0.97	0.11	98,98,98,98	0
57	MG	13	1725	1/1	0.97	0.06	99,99,99,99	0
57	MG	1G	1658	1/1	0.97	0.05	97,97,97,97	0
57	MG	14	3350	1/1	0.97	0.05	88,88,88,88	0
57	MG	16	211	1/1	0.97	0.05	93,93,93,93	0
57	MG	1H	3477	1/1	0.97	0.16	91,91,91,91	0
57	MG	14	3354	1/1	0.97	0.08	80,80,80,80	0
57	MG	1G	1662	1/1	0.97	0.08	118,118,118,118	0
57	MG	13	1707	1/1	0.97	0.05	88,88,88,88	0
57	MG	14	3026	1/1	0.97	0.10	74,74,74,74	0
57	MG	1H	3385	1/1	0.97	0.13	94,94,94,94	0
57	MG	13	1698	1/1	0.97	0.12	93,93,93,93	0
57	MG	14	3361	1/1	0.97	0.05	87,87,87,87	0
57	MG	13	1682	1/1	0.97	0.06	109,109,109,109	0
57	MG	1H	3317	1/1	0.97	0.07	70,70,70,70	0
57	MG	1G	1672	1/1	0.97	0.09	117,117,117,117	0
57	MG	14	3369	1/1	0.97	0.05	90,90,90,90	0
57	MG	1G	1673	1/1	0.97	0.07	80,80,80,80	0
57	MG	1H	3321	1/1	0.97	0.08	55,55,55,55	0
57	MG	1G	1675	1/1	0.97	0.05	86,86,86,86	0
57	MG	1G	1676	1/1	0.97	0.04	104,104,104,104	0
57	MG	1H	3325	1/1	0.97	0.06	88,88,88,88	0
57	MG	1H	3395	1/1	0.97	0.05	92,92,92,92	0
57	MG	1H	3243	1/1	0.97	0.05	63,63,63,63	0
57	MG	1H	3328	1/1	0.97	0.07	81,81,81,81	0
57	MG	14	3041	1/1	0.97	0.10	66,66,66,66	0
57	MG	13	1714	1/1	0.97	0.06	94,94,94,94	0
57	MG	13	1733	1/1	0.97	0.04	118,118,118,118	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	13	1700	1/1	0.97	0.04	110,110,110,110	0
57	MG	13	1604	1/1	0.97	0.07	79,79,79,79	0
57	MG	1G	1691	1/1	0.97	0.06	104,104,104,104	0
57	MG	14	3210	1/1	0.97	0.06	78,78,78,78	0
57	MG	14	3211	1/1	0.97	0.07	67,67,67,67	0
57	MG	14	3213	1/1	0.97	0.10	70,70,70,70	0
57	MG	1H	3501	1/1	0.97	0.05	108,108,108,108	0
57	MG	1H	3262	1/1	0.97	0.06	59,59,59,59	0
57	MG	1H	3503	1/1	0.97	0.07	104,104,104,104	0
57	MG	1H	3405	1/1	0.97	0.07	75,75,75,75	0
57	MG	14	3396	1/1	0.97	0.05	71,71,71,71	0
57	MG	1H	3408	1/1	0.97	0.05	87,87,87,87	0
57	MG	1H	3339	1/1	0.97	0.06	99,99,99,99	0
57	MG	14	3229	1/1	0.97	0.07	74,74,74,74	0
57	MG	14	3230	1/1	0.97	0.05	56,56,56,56	0
57	MG	14	3233	1/1	0.97	0.09	85,85,85,85	0
57	MG	14	3238	1/1	0.97	0.08	67,67,67,67	0
57	MG	14	3241	1/1	0.97	0.07	61,61,61,61	0
57	MG	14	3407	1/1	0.97	0.14	111,111,111,111	0
57	MG	1H	3507	1/1	0.97	0.14	90,90,90,90	0
57	MG	14	3411	1/1	0.97	0.04	115,115,115,115	0
57	MG	1H	3508	1/1	0.97	0.17	144,144,144,144	0
57	MG	14	3247	1/1	0.97	0.12	87,87,87,87	0
57	MG	13	1619	1/1	0.97	0.08	54,54,54,54	0
57	MG	1H	3343	1/1	0.97	0.07	115,115,115,115	0
57	MG	1H	3067	1/1	0.97	0.06	55,55,55,55	0
57	MG	1H	3104	1/1	0.97	0.12	68,68,68,68	0
57	MG	14	3256	1/1	0.97	0.08	99,99,99,99	0
57	MG	1H	3348	1/1	0.97	0.05	66,66,66,66	0
57	MG	14	3060	1/1	0.97	0.11	65,65,65,65	0
57	MG	14	3260	1/1	0.97	0.16	77,77,77,77	0
57	MG	1H	3350	1/1	0.97	0.06	58,58,58,58	0
57	MG	1H	3516	1/1	0.97	0.04	122,122,122,122	0
57	MG	14	3426	1/1	0.97	0.05	99,99,99,99	0
57	MG	1H	3351	1/1	0.97	0.14	66,66,66,66	0
57	MG	14	3428	1/1	0.97	0.04	110,110,110,110	0
57	MG	1H	3522	1/1	0.97	0.05	112,112,112,112	0
57	MG	14	3268	1/1	0.97	0.18	89,89,89,89	0
57	MG	1H	3271	1/1	0.97	0.07	84,84,84,84	0
57	MG	1H	3272	1/1	0.97	0.11	79,79,79,79	0
57	MG	14	3146	1/1	0.97	0.05	62,62,62,62	0
57	MG	1H	3355	1/1	0.97	0.07	58,58,58,58	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	14	3437	1/1	0.97	0.07	111,111,111,111	0
57	MG	1H	3033	1/1	0.97	0.11	63,63,63,63	0
57	MG	14	3278	1/1	0.97	0.05	83,83,83,83	0
57	MG	14	3279	1/1	0.97	0.06	93,93,93,93	0
57	MG	1H	3428	1/1	0.97	0.06	93,93,93,93	0
57	MG	14	3282	1/1	0.97	0.06	82,82,82,82	0
57	MG	1H	3431	1/1	0.97	0.05	102,102,102,102	0
57	MG	14	3446	1/1	0.97	0.04	118,118,118,118	0
57	MG	14	3286	1/1	0.97	0.06	58,58,58,58	0
57	MG	1H	3531	1/1	0.97	0.05	114,114,114,114	0
57	MG	14	3288	1/1	0.97	0.07	59,59,59,59	0
57	MG	1H	3277	1/1	0.97	0.09	79,79,79,79	0
57	MG	1H	3433	1/1	0.97	0.06	98,98,98,98	0
57	MG	13	1720	1/1	0.97	0.04	121,121,121,121	0
57	MG	13	1694	1/1	0.97	0.06	92,92,92,92	0
57	MG	1H	3231	1/1	0.97	0.06	103,103,103,103	0
57	MG	14	3077	1/1	0.97	0.15	85,85,85,85	0
57	MG	14	3296	1/1	0.97	0.06	76,76,76,76	0
57	MG	14	3297	1/1	0.97	0.06	90,90,90,90	0
57	MG	1H	3442	1/1	0.97	0.04	107,107,107,107	0
57	MG	1H	3443	1/1	0.97	0.05	112,112,112,112	0
57	MG	13	1685	1/1	0.97	0.06	79,79,79,79	0
57	MG	14	3305	1/1	0.97	0.07	64,64,64,64	0
57	MG	1H	3037	1/1	0.97	0.08	57,57,57,57	0
57	MG	1H	3446	1/1	0.97	0.04	100,100,100,100	0
57	MG	1H	3544	1/1	0.97	0.06	105,105,105,105	0
57	MG	1J	206	1/1	0.97	0.04	99,99,99,99	0
57	MG	14	3164	1/1	0.97	0.04	83,83,83,83	0
57	MG	1H	3295	1/1	0.97	0.06	58,58,58,58	0
57	MG	1H	3296	1/1	0.97	0.06	56,56,56,56	0
57	MG	1H	3038	1/1	0.97	0.07	61,61,61,61	0
57	MG	14	3320	1/1	0.97	0.07	70,70,70,70	0
57	MG	14	3321	1/1	0.97	0.08	89,89,89,89	0
57	MG	1H	3372	1/1	0.97	0.17	66,66,66,66	0
57	MG	1H	3373	1/1	0.97	0.12	79,79,79,79	0
57	MG	14	3326	1/1	0.97	0.11	87,87,87,87	0
57	MG	1H	3375	1/1	0.97	0.05	80,80,80,80	0
57	MG	1H	3457	1/1	0.97	0.06	102,102,102,102	0
57	MG	1H	3132	1/1	0.97	0.14	55,55,55,55	0
57	MG	1H	3039	1/1	0.97	0.05	56,56,56,56	0
57	MG	1H	3462	1/1	0.97	0.05	99,99,99,99	0
57	MG	M5	101	1/1	0.97	0.26	81,81,81,81	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	14	3337	1/1	0.97	0.04	116,116,116,116	0
57	MG	13	1680	1/1	0.97	0.06	89,89,89,89	0
57	MG	1H	3465	1/1	0.97	0.07	112,112,112,112	0
57	MG	1H	3381	1/1	0.97	0.06	58,58,58,58	0
57	MG	13	1738	1/1	0.98	0.06	138,138,138,138	0
57	MG	14	3342	1/1	0.98	0.05	105,105,105,105	0
57	MG	1H	3409	1/1	0.98	0.07	83,83,83,83	0
57	MG	1H	3275	1/1	0.98	0.06	72,72,72,72	0
57	MG	13	1730	1/1	0.98	0.05	110,110,110,110	0
57	MG	1H	3475	1/1	0.98	0.05	99,99,99,99	0
57	MG	1H	3476	1/1	0.98	0.13	94,94,94,94	0
57	MG	1H	3412	1/1	0.98	0.07	90,90,90,90	0
57	MG	1H	3478	1/1	0.98	0.07	79,79,79,79	0
57	MG	1H	3319	1/1	0.98	0.04	58,58,58,58	0
57	MG	1H	3366	1/1	0.98	0.04	56,56,56,56	0
57	MG	14	3013	1/1	0.98	0.11	56,56,56,56	0
57	MG	14	3353	1/1	0.98	0.11	89,89,89,89	0
57	MG	1H	3483	1/1	0.98	0.04	99,99,99,99	0
57	MG	1H	3416	1/1	0.98	0.04	80,80,80,80	0
57	MG	13	1716	1/1	0.98	0.07	116,116,116,116	0
57	MG	1H	3323	1/1	0.98	0.08	78,78,78,78	0
57	MG	1H	3487	1/1	0.98	0.04	108,108,108,108	0
57	MG	1H	3324	1/1	0.98	0.06	69,69,69,69	0
57	MG	1H	3278	1/1	0.98	0.04	86,86,86,86	0
57	MG	1G	1661	1/1	0.98	0.15	118,118,118,118	0
57	MG	14	3364	1/1	0.98	0.03	98,98,98,98	0
57	MG	1H	3490	1/1	0.98	0.10	95,95,95,95	0
57	MG	14	3366	1/1	0.98	0.04	99,99,99,99	0
57	MG	14	3367	1/1	0.98	0.07	101,101,101,101	0
57	MG	1H	3242	1/1	0.98	0.04	50,50,50,50	0
57	MG	1G	1664	1/1	0.98	0.06	82,82,82,82	0
57	MG	1G	1665	1/1	0.98	0.06	82,82,82,82	0
57	MG	14	3216	1/1	0.98	0.12	62,62,62,62	0
57	MG	14	3217	1/1	0.98	0.04	76,76,76,76	0
57	MG	1H	3106	1/1	0.98	0.09	73,73,73,73	0
57	MG	1H	3376	1/1	0.98	0.04	71,71,71,71	0
57	MG	14	3223	1/1	0.98	0.10	61,61,61,61	0
57	MG	14	3376	1/1	0.98	0.05	82,82,82,82	0
57	MG	14	3224	1/1	0.98	0.05	76,76,76,76	0
57	MG	1G	1668	1/1	0.98	0.06	106,106,106,106	0
57	MG	1H	3426	1/1	0.98	0.14	82,82,82,82	0
57	MG	14	3380	1/1	0.98	0.09	106,106,106,106	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	1H	3284	1/1	0.98	0.05	62,62,62,62	0
57	MG	14	3031	1/1	0.98	0.14	51,51,51,51	0
57	MG	14	3231	1/1	0.98	0.06	78,78,78,78	0
57	MG	1G	1671	1/1	0.98	0.05	101,101,101,101	0
57	MG	14	3236	1/1	0.98	0.05	69,69,69,69	0
57	MG	14	3386	1/1	0.98	0.12	65,65,65,65	0
57	MG	1H	3498	1/1	0.98	0.04	113,113,113,113	0
57	MG	14	3239	1/1	0.98	0.06	60,60,60,60	0
57	MG	1H	3118	1/1	0.98	0.07	63,63,63,63	0
57	MG	F8	101	1/1	0.98	0.10	85,85,85,85	0
57	MG	14	3244	1/1	0.98	0.06	68,68,68,68	0
57	MG	14	3393	1/1	0.98	0.06	89,89,89,89	0
57	MG	I8	101	1/1	0.98	0.07	95,95,95,95	0
57	MG	1H	3429	1/1	0.98	0.05	87,87,87,87	0
57	MG	1H	3430	1/1	0.98	0.08	94,94,94,94	0
57	MG	1G	1679	1/1	0.98	0.14	105,105,105,105	0
57	MG	14	3252	1/1	0.98	0.04	69,69,69,69	0
57	MG	1H	3248	1/1	0.98	0.05	57,57,57,57	0
57	MG	1H	3336	1/1	0.98	0.04	88,88,88,88	0
57	MG	14	3401	1/1	0.98	0.15	89,89,89,89	0
57	MG	14	3402	1/1	0.98	0.05	111,111,111,111	0
57	MG	14	3403	1/1	0.98	0.04	78,78,78,78	0
57	MG	1G	1682	1/1	0.98	0.09	123,123,123,123	0
57	MG	13	1717	1/1	0.98	0.07	93,93,93,93	0
57	MG	14	3258	1/1	0.98	0.07	97,97,97,97	0
57	MG	1H	3289	1/1	0.98	0.05	91,91,91,91	0
57	MG	14	3408	1/1	0.98	0.04	77,77,77,77	0
57	MG	14	3409	1/1	0.98	0.10	87,87,87,87	0
57	MG	1G	1685	1/1	0.98	0.05	129,129,129,129	0
57	MG	14	3261	1/1	0.98	0.07	64,64,64,64	0
57	MG	1H	3291	1/1	0.98	0.05	57,57,57,57	0
57	MG	1H	3340	1/1	0.98	0.04	109,109,109,109	0
57	MG	14	3264	1/1	0.98	0.07	88,88,88,88	0
57	MG	1H	3437	1/1	0.98	0.07	76,76,76,76	0
57	MG	14	3416	1/1	0.98	0.04	87,87,87,87	0
57	MG	14	3266	1/1	0.98	0.04	77,77,77,77	0
57	MG	14	3418	1/1	0.98	0.05	97,97,97,97	0
57	MG	1G	1689	1/1	0.98	0.07	92,92,92,92	0
57	MG	1G	1690	1/1	0.98	0.07	113,113,113,113	0
57	MG	14	3269	1/1	0.98	0.05	104,104,104,104	0
57	MG	1H	3441	1/1	0.98	0.06	100,100,100,100	0
57	MG	14	3271	1/1	0.98	0.05	67,67,67,67	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	1H	3294	1/1	0.98	0.12	68,68,68,68	0
57	MG	13	1690	1/1	0.98	0.04	117,117,117,117	0
57	MG	14	3274	1/1	0.98	0.07	62,62,62,62	0
57	MG	1H	3390	1/1	0.98	0.08	48,48,48,48	0
57	MG	1G	1695	1/1	0.98	0.09	126,126,126,126	0
57	MG	1H	3345	1/1	0.98	0.09	85,85,85,85	0
57	MG	13	1687	1/1	0.98	0.07	89,89,89,89	0
57	MG	1H	3515	1/1	0.98	0.07	78,78,78,78	0
57	MG	14	3432	1/1	0.98	0.12	103,103,103,103	0
57	MG	14	3281	1/1	0.98	0.10	75,75,75,75	0
57	MG	1H	3447	1/1	0.98	0.03	98,98,98,98	0
57	MG	14	3435	1/1	0.98	0.04	122,122,122,122	0
57	MG	1H	3517	1/1	0.98	0.20	85,85,85,85	0
57	MG	14	3285	1/1	0.98	0.05	89,89,89,89	0
57	MG	1H	3297	1/1	0.98	0.06	56,56,56,56	0
57	MG	1H	3520	1/1	0.98	0.06	88,88,88,88	0
57	MG	14	3440	1/1	0.98	0.15	87,87,87,87	0
57	MG	14	3441	1/1	0.98	0.13	103,103,103,103	0
57	MG	1H	3521	1/1	0.98	0.04	65,65,65,65	0
57	MG	1H	3449	1/1	0.98	0.11	92,92,92,92	0
57	MG	1G	1705	1/1	0.98	0.03	117,117,117,117	0
57	MG	1H	3450	1/1	0.98	0.07	87,87,87,87	0
57	MG	13	1726	1/1	0.98	0.06	107,107,107,107	0
57	MG	2K	102	1/1	0.98	0.11	99,99,99,99	0
57	MG	1H	3302	1/1	0.98	0.05	54,54,54,54	0
57	MG	14	3449	1/1	0.98	0.05	105,105,105,105	0
57	MG	1G	1710	1/1	0.98	0.04	113,113,113,113	0
57	MG	1H	3527	1/1	0.98	0.04	97,97,97,97	0
57	MG	1H	3398	1/1	0.98	0.04	86,86,86,86	0
57	MG	1H	3529	1/1	0.98	0.04	110,110,110,110	0
57	MG	1H	3266	1/1	0.98	0.10	92,92,92,92	0
57	MG	14	3303	1/1	0.98	0.04	52,52,52,52	0
57	MG	1G	1715	1/1	0.98	0.05	110,110,110,110	0
57	MG	1H	3305	1/1	0.98	0.07	72,72,72,72	0
57	MG	1G	1717	1/1	0.98	0.04	126,126,126,126	0
57	MG	14	3309	1/1	0.98	0.04	48,48,48,48	0
57	MG	14	3310	1/1	0.98	0.04	71,71,71,71	0
57	MG	1G	1718	1/1	0.98	0.04	124,124,124,124	0
57	MG	1H	3458	1/1	0.98	0.12	89,89,89,89	0
57	MG	14	3313	1/1	0.98	0.06	67,67,67,67	0
57	MG	13	1695	1/1	0.98	0.05	91,91,91,91	0
57	MG	1H	3198	1/1	0.98	0.24	75,75,75,75	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	1H	3461	1/1	0.98	0.05	80,80,80,80	0
57	MG	14	3319	1/1	0.98	0.09	72,72,72,72	0
57	MG	1H	3403	1/1	0.98	0.07	68,68,68,68	0
57	MG	1G	1724	1/1	0.98	0.06	126,126,126,126	0
57	MG	1H	3308	1/1	0.98	0.06	62,62,62,62	0
57	MG	1H	3538	1/1	0.98	0.05	107,107,107,107	0
57	MG	14	3325	1/1	0.98	0.04	88,88,88,88	0
57	MG	1H	3464	1/1	0.98	0.12	57,57,57,57	0
57	MG	14	3327	1/1	0.98	0.05	108,108,108,108	0
57	MG	13	1721	1/1	0.98	0.11	77,77,77,77	0
57	MG	14	3329	1/1	0.98	0.13	93,93,93,93	0
57	MG	14	3332	1/1	0.98	0.08	63,63,63,63	0
57	MG	1H	3406	1/1	0.98	0.03	95,95,95,95	0
57	MG	7A	101	1/1	0.98	0.16	110,110,110,110	0
57	MG	1H	3542	1/1	0.98	0.04	103,103,103,103	0
57	MG	1H	3468	1/1	0.98	0.05	82,82,82,82	0
58	SF4	3E	301	8/8	0.98	0.04	95,98,106,108	0
57	MG	1H	3469	1/1	0.98	0.06	84,84,84,84	0
57	MG	14	3001	1/1	0.98	0.05	51,51,51,51	0
57	MG	1H	3470	1/1	0.98	0.11	105,105,105,105	0
57	MG	14	3340	1/1	0.98	0.06	63,63,63,63	0
57	MG	1H	3273	1/1	0.99	0.07	56,56,56,56	0
57	MG	1H	3318	1/1	0.99	0.08	74,74,74,74	0
57	MG	1H	3274	1/1	0.99	0.03	48,48,48,48	0
57	MG	1H	3378	1/1	0.99	0.04	54,54,54,54	0
57	MG	14	3277	1/1	0.99	0.11	64,64,64,64	0
57	MG	1H	3320	1/1	0.99	0.03	71,71,71,71	0
57	MG	13	1729	1/1	0.99	0.04	110,110,110,110	0
57	MG	14	3387	1/1	0.99	0.08	83,83,83,83	0
57	MG	1H	3244	1/1	0.99	0.04	47,47,47,47	0
57	MG	1H	3245	1/1	0.99	0.08	58,58,58,58	0
57	MG	13	1688	1/1	0.99	0.04	96,96,96,96	0
57	MG	14	3283	1/1	0.99	0.05	105,105,105,105	0
57	MG	1H	3247	1/1	0.99	0.05	67,67,67,67	0
57	MG	1H	3327	1/1	0.99	0.10	81,81,81,81	0
57	MG	1H	3280	1/1	0.99	0.03	47,47,47,47	0
57	MG	1H	3329	1/1	0.99	0.04	53,53,53,53	0
57	MG	14	3192	1/1	0.99	0.03	80,80,80,80	0
57	MG	1H	3388	1/1	0.99	0.10	49,49,49,49	0
57	MG	1H	3330	1/1	0.99	0.03	74,74,74,74	0
57	MG	1H	3331	1/1	0.99	0.03	88,88,88,88	0
57	MG	14	3292	1/1	0.99	0.08	71,71,71,71	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	13	1708	1/1	0.99	0.03	91,91,91,91	0
57	MG	1H	3393	1/1	0.99	0.04	63,63,63,63	0
57	MG	1H	3282	1/1	0.99	0.10	54,54,54,54	0
57	MG	13	1676	1/1	0.99	0.03	67,67,67,67	0
57	MG	1H	3250	1/1	0.99	0.04	54,54,54,54	0
57	MG	14	3298	1/1	0.99	0.03	95,95,95,95	0
57	MG	1H	3252	1/1	0.99	0.04	52,52,52,52	0
57	MG	1H	3253	1/1	0.99	0.04	58,58,58,58	0
57	MG	1H	3288	1/1	0.99	0.04	58,58,58,58	0
57	MG	1H	3467	1/1	0.99	0.12	74,74,74,74	0
57	MG	14	3304	1/1	0.99	0.04	61,61,61,61	0
57	MG	1H	3254	1/1	0.99	0.04	49,49,49,49	0
57	MG	1H	3290	1/1	0.99	0.08	87,87,87,87	0
57	MG	1H	3342	1/1	0.99	0.05	83,83,83,83	0
57	MG	14	3308	1/1	0.99	0.06	64,64,64,64	0
57	MG	14	3208	1/1	0.99	0.10	63,63,63,63	0
57	MG	14	3209	1/1	0.99	0.05	61,61,61,61	0
57	MG	13	1710	1/1	0.99	0.08	73,73,73,73	0
57	MG	1H	3344	1/1	0.99	0.04	60,60,60,60	0
57	MG	14	3212	1/1	0.99	0.05	60,60,60,60	0
57	MG	1H	3292	1/1	0.99	0.03	62,62,62,62	0
57	MG	1H	3546	1/1	0.99	0.06	105,105,105,105	0
57	MG	14	3316	1/1	0.99	0.03	100,100,100,100	0
57	MG	14	3317	1/1	0.99	0.03	100,100,100,100	0
57	MG	1H	3258	1/1	0.99	0.04	56,56,56,56	0
57	MG	1H	3407	1/1	0.99	0.04	69,69,69,69	0
57	MG	1H	3259	1/1	0.99	0.04	59,59,59,59	0
57	MG	14	3218	1/1	0.99	0.04	55,55,55,55	0
57	MG	14	3322	1/1	0.99	0.03	58,58,58,58	0
57	MG	14	3219	1/1	0.99	0.02	59,59,59,59	0
57	MG	14	3220	1/1	0.99	0.06	65,65,65,65	0
57	MG	1H	3260	1/1	0.99	0.05	70,70,70,70	0
57	MG	1H	3349	1/1	0.99	0.04	61,61,61,61	0
57	MG	1H	3479	1/1	0.99	0.03	95,95,95,95	0
57	MG	13	1711	1/1	0.99	0.04	70,70,70,70	0
57	MG	13	1702	1/1	0.99	0.04	70,70,70,70	0
57	MG	14	3330	1/1	0.99	0.04	94,94,94,94	0
57	MG	14	3331	1/1	0.99	0.02	56,56,56,56	0
57	MG	14	3227	1/1	0.99	0.04	52,52,52,52	0
57	MG	1H	3482	1/1	0.99	0.06	107,107,107,107	0
57	MG	1H	3352	1/1	0.99	0.04	70,70,70,70	0
57	MG	1H	3414	1/1	0.99	0.06	52,52,52,52	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	1H	3300	1/1	0.99	0.04	73,73,73,73	0
57	MG	14	3232	1/1	0.99	0.04	75,75,75,75	0
57	MG	1H	3263	1/1	0.99	0.06	53,53,53,53	0
57	MG	14	3234	1/1	0.99	0.03	62,62,62,62	0
57	MG	14	3235	1/1	0.99	0.03	55,55,55,55	0
57	MG	1H	3417	1/1	0.99	0.03	100,100,100,100	0
57	MG	14	3237	1/1	0.99	0.04	67,67,67,67	0
57	MG	13	1713	1/1	0.99	0.05	96,96,96,96	0
57	MG	1H	3265	1/1	0.99	0.06	74,74,74,74	0
57	MG	14	3240	1/1	0.99	0.11	63,63,63,63	0
57	MG	1H	3357	1/1	0.99	0.07	64,64,64,64	0
57	MG	14	3242	1/1	0.99	0.04	82,82,82,82	0
57	MG	16	212	1/1	0.99	0.02	78,78,78,78	0
57	MG	13	1681	1/1	0.99	0.11	91,91,91,91	0
57	MG	1H	3359	1/1	0.99	0.06	92,92,92,92	0
57	MG	14	3246	1/1	0.99	0.10	93,93,93,93	0
57	MG	1H	3267	1/1	0.99	0.05	103,103,103,103	0
57	MG	1H	3361	1/1	0.99	0.04	53,53,53,53	0
57	MG	14	3249	1/1	0.99	0.09	85,85,85,85	0
57	MG	1H	3495	1/1	0.99	0.05	87,87,87,87	0
57	MG	14	3251	1/1	0.99	0.15	113,113,113,113	0
57	MG	1H	3496	1/1	0.99	0.09	89,89,89,89	0
57	MG	14	3358	1/1	0.99	0.08	78,78,78,78	0
57	MG	14	3253	1/1	0.99	0.03	79,79,79,79	0
57	MG	1H	3425	1/1	0.99	0.04	81,81,81,81	0
57	MG	13	1677	1/1	0.99	0.04	90,90,90,90	0
57	MG	1H	3269	1/1	0.99	0.05	83,83,83,83	0
57	MG	14	3363	1/1	0.99	0.02	83,83,83,83	0
57	MG	1H	3309	1/1	0.99	0.03	73,73,73,73	0
57	MG	I8	102	1/1	0.99	0.09	70,70,70,70	0
57	MG	1H	3310	1/1	0.99	0.02	76,76,76,76	0
57	MG	1H	3005	1/1	0.99	0.10	67,67,67,67	0
57	MG	1H	3367	1/1	0.99	0.08	69,69,69,69	0
57	MG	1H	3368	1/1	0.99	0.09	72,72,72,72	0
57	MG	1G	1677	1/1	0.99	0.03	83,83,83,83	0
57	MG	13	1620	1/1	0.99	0.05	68,68,68,68	0
57	MG	13	1693	1/1	0.99	0.08	95,95,95,95	0
57	MG	1H	3314	1/1	0.99	0.09	65,65,65,65	0
57	MG	1H	3315	1/1	0.99	0.04	61,61,61,61	0
57	MG	1H	3316	1/1	0.99	0.04	76,76,76,76	0
58	SF4	32	302	8/8	0.99	0.04	115,120,128,136	0
57	MG	1H	3438	1/1	0.99	0.03	95,95,95,95	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
59	ZN	5A	101	1/1	0.99	0.04	129,129,129,129	0
57	MG	1H	3439	1/1	0.99	0.04	76,76,76,76	0
57	MG	1H	3440	1/1	0.99	0.08	83,83,83,83	0
57	MG	1H	3374	1/1	0.99	0.08	57,57,57,57	0
57	MG	1H	3332	1/1	1.00	0.03	84,84,84,84	0
57	MG	1H	3322	1/1	1.00	0.03	59,59,59,59	0
57	MG	14	3299	1/1	1.00	0.05	63,63,63,63	0
57	MG	1H	3389	1/1	1.00	0.05	63,63,63,63	0
57	MG	1H	3257	1/1	1.00	0.03	49,49,49,49	0
57	MG	14	3226	1/1	1.00	0.03	54,54,54,54	0
57	MG	1H	3451	1/1	1.00	0.01	55,55,55,55	0
57	MG	1H	3283	1/1	1.00	0.03	59,59,59,59	0
57	MG	1H	3518	1/1	1.00	0.03	57,57,57,57	0
57	MG	1H	3186	1/1	1.00	0.02	56,56,56,56	0
57	MG	1H	3298	1/1	1.00	0.03	52,52,52,52	0
59	ZN	5I	101	1/1	1.00	0.02	94,94,94,94	0
57	MG	1H	3251	1/1	1.00	0.05	49,49,49,49	0
57	MG	13	1679	1/1	1.00	0.03	89,89,89,89	0
57	MG	1H	3293	1/1	1.00	0.02	60,60,60,60	0
57	MG	1H	3256	1/1	1.00	0.02	48,48,48,48	0
57	MG	1H	3303	1/1	1.00	0.03	49,49,49,49	0

5.5 Other polymers (i)

There are no such residues in this entry.