Full wwPDB X-ray Structure Validation Report (i)

Sep 16, 2026 – 06:49 am BST

PDB ID	:	5E81 / pdb_00005e81
Title	:	Structure of T. thermophilus 70S ribosome complex with mRNA and tRNALys in the A-site with wobble pair
Authors	:	Rozov, A.; Demeshkina, N.; Khusainov, I.; Yusupov, M.; Yusupova, G.
Deposited on	:	2015-10-13
Resolution	:	2.95 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:

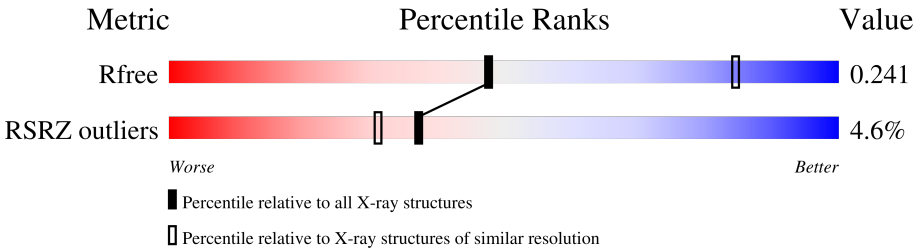
MolProbity	:	FAILED
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 2.95 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	1130 (2.98-2.94)
RSRZ outliers	180081	1130 (2.98-2.94)

MolProbity failed to run properly - the sequence quality summary graphics cannot be shown.

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
56	MG	13	1655	-	-	-	X
56	MG	14	3028	-	-	-	X
56	MG	14	3149	-	-	-	X
56	MG	14	3212	-	-	-	X
56	MG	1G	1641	-	-	-	X
56	MG	1G	1656	-	-	-	X
56	MG	1H	3015	-	-	-	X
56	MG	1H	3258	-	-	-	X

2 Entry composition (i)

There are 59 unique types of molecules in this entry. The entry contains 297904 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	1496	Total	C	N	O	P	0	0	0
			32157	14313	5960	10388	1496			
1	1G	1506	Total	C	N	O	P	0	0	0
			32371	14409	6001	10456	1505			

- 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			
4	32	208	Total	C	N	O	S	0	0	0
			1702	1066	339	290	7			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	4E	149	Total	C	N	O	S	0	0	0
			1142	722	216	200	4			
5	42	149	Total	C	N	O	S	0	0	0
			1139	721	216	198	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	140	Total	C	N	O	S	0	0	0
			1120	695	223	196	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	95	Total	C	N	O	S	0	0	0
			754	471	148	134	1			

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
10	1A	80	Total 646	C 403	N 129	O 114	0	0	0

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	4I	119	Total 942	C 582	N 194	O 164	S 2	0	0	0
13	4A	111	Total 893	C 552	N 183	O 156	S 2	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	5I	60	Total 491	C 312	N 104	O 71	S 4	0	0	0
14	5A	59	Total 486	C 309	N 103	O 70	S 4	0	0	0

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

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

- 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	62	Total	C	N	O	S	0	0	0
			481	306	85	88	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	BI	97	Total	C	N	O	S	0	0	0
			746	461	157	126	2			
20	BA	99	Total	C	N	O	S	0	0	0
			762	470	162	128	2			

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

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

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

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
22	1K	72	Total	C	N	O	P	S	0	0	0
			1542	691	269	509	72	1			
22	1L	69	Total	C	N	O	P	S	0	0	0
			1477	662	257	488	69	1			

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	3K	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	21	Total	C	N	O	P	0	0	0
			464	208	99	136	21			
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	2885	Total	C	N	O	P	0	3	0
			62204	27685	11631	20000	2888			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	14	2855	Total	C	N	O	P	0	0	0
			61505	27372	11512	19766	2855			

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	133	Total	C	N	O	S	0	0	0
			1033	651	194	187	1			
28	79	57	Total	C	N	O		0	0	0
			456	283	91	82				

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

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

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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
			1558	985	298	269	6			
30	29	204	Total	C	N	O	S	0	0	0
			1563	988	299	270	6			

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
32	41	179	Total	C	N	O	S	0	0	0
			1457	931	265	257	4			
32	49	181	Total	C	N	O	S	0	0	0
			1468	937	268	259	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	70	Total	C	N	O		0	0	0
			543	341	110	92				

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
34	61	146	Total	C	N	O	S	0	0	0
			1136	726	201	208	1			
34	69	145	Total	C	N	O	S	0	0	0
			1131	723	200	207	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
35	58	137	Total	C	N	O	S	0	0	0
			1096	706	205	181	4			
35	15	138	Total	C	N	O	S	0	0	0
			1104	712	206	182	4			

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
38	88	141	Total	C	N	O	S	0	0	0
			1117	712	211	187	7			
38	45	139	Total	C	N	O	S	0	0	0
			1104	705	209	184	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	136	Total 1124	C 700	N 231	O 192	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 743	C 482	N 134	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	133	Total	C	N	O	S	0	0	0
			1079	694	194	189	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	94	Total	C	N	O	S	0	0	0
			737	463	146	127	1			
49	F5	94	Total	C	N	O	S	0	0	0
			737	463	146	127	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
50	K8	68	Total	C	N	O	S	0	0	0
			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	49	Total	C	N	O	S	0	0	0
			376	240	63	68	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 MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	13	161	Total	Mg	0	0
			161	161		

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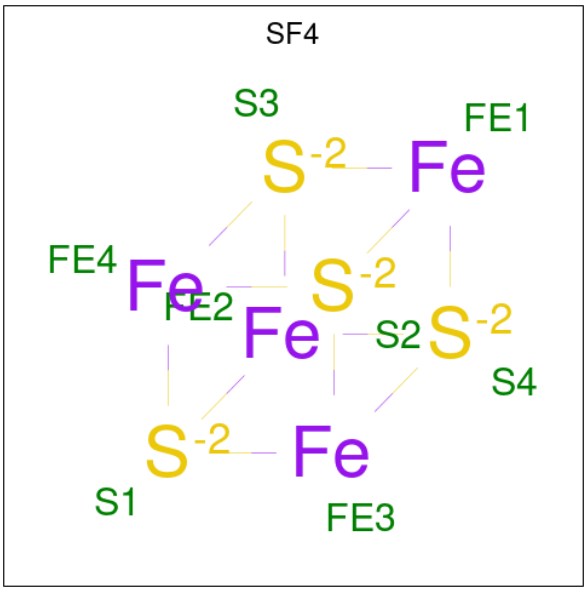
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
56	5E	1	Total Mg 1 1	0	0
56	5I	1	Total Mg 1 1	0	0
56	1K	1	Total Mg 1 1	0	0
56	2K	3	Total Mg 3 3	0	0
56	4K	1	Total Mg 1 1	0	0
56	1H	572	Total Mg 572 572	0	0
56	16	13	Total Mg 13 13	0	0
56	11	3	Total Mg 3 3	0	0
56	21	3	Total Mg 3 3	0	0
56	41	2	Total Mg 2 2	0	0
56	78	2	Total Mg 2 2	0	0
56	88	3	Total Mg 3 3	0	0
56	98	1	Total Mg 1 1	0	0
56	F8	1	Total Mg 1 1	0	0
56	I8	1	Total Mg 1 1	0	0
56	L8	1	Total Mg 1 1	0	0
56	P8	1	Total Mg 1 1	0	0
56	Q8	1	Total Mg 1 1	0	0
56	1G	126	Total Mg 126 126	0	0
56	32	1	Total Mg 1 1	0	0
56	42	2	Total Mg 2 2	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
56	52	1	Total Mg 1 1	0	0
56	2A	1	Total Mg 1 1	0	0
56	2L	3	Total Mg 3 3	0	0
56	14	471	Total Mg 471 471	0	0
56	1J	11	Total Mg 11 11	0	0
56	29	1	Total Mg 1 1	0	0
56	39	2	Total Mg 2 2	0	0
56	25	2	Total Mg 2 2	0	0
56	35	3	Total Mg 3 3	0	0
56	45	2	Total Mg 2 2	0	0
56	B5	1	Total Mg 1 1	0	0
56	E5	3	Total Mg 3 3	0	0
56	M5	1	Total Mg 1 1	0	0

- Molecule 57 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
57	3E	1	Total Fe S 8 4 4	0	0
57	32	1	Total Fe S 8 4 4	0	0

- Molecule 58 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
58	5I	1	Total Zn 1 1	0	0
58	G8	1	Total Zn 1 1	0	0
58	5A	1	Total Zn 1 1	0	0
58	C5	1	Total Zn 1 1	0	0

- Molecule 59 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
59	13	389	Total O 389 389	0	0
59	1E	1	Total O 1 1	0	0
59	3E	2	Total O 2 2	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
59	4E	1	Total O 1 1	0	0
59	8E	3	Total O 3 3	0	0
59	1I	2	Total O 2 2	0	0
59	3I	2	Total O 2 2	0	0
59	4I	2	Total O 2 2	0	0
59	5I	2	Total O 2 2	0	0
59	6I	3	Total O 3 3	0	0
59	7I	1	Total O 1 1	0	0
59	1F	2	Total O 2 2	0	0
59	1K	8	Total O 8 8	0	0
59	2K	6	Total O 6 6	0	0
59	3K	1	Total O 1 1	0	0
59	4K	5	Total O 5 5	0	0
59	1H	1539	Total O 1539 1539	0	0
59	16	35	Total O 35 35	0	0
59	11	16	Total O 16 16	0	0
59	21	7	Total O 7 7	0	0
59	31	6	Total O 6 6	0	0
59	41	1	Total O 1 1	0	0
59	58	2	Total O 2 2	0	0
59	68	2	Total O 2 2	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
59	78	8	Total O 8 8	0	0
59	88	8	Total O 8 8	0	0
59	C8	4	Total O 4 4	0	0
59	D8	2	Total O 2 2	0	0
59	F8	2	Total O 2 2	0	0
59	G8	1	Total O 1 1	0	0
59	I8	7	Total O 7 7	0	0
59	J8	2	Total O 2 2	0	0
59	K8	1	Total O 1 1	0	0
59	L8	3	Total O 3 3	0	0
59	P8	1	Total O 1 1	0	0
59	Q8	8	Total O 8 8	0	0
59	1G	297	Total O 297 297	0	0
59	32	2	Total O 2 2	0	0
59	42	1	Total O 1 1	0	0
59	52	4	Total O 4 4	0	0
59	62	3	Total O 3 3	0	0
59	2A	3	Total O 3 3	0	0
59	3A	1	Total O 1 1	0	0
59	6A	1	Total O 1 1	0	0
59	7A	6	Total O 6 6	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
59	9A	2	Total O 2 2	0	0
59	BA	5	Total O 5 5	0	0
59	1L	1	Total O 1 1	0	0
59	2L	6	Total O 6 6	0	0
59	4L	5	Total O 5 5	0	0
59	14	1225	Total O 1225 1225	0	0
59	1J	12	Total O 12 12	0	0
59	19	11	Total O 11 11	0	0
59	29	5	Total O 5 5	0	0
59	39	7	Total O 7 7	0	0
59	25	6	Total O 6 6	0	0
59	35	8	Total O 8 8	0	0
59	45	4	Total O 4 4	0	0
59	55	3	Total O 3 3	0	0
59	85	1	Total O 1 1	0	0
59	95	1	Total O 1 1	0	0
59	A5	1	Total O 1 1	0	0
59	B5	1	Total O 1 1	0	0
59	C5	3	Total O 3 3	0	0
59	F5	1	Total O 1 1	0	0
59	H5	2	Total O 2 2	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
59	L5	3	Total O 3 3	0	0
59	M5	6	Total O 6 6	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	209.20Å 448.50Å 619.90Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	147.01 – 2.95 147.01 – 2.95	Depositor EDS
% Data completeness (in resolution range)	100.0 (147.01-2.95) 91.6 (147.01-2.95)	Depositor EDS
R_{merge}	0.32	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	0.91 (at 2.96Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.196 , 0.242 0.197 , 0.241	Depositor DCC
R_{free} test set	2000 reflections (0.17%)	wwPDB-VP
Wilson B-factor (Å^2)	77.9	Xtriage
Anisotropy	0.354	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 66.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	297904	wwPDB-VP
Average B, all atoms (Å^2)	98.0	wwPDB-VP

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

[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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
22	PSU	1L	55	22	18,21,22	1.18	2 (11%)	22,30,33	1.51	4 (18%)
22	T6A	1K	37	22	31,34,35	2.16	9 (29%)	44,49,52	2.19	14 (31%)
22	U8U	1L	34	22,25	19,24,25	2.54	7 (36%)	23,34,37	1.22	3 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
23	PSU	2K	56	23	18,21,22	1.32	2 (11%)	22,30,33	2.18	6 (27%)
23	4SU	2K	8	23	18,21,22	1.93	3 (16%)	26,30,33	2.60	5 (19%)
22	PSU	1K	39	22	18,21,22	1.00	1 (5%)	22,30,33	1.50	3 (13%)
23	PSU	2L	56	23	18,21,22	1.20	1 (5%)	22,30,33	1.56	2 (9%)
23	4SU	2L	8	23	18,21,22	1.91	3 (16%)	26,30,33	2.67	5 (19%)
23	OMC	2L	33	23	19,22,23	1.59	3 (15%)	26,31,34	1.11	1 (3%)
22	5MU	1K	54	22	19,22,23	3.83	5 (26%)	28,32,35	2.78	8 (28%)
22	PSU	1K	55	22	18,21,22	1.26	1 (5%)	22,30,33	1.63	4 (18%)
22	PSU	1L	39	22	18,21,22	1.08	1 (5%)	22,30,33	1.43	3 (13%)
23	5MU	2L	55	23	19,22,23	3.82	5 (26%)	28,32,35	3.43	9 (32%)
23	5MU	2K	55	23	19,22,23	3.90	5 (26%)	28,32,35	3.33	7 (25%)
23	OMC	2K	33	23	19,22,23	1.59	3 (15%)	26,31,34	1.05	3 (11%)
23	G7M	2K	47	23	23,26,27	4.41	7 (30%)	35,39,42	3.18	14 (40%)
22	5MU	1L	54	22	19,22,23	3.92	5 (26%)	28,32,35	3.33	7 (25%)
22	T6A	1L	37	22	31,34,35	2.11	7 (22%)	44,49,52	2.27	12 (27%)
23	G7M	2L	47	23	23,26,27	4.52	8 (34%)	35,39,42	3.26	14 (40%)
22	U8U	1K	34	22,25	19,24,25	2.35	7 (36%)	23,34,37	1.15	2 (8%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	PSU	1L	55	22	-	1/7/25/26	0/2/2/2
22	T6A	1K	37	22	-	2/23/41/42	0/3/3/3
22	U8U	1L	34	22,25	-	4/9/28/29	0/2/2/2
23	PSU	2K	56	23	-	1/7/25/26	0/2/2/2
23	4SU	2K	8	23	-	0/7/25/26	0/2/2/2
22	PSU	1K	39	22	-	0/7/25/26	0/2/2/2
23	PSU	2L	56	23	-	1/7/25/26	0/2/2/2
23	4SU	2L	8	23	-	0/7/25/26	0/2/2/2
23	OMC	2L	33	23	-	1/9/27/28	0/2/2/2
22	5MU	1K	54	22	-	0/7/25/26	0/2/2/2
22	PSU	1K	55	22	-	0/7/25/26	0/2/2/2
22	PSU	1L	39	22	-	2/7/25/26	0/2/2/2
23	5MU	2L	55	23	-	0/7/25/26	0/2/2/2
23	5MU	2K	55	23	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	OMC	2K	33	23	-	1/9/27/28	0/2/2/2
23	G7M	2K	47	23	-	0/7/25/26	0/3/3/3
22	5MU	1L	54	22	-	0/7/25/26	0/2/2/2
22	T6A	1L	37	22	-	1/23/41/42	0/3/3/3
23	G7M	2L	47	23	-	2/7/25/26	0/3/3/3
22	U8U	1K	34	22,25	-	0/9/28/29	0/2/2/2

All (85) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	2L	47	G7M	C8-N7	17.97	1.65	1.33
23	2K	47	G7M	C8-N7	17.54	1.64	1.33
22	1L	54	5MU	C2-N1	12.90	1.59	1.38
23	2K	55	5MU	C2-N1	12.73	1.58	1.38
22	1K	54	5MU	C2-N1	12.30	1.58	1.38
23	2L	55	5MU	C2-N1	12.29	1.58	1.38
22	1L	37	T6A	C10-N11	6.50	1.49	1.35
23	2K	55	5MU	C2-N3	6.41	1.49	1.38
22	1K	54	5MU	C2-N3	6.28	1.49	1.38
22	1L	54	5MU	C4-N3	-6.25	1.27	1.38
23	2L	55	5MU	C4-N3	-6.20	1.27	1.38
22	1K	37	T6A	C10-N11	6.16	1.48	1.35
23	2L	47	G7M	C4-N3	6.05	1.48	1.34
23	2K	47	G7M	C4-N3	6.04	1.48	1.34
23	2K	8	4SU	C5-C4	5.95	1.50	1.42
23	2K	47	G7M	C5-C4	-5.85	1.23	1.38
22	1K	37	T6A	C10-N6	5.77	1.49	1.37
22	1L	54	5MU	C6-N1	5.75	1.47	1.38
23	2L	47	G7M	C5-N7	5.71	1.45	1.39
22	1L	54	5MU	C2-N3	5.71	1.48	1.38
23	2L	47	G7M	C5-C4	-5.68	1.23	1.38
22	1L	34	U8U	C2-N3	5.66	1.50	1.37
23	2K	55	5MU	C4-N3	-5.62	1.28	1.38
22	1K	54	5MU	C6-N1	5.62	1.47	1.38
23	2L	8	4SU	C5-C4	5.60	1.49	1.42
23	2L	55	5MU	C2-N3	5.56	1.47	1.38
22	1L	37	T6A	C10-N6	5.48	1.48	1.37
22	1K	54	5MU	C4-N3	-5.39	1.28	1.38
23	2K	55	5MU	C6-N1	5.33	1.47	1.38
23	2L	55	5MU	C6-N1	5.22	1.47	1.38
22	1L	37	T6A	C6-N6	5.15	1.49	1.39
22	1L	34	U8U	C6-C5	5.14	1.49	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	2L	55	5MU	C4-C5	5.04	1.53	1.44
22	1K	34	U8U	C2-N3	4.91	1.48	1.37
22	1K	54	5MU	C4-C5	4.84	1.52	1.44
23	2K	55	5MU	C4-C5	4.75	1.52	1.44
22	1K	34	U8U	C6-C5	4.68	1.48	1.34
22	1L	34	U8U	C6-N1	4.56	1.45	1.38
23	2K	47	G7M	C5-N7	4.52	1.44	1.39
22	1K	37	T6A	C6-N6	4.41	1.48	1.39
23	2L	33	OMC	C2-N3	4.40	1.45	1.36
23	2K	33	OMC	C2-N3	4.27	1.45	1.36
22	1K	55	PSU	C6-C5	4.21	1.40	1.35
23	2K	8	4SU	C2-N1	4.18	1.45	1.38
22	1K	34	U8U	C6-N1	4.18	1.45	1.38
23	2L	47	G7M	C8-N9	4.09	1.47	1.35
22	1L	34	U8U	C2-S2	-4.07	1.61	1.67
22	1L	54	5MU	C4-C5	4.05	1.51	1.44
22	1K	34	U8U	C2-S2	-4.01	1.61	1.67
22	1L	34	U8U	C4-N3	3.98	1.46	1.38
23	2L	56	PSU	C6-C5	3.95	1.39	1.35
23	2K	33	OMC	C4-N4	3.82	1.42	1.33
23	2L	8	4SU	C2-N1	3.78	1.44	1.38
23	2K	47	G7M	C8-N9	3.75	1.46	1.35
22	1L	55	PSU	C6-C5	3.74	1.39	1.35
23	2K	56	PSU	C6-C5	3.71	1.39	1.35
23	2L	33	OMC	C4-N4	3.68	1.42	1.33
23	2K	47	G7M	C2-N2	3.63	1.42	1.34
22	1L	39	PSU	C6-C5	3.54	1.39	1.35
23	2K	47	G7M	C4-N9	-3.43	1.29	1.38
23	2L	47	G7M	C4-N9	-3.39	1.29	1.38
22	1K	34	U8U	C4-N3	3.26	1.44	1.38
23	2L	8	4SU	C6-N1	3.07	1.45	1.38
22	1K	37	T6A	C5-C4	-2.99	1.33	1.39
22	1K	37	T6A	C6-N1	-2.99	1.30	1.35
23	2K	33	OMC	C5-C4	2.87	1.49	1.42
23	2L	47	G7M	C2-N2	2.86	1.41	1.34
23	2L	33	OMC	C5-C4	2.84	1.49	1.42
22	1K	37	T6A	C5-N7	-2.73	1.33	1.39
23	2K	56	PSU	C4-C5	-2.73	1.36	1.44
22	1K	39	PSU	C6-C5	2.69	1.38	1.35
23	2K	8	4SU	C6-N1	2.44	1.43	1.38
22	1L	37	T6A	ODB-C13	-2.38	1.22	1.30
22	1K	37	T6A	ODB-C13	-2.31	1.23	1.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	1K	37	T6A	C4-N9	-2.28	1.32	1.37
22	1L	34	U8U	O4-C4	-2.28	1.19	1.23
22	1K	34	U8U	C4-C5	2.26	1.50	1.45
22	1L	37	T6A	C5-C4	-2.21	1.34	1.39
22	1L	37	T6A	C5-N7	-2.21	1.34	1.39
22	1L	55	PSU	C2-N1	2.20	1.39	1.36
22	1L	37	T6A	C4-N9	-2.15	1.32	1.37
22	1K	34	U8U	O4-C4	-2.09	1.19	1.23
23	2L	47	G7M	C5-C6	2.03	1.48	1.43
22	1L	34	U8U	C4-C5	2.01	1.49	1.45
22	1K	37	T6A	ODA-C13	2.01	1.28	1.22

All (126) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	2L	47	G7M	CN7-N7-C5	11.68	141.28	126.77
22	1L	54	5MU	C5-C4-N3	11.37	125.02	115.31
23	2K	47	G7M	CN7-N7-C5	10.83	140.23	126.77
23	2L	55	5MU	C5-C4-N3	10.81	124.54	115.31
23	2K	55	5MU	C5-C4-N3	10.47	124.25	115.31
22	1K	54	5MU	C5-C4-N3	9.27	123.22	115.31
23	2K	8	4SU	C4-N3-C2	-8.95	118.65	127.34
23	2L	8	4SU	C4-N3-C2	-8.65	118.94	127.34
23	2L	8	4SU	C5-C4-N3	7.85	121.97	114.69
23	2L	55	5MU	C5-C6-N1	-7.16	115.97	123.34
23	2K	8	4SU	C5-C4-N3	7.11	121.28	114.69
23	2L	55	5MU	C4-N3-C2	-6.93	118.37	127.35
23	2K	47	G7M	C6-C5-N7	-6.51	124.37	132.25
22	1L	54	5MU	O4-C4-C5	-6.47	117.41	124.90
23	2L	55	5MU	C6-C5-C4	6.39	123.38	118.03
23	2K	55	5MU	C4-N3-C2	-6.36	119.12	127.35
23	2K	55	5MU	C5-C6-N1	-6.33	116.83	123.34
22	1L	54	5MU	C4-N3-C2	-6.30	119.19	127.35
23	2L	47	G7M	C8-N7-C5	-6.29	99.92	107.78
23	2K	55	5MU	C6-C5-C4	6.20	123.22	118.03
23	2K	47	G7M	C8-N7-C5	-6.18	100.06	107.78
22	1L	37	T6A	C12-N11-C10	5.87	131.72	121.94
23	2K	55	5MU	O4-C4-C5	-5.85	118.12	124.90
22	1L	37	T6A	N3-C2-N1	-5.81	119.52	128.60
23	2K	47	G7M	N9-C8-N7	-5.67	98.19	112.21
23	2L	47	G7M	N9-C8-N7	-5.58	98.40	112.21
22	1L	54	5MU	C5-C6-N1	-5.56	117.62	123.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	2K	56	PSU	N1-C2-N3	5.50	121.37	115.13
23	2L	47	G7M	C6-C5-N7	-5.38	125.74	132.25
22	1L	54	5MU	C6-C5-C4	5.36	122.51	118.03
22	1K	37	T6A	N3-C2-N1	-5.24	120.40	128.60
22	1K	37	T6A	C5-C4-N3	-5.18	119.99	126.75
22	1K	37	T6A	C4-C5-C6	5.12	120.78	116.81
23	2K	56	PSU	C4-N3-C2	-5.09	119.00	126.34
23	2K	55	5MU	C5M-C5-C6	-5.01	116.16	122.85
22	1K	54	5MU	O4-C4-C5	-4.98	119.13	124.90
23	2L	55	5MU	O4-C4-C5	-4.94	119.17	124.90
22	1K	54	5MU	C5-C6-N1	-4.79	118.41	123.34
22	1L	37	T6A	C5-C4-N3	-4.77	120.53	126.75
22	1K	54	5MU	C4-N3-C2	-4.66	121.32	127.35
22	1K	54	5MU	C6-C5-C4	4.63	121.90	118.03
22	1K	37	T6A	N9-C8-N7	-4.53	107.72	113.91
23	2L	8	4SU	C5-C4-S4	-4.52	118.64	124.47
22	1K	37	T6A	N6-C10-N11	4.45	119.98	113.76
22	1K	39	PSU	C4-N3-C2	-4.41	119.99	126.34
23	2K	47	G7M	C4-C5-N7	4.40	114.86	107.67
22	1K	54	5MU	C5M-C5-C6	-4.40	116.98	122.85
23	2K	56	PSU	C6-N1-C2	-4.28	118.31	122.68
23	2L	55	5MU	C5M-C5-C6	-4.27	117.15	122.85
22	1L	55	PSU	C4-N3-C2	-4.22	120.26	126.34
22	1L	37	T6A	C4-C5-C6	4.16	120.04	116.81
23	2L	47	G7M	C4-C5-N7	4.14	114.43	107.67
23	2L	56	PSU	C4-N3-C2	-4.10	120.44	126.34
23	2K	8	4SU	C5-C4-S4	-4.07	119.23	124.47
22	1K	55	PSU	N1-C2-N3	3.97	119.63	115.13
23	2K	47	G7M	O6-C6-C5	-3.93	119.19	128.06
23	2L	47	G7M	C2-N3-C4	3.92	119.28	112.30
23	2L	47	G7M	CN7-N7-C8	-3.91	118.80	124.84
23	2L	47	G7M	O6-C6-C5	-3.88	119.32	128.06
22	1L	37	T6A	N9-C8-N7	-3.87	108.61	113.91
22	1K	55	PSU	C4-N3-C2	-3.83	120.83	126.34
22	1L	39	PSU	C4-N3-C2	-3.82	120.83	126.34
22	1L	37	T6A	N6-C10-N11	3.78	119.05	113.76
22	1L	37	T6A	O10-C10-N6	-3.76	117.27	123.62
23	2L	47	G7M	C5-C6-N1	3.73	119.58	111.79
23	2K	47	G7M	C5-C4-N3	-3.67	121.10	128.15
23	2L	47	G7M	C5-C4-N9	3.66	113.92	105.89
23	2K	47	G7M	C2-N3-C4	3.65	118.81	112.30
22	1L	37	T6A	C13-C12-N11	-3.62	102.38	110.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	2L	47	G7M	C5-C4-N3	-3.61	121.23	128.15
23	2K	8	4SU	N3-C2-N1	3.52	119.56	114.89
22	1L	54	5MU	C5M-C5-C6	-3.49	118.18	122.85
23	2L	8	4SU	N3-C2-N1	3.47	119.50	114.89
23	2L	56	PSU	N1-C2-N3	3.44	119.03	115.13
23	2K	47	G7M	C5-C6-N1	3.40	118.89	111.79
22	1L	37	T6A	C2-N3-C4	3.40	119.78	111.75
23	2K	47	G7M	C5-C4-N9	3.34	113.20	105.89
23	2K	47	G7M	CN7-N7-C8	-3.32	119.71	124.84
22	1K	37	T6A	C2-N3-C4	3.26	119.45	111.75
22	1K	37	T6A	C5-N7-C8	3.20	108.06	103.51
22	1K	34	U8U	C5-C4-N3	3.19	119.45	114.97
22	1L	34	U8U	C1'-N1-C6	-3.15	115.88	121.12
22	1L	54	5MU	C6-N1-C2	-3.11	118.14	121.30
23	2L	47	G7M	C2-N1-C6	-3.06	119.51	125.10
22	1L	34	U8U	O4-C4-C5	-3.04	120.44	124.96
22	1L	39	PSU	N1-C2-N3	3.01	118.54	115.13
22	1K	39	PSU	N1-C2-N3	3.00	118.53	115.13
22	1K	55	PSU	C6-N1-C2	-2.93	119.69	122.68
22	1L	55	PSU	N1-C2-N3	2.92	118.44	115.13
22	1K	37	T6A	N3-C4-N9	2.90	131.87	127.08
22	1K	55	PSU	O2-C2-N1	-2.90	119.60	122.79
22	1K	37	T6A	C14-C12-N11	-2.89	104.33	111.72
22	1K	37	T6A	O10-C10-N6	-2.79	118.90	123.62
22	1L	37	T6A	N3-C4-N9	2.79	131.69	127.08
22	1L	37	T6A	C5-N7-C8	2.79	107.48	103.51
22	1L	34	U8U	C5-C4-N3	2.74	118.81	114.97
23	2L	55	5MU	N3-C2-N1	2.72	118.50	114.89
23	2K	47	G7M	C2-N1-C6	-2.60	120.36	125.10
23	2K	47	G7M	C8-N9-C4	2.56	113.65	107.16
23	2K	56	PSU	O2-C2-N1	-2.44	120.11	122.79
23	2L	47	G7M	C8-N9-C4	2.44	113.33	107.16
23	2K	33	OMC	C1'-N1-C6	-2.36	115.70	120.84
22	1K	37	T6A	ODB-C13-ODA	-2.35	118.75	124.09
23	2L	33	OMC	C1'-N1-C6	-2.33	115.75	120.84
23	2K	8	4SU	C5-C6-N1	-2.29	117.97	121.81
23	2L	47	G7M	C1'-N9-C4	-2.26	119.80	126.50
23	2K	56	PSU	O4-C4-C5	-2.24	118.18	124.05
22	1L	39	PSU	O2-C2-N1	-2.23	120.33	122.79
23	2K	55	5MU	O2-C2-N1	-2.22	119.84	122.79
22	1K	37	T6A	C13-C12-N11	2.20	115.07	110.28
22	1K	54	5MU	C6-N1-C2	-2.16	119.11	121.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	1K	39	PSU	C5-C4-N3	2.14	121.43	116.58
22	1K	54	5MU	C5M-C5-C4	2.14	121.12	118.77
23	2L	55	5MU	O2-C2-N1	-2.13	119.96	122.79
23	2L	8	4SU	C1'-N1-C2	2.12	121.41	117.57
22	1K	34	U8U	C-C5-C6	-2.10	118.06	121.21
23	2K	33	OMC	C1'-N1-C2	2.09	123.09	118.42
22	1L	37	T6A	C14-C12-C13	2.09	113.76	110.19
23	2K	33	OMC	N4-C4-N3	2.07	121.60	117.97
22	1L	55	PSU	O4'-C1'-C2'	2.05	108.04	105.14
23	2L	55	5MU	C6-N1-C2	-2.04	119.23	121.30
22	1K	37	T6A	C5-C4-N9	2.03	108.14	105.78
23	2K	47	G7M	C1'-N9-C4	-2.02	120.50	126.50
22	1K	37	T6A	C15-C14-C12	-2.02	108.22	112.29
23	2K	56	PSU	C6-C5-C4	2.01	119.60	118.20
22	1L	55	PSU	O4-C4-C5	-2.00	118.81	124.05

There are no chirality outliers.

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
22	1L	34	U8U	N-C-C5-C4
22	1L	34	U8U	O4'-C4'-C5'-O5'
23	2K	33	OMC	C1'-C2'-O2'-CM2
22	1L	34	U8U	C3'-C4'-C5'-O5'
23	2L	47	G7M	O4'-C4'-C5'-O5'
22	1L	37	T6A	C14-C12-N11-C10
22	1K	37	T6A	O4'-C4'-C5'-O5'
22	1K	37	T6A	C3'-C4'-C5'-O5'
22	1L	55	PSU	C4'-C5'-O5'-P
23	2L	56	PSU	C4'-C5'-O5'-P
23	2L	47	G7M	C3'-C4'-C5'-O5'
22	1L	39	PSU	O4'-C1'-C5-C4
22	1L	39	PSU	O4'-C1'-C5-C6
23	2L	33	OMC	C2'-C1'-N1-C2
23	2K	56	PSU	O4'-C4'-C5'-O5'
22	1L	34	U8U	N-C-C5-C6

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 1409 ligands modelled in this entry, 1407 are monoatomic - leaving 2 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
57	SF4	3E	301	4	0,12,12	-	-	-		
57	SF4	32	302	4	0,12,12	-	-	-		

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
57	SF4	3E	301	4	-	-	0/6/5/5
57	SF4	32	302	4	-	-	0/6/5/5

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

4.7 Other polymers (i)

There are no such residues in this entry.

4.8 Polymer linkage issues

The following chains have linkage breaks:

Mol	Chain	Number of breaks
25	4K	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	4K	25:A	O3'	26:A	P	3.07

5 Fit of model and data

5.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	1496/1519 (98%)	-0.12	32 (2%) 63 55	52, 95, 168, 235	0
1	1G	1506/1519 (99%)	-0.10	32 (2%) 63 55	67, 112, 176, 243	0
2	12	207/256 (80%)	0.85	24 (11%) 9 8	128, 159, 178, 183	0
2	1E	231/256 (90%)	0.85	24 (10%) 11 10	108, 138, 168, 172	0
3	22	195/239 (81%)	0.56	10 (5%) 33 28	119, 140, 163, 172	0
3	2E	205/239 (85%)	0.36	5 (2%) 59 51	82, 105, 135, 142	0
4	32	208/209 (99%)	0.63	13 (6%) 26 22	92, 113, 135, 140	0
4	3E	207/209 (99%)	0.58	11 (5%) 32 27	77, 104, 125, 136	0
5	42	149/162 (91%)	0.63	11 (7%) 20 18	97, 118, 134, 142	0
5	4E	149/162 (91%)	0.56	9 (6%) 27 23	76, 96, 115, 122	0
6	52	101/101 (100%)	0.54	4 (3%) 42 35	81, 99, 115, 130	0
6	5E	100/101 (99%)	0.50	5 (5%) 34 28	76, 97, 116, 122	0
7	62	140/156 (89%)	0.48	12 (8%) 16 14	108, 126, 138, 140	0
7	6E	154/156 (98%)	0.28	7 (4%) 38 31	96, 114, 144, 165	0
8	72	137/138 (99%)	0.65	11 (8%) 18 16	95, 123, 136, 143	0
8	7E	138/138 (100%)	0.56	8 (5%) 29 24	84, 104, 116, 127	0
9	82	121/128 (94%)	0.96	19 (15%) 5 5	109, 156, 170, 181	0
9	8E	126/128 (98%)	0.78	15 (11%) 9 8	80, 133, 153, 158	0
10	1A	80/105 (76%)	1.68	24 (30%) 1 1	114, 151, 163, 163	0
10	1I	95/105 (90%)	0.63	5 (5%) 32 27	76, 120, 160, 164	0
11	2A	113/129 (87%)	0.63	9 (7%) 18 16	78, 106, 120, 129	0
11	2I	111/129 (86%)	0.40	6 (5%) 31 26	69, 102, 117, 129	0
12	3A	122/132 (92%)	0.89	19 (15%) 5 5	80, 96, 120, 140	0
12	3I	122/132 (92%)	0.38	11 (9%) 15 13	61, 72, 100, 126	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
13	4A	111/126 (88%)	0.91	24 (21%) 2 2	112, 142, 159, 167	0
13	4I	119/126 (94%)	0.59	13 (10%) 10 9	81, 108, 129, 137	0
14	5A	59/61 (96%)	0.94	9 (15%) 5 5	124, 137, 150, 154	0
14	5I	60/61 (98%)	0.39	3 (5%) 34 28	77, 93, 107, 120	0
15	6A	87/89 (97%)	-0.01	2 (2%) 61 53	78, 106, 118, 120	0
15	6I	87/89 (97%)	0.09	2 (2%) 61 53	73, 92, 109, 116	0
16	7A	84/88 (95%)	0.78	9 (10%) 11 10	88, 101, 121, 145	0
16	7I	83/88 (94%)	0.96	8 (9%) 13 12	93, 106, 134, 154	0
17	8A	99/105 (94%)	0.29	6 (6%) 27 22	90, 105, 120, 124	0
17	8I	100/105 (95%)	0.36	4 (4%) 42 35	85, 101, 110, 115	0
18	9A	67/88 (76%)	0.70	7 (10%) 11 10	89, 107, 126, 130	0
18	9I	68/88 (77%)	0.54	4 (5%) 28 23	83, 102, 124, 127	0
19	AA	62/93 (66%)	1.18	13 (20%) 2 2	132, 153, 166, 171	0
19	AI	82/93 (88%)	0.37	4 (4%) 35 29	83, 106, 127, 139	0
20	BA	99/106 (93%)	0.21	4 (4%) 42 35	84, 104, 131, 142	0
20	BI	97/106 (91%)	0.45	6 (6%) 26 22	98, 116, 141, 150	0
21	1B	22/27 (81%)	0.77	3 (13%) 7 6	118, 127, 133, 141	0
21	1F	23/27 (85%)	0.00	0 100 100	84, 95, 101, 111	0
22	1K	67/76 (88%)	1.46	14 (20%) 2 2	76, 147, 198, 203	0
22	1L	64/76 (84%)	2.05	21 (32%) 1 1	108, 196, 215, 219	0
23	2K	72/77 (93%)	0.10	1 (1%) 73 67	64, 86, 118, 128	0
23	2L	72/77 (93%)	0.55	6 (8%) 17 15	73, 105, 137, 148	0
24	3K	70/76 (92%)	1.38	14 (20%) 3 3	71, 198, 240, 244	0
24	3L	72/76 (94%)	1.29	17 (23%) 2 2	77, 194, 224, 230	0
25	4K	21/27 (77%)	1.12	7 (33%) 1 1	67, 124, 208, 209	0
25	4L	19/27 (70%)	1.12	6 (31%) 1 1	86, 143, 217, 218	0
26	14	2855/2917 (97%)	-0.32	39 (1%) 73 67	45, 78, 200, 265	0
26	1H	2885/2917 (98%)	-0.50	21 (0%) 84 80	31, 66, 193, 330	3 (0%)
27	16	122/122 (100%)	-0.63	0 100 100	57, 82, 103, 188	0
27	1J	122/122 (100%)	-0.09	2 (1%) 70 63	78, 110, 130, 191	0
28	71	133/229 (58%)	1.08	21 (15%) 5 4	146, 216, 237, 244	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
28	79	57/229 (24%)	1.67	16 (28%) 1 1	146, 199, 221, 227	0
29	11	273/276 (98%)	-0.01	4 (1%) 72 65	37, 59, 76, 92	0
29	19	274/276 (99%)	0.33	12 (4%) 39 32	46, 69, 87, 106	0
30	21	203/206 (98%)	0.39	9 (4%) 39 32	46, 80, 123, 134	0
30	29	204/206 (99%)	0.39	11 (5%) 31 26	53, 88, 124, 134	0
31	31	202/210 (96%)	-0.08	2 (0%) 79 74	43, 72, 107, 128	0
31	39	204/210 (97%)	0.34	12 (5%) 28 23	51, 98, 144, 167	0
32	41	179/182 (98%)	0.14	3 (1%) 69 62	72, 93, 130, 142	0
32	49	181/182 (99%)	0.53	11 (6%) 27 22	106, 125, 148, 166	0
33	51	174/180 (96%)	0.50	11 (6%) 26 22	75, 98, 112, 124	0
33	59	70/180 (38%)	1.84	23 (32%) 1 1	136, 156, 178, 182	0
34	61	146/148 (98%)	0.42	6 (4%) 41 34	73, 123, 144, 151	0
34	69	145/148 (97%)	0.68	18 (12%) 8 8	83, 118, 146, 155	0
35	15	138/140 (98%)	1.03	20 (14%) 6 5	73, 99, 128, 143	0
35	58	137/140 (97%)	0.54	7 (5%) 33 28	61, 83, 118, 132	0
36	25	122/122 (100%)	0.07	5 (4%) 41 34	64, 81, 99, 111	0
36	68	122/122 (100%)	-0.07	1 (0%) 82 78	53, 68, 85, 93	0
37	35	147/150 (98%)	0.36	6 (4%) 41 34	52, 95, 126, 140	0
37	78	147/150 (98%)	-0.13	1 (0%) 84 80	42, 74, 98, 107	0
38	45	139/141 (98%)	0.57	9 (6%) 25 21	64, 95, 114, 130	0
38	88	141/141 (100%)	-0.11	1 (0%) 84 80	49, 70, 92, 112	0
39	55	118/118 (100%)	-0.07	1 (0%) 82 78	59, 74, 88, 106	0
39	98	118/118 (100%)	0.07	1 (0%) 82 78	58, 76, 93, 107	0
40	65	110/112 (98%)	0.60	9 (8%) 17 15	82, 104, 124, 131	0
40	A8	111/112 (99%)	-0.05	2 (1%) 67 59	66, 82, 103, 110	0
41	75	133/146 (91%)	0.34	7 (5%) 32 27	77, 91, 124, 144	0
41	B8	136/146 (93%)	0.51	17 (12%) 8 7	64, 83, 122, 132	0
42	85	116/118 (98%)	0.61	7 (6%) 27 23	60, 87, 118, 120	0
42	C8	115/118 (97%)	0.29	3 (2%) 57 49	50, 73, 102, 109	0
43	95	100/101 (99%)	0.69	6 (6%) 27 23	58, 109, 127, 135	0
43	D8	100/101 (99%)	0.63	4 (4%) 42 35	52, 96, 116, 127	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
44	A5	111/113 (98%)	0.11	3 (2%) 56 48	55, 70, 94, 135	0
44	E8	110/113 (97%)	-0.04	3 (2%) 56 48	51, 67, 91, 104	0
45	B5	94/96 (97%)	0.17	2 (2%) 63 55	62, 78, 98, 110	0
45	F8	95/96 (98%)	-0.03	1 (1%) 78 73	47, 63, 90, 97	0
46	C5	104/110 (94%)	1.41	28 (26%) 1 1	85, 113, 147, 155	0
46	G8	103/110 (93%)	0.81	10 (9%) 13 12	66, 88, 118, 129	0
47	D5	133/206 (64%)	0.51	7 (5%) 32 27	102, 130, 153, 163	0
47	H8	170/206 (82%)	0.19	4 (2%) 59 51	76, 111, 188, 193	0
48	E5	76/85 (89%)	0.24	2 (2%) 57 49	56, 83, 96, 104	0
48	I8	77/85 (90%)	-0.13	3 (3%) 43 35	45, 65, 78, 93	0
49	F5	94/98 (95%)	0.46	7 (7%) 20 18	59, 76, 106, 129	0
49	J8	94/98 (95%)	0.43	8 (8%) 16 15	46, 67, 110, 116	0
50	G5	69/72 (95%)	0.30	3 (4%) 40 32	77, 96, 116, 124	0
50	K8	68/72 (94%)	0.16	3 (4%) 39 32	54, 72, 92, 114	0
51	H5	58/60 (96%)	0.19	0 100 100	70, 90, 116, 124	0
51	L8	58/60 (96%)	-0.08	0 100 100	55, 74, 99, 111	0
52	M8	49/71 (69%)	0.84	6 (12%) 8 8	94, 136, 150, 166	0
53	J5	56/60 (93%)	0.27	1 (1%) 67 59	52, 77, 126, 137	0
53	N8	48/60 (80%)	-0.09	1 (2%) 63 55	44, 77, 124, 127	0
54	L5	47/49 (95%)	-0.37	1 (2%) 63 55	44, 55, 77, 97	0
54	P8	47/49 (95%)	-0.42	2 (4%) 40 32	40, 46, 68, 76	0
55	M5	64/65 (98%)	0.20	3 (4%) 36 30	62, 73, 88, 112	0
55	Q8	64/65 (98%)	-0.24	0 100 100	47, 60, 76, 88	0
All	All	20647/21961 (94%)	0.13	959 (4%) 37 31	31, 93, 171, 330	3 (0%)

All (959) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
22	1L	76	A	13.1
22	1K	76	A	9.5
43	D8	37	VAL	8.9
33	59	170	ARG	8.0
9	82	115	GLY	7.8
22	1L	75	C	7.7

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Mol	Chain	Res	Type	RSRZ
28	79	209	LEU	7.7
41	B8	104	ASN	7.7
22	1L	71	C	7.6
33	59	169	VAL	7.6
10	1A	47	PHE	7.2
34	69	20	ASP	7.1
13	4A	95	GLY	7.1
10	1A	62	HIS	6.7
24	3L	34	U	6.7
24	3L	35	U	6.5
13	4A	102	ARG	6.5
40	65	20	ARG	6.5
13	4A	117	VAL	6.4
33	59	168	PRO	6.4
28	71	193	ILE	6.4
22	1L	74	C	6.3
41	B8	106	SER	6.1
12	3A	28	LYS	6.0
33	59	171	LEU	5.9
9	8E	126	SER	5.9
12	3A	27	LEU	5.7
26	14	880	G	5.6
10	1A	58	ASP	5.5
46	C5	49	VAL	5.5
13	4I	120	LYS	5.5
29	19	262	ARG	5.5
29	19	27	THR	5.5
22	1K	74	C	5.5
22	1L	72	C	5.4
9	8E	127	LYS	5.4
35	15	84	LYS	5.4
33	59	162	ILE	5.3
10	1A	49	VAL	5.3
10	1A	59	SER	5.2
2	1E	29	ALA	5.2
22	1K	75	C	5.1
46	C5	59	GLY	5.1
2	1E	81	VAL	5.1
34	69	1	MET	5.0
41	75	106	SER	5.0
20	BI	12	ALA	5.0
12	3A	64	TYR	5.0

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Mol	Chain	Res	Type	RSRZ
48	E5	8	GLY	5.0
46	G8	104	GLY	4.9
50	G5	44	LEU	4.9
33	51	9	ILE	4.9
10	1A	85	LEU	4.9
38	45	2	LEU	4.9
14	5I	2	ALA	4.9
24	3K	34	U	4.9
24	3K	36	U	4.9
54	L5	47	ARG	4.9
20	BA	9	ASN	4.9
12	3A	20	LYS	4.9
22	1L	1	G	4.8
46	C5	29	GLU	4.8
28	79	47	LEU	4.8
13	4I	102	ARG	4.7
22	1K	73	A	4.7
42	C8	116	ALA	4.7
27	1J	88	C	4.7
34	69	3	VAL	4.7
34	61	116	LEU	4.7
12	3I	17	LYS	4.7
12	3A	21	LYS	4.7
25	4K	13	A	4.6
46	C5	47	LYS	4.6
4	3E	96	LEU	4.6
13	4I	118	ALA	4.6
46	C5	105	ALA	4.6
2	12	102	LEU	4.5
12	3A	26	ALA	4.5
10	1A	57	LYS	4.5
22	1K	31	A	4.5
26	14	2902	C	4.5
10	1A	46	ARG	4.5
12	3A	19	ARG	4.5
35	15	9	VAL	4.5
22	1L	73	A	4.5
30	29	116	VAL	4.4
26	14	229	A	4.4
10	1A	56	HIS	4.4
10	1A	63	PHE	4.4
46	C5	63	LYS	4.4

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Mol	Chain	Res	Type	RSRZ
13	4I	96	LEU	4.3
26	14	2901	C	4.3
46	C5	58	GLY	4.3
47	D5	171	ILE	4.3
10	1A	65	LEU	4.3
13	4A	111	LYS	4.3
46	G8	89	PHE	4.3
35	15	92	ALA	4.3
33	59	155	SER	4.2
23	2L	1	C	4.2
55	M5	40	GLU	4.2
41	75	104	ASN	4.2
22	1L	40	C	4.2
24	3K	70	C	4.2
55	M5	34	TRP	4.2
46	C5	46	LYS	4.2
12	3I	28	LYS	4.2
3	22	39	ILE	4.2
7	62	37	ASN	4.1
2	12	70	PHE	4.1
17	8I	29	HIS	4.1
28	79	171	ILE	4.1
37	35	110	TYR	4.1
13	4A	100	GLY	4.1
12	3I	19	ARG	4.1
22	1K	72	C	4.1
41	B8	109	GLU	4.1
13	4A	118	ALA	4.0
13	4A	104	ARG	4.0
13	4A	107	ALA	4.0
33	51	170	ARG	4.0
44	E8	92	ARG	4.0
1	1G	1202	G	4.0
7	62	85	TYR	4.0
46	C5	44	ILE	3.9
10	1A	54	PHE	3.9
35	15	132	ALA	3.9
9	8E	115	GLY	3.9
22	1L	14	A	3.9
40	A8	110	LEU	3.9
26	1H	893	C	3.9
8	72	91	ARG	3.9

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Mol	Chain	Res	Type	RSRZ
35	58	72	TYR	3.9
46	C5	45	VAL	3.9
24	3K	71	C	3.9
29	19	5	LYS	3.8
14	5A	39	LEU	3.8
40	65	60	GLY	3.8
9	82	109	VAL	3.8
26	14	1026	U	3.8
8	72	86	ILE	3.8
3	2E	193	TYR	3.8
35	15	129	PRO	3.8
24	3L	1	G	3.8
5	42	5	ASP	3.8
1	1G	883	C	3.8
2	12	13	ALA	3.8
19	AA	58	VAL	3.7
19	AA	76	PRO	3.7
30	21	195	LEU	3.7
43	95	74	LYS	3.7
11	2A	89	ALA	3.7
31	39	72	ARG	3.7
26	14	896	A	3.7
33	59	165	ALA	3.7
45	B5	69	TYR	3.7
49	J8	92	LYS	3.7
26	1H	1762[A]	A	3.6
43	95	81	TYR	3.6
33	59	76	VAL	3.6
22	1K	32	C	3.6
9	8E	121	ARG	3.6
46	G8	98	VAL	3.6
44	A5	111	HIS	3.6
5	4E	88	LYS	3.6
5	4E	81	GLU	3.6
33	59	79	VAL	3.6
32	49	34	LEU	3.6
9	8E	117	HIS	3.6
2	12	163	PHE	3.6
28	71	202	GLU	3.6
9	82	47	LEU	3.6
35	58	137	LYS	3.5
18	9I	20	ALA	3.5

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Mol	Chain	Res	Type	RSRZ
49	J8	77	ALA	3.5
33	59	148	ILE	3.5
45	B5	94	GLY	3.5
11	2A	25	TYR	3.5
18	9A	84	LYS	3.5
22	1L	69	A	3.5
13	4A	93	ARG	3.5
5	42	153	LYS	3.5
13	4I	114	ARG	3.5
41	B8	112	ARG	3.5
28	71	208	PHE	3.5
11	2I	25	TYR	3.5
1	13	230	G	3.5
12	3I	11	VAL	3.5
24	3L	70	C	3.5
24	3L	72	C	3.5
42	85	25	TRP	3.5
12	3I	7	ILE	3.4
38	88	104	PHE	3.4
28	71	175	VAL	3.4
29	19	26	LYS	3.4
34	69	18	VAL	3.4
10	1A	61	GLU	3.4
12	3I	16	GLU	3.4
1	1G	975	A	3.4
37	35	47	ASP	3.4
16	7A	84	ALA	3.4
35	15	85	ILE	3.4
15	6I	60	VAL	3.4
46	C5	51	VAL	3.4
35	58	129	PRO	3.4
2	1E	80	ILE	3.4
30	21	72	VAL	3.4
41	B8	108	ARG	3.4
1	13	76	G	3.4
18	9A	20	ALA	3.4
26	14	2900	A	3.4
19	AA	56	GLN	3.4
55	M5	35	GLN	3.4
2	1E	33	TYR	3.4
22	1L	31	A	3.4
49	J8	94	LEU	3.3

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Mol	Chain	Res	Type	RSRZ
1	1G	966	G	3.3
22	1L	3	G	3.3
2	1E	13	ALA	3.3
13	4A	116	THR	3.3
3	2E	94	LEU	3.3
14	5A	44	LEU	3.3
38	45	93	TYR	3.3
28	79	165	ASN	3.3
34	69	11	ASN	3.3
30	29	77	ILE	3.3
26	14	614	U	3.3
48	I8	9	SER	3.3
13	4A	114	ARG	3.3
49	F5	91	LYS	3.3
2	1E	208	ILE	3.3
47	D5	57	ILE	3.3
25	4L	7	G	3.3
26	1H	254	G	3.3
32	41	3	LEU	3.3
34	69	12	LEU	3.3
13	4A	103	THR	3.3
2	1E	14	GLY	3.3
9	82	125	TYR	3.3
24	3L	33	U	3.3
24	3L	37	A	3.3
25	4K	14	A	3.3
28	79	198	ALA	3.3
9	8E	128	ARG	3.3
30	29	76	ARG	3.3
4	32	23	GLY	3.3
22	1L	2	G	3.3
46	G8	93	GLY	3.3
9	8E	125	TYR	3.2
13	4A	87	TYR	3.2
28	79	202	GLU	3.2
10	1A	91	PRO	3.2
8	72	9	MET	3.2
1	1G	915	A	3.2
26	1H	529	A	3.2
52	M8	49	PHE	3.2
14	5A	38	GLY	3.2
10	1A	64	GLU	3.2

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Mol	Chain	Res	Type	RSRZ
16	7A	29	ASP	3.2
20	BI	72	LEU	3.2
31	39	12	LEU	3.2
29	19	35	LYS	3.2
23	2L	40	C	3.2
10	1A	74	ILE	3.2
6	5E	46	ARG	3.2
19	AA	75	ALA	3.2
22	1L	18	G	3.2
40	65	112	PHE	3.2
19	AA	60	VAL	3.2
30	21	203	LYS	3.2
3	22	155	GLY	3.2
1	1G	974	A	3.2
33	59	159	GLU	3.2
31	39	65	TRP	3.2
9	8E	114	TYR	3.2
16	7A	32	TYR	3.2
22	1K	40	C	3.2
28	71	43	VAL	3.2
30	21	64	LYS	3.2
1	1G	887	G	3.2
26	14	2899	G	3.2
10	1A	48	THR	3.2
38	45	105	GLU	3.2
1	1G	968	A	3.1
41	B8	115	ARG	3.1
2	12	218	ALA	3.1
5	4E	21	ALA	3.1
17	8A	33	GLY	3.1
35	15	73	THR	3.1
46	C5	61	ILE	3.1
30	29	151	TYR	3.1
46	G8	92	ASN	3.1
19	AI	67	VAL	3.1
13	4I	100	GLY	3.1
3	2E	91	LEU	3.1
7	62	32	ARG	3.1
33	59	144	VAL	3.1
1	13	1531	A	3.1
3	22	158	GLY	3.1
7	6E	81	GLY	3.1

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Mol	Chain	Res	Type	RSRZ
16	7I	83	GLU	3.1
17	8I	36	ILE	3.1
1	13	307	C	3.1
1	1G	1367	C	3.1
11	2A	126	ARG	3.1
46	C5	60	PHE	3.1
11	2A	36	ASP	3.1
49	F5	8	SER	3.1
33	59	151	ILE	3.1
3	22	91	LEU	3.1
9	8E	118	LYS	3.1
34	69	38	LEU	3.1
10	1I	92	THR	3.1
41	75	101	PHE	3.0
13	4A	108	ARG	3.0
46	G8	86	ARG	3.0
47	D5	138	GLU	3.0
1	1G	815	A	3.0
26	14	1088	A	3.0
26	1H	615	G	3.0
7	6E	83	ALA	3.0
5	42	6	PHE	3.0
28	79	43	VAL	3.0
22	1K	71	C	3.0
22	1L	70	C	3.0
41	B8	111	ARG	3.0
41	75	103	ARG	3.0
2	12	215	LEU	3.0
29	19	40	THR	3.0
32	49	50	ALA	3.0
24	3K	27	G	3.0
2	1E	211	ILE	3.0
3	22	84	ILE	3.0
16	7I	28	ARG	3.0
34	69	75	LEU	3.0
11	2I	125	PHE	3.0
1	1G	969	A	3.0
1	1G	1227	A	3.0
26	14	1073	A	3.0
12	3A	16	GLU	3.0
26	14	1076	C	3.0
47	D5	170	THR	3.0

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Mol	Chain	Res	Type	RSRZ
31	39	11	VAL	3.0
34	69	21	VAL	3.0
28	79	199	HIS	3.0
10	1A	55	LYS	2.9
40	65	19	LYS	2.9
10	1A	60	ARG	2.9
22	1L	41	A	2.9
34	69	4	ILE	2.9
2	12	14	GLY	2.9
28	71	209	LEU	2.9
42	C8	95	LEU	2.9
13	4A	101	GLN	2.9
26	14	879	G	2.9
1	1G	1226	C	2.9
1	1G	1535	C	2.9
9	82	106	ALA	2.9
26	1H	34	C	2.9
10	1I	55	LYS	2.9
33	59	153	LYS	2.9
26	1H	614	U	2.9
44	A5	92	ARG	2.9
35	15	138	LEU	2.9
12	3I	64	TYR	2.9
33	51	86	GLU	2.9
26	14	1063	G	2.9
33	59	166	GLY	2.9
30	29	64	LYS	2.9
32	41	23	PHE	2.9
10	1I	60	ARG	2.9
46	C5	53	PRO	2.9
17	8A	100	LYS	2.9
30	21	89	ASP	2.9
46	C5	42	VAL	2.9
26	14	878	A	2.9
28	71	52	ARG	2.9
34	61	109	ILE	2.9
49	J8	85	LEU	2.9
1	1G	973	G	2.8
2	12	34	ALA	2.8
26	1H	882	G	2.8
14	5A	37	PHE	2.8
4	3E	89	THR	2.8

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Mol	Chain	Res	Type	RSRZ
14	5I	13	THR	2.8
38	45	103	MET	2.8
4	3E	172	PRO	2.8
14	5A	34	TYR	2.8
24	3K	35	U	2.8
1	13	311	C	2.8
1	13	1536	C	2.8
24	3K	5	C	2.8
39	55	101	ALA	2.8
10	1A	50	ILE	2.8
24	3K	1	G	2.8
2	1E	26	PRO	2.8
52	M8	41	PRO	2.8
24	3K	33	U	2.8
6	5E	55	ASP	2.8
24	3K	72	C	2.8
33	51	16	SER	2.8
31	31	131	GLY	2.8
1	13	1508	G	2.8
12	3A	5	PRO	2.8
33	51	39	PRO	2.8
47	D5	103	ARG	2.8
47	H8	116	VAL	2.8
9	8E	119	ALA	2.8
13	4A	90	LEU	2.8
18	9A	44	LEU	2.8
6	5E	54	LYS	2.8
37	35	46	LYS	2.8
12	3A	62	SER	2.8
50	K8	69	ARG	2.7
28	71	58	VAL	2.7
1	13	965	A	2.7
7	62	147	ALA	2.7
32	41	80	PHE	2.7
17	8A	32	TYR	2.7
35	15	90	MET	2.7
6	5E	11	ASN	2.7
12	3A	29	GLY	2.7
30	29	65	GLY	2.7
13	4A	94	ARG	2.7
54	P8	47	ARG	2.7
22	1K	70	C	2.7

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Mol	Chain	Res	Type	RSRZ
26	1H	856	C	2.7
38	45	102	VAL	2.7
2	1E	41	ILE	2.7
28	71	19	ILE	2.7
35	15	75	TYR	2.7
1	1G	1225	A	2.7
1	1G	630	G	2.7
22	1L	45	G	2.7
11	2I	126	ARG	2.7
43	95	73	SER	2.7
34	69	19	VAL	2.7
28	79	45	ALA	2.7
37	78	141	ALA	2.7
16	7I	32	TYR	2.7
36	25	1	MET	2.7
11	2A	87	THR	2.7
9	82	123	PRO	2.7
25	4K	10	G	2.7
28	71	197	GLU	2.7
3	22	157	ILE	2.7
13	4I	56	LEU	2.7
18	9I	78	LEU	2.7
28	79	224	ILE	2.7
42	85	40	PHE	2.7
8	7E	102	ARG	2.7
29	19	36	PRO	2.7
34	61	134	PRO	2.7
35	58	73	THR	2.7
40	65	109	GLY	2.7
1	1G	82	U	2.7
1	1G	884	U	2.7
24	3L	36	U	2.7
26	1H	1026	U	2.7
26	1H	2062	A	2.7
26	14	2797	U	2.7
33	59	167	GLU	2.7
5	42	131	ILE	2.6
14	5A	6	LEU	2.7
12	3A	23	LYS	2.6
43	95	77	ALA	2.6
24	3L	32	C	2.6
21	1B	2	GLY	2.6

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Mol	Chain	Res	Type	RSRZ
28	71	203	GLY	2.6
5	4E	67	VAL	2.6
9	8E	116	LYS	2.6
20	BI	13	LEU	2.6
34	69	35	LEU	2.6
22	1K	15	G	2.6
28	79	48	GLY	2.6
9	82	116	LYS	2.6
4	3E	176	LEU	2.6
7	6E	84	ASN	2.6
24	3L	71	C	2.6
29	19	275	LYS	2.6
33	51	175	LYS	2.6
33	51	7	LEU	2.6
33	59	50	VAL	2.6
34	69	145	VAL	2.6
35	15	46	VAL	2.6
31	39	96	ASP	2.6
49	F5	77	ALA	2.6
24	3K	37	A	2.6
2	12	26	PRO	2.6
49	J8	79	GLY	2.6
11	2A	124	LYS	2.6
12	3A	61	THR	2.6
26	14	530	G	2.6
28	71	47	LEU	2.6
28	71	196	LEU	2.6
30	29	150	VAL	2.6
39	98	114	VAL	2.6
40	65	98	VAL	2.6
19	AA	24	ALA	2.6
22	1L	48	C	2.6
23	2K	1	C	2.6
26	14	2611	U	2.6
10	1A	51	ARG	2.6
10	1A	66	ARG	2.6
1	13	815	A	2.6
21	1B	14	TRP	2.6
33	59	172	LYS	2.6
5	42	90	VAL	2.6
13	4A	54	VAL	2.6
1	13	1516	G	2.5

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Mol	Chain	Res	Type	RSRZ
26	14	2506	U	2.5
49	J8	91	LYS	2.5
25	4L	8	A	2.5
35	15	86	PRO	2.5
32	49	82	LEU	2.5
41	75	105	LEU	2.5
2	12	42	ILE	2.5
17	8A	23	VAL	2.5
28	71	49	ILE	2.5
36	25	96	THR	2.5
2	1E	96	ARG	2.5
8	7E	84	ARG	2.5
36	25	80	ASP	2.5
22	1L	17	U	2.5
1	1G	1365	G	2.5
23	2L	35	C	2.5
3	22	7	PRO	2.5
33	51	5	GLY	2.5
33	59	142	GLY	2.5
38	45	79	LEU	2.5
40	65	110	LEU	2.5
28	79	49	ILE	2.5
37	35	71	VAL	2.5
4	3E	195	ALA	2.5
7	6E	2	ALA	2.5
46	C5	65	ALA	2.5
46	C5	50	ARG	2.5
30	29	132	HIS	2.5
9	82	75	ASP	2.5
19	AA	32	LYS	2.5
35	58	84	LYS	2.5
1	13	93	U	2.5
4	32	157	LEU	2.5
16	7I	6	LEU	2.5
34	69	77	LEU	2.5
28	79	22	ILE	2.5
31	39	9	ILE	2.5
44	E8	91	GLY	2.5
48	I8	8	GLY	2.5
2	12	219	VAL	2.5
1	13	1461	G	2.5
23	2L	71	G	2.5

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Mol	Chain	Res	Type	RSRZ
25	4K	6	G	2.5
2	1E	17	PHE	2.5
41	B8	101	PHE	2.5
4	32	169	LYS	2.5
19	AA	53	ASN	2.5
8	7E	72	PRO	2.5
19	AA	59	PRO	2.5
31	31	66	PRO	2.5
2	12	39	ILE	2.5
12	3I	29	GLY	2.5
28	71	171	ILE	2.5
30	21	88	GLY	2.5
3	2E	184	TYR	2.5
7	62	39	ALA	2.5
8	7E	88	LYS	2.5
12	3I	13	LYS	2.5
26	1H	591	C	2.5
26	1H	881	G	2.5
26	14	1131	G	2.5
1	13	1394	A	2.5
25	4K	15	A	2.5
46	G8	99	CYS	2.5
2	12	44	LEU	2.4
5	42	12	LEU	2.4
16	7I	29	ASP	2.4
17	8I	31	LEU	2.4
41	B8	110	ILE	2.4
53	N8	50	GLY	2.4
8	72	87	SER	2.4
14	5A	3	ARG	2.4
28	71	192	PHE	2.4
35	15	72	TYR	2.4
30	21	90	THR	2.4
18	9I	76	LEU	2.4
22	1K	41	A	2.4
22	1K	69	A	2.4
25	4K	26	A	2.4
26	14	2015	A	2.4
1	1G	886	G	2.4
16	7I	66	PRO	2.4
52	M8	22	ILE	2.4
8	72	93	VAL	2.4

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Mol	Chain	Res	Type	RSRZ
12	3A	18	VAL	2.4
14	5I	25	VAL	2.4
4	32	73	ARG	2.4
8	72	84	ARG	2.4
24	3K	28	U	2.4
18	9I	24	ALA	2.4
7	62	31	MET	2.4
32	49	133	LEU	2.4
34	61	140	LEU	2.4
45	F8	95	LEU	2.4
4	32	5	ILE	2.4
6	52	56	PRO	2.4
10	1I	75	ILE	2.4
12	3I	5	PRO	2.4
12	3A	85	ILE	2.4
30	29	75	VAL	2.4
36	25	81	ASP	2.4
1	1G	1531	A	2.4
25	4L	15	A	2.4
20	BI	70	SER	2.4
25	4L	9	G	2.4
30	21	51	PHE	2.4
34	61	117	GLU	2.4
1	13	1159	U	2.4
2	1E	31	TYR	2.4
35	15	130	HIS	2.4
30	21	78	LEU	2.4
41	B8	105	LEU	2.4
49	F5	80	LEU	2.4
5	42	109	ILE	2.4
29	19	270	ILE	2.4
9	8E	123	PRO	2.4
34	61	111	PRO	2.4
16	7A	50	LYS	2.4
33	59	5	GLY	2.4
28	79	55	ASP	2.4
33	51	51	ARG	2.4
49	J8	78	LYS	2.4
1	13	328	C	2.4
1	1G	412	A	2.4
24	3L	69	A	2.4
24	3L	73	A	2.4

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Mol	Chain	Res	Type	RSRZ
41	B8	94	ALA	2.4
1	13	108	G	2.4
2	1E	73	THR	2.4
17	8I	32	TYR	2.4
26	14	615	G	2.4
26	14	2024	G	2.4
35	15	63	THR	2.4
9	82	19	LEU	2.4
15	6A	57	LEU	2.4
46	C5	90	LEU	2.4
2	1E	71	VAL	2.3
7	6E	5	ARG	2.3
31	39	93	LYS	2.3
43	95	72	VAL	2.3
13	4A	85	GLY	2.3
43	95	75	PHE	2.3
9	82	52	ALA	2.3
23	2L	72	C	2.3
35	15	131	GLN	2.3
26	1H	590	A	2.3
2	1E	196	LEU	2.3
2	12	61	LEU	2.3
35	58	22	THR	2.3
46	G8	90	LEU	2.3
29	11	274	ARG	2.3
49	J8	21	ARG	2.3
16	7I	30	GLY	2.3
53	J5	50	GLY	2.3
16	7A	80	PHE	2.3
42	85	97	ASP	2.3
19	AI	75	ALA	2.3
38	45	7	MET	2.3
31	39	13	SER	2.3
23	2L	17	C	2.3
24	3L	5	C	2.3
25	4K	12	A	2.3
31	39	97	TYR	2.3
46	G8	83	THR	2.3
46	C5	55	TYR	2.3
18	9A	41	LYS	2.3
1	1G	1062	U	2.3
4	3E	29	PRO	2.3

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Mol	Chain	Res	Type	RSRZ
13	4A	113	PRO	2.3
46	C5	77	PRO	2.3
2	12	164	VAL	2.3
7	62	141	VAL	2.3
28	71	62	VAL	2.3
33	51	44	VAL	2.3
38	45	90	VAL	2.3
32	49	177	GLY	2.3
13	4A	106	ASN	2.3
32	49	178	PHE	2.3
1	1G	1061	G	2.3
7	62	2	ALA	2.3
26	14	2023	G	2.3
42	85	48	ALA	2.3
2	12	22	LYS	2.3
9	82	71	SER	2.3
12	3A	13	LYS	2.3
48	E5	16	SER	2.3
9	8E	120	ARG	2.3
18	9A	86	VAL	2.3
2	1E	45	GLN	2.3
6	52	83	ASP	2.3
16	7A	76	GLN	2.3
50	G5	43	GLN	2.3
2	1E	74	LYS	2.3
34	69	2	LYS	2.3
1	13	966	G	2.3
1	1G	631	G	2.3
24	3K	6	G	2.3
26	1H	592	G	2.3
41	75	50	ILE	2.3
13	4I	104	ARG	2.3
19	AA	33	THR	2.3
47	D5	79	ARG	2.3
4	32	68	TYR	2.3
13	4I	87	TYR	2.3
43	D8	81	TYR	2.3
4	32	170	VAL	2.3
11	2A	105	VAL	2.3
12	3A	39	VAL	2.3
12	3A	43	VAL	2.3
8	72	131	GLY	2.3

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Mol	Chain	Res	Type	RSRZ
26	14	958	U	2.3
1	13	1437	C	2.2
4	32	79	PHE	2.2
22	1L	32	C	2.2
5	4E	68	GLU	2.2
7	62	16	LEU	2.2
8	72	133	LEU	2.2
2	12	214	ILE	2.2
4	32	168	ARG	2.2
37	35	35	HIS	2.2
32	49	25	TYR	2.2
1	13	346	G	2.2
26	1H	669	G	2.2
15	6A	86	GLY	2.2
42	85	99	ALA	2.2
10	1I	85	LEU	2.2
13	4A	115	LYS	2.2
25	4L	13	A	2.2
26	14	2619	C	2.2
32	49	39	ILE	2.2
47	H8	146	ILE	2.2
28	79	210	ARG	2.2
44	A5	90	ARG	2.2
46	C5	2	ARG	2.2
4	3E	178	VAL	2.2
13	4A	105	THR	2.2
14	5A	18	VAL	2.2
16	7I	59	TRP	2.2
36	25	50	GLY	2.2
47	D5	12	GLY	2.2
12	3A	68	ALA	2.2
16	7A	64	ALA	2.2
29	11	39	LYS	2.2
35	15	104	LYS	2.2
41	B8	114	LEU	2.2
48	I8	84	LEU	2.2
50	K8	15	LYS	2.2
26	14	382	G	2.2
5	42	130	ASN	2.2
41	B8	2	ASN	2.2
20	BA	17	ARG	2.2
20	BA	23	ARG	2.2

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Mol	Chain	Res	Type	RSRZ
30	29	134	ILE	2.2
44	E8	96	ILE	2.2
46	C5	57	GLN	2.2
54	P8	36	GLN	2.2
1	13	389	A	2.2
1	1G	553	A	2.2
26	14	2062	A	2.2
1	13	562	C	2.2
17	8A	11	VAL	2.2
52	M8	21	VAL	2.2
13	4I	103	THR	2.2
4	3E	23	GLY	2.2
29	19	67	PHE	2.2
32	49	23	PHE	2.2
49	F5	60	PHE	2.2
2	12	196	LEU	2.2
9	82	50	LEU	2.2
8	7E	105	ARG	2.2
10	1A	23	ILE	2.2
13	4I	4	ILE	2.2
13	4I	108	ARG	2.2
15	6I	3	ILE	2.2
37	35	50	ARG	2.2
46	C5	97	ARG	2.2
22	1L	68	G	2.2
24	3L	15	G	2.2
8	7E	93	VAL	2.2
19	AI	76	PRO	2.2
36	68	81	ASP	2.2
1	13	308	C	2.2
26	1H	2612	C	2.2
26	14	1075	C	2.2
20	BI	74	LYS	2.2
49	F5	28	GLY	2.2
3	22	23	TYR	2.2
5	42	123	LEU	2.2
8	7E	119	LEU	2.2
8	72	112	LEU	2.2
34	69	36	ALA	2.2
14	5A	41	ARG	2.1
3	22	3	ASN	2.1
19	AA	57	HIS	2.1

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Mol	Chain	Res	Type	RSRZ
26	1H	895	U	2.1
4	3E	203	VAL	2.1
11	2I	82	VAL	2.1
32	49	160	VAL	2.1
46	C5	98	VAL	2.1
5	4E	5	ASP	2.1
1	13	968	A	2.1
1	13	1182	G	2.1
8	72	88	LYS	2.1
11	2A	86	GLY	2.1
25	4L	25	A	2.1
29	11	40	THR	2.1
41	75	4	GLY	2.1
1	13	1514	C	2.1
1	1G	1509	C	2.1
2	12	152	PHE	2.1
5	42	45	PHE	2.1
22	1K	5	C	2.1
26	14	2896	C	2.1
30	29	63	LEU	2.1
31	39	83	PHE	2.1
35	15	82	LEU	2.1
43	D8	38	LEU	2.1
33	59	80	SER	2.1
33	59	156	ALA	2.1
3	2E	166	GLU	2.1
8	7E	91	ARG	2.1
16	7A	26	ARG	2.1
29	19	273	ARG	2.1
46	C5	62	GLU	2.1
7	62	42	ILE	2.1
19	AI	56	GLN	2.1
41	B8	136	GLN	2.1
32	49	108	ASN	2.1
5	4E	128	PRO	2.1
26	14	2897	U	2.1
35	15	98	VAL	2.1
47	H8	165	VAL	2.1
2	1E	46	LYS	2.1
2	12	43	ASP	2.1
19	AA	77	THR	2.1
49	F5	79	GLY	2.1

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Mol	Chain	Res	Type	RSRZ
2	1E	121	LEU	2.1
18	9A	43	PHE	2.1
1	13	792	A	2.1
1	1G	1349	A	2.1
5	4E	152	ARG	2.1
27	1J	1(M)	A	2.1
28	71	164	ARG	2.1
42	85	101	ARG	2.1
1	13	377	G	2.1
4	32	34	GLU	2.1
21	1B	13	ILE	2.1
26	1H	530	G	2.1
26	14	897	C	2.1
3	22	198	VAL	2.1
7	62	17	VAL	2.1
8	72	89	PRO	2.1
13	4I	111	LYS	2.1
33	51	11	VAL	2.1
46	C5	54	LYS	2.1
1	13	4	U	2.1
26	1H	2506	U	2.1
40	A8	109	GLY	2.1
2	1E	122	PHE	2.1
5	4E	24	ARG	2.1
7	6E	79	ARG	2.1
33	59	152	ARG	2.1
11	2A	75	TYR	2.1
31	39	82	ILE	2.1
52	M8	37	SER	2.1
1	1G	466	C	2.1
20	BA	16	HIS	2.1
1	1G	888	G	2.1
24	3K	25	C	2.1
24	3L	74	C	2.1
9	8E	44	VAL	2.1
9	82	26	VAL	2.1
26	14	214	G	2.1
34	69	37	VAL	2.1
42	85	44	ASN	2.1
2	12	118	LEU	2.1
2	12	187	LEU	2.1
6	52	45	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
17	8A	22	LEU	2.1
28	71	28	LEU	2.1
28	71	64	LEU	2.1
29	19	37	LEU	2.1
31	39	20	LEU	2.1
4	32	87	GLY	2.1
16	7A	10	GLY	2.1
41	B8	25	GLY	2.1
4	3E	50	ARG	2.1
35	58	74	ARG	2.1
7	62	40	ALA	2.1
9	82	45	ALA	2.1
9	82	74	ILE	2.1
41	B8	48	ILE	2.1
50	G5	41	ILE	2.1
29	11	30	GLU	2.1
9	82	62	TYR	2.1
12	3I	62	SER	2.0
1	13	134	A	2.0
13	4A	98	VAL	2.0
26	14	899	A	2.0
42	C8	90	VAL	2.0
10	1A	37	PRO	2.0
6	5E	21	LEU	2.0
11	2I	98	LEU	2.0
26	14	574	C	2.0
26	14	654(R)	C	2.0
43	D8	35	LEU	2.0
50	K8	3	LEU	2.0
1	13	266	G	2.0
4	3E	110	PHE	2.0
34	69	16	GLY	2.0
46	C5	89	PHE	2.0
40	65	21	THR	2.0
2	1E	43	ASP	2.0
28	71	45	ALA	2.0
7	6E	85	TYR	2.0
40	65	57	LYS	2.0
46	G8	94	LYS	2.0
47	H8	38	TYR	2.0
19	AA	44	MET	2.0
2	1E	165	VAL	2.0

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Mol	Chain	Res	Type	RSRZ
2	12	165	VAL	2.0
4	32	178	VAL	2.0
41	B8	70	VAL	2.0
1	13	969	A	2.0
9	82	79	LEU	2.0
20	BI	10	LEU	2.0
26	14	6	A	2.0
26	14	1536	A	2.0
28	79	52	ARG	2.0
38	45	10	ARG	2.0
2	12	17	PHE	2.0
5	42	84	PHE	2.0
9	8E	8	GLY	2.0
35	15	80	GLY	2.0
1	13	269	C	2.0
24	3L	61	C	2.0
26	1H	897	C	2.0
2	1E	188	ALA	2.0
1	1G	4	U	2.0
6	52	54	LYS	2.0
11	2I	123	LYS	2.0
18	9A	46	GLU	2.0
24	3L	6	G	2.0
26	14	561	G	2.0
4	32	207	TYR	2.0
9	82	114	TYR	2.0
52	M8	25	TYR	2.0
9	82	41	VAL	2.0
46	C5	30	VAL	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	PSU	1L	55	20/21	0.78	0.09	113,126,140,141	0
22	5MU	1L	54	21/22	0.84	0.09	113,125,134,142	0
22	PSU	1K	55	20/21	0.84	0.10	95,109,120,124	0
22	U8U	1L	34	23/24	0.88	0.17	102,117,122,124	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
23	5MU	2L	55	21/22	0.88	0.09	99,108,115,124	0
23	PSU	2L	56	20/21	0.89	0.08	98,105,111,115	0
23	G7M	2L	47	24/25	0.90	0.11	110,117,123,127	0
23	5MU	2K	55	21/22	0.90	0.08	89,95,100,103	0
22	5MU	1K	54	21/22	0.90	0.08	93,106,119,128	0
23	4SU	2L	8	20/21	0.90	0.13	94,104,108,112	0
23	PSU	2K	56	20/21	0.91	0.07	86,90,100,104	0
23	G7M	2K	47	24/25	0.92	0.08	86,95,107,113	0
22	T6A	1L	37	32/33	0.92	0.17	91,110,116,118	0
22	PSU	1L	39	20/21	0.94	0.18	88,116,127,129	0
22	U8U	1K	34	23/24	0.94	0.11	76,81,86,100	0
23	OMC	2K	33	21/22	0.95	0.17	67,74,78,82	0
23	OMC	2L	33	21/22	0.95	0.11	88,93,99,103	0
23	4SU	2K	8	20/21	0.95	0.11	75,83,88,90	0
22	PSU	1K	39	20/21	0.95	0.15	74,91,100,100	0
22	T6A	1K	37	32/33	0.96	0.13	58,79,98,99	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
56	MG	1G	1661	1/1	0.44	0.39	92,92,92,92	0
56	MG	1H	3263	1/1	0.48	0.37	91,91,91,91	0
56	MG	1H	3231	1/1	0.49	0.26	106,106,106,106	0
56	MG	1G	1631	1/1	0.53	0.34	99,99,99,99	0
56	MG	1H	3011	1/1	0.56	0.25	119,119,119,119	0
56	MG	1H	3208	1/1	0.57	0.22	141,141,141,141	0
56	MG	14	3151	1/1	0.58	0.34	107,107,107,107	0
56	MG	1H	3219	1/1	0.61	0.16	79,79,79,79	0
56	MG	1G	1632	1/1	0.61	0.35	92,92,92,92	0
56	MG	13	1640	1/1	0.62	0.33	99,99,99,99	0
56	MG	42	201	1/1	0.62	0.32	111,111,111,111	0
56	MG	1G	1635	1/1	0.62	0.22	101,101,101,101	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	1G	1645	1/1	0.63	0.25	113,113,113,113	0
56	MG	2K	101	1/1	0.63	0.27	91,91,91,91	0
56	MG	1G	1643	1/1	0.64	0.29	106,106,106,106	0
56	MG	14	3178	1/1	0.64	0.30	114,114,114,114	0
56	MG	1H	3177	1/1	0.65	0.39	75,75,75,75	0
56	MG	1H	3015	1/1	0.65	0.41	82,82,82,82	0
56	MG	13	1628	1/1	0.66	0.27	89,89,89,89	0
56	MG	4K	101	1/1	0.66	0.36	96,96,96,96	0
56	MG	14	3209	1/1	0.66	0.30	90,90,90,90	0
56	MG	13	1658	1/1	0.67	0.13	116,116,116,116	0
56	MG	1H	3286	1/1	0.67	0.22	119,119,119,119	0
56	MG	1G	1637	1/1	0.68	0.35	89,89,89,89	0
56	MG	13	1653	1/1	0.68	0.34	80,80,80,80	0
56	MG	1J	207	1/1	0.68	0.16	88,88,88,88	0
56	MG	1H	3158	1/1	0.69	0.24	72,72,72,72	0
56	MG	1G	1656	1/1	0.70	0.43	89,89,89,89	0
56	MG	1H	3210	1/1	0.70	0.32	75,75,75,75	0
56	MG	1G	1668	1/1	0.70	0.28	96,96,96,96	0
56	MG	1H	3144	1/1	0.70	0.31	86,86,86,86	0
56	MG	1H	3455	1/1	0.70	0.12	76,76,76,76	0
56	MG	14	3166	1/1	0.70	0.31	85,85,85,85	0
56	MG	1G	1619	1/1	0.70	0.34	103,103,103,103	0
56	MG	13	1679	1/1	0.70	0.27	81,81,81,81	0
56	MG	14	3212	1/1	0.70	0.41	82,82,82,82	0
56	MG	1G	1655	1/1	0.70	0.27	106,106,106,106	0
56	MG	13	1668	1/1	0.71	0.26	105,105,105,105	0
56	MG	13	1662	1/1	0.71	0.25	114,114,114,114	0
56	MG	1H	3096	1/1	0.71	0.28	77,77,77,77	0
56	MG	14	3214	1/1	0.71	0.31	113,113,113,113	0
56	MG	1H	3143	1/1	0.71	0.37	84,84,84,84	0
56	MG	14	3180	1/1	0.72	0.31	74,74,74,74	0
56	MG	1H	3228	1/1	0.72	0.29	79,79,79,79	0
56	MG	1G	1638	1/1	0.72	0.35	92,92,92,92	0
56	MG	1H	3207	1/1	0.72	0.22	119,119,119,119	0
56	MG	1H	3194	1/1	0.72	0.33	83,83,83,83	0
56	MG	1H	3169	1/1	0.73	0.26	111,111,111,111	0
56	MG	14	3158	1/1	0.73	0.37	91,91,91,91	0
56	MG	1H	3258	1/1	0.73	0.48	97,97,97,97	0
56	MG	1G	1604	1/1	0.73	0.30	102,102,102,102	0
56	MG	13	1655	1/1	0.73	0.43	99,99,99,99	0
56	MG	14	3192	1/1	0.73	0.26	81,81,81,81	0
56	MG	1G	1642	1/1	0.73	0.21	102,102,102,102	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	1H	3276	1/1	0.73	0.26	78,78,78,78	0
56	MG	14	3118	1/1	0.73	0.30	89,89,89,89	0
56	MG	14	3148	1/1	0.73	0.20	78,78,78,78	0
56	MG	1H	3077	1/1	0.74	0.15	70,70,70,70	0
56	MG	14	3179	1/1	0.74	0.24	92,92,92,92	0
56	MG	13	1627	1/1	0.74	0.33	82,82,82,82	0
56	MG	14	3183	1/1	0.74	0.26	87,87,87,87	0
56	MG	1H	3270	1/1	0.74	0.34	78,78,78,78	0
56	MG	14	3205	1/1	0.74	0.29	87,87,87,87	0
56	MG	1G	1614	1/1	0.74	0.29	91,91,91,91	0
56	MG	1H	3256	1/1	0.74	0.30	100,100,100,100	0
56	MG	14	3161	1/1	0.74	0.34	86,86,86,86	0
56	MG	1G	1624	1/1	0.74	0.23	87,87,87,87	0
56	MG	39	302	1/1	0.74	0.14	73,73,73,73	0
56	MG	13	1676	1/1	0.75	0.15	92,92,92,92	0
56	MG	14	3124	1/1	0.75	0.12	62,62,62,62	0
56	MG	14	3190	1/1	0.75	0.17	81,81,81,81	0
56	MG	1H	3203	1/1	0.75	0.23	68,68,68,68	0
56	MG	13	1601	1/1	0.75	0.29	102,102,102,102	0
56	MG	1H	3153	1/1	0.75	0.33	88,88,88,88	0
56	MG	13	1685	1/1	0.75	0.31	100,100,100,100	0
56	MG	13	1688	1/1	0.75	0.24	92,92,92,92	0
56	MG	1J	202	1/1	0.75	0.20	91,91,91,91	0
56	MG	13	1661	1/1	0.75	0.31	73,73,73,73	0
56	MG	1H	3181	1/1	0.75	0.24	88,88,88,88	0
56	MG	14	3116	1/1	0.76	0.28	89,89,89,89	0
56	MG	13	1673	1/1	0.76	0.31	93,93,93,93	0
56	MG	1H	3195	1/1	0.76	0.15	69,69,69,69	0
56	MG	1H	3217	1/1	0.76	0.10	61,61,61,61	0
56	MG	1J	206	1/1	0.76	0.21	86,86,86,86	0
56	MG	14	3177	1/1	0.76	0.26	91,91,91,91	0
56	MG	14	3149	1/1	0.76	0.41	89,89,89,89	0
56	MG	1H	3234	1/1	0.77	0.30	90,90,90,90	0
56	MG	13	1672	1/1	0.77	0.22	79,79,79,79	0
56	MG	1H	3161	1/1	0.77	0.18	82,82,82,82	0
56	MG	13	1687	1/1	0.77	0.26	82,82,82,82	0
56	MG	1H	3170	1/1	0.77	0.22	115,115,115,115	0
56	MG	13	1624	1/1	0.77	0.29	80,80,80,80	0
56	MG	13	1663	1/1	0.77	0.29	90,90,90,90	0
56	MG	42	202	1/1	0.77	0.22	110,110,110,110	0
56	MG	14	3081	1/1	0.77	0.30	89,89,89,89	0
56	MG	13	1677	1/1	0.77	0.21	77,77,77,77	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	13	1643	1/1	0.77	0.31	69,69,69,69	0
56	MG	1G	1641	1/1	0.78	0.46	91,91,91,91	0
56	MG	1H	3230	1/1	0.78	0.31	89,89,89,89	0
56	MG	13	1667	1/1	0.78	0.17	105,105,105,105	0
56	MG	14	3027	1/1	0.78	0.23	86,86,86,86	0
56	MG	14	3028	1/1	0.78	0.43	83,83,83,83	0
56	MG	16	203	1/1	0.78	0.20	78,78,78,78	0
56	MG	14	3175	1/1	0.78	0.15	74,74,74,74	0
56	MG	1H	3264	1/1	0.78	0.20	80,80,80,80	0
56	MG	1H	3209	1/1	0.78	0.17	65,65,65,65	0
56	MG	1H	3079	1/1	0.78	0.32	88,88,88,88	0
56	MG	14	3141	1/1	0.78	0.32	86,86,86,86	0
56	MG	1G	1660	1/1	0.79	0.23	92,92,92,92	0
56	MG	13	1629	1/1	0.79	0.17	85,85,85,85	0
56	MG	14	3140	1/1	0.79	0.24	78,78,78,78	0
56	MG	1G	1667	1/1	0.79	0.28	97,97,97,97	0
56	MG	1G	1639	1/1	0.79	0.23	87,87,87,87	0
56	MG	1H	3204	1/1	0.79	0.32	74,74,74,74	0
56	MG	13	1602	1/1	0.79	0.27	61,61,61,61	0
56	MG	1H	3227	1/1	0.79	0.15	79,79,79,79	0
56	MG	16	202	1/1	0.79	0.16	66,66,66,66	0
56	MG	14	3049	1/1	0.79	0.34	79,79,79,79	0
56	MG	14	3050	1/1	0.79	0.28	76,76,76,76	0
56	MG	1H	3105	1/1	0.79	0.39	72,72,72,72	0
56	MG	1H	3156	1/1	0.79	0.08	55,55,55,55	0
56	MG	1H	3107	1/1	0.80	0.27	73,73,73,73	0
56	MG	1H	3180	1/1	0.80	0.28	87,87,87,87	0
56	MG	14	3186	1/1	0.80	0.29	80,80,80,80	0
56	MG	1H	3089	1/1	0.80	0.28	82,82,82,82	0
56	MG	13	1730	1/1	0.80	0.12	102,102,102,102	0
56	MG	14	3199	1/1	0.80	0.32	89,89,89,89	0
56	MG	1G	1607	1/1	0.80	0.18	120,120,120,120	0
56	MG	1H	3145	1/1	0.80	0.32	82,82,82,82	0
56	MG	14	3163	1/1	0.80	0.31	76,76,76,76	0
56	MG	14	3213	1/1	0.80	0.33	78,78,78,78	0
56	MG	1H	3082	1/1	0.80	0.16	55,55,55,55	0
56	MG	14	3244	1/1	0.80	0.27	71,71,71,71	0
56	MG	1G	1620	1/1	0.80	0.28	85,85,85,85	0
56	MG	14	3129	1/1	0.80	0.16	62,62,62,62	0
56	MG	14	3131	1/1	0.80	0.17	62,62,62,62	0
56	MG	1J	209	1/1	0.80	0.22	93,93,93,93	0
56	MG	1H	3254	1/1	0.80	0.20	69,69,69,69	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	16	201	1/1	0.81	0.27	84,84,84,84	0
56	MG	1G	1617	1/1	0.81	0.37	86,86,86,86	0
56	MG	14	3197	1/1	0.81	0.13	44,44,44,44	0
56	MG	1H	3186	1/1	0.81	0.28	76,76,76,76	0
56	MG	1H	3281	1/1	0.81	0.14	82,82,82,82	0
56	MG	88	201	1/1	0.81	0.30	73,73,73,73	0
56	MG	14	3127	1/1	0.81	0.16	85,85,85,85	0
56	MG	1G	1602	1/1	0.81	0.28	87,87,87,87	0
56	MG	14	3130	1/1	0.81	0.15	75,75,75,75	0
56	MG	14	3221	1/1	0.81	0.32	86,86,86,86	0
56	MG	1H	3213	1/1	0.81	0.30	96,96,96,96	0
56	MG	14	3432	1/1	0.81	0.16	92,92,92,92	0
56	MG	1G	1651	1/1	0.81	0.16	84,84,84,84	0
56	MG	1G	1654	1/1	0.81	0.25	99,99,99,99	0
56	MG	14	3143	1/1	0.81	0.33	86,86,86,86	0
56	MG	1J	208	1/1	0.81	0.25	90,90,90,90	0
56	MG	1H	3059	1/1	0.81	0.32	73,73,73,73	0
56	MG	14	3187	1/1	0.81	0.44	81,81,81,81	0
56	MG	13	1654	1/1	0.82	0.18	91,91,91,91	0
56	MG	14	3075	1/1	0.82	0.22	78,78,78,78	0
56	MG	5I	101	1/1	0.82	0.16	77,77,77,77	0
56	MG	16	206	1/1	0.82	0.19	81,81,81,81	0
56	MG	13	1678	1/1	0.82	0.36	83,83,83,83	0
56	MG	1H	3251	1/1	0.82	0.28	80,80,80,80	0
56	MG	1H	3157	1/1	0.82	0.15	96,96,96,96	0
56	MG	13	1671	1/1	0.82	0.22	79,79,79,79	0
56	MG	1G	1608	1/1	0.82	0.33	96,96,96,96	0
56	MG	1G	1613	1/1	0.82	0.16	85,85,85,85	0
56	MG	13	1644	1/1	0.82	0.23	94,94,94,94	0
56	MG	13	1657	1/1	0.82	0.27	89,89,89,89	0
56	MG	1H	3040	1/1	0.82	0.27	71,71,71,71	0
56	MG	1H	3211	1/1	0.82	0.16	90,90,90,90	0
56	MG	1H	3128	1/1	0.82	0.28	76,76,76,76	0
56	MG	1G	1630	1/1	0.82	0.28	97,97,97,97	0
56	MG	14	3225	1/1	0.82	0.32	84,84,84,84	0
56	MG	14	3231	1/1	0.82	0.28	69,69,69,69	0
56	MG	14	3236	1/1	0.82	0.17	94,94,94,94	0
56	MG	14	3238	1/1	0.82	0.29	83,83,83,83	0
56	MG	14	3157	1/1	0.82	0.20	76,76,76,76	0
56	MG	1H	3132	1/1	0.82	0.19	58,58,58,58	0
56	MG	14	3019	1/1	0.82	0.19	48,48,48,48	0
56	MG	1J	204	1/1	0.82	0.29	90,90,90,90	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	1H	3041	1/1	0.82	0.18	86,86,86,86	0
56	MG	13	1622	1/1	0.82	0.26	104,104,104,104	0
56	MG	14	3173	1/1	0.82	0.28	93,93,93,93	0
56	MG	14	3045	1/1	0.82	0.14	67,67,67,67	0
56	MG	1H	3193	1/1	0.82	0.19	78,78,78,78	0
56	MG	25	201	1/1	0.82	0.23	93,93,93,93	0
56	MG	14	3224	1/1	0.83	0.31	82,82,82,82	0
56	MG	14	3109	1/1	0.83	0.22	86,86,86,86	0
56	MG	1G	1644	1/1	0.83	0.22	92,92,92,92	0
56	MG	13	1681	1/1	0.83	0.21	83,83,83,83	0
56	MG	14	3152	1/1	0.83	0.20	85,85,85,85	0
56	MG	1G	1646	1/1	0.83	0.15	119,119,119,119	0
56	MG	1H	3094	1/1	0.83	0.24	61,61,61,61	0
56	MG	13	1617	1/1	0.83	0.11	53,53,53,53	0
56	MG	14	3058	1/1	0.83	0.23	93,93,93,93	0
56	MG	13	1674	1/1	0.83	0.24	67,67,67,67	0
56	MG	14	3137	1/1	0.83	0.25	61,61,61,61	0
56	MG	14	3138	1/1	0.83	0.15	71,71,71,71	0
56	MG	14	3079	1/1	0.83	0.20	75,75,75,75	0
56	MG	13	1648	1/1	0.83	0.17	105,105,105,105	0
56	MG	14	3103	1/1	0.83	0.23	81,81,81,81	0
56	MG	13	1631	1/1	0.84	0.22	89,89,89,89	0
56	MG	14	3215	1/1	0.84	0.10	79,79,79,79	0
56	MG	14	3048	1/1	0.84	0.15	68,68,68,68	0
56	MG	1H	3172	1/1	0.84	0.33	70,70,70,70	0
56	MG	2K	103	1/1	0.84	0.20	56,56,56,56	0
56	MG	1G	1659	1/1	0.84	0.24	85,85,85,85	0
56	MG	14	3234	1/1	0.84	0.20	71,71,71,71	0
56	MG	14	3064	1/1	0.84	0.26	62,62,62,62	0
56	MG	1H	3127	1/1	0.84	0.18	44,44,44,44	0
56	MG	14	3240	1/1	0.84	0.21	83,83,83,83	0
56	MG	13	1639	1/1	0.84	0.31	91,91,91,91	0
56	MG	14	3298	1/1	0.84	0.13	105,105,105,105	0
56	MG	14	3328	1/1	0.84	0.16	83,83,83,83	0
56	MG	1H	3050	1/1	0.84	0.13	49,49,49,49	0
56	MG	1H	3241	1/1	0.84	0.40	81,81,81,81	0
56	MG	1H	3247	1/1	0.84	0.27	62,62,62,62	0
56	MG	1J	205	1/1	0.84	0.25	90,90,90,90	0
56	MG	13	1626	1/1	0.84	0.18	60,60,60,60	0
56	MG	1H	3162	1/1	0.84	0.20	66,66,66,66	0
56	MG	1H	3215	1/1	0.84	0.27	83,83,83,83	0
56	MG	1H	3066	1/1	0.84	0.23	57,57,57,57	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	14	3029	1/1	0.84	0.20	68,68,68,68	0
56	MG	14	3171	1/1	0.84	0.27	84,84,84,84	0
56	MG	1G	1664	1/1	0.85	0.17	126,126,126,126	0
56	MG	1H	3431	1/1	0.85	0.18	74,74,74,74	0
56	MG	14	3128	1/1	0.85	0.12	49,49,49,49	0
56	MG	14	3193	1/1	0.85	0.16	74,74,74,74	0
56	MG	1H	3115	1/1	0.85	0.28	59,59,59,59	0
56	MG	14	3198	1/1	0.85	0.37	84,84,84,84	0
56	MG	1H	3238	1/1	0.85	0.13	76,76,76,76	0
56	MG	14	3200	1/1	0.85	0.29	94,94,94,94	0
56	MG	13	1636	1/1	0.85	0.29	70,70,70,70	0
56	MG	14	3206	1/1	0.85	0.25	72,72,72,72	0
56	MG	14	3208	1/1	0.85	0.31	77,77,77,77	0
56	MG	14	3134	1/1	0.85	0.31	88,88,88,88	0
56	MG	14	3211	1/1	0.85	0.25	70,70,70,70	0
56	MG	14	3136	1/1	0.85	0.12	83,83,83,83	0
56	MG	14	3005	1/1	0.85	0.20	73,73,73,73	0
56	MG	1G	1636	1/1	0.85	0.20	91,91,91,91	0
56	MG	1H	3084	1/1	0.85	0.22	58,58,58,58	0
56	MG	14	3217	1/1	0.85	0.35	94,94,94,94	0
56	MG	13	1642	1/1	0.85	0.22	78,78,78,78	0
56	MG	1H	3212	1/1	0.85	0.21	90,90,90,90	0
56	MG	1H	3012	1/1	0.85	0.24	78,78,78,78	0
56	MG	1H	3164	1/1	0.85	0.08	53,53,53,53	0
56	MG	1H	3260	1/1	0.85	0.25	74,74,74,74	0
56	MG	1H	3013	1/1	0.85	0.25	69,69,69,69	0
56	MG	14	3154	1/1	0.85	0.13	60,60,60,60	0
56	MG	14	3239	1/1	0.85	0.36	82,82,82,82	0
56	MG	14	3056	1/1	0.85	0.47	69,69,69,69	0
56	MG	14	3241	1/1	0.85	0.15	77,77,77,77	0
56	MG	1G	1612	1/1	0.85	0.36	76,76,76,76	0
56	MG	14	3062	1/1	0.85	0.22	80,80,80,80	0
56	MG	14	3311	1/1	0.85	0.15	73,73,73,73	0
56	MG	1H	3201	1/1	0.85	0.39	82,82,82,82	0
56	MG	13	1633	1/1	0.85	0.10	80,80,80,80	0
56	MG	1H	3171	1/1	0.85	0.37	67,67,67,67	0
56	MG	1G	1618	1/1	0.85	0.27	88,88,88,88	0
56	MG	14	3095	1/1	0.85	0.30	76,76,76,76	0
56	MG	1H	3205	1/1	0.85	0.29	73,73,73,73	0
56	MG	13	1669	1/1	0.85	0.27	95,95,95,95	0
56	MG	14	3110	1/1	0.85	0.22	51,51,51,51	0
56	MG	14	3112	1/1	0.85	0.20	69,69,69,69	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	1H	3287	1/1	0.85	0.20	121,121,121,121	0
56	MG	1G	1629	1/1	0.85	0.26	69,69,69,69	0
56	MG	14	3119	1/1	0.86	0.21	67,67,67,67	0
56	MG	14	3169	1/1	0.86	0.37	81,81,81,81	0
56	MG	14	3033	1/1	0.86	0.22	63,63,63,63	0
56	MG	1G	1648	1/1	0.86	0.16	94,94,94,94	0
56	MG	13	1646	1/1	0.86	0.18	89,89,89,89	0
56	MG	1H	3027	1/1	0.86	0.21	68,68,68,68	0
56	MG	1H	3199	1/1	0.86	0.22	74,74,74,74	0
56	MG	1H	3232	1/1	0.86	0.32	77,77,77,77	0
56	MG	14	3133	1/1	0.86	0.26	72,72,72,72	0
56	MG	16	205	1/1	0.86	0.20	83,83,83,83	0
56	MG	14	3184	1/1	0.86	0.17	70,70,70,70	0
56	MG	1H	3102	1/1	0.86	0.23	63,63,63,63	0
56	MG	1H	3014	1/1	0.86	0.23	75,75,75,75	0
56	MG	1H	3165	1/1	0.86	0.22	63,63,63,63	0
56	MG	14	3078	1/1	0.86	0.22	80,80,80,80	0
56	MG	1H	3278	1/1	0.86	0.24	76,76,76,76	0
56	MG	1H	3106	1/1	0.86	0.26	55,55,55,55	0
56	MG	14	3084	1/1	0.86	0.28	77,77,77,77	0
56	MG	1H	3284	1/1	0.86	0.29	44,44,44,44	0
56	MG	1H	3190	1/1	0.86	0.09	60,60,60,60	0
56	MG	1H	3252	1/1	0.86	0.37	75,75,75,75	0
56	MG	14	3153	1/1	0.86	0.38	74,74,74,74	0
56	MG	1H	3363	1/1	0.86	0.15	78,78,78,78	0
56	MG	14	3111	1/1	0.86	0.25	73,73,73,73	0
56	MG	1H	3407	1/1	0.86	0.14	89,89,89,89	0
56	MG	1H	3133	1/1	0.86	0.26	64,64,64,64	0
56	MG	1H	3444	1/1	0.86	0.14	82,82,82,82	0
56	MG	1H	3220	1/1	0.87	0.36	71,71,71,71	0
56	MG	14	3189	1/1	0.87	0.11	60,60,60,60	0
56	MG	1H	3479	1/1	0.87	0.13	99,99,99,99	0
56	MG	1H	3495	1/1	0.87	0.08	100,100,100,100	0
56	MG	14	3004	1/1	0.87	0.28	58,58,58,58	0
56	MG	1H	3540	1/1	0.87	0.08	78,78,78,78	0
56	MG	14	3013	1/1	0.87	0.20	60,60,60,60	0
56	MG	14	3016	1/1	0.87	0.26	55,55,55,55	0
56	MG	1H	3257	1/1	0.87	0.22	83,83,83,83	0
56	MG	14	3201	1/1	0.87	0.08	84,84,84,84	0
56	MG	14	3024	1/1	0.87	0.21	65,65,65,65	0
56	MG	13	1686	1/1	0.87	0.14	98,98,98,98	0
56	MG	1H	3191	1/1	0.87	0.12	59,59,59,59	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	1H	3137	1/1	0.87	0.20	70,70,70,70	0
56	MG	1H	3138	1/1	0.87	0.18	59,59,59,59	0
56	MG	1G	1640	1/1	0.87	0.20	95,95,95,95	0
56	MG	11	302	1/1	0.87	0.14	55,55,55,55	0
56	MG	1H	3160	1/1	0.87	0.21	70,70,70,70	0
56	MG	1H	3123	1/1	0.87	0.24	65,65,65,65	0
56	MG	14	3052	1/1	0.87	0.35	71,71,71,71	0
56	MG	14	3219	1/1	0.87	0.30	86,86,86,86	0
56	MG	14	3053	1/1	0.87	0.25	53,53,53,53	0
56	MG	1H	3236	1/1	0.87	0.29	78,78,78,78	0
56	MG	1G	1605	1/1	0.87	0.22	76,76,76,76	0
56	MG	1H	3019	1/1	0.87	0.22	39,39,39,39	0
56	MG	14	3063	1/1	0.87	0.21	82,82,82,82	0
56	MG	1H	3240	1/1	0.87	0.15	75,75,75,75	0
56	MG	14	3072	1/1	0.87	0.27	67,67,67,67	0
56	MG	14	3160	1/1	0.87	0.39	78,78,78,78	0
56	MG	1G	1650	1/1	0.87	0.15	89,89,89,89	0
56	MG	14	3076	1/1	0.87	0.27	68,68,68,68	0
56	MG	1H	3285	1/1	0.87	0.28	50,50,50,50	0
56	MG	14	3167	1/1	0.87	0.09	54,54,54,54	0
56	MG	1H	3214	1/1	0.87	0.37	83,83,83,83	0
56	MG	13	1635	1/1	0.87	0.18	72,72,72,72	0
56	MG	14	3400	1/1	0.87	0.12	90,90,90,90	0
56	MG	1H	3345	1/1	0.87	0.11	91,91,91,91	0
56	MG	14	3463	1/1	0.87	0.19	97,97,97,97	0
56	MG	14	3470	1/1	0.87	0.16	79,79,79,79	0
56	MG	14	3093	1/1	0.87	0.13	71,71,71,71	0
56	MG	1G	1658	1/1	0.87	0.17	79,79,79,79	0
56	MG	14	3097	1/1	0.87	0.25	70,70,70,70	0
56	MG	1H	3034	1/1	0.87	0.24	63,63,63,63	0
56	MG	1H	3218	1/1	0.87	0.19	65,65,65,65	0
56	MG	14	3181	1/1	0.87	0.23	76,76,76,76	0
56	MG	1H	3253	1/1	0.87	0.16	62,62,62,62	0
56	MG	1H	3187	1/1	0.87	0.29	77,77,77,77	0
56	MG	1G	1627	1/1	0.87	0.09	139,139,139,139	0
56	MG	35	201	1/1	0.87	0.12	74,74,74,74	0
56	MG	E5	103	1/1	0.87	0.32	80,80,80,80	0
56	MG	13	1734	1/1	0.88	0.08	105,105,105,105	0
56	MG	13	1747	1/1	0.88	0.08	107,107,107,107	0
56	MG	98	201	1/1	0.88	0.31	67,67,67,67	0
56	MG	14	3185	1/1	0.88	0.24	71,71,71,71	0
56	MG	1H	3048	1/1	0.88	0.15	45,45,45,45	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	14	3237	1/1	0.88	0.15	88,88,88,88	0
56	MG	13	1613	1/1	0.88	0.26	86,86,86,86	0
56	MG	1H	3147	1/1	0.88	0.13	43,43,43,43	0
56	MG	14	3150	1/1	0.88	0.39	84,84,84,84	0
56	MG	1H	3151	1/1	0.88	0.13	52,52,52,52	0
56	MG	1H	3245	1/1	0.88	0.10	58,58,58,58	0
56	MG	1H	3246	1/1	0.88	0.22	71,71,71,71	0
56	MG	14	3308	1/1	0.88	0.13	90,90,90,90	0
56	MG	13	1620	1/1	0.88	0.35	74,74,74,74	0
56	MG	1H	3065	1/1	0.88	0.18	61,61,61,61	0
56	MG	13	1614	1/1	0.88	0.31	73,73,73,73	0
56	MG	1H	3016	1/1	0.88	0.22	72,72,72,72	0
56	MG	14	3435	1/1	0.88	0.15	93,93,93,93	0
56	MG	13	1638	1/1	0.88	0.20	71,71,71,71	0
56	MG	1H	3473	1/1	0.88	0.15	88,88,88,88	0
56	MG	1H	3124	1/1	0.88	0.24	70,70,70,70	0
56	MG	1G	1625	1/1	0.88	0.17	81,81,81,81	0
56	MG	1H	3080	1/1	0.88	0.23	74,74,74,74	0
56	MG	1H	3005	1/1	0.88	0.32	83,83,83,83	0
56	MG	1H	3083	1/1	0.88	0.18	81,81,81,81	0
56	MG	1H	3229	1/1	0.88	0.10	59,59,59,59	0
56	MG	1H	3008	1/1	0.88	0.23	61,61,61,61	0
56	MG	1H	3087	1/1	0.88	0.20	66,66,66,66	0
56	MG	1G	1695	1/1	0.88	0.10	99,99,99,99	0
56	MG	14	3220	1/1	0.88	0.21	74,74,74,74	0
56	MG	1H	3271	1/1	0.88	0.18	63,63,63,63	0
56	MG	13	1607	1/1	0.89	0.09	74,74,74,74	0
56	MG	1H	3196	1/1	0.89	0.19	62,62,62,62	0
56	MG	14	3203	1/1	0.89	0.19	69,69,69,69	0
56	MG	1H	3267	1/1	0.89	0.39	90,90,90,90	0
56	MG	1H	3141	1/1	0.89	0.12	53,53,53,53	0
56	MG	14	3038	1/1	0.89	0.20	81,81,81,81	0
56	MG	1H	3167	1/1	0.89	0.13	45,45,45,45	0
56	MG	1H	3275	1/1	0.89	0.20	68,68,68,68	0
56	MG	41	202	1/1	0.89	0.17	75,75,75,75	0
56	MG	1H	3168	1/1	0.89	0.36	75,75,75,75	0
56	MG	1H	3277	1/1	0.89	0.34	81,81,81,81	0
56	MG	P8	101	1/1	0.89	0.24	66,66,66,66	0
56	MG	1H	3023	1/1	0.89	0.22	56,56,56,56	0
56	MG	1H	3279	1/1	0.89	0.11	67,67,67,67	0
56	MG	1H	3049	1/1	0.89	0.11	50,50,50,50	0
56	MG	1H	3009	1/1	0.89	0.23	74,74,74,74	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	1G	1653	1/1	0.89	0.24	82,82,82,82	0
56	MG	14	3067	1/1	0.89	0.22	85,85,85,85	0
56	MG	1H	3146	1/1	0.89	0.39	90,90,90,90	0
56	MG	14	3232	1/1	0.89	0.15	88,88,88,88	0
56	MG	14	3074	1/1	0.89	0.26	76,76,76,76	0
56	MG	14	3235	1/1	0.89	0.23	83,83,83,83	0
56	MG	1H	3176	1/1	0.89	0.27	51,51,51,51	0
56	MG	1H	3118	1/1	0.89	0.26	52,52,52,52	0
56	MG	14	3164	1/1	0.89	0.32	64,64,64,64	0
56	MG	1H	3311	1/1	0.89	0.17	56,56,56,56	0
56	MG	1H	3032	1/1	0.89	0.28	68,68,68,68	0
56	MG	14	3168	1/1	0.89	0.21	52,52,52,52	0
56	MG	1H	3064	1/1	0.89	0.32	76,76,76,76	0
56	MG	1H	3369	1/1	0.89	0.11	57,57,57,57	0
56	MG	14	3087	1/1	0.89	0.20	73,73,73,73	0
56	MG	1H	3183	1/1	0.89	0.23	74,74,74,74	0
56	MG	14	3319	1/1	0.89	0.15	84,84,84,84	0
56	MG	1G	1665	1/1	0.89	0.10	104,104,104,104	0
56	MG	13	1649	1/1	0.89	0.33	87,87,87,87	0
56	MG	1H	3039	1/1	0.89	0.24	74,74,74,74	0
56	MG	1G	1626	1/1	0.89	0.18	78,78,78,78	0
56	MG	14	3447	1/1	0.89	0.11	116,116,116,116	0
56	MG	1G	1702	1/1	0.89	0.15	100,100,100,100	0
56	MG	1H	3068	1/1	0.89	0.19	50,50,50,50	0
56	MG	1G	1628	1/1	0.89	0.24	77,77,77,77	0
56	MG	2L	103	1/1	0.89	0.26	70,70,70,70	0
56	MG	14	3002	1/1	0.89	0.15	61,61,61,61	0
56	MG	13	1682	1/1	0.89	0.09	91,91,91,91	0
56	MG	14	3122	1/1	0.89	0.24	53,53,53,53	0
56	MG	1H	3192	1/1	0.89	0.31	61,61,61,61	0
56	MG	14	3125	1/1	0.89	0.25	76,76,76,76	0
56	MG	1H	3135	1/1	0.89	0.23	54,54,54,54	0
56	MG	1H	3104	1/1	0.89	0.16	65,65,65,65	0
56	MG	1G	1634	1/1	0.89	0.16	91,91,91,91	0
56	MG	35	203	1/1	0.89	0.18	83,83,83,83	0
56	MG	1H	3551	1/1	0.89	0.11	105,105,105,105	0
56	MG	1H	3556	1/1	0.90	0.09	101,101,101,101	0
56	MG	1H	3557	1/1	0.90	0.10	84,84,84,84	0
56	MG	1H	3283	1/1	0.90	0.10	58,58,58,58	0
56	MG	1G	1621	1/1	0.90	0.20	76,76,76,76	0
56	MG	13	1659	1/1	0.90	0.24	57,57,57,57	0
56	MG	14	3018	1/1	0.90	0.23	75,75,75,75	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	1H	3090	1/1	0.90	0.21	50,50,50,50	0
56	MG	14	3144	1/1	0.90	0.25	60,60,60,60	0
56	MG	14	3085	1/1	0.90	0.20	64,64,64,64	0
56	MG	14	3191	1/1	0.90	0.14	66,66,66,66	0
56	MG	14	3242	1/1	0.90	0.24	83,83,83,83	0
56	MG	1H	3018	1/1	0.90	0.29	51,51,51,51	0
56	MG	14	3245	1/1	0.90	0.12	61,61,61,61	0
56	MG	14	3089	1/1	0.90	0.12	53,53,53,53	0
56	MG	14	3025	1/1	0.90	0.19	59,59,59,59	0
56	MG	1H	3233	1/1	0.90	0.21	57,57,57,57	0
56	MG	14	3316	1/1	0.90	0.12	79,79,79,79	0
56	MG	1H	3173	1/1	0.90	0.16	67,67,67,67	0
56	MG	1H	3262	1/1	0.90	0.39	86,86,86,86	0
56	MG	14	3155	1/1	0.90	0.21	73,73,73,73	0
56	MG	14	3032	1/1	0.90	0.27	50,50,50,50	0
56	MG	1H	3159	1/1	0.90	0.08	69,69,69,69	0
56	MG	88	203	1/1	0.90	0.22	87,87,87,87	0
56	MG	13	1645	1/1	0.90	0.27	84,84,84,84	0
56	MG	1H	3239	1/1	0.90	0.34	69,69,69,69	0
56	MG	1H	3125	1/1	0.90	0.17	50,50,50,50	0
56	MG	1H	3020	1/1	0.90	0.19	56,56,56,56	0
56	MG	13	1612	1/1	0.90	0.13	78,78,78,78	0
56	MG	1H	3470	1/1	0.90	0.14	82,82,82,82	0
56	MG	1H	3047	1/1	0.90	0.30	76,76,76,76	0
56	MG	1H	3224	1/1	0.90	0.15	74,74,74,74	0
56	MG	1G	1726	1/1	0.90	0.20	92,92,92,92	0
56	MG	1H	3085	1/1	0.90	0.19	85,85,85,85	0
56	MG	13	1625	1/1	0.90	0.22	78,78,78,78	0
56	MG	14	3222	1/1	0.90	0.20	88,88,88,88	0
56	MG	2L	101	1/1	0.90	0.27	71,71,71,71	0
56	MG	45	201	1/1	0.90	0.19	87,87,87,87	0
56	MG	1H	3155	1/1	0.90	0.20	80,80,80,80	0
56	MG	1H	3273	1/1	0.91	0.21	76,76,76,76	0
56	MG	1H	3108	1/1	0.91	0.20	34,34,34,34	0
56	MG	16	211	1/1	0.91	0.15	92,92,92,92	0
56	MG	14	3204	1/1	0.91	0.20	63,63,63,63	0
56	MG	1H	3112	1/1	0.91	0.10	53,53,53,53	0
56	MG	14	3037	1/1	0.91	0.22	61,61,61,61	0
56	MG	13	1632	1/1	0.91	0.17	69,69,69,69	0
56	MG	1H	3117	1/1	0.91	0.12	61,61,61,61	0
56	MG	1H	3081	1/1	0.91	0.36	76,76,76,76	0
56	MG	14	3139	1/1	0.91	0.28	75,75,75,75	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	1H	3121	1/1	0.91	0.39	64,64,64,64	0
56	MG	13	1605	1/1	0.91	0.16	79,79,79,79	0
56	MG	13	1683	1/1	0.91	0.19	92,92,92,92	0
56	MG	14	3216	1/1	0.91	0.30	79,79,79,79	0
56	MG	1G	1652	1/1	0.91	0.29	76,76,76,76	0
56	MG	14	3145	1/1	0.91	0.20	75,75,75,75	0
56	MG	14	3146	1/1	0.91	0.21	72,72,72,72	0
56	MG	13	1684	1/1	0.91	0.23	71,71,71,71	0
56	MG	13	1650	1/1	0.91	0.15	121,121,121,121	0
56	MG	14	3059	1/1	0.91	0.16	53,53,53,53	0
56	MG	1H	3054	1/1	0.91	0.45	70,70,70,70	0
56	MG	14	3227	1/1	0.91	0.23	70,70,70,70	0
56	MG	1H	3001	1/1	0.91	0.12	61,61,61,61	0
56	MG	13	1675	1/1	0.91	0.11	65,65,65,65	0
56	MG	1H	3134	1/1	0.91	0.16	74,74,74,74	0
56	MG	13	1651	1/1	0.91	0.29	82,82,82,82	0
56	MG	1G	1615	1/1	0.91	0.12	93,93,93,93	0
56	MG	13	1652	1/1	0.91	0.34	91,91,91,91	0
56	MG	1H	3421	1/1	0.91	0.09	98,98,98,98	0
56	MG	1H	3100	1/1	0.91	0.25	59,59,59,59	0
56	MG	1H	3101	1/1	0.91	0.15	79,79,79,79	0
56	MG	1H	3142	1/1	0.91	0.11	74,74,74,74	0
56	MG	14	3083	1/1	0.91	0.15	74,74,74,74	0
56	MG	14	3243	1/1	0.91	0.29	60,60,60,60	0
56	MG	1G	1622	1/1	0.91	0.24	73,73,73,73	0
56	MG	13	1712	1/1	0.91	0.14	96,96,96,96	0
56	MG	14	3284	1/1	0.91	0.21	87,87,87,87	0
56	MG	1H	3471	1/1	0.91	0.08	91,91,91,91	0
56	MG	14	3170	1/1	0.91	0.10	63,63,63,63	0
56	MG	1H	3069	1/1	0.91	0.21	45,45,45,45	0
56	MG	14	3313	1/1	0.91	0.10	53,53,53,53	0
56	MG	14	3172	1/1	0.91	0.28	82,82,82,82	0
56	MG	14	3091	1/1	0.91	0.16	44,44,44,44	0
56	MG	1H	3178	1/1	0.91	0.32	69,69,69,69	0
56	MG	14	3176	1/1	0.91	0.22	72,72,72,72	0
56	MG	1H	3216	1/1	0.91	0.18	71,71,71,71	0
56	MG	1H	3498	1/1	0.91	0.12	85,85,85,85	0
56	MG	13	1670	1/1	0.91	0.27	80,80,80,80	0
56	MG	14	3455	1/1	0.91	0.20	87,87,87,87	0
56	MG	14	3462	1/1	0.91	0.12	99,99,99,99	0
56	MG	14	3106	1/1	0.91	0.31	75,75,75,75	0
56	MG	1H	3549	1/1	0.91	0.14	75,75,75,75	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	14	3006	1/1	0.91	0.22	67,67,67,67	0
56	MG	1H	3078	1/1	0.91	0.24	70,70,70,70	0
56	MG	14	3015	1/1	0.91	0.18	80,80,80,80	0
56	MG	14	3113	1/1	0.91	0.10	67,67,67,67	0
56	MG	14	3115	1/1	0.91	0.23	64,64,64,64	0
56	MG	13	1606	1/1	0.91	0.19	71,71,71,71	0
56	MG	1H	3184	1/1	0.91	0.12	57,57,57,57	0
56	MG	1H	3222	1/1	0.91	0.13	72,72,72,72	0
56	MG	14	3020	1/1	0.91	0.21	73,73,73,73	0
56	MG	1H	3223	1/1	0.91	0.23	76,76,76,76	0
56	MG	1H	3149	1/1	0.91	0.13	54,54,54,54	0
56	MG	14	3026	1/1	0.91	0.24	70,70,70,70	0
56	MG	E5	101	1/1	0.91	0.36	74,74,74,74	0
56	MG	E5	102	1/1	0.91	0.34	72,72,72,72	0
56	MG	16	204	1/1	0.91	0.12	57,57,57,57	0
58	ZN	G8	201	1/1	0.91	0.16	143,143,143,143	0
56	MG	14	3223	1/1	0.92	0.20	78,78,78,78	0
56	MG	1H	3445	1/1	0.92	0.08	90,90,90,90	0
56	MG	1H	3221	1/1	0.92	0.12	65,65,65,65	0
56	MG	13	1758	1/1	0.92	0.09	137,137,137,137	0
56	MG	14	3230	1/1	0.92	0.17	74,74,74,74	0
56	MG	1H	3166	1/1	0.92	0.07	52,52,52,52	0
56	MG	13	1761	1/1	0.92	0.18	75,75,75,75	0
56	MG	1H	3225	1/1	0.92	0.11	60,60,60,60	0
56	MG	1H	3198	1/1	0.92	0.19	65,65,65,65	0
56	MG	14	3034	1/1	0.92	0.32	72,72,72,72	0
56	MG	14	3117	1/1	0.92	0.22	79,79,79,79	0
56	MG	13	1630	1/1	0.92	0.39	81,81,81,81	0
56	MG	1H	3504	1/1	0.92	0.07	86,86,86,86	0
56	MG	14	3120	1/1	0.92	0.14	72,72,72,72	0
56	MG	1H	3519	1/1	0.92	0.13	78,78,78,78	0
56	MG	1H	3530	1/1	0.92	0.24	81,81,81,81	0
56	MG	1H	3533	1/1	0.92	0.15	86,86,86,86	0
56	MG	1G	1663	1/1	0.92	0.10	85,85,85,85	0
56	MG	1H	3200	1/1	0.92	0.27	70,70,70,70	0
56	MG	13	1615	1/1	0.92	0.16	94,94,94,94	0
56	MG	1H	3202	1/1	0.92	0.21	63,63,63,63	0
56	MG	14	3305	1/1	0.92	0.09	96,96,96,96	0
56	MG	13	1623	1/1	0.92	0.25	62,62,62,62	0
56	MG	1G	1694	1/1	0.92	0.12	103,103,103,103	0
56	MG	1H	3053	1/1	0.92	0.19	40,40,40,40	0
56	MG	13	1637	1/1	0.92	0.09	73,73,73,73	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	1G	1723	1/1	0.92	0.10	106,106,106,106	0
56	MG	1H	3086	1/1	0.92	0.17	65,65,65,65	0
56	MG	14	3360	1/1	0.92	0.09	88,88,88,88	0
56	MG	14	3196	1/1	0.92	0.07	77,77,77,77	0
56	MG	14	3071	1/1	0.92	0.24	52,52,52,52	0
56	MG	13	1664	1/1	0.92	0.34	69,69,69,69	0
56	MG	14	3437	1/1	0.92	0.06	115,115,115,115	0
56	MG	1H	3122	1/1	0.92	0.17	58,58,58,58	0
56	MG	13	1665	1/1	0.92	0.31	76,76,76,76	0
56	MG	13	1666	1/1	0.92	0.29	79,79,79,79	0
56	MG	1H	3030	1/1	0.92	0.17	49,49,49,49	0
56	MG	14	3465	1/1	0.92	0.14	85,85,85,85	0
56	MG	14	3468	1/1	0.92	0.20	58,58,58,58	0
56	MG	1H	3095	1/1	0.92	0.23	66,66,66,66	0
56	MG	21	301	1/1	0.92	0.21	62,62,62,62	0
56	MG	13	1647	1/1	0.92	0.12	73,73,73,73	0
56	MG	14	3207	1/1	0.92	0.23	63,63,63,63	0
56	MG	14	3012	1/1	0.92	0.20	56,56,56,56	0
56	MG	1H	3129	1/1	0.92	0.20	66,66,66,66	0
56	MG	14	3086	1/1	0.92	0.14	61,61,61,61	0
56	MG	1H	3131	1/1	0.92	0.11	54,54,54,54	0
56	MG	39	301	1/1	0.92	0.15	92,92,92,92	0
56	MG	1H	3010	1/1	0.92	0.12	53,53,53,53	0
56	MG	14	3017	1/1	0.92	0.25	54,54,54,54	0
56	MG	1H	3070	1/1	0.92	0.27	54,54,54,54	0
56	MG	35	202	1/1	0.92	0.20	78,78,78,78	0
56	MG	14	3094	1/1	0.92	0.21	73,73,73,73	0
56	MG	14	3159	1/1	0.92	0.15	70,70,70,70	0
56	MG	1H	3255	1/1	0.92	0.09	75,75,75,75	0
56	MG	13	1750	1/1	0.92	0.12	101,101,101,101	0
56	MG	13	1752	1/1	0.92	0.08	108,108,108,108	0
56	MG	14	3104	1/1	0.92	0.45	74,74,74,74	0
56	MG	1H	3033	1/1	0.93	0.24	67,67,67,67	0
56	MG	1H	3348	1/1	0.93	0.16	78,78,78,78	0
56	MG	1H	3002	1/1	0.93	0.15	59,59,59,59	0
56	MG	14	3080	1/1	0.93	0.15	53,53,53,53	0
56	MG	1G	1633	1/1	0.93	0.14	92,92,92,92	0
56	MG	14	3229	1/1	0.93	0.13	66,66,66,66	0
56	MG	1H	3057	1/1	0.93	0.21	63,63,63,63	0
56	MG	14	3003	1/1	0.93	0.15	43,43,43,43	0
56	MG	1H	3405	1/1	0.93	0.08	91,91,91,91	0
56	MG	14	3233	1/1	0.93	0.09	61,61,61,61	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	16	210	1/1	0.93	0.10	89,89,89,89	0
56	MG	1H	3103	1/1	0.93	0.16	62,62,62,62	0
56	MG	14	3008	1/1	0.93	0.17	84,84,84,84	0
56	MG	14	3090	1/1	0.93	0.22	55,55,55,55	0
56	MG	1H	3419	1/1	0.93	0.08	78,78,78,78	0
56	MG	1H	3058	1/1	0.93	0.18	69,69,69,69	0
56	MG	21	302	1/1	0.93	0.25	75,75,75,75	0
56	MG	13	1723	1/1	0.93	0.11	75,75,75,75	0
56	MG	1H	3060	1/1	0.93	0.08	54,54,54,54	0
56	MG	14	3100	1/1	0.93	0.14	77,77,77,77	0
56	MG	14	3102	1/1	0.93	0.18	60,60,60,60	0
56	MG	88	202	1/1	0.93	0.22	67,67,67,67	0
56	MG	13	1689	1/1	0.93	0.08	65,65,65,65	0
56	MG	1H	3136	1/1	0.93	0.51	76,76,76,76	0
56	MG	14	3302	1/1	0.93	0.09	96,96,96,96	0
56	MG	14	3021	1/1	0.93	0.18	36,36,36,36	0
56	MG	F8	101	1/1	0.93	0.11	63,63,63,63	0
56	MG	1G	1647	1/1	0.93	0.14	82,82,82,82	0
56	MG	1H	3461	1/1	0.93	0.07	90,90,90,90	0
56	MG	1H	3163	1/1	0.93	0.38	83,83,83,83	0
56	MG	14	3114	1/1	0.93	0.17	68,68,68,68	0
56	MG	14	3327	1/1	0.93	0.09	60,60,60,60	0
56	MG	1H	3272	1/1	0.93	0.51	67,67,67,67	0
56	MG	14	3331	1/1	0.93	0.15	65,65,65,65	0
56	MG	14	3346	1/1	0.93	0.10	74,74,74,74	0
56	MG	1H	3026	1/1	0.93	0.18	71,71,71,71	0
56	MG	1H	3110	1/1	0.93	0.18	44,44,44,44	0
56	MG	1H	3482	1/1	0.93	0.09	85,85,85,85	0
56	MG	1H	3043	1/1	0.93	0.14	47,47,47,47	0
56	MG	14	3035	1/1	0.93	0.23	67,67,67,67	0
56	MG	13	1616	1/1	0.93	0.29	77,77,77,77	0
56	MG	14	3449	1/1	0.93	0.10	88,88,88,88	0
56	MG	14	3454	1/1	0.93	0.20	78,78,78,78	0
56	MG	1H	3088	1/1	0.93	0.37	74,74,74,74	0
56	MG	14	3457	1/1	0.93	0.07	92,92,92,92	0
56	MG	14	3459	1/1	0.93	0.06	97,97,97,97	0
56	MG	1H	3509	1/1	0.93	0.16	46,46,46,46	0
56	MG	13	1719	1/1	0.93	0.13	89,89,89,89	0
56	MG	1H	3524	1/1	0.93	0.08	96,96,96,96	0
56	MG	1G	1662	1/1	0.93	0.19	94,94,94,94	0
56	MG	1H	3280	1/1	0.93	0.21	76,76,76,76	0
56	MG	1H	3248	1/1	0.93	0.19	72,72,72,72	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	14	3132	1/1	0.93	0.35	56,56,56,56	0
56	MG	14	3054	1/1	0.93	0.17	55,55,55,55	0
56	MG	1H	3249	1/1	0.93	0.33	67,67,67,67	0
56	MG	14	3057	1/1	0.93	0.21	61,61,61,61	0
56	MG	1H	3031	1/1	0.93	0.21	74,74,74,74	0
56	MG	1H	3092	1/1	0.93	0.23	55,55,55,55	0
56	MG	1G	1672	1/1	0.93	0.07	109,109,109,109	0
56	MG	1H	3554	1/1	0.93	0.13	100,100,100,100	0
56	MG	1H	3075	1/1	0.93	0.23	80,80,80,80	0
56	MG	14	3066	1/1	0.93	0.15	49,49,49,49	0
56	MG	1G	1700	1/1	0.93	0.08	87,87,87,87	0
56	MG	14	3068	1/1	0.93	0.18	59,59,59,59	0
56	MG	1H	3076	1/1	0.93	0.24	60,60,60,60	0
56	MG	1G	1713	1/1	0.93	0.07	112,112,112,112	0
56	MG	14	3073	1/1	0.93	0.25	65,65,65,65	0
56	MG	1H	3563	1/1	0.93	0.19	75,75,75,75	0
56	MG	5E	201	1/1	0.93	0.13	71,71,71,71	0
56	MG	14	3105	1/1	0.94	0.09	72,72,72,72	0
56	MG	1H	3061	1/1	0.94	0.20	41,41,41,41	0
56	MG	1H	3097	1/1	0.94	0.22	53,53,53,53	0
56	MG	1G	1616	1/1	0.94	0.26	71,71,71,71	0
56	MG	14	3036	1/1	0.94	0.18	39,39,39,39	0
56	MG	1H	3098	1/1	0.94	0.13	58,58,58,58	0
56	MG	13	1610	1/1	0.94	0.13	77,77,77,77	0
56	MG	14	3043	1/1	0.94	0.17	68,68,68,68	0
56	MG	13	1756	1/1	0.94	0.05	120,120,120,120	0
56	MG	14	3046	1/1	0.94	0.14	52,52,52,52	0
56	MG	1H	3226	1/1	0.94	0.19	78,78,78,78	0
56	MG	14	3254	1/1	0.94	0.07	92,92,92,92	0
56	MG	1H	3331	1/1	0.94	0.08	49,49,49,49	0
56	MG	14	3296	1/1	0.94	0.12	70,70,70,70	0
56	MG	13	1634	1/1	0.94	0.07	68,68,68,68	0
56	MG	14	3051	1/1	0.94	0.19	62,62,62,62	0
56	MG	1G	1623	1/1	0.94	0.12	77,77,77,77	0
56	MG	1H	3067	1/1	0.94	0.27	75,75,75,75	0
56	MG	1G	1691	1/1	0.94	0.07	110,110,110,110	0
56	MG	1H	3179	1/1	0.94	0.15	47,47,47,47	0
56	MG	13	1611	1/1	0.94	0.20	64,64,64,64	0
56	MG	1G	1697	1/1	0.94	0.11	94,94,94,94	0
56	MG	14	3324	1/1	0.94	0.12	70,70,70,70	0
56	MG	1H	3390	1/1	0.94	0.07	102,102,102,102	0
56	MG	1H	3401	1/1	0.94	0.10	46,46,46,46	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	1H	3261	1/1	0.94	0.24	65,65,65,65	0
56	MG	14	3342	1/1	0.94	0.10	75,75,75,75	0
56	MG	1G	1719	1/1	0.94	0.07	100,100,100,100	0
56	MG	14	3349	1/1	0.94	0.10	65,65,65,65	0
56	MG	14	3357	1/1	0.94	0.10	79,79,79,79	0
56	MG	1H	3051	1/1	0.94	0.17	46,46,46,46	0
56	MG	14	3368	1/1	0.94	0.07	75,75,75,75	0
56	MG	14	3390	1/1	0.94	0.12	72,72,72,72	0
56	MG	14	3395	1/1	0.94	0.07	69,69,69,69	0
56	MG	14	3396	1/1	0.94	0.06	102,102,102,102	0
56	MG	1H	3411	1/1	0.94	0.11	65,65,65,65	0
56	MG	14	3405	1/1	0.94	0.05	106,106,106,106	0
56	MG	14	3417	1/1	0.94	0.09	116,116,116,116	0
56	MG	1H	3182	1/1	0.94	0.18	56,56,56,56	0
56	MG	14	3202	1/1	0.94	0.11	65,65,65,65	0
56	MG	1H	3037	1/1	0.94	0.32	63,63,63,63	0
56	MG	1H	3265	1/1	0.94	0.07	69,69,69,69	0
56	MG	1H	3438	1/1	0.94	0.07	71,71,71,71	0
56	MG	1H	3440	1/1	0.94	0.08	72,72,72,72	0
56	MG	14	3142	1/1	0.94	0.14	83,83,83,83	0
56	MG	1H	3074	1/1	0.94	0.05	52,52,52,52	0
56	MG	1H	3235	1/1	0.94	0.25	65,65,65,65	0
56	MG	14	3210	1/1	0.94	0.26	74,74,74,74	0
56	MG	78	201	1/1	0.94	0.20	70,70,70,70	0
56	MG	14	3464	1/1	0.94	0.09	105,105,105,105	0
56	MG	1H	3451	1/1	0.94	0.09	78,78,78,78	0
56	MG	1H	3452	1/1	0.94	0.07	72,72,72,72	0
56	MG	1H	3025	1/1	0.94	0.17	32,32,32,32	0
56	MG	13	1604	1/1	0.94	0.14	66,66,66,66	0
56	MG	1H	3111	1/1	0.94	0.17	57,57,57,57	0
56	MG	L8	101	1/1	0.94	0.19	80,80,80,80	0
56	MG	1H	3274	1/1	0.94	0.19	48,48,48,48	0
56	MG	1H	3091	1/1	0.94	0.12	65,65,65,65	0
56	MG	13	1603	1/1	0.94	0.15	72,72,72,72	0
56	MG	1G	1649	1/1	0.94	0.11	83,83,83,83	0
56	MG	1H	3243	1/1	0.94	0.14	54,54,54,54	0
56	MG	14	3022	1/1	0.94	0.21	73,73,73,73	0
56	MG	1G	1606	1/1	0.94	0.09	80,80,80,80	0
56	MG	14	3226	1/1	0.94	0.12	51,51,51,51	0
56	MG	1H	3093	1/1	0.94	0.15	60,60,60,60	0
56	MG	13	1608	1/1	0.94	0.17	71,71,71,71	0
56	MG	1G	1611	1/1	0.94	0.13	84,84,84,84	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	B5	101	1/1	0.94	0.08	76,76,76,76	0
56	MG	14	3101	1/1	0.94	0.18	70,70,70,70	0
56	MG	1H	3120	1/1	0.94	0.07	39,39,39,39	0
56	MG	1H	3046	1/1	0.94	0.15	59,59,59,59	0
56	MG	1G	1657	1/1	0.94	0.24	77,77,77,77	0
56	MG	1H	3435	1/1	0.95	0.06	55,55,55,55	0
56	MG	14	3253	1/1	0.95	0.06	57,57,57,57	0
56	MG	1H	3035	1/1	0.95	0.09	64,64,64,64	0
56	MG	14	3263	1/1	0.95	0.07	64,64,64,64	0
56	MG	14	3269	1/1	0.95	0.09	60,60,60,60	0
56	MG	1H	3439	1/1	0.95	0.07	55,55,55,55	0
56	MG	13	1744	1/1	0.95	0.06	111,111,111,111	0
56	MG	1H	3442	1/1	0.95	0.15	64,64,64,64	0
56	MG	13	1746	1/1	0.95	0.06	102,102,102,102	0
56	MG	1H	3126	1/1	0.95	0.16	64,64,64,64	0
56	MG	14	3188	1/1	0.95	0.09	61,61,61,61	0
56	MG	1G	1709	1/1	0.95	0.10	99,99,99,99	0
56	MG	1G	1710	1/1	0.95	0.06	95,95,95,95	0
56	MG	14	3314	1/1	0.95	0.10	46,46,46,46	0
56	MG	1H	3188	1/1	0.95	0.22	69,69,69,69	0
56	MG	11	301	1/1	0.95	0.08	77,77,77,77	0
56	MG	1G	1722	1/1	0.95	0.06	102,102,102,102	0
56	MG	14	3195	1/1	0.95	0.18	71,71,71,71	0
56	MG	13	1680	1/1	0.95	0.29	73,73,73,73	0
56	MG	1H	3454	1/1	0.95	0.17	67,67,67,67	0
56	MG	14	3335	1/1	0.95	0.12	78,78,78,78	0
56	MG	14	3341	1/1	0.95	0.10	76,76,76,76	0
56	MG	1H	3017	1/1	0.95	0.26	55,55,55,55	0
56	MG	14	3345	1/1	0.95	0.07	66,66,66,66	0
56	MG	1H	3148	1/1	0.95	0.08	56,56,56,56	0
56	MG	14	3065	1/1	0.95	0.16	58,58,58,58	0
56	MG	14	3354	1/1	0.95	0.07	63,63,63,63	0
56	MG	1H	3468	1/1	0.95	0.09	68,68,68,68	0
56	MG	1H	3073	1/1	0.95	0.14	39,39,39,39	0
56	MG	14	3363	1/1	0.95	0.06	54,54,54,54	0
56	MG	1H	3150	1/1	0.95	0.18	51,51,51,51	0
56	MG	13	1618	1/1	0.95	0.10	45,45,45,45	0
56	MG	1H	3114	1/1	0.95	0.15	66,66,66,66	0
56	MG	1H	3341	1/1	0.95	0.09	43,43,43,43	0
56	MG	1H	3491	1/1	0.95	0.19	73,73,73,73	0
56	MG	1H	3154	1/1	0.95	0.21	60,60,60,60	0
56	MG	14	3407	1/1	0.95	0.12	79,79,79,79	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	14	3010	1/1	0.95	0.18	50,50,50,50	0
56	MG	14	3077	1/1	0.95	0.19	45,45,45,45	0
56	MG	1H	3099	1/1	0.95	0.32	80,80,80,80	0
56	MG	1G	1603	1/1	0.95	0.13	85,85,85,85	0
56	MG	1H	3242	1/1	0.95	0.20	70,70,70,70	0
56	MG	1H	3268	1/1	0.95	0.16	78,78,78,78	0
56	MG	1H	3386	1/1	0.95	0.06	88,88,88,88	0
56	MG	1H	3520	1/1	0.95	0.16	98,98,98,98	0
56	MG	1H	3269	1/1	0.95	0.17	61,61,61,61	0
56	MG	14	3218	1/1	0.95	0.10	74,74,74,74	0
56	MG	1G	1609	1/1	0.95	0.13	70,70,70,70	0
56	MG	1H	3526	1/1	0.95	0.10	73,73,73,73	0
56	MG	1H	3044	1/1	0.95	0.14	39,39,39,39	0
56	MG	14	3156	1/1	0.95	0.40	86,86,86,86	0
56	MG	14	3467	1/1	0.95	0.20	71,71,71,71	0
56	MG	14	3023	1/1	0.95	0.14	69,69,69,69	0
56	MG	1H	3244	1/1	0.95	0.10	67,67,67,67	0
56	MG	14	3471	1/1	0.95	0.10	68,68,68,68	0
56	MG	1J	201	1/1	0.95	0.05	70,70,70,70	0
56	MG	13	1656	1/1	0.95	0.10	60,60,60,60	0
56	MG	1J	203	1/1	0.95	0.18	70,70,70,70	0
56	MG	1H	3546	1/1	0.95	0.07	93,93,93,93	0
56	MG	1H	3119	1/1	0.95	0.10	46,46,46,46	0
56	MG	14	3096	1/1	0.95	0.12	48,48,48,48	0
56	MG	1H	3415	1/1	0.95	0.13	73,73,73,73	0
56	MG	14	3165	1/1	0.95	0.18	67,67,67,67	0
56	MG	14	3098	1/1	0.95	0.17	68,68,68,68	0
56	MG	29	301	1/1	0.95	0.16	49,49,49,49	0
56	MG	1K	101	1/1	0.95	0.08	119,119,119,119	0
56	MG	14	3030	1/1	0.95	0.16	38,38,38,38	0
56	MG	1H	3021	1/1	0.95	0.17	43,43,43,43	0
56	MG	1H	3426	1/1	0.95	0.12	77,77,77,77	0
56	MG	1H	3562	1/1	0.95	0.15	69,69,69,69	0
56	MG	1H	3022	1/1	0.95	0.16	45,45,45,45	0
56	MG	1G	1666	1/1	0.95	0.07	100,100,100,100	0
56	MG	1H	3568	1/1	0.95	0.14	94,94,94,94	0
56	MG	1H	3572	1/1	0.95	0.18	54,54,54,54	0
56	MG	14	3042	1/1	0.95	0.20	85,85,85,85	0
56	MG	1G	1669	1/1	0.95	0.08	81,81,81,81	0
56	MG	14	3044	1/1	0.95	0.30	78,78,78,78	0
56	MG	1H	3062	1/1	0.96	0.06	29,29,29,29	0
56	MG	13	1749	1/1	0.96	0.06	106,106,106,106	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	1H	3522	1/1	0.96	0.05	98,98,98,98	0
56	MG	14	3174	1/1	0.96	0.16	64,64,64,64	0
56	MG	1H	3045	1/1	0.96	0.14	42,42,42,42	0
56	MG	1G	1610	1/1	0.96	0.08	70,70,70,70	0
56	MG	14	3299	1/1	0.96	0.05	99,99,99,99	0
56	MG	14	3301	1/1	0.96	0.10	111,111,111,111	0
56	MG	1H	3424	1/1	0.96	0.08	44,44,44,44	0
56	MG	1H	3028	1/1	0.96	0.11	49,49,49,49	0
56	MG	14	3031	1/1	0.96	0.20	48,48,48,48	0
56	MG	1H	3427	1/1	0.96	0.10	60,60,60,60	0
56	MG	1H	3534	1/1	0.96	0.06	85,85,85,85	0
56	MG	14	3107	1/1	0.96	0.08	61,61,61,61	0
56	MG	14	3315	1/1	0.96	0.07	56,56,56,56	0
56	MG	14	3108	1/1	0.96	0.04	67,67,67,67	0
56	MG	14	3318	1/1	0.96	0.06	65,65,65,65	0
56	MG	1H	3536	1/1	0.96	0.07	98,98,98,98	0
56	MG	14	3321	1/1	0.96	0.06	88,88,88,88	0
56	MG	14	3322	1/1	0.96	0.13	77,77,77,77	0
56	MG	1H	3538	1/1	0.96	0.20	78,78,78,78	0
56	MG	1H	3428	1/1	0.96	0.06	64,64,64,64	0
56	MG	1H	3029	1/1	0.96	0.10	48,48,48,48	0
56	MG	1H	3432	1/1	0.96	0.05	44,44,44,44	0
56	MG	14	3333	1/1	0.96	0.10	64,64,64,64	0
56	MG	14	3334	1/1	0.96	0.09	69,69,69,69	0
56	MG	14	3040	1/1	0.96	0.12	58,58,58,58	0
56	MG	1H	3282	1/1	0.96	0.14	66,66,66,66	0
56	MG	1G	1682	1/1	0.96	0.16	117,117,117,117	0
56	MG	1G	1688	1/1	0.96	0.08	81,81,81,81	0
56	MG	14	3194	1/1	0.96	0.31	79,79,79,79	0
56	MG	14	3347	1/1	0.96	0.10	74,74,74,74	0
56	MG	1H	3189	1/1	0.96	0.13	53,53,53,53	0
56	MG	1H	3555	1/1	0.96	0.21	70,70,70,70	0
56	MG	13	1641	1/1	0.96	0.10	78,78,78,78	0
56	MG	14	3121	1/1	0.96	0.15	45,45,45,45	0
56	MG	1G	1696	1/1	0.96	0.07	107,107,107,107	0
56	MG	14	3123	1/1	0.96	0.08	60,60,60,60	0
56	MG	14	3376	1/1	0.96	0.11	91,91,91,91	0
56	MG	14	3383	1/1	0.96	0.05	102,102,102,102	0
56	MG	14	3384	1/1	0.96	0.09	79,79,79,79	0
56	MG	14	3385	1/1	0.96	0.07	80,80,80,80	0
56	MG	13	1733	1/1	0.96	0.10	102,102,102,102	0
56	MG	14	3392	1/1	0.96	0.06	85,85,85,85	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	1G	1698	1/1	0.96	0.06	102,102,102,102	0
56	MG	1H	3560	1/1	0.96	0.11	85,85,85,85	0
56	MG	13	1754	1/1	0.96	0.07	80,80,80,80	0
56	MG	1G	1703	1/1	0.96	0.13	85,85,85,85	0
56	MG	14	3055	1/1	0.96	0.19	50,50,50,50	0
56	MG	14	3413	1/1	0.96	0.12	64,64,64,64	0
56	MG	1H	3071	1/1	0.96	0.10	57,57,57,57	0
56	MG	14	3424	1/1	0.96	0.05	81,81,81,81	0
56	MG	14	3429	1/1	0.96	0.10	68,68,68,68	0
56	MG	1H	3293	1/1	0.96	0.06	41,41,41,41	0
56	MG	1G	1712	1/1	0.96	0.05	122,122,122,122	0
56	MG	14	3436	1/1	0.96	0.08	98,98,98,98	0
56	MG	1H	3447	1/1	0.96	0.07	59,59,59,59	0
56	MG	14	3061	1/1	0.96	0.18	47,47,47,47	0
56	MG	1G	1717	1/1	0.96	0.06	118,118,118,118	0
56	MG	14	3451	1/1	0.96	0.07	88,88,88,88	0
56	MG	1H	3449	1/1	0.96	0.12	53,53,53,53	0
56	MG	1H	3130	1/1	0.96	0.09	54,54,54,54	0
56	MG	1H	3326	1/1	0.96	0.09	56,56,56,56	0
56	MG	13	1713	1/1	0.96	0.17	82,82,82,82	0
56	MG	14	3461	1/1	0.96	0.11	80,80,80,80	0
56	MG	1H	3266	1/1	0.96	0.11	61,61,61,61	0
56	MG	1H	3456	1/1	0.96	0.12	102,102,102,102	0
56	MG	52	201	1/1	0.96	0.05	109,109,109,109	0
56	MG	1H	3006	1/1	0.96	0.20	43,43,43,43	0
56	MG	14	3466	1/1	0.96	0.10	92,92,92,92	0
56	MG	1H	3463	1/1	0.96	0.07	78,78,78,78	0
56	MG	14	3147	1/1	0.96	0.11	66,66,66,66	0
56	MG	1H	3467	1/1	0.96	0.06	95,95,95,95	0
56	MG	1H	3197	1/1	0.96	0.13	69,69,69,69	0
56	MG	1H	3469	1/1	0.96	0.05	79,79,79,79	0
56	MG	1H	3174	1/1	0.96	0.17	50,50,50,50	0
56	MG	13	1740	1/1	0.96	0.06	96,96,96,96	0
56	MG	1H	3372	1/1	0.96	0.06	54,54,54,54	0
56	MG	1H	3379	1/1	0.96	0.05	86,86,86,86	0
56	MG	14	3011	1/1	0.96	0.20	50,50,50,50	0
56	MG	14	3082	1/1	0.96	0.10	73,73,73,73	0
56	MG	1H	3055	1/1	0.96	0.14	43,43,43,43	0
56	MG	1H	3484	1/1	0.96	0.06	88,88,88,88	0
56	MG	1J	210	1/1	0.96	0.08	91,91,91,91	0
56	MG	13	1741	1/1	0.96	0.06	110,110,110,110	0
56	MG	13	1621	1/1	0.96	0.14	84,84,84,84	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	13	1609	1/1	0.96	0.19	64,64,64,64	0
56	MG	14	3162	1/1	0.96	0.06	50,50,50,50	0
56	MG	14	3088	1/1	0.96	0.07	105,105,105,105	0
56	MG	1H	3501	1/1	0.96	0.06	76,76,76,76	0
56	MG	Q8	101	1/1	0.96	0.15	71,71,71,71	0
56	MG	13	1724	1/1	0.96	0.06	94,94,94,94	0
56	MG	14	3092	1/1	0.96	0.14	43,43,43,43	0
56	MG	1H	3505	1/1	0.96	0.18	82,82,82,82	0
56	MG	13	1748	1/1	0.96	0.12	102,102,102,102	0
56	MG	14	3252	1/1	0.96	0.06	52,52,52,52	0
56	MG	M5	101	1/1	0.96	0.14	81,81,81,81	0
56	MG	1H	3518	1/1	0.96	0.11	76,76,76,76	0
58	ZN	C5	201	1/1	0.96	0.05	156,156,156,156	0
56	MG	1H	3332	1/1	0.97	0.05	50,50,50,50	0
56	MG	14	3268	1/1	0.97	0.06	64,64,64,64	0
56	MG	1G	1675	1/1	0.97	0.09	101,101,101,101	0
56	MG	14	3270	1/1	0.97	0.05	80,80,80,80	0
56	MG	14	3272	1/1	0.97	0.05	68,68,68,68	0
56	MG	1G	1677	1/1	0.97	0.06	93,93,93,93	0
56	MG	14	3290	1/1	0.97	0.06	67,67,67,67	0
56	MG	14	3291	1/1	0.97	0.10	82,82,82,82	0
56	MG	1G	1678	1/1	0.97	0.10	93,93,93,93	0
56	MG	14	3297	1/1	0.97	0.06	91,91,91,91	0
56	MG	1G	1681	1/1	0.97	0.05	99,99,99,99	0
56	MG	1H	3340	1/1	0.97	0.10	65,65,65,65	0
56	MG	14	3300	1/1	0.97	0.04	76,76,76,76	0
56	MG	1G	1684	1/1	0.97	0.05	98,98,98,98	0
56	MG	1G	1687	1/1	0.97	0.06	75,75,75,75	0
56	MG	1H	3152	1/1	0.97	0.14	87,87,87,87	0
56	MG	1G	1689	1/1	0.97	0.06	79,79,79,79	0
56	MG	14	3310	1/1	0.97	0.08	98,98,98,98	0
56	MG	13	1736	1/1	0.97	0.12	99,99,99,99	0
56	MG	13	1710	1/1	0.97	0.09	85,85,85,85	0
56	MG	1H	3477	1/1	0.97	0.04	91,91,91,91	0
56	MG	1G	1601	1/1	0.97	0.09	78,78,78,78	0
56	MG	1H	3353	1/1	0.97	0.05	68,68,68,68	0
56	MG	1H	3360	1/1	0.97	0.06	59,59,59,59	0
56	MG	1H	3362	1/1	0.97	0.06	55,55,55,55	0
56	MG	1H	3485	1/1	0.97	0.05	97,97,97,97	0
56	MG	1H	3488	1/1	0.97	0.07	85,85,85,85	0
56	MG	1G	1705	1/1	0.97	0.06	116,116,116,116	0
56	MG	14	3326	1/1	0.97	0.04	81,81,81,81	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	1G	1708	1/1	0.97	0.10	84,84,84,84	0
56	MG	1H	3490	1/1	0.97	0.07	95,95,95,95	0
56	MG	14	3330	1/1	0.97	0.04	77,77,77,77	0
56	MG	13	1660	1/1	0.97	0.14	55,55,55,55	0
56	MG	1H	3366	1/1	0.97	0.12	67,67,67,67	0
56	MG	1H	3496	1/1	0.97	0.15	76,76,76,76	0
56	MG	1H	3497	1/1	0.97	0.07	75,75,75,75	0
56	MG	14	3336	1/1	0.97	0.06	75,75,75,75	0
56	MG	13	1742	1/1	0.97	0.05	105,105,105,105	0
56	MG	1G	1720	1/1	0.97	0.10	129,129,129,129	0
56	MG	14	3182	1/1	0.97	0.04	66,66,66,66	0
56	MG	1H	3499	1/1	0.97	0.17	82,82,82,82	0
56	MG	13	1743	1/1	0.97	0.06	102,102,102,102	0
56	MG	14	3348	1/1	0.97	0.05	51,51,51,51	0
56	MG	1G	1724	1/1	0.97	0.09	102,102,102,102	0
56	MG	14	3350	1/1	0.97	0.06	44,44,44,44	0
56	MG	14	3353	1/1	0.97	0.05	91,91,91,91	0
56	MG	1G	1725	1/1	0.97	0.06	95,95,95,95	0
56	MG	14	3356	1/1	0.97	0.05	60,60,60,60	0
56	MG	1H	3503	1/1	0.97	0.10	75,75,75,75	0
56	MG	1H	3375	1/1	0.97	0.06	85,85,85,85	0
56	MG	1H	3377	1/1	0.97	0.04	49,49,49,49	0
56	MG	13	1619	1/1	0.97	0.07	51,51,51,51	0
56	MG	14	3373	1/1	0.97	0.07	58,58,58,58	0
56	MG	1H	3513	1/1	0.97	0.15	64,64,64,64	0
56	MG	14	3379	1/1	0.97	0.04	94,94,94,94	0
56	MG	1H	3185	1/1	0.97	0.22	54,54,54,54	0
56	MG	1H	3388	1/1	0.97	0.05	97,97,97,97	0
56	MG	14	3099	1/1	0.97	0.21	51,51,51,51	0
56	MG	14	3387	1/1	0.97	0.05	87,87,87,87	0
56	MG	14	3388	1/1	0.97	0.04	90,90,90,90	0
56	MG	1H	3063	1/1	0.97	0.10	43,43,43,43	0
56	MG	14	3391	1/1	0.97	0.06	73,73,73,73	0
56	MG	1H	3397	1/1	0.97	0.06	46,46,46,46	0
56	MG	14	3393	1/1	0.97	0.05	98,98,98,98	0
56	MG	1H	3398	1/1	0.97	0.06	55,55,55,55	0
56	MG	1H	3042	1/1	0.97	0.06	43,43,43,43	0
56	MG	14	3398	1/1	0.97	0.06	84,84,84,84	0
56	MG	13	1716	1/1	0.97	0.04	108,108,108,108	0
56	MG	14	3009	1/1	0.97	0.10	41,41,41,41	0
56	MG	1H	3532	1/1	0.97	0.05	96,96,96,96	0
56	MG	14	3408	1/1	0.97	0.05	94,94,94,94	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	14	3410	1/1	0.97	0.09	83,83,83,83	0
56	MG	14	3412	1/1	0.97	0.06	76,76,76,76	0
56	MG	13	1718	1/1	0.97	0.08	54,54,54,54	0
56	MG	1H	3409	1/1	0.97	0.09	65,65,65,65	0
56	MG	14	3422	1/1	0.97	0.14	70,70,70,70	0
56	MG	1H	3113	1/1	0.97	0.05	37,37,37,37	0
56	MG	14	3425	1/1	0.97	0.09	96,96,96,96	0
56	MG	1H	3537	1/1	0.97	0.08	79,79,79,79	0
56	MG	14	3431	1/1	0.97	0.06	84,84,84,84	0
56	MG	1H	3003	1/1	0.97	0.14	44,44,44,44	0
56	MG	14	3433	1/1	0.97	0.10	143,143,143,143	0
56	MG	1H	3417	1/1	0.97	0.07	71,71,71,71	0
56	MG	1H	3543	1/1	0.97	0.11	81,81,81,81	0
56	MG	1H	3544	1/1	0.97	0.07	81,81,81,81	0
56	MG	14	3438	1/1	0.97	0.05	115,115,115,115	0
56	MG	14	3440	1/1	0.97	0.05	95,95,95,95	0
56	MG	14	3442	1/1	0.97	0.07	96,96,96,96	0
56	MG	14	3443	1/1	0.97	0.06	91,91,91,91	0
56	MG	14	3444	1/1	0.97	0.09	90,90,90,90	0
56	MG	14	3446	1/1	0.97	0.07	98,98,98,98	0
56	MG	1H	3545	1/1	0.97	0.08	88,88,88,88	0
56	MG	1H	3418	1/1	0.97	0.16	68,68,68,68	0
56	MG	1H	3547	1/1	0.97	0.11	91,91,91,91	0
56	MG	1H	3140	1/1	0.97	0.16	50,50,50,50	0
56	MG	1H	3420	1/1	0.97	0.11	55,55,55,55	0
56	MG	13	1691	1/1	0.97	0.06	76,76,76,76	0
56	MG	1H	3250	1/1	0.97	0.13	64,64,64,64	0
56	MG	14	3460	1/1	0.97	0.09	93,93,93,93	0
56	MG	13	1695	1/1	0.97	0.07	78,78,78,78	0
56	MG	13	1701	1/1	0.97	0.08	100,100,100,100	0
56	MG	1H	3559	1/1	0.97	0.07	73,73,73,73	0
56	MG	13	1704	1/1	0.97	0.14	73,73,73,73	0
56	MG	14	3126	1/1	0.97	0.04	55,55,55,55	0
56	MG	13	1732	1/1	0.97	0.05	113,113,113,113	0
56	MG	13	1706	1/1	0.97	0.04	92,92,92,92	0
56	MG	1H	3565	1/1	0.97	0.14	60,60,60,60	0
56	MG	14	3469	1/1	0.97	0.05	55,55,55,55	0
56	MG	1H	3052	1/1	0.97	0.08	59,59,59,59	0
56	MG	1H	3570	1/1	0.97	0.07	48,48,48,48	0
56	MG	13	1707	1/1	0.97	0.05	63,63,63,63	0
56	MG	14	3228	1/1	0.97	0.20	63,63,63,63	0
56	MG	13	1759	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
56	MG	1H	3288	1/1	0.97	0.05	38,38,38,38	0
56	MG	14	3039	1/1	0.97	0.08	63,63,63,63	0
56	MG	1H	3292	1/1	0.97	0.05	38,38,38,38	0
56	MG	14	3041	1/1	0.97	0.11	44,44,44,44	0
56	MG	1H	3259	1/1	0.97	0.11	58,58,58,58	0
56	MG	1H	3294	1/1	0.97	0.06	43,43,43,43	0
56	MG	1H	3296	1/1	0.97	0.06	43,43,43,43	0
56	MG	16	208	1/1	0.97	0.18	80,80,80,80	0
56	MG	1H	3448	1/1	0.97	0.08	74,74,74,74	0
56	MG	14	3047	1/1	0.97	0.13	46,46,46,46	0
56	MG	1H	3305	1/1	0.97	0.05	48,48,48,48	0
56	MG	1H	3175	1/1	0.97	0.10	55,55,55,55	0
56	MG	1H	3312	1/1	0.97	0.09	49,49,49,49	0
56	MG	1H	3315	1/1	0.97	0.05	85,85,85,85	0
56	MG	1H	3316	1/1	0.97	0.06	60,60,60,60	0
56	MG	1H	3320	1/1	0.97	0.08	43,43,43,43	0
56	MG	14	3247	1/1	0.97	0.06	58,58,58,58	0
56	MG	14	3251	1/1	0.97	0.05	48,48,48,48	0
56	MG	13	1735	1/1	0.97	0.04	109,109,109,109	0
56	MG	1H	3327	1/1	0.97	0.09	68,68,68,68	0
56	MG	1H	3056	1/1	0.97	0.14	28,28,28,28	0
56	MG	14	3259	1/1	0.97	0.06	57,57,57,57	0
56	MG	13	1757	1/1	0.98	0.12	84,84,84,84	0
56	MG	14	3303	1/1	0.98	0.04	68,68,68,68	0
56	MG	1H	3465	1/1	0.98	0.04	58,58,58,58	0
56	MG	14	3306	1/1	0.98	0.17	76,76,76,76	0
56	MG	1H	3373	1/1	0.98	0.12	100,100,100,100	0
56	MG	14	3309	1/1	0.98	0.04	76,76,76,76	0
56	MG	13	1692	1/1	0.98	0.04	79,79,79,79	0
56	MG	1H	3376	1/1	0.98	0.05	50,50,50,50	0
56	MG	14	3312	1/1	0.98	0.08	47,47,47,47	0
56	MG	13	1726	1/1	0.98	0.04	64,64,64,64	0
56	MG	1H	3378	1/1	0.98	0.06	83,83,83,83	0
56	MG	16	207	1/1	0.98	0.04	60,60,60,60	0
56	MG	1H	3472	1/1	0.98	0.04	82,82,82,82	0
56	MG	14	3317	1/1	0.98	0.11	119,119,119,119	0
56	MG	16	209	1/1	0.98	0.04	67,67,67,67	0
56	MG	1G	1671	1/1	0.98	0.05	82,82,82,82	0
56	MG	13	1760	1/1	0.98	0.04	113,113,113,113	0
56	MG	1G	1673	1/1	0.98	0.08	86,86,86,86	0
56	MG	14	3323	1/1	0.98	0.04	57,57,57,57	0
56	MG	1H	3291	1/1	0.98	0.06	44,44,44,44	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	1G	1676	1/1	0.98	0.12	97,97,97,97	0
56	MG	14	3060	1/1	0.98	0.06	47,47,47,47	0
56	MG	16	212	1/1	0.98	0.07	68,68,68,68	0
56	MG	14	3329	1/1	0.98	0.07	54,54,54,54	0
56	MG	16	213	1/1	0.98	0.08	87,87,87,87	0
56	MG	1G	1679	1/1	0.98	0.04	70,70,70,70	0
56	MG	1H	3387	1/1	0.98	0.04	96,96,96,96	0
56	MG	1H	3206	1/1	0.98	0.07	53,53,53,53	0
56	MG	13	1727	1/1	0.98	0.07	87,87,87,87	0
56	MG	1G	1685	1/1	0.98	0.06	63,63,63,63	0
56	MG	14	3337	1/1	0.98	0.07	70,70,70,70	0
56	MG	1H	3391	1/1	0.98	0.04	56,56,56,56	0
56	MG	14	3070	1/1	0.98	0.10	49,49,49,49	0
56	MG	41	201	1/1	0.98	0.06	62,62,62,62	0
56	MG	1H	3486	1/1	0.98	0.09	95,95,95,95	0
56	MG	1H	3487	1/1	0.98	0.10	71,71,71,71	0
56	MG	1G	1693	1/1	0.98	0.05	114,114,114,114	0
56	MG	78	202	1/1	0.98	0.08	63,63,63,63	0
56	MG	1H	3395	1/1	0.98	0.04	47,47,47,47	0
56	MG	14	3352	1/1	0.98	0.04	66,66,66,66	0
56	MG	1H	3036	1/1	0.98	0.11	45,45,45,45	0
56	MG	1H	3295	1/1	0.98	0.05	55,55,55,55	0
56	MG	1H	3493	1/1	0.98	0.06	87,87,87,87	0
56	MG	1H	3400	1/1	0.98	0.06	48,48,48,48	0
56	MG	14	3359	1/1	0.98	0.09	57,57,57,57	0
56	MG	13	1729	1/1	0.98	0.10	88,88,88,88	0
56	MG	14	3362	1/1	0.98	0.08	65,65,65,65	0
56	MG	1H	3402	1/1	0.98	0.05	40,40,40,40	0
56	MG	14	3364	1/1	0.98	0.07	83,83,83,83	0
56	MG	14	3366	1/1	0.98	0.05	65,65,65,65	0
56	MG	1H	3303	1/1	0.98	0.11	57,57,57,57	0
56	MG	14	3372	1/1	0.98	0.04	45,45,45,45	0
56	MG	1G	1707	1/1	0.98	0.08	114,114,114,114	0
56	MG	14	3374	1/1	0.98	0.04	68,68,68,68	0
56	MG	14	3375	1/1	0.98	0.07	87,87,87,87	0
56	MG	1H	3237	1/1	0.98	0.04	41,41,41,41	0
56	MG	14	3377	1/1	0.98	0.05	77,77,77,77	0
56	MG	14	3378	1/1	0.98	0.04	96,96,96,96	0
56	MG	1H	3500	1/1	0.98	0.04	103,103,103,103	0
56	MG	14	3381	1/1	0.98	0.06	101,101,101,101	0
56	MG	1H	3408	1/1	0.98	0.06	42,42,42,42	0
56	MG	1G	1711	1/1	0.98	0.04	102,102,102,102	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	1H	3502	1/1	0.98	0.04	87,87,87,87	0
56	MG	1H	3310	1/1	0.98	0.05	43,43,43,43	0
56	MG	1G	1714	1/1	0.98	0.04	101,101,101,101	0
56	MG	1G	1715	1/1	0.98	0.05	116,116,116,116	0
56	MG	1H	3410	1/1	0.98	0.05	57,57,57,57	0
56	MG	1G	1718	1/1	0.98	0.05	89,89,89,89	0
56	MG	1H	3038	1/1	0.98	0.04	70,70,70,70	0
56	MG	1H	3508	1/1	0.98	0.06	37,37,37,37	0
56	MG	1G	1721	1/1	0.98	0.09	84,84,84,84	0
56	MG	14	3397	1/1	0.98	0.04	95,95,95,95	0
56	MG	1H	3412	1/1	0.98	0.05	39,39,39,39	0
56	MG	14	3399	1/1	0.98	0.04	82,82,82,82	0
56	MG	13	1703	1/1	0.98	0.04	75,75,75,75	0
56	MG	14	3401	1/1	0.98	0.04	75,75,75,75	0
56	MG	14	3402	1/1	0.98	0.04	94,94,94,94	0
56	MG	1H	3516	1/1	0.98	0.06	81,81,81,81	0
56	MG	14	3406	1/1	0.98	0.16	86,86,86,86	0
56	MG	1H	3517	1/1	0.98	0.07	84,84,84,84	0
56	MG	1H	3416	1/1	0.98	0.05	70,70,70,70	0
56	MG	32	301	1/1	0.98	0.06	112,112,112,112	0
56	MG	14	3411	1/1	0.98	0.05	101,101,101,101	0
56	MG	13	1745	1/1	0.98	0.03	99,99,99,99	0
56	MG	1H	3109	1/1	0.98	0.17	34,34,34,34	0
56	MG	14	3414	1/1	0.98	0.04	78,78,78,78	0
56	MG	1H	3317	1/1	0.98	0.07	63,63,63,63	0
56	MG	14	3419	1/1	0.98	0.07	97,97,97,97	0
56	MG	14	3420	1/1	0.98	0.08	66,66,66,66	0
56	MG	14	3421	1/1	0.98	0.04	84,84,84,84	0
56	MG	2A	201	1/1	0.98	0.09	103,103,103,103	0
56	MG	14	3423	1/1	0.98	0.06	52,52,52,52	0
56	MG	1H	3523	1/1	0.98	0.13	76,76,76,76	0
56	MG	2L	102	1/1	0.98	0.06	88,88,88,88	0
56	MG	1H	3319	1/1	0.98	0.05	51,51,51,51	0
56	MG	14	3430	1/1	0.98	0.07	86,86,86,86	0
56	MG	14	3001	1/1	0.98	0.05	51,51,51,51	0
56	MG	1H	3525	1/1	0.98	0.16	71,71,71,71	0
56	MG	13	1731	1/1	0.98	0.08	83,83,83,83	0
56	MG	14	3434	1/1	0.98	0.05	77,77,77,77	0
56	MG	1H	3527	1/1	0.98	0.04	86,86,86,86	0
56	MG	1H	3529	1/1	0.98	0.04	102,102,102,102	0
56	MG	1H	3325	1/1	0.98	0.10	56,56,56,56	0
56	MG	14	3007	1/1	0.98	0.04	55,55,55,55	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	2K	102	1/1	0.98	0.08	83,83,83,83	0
56	MG	14	3441	1/1	0.98	0.04	95,95,95,95	0
56	MG	13	1717	1/1	0.98	0.06	51,51,51,51	0
56	MG	13	1699	1/1	0.98	0.05	75,75,75,75	0
56	MG	1H	3430	1/1	0.98	0.04	46,46,46,46	0
56	MG	14	3445	1/1	0.98	0.09	89,89,89,89	0
56	MG	1H	3139	1/1	0.98	0.10	52,52,52,52	0
56	MG	1H	3333	1/1	0.98	0.05	53,53,53,53	0
56	MG	14	3448	1/1	0.98	0.17	72,72,72,72	0
56	MG	14	3014	1/1	0.98	0.11	64,64,64,64	0
56	MG	14	3450	1/1	0.98	0.04	100,100,100,100	0
56	MG	1H	3434	1/1	0.98	0.06	47,47,47,47	0
56	MG	14	3453	1/1	0.98	0.04	102,102,102,102	0
56	MG	1H	3541	1/1	0.98	0.04	85,85,85,85	0
56	MG	1H	3542	1/1	0.98	0.05	81,81,81,81	0
56	MG	14	3456	1/1	0.98	0.07	99,99,99,99	0
56	MG	1H	3334	1/1	0.98	0.06	59,59,59,59	0
56	MG	14	3458	1/1	0.98	0.12	91,91,91,91	0
56	MG	1H	3335	1/1	0.98	0.04	77,77,77,77	0
56	MG	1H	3336	1/1	0.98	0.08	86,86,86,86	0
56	MG	1H	3339	1/1	0.98	0.04	41,41,41,41	0
56	MG	1H	3441	1/1	0.98	0.08	76,76,76,76	0
56	MG	1H	3548	1/1	0.98	0.07	98,98,98,98	0
56	MG	13	1711	1/1	0.98	0.08	101,101,101,101	0
56	MG	14	3135	1/1	0.98	0.04	59,59,59,59	0
56	MG	14	3246	1/1	0.98	0.11	57,57,57,57	0
56	MG	1H	3550	1/1	0.98	0.14	125,125,125,125	0
56	MG	14	3249	1/1	0.98	0.04	64,64,64,64	0
56	MG	13	1722	1/1	0.98	0.04	78,78,78,78	0
56	MG	1H	3552	1/1	0.98	0.15	73,73,73,73	0
56	MG	1H	3116	1/1	0.98	0.03	64,64,64,64	0
56	MG	1H	3446	1/1	0.98	0.06	64,64,64,64	0
56	MG	14	3258	1/1	0.98	0.07	52,52,52,52	0
56	MG	13	1751	1/1	0.98	0.09	76,76,76,76	0
56	MG	14	3260	1/1	0.98	0.04	52,52,52,52	0
56	MG	14	3261	1/1	0.98	0.04	57,57,57,57	0
56	MG	13	1705	1/1	0.98	0.04	102,102,102,102	0
56	MG	14	3267	1/1	0.98	0.04	50,50,50,50	0
56	MG	1H	3558	1/1	0.98	0.03	99,99,99,99	0
56	MG	1H	3355	1/1	0.98	0.04	40,40,40,40	0
56	MG	1H	3356	1/1	0.98	0.09	64,64,64,64	0
56	MG	14	3271	1/1	0.98	0.05	60,60,60,60	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	1H	3561	1/1	0.98	0.05	87,87,87,87	0
56	MG	14	3275	1/1	0.98	0.05	47,47,47,47	0
56	MG	14	3282	1/1	0.98	0.04	92,92,92,92	0
56	MG	25	202	1/1	0.98	0.05	108,108,108,108	0
56	MG	13	1737	1/1	0.98	0.04	83,83,83,83	0
56	MG	1H	3072	1/1	0.98	0.13	33,33,33,33	0
56	MG	1H	3564	1/1	0.98	0.04	95,95,95,95	0
56	MG	14	3293	1/1	0.98	0.07	94,94,94,94	0
56	MG	14	3294	1/1	0.98	0.05	59,59,59,59	0
56	MG	1H	3007	1/1	0.98	0.11	60,60,60,60	0
56	MG	1H	3566	1/1	0.98	0.04	105,105,105,105	0
56	MG	1H	3567	1/1	0.98	0.05	42,42,42,42	0
56	MG	13	1755	1/1	0.98	0.04	101,101,101,101	0
57	SF4	3E	301	8/8	0.98	0.03	75,82,92,93	0
56	MG	1H	3569	1/1	0.98	0.07	85,85,85,85	0
56	MG	13	1738	1/1	0.98	0.07	71,71,71,71	0
56	MG	14	3325	1/1	0.99	0.05	66,66,66,66	0
56	MG	1H	3462	1/1	0.99	0.03	66,66,66,66	0
56	MG	1H	3380	1/1	0.99	0.04	69,69,69,69	0
56	MG	1G	1674	1/1	0.99	0.05	97,97,97,97	0
56	MG	1H	3464	1/1	0.99	0.04	40,40,40,40	0
56	MG	1H	3381	1/1	0.99	0.02	74,74,74,74	0
56	MG	1H	3571	1/1	0.99	0.03	39,39,39,39	0
56	MG	14	3332	1/1	0.99	0.06	70,70,70,70	0
56	MG	1H	3466	1/1	0.99	0.08	74,74,74,74	0
56	MG	1H	3382	1/1	0.99	0.05	70,70,70,70	0
56	MG	1G	1680	1/1	0.99	0.07	68,68,68,68	0
56	MG	1H	3383	1/1	0.99	0.03	61,61,61,61	0
56	MG	1H	3384	1/1	0.99	0.05	77,77,77,77	0
56	MG	14	3338	1/1	0.99	0.05	83,83,83,83	0
56	MG	14	3339	1/1	0.99	0.04	73,73,73,73	0
56	MG	1G	1683	1/1	0.99	0.03	89,89,89,89	0
56	MG	14	3069	1/1	0.99	0.02	47,47,47,47	0
56	MG	14	3343	1/1	0.99	0.02	42,42,42,42	0
56	MG	14	3344	1/1	0.99	0.04	56,56,56,56	0
56	MG	1H	3385	1/1	0.99	0.03	74,74,74,74	0
56	MG	1H	3321	1/1	0.99	0.04	59,59,59,59	0
56	MG	1G	1686	1/1	0.99	0.03	90,90,90,90	0
56	MG	1H	3322	1/1	0.99	0.11	67,67,67,67	0
56	MG	1H	3324	1/1	0.99	0.04	70,70,70,70	0
56	MG	1H	3474	1/1	0.99	0.07	79,79,79,79	0
56	MG	14	3351	1/1	0.99	0.05	54,54,54,54	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	1G	1690	1/1	0.99	0.03	90,90,90,90	0
56	MG	1H	3475	1/1	0.99	0.07	73,73,73,73	0
56	MG	1G	1692	1/1	0.99	0.03	106,106,106,106	0
56	MG	1H	3476	1/1	0.99	0.04	91,91,91,91	0
56	MG	1H	3389	1/1	0.99	0.06	46,46,46,46	0
56	MG	14	3358	1/1	0.99	0.05	76,76,76,76	0
56	MG	1H	3478	1/1	0.99	0.05	78,78,78,78	0
56	MG	13	1690	1/1	0.99	0.05	56,56,56,56	0
56	MG	14	3361	1/1	0.99	0.03	41,41,41,41	0
56	MG	1H	3480	1/1	0.99	0.07	66,66,66,66	0
56	MG	1H	3481	1/1	0.99	0.03	59,59,59,59	0
56	MG	1G	1699	1/1	0.99	0.04	86,86,86,86	0
56	MG	14	3365	1/1	0.99	0.03	44,44,44,44	0
56	MG	11	303	1/1	0.99	0.03	49,49,49,49	0
56	MG	14	3367	1/1	0.99	0.04	75,75,75,75	0
56	MG	1G	1701	1/1	0.99	0.06	106,106,106,106	0
56	MG	14	3369	1/1	0.99	0.05	93,93,93,93	0
56	MG	14	3370	1/1	0.99	0.09	83,83,83,83	0
56	MG	14	3371	1/1	0.99	0.09	75,75,75,75	0
56	MG	13	1753	1/1	0.99	0.05	64,64,64,64	0
56	MG	1H	3483	1/1	0.99	0.12	76,76,76,76	0
56	MG	1G	1704	1/1	0.99	0.06	99,99,99,99	0
56	MG	1H	3392	1/1	0.99	0.03	63,63,63,63	0
56	MG	1G	1706	1/1	0.99	0.07	82,82,82,82	0
56	MG	1H	3393	1/1	0.99	0.08	61,61,61,61	0
56	MG	1H	3394	1/1	0.99	0.04	40,40,40,40	0
56	MG	1H	3289	1/1	0.99	0.05	48,48,48,48	0
56	MG	14	3380	1/1	0.99	0.05	95,95,95,95	0
56	MG	1H	3396	1/1	0.99	0.03	41,41,41,41	0
56	MG	14	3382	1/1	0.99	0.04	47,47,47,47	0
56	MG	1H	3489	1/1	0.99	0.07	87,87,87,87	0
56	MG	1H	3328	1/1	0.99	0.10	48,48,48,48	0
56	MG	1H	3329	1/1	0.99	0.03	41,41,41,41	0
56	MG	14	3386	1/1	0.99	0.07	81,81,81,81	0
56	MG	1H	3492	1/1	0.99	0.07	74,74,74,74	0
56	MG	I8	101	1/1	0.99	0.08	55,55,55,55	0
56	MG	14	3389	1/1	0.99	0.04	82,82,82,82	0
56	MG	1G	1716	1/1	0.99	0.06	88,88,88,88	0
56	MG	1H	3330	1/1	0.99	0.02	46,46,46,46	0
56	MG	1H	3494	1/1	0.99	0.03	53,53,53,53	0
56	MG	1H	3290	1/1	0.99	0.07	40,40,40,40	0
56	MG	14	3394	1/1	0.99	0.09	63,63,63,63	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	13	1697	1/1	0.99	0.03	91,91,91,91	0
56	MG	1H	3403	1/1	0.99	0.04	71,71,71,71	0
56	MG	13	1739	1/1	0.99	0.04	79,79,79,79	0
56	MG	1H	3406	1/1	0.99	0.13	52,52,52,52	0
56	MG	1H	3004	1/1	0.99	0.07	46,46,46,46	0
56	MG	13	1725	1/1	0.99	0.10	65,65,65,65	0
56	MG	13	1698	1/1	0.99	0.08	98,98,98,98	0
56	MG	1H	3338	1/1	0.99	0.06	45,45,45,45	0
56	MG	14	3403	1/1	0.99	0.11	80,80,80,80	0
56	MG	14	3404	1/1	0.99	0.03	77,77,77,77	0
56	MG	1H	3024	1/1	0.99	0.06	47,47,47,47	0
56	MG	1H	3297	1/1	0.99	0.04	52,52,52,52	0
56	MG	1H	3506	1/1	0.99	0.02	58,58,58,58	0
56	MG	1H	3507	1/1	0.99	0.05	84,84,84,84	0
56	MG	1H	3413	1/1	0.99	0.03	59,59,59,59	0
56	MG	1H	3414	1/1	0.99	0.08	68,68,68,68	0
56	MG	1H	3510	1/1	0.99	0.06	92,92,92,92	0
56	MG	1H	3511	1/1	0.99	0.04	78,78,78,78	0
56	MG	1H	3512	1/1	0.99	0.04	60,60,60,60	0
56	MG	14	3415	1/1	0.99	0.03	78,78,78,78	0
56	MG	14	3416	1/1	0.99	0.05	80,80,80,80	0
56	MG	1H	3299	1/1	0.99	0.06	35,35,35,35	0
56	MG	14	3418	1/1	0.99	0.11	75,75,75,75	0
56	MG	1H	3514	1/1	0.99	0.04	69,69,69,69	0
56	MG	1H	3515	1/1	0.99	0.14	57,57,57,57	0
56	MG	1H	3343	1/1	0.99	0.07	39,39,39,39	0
56	MG	1H	3344	1/1	0.99	0.02	42,42,42,42	0
56	MG	14	3248	1/1	0.99	0.06	47,47,47,47	0
56	MG	1H	3301	1/1	0.99	0.03	42,42,42,42	0
56	MG	14	3250	1/1	0.99	0.04	55,55,55,55	0
56	MG	14	3427	1/1	0.99	0.12	69,69,69,69	0
56	MG	14	3428	1/1	0.99	0.11	59,59,59,59	0
56	MG	1H	3347	1/1	0.99	0.05	72,72,72,72	0
56	MG	1H	3302	1/1	0.99	0.06	52,52,52,52	0
56	MG	1H	3350	1/1	0.99	0.02	43,43,43,43	0
56	MG	1H	3422	1/1	0.99	0.04	42,42,42,42	0
56	MG	14	3256	1/1	0.99	0.03	65,65,65,65	0
56	MG	14	3257	1/1	0.99	0.03	42,42,42,42	0
56	MG	1H	3423	1/1	0.99	0.07	33,33,33,33	0
56	MG	1H	3351	1/1	0.99	0.03	50,50,50,50	0
56	MG	1H	3425	1/1	0.99	0.03	39,39,39,39	0
56	MG	1H	3352	1/1	0.99	0.03	57,57,57,57	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	14	3439	1/1	0.99	0.10	86,86,86,86	0
56	MG	14	3262	1/1	0.99	0.04	54,54,54,54	0
56	MG	1H	3528	1/1	0.99	0.09	72,72,72,72	0
56	MG	14	3264	1/1	0.99	0.04	59,59,59,59	0
56	MG	13	1714	1/1	0.99	0.03	59,59,59,59	0
56	MG	1H	3354	1/1	0.99	0.04	45,45,45,45	0
56	MG	1H	3531	1/1	0.99	0.14	56,56,56,56	0
56	MG	1H	3429	1/1	0.99	0.04	49,49,49,49	0
56	MG	13	1728	1/1	0.99	0.04	77,77,77,77	0
56	MG	1H	3306	1/1	0.99	0.03	38,38,38,38	0
56	MG	14	3273	1/1	0.99	0.06	55,55,55,55	0
56	MG	14	3274	1/1	0.99	0.06	50,50,50,50	0
56	MG	1H	3535	1/1	0.99	0.04	70,70,70,70	0
56	MG	14	3452	1/1	0.99	0.03	90,90,90,90	0
56	MG	14	3276	1/1	0.99	0.03	56,56,56,56	0
56	MG	14	3278	1/1	0.99	0.04	50,50,50,50	0
56	MG	14	3279	1/1	0.99	0.10	45,45,45,45	0
56	MG	14	3280	1/1	0.99	0.04	47,47,47,47	0
56	MG	1H	3357	1/1	0.99	0.02	66,66,66,66	0
56	MG	14	3283	1/1	0.99	0.05	79,79,79,79	0
56	MG	1H	3433	1/1	0.99	0.04	37,37,37,37	0
56	MG	14	3285	1/1	0.99	0.02	55,55,55,55	0
56	MG	14	3286	1/1	0.99	0.03	68,68,68,68	0
56	MG	14	3287	1/1	0.99	0.10	71,71,71,71	0
56	MG	14	3288	1/1	0.99	0.05	76,76,76,76	0
56	MG	14	3289	1/1	0.99	0.07	64,64,64,64	0
56	MG	1H	3359	1/1	0.99	0.06	59,59,59,59	0
56	MG	1H	3539	1/1	0.99	0.05	90,90,90,90	0
56	MG	14	3292	1/1	0.99	0.10	63,63,63,63	0
56	MG	1H	3307	1/1	0.99	0.03	50,50,50,50	0
56	MG	1H	3436	1/1	0.99	0.06	64,64,64,64	0
56	MG	14	3295	1/1	0.99	0.03	73,73,73,73	0
56	MG	1H	3437	1/1	0.99	0.03	62,62,62,62	0
56	MG	1H	3308	1/1	0.99	0.08	49,49,49,49	0
56	MG	13	1715	1/1	0.99	0.04	94,94,94,94	0
56	MG	1H	3364	1/1	0.99	0.04	51,51,51,51	0
56	MG	1H	3365	1/1	0.99	0.07	50,50,50,50	0
56	MG	13	1693	1/1	0.99	0.02	80,80,80,80	0
56	MG	1H	3443	1/1	0.99	0.04	72,72,72,72	0
56	MG	1H	3368	1/1	0.99	0.03	49,49,49,49	0
56	MG	13	1700	1/1	0.99	0.04	64,64,64,64	0
56	MG	1H	3370	1/1	0.99	0.03	37,37,37,37	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	14	3307	1/1	0.99	0.16	60,60,60,60	0
56	MG	1J	211	1/1	0.99	0.03	85,85,85,85	0
56	MG	1H	3371	1/1	0.99	0.07	64,64,64,64	0
56	MG	1H	3553	1/1	0.99	0.05	78,78,78,78	0
56	MG	1H	3314	1/1	0.99	0.06	74,74,74,74	0
56	MG	13	1708	1/1	0.99	0.04	80,80,80,80	0
56	MG	1H	3374	1/1	0.99	0.08	68,68,68,68	0
56	MG	13	1709	1/1	0.99	0.07	68,68,68,68	0
56	MG	1H	3453	1/1	0.99	0.05	81,81,81,81	0
56	MG	13	1720	1/1	0.99	0.08	66,66,66,66	0
56	MG	1H	3318	1/1	0.99	0.03	72,72,72,72	0
56	MG	45	202	1/1	0.99	0.11	66,66,66,66	0
56	MG	13	1721	1/1	0.99	0.02	82,82,82,82	0
56	MG	1H	3457	1/1	0.99	0.02	78,78,78,78	0
56	MG	1H	3458	1/1	0.99	0.06	56,56,56,56	0
56	MG	14	3320	1/1	0.99	0.06	79,79,79,79	0
56	MG	1H	3459	1/1	0.99	0.05	69,69,69,69	0
56	MG	1H	3460	1/1	0.99	0.07	75,75,75,75	0
57	SF4	32	302	8/8	0.99	0.04	99,104,114,118	0
58	ZN	5I	102	1/1	0.99	0.02	87,87,87,87	0
56	MG	1G	1670	1/1	0.99	0.06	71,71,71,71	0
58	ZN	5A	101	1/1	0.99	0.04	130,130,130,130	0
56	MG	13	1694	1/1	0.99	0.06	79,79,79,79	0
56	MG	1H	3337	1/1	1.00	0.03	41,41,41,41	0
56	MG	14	3304	1/1	1.00	0.04	64,64,64,64	0
56	MG	14	3255	1/1	1.00	0.03	42,42,42,42	0
56	MG	1H	3349	1/1	1.00	0.02	42,42,42,42	0
56	MG	14	3281	1/1	1.00	0.04	69,69,69,69	0
56	MG	1H	3298	1/1	1.00	0.03	46,46,46,46	0
56	MG	13	1702	1/1	1.00	0.04	64,64,64,64	0
56	MG	1H	3323	1/1	1.00	0.03	64,64,64,64	0
56	MG	1H	3367	1/1	1.00	0.03	40,40,40,40	0
56	MG	1H	3521	1/1	1.00	0.07	79,79,79,79	0
56	MG	1H	3309	1/1	1.00	0.03	47,47,47,47	0
56	MG	14	3340	1/1	1.00	0.02	54,54,54,54	0
56	MG	14	3426	1/1	1.00	0.06	75,75,75,75	0
56	MG	1H	3450	1/1	1.00	0.08	45,45,45,45	0
56	MG	1H	3399	1/1	1.00	0.02	52,52,52,52	0
56	MG	14	3265	1/1	1.00	0.04	51,51,51,51	0
56	MG	14	3266	1/1	1.00	0.07	43,43,43,43	0
56	MG	1H	3342	1/1	1.00	0.01	44,44,44,44	0
56	MG	1H	3304	1/1	1.00	0.03	42,42,42,42	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	1H	3300	1/1	1.00	0.03	41,41,41,41	0
56	MG	13	1696	1/1	1.00	0.07	72,72,72,72	0
56	MG	1H	3404	1/1	1.00	0.03	45,45,45,45	0
56	MG	1H	3358	1/1	1.00	0.06	78,78,78,78	0
56	MG	1H	3346	1/1	1.00	0.07	60,60,60,60	0
56	MG	1H	3313	1/1	1.00	0.10	58,58,58,58	0
56	MG	14	3409	1/1	1.00	0.03	73,73,73,73	0
56	MG	1H	3361	1/1	1.00	0.08	56,56,56,56	0
56	MG	21	303	1/1	1.00	0.02	42,42,42,42	0
56	MG	14	3355	1/1	1.00	0.07	52,52,52,52	0
56	MG	14	3277	1/1	1.00	0.02	57,57,57,57	0

5.5 Other polymers (i)

There are no such residues in this entry.