



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 20, 2026 – 08:00 AM UTC

PDB ID : 8CRE / pdb_00008cre
Title : Crystal structure of the Candida albicans 80S ribosome in complex with geneticin G418
Authors : Kolosova, O.; Zgadzay, Y.; Yusupov, M.
Deposited on : 2023-03-08
Resolution : 3.00 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : **FAILED**
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

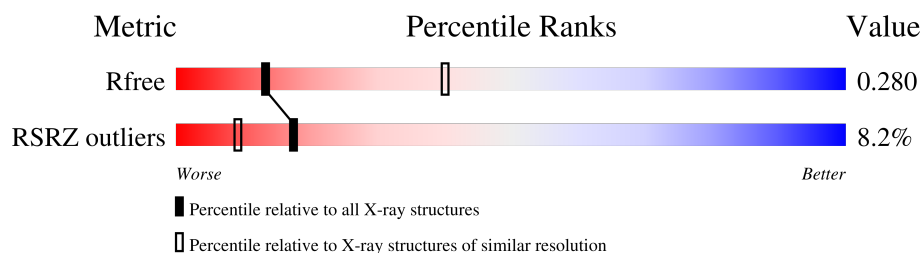
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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	2672 (3.00-3.00)
RSRZ outliers	180081	2671 (3.00-3.00)

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
83	MG	9	202	-	-	-	X
83	MG	AS	3421	-	-	-	X
83	MG	AS	3434	-	-	-	X
83	MG	AS	3522	-	-	-	X
83	MG	B	1839	-	-	-	X
83	MG	B	1876	-	-	-	X
83	MG	B	1892	-	-	-	X
83	MG	CL	302	-	-	-	X

2 Entry composition [i](#)

There are 87 unique types of molecules in this entry. The entry contains 409812 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 25S.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	1	3216	Total	C	N	O	P	0	0	0
			68751	30713	12360	22462	3216			
1	AS	3229	Total	C	N	O	P	0	0	0
			69025	30835	12406	22555	3229			

- Molecule 2 is a RNA chain called 5S.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	3	121	Total	C	N	O	P	0	0	0
			2579	1153	463	842	121			
2	AT	121	Total	C	N	O	P	0	0	0
			2579	1153	463	842	121			

- Molecule 3 is a RNA chain called 5.8S.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	4	157	Total	C	N	O	P	0	0	0
			3333	1491	583	1102	157			
3	AU	158	Total	C	N	O	P	0	0	0
			3353	1500	585	1110	158			

- Molecule 4 is a protein called 60S ribosomal protein L2-B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	j	249	Total	C	N	O	S	0	0	0
			1888	1180	376	330	2			
4	AW	249	Total	C	N	O	S	0	0	0
			1888	1180	376	330	2			

- Molecule 5 is a protein called 60S ribosomal protein L3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	k	386	Total	C	N	O	S	0	0	0
			3077	1950	582	538	7			
5	AX	386	Total	C	N	O	S	0	0	0
			3077	1950	582	538	7			

- Molecule 6 is a protein called 60S ribosomal protein L4-B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	l	361	Total	C	N	O	S	0	0	0
			2751	1729	529	490	3			
6	AY	361	Total	C	N	O	S	0	0	0
			2751	1729	529	490	3			

- Molecule 7 is a protein called Uncharacterized protein CaJ7.0206.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	m	296	Total	C	N	O	S	0	0	0
			2426	1544	422	458	2			
7	AZ	292	Total	C	N	O	S	0	0	0
			2394	1526	416	450	2			

- Molecule 8 is a protein called 60S ribosomal protein L6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	n	157	Total	C	N	O	S	0	0	0
			1242	796	226	219	1			
8	BA	153	Total	C	N	O		0	0	0
			1210	777	221	212				

- Molecule 9 is a protein called 60S ribosomal protein L7-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	o	234	Total	C	N	O	S	0	0	0
			1885	1208	345	331	1			
9	BB	234	Total	C	N	O	S	0	0	0
			1885	1208	345	331	1			

- Molecule 10 is a protein called 60S ribosomal protein L8.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	p	238	Total	C	N	O	S	0	0	0
			1839	1175	327	334	3			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	BC	233	Total	C	N	O	S	0	0	0
			1805	1156	321	325	3			

- Molecule 11 is a protein called 60S ribosomal protein L9-B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	q	190	Total	C	N	O	S	0	0	0
			1519	958	276	281	4			
11	BD	190	Total	C	N	O	S	0	0	0
			1519	958	276	281	4			

- Molecule 12 is a protein called 60S ribosomal protein L10.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	r	208	Total	C	N	O	S	0	0	0
			1689	1069	322	291	7			
12	BE	208	Total	C	N	O	S	0	0	0
			1689	1069	322	291	7			

- Molecule 13 is a protein called 60S ribosomal protein L11-B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	s	171	Total	C	N	O	S	0	0	0
			1371	857	260	250	4			
13	BF	171	Total	C	N	O	S	0	0	0
			1371	857	260	250	4			

- Molecule 14 is a protein called 60S ribosomal protein L13.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
14	t	200	Total	C	N	O	0	0	0
			1610	1009	318	283			
14	BG	200	Total	C	N	O	0	0	0
			1610	1009	318	283			

- Molecule 15 is a protein called 60S ribosomal protein L14-B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	u	130	Total	C	N	O	S	0	0	0
			1029	660	193	175	1			
15	BH	130	Total	C	N	O	S	0	0	0
			1029	660	193	175	1			

- Molecule 16 is a protein called 60S ribosomal protein L15-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	v	203	Total	C	N	O	S	0	0	0
			1713	1075	356	280	2			
16	BI	203	Total	C	N	O	S	0	0	0
			1713	1075	356	280	2			

- Molecule 17 is a protein called Ribosomal protein L13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	w	199	Total	C	N	O	S	0	0	0
			1590	1025	294	269	2			
17	BJ	199	Total	C	N	O	S	0	0	0
			1590	1025	294	269	2			

- Molecule 18 is a protein called Ribosomal protein L22.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
18	x	173	Total	C	N	O	0	0	0
			1387	856	280	251			
18	BK	176	Total	C	N	O	0	0	0
			1406	868	284	254			

- Molecule 19 is a protein called 60S ribosomal protein L18-A.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
19	y	185	Total	C	N	O	0	0	0
			1458	916	297	245			
19	BL	185	Total	C	N	O	0	0	0
			1458	916	297	245			

- Molecule 20 is a protein called 60S ribosomal protein L19-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	z	179	Total	C	N	O	S	0	0	0
			1457	901	310	243	3			
20	BM	179	Total	C	N	O	S	0	0	0
			1457	901	310	243	3			

- Molecule 21 is a protein called 60S ribosomal protein L20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
21	0	170	Total	C	N	O	S	0	0	0
			1423	921	258	241	3			
21	BN	170	Total	C	N	O	S	0	0	0
			1423	921	258	241	3			

- Molecule 22 is a protein called 60S ribosomal protein L21-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	2	159	Total	C	N	O	S	0	0	0
			1262	798	241	221	2			
22	BO	159	Total	C	N	O	S	0	0	0
			1262	798	241	221	2			

- Molecule 23 is a protein called 60S ribosomal protein L22-B.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
23	5	103	Total	C	N	O	0	0	0
			831	539	138	154			
23	BP	102	Total	C	N	O	0	0	0
			826	536	137	153			

- Molecule 24 is a protein called 60S ribosomal protein L23-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	6	131	Total	C	N	O	S	0	0	0
			977	615	183	171	8			
24	BQ	131	Total	C	N	O	S	0	0	0
			977	615	183	171	8			

- Molecule 25 is a protein called 60S ribosomal protein L24-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
25	7	118	Total	C	N	O	S	0	0	0
			945	591	192	161	1			
25	BR	98	Total	C	N	O	S	0	0	0
			801	501	162	137	1			

- Molecule 26 is a protein called 60S ribosomal protein L25.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	8	121	Total	C	N	O	S	0	0	0
			974	622	175	176	1			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	BS	119	Total	C	N	O	S	0	0	0
			960	613	172	174	1			

- Molecule 27 is a protein called Ribosomal protein L24.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
27	9	126	Total	C	N	O		0	0	0
			989	618	190	181				
27	BT	126	Total	C	N	O		0	0	0
			989	618	190	181				

- Molecule 28 is a protein called 60S ribosomal protein L27.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
28	AA	135	Total	C	N	O	S	0	0	0
			1087	705	197	183	2			
28	BU	135	Total	C	N	O	S	0	0	0
			1087	705	197	183	2			

- Molecule 29 is a protein called 60S ribosomal protein L28.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
29	AB	148	Total	C	N	O	S	0	0	0
			1170	741	231	197	1			
29	BV	148	Total	C	N	O	S	0	0	0
			1170	741	231	197	1			

- Molecule 30 is a protein called 60S ribosomal protein L29.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
30	AC	62	Total	C	N	O		0	0	0
			493	307	105	81				
30	BW	61	Total	C	N	O		0	0	0
			488	304	104	80				

- Molecule 31 is a protein called 60S ribosomal protein L30.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
31	AD	96	Total	C	N	O	S	0	0	0
			729	469	121	137	2			
31	BX	96	Total	C	N	O	S	0	0	0
			729	469	121	137	2			

- Molecule 32 is a protein called 60S ribosomal protein L31-B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
32	AE	110	Total	C	N	O	S	0	0	0
			894	565	168	159	2			
32	BY	110	Total	C	N	O	S	0	0	0
			894	565	168	159	2			

- Molecule 33 is a protein called 60S ribosomal protein L32.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
33	AF	124	Total	C	N	O	S	0	0	0
			1000	638	194	167	1			
33	BZ	124	Total	C	N	O	S	0	0	0
			1004	641	195	167	1			

- Molecule 34 is a protein called 60S ribosomal protein L33-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
34	AG	106	Total	C	N	O	S	0	0	0
			847	543	161	142	1			
34	CA	106	Total	C	N	O	S	0	0	0
			847	543	161	142	1			

- Molecule 35 is a protein called 60S ribosomal protein L34-B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
35	AH	112	Total	C	N	O	S	0	0	0
			887	547	182	154	4			
35	CB	112	Total	C	N	O	S	0	0	0
			887	547	182	154	4			

- Molecule 36 is a protein called Ribosomal protein L29.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
36	AI	120	Total	C	N	O	S	0	0	0
			992	629	195	167	1			
36	CC	118	Total	C	N	O		0	0	0
			979	621	193	165				

- Molecule 37 is a protein called 60S ribosomal protein L36.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
37	AJ	97	Total	C	N	O	S	0	0	0
			758	471	156	130	1			
37	CD	97	Total	C	N	O	S	0	0	0
			758	471	156	130	1			

- Molecule 38 is a protein called 60S ribosomal protein L37-B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
38	AK	86	Total	C	N	O	S	0	0	0
			677	413	148	110	6			
38	CE	86	Total	C	N	O	S	0	0	0
			677	413	148	110	6			

- Molecule 39 is a protein called 60S ribosomal protein L38.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
39	AL	77	Total	C	N	O	0	0	0
			617	393	115	109			
39	CF	77	Total	C	N	O	0	0	0
			617	393	115	109			

- Molecule 40 is a protein called 60S ribosomal protein L39.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
40	AM	50	Total	C	N	O	0	0	0
			438	275	97	66			
40	CG	50	Total	C	N	O	0	0	0
			438	275	97	66			

- Molecule 41 is a protein called 60S ribosomal protein L40-B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
41	AN	52	Total	C	N	O	S	0	0	0
			419	260	86	67	6			
41	CH	51	Total	C	N	O	S	0	0	0
			411	255	85	66	5			

- Molecule 42 is a protein called 60S ribosomal protein L41.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
42	AO	25	Total	C	N	O	S	0	0	0
			236	144	63	28	1			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
42	CI	24	Total	C	N	O	S	0	0	0
			227	138	61	27	1			

- Molecule 43 is a protein called 60S ribosomal protein L42-B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
43	AP	103	Total	C	N	O	S	0	0	0
			828	521	165	137	5			
43	CJ	103	Total	C	N	O	S	0	0	0
			828	521	165	137	5			

- Molecule 44 is a protein called 60S ribosomal protein L43-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
44	AQ	91	Total	C	N	O	S	0	0	0
			698	430	140	124	4			
44	CK	91	Total	C	N	O	S	0	0	0
			698	430	140	124	4			

- Molecule 45 is a protein called 60S ribosomal protein CAALFM_C304810CA.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
45	i	121	Total	C	N	O	0	0	0
			931	563	166	202			
45	CL	121	Total	C	N	O	0	0	0
			931	563	166	202			

- Molecule 46 is a RNA chain called 18S.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
46	B	1761	Total	C	N	O	P	0	0	0
			37537	16780	6656	12340	1761			
46	CM	1765	Total	C	N	O	P	0	0	0
			37621	16818	6670	12368	1765			

- Molecule 47 is a protein called 40S ribosomal protein S0.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
47	C	208	Total	C	N	O	S	0	0	0
			1627	1041	284	297	5			
47	CN	208	Total	C	N	O	S	0	0	0
			1627	1041	284	297	5			

- Molecule 48 is a protein called 40S ribosomal protein S1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
48	D	214	Total	C	N	O	S	0	0	0
			1724	1094	313	313	4			
48	CO	214	Total	C	N	O	S	0	0	0
			1724	1094	313	313	4			

- Molecule 49 is a protein called Ribosomal protein S5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
49	E	217	Total	C	N	O	S	0	0	0
			1629	1039	289	296	5			
49	CP	217	Total	C	N	O	S	0	0	0
			1629	1039	289	296	5			

- Molecule 50 is a protein called Ribosomal protein S3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
50	F	223	Total	C	N	O	S	0	0	0
			1707	1087	311	305	4			
50	CQ	223	Total	C	N	O	S	0	0	0
			1707	1087	311	305	4			

- Molecule 51 is a protein called 40S ribosomal protein S4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
51	G	259	Total	C	N	O	S	0	0	0
			2051	1304	385	357	5			
51	CR	260	Total	C	N	O	S	0	0	0
			2055	1306	386	358	5			

- Molecule 52 is a protein called Ribosomal protein S7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
52	H	206	Total	C	N	O	S	0	0	0
			1614	1008	301	301	4			
52	CS	206	Total	C	N	O	S	0	0	0
			1614	1008	301	301	4			

- Molecule 53 is a protein called 40S ribosomal protein S6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
53	I	226	Total	C	N	O	S	0	0	0
			1820	1133	351	330	6			
53	CT	236	Total	C	N	O	S	0	0	0
			1904	1184	369	345	6			

- Molecule 54 is a protein called 40S ribosomal protein S7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
54	J	185	Total	C	N	O	S	0	0	0
			1491	953	269	269				
54	CU	183	Total	C	N	O	S	0	0	0
			1475	944	265	266				

- Molecule 55 is a protein called 40S ribosomal protein S8.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
55	K	203	Total	C	N	O	S	0	0	0
			1579	973	322	283	1			
55	CV	203	Total	C	N	O	S	0	0	0
			1579	973	322	283	1			

- Molecule 56 is a protein called Ribosomal protein S4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
56	L	178	Total	C	N	O	S	0	0	0
			1453	918	286	248	1			
56	CW	178	Total	C	N	O	S	0	0	0
			1453	918	286	248	1			

- Molecule 57 is a protein called 40S ribosomal protein S10-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
57	M	98	Total	C	N	O	S	0	0	0
			817	531	135	150	1			
57	CX	94	Total	C	N	O	S	0	0	0
			791	515	131	144	1			

- Molecule 58 is a protein called 40S ribosomal protein S11A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
58	N	144	Total	C	N	O	S	0	0	0
			1150	734	215	198	3			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
58	CY	141	Total	C	N	O	S	0	0	0
			1129	722	212	192	3			

- Molecule 59 is a protein called 40S ribosomal protein S12.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
59	O	116	Total	C	N	O	S	0	0	0
			885	550	158	172	5			
59	CZ	119	Total	C	N	O	S	0	0	0
			913	566	163	179	5			

- Molecule 60 is a protein called 40S ribosomal protein S13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
60	P	150	Total	C	N	O	S	0	0	0
			1187	757	219	210	1			
60	DA	150	Total	C	N	O	S	0	0	0
			1187	757	219	210	1			

- Molecule 61 is a protein called 40S ribosomal protein S14-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
61	Q	127	Total	C	N	O	S	0	0	0
			942	579	186	174	3			
61	DB	127	Total	C	N	O	S	0	0	0
			942	579	186	174	3			

- Molecule 62 is a protein called 40S ribosomal protein S15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
62	R	129	Total	C	N	O	S	0	0	0
			1018	649	185	177	7			
62	DC	130	Total	C	N	O	S	0	0	0
			1029	655	189	178	7			

- Molecule 63 is a protein called 40S ribosomal protein S16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
63	S	140	Total	C	N	O	S	0	0	0
			1091	700	198	192	1			
63	DD	140	Total	C	N	O	S	0	0	0
			1091	700	198	192	1			

- Molecule 64 is a protein called 40S ribosomal protein S17-B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
64	T	124	Total	C	N	O	S	0	0	0
			997	628	183	185	1			
64	DE	124	Total	C	N	O	S	0	0	0
			997	628	183	185	1			

- Molecule 65 is a protein called 40S ribosomal protein S18-B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
65	U	144	Total	C	N	O	S	0	0	0
			1187	744	233	207	3			
65	DF	141	Total	C	N	O	S	0	0	0
			1161	727	227	204	3			

- Molecule 66 is a protein called 40S ribosomal protein S19-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
66	V	141	Total	C	N	O	S	0	0	0
			1100	689	210	200	1			
66	DG	141	Total	C	N	O	S	0	0	0
			1100	689	210	200	1			

- Molecule 67 is a protein called Ribosomal protein S10.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
67	W	102	Total	C	N	O	S	0	0	0
			808	509	150	147	2			
67	DH	97	Total	C	N	O	S	0	0	0
			763	481	140	140	2			

- Molecule 68 is a protein called 40S ribosomal protein S21.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
68	X	87	Total	C	N	O	S	0	0	0
			676	415	126	133	2			
68	DI	87	Total	C	N	O	S	0	0	0
			676	415	126	133	2			

- Molecule 69 is a protein called 40S ribosomal protein S22-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
69	Y	129	Total	C	N	O	S	0	0	0
			1032	655	191	183	3			
69	DJ	129	Total	C	N	O	S	0	0	0
			1032	655	191	183	3			

- Molecule 70 is a protein called Ribosomal protein S23 (S12).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
70	Z	143	Total	C	N	O	S	0	0	0
			1110	701	219	188	2			
70	DK	143	Total	C	N	O	S	0	0	0
			1110	701	219	188	2			

- Molecule 71 is a protein called 40S ribosomal protein S24.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
71	a	134	Total	C	N	O		0	0	0
			1086	677	218	191				
71	DL	132	Total	C	N	O		0	0	0
			1072	670	216	186				

- Molecule 72 is a protein called 40S ribosomal protein S25.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
72	b	72	Total	C	N	O		0	0	0
			578	369	103	106				
72	DM	71	Total	C	N	O		0	0	0
			570	365	102	103				

- Molecule 73 is a protein called 40S ribosomal protein S26.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
73	c	98	Total	C	N	O	S	0	0	0
			779	482	163	128	6			
73	DN	98	Total	C	N	O	S	0	0	0
			779	482	163	128	6			

- Molecule 74 is a protein called 40S ribosomal protein S27.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
74	d	81	Total	C	N	O	S	0	0	0
			614	383	110	114	7			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
74	DO	81	Total	C	N	O	S	0	0	0
			614	383	110	114	7			

- Molecule 75 is a protein called 40S ribosomal protein S28-B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
75	e	62	Total	C	N	O	S	0	0	0
			487	299	98	88	2			
75	DP	61	Total	C	N	O	S	0	0	0
			476	293	94	87	2			

- Molecule 76 is a protein called 40S ribosomal protein S29A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
76	f	55	Total	C	N	O	S	0	0	0
			454	281	94	75	4			
76	DQ	54	Total	C	N	O	S	0	0	0
			449	278	93	74	4			

- Molecule 77 is a protein called 40S ribosomal protein S30.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
77	g	60	Total	C	N	O	S	0	0	0
			474	297	96	79	2			
77	DR	58	Total	C	N	O	S	0	0	0
			461	289	93	77	2			

- Molecule 78 is a protein called Ubiquitin-40S ribosomal protein S31 fusion protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
78	h	70	Total	C	N	O	S	0	0	0
			574	362	113	93	6			
78	DS	69	Total	C	N	O	S	0	0	0
			563	356	109	92	6			

- Molecule 79 is a protein called Guanine nucleotide-binding protein subunit beta-like protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
79	AR	311	Total	C	N	O	S	0	0	0
			2398	1519	412	462	5			
79	DT	311	Total	C	N	O	S	0	0	0
			2398	1519	412	462	5			

- Molecule 80 is a protein called 60S acidic ribosomal protein P0.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
80	P0	107	Total	C	N	O	S	0	0	0
			845	542	150	150	3			
80	p0	107	Total	C	N	O	S	0	0	0
			845	542	150	150	3			

- Molecule 81 is a protein called 60S ribosomal protein L12-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
81	12	63	Total	C	N	O	S	0	0	0
			480	297	85	96	2			

- Molecule 82 is a protein called Ribosomal protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
82	L1	217	Total	C	N	O	S	0	0	0
			1711	1096	294	312	9			
82	11	217	Total	C	N	O	S	0	0	0
			1711	1096	294	312	9			

- Molecule 83 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
83	1	531	Total	Mg	0	0
			531	531		
83	3	13	Total	Mg	0	0
			13	13		
83	4	11	Total	Mg	0	0
			11	11		
83	j	4	Total	Mg	0	0
			4	4		
83	k	4	Total	Mg	0	0
			4	4		
83	m	1	Total	Mg	0	0
			1	1		
83	o	3	Total	Mg	0	0
			3	3		
83	r	3	Total	Mg	0	0
			3	3		
83	s	1	Total	Mg	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
83	u	1	Total 1	Mg 1	0	0
83	v	4	Total 4	Mg 4	0	0
83	w	3	Total 3	Mg 3	0	0
83	x	3	Total 3	Mg 3	0	0
83	z	1	Total 1	Mg 1	0	0
83	0	5	Total 5	Mg 5	0	0
83	2	2	Total 2	Mg 2	0	0
83	6	2	Total 2	Mg 2	0	0
83	7	1	Total 1	Mg 1	0	0
83	8	2	Total 2	Mg 2	0	0
83	9	3	Total 3	Mg 3	0	0
83	AB	1	Total 1	Mg 1	0	0
83	AC	1	Total 1	Mg 1	0	0
83	AD	1	Total 1	Mg 1	0	0
83	AE	2	Total 2	Mg 2	0	0
83	AF	1	Total 1	Mg 1	0	0
83	AG	2	Total 2	Mg 2	0	0
83	AH	2	Total 2	Mg 2	0	0
83	AM	2	Total 2	Mg 2	0	0
83	AP	2	Total 2	Mg 2	0	0
83	i	1	Total 1	Mg 1	0	0

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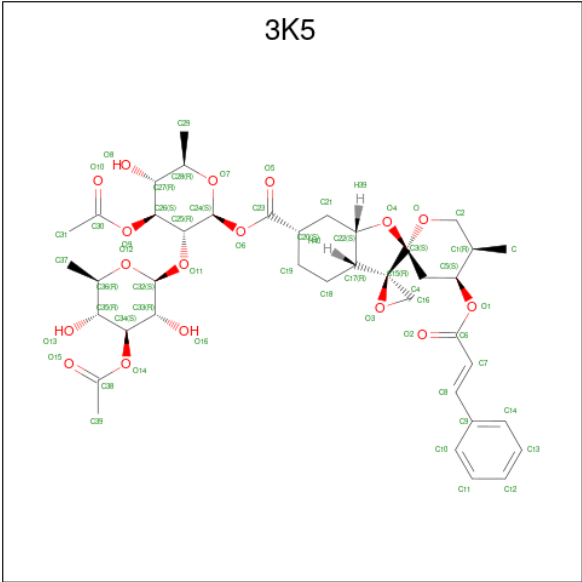
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
83	B	152	Total 152	Mg 152	0	0
83	D	1	Total 1	Mg 1	0	0
83	G	1	Total 1	Mg 1	0	0
83	I	1	Total 1	Mg 1	0	0
83	J	1	Total 1	Mg 1	0	0
83	K	1	Total 1	Mg 1	0	0
83	L	1	Total 1	Mg 1	0	0
83	Q	3	Total 3	Mg 3	0	0
83	R	1	Total 1	Mg 1	0	0
83	Y	3	Total 3	Mg 3	0	0
83	Z	3	Total 3	Mg 3	0	0
83	a	1	Total 1	Mg 1	0	0
83	f	1	Total 1	Mg 1	0	0
83	AR	2	Total 2	Mg 2	0	0
83	AS	274	Total 274	Mg 274	0	0
83	AT	10	Total 10	Mg 10	0	0
83	AU	2	Total 2	Mg 2	0	0
83	AW	4	Total 4	Mg 4	0	0
83	BB	4	Total 4	Mg 4	0	0
83	BE	3	Total 3	Mg 3	0	0
83	BF	1	Total 1	Mg 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
83	BH	1	Total 1	Mg 1	0	0
83	BJ	2	Total 2	Mg 2	0	0
83	BK	1	Total 1	Mg 1	0	0
83	BN	1	Total 1	Mg 1	0	0
83	BV	1	Total 1	Mg 1	0	0
83	BZ	3	Total 3	Mg 3	0	0
83	CA	1	Total 1	Mg 1	0	0
83	CJ	1	Total 1	Mg 1	0	0
83	CK	2	Total 2	Mg 2	0	0
83	CL	3	Total 3	Mg 3	0	0
83	CM	103	Total 103	Mg 103	0	0
83	CN	1	Total 1	Mg 1	0	0
83	CP	1	Total 1	Mg 1	0	0
83	CQ	1	Total 1	Mg 1	0	0
83	DA	1	Total 1	Mg 1	0	0
83	DB	3	Total 3	Mg 3	0	0
83	DQ	1	Total 1	Mg 1	0	0

- Molecule 84 is 3-O-acetyl-2-O-(3-O-acetyl-6-deoxy-beta-D-glucopyranosyl)-6-deoxy-1-O- $\{[(2R,2'S,3a'R,4''S,5''R,6'S,7a'S)-5''\text{-methyl-4''-}\{[(2E)\text{-3-phenylprop-2-enoyl}]\text{oxy}\}\text{decahydrodispiro[oxirane-2,3'-[1]benzofuran-2',2''-pyran]-6'-yl}]\text{carbonyl}\}$ -beta-D-glucopyranose (CCD ID: 3K5) (formula: C₄₀H₅₂O₁₇).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
84	1	1	Total	C	O	0	0
			57	40	17		
84	AS	1	Total	C	O	0	0
			57	40	17		

- Molecule 85 is ZINC ION (CCD ID: ZN) (formula: Zn).

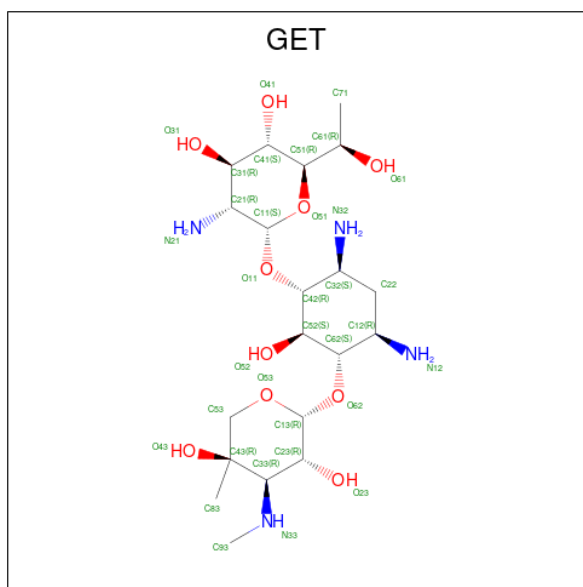
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
85	AH	1	Total	Zn	0	0
			1	1		
85	AK	1	Total	Zn	0	0
			1	1		
85	AN	1	Total	Zn	0	0
			1	1		
85	AP	1	Total	Zn	0	0
			1	1		
85	AQ	1	Total	Zn	0	0
			1	1		
85	c	1	Total	Zn	0	0
			1	1		
85	d	1	Total	Zn	0	0
			1	1		
85	f	1	Total	Zn	0	0
			1	1		
85	h	1	Total	Zn	0	0
			1	1		
85	CB	1	Total	Zn	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
85	CE	1	Total	Zn	0	0
			1	1		
85	CH	1	Total	Zn	0	0
			1	1		
85	CJ	1	Total	Zn	0	0
			1	1		
85	CK	1	Total	Zn	0	0
			1	1		
85	DN	1	Total	Zn	0	0
			1	1		
85	DO	1	Total	Zn	0	0
			1	1		
85	DQ	1	Total	Zn	0	0
			1	1		
85	DS	1	Total	Zn	0	0
			1	1		

- Molecule 86 is GENETICIN (CCD ID: GET) (formula: $C_{20}H_{40}N_4O_{10}$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
86	B	1	Total	C	N	O	0	0
			34	20	4	10		
86	CM	1	Total	C	N	O	0	0
			34	20	4	10		

- Molecule 87 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
87	1	9	Total 9	O 9	0	0
87	4	3	Total 3	O 3	0	0
87	B	5	Total 5	O 5	0	0
87	G	1	Total 1	O 1	0	0
87	AS	12	Total 12	O 12	0	0

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

3 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	299.18Å 294.18Å 450.09Å 90.00° 100.05° 90.00°	Depositor
Resolution (Å)	162.01 – 3.00 162.01 – 3.00	Depositor EDS
% Data completeness (in resolution range)	99.3 (162.01-3.00) 88.2 (162.01-3.00)	Depositor EDS
R_{merge}	0.64	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.88 (at 3.01Å)	Xtriage
Refinement program	PHENIX 1.19rc4_4035	Depositor
R, R_{free}	0.264 , 0.281 0.264 , 0.280	Depositor DCC
R_{free} test set	2000 reflections (0.13%)	wwPDB-VP
Wilson B-factor (Å ²)	54.0	Xtriage
Anisotropy	0.116	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 41.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	409812	wwPDB-VP
Average B, all atoms (Å ²)	92.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.46% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

4 Model quality [i](#)

4.1 Standard geometry [i](#)

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

4.2 Too-close contacts [i](#)

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

4.3 Torsion angles [i](#)

4.3.1 Protein backbone [i](#)

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

4.3.2 Protein sidechains [i](#)

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

4.3.3 RNA [i](#)

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

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

There are no non-standard protein/DNA/RNA residues in this entry.

4.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

4.6 Ligand geometry [i](#)

Of 1232 ligands modelled in this entry, 1228 are monoatomic - leaving 4 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond

length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
84	3K5	AS	3401	-	63,63,63	2.77	27 (42%)	84,95,95	1.69	14 (16%)
86	GET	CM	1904	-	35,36,36	1.92	1 (2%)	43,55,55	1.50	7 (16%)
86	GET	B	1801	-	35,36,36	0.90	1 (2%)	43,55,55	1.60	6 (13%)
84	3K5	1	3402	-	63,63,63	2.83	29 (46%)	84,95,95	1.73	18 (21%)

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
84	3K5	AS	3401	-	-	11/29/121/121	0/7/7/7
86	GET	CM	1904	-	-	3/13/74/74	0/3/3/3
86	GET	B	1801	-	-	4/13/74/74	0/3/3/3
84	3K5	1	3402	-	-	10/29/121/121	0/7/7/7

The worst 5 of 58 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
86	CM	1904	GET	C33-N33	-10.96	1.31	1.45
84	1	3402	3K5	C17-C22	-8.45	1.36	1.53
84	1	3402	3K5	O4-C22	7.37	1.60	1.43
84	AS	3401	3K5	C17-C22	-7.10	1.39	1.53
84	AS	3401	3K5	O4-C22	6.91	1.59	1.43

The worst 5 of 45 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
84	AS	3401	3K5	C2-O-C3	-6.94	109.05	113.51
86	B	1801	GET	C53-O53-C13	6.77	121.94	111.53
84	1	3402	3K5	O14-C38-C39	4.91	119.84	111.09
84	AS	3401	3K5	O9-C30-C31	4.59	119.28	111.09
84	AS	3401	3K5	O14-C38-C39	4.54	119.19	111.09

There are no chirality outliers.

5 of 28 torsion outliers are listed below:

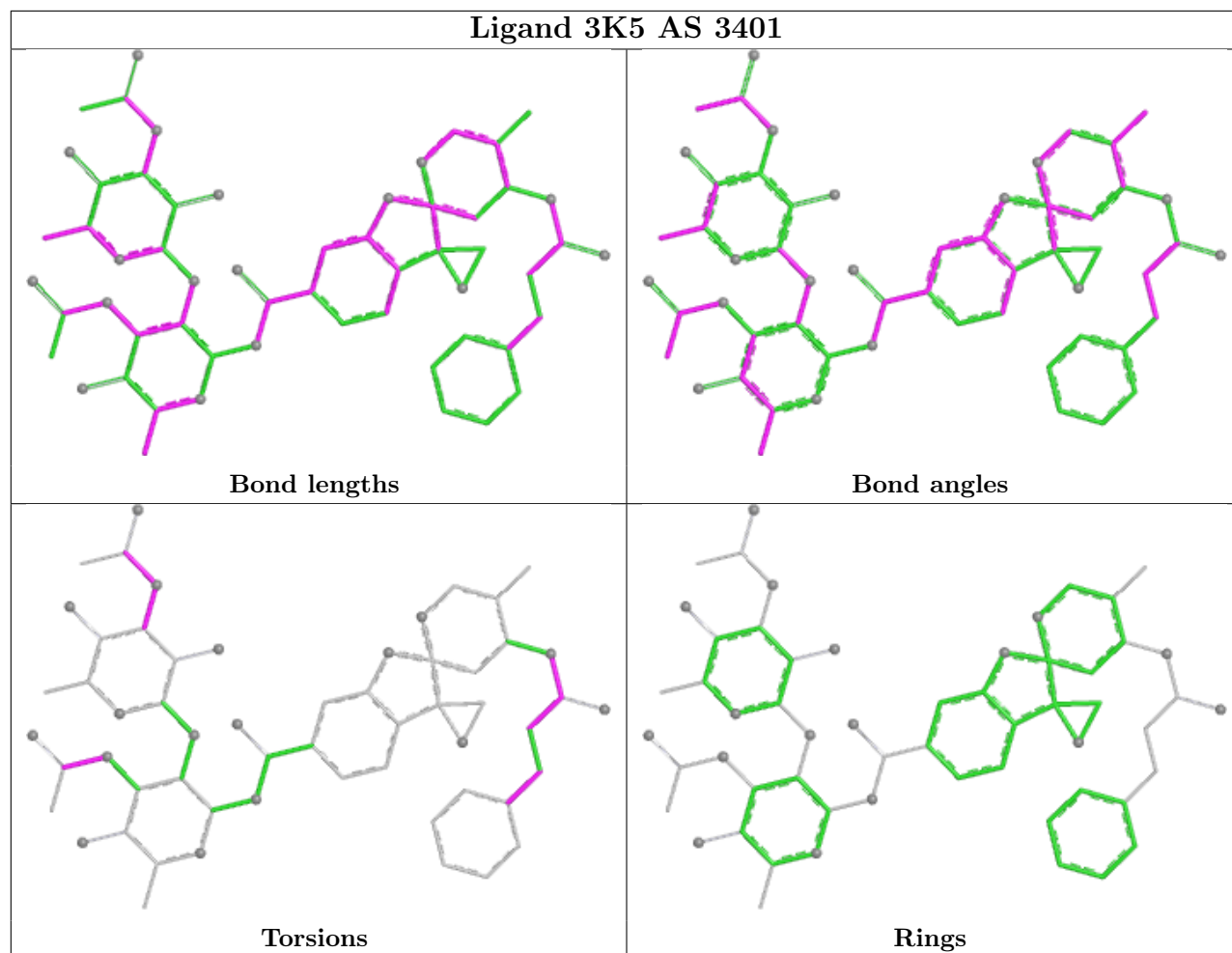
Mol	Chain	Res	Type	Atoms
84	1	3402	3K5	C4-C5-O1-C6
84	1	3402	3K5	C7-C6-O1-C5
84	1	3402	3K5	C39-C38-O14-C34
84	AS	3401	3K5	C39-C38-O14-C34
84	AS	3401	3K5	C35-C34-O14-C38

There are no ring outliers.

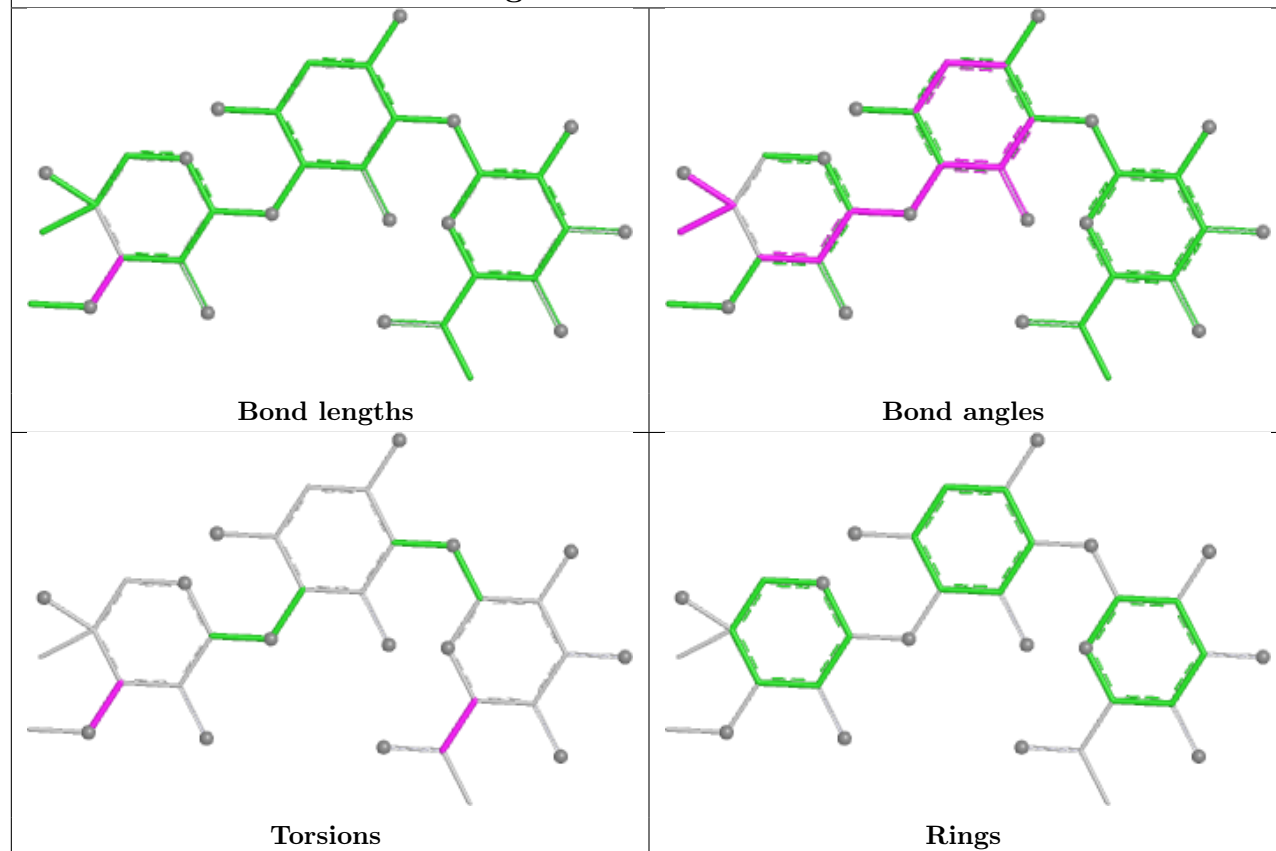
No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

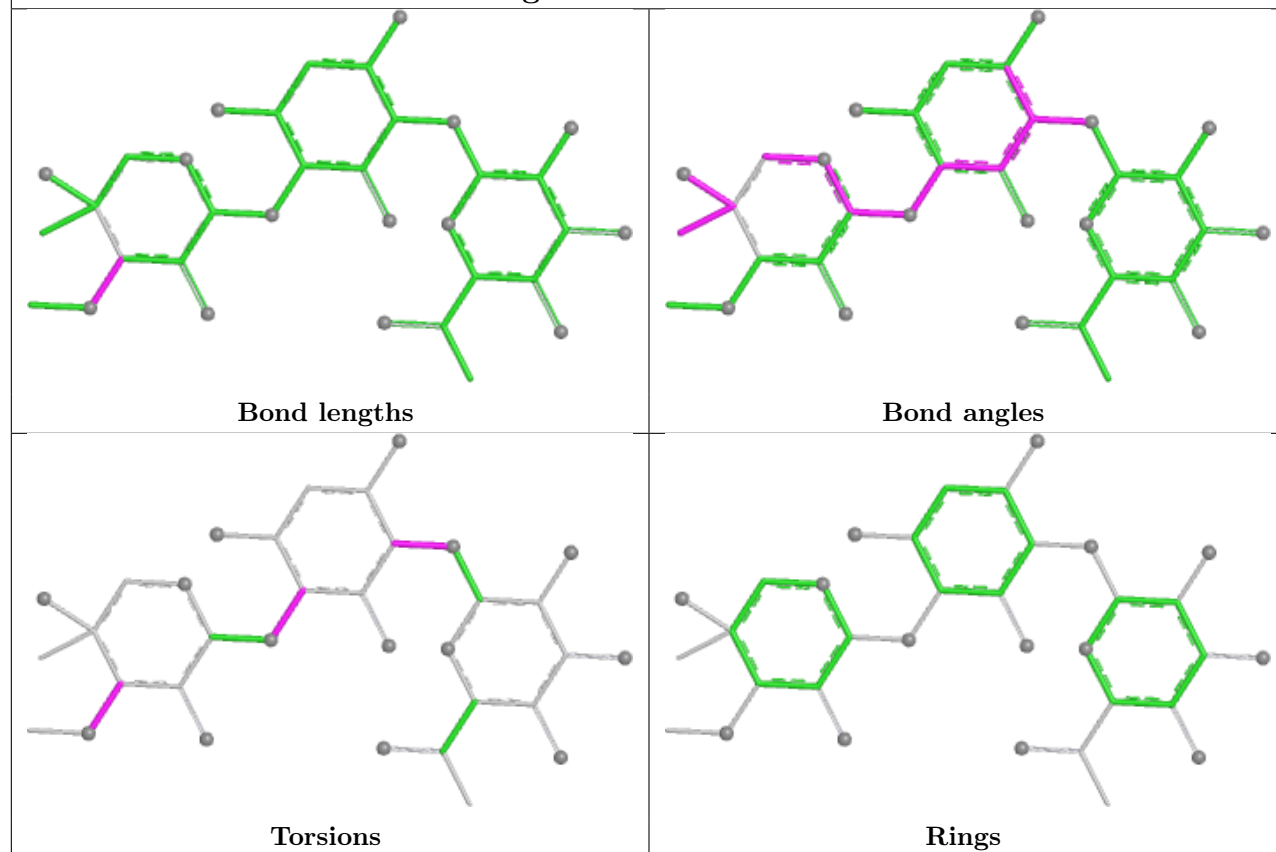
Ligand 3K5 AS 3401

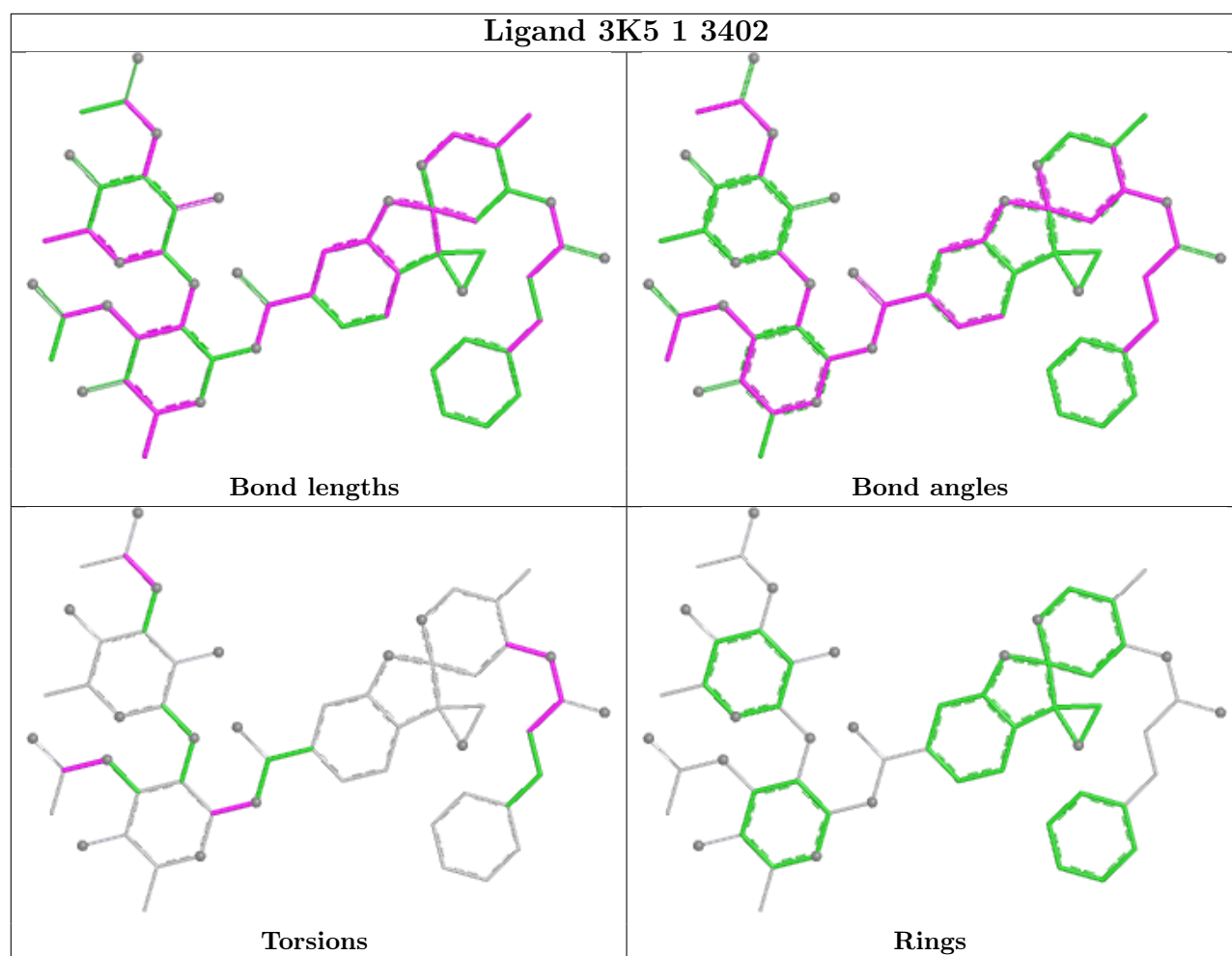


Ligand GET CM 1904



Ligand GET B 1801





4.7 Other polymers [i](#)

There are no such residues in this entry.

4.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

5 Fit of model and data ⓘ

5.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	1	3216/3359 (95%)	0.01	48 (1%) 72 49	34, 65, 184, 386	0
1	AS	3229/3359 (96%)	0.22	89 (2%) 55 32	39, 76, 213, 334	0
2	3	121/121 (100%)	-0.20	1 (0%) 82 64	45, 80, 101, 132	0
2	AT	121/121 (100%)	-0.06	1 (0%) 82 64	40, 75, 101, 149	0
3	4	157/158 (99%)	-0.07	1 (0%) 85 69	49, 69, 121, 183	0
3	AU	158/158 (100%)	0.37	5 (3%) 50 29	61, 99, 147, 227	0
4	AW	249/254 (98%)	0.83	21 (8%) 17 9	44, 81, 108, 126	0
4	j	249/254 (98%)	0.60	9 (3%) 46 26	30, 56, 80, 157	0
5	AX	386/389 (99%)	0.44	11 (2%) 55 32	41, 64, 98, 158	0
5	k	386/389 (99%)	0.45	9 (2%) 61 38	39, 61, 84, 132	0
6	AY	361/363 (99%)	1.09	55 (15%) 5 3	54, 81, 112, 138	0
6	l	361/363 (99%)	0.65	16 (4%) 39 21	38, 72, 109, 144	0
7	AZ	292/298 (97%)	1.32	58 (19%) 3 2	49, 100, 135, 157	0
7	m	296/298 (99%)	0.84	25 (8%) 17 9	53, 91, 124, 149	0
8	BA	153/176 (86%)	0.93	13 (8%) 16 8	58, 79, 111, 146	0
8	n	157/176 (89%)	0.66	12 (7%) 20 10	60, 81, 115, 150	0
9	BB	234/241 (97%)	0.54	5 (2%) 63 40	44, 62, 119, 178	0
9	o	234/241 (97%)	0.38	2 (0%) 81 61	43, 63, 124, 170	0
10	BC	233/262 (88%)	1.19	35 (15%) 5 3	99, 131, 170, 188	0
10	p	238/262 (90%)	0.75	9 (3%) 44 24	62, 83, 139, 178	0
11	BD	190/191 (99%)	0.81	10 (5%) 32 16	63, 82, 113, 157	0
11	q	190/191 (99%)	0.77	7 (3%) 45 25	62, 81, 107, 138	0
12	BE	208/220 (94%)	0.23	2 (0%) 79 59	37, 56, 109, 150	0
12	r	208/220 (94%)	0.52	7 (3%) 48 27	42, 62, 102, 121	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	BF	171/174 (98%)	0.74	12 (7%) 22 12	62, 91, 124, 140	0
13	s	171/174 (98%)	0.83	6 (3%) 47 27	62, 92, 119, 131	0
14	BG	200/202 (99%)	1.04	19 (9%) 14 7	54, 102, 139, 158	0
14	t	200/202 (99%)	0.53	5 (2%) 58 35	47, 77, 121, 145	0
15	BH	130/131 (99%)	0.74	9 (6%) 23 12	55, 74, 102, 126	0
15	u	130/131 (99%)	0.34	3 (2%) 61 38	58, 72, 97, 120	0
16	BI	203/204 (99%)	1.48	44 (21%) 2 1	61, 94, 114, 123	0
16	v	203/204 (99%)	0.70	6 (2%) 52 30	38, 58, 75, 87	0
17	BJ	199/200 (99%)	0.49	4 (2%) 65 41	38, 56, 97, 133	0
17	w	199/200 (99%)	0.50	3 (1%) 72 49	42, 58, 91, 117	0
18	BK	176/185 (95%)	1.02	16 (9%) 15 8	53, 70, 102, 139	0
18	x	173/185 (93%)	0.85	13 (7%) 20 10	44, 61, 99, 127	0
19	BL	185/186 (99%)	0.82	12 (6%) 25 13	56, 76, 94, 108	0
19	y	185/186 (99%)	0.84	14 (7%) 20 10	47, 67, 86, 99	0
20	BM	179/190 (94%)	0.98	9 (5%) 34 18	65, 90, 149, 183	0
20	z	179/190 (94%)	0.82	14 (7%) 19 10	56, 74, 136, 153	0
21	0	170/172 (98%)	0.40	2 (1%) 76 55	50, 64, 85, 145	0
21	BN	170/172 (98%)	0.64	5 (2%) 53 31	44, 64, 88, 118	0
22	2	159/160 (99%)	0.60	9 (5%) 29 15	46, 61, 124, 152	0
22	BO	159/160 (99%)	0.93	13 (8%) 17 9	43, 64, 122, 154	0
23	5	103/124 (83%)	0.84	4 (3%) 43 24	88, 121, 152, 169	0
23	BP	102/124 (82%)	0.98	4 (3%) 43 24	102, 137, 160, 173	0
24	6	131/137 (95%)	0.45	3 (2%) 61 38	43, 56, 79, 100	0
24	BQ	131/137 (95%)	0.66	2 (1%) 72 49	40, 56, 87, 106	0
25	7	118/155 (76%)	0.70	7 (5%) 28 14	41, 82, 134, 147	0
25	BR	98/155 (63%)	1.12	10 (10%) 12 6	52, 74, 132, 146	0
26	8	121/142 (85%)	0.73	4 (3%) 49 28	60, 77, 97, 131	0
26	BS	119/142 (83%)	1.34	24 (20%) 3 2	74, 105, 126, 134	0
27	9	126/127 (99%)	1.12	14 (11%) 10 6	54, 82, 105, 137	0
27	BT	126/127 (99%)	1.02	13 (10%) 12 6	70, 102, 136, 156	0
28	AA	135/136 (99%)	0.88	8 (5%) 28 14	69, 96, 115, 151	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
28	BU	135/136 (99%)	1.18	18 (13%) 7 4	100, 128, 152, 180	0
29	AB	148/149 (99%)	0.67	5 (3%) 48 27	37, 64, 93, 131	0
29	BV	148/149 (99%)	1.09	13 (8%) 15 8	51, 83, 106, 123	0
30	AC	62/63 (98%)	1.15	11 (17%) 4 2	44, 77, 136, 150	0
30	BW	61/63 (96%)	1.52	14 (22%) 2 1	48, 83, 131, 149	0
31	AD	96/106 (90%)	0.53	2 (2%) 63 40	63, 84, 106, 118	0
31	BX	96/106 (90%)	1.16	16 (16%) 4 3	87, 123, 144, 157	0
32	AE	110/112 (98%)	0.65	1 (0%) 81 61	52, 70, 119, 151	0
32	BY	110/112 (98%)	0.93	7 (6%) 25 13	56, 83, 128, 158	0
33	AF	124/131 (94%)	0.69	8 (6%) 25 13	42, 67, 84, 100	0
33	BZ	124/131 (94%)	0.89	13 (10%) 11 6	45, 71, 100, 117	0
34	AG	106/107 (99%)	0.53	1 (0%) 81 61	49, 62, 78, 98	0
34	CA	106/107 (99%)	0.44	1 (0%) 81 61	42, 57, 77, 92	0
35	AH	112/122 (91%)	1.04	14 (12%) 8 5	52, 76, 124, 146	0
35	CB	112/122 (91%)	1.68	36 (32%) 1 1	74, 106, 148, 166	0
36	AI	120/120 (100%)	0.98	12 (10%) 12 7	68, 86, 118, 138	0
36	CC	118/120 (98%)	1.44	26 (22%) 2 1	88, 114, 138, 150	0
37	AJ	97/99 (97%)	0.67	4 (4%) 41 23	58, 75, 109, 177	0
37	CD	97/99 (97%)	1.30	19 (19%) 3 2	86, 107, 137, 156	0
38	AK	86/90 (95%)	0.78	1 (1%) 76 55	42, 56, 96, 121	0
38	CE	86/90 (95%)	1.06	10 (11%) 9 5	53, 76, 122, 141	0
39	AL	77/78 (98%)	1.10	6 (7%) 19 10	81, 106, 140, 165	0
39	CF	77/78 (98%)	1.40	17 (22%) 2 1	100, 130, 164, 170	0
40	AM	50/51 (98%)	0.78	4 (8%) 18 9	48, 63, 87, 91	0
40	CG	50/51 (98%)	1.42	9 (18%) 3 2	63, 84, 98, 108	0
41	AN	52/52 (100%)	1.95	26 (50%) 0 0	95, 121, 135, 144	0
41	CH	51/52 (98%)	1.98	23 (45%) 0 0	92, 125, 142, 145	0
42	AO	25/25 (100%)	1.28	3 (12%) 9 5	62, 69, 80, 89	0
42	CI	24/25 (96%)	1.26	4 (16%) 4 3	54, 63, 74, 84	0
43	AP	103/106 (97%)	0.51	5 (4%) 35 18	35, 62, 111, 126	0
43	CJ	103/106 (97%)	0.74	5 (4%) 35 18	48, 75, 123, 136	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å ²)	Q<0.9
44	AQ	91/92 (98%)	0.62	4 (4%)	39 21	45, 64, 95, 126	0
44	CK	91/92 (98%)	0.81	5 (5%)	30 15	54, 84, 121, 131	0
45	CL	121/267 (45%)	1.43	32 (26%)	1 1	63, 100, 135, 150	0
45	i	121/267 (45%)	1.63	35 (28%)	1 1	75, 111, 143, 150	0
46	B	1761/1787 (98%)	0.36	51 (2%)	53 31	48, 93, 186, 464	0
46	CM	1765/1787 (98%)	0.30	52 (2%)	53 31	40, 82, 188, 472	0
47	C	208/261 (79%)	1.15	27 (12%)	7 4	91, 123, 148, 166	0
47	CN	208/261 (79%)	1.01	26 (12%)	8 5	67, 105, 139, 177	0
48	CO	214/256 (83%)	1.17	28 (13%)	7 4	79, 126, 149, 177	0
48	D	214/256 (83%)	0.72	9 (4%)	40 22	74, 98, 120, 131	0
49	CP	217/249 (87%)	0.49	9 (4%)	41 23	48, 74, 104, 128	0
49	E	217/249 (87%)	1.08	32 (14%)	6 3	76, 102, 125, 145	0
50	CQ	223/251 (88%)	0.71	9 (4%)	42 23	58, 80, 146, 173	0
50	F	223/251 (88%)	1.07	27 (12%)	8 5	81, 111, 159, 181	0
51	CR	260/262 (99%)	0.98	23 (8%)	15 8	62, 88, 115, 155	0
51	G	259/262 (98%)	1.44	57 (22%)	2 1	74, 104, 128, 156	0
52	CS	206/225 (91%)	1.06	29 (14%)	6 4	80, 109, 152, 202	0
52	H	206/225 (91%)	1.15	31 (15%)	5 3	81, 109, 142, 175	0
53	CT	236/236 (100%)	0.89	23 (9%)	13 7	60, 103, 147, 168	0
53	I	226/236 (95%)	1.01	29 (12%)	7 5	65, 105, 146, 185	0
54	CU	183/186 (98%)	1.06	27 (14%)	5 3	71, 136, 176, 185	0
54	J	185/186 (99%)	1.51	50 (27%)	1 1	84, 136, 165, 176	0
55	CV	203/206 (98%)	1.00	22 (10%)	11 6	46, 75, 131, 165	0
55	K	203/206 (98%)	0.98	24 (11%)	9 5	53, 87, 130, 156	0
56	CW	178/189 (94%)	1.18	25 (14%)	6 4	64, 95, 126, 144	0
56	L	178/189 (94%)	1.80	67 (37%)	1 1	77, 114, 131, 147	0
57	CX	94/118 (79%)	0.74	5 (5%)	32 16	61, 94, 136, 150	0
57	M	98/118 (83%)	1.10	8 (8%)	17 9	87, 120, 149, 161	0
58	CY	141/155 (90%)	0.75	11 (7%)	19 10	47, 67, 98, 158	0
58	N	144/155 (92%)	1.03	19 (13%)	7 4	56, 83, 120, 152	0
59	CZ	119/143 (83%)	1.19	15 (12%)	8 5	147, 171, 185, 192	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
59	O	116/143 (81%)	1.14	16 (13%) 6 4	156, 188, 199, 207	0
60	DA	150/151 (99%)	1.07	11 (7%) 21 11	59, 97, 127, 146	0
60	P	150/151 (99%)	1.16	23 (15%) 5 3	64, 98, 119, 132	0
61	DB	127/132 (96%)	1.00	11 (8%) 16 8	60, 105, 132, 140	0
61	Q	127/132 (96%)	0.62	8 (6%) 26 13	56, 84, 105, 113	0
62	DC	130/142 (91%)	1.36	24 (18%) 3 2	64, 101, 133, 157	0
62	R	129/142 (90%)	1.08	16 (12%) 8 5	79, 102, 136, 157	0
63	DD	140/142 (98%)	1.42	33 (23%) 2 1	67, 104, 140, 152	0
63	S	140/142 (98%)	1.61	42 (30%) 1 1	82, 115, 148, 163	0
64	DE	124/137 (90%)	1.28	21 (16%) 4 3	69, 122, 170, 177	0
64	T	124/137 (90%)	1.49	34 (27%) 1 1	97, 129, 174, 180	0
65	DF	141/145 (97%)	1.12	13 (9%) 14 8	63, 102, 137, 165	0
65	U	144/145 (99%)	0.74	9 (6%) 26 13	73, 91, 124, 154	0
66	DG	141/145 (97%)	1.22	16 (11%) 10 6	69, 100, 129, 154	0
66	V	141/145 (97%)	1.11	23 (16%) 4 3	85, 108, 141, 157	0
67	DH	97/119 (81%)	1.13	9 (9%) 14 7	53, 104, 128, 146	0
67	W	102/119 (85%)	1.28	17 (16%) 4 3	78, 129, 154, 164	0
68	DI	87/87 (100%)	0.70	3 (3%) 48 27	68, 90, 126, 152	0
68	X	87/87 (100%)	1.05	12 (13%) 6 4	83, 110, 136, 141	0
69	DJ	129/130 (99%)	0.69	3 (2%) 61 38	52, 69, 87, 99	0
69	Y	129/130 (99%)	1.34	27 (20%) 2 2	77, 91, 110, 119	0
70	DK	143/145 (98%)	0.91	13 (9%) 15 8	46, 66, 88, 120	0
70	Z	143/145 (98%)	0.80	13 (9%) 15 8	63, 78, 95, 118	0
71	DL	132/135 (97%)	0.84	9 (6%) 23 12	84, 111, 140, 184	0
71	a	134/135 (99%)	1.18	20 (14%) 5 3	80, 119, 138, 158	0
72	DM	71/105 (67%)	0.94	7 (9%) 13 7	106, 132, 150, 159	0
72	b	72/105 (68%)	0.59	0 100 100	95, 114, 138, 154	0
73	DN	98/119 (82%)	1.10	11 (11%) 10 6	64, 83, 139, 147	0
73	c	98/119 (82%)	1.20	21 (21%) 2 1	68, 88, 130, 148	0
74	DO	81/82 (98%)	1.07	9 (11%) 10 6	77, 107, 173, 189	0
74	d	81/82 (98%)	0.89	4 (4%) 35 18	87, 107, 163, 179	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
75	DP	61/67 (91%)	0.68	3 (4%) 35 18	88, 112, 140, 161	0
75	e	62/67 (92%)	1.16	13 (20%) 2 1	96, 117, 142, 152	0
76	DQ	54/56 (96%)	0.95	5 (9%) 14 7	55, 70, 100, 118	0
76	f	55/56 (98%)	1.22	7 (12%) 8 5	82, 93, 120, 138	0
77	DR	58/63 (92%)	1.47	16 (27%) 1 1	69, 103, 170, 187	0
77	g	60/63 (95%)	1.24	10 (16%) 4 3	82, 113, 159, 176	0
78	DS	69/193 (35%)	2.35	39 (56%) 0 0	127, 179, 197, 217	0
78	h	70/193 (36%)	1.25	14 (20%) 3 2	132, 176, 195, 200	0
79	AR	311/317 (98%)	1.22	50 (16%) 4 3	130, 163, 185, 198	0
79	DT	311/317 (98%)	1.30	60 (19%) 3 2	114, 157, 182, 197	0
80	P0	107/312 (34%)	1.43	22 (20%) 2 2	115, 131, 144, 164	0
80	p0	107/312 (34%)	2.13	50 (46%) 0 0	123, 138, 154, 166	0
81	12	63/165 (38%)	1.05	9 (14%) 6 3	111, 134, 150, 158	0
82	L1	217/217 (100%)	1.08	29 (13%) 7 4	107, 133, 170, 237	0
82	l1	217/217 (100%)	1.29	42 (19%) 3 2	115, 140, 163, 206	0
All	All	33667/36349 (92%)	0.71	2754 (8%) 17 9	30, 86, 164, 472	0

The worst 5 of 2754 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
78	DS	127	TYR	9.6
4	j	250	GLN	7.3
6	AY	363	ASN	7.1
1	AS	1263	U	6.9
1	AS	1262	G	6.8

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
83	MG	1	3628	1/1	0.03	0.24	170,170,170,170	0
83	MG	B	1928	1/1	0.16	0.33	143,143,143,143	0
83	MG	B	1943	1/1	0.31	0.15	93,93,93,93	0
83	MG	I	301	1/1	0.32	0.37	123,123,123,123	0
83	MG	1	3922	1/1	0.33	0.19	84,84,84,84	0
83	MG	B	1952	1/1	0.36	0.16	75,75,75,75	0
83	MG	1	3782	1/1	0.39	0.31	68,68,68,68	0
83	MG	1	3594	1/1	0.39	0.30	84,84,84,84	0
83	MG	J	201	1/1	0.40	0.16	144,144,144,144	0
83	MG	1	3624	1/1	0.42	0.16	70,70,70,70	0
83	MG	1	3903	1/1	0.48	0.14	40,40,40,40	0
83	MG	Y	203	1/1	0.49	0.26	89,89,89,89	0
83	MG	B	1918	1/1	0.51	0.31	68,68,68,68	0
83	MG	B	1896	1/1	0.53	0.27	59,59,59,59	0
83	MG	1	3915	1/1	0.53	0.15	75,75,75,75	0
83	MG	1	3864	1/1	0.53	0.26	99,99,99,99	0
83	MG	3	211	1/1	0.53	0.24	86,86,86,86	0
83	MG	AT	203	1/1	0.54	0.35	68,68,68,68	0
83	MG	1	3856	1/1	0.55	0.26	67,67,67,67	0
83	MG	1	3804	1/1	0.55	0.23	63,63,63,63	0
83	MG	AD	201	1/1	0.55	0.20	81,81,81,81	0
85	ZN	DO	101	1/1	0.55	0.11	247,247,247,247	0
83	MG	B	1939	1/1	0.56	0.20	117,117,117,117	0
83	MG	B	1876	1/1	0.56	0.41	82,82,82,82	0
83	MG	1	3721	1/1	0.57	0.18	101,101,101,101	0
83	MG	AS	3575	1/1	0.58	0.27	57,57,57,57	0
83	MG	1	3809	1/1	0.59	0.23	61,61,61,61	0
83	MG	B	1945	1/1	0.60	0.22	103,103,103,103	0
83	MG	1	3758	1/1	0.60	0.39	77,77,77,77	0
83	MG	1	3920	1/1	0.60	0.18	60,60,60,60	0
83	MG	1	3607	1/1	0.60	0.15	58,58,58,58	0
83	MG	1	3801	1/1	0.60	0.26	102,102,102,102	0
83	MG	1	3601	1/1	0.60	0.24	73,73,73,73	0
83	MG	AS	3622	1/1	0.60	0.31	66,66,66,66	0
83	MG	B	1942	1/1	0.60	0.20	79,79,79,79	0
83	MG	AT	204	1/1	0.60	0.28	78,78,78,78	0
83	MG	B	1864	1/1	0.60	0.17	87,87,87,87	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
83	MG	1	3846	1/1	0.61	0.11	63,63,63,63	0
83	MG	AS	3645	1/1	0.61	0.16	54,54,54,54	0
83	MG	1	3926	1/1	0.61	0.14	50,50,50,50	0
83	MG	1	3463	1/1	0.61	0.38	57,57,57,57	0
83	MG	AS	3601	1/1	0.61	0.21	51,51,51,51	0
83	MG	1	3800	1/1	0.62	0.26	73,73,73,73	0
83	MG	AS	3492	1/1	0.62	0.22	43,43,43,43	0
83	MG	1	3908	1/1	0.62	0.27	59,59,59,59	0
83	MG	AS	3591	1/1	0.62	0.30	85,85,85,85	0
83	MG	B	1846	1/1	0.62	0.14	70,70,70,70	0
83	MG	B	1806	1/1	0.63	0.34	67,67,67,67	0
83	MG	AS	3672	1/1	0.63	0.30	57,57,57,57	0
83	MG	1	3917	1/1	0.63	0.13	62,62,62,62	0
83	MG	1	3930	1/1	0.63	0.20	88,88,88,88	0
83	MG	CM	1877	1/1	0.63	0.22	86,86,86,86	0
83	MG	B	1804	1/1	0.63	0.29	74,74,74,74	0
83	MG	1	3696	1/1	0.64	0.14	202,202,202,202	0
83	MG	1	3889	1/1	0.64	0.16	58,58,58,58	0
83	MG	AW	303	1/1	0.64	0.22	53,53,53,53	0
83	MG	B	1823	1/1	0.64	0.31	59,59,59,59	0
83	MG	AE	202	1/1	0.64	0.15	90,90,90,90	0
83	MG	AS	3522	1/1	0.65	0.46	60,60,60,60	0
83	MG	1	3668	1/1	0.65	0.14	50,50,50,50	0
85	ZN	d	101	1/1	0.65	0.15	257,257,257,257	0
83	MG	AS	3670	1/1	0.65	0.19	62,62,62,62	0
83	MG	AS	3675	1/1	0.66	0.20	64,64,64,64	0
83	MG	1	3785	1/1	0.66	0.18	83,83,83,83	0
83	MG	1	3857	1/1	0.66	0.12	59,59,59,59	0
83	MG	AS	3571	1/1	0.66	0.17	46,46,46,46	0
83	MG	AS	3667	1/1	0.66	0.12	44,44,44,44	0
83	MG	B	1949	1/1	0.66	0.30	65,65,65,65	0
83	MG	B	1951	1/1	0.66	0.20	77,77,77,77	0
83	MG	1	3583	1/1	0.67	0.18	61,61,61,61	0
83	MG	AS	3533	1/1	0.67	0.25	59,59,59,59	0
83	MG	CL	302	1/1	0.67	0.47	78,78,78,78	0
83	MG	CM	1819	1/1	0.67	0.26	65,65,65,65	0
83	MG	1	3727	1/1	0.67	0.16	60,60,60,60	0
83	MG	AS	3636	1/1	0.67	0.21	66,66,66,66	0
83	MG	1	3564	1/1	0.67	0.20	70,70,70,70	0
83	MG	AS	3454	1/1	0.68	0.27	59,59,59,59	0
83	MG	4	202	1/1	0.68	0.22	62,62,62,62	0
83	MG	AS	3647	1/1	0.68	0.16	55,55,55,55	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
83	MG	AS	3611	1/1	0.68	0.22	55,55,55,55	0
83	MG	B	1837	1/1	0.68	0.09	319,319,319,319	0
83	MG	B	1835	1/1	0.69	0.22	71,71,71,71	0
83	MG	K	301	1/1	0.69	0.15	57,57,57,57	0
83	MG	9	203	1/1	0.69	0.23	82,82,82,82	0
83	MG	B	1817	1/1	0.69	0.28	67,67,67,67	0
83	MG	DA	201	1/1	0.69	0.28	65,65,65,65	0
83	MG	0	201	1/1	0.69	0.19	76,76,76,76	0
83	MG	AS	3597	1/1	0.69	0.20	136,136,136,136	0
83	MG	3	202	1/1	0.70	0.16	75,75,75,75	0
83	MG	AS	3609	1/1	0.70	0.19	56,56,56,56	0
83	MG	CN	301	1/1	0.70	0.27	65,65,65,65	0
83	MG	1	3821	1/1	0.70	0.21	44,44,44,44	0
83	MG	B	1898	1/1	0.70	0.19	75,75,75,75	0
83	MG	1	3819	1/1	0.70	0.23	54,54,54,54	0
83	MG	1	3842	1/1	0.71	0.23	69,69,69,69	0
83	MG	1	3892	1/1	0.71	0.14	50,50,50,50	0
83	MG	9	202	1/1	0.71	0.60	65,65,65,65	0
83	MG	AS	3520	1/1	0.71	0.33	53,53,53,53	0
83	MG	AS	3631	1/1	0.71	0.24	49,49,49,49	0
83	MG	1	3676	1/1	0.71	0.22	81,81,81,81	0
83	MG	1	3679	1/1	0.71	0.18	70,70,70,70	0
83	MG	B	1953	1/1	0.71	0.24	60,60,60,60	0
83	MG	B	1936	1/1	0.71	0.19	73,73,73,73	0
83	MG	1	3731	1/1	0.71	0.28	56,56,56,56	0
83	MG	1	3614	1/1	0.71	0.27	73,73,73,73	0
83	MG	B	1839	1/1	0.72	0.43	74,74,74,74	0
83	MG	CJ	202	1/1	0.72	0.21	62,62,62,62	0
83	MG	B	1897	1/1	0.72	0.20	70,70,70,70	0
83	MG	1	3599	1/1	0.72	0.23	53,53,53,53	0
83	MG	CM	1854	1/1	0.72	0.26	68,68,68,68	0
83	MG	CM	1872	1/1	0.72	0.23	73,73,73,73	0
83	MG	AS	3434	1/1	0.72	0.46	57,57,57,57	0
83	MG	CM	1885	1/1	0.72	0.27	68,68,68,68	0
83	MG	1	3736	1/1	0.72	0.23	59,59,59,59	0
83	MG	AS	3628	1/1	0.72	0.29	64,64,64,64	0
83	MG	AS	3587	1/1	0.72	0.24	83,83,83,83	0
83	MG	1	3878	1/1	0.72	0.20	69,69,69,69	0
83	MG	1	3580	1/1	0.73	0.21	71,71,71,71	0
83	MG	B	1922	1/1	0.73	0.18	67,67,67,67	0
83	MG	CM	1870	1/1	0.73	0.26	91,91,91,91	0
83	MG	4	211	1/1	0.73	0.10	68,68,68,68	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
83	MG	1	3671	1/1	0.73	0.16	61,61,61,61	0
83	MG	1	3449	1/1	0.73	0.23	43,43,43,43	0
83	MG	AS	3509	1/1	0.73	0.21	63,63,63,63	0
83	MG	BZ	203	1/1	0.73	0.17	88,88,88,88	0
83	MG	1	3565	1/1	0.73	0.26	66,66,66,66	0
83	MG	B	1912	1/1	0.73	0.16	71,71,71,71	0
83	MG	1	3450	1/1	0.74	0.33	45,45,45,45	0
83	MG	4	205	1/1	0.74	0.15	39,39,39,39	0
83	MG	1	3841	1/1	0.74	0.17	48,48,48,48	0
83	MG	CM	1866	1/1	0.74	0.20	68,68,68,68	0
83	MG	1	3722	1/1	0.74	0.26	60,60,60,60	0
83	MG	B	1832	1/1	0.74	0.34	63,63,63,63	0
83	MG	1	3681	1/1	0.74	0.17	35,35,35,35	0
83	MG	1	3847	1/1	0.74	0.36	63,63,63,63	0
83	MG	B	1838	1/1	0.74	0.27	47,47,47,47	0
83	MG	1	3539	1/1	0.74	0.24	55,55,55,55	0
83	MG	AS	3536	1/1	0.74	0.27	76,76,76,76	0
85	ZN	CB	201	1/1	0.74	0.13	235,235,235,235	0
83	MG	1	3794	1/1	0.74	0.17	42,42,42,42	0
83	MG	CM	1822	1/1	0.75	0.20	51,51,51,51	0
83	MG	AH	203	1/1	0.75	0.29	77,77,77,77	0
83	MG	1	3598	1/1	0.75	0.29	75,75,75,75	0
83	MG	1	3858	1/1	0.75	0.21	79,79,79,79	0
83	MG	0	203	1/1	0.75	0.18	55,55,55,55	0
83	MG	B	1866	1/1	0.75	0.26	73,73,73,73	0
83	MG	B	1937	1/1	0.75	0.13	56,56,56,56	0
83	MG	1	3808	1/1	0.75	0.28	100,100,100,100	0
83	MG	AS	3634	1/1	0.75	0.28	66,66,66,66	0
83	MG	1	3460	1/1	0.75	0.27	41,41,41,41	0
83	MG	1	3575	1/1	0.75	0.21	65,65,65,65	0
83	MG	1	3577	1/1	0.75	0.26	45,45,45,45	0
83	MG	1	3569	1/1	0.76	0.20	48,48,48,48	0
83	MG	1	3527	1/1	0.76	0.14	56,56,56,56	0
83	MG	1	3558	1/1	0.76	0.27	68,68,68,68	0
83	MG	B	1934	1/1	0.76	0.15	98,98,98,98	0
83	MG	B	1892	1/1	0.76	0.44	64,64,64,64	0
83	MG	w	302	1/1	0.76	0.21	51,51,51,51	0
83	MG	1	3650	1/1	0.76	0.28	55,55,55,55	0
83	MG	1	3871	1/1	0.76	0.19	51,51,51,51	0
83	MG	CM	1834	1/1	0.76	0.30	49,49,49,49	0
83	MG	1	3595	1/1	0.76	0.12	57,57,57,57	0
83	MG	AS	3421	1/1	0.77	0.48	50,50,50,50	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
83	MG	1	3905	1/1	0.77	0.11	39,39,39,39	0
83	MG	1	3925	1/1	0.77	0.19	73,73,73,73	0
83	MG	AS	3490	1/1	0.77	0.25	55,55,55,55	0
83	MG	AG	202	1/1	0.77	0.13	56,56,56,56	0
83	MG	B	1902	1/1	0.77	0.23	94,94,94,94	0
83	MG	1	3717	1/1	0.77	0.18	54,54,54,54	0
83	MG	B	1841	1/1	0.77	0.21	48,48,48,48	0
83	MG	1	3684	1/1	0.77	0.18	86,86,86,86	0
83	MG	AS	3642	1/1	0.77	0.19	58,58,58,58	0
83	MG	AS	3534	1/1	0.77	0.31	64,64,64,64	0
83	MG	AS	3535	1/1	0.77	0.23	65,65,65,65	0
83	MG	B	1927	1/1	0.77	0.13	49,49,49,49	0
83	MG	1	3931	1/1	0.77	0.14	71,71,71,71	0
83	MG	1	3932	1/1	0.77	0.15	71,71,71,71	0
83	MG	AS	3583	1/1	0.77	0.19	59,59,59,59	0
83	MG	1	3563	1/1	0.77	0.19	52,52,52,52	0
83	MG	1	3754	1/1	0.77	0.27	66,66,66,66	0
83	MG	BH	201	1/1	0.78	0.15	52,52,52,52	0
83	MG	1	3894	1/1	0.78	0.18	73,73,73,73	0
83	MG	B	1844	1/1	0.78	0.10	67,67,67,67	0
83	MG	AS	3540	1/1	0.78	0.18	42,42,42,42	0
83	MG	AS	3461	1/1	0.78	0.29	63,63,63,63	0
83	MG	AS	3641	1/1	0.78	0.21	63,63,63,63	0
83	MG	AS	3481	1/1	0.78	0.23	96,96,96,96	0
83	MG	1	3814	1/1	0.78	0.23	54,54,54,54	0
83	MG	m	301	1/1	0.78	0.15	65,65,65,65	0
83	MG	1	3921	1/1	0.78	0.27	68,68,68,68	0
83	MG	AS	3514	1/1	0.78	0.32	63,63,63,63	0
83	MG	1	3784	1/1	0.78	0.21	51,51,51,51	0
83	MG	Q	203	1/1	0.78	0.24	64,64,64,64	0
83	MG	1	3737	1/1	0.78	0.18	29,29,29,29	0
83	MG	1	3836	1/1	0.78	0.21	81,81,81,81	0
83	MG	AS	3623	1/1	0.78	0.16	59,59,59,59	0
83	MG	BE	303	1/1	0.78	0.10	45,45,45,45	0
83	MG	BF	201	1/1	0.78	0.14	70,70,70,70	0
83	MG	B	1861	1/1	0.79	0.16	83,83,83,83	0
83	MG	1	3767	1/1	0.79	0.21	36,36,36,36	0
83	MG	1	3928	1/1	0.79	0.13	52,52,52,52	0
83	MG	1	3815	1/1	0.79	0.17	73,73,73,73	0
83	MG	B	1887	1/1	0.79	0.30	74,74,74,74	0
83	MG	1	3724	1/1	0.79	0.11	34,34,34,34	0
83	MG	B	1895	1/1	0.79	0.12	55,55,55,55	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
83	MG	1	3470	1/1	0.79	0.21	37,37,37,37	0
83	MG	BN	201	1/1	0.79	0.08	71,71,71,71	0
83	MG	1	3584	1/1	0.79	0.17	54,54,54,54	0
83	MG	3	208	1/1	0.79	0.23	74,74,74,74	0
83	MG	1	3518	1/1	0.79	0.20	60,60,60,60	0
83	MG	CM	1806	1/1	0.79	0.16	52,52,52,52	0
83	MG	B	1903	1/1	0.79	0.19	70,70,70,70	0
83	MG	B	1907	1/1	0.79	0.38	56,56,56,56	0
83	MG	AS	3450	1/1	0.79	0.23	32,32,32,32	0
83	MG	3	212	1/1	0.79	0.20	60,60,60,60	0
83	MG	1	3797	1/1	0.79	0.34	52,52,52,52	0
83	MG	AS	3466	1/1	0.79	0.15	58,58,58,58	0
83	MG	1	3609	1/1	0.79	0.14	47,47,47,47	0
83	MG	1	3750	1/1	0.79	0.11	46,46,46,46	0
83	MG	1	3803	1/1	0.79	0.17	39,39,39,39	0
83	MG	1	3432	1/1	0.79	0.22	59,59,59,59	0
83	MG	B	1840	1/1	0.79	0.22	75,75,75,75	0
85	ZN	AP	201	1/1	0.79	0.19	209,209,209,209	0
83	MG	1	3755	1/1	0.79	0.24	63,63,63,63	0
83	MG	1	3453	1/1	0.79	0.16	46,46,46,46	0
85	ZN	CJ	201	1/1	0.79	0.17	222,222,222,222	0
83	MG	1	3869	1/1	0.79	0.12	66,66,66,66	0
83	MG	AS	3437	1/1	0.80	0.20	48,48,48,48	0
83	MG	1	3592	1/1	0.80	0.29	64,64,64,64	0
83	MG	AS	3584	1/1	0.80	0.16	46,46,46,46	0
83	MG	1	3481	1/1	0.80	0.30	41,41,41,41	0
83	MG	AS	3589	1/1	0.80	0.22	51,51,51,51	0
83	MG	AS	3458	1/1	0.80	0.20	80,80,80,80	0
83	MG	1	3531	1/1	0.80	0.19	43,43,43,43	0
83	MG	1	3581	1/1	0.80	0.19	57,57,57,57	0
83	MG	AS	3470	1/1	0.80	0.22	72,72,72,72	0
83	MG	1	3574	1/1	0.80	0.22	55,55,55,55	0
83	MG	CM	1813	1/1	0.80	0.37	60,60,60,60	0
83	MG	AS	3483	1/1	0.80	0.12	54,54,54,54	0
83	MG	1	3633	1/1	0.80	0.25	45,45,45,45	0
83	MG	1	3876	1/1	0.80	0.11	45,45,45,45	0
83	MG	CM	1840	1/1	0.80	0.17	48,48,48,48	0
83	MG	AS	3493	1/1	0.80	0.16	50,50,50,50	0
83	MG	1	3805	1/1	0.80	0.17	45,45,45,45	0
83	MG	B	1916	1/1	0.80	0.28	66,66,66,66	0
83	MG	AS	3517	1/1	0.80	0.31	50,50,50,50	0
83	MG	CM	1876	1/1	0.80	0.27	38,38,38,38	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
83	MG	1	3883	1/1	0.80	0.20	46,46,46,46	0
83	MG	CM	1884	1/1	0.80	0.13	46,46,46,46	0
83	MG	AS	3643	1/1	0.80	0.20	37,37,37,37	0
83	MG	CM	1901	1/1	0.80	0.11	45,45,45,45	0
83	MG	1	3923	1/1	0.80	0.31	64,64,64,64	0
83	MG	B	1923	1/1	0.80	0.17	78,78,78,78	0
83	MG	1	3924	1/1	0.80	0.28	67,67,67,67	0
83	MG	1	3418	1/1	0.80	0.10	47,47,47,47	0
83	MG	AS	3419	1/1	0.80	0.26	39,39,39,39	0
83	MG	B	1831	1/1	0.80	0.37	52,52,52,52	0
83	MG	1	3703	1/1	0.80	0.11	63,63,63,63	0
83	MG	B	1911	1/1	0.81	0.25	63,63,63,63	0
83	MG	1	3540	1/1	0.81	0.30	51,51,51,51	0
83	MG	1	3734	1/1	0.81	0.45	59,59,59,59	0
83	MG	1	3929	1/1	0.81	0.22	71,71,71,71	0
83	MG	AS	3427	1/1	0.81	0.20	66,66,66,66	0
83	MG	1	3686	1/1	0.81	0.08	100,100,100,100	0
83	MG	B	1857	1/1	0.81	0.09	55,55,55,55	0
83	MG	B	1860	1/1	0.81	0.14	68,68,68,68	0
83	MG	1	3899	1/1	0.81	0.20	59,59,59,59	0
83	MG	AS	3455	1/1	0.81	0.39	46,46,46,46	0
83	MG	1	3687	1/1	0.81	0.21	64,64,64,64	0
83	MG	AS	3593	1/1	0.81	0.08	41,41,41,41	0
83	MG	B	1935	1/1	0.81	0.19	88,88,88,88	0
83	MG	1	3691	1/1	0.81	0.18	87,87,87,87	0
83	MG	1	3570	1/1	0.81	0.22	47,47,47,47	0
83	MG	AS	3480	1/1	0.81	0.20	52,52,52,52	0
83	MG	B	1882	1/1	0.81	0.19	36,36,36,36	0
83	MG	1	3405	1/1	0.81	0.36	40,40,40,40	0
83	MG	AS	3625	1/1	0.81	0.16	85,85,85,85	0
83	MG	CM	1864	1/1	0.81	0.26	67,67,67,67	0
83	MG	1	3861	1/1	0.81	0.10	81,81,81,81	0
83	MG	1	3530	1/1	0.81	0.25	54,54,54,54	0
83	MG	AS	3633	1/1	0.81	0.22	99,99,99,99	0
83	MG	1	3673	1/1	0.81	0.14	59,59,59,59	0
83	MG	AS	3505	1/1	0.81	0.30	59,59,59,59	0
83	MG	CM	1879	1/1	0.81	0.19	54,54,54,54	0
83	MG	CM	1883	1/1	0.81	0.24	63,63,63,63	0
83	MG	1	3576	1/1	0.81	0.27	69,69,69,69	0
83	MG	j	302	1/1	0.81	0.13	69,69,69,69	0
83	MG	B	1900	1/1	0.81	0.24	88,88,88,88	0
83	MG	AS	3644	1/1	0.81	0.22	54,54,54,54	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
83	MG	1	3445	1/1	0.81	0.34	53,53,53,53	0
83	MG	DB	203	1/1	0.81	0.21	56,56,56,56	0
85	ZN	AH	201	1/1	0.81	0.09	179,179,179,179	0
83	MG	AS	3521	1/1	0.81	0.26	56,56,56,56	0
83	MG	AS	3655	1/1	0.81	0.18	49,49,49,49	0
83	MG	AS	3662	1/1	0.81	0.15	103,103,103,103	0
83	MG	1	3521	1/1	0.81	0.27	52,52,52,52	0
83	MG	1	3730	1/1	0.81	0.26	48,48,48,48	0
83	MG	1	3852	1/1	0.82	0.16	64,64,64,64	0
83	MG	B	1850	1/1	0.82	0.16	43,43,43,43	0
83	MG	B	1855	1/1	0.82	0.14	71,71,71,71	0
83	MG	1	3579	1/1	0.82	0.11	38,38,38,38	0
83	MG	1	3900	1/1	0.82	0.23	52,52,52,52	0
83	MG	AE	201	1/1	0.82	0.12	88,88,88,88	0
83	MG	AS	3610	1/1	0.82	0.15	31,31,31,31	0
83	MG	1	3799	1/1	0.82	0.31	68,68,68,68	0
83	MG	1	3818	1/1	0.82	0.15	46,46,46,46	0
83	MG	1	3646	1/1	0.82	0.15	48,48,48,48	0
83	MG	B	1881	1/1	0.82	0.21	64,64,64,64	0
83	MG	1	3497	1/1	0.82	0.26	45,45,45,45	0
83	MG	B	1885	1/1	0.82	0.14	92,92,92,92	0
83	MG	B	1946	1/1	0.82	0.25	69,69,69,69	0
83	MG	1	3694	1/1	0.82	0.26	29,29,29,29	0
83	MG	1	3839	1/1	0.82	0.15	43,43,43,43	0
83	MG	4	203	1/1	0.82	0.27	69,69,69,69	0
83	MG	B	1826	1/1	0.82	0.16	51,51,51,51	0
83	MG	G	301	1/1	0.82	0.14	66,66,66,66	0
83	MG	B	1830	1/1	0.82	0.28	59,59,59,59	0
83	MG	1	3875	1/1	0.82	0.10	53,53,53,53	0
83	MG	4	207	1/1	0.82	0.17	48,48,48,48	0
83	MG	1	3840	1/1	0.82	0.19	49,49,49,49	0
83	MG	1	3738	1/1	0.82	0.31	24,24,24,24	0
83	MG	k	403	1/1	0.82	0.16	60,60,60,60	0
83	MG	AS	3669	1/1	0.82	0.14	64,64,64,64	0
83	MG	1	3881	1/1	0.82	0.15	64,64,64,64	0
83	MG	1	3422	1/1	0.82	0.33	28,28,28,28	0
83	MG	AS	3674	1/1	0.82	0.13	49,49,49,49	0
83	MG	B	1914	1/1	0.82	0.13	56,56,56,56	0
83	MG	1	3790	1/1	0.82	0.26	52,52,52,52	0
83	MG	AS	3586	1/1	0.82	0.25	52,52,52,52	0
83	MG	AU	201	1/1	0.82	0.14	66,66,66,66	0
83	MG	1	3417	1/1	0.82	0.20	41,41,41,41	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
83	MG	AT	207	1/1	0.83	0.19	58,58,58,58	0
83	MG	AT	210	1/1	0.83	0.21	69,69,69,69	0
83	MG	1	3647	1/1	0.83	0.23	50,50,50,50	0
83	MG	1	3618	1/1	0.83	0.22	55,55,55,55	0
83	MG	1	3891	1/1	0.83	0.18	75,75,75,75	0
83	MG	1	3652	1/1	0.83	0.19	70,70,70,70	0
83	MG	AS	3459	1/1	0.83	0.19	63,63,63,63	0
83	MG	AS	3600	1/1	0.83	0.29	51,51,51,51	0
83	MG	1	3619	1/1	0.83	0.13	44,44,44,44	0
83	MG	AG	201	1/1	0.83	0.17	80,80,80,80	0
83	MG	1	3623	1/1	0.83	0.17	56,56,56,56	0
83	MG	1	3697	1/1	0.83	0.13	55,55,55,55	0
83	MG	CM	1809	1/1	0.83	0.30	95,95,95,95	0
83	MG	B	1941	1/1	0.83	0.10	86,86,86,86	0
83	MG	1	3901	1/1	0.83	0.15	41,41,41,41	0
83	MG	B	1805	1/1	0.83	0.21	76,76,76,76	0
83	MG	CM	1823	1/1	0.83	0.24	41,41,41,41	0
83	MG	1	3745	1/1	0.83	0.21	45,45,45,45	0
83	MG	B	1891	1/1	0.83	0.17	52,52,52,52	0
83	MG	CM	1848	1/1	0.83	0.23	46,46,46,46	0
83	MG	1	3499	1/1	0.83	0.23	33,33,33,33	0
83	MG	1	3626	1/1	0.83	0.16	60,60,60,60	0
83	MG	1	3718	1/1	0.83	0.12	43,43,43,43	0
83	MG	1	3468	1/1	0.83	0.28	50,50,50,50	0
83	MG	1	3765	1/1	0.83	0.19	38,38,38,38	0
83	MG	1	3680	1/1	0.83	0.24	34,34,34,34	0
83	MG	1	3773	1/1	0.83	0.22	39,39,39,39	0
83	MG	AS	3530	1/1	0.83	0.24	38,38,38,38	0
83	MG	1	3586	1/1	0.83	0.12	64,64,64,64	0
83	MG	AS	3648	1/1	0.83	0.11	58,58,58,58	0
83	MG	AS	3651	1/1	0.83	0.15	59,59,59,59	0
83	MG	o	301	1/1	0.83	0.17	42,42,42,42	0
83	MG	v	301	1/1	0.83	0.20	39,39,39,39	0
83	MG	CQ	301	1/1	0.83	0.22	57,57,57,57	0
83	MG	AS	3413	1/1	0.83	0.17	51,51,51,51	0
83	MG	1	3475	1/1	0.83	0.15	50,50,50,50	0
83	MG	AS	3567	1/1	0.83	0.21	34,34,34,34	0
83	MG	1	3835	1/1	0.83	0.14	49,49,49,49	0
83	MG	1	3728	1/1	0.83	0.09	54,54,54,54	0
83	MG	AS	3428	1/1	0.83	0.19	32,32,32,32	0
83	MG	2	202	1/1	0.83	0.19	52,52,52,52	0
83	MG	8	202	1/1	0.83	0.16	60,60,60,60	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
83	MG	1	3862	1/1	0.84	0.12	56,56,56,56	0
83	MG	L	201	1/1	0.84	0.33	73,73,73,73	0
83	MG	1	3863	1/1	0.84	0.10	62,62,62,62	0
83	MG	1	3641	1/1	0.84	0.33	56,56,56,56	0
83	MG	a	201	1/1	0.84	0.12	75,75,75,75	0
83	MG	CM	1839	1/1	0.84	0.41	62,62,62,62	0
83	MG	1	3825	1/1	0.84	0.11	29,29,29,29	0
83	MG	AS	3496	1/1	0.84	0.22	49,49,49,49	0
83	MG	AS	3503	1/1	0.84	0.36	58,58,58,58	0
83	MG	1	3896	1/1	0.84	0.18	49,49,49,49	0
83	MG	AS	3599	1/1	0.84	0.25	61,61,61,61	0
83	MG	B	1906	1/1	0.84	0.12	46,46,46,46	0
83	MG	AS	3512	1/1	0.84	0.25	35,35,35,35	0
83	MG	1	3543	1/1	0.84	0.17	52,52,52,52	0
83	MG	AS	3516	1/1	0.84	0.23	43,43,43,43	0
83	MG	B	1909	1/1	0.84	0.09	62,62,62,62	0
83	MG	AS	3617	1/1	0.84	0.18	55,55,55,55	0
83	MG	AS	3621	1/1	0.84	0.25	60,60,60,60	0
83	MG	B	1944	1/1	0.84	0.08	87,87,87,87	0
83	MG	1	3874	1/1	0.84	0.17	57,57,57,57	0
83	MG	1	3591	1/1	0.84	0.18	51,51,51,51	0
83	MG	1	3837	1/1	0.84	0.20	61,61,61,61	0
83	MG	1	3817	1/1	0.84	0.12	31,31,31,31	0
83	MG	1	3503	1/1	0.84	0.34	48,48,48,48	0
83	MG	1	3882	1/1	0.84	0.21	49,49,49,49	0
83	MG	1	3786	1/1	0.84	0.12	40,40,40,40	0
83	MG	1	3919	1/1	0.84	0.11	58,58,58,58	0
83	MG	CM	1804	1/1	0.84	0.27	40,40,40,40	0
83	MG	AS	3469	1/1	0.84	0.27	54,54,54,54	0
83	MG	B	1814	1/1	0.84	0.33	64,64,64,64	0
83	MG	AS	3471	1/1	0.85	0.24	48,48,48,48	0
83	MG	1	3454	1/1	0.85	0.29	26,26,26,26	0
83	MG	1	3653	1/1	0.85	0.11	40,40,40,40	0
83	MG	AU	202	1/1	0.85	0.22	50,50,50,50	0
83	MG	AS	3596	1/1	0.85	0.24	56,56,56,56	0
83	MG	B	1836	1/1	0.85	0.18	49,49,49,49	0
83	MG	1	3548	1/1	0.85	0.24	40,40,40,40	0
83	MG	1	3556	1/1	0.85	0.10	64,64,64,64	0
83	MG	1	3860	1/1	0.85	0.23	58,58,58,58	0
83	MG	AS	3606	1/1	0.85	0.10	52,52,52,52	0
83	MG	1	3700	1/1	0.85	0.08	49,49,49,49	0
83	MG	AS	3498	1/1	0.85	0.12	25,25,25,25	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
83	MG	AS	3501	1/1	0.85	0.21	49,49,49,49	0
83	MG	1	3822	1/1	0.85	0.24	52,52,52,52	0
83	MG	AS	3620	1/1	0.85	0.12	45,45,45,45	0
83	MG	AS	3504	1/1	0.85	0.28	37,37,37,37	0
83	MG	CM	1817	1/1	0.85	0.27	38,38,38,38	0
83	MG	1	3627	1/1	0.85	0.13	57,57,57,57	0
83	MG	AB	201	1/1	0.85	0.16	57,57,57,57	0
83	MG	1	3832	1/1	0.85	0.13	36,36,36,36	0
83	MG	CM	1829	1/1	0.85	0.28	47,47,47,47	0
83	MG	1	3747	1/1	0.85	0.17	47,47,47,47	0
83	MG	1	3870	1/1	0.85	0.23	50,50,50,50	0
83	MG	AS	3414	1/1	0.85	0.36	65,65,65,65	0
83	MG	4	201	1/1	0.85	0.15	76,76,76,76	0
83	MG	1	3603	1/1	0.85	0.08	51,51,51,51	0
83	MG	CM	1861	1/1	0.85	0.34	50,50,50,50	0
83	MG	1	3446	1/1	0.85	0.33	32,32,32,32	0
83	MG	1	3918	1/1	0.85	0.10	67,67,67,67	0
83	MG	AS	3433	1/1	0.85	0.28	31,31,31,31	0
83	MG	B	1869	1/1	0.85	0.24	55,55,55,55	0
83	MG	B	1872	1/1	0.85	0.27	70,70,70,70	0
83	MG	AS	3646	1/1	0.85	0.10	49,49,49,49	0
83	MG	CM	1878	1/1	0.85	0.21	47,47,47,47	0
83	MG	1	3637	1/1	0.85	0.10	39,39,39,39	0
83	MG	1	3559	1/1	0.85	0.19	64,64,64,64	0
83	MG	AS	3649	1/1	0.85	0.13	76,76,76,76	0
83	MG	AS	3543	1/1	0.85	0.27	53,53,53,53	0
83	MG	CM	1896	1/1	0.85	0.27	40,40,40,40	0
83	MG	AS	3545	1/1	0.85	0.14	49,49,49,49	0
83	MG	AS	3661	1/1	0.85	0.24	71,71,71,71	0
83	MG	CP	301	1/1	0.85	0.22	41,41,41,41	0
83	MG	AS	3564	1/1	0.85	0.16	46,46,46,46	0
83	MG	B	1809	1/1	0.85	0.23	50,50,50,50	0
83	MG	1	3443	1/1	0.85	0.23	56,56,56,56	0
83	MG	1	3465	1/1	0.85	0.17	45,45,45,45	0
83	MG	AS	3579	1/1	0.85	0.27	51,51,51,51	0
83	MG	1	3484	1/1	0.85	0.13	44,44,44,44	0
85	ZN	h	201	1/1	0.85	0.10	228,228,228,228	0
83	MG	1	3690	1/1	0.85	0.14	47,47,47,47	0
83	MG	r	303	1/1	0.85	0.11	53,53,53,53	0
83	MG	s	201	1/1	0.85	0.21	52,52,52,52	0
83	MG	1	3774	1/1	0.86	0.12	50,50,50,50	0
83	MG	1	3781	1/1	0.86	0.24	32,32,32,32	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
83	MG	B	1884	1/1	0.86	0.12	81,81,81,81	0
83	MG	AS	3544	1/1	0.86	0.19	56,56,56,56	0
83	MG	1	3826	1/1	0.86	0.23	47,47,47,47	0
83	MG	AS	3557	1/1	0.86	0.24	49,49,49,49	0
83	MG	AT	209	1/1	0.86	0.25	51,51,51,51	0
83	MG	AS	3559	1/1	0.86	0.26	46,46,46,46	0
83	MG	1	3504	1/1	0.86	0.14	43,43,43,43	0
83	MG	AS	3411	1/1	0.86	0.31	25,25,25,25	0
83	MG	1	3483	1/1	0.86	0.19	54,54,54,54	0
83	MG	BB	303	1/1	0.86	0.15	38,38,38,38	0
83	MG	BB	304	1/1	0.86	0.32	71,71,71,71	0
83	MG	1	3573	1/1	0.86	0.15	40,40,40,40	0
83	MG	1	3544	1/1	0.86	0.22	46,46,46,46	0
83	MG	AM	101	1/1	0.86	0.22	45,45,45,45	0
83	MG	i	301	1/1	0.86	0.21	54,54,54,54	0
83	MG	1	3787	1/1	0.86	0.22	47,47,47,47	0
83	MG	CA	201	1/1	0.86	0.10	56,56,56,56	0
83	MG	3	209	1/1	0.86	0.22	54,54,54,54	0
83	MG	1	3433	1/1	0.86	0.26	33,33,33,33	0
83	MG	1	3631	1/1	0.86	0.09	30,30,30,30	0
83	MG	AS	3592	1/1	0.86	0.20	62,62,62,62	0
83	MG	CM	1808	1/1	0.86	0.32	91,91,91,91	0
83	MG	3	213	1/1	0.86	0.19	69,69,69,69	0
83	MG	1	3893	1/1	0.86	0.15	50,50,50,50	0
83	MG	CM	1814	1/1	0.86	0.22	43,43,43,43	0
83	MG	1	3550	1/1	0.86	0.21	57,57,57,57	0
83	MG	B	1825	1/1	0.86	0.26	57,57,57,57	0
83	MG	1	3555	1/1	0.86	0.12	36,36,36,36	0
83	MG	B	1828	1/1	0.86	0.14	62,62,62,62	0
83	MG	B	1915	1/1	0.86	0.16	59,59,59,59	0
83	MG	1	3897	1/1	0.86	0.21	53,53,53,53	0
83	MG	1	3735	1/1	0.86	0.24	58,58,58,58	0
83	MG	B	1919	1/1	0.86	0.22	72,72,72,72	0
83	MG	1	3638	1/1	0.86	0.13	48,48,48,48	0
83	MG	CM	1853	1/1	0.86	0.12	33,33,33,33	0
83	MG	1	3853	1/1	0.86	0.19	50,50,50,50	0
83	MG	CM	1858	1/1	0.86	0.12	35,35,35,35	0
83	MG	1	3688	1/1	0.86	0.16	33,33,33,33	0
83	MG	AS	3486	1/1	0.86	0.25	30,30,30,30	0
83	MG	k	404	1/1	0.86	0.20	80,80,80,80	0
83	MG	1	3640	1/1	0.86	0.12	51,51,51,51	0
83	MG	1	3524	1/1	0.86	0.20	43,43,43,43	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
83	MG	1	3526	1/1	0.86	0.19	53,53,53,53	0
83	MG	1	3494	1/1	0.86	0.18	66,66,66,66	0
83	MG	1	3439	1/1	0.86	0.21	35,35,35,35	0
83	MG	B	1940	1/1	0.86	0.16	83,83,83,83	0
83	MG	v	304	1/1	0.86	0.21	76,76,76,76	0
83	MG	1	3423	1/1	0.86	0.21	61,61,61,61	0
83	MG	z	201	1/1	0.86	0.11	69,69,69,69	0
83	MG	CM	1893	1/1	0.86	0.23	37,37,37,37	0
83	MG	CM	1895	1/1	0.86	0.25	47,47,47,47	0
83	MG	1	3702	1/1	0.86	0.09	46,46,46,46	0
83	MG	1	3419	1/1	0.86	0.11	56,56,56,56	0
83	MG	0	205	1/1	0.86	0.21	59,59,59,59	0
83	MG	2	201	1/1	0.86	0.28	102,102,102,102	0
83	MG	AS	3518	1/1	0.86	0.26	36,36,36,36	0
83	MG	1	3622	1/1	0.86	0.25	47,47,47,47	0
83	MG	1	3669	1/1	0.86	0.08	34,34,34,34	0
83	MG	1	3872	1/1	0.86	0.13	51,51,51,51	0
83	MG	AS	3524	1/1	0.86	0.12	46,46,46,46	0
83	MG	D	301	1/1	0.86	0.25	61,61,61,61	0
83	MG	AS	3665	1/1	0.86	0.39	63,63,63,63	0
83	MG	1	3873	1/1	0.86	0.15	41,41,41,41	0
83	MG	B	1878	1/1	0.86	0.24	60,60,60,60	0
83	MG	B	1879	1/1	0.86	0.23	43,43,43,43	0
83	MG	1	3525	1/1	0.87	0.23	58,58,58,58	0
83	MG	1	3582	1/1	0.87	0.28	55,55,55,55	0
83	MG	1	3629	1/1	0.87	0.22	37,37,37,37	0
83	MG	AS	3422	1/1	0.87	0.21	51,51,51,51	0
83	MG	AF	201	1/1	0.87	0.10	46,46,46,46	0
83	MG	1	3551	1/1	0.87	0.18	50,50,50,50	0
83	MG	AS	3513	1/1	0.87	0.27	50,50,50,50	0
83	MG	AS	3598	1/1	0.87	0.11	74,74,74,74	0
83	MG	1	3438	1/1	0.87	0.21	31,31,31,31	0
83	MG	1	3620	1/1	0.87	0.13	44,44,44,44	0
83	MG	AS	3436	1/1	0.87	0.34	43,43,43,43	0
83	MG	CM	1863	1/1	0.87	0.31	56,56,56,56	0
83	MG	1	3693	1/1	0.87	0.15	42,42,42,42	0
83	MG	AS	3441	1/1	0.87	0.30	52,52,52,52	0
83	MG	AS	3443	1/1	0.87	0.26	33,33,33,33	0
83	MG	1	3729	1/1	0.87	0.23	53,53,53,53	0
83	MG	CM	1875	1/1	0.87	0.18	71,71,71,71	0
83	MG	1	3621	1/1	0.87	0.11	60,60,60,60	0
83	MG	AS	3618	1/1	0.87	0.11	49,49,49,49	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
83	MG	1	3455	1/1	0.87	0.22	31,31,31,31	0
83	MG	B	1858	1/1	0.87	0.25	53,53,53,53	0
83	MG	1	3904	1/1	0.87	0.13	68,68,68,68	0
83	MG	3	203	1/1	0.87	0.25	46,46,46,46	0
83	MG	1	3602	1/1	0.87	0.19	50,50,50,50	0
83	MG	B	1913	1/1	0.87	0.15	62,62,62,62	0
83	MG	AS	3630	1/1	0.87	0.12	64,64,64,64	0
83	MG	1	3812	1/1	0.87	0.13	51,51,51,51	0
83	MG	CM	1897	1/1	0.87	0.31	35,35,35,35	0
83	MG	1	3909	1/1	0.87	0.15	40,40,40,40	0
83	MG	CM	1903	1/1	0.87	0.12	43,43,43,43	0
83	MG	B	1824	1/1	0.87	0.17	36,36,36,36	0
83	MG	1	3457	1/1	0.87	0.29	21,21,21,21	0
83	MG	1	3488	1/1	0.87	0.14	56,56,56,56	0
83	MG	AS	3484	1/1	0.87	0.22	40,40,40,40	0
83	MG	DB	202	1/1	0.87	0.21	77,77,77,77	0
83	MG	1	3683	1/1	0.87	0.23	64,64,64,64	0
83	MG	R	201	1/1	0.87	0.13	92,92,92,92	0
83	MG	1	3706	1/1	0.87	0.21	42,42,42,42	0
83	MG	CM	1810	1/1	0.87	0.19	32,32,32,32	0
83	MG	1	3742	1/1	0.87	0.24	27,27,27,27	0
83	MG	4	204	1/1	0.87	0.16	50,50,50,50	0
83	MG	1	3788	1/1	0.87	0.19	48,48,48,48	0
83	MG	AS	3500	1/1	0.87	0.20	63,63,63,63	0
83	MG	BZ	202	1/1	0.88	0.33	64,64,64,64	0
83	MG	1	3844	1/1	0.88	0.10	33,33,33,33	0
83	MG	AS	3602	1/1	0.88	0.33	47,47,47,47	0
83	MG	1	3566	1/1	0.88	0.23	25,25,25,25	0
83	MG	Y	201	1/1	0.88	0.06	39,39,39,39	0
83	MG	1	3751	1/1	0.88	0.10	48,48,48,48	0
83	MG	1	3585	1/1	0.88	0.18	47,47,47,47	0
83	MG	CM	1807	1/1	0.88	0.28	50,50,50,50	0
83	MG	AR	401	1/1	0.88	0.29	73,73,73,73	0
83	MG	AS	3404	1/1	0.88	0.35	28,28,28,28	0
83	MG	1	3720	1/1	0.88	0.15	45,45,45,45	0
83	MG	1	3545	1/1	0.88	0.09	38,38,38,38	0
83	MG	B	1842	1/1	0.88	0.17	32,32,32,32	0
83	MG	1	3763	1/1	0.88	0.12	43,43,43,43	0
83	MG	1	3451	1/1	0.88	0.25	27,27,27,27	0
83	MG	CM	1820	1/1	0.88	0.28	42,42,42,42	0
83	MG	1	3766	1/1	0.88	0.23	54,54,54,54	0
83	MG	AS	3425	1/1	0.88	0.26	30,30,30,30	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
83	MG	CM	1825	1/1	0.88	0.25	44,44,44,44	0
83	MG	1	3496	1/1	0.88	0.33	34,34,34,34	0
83	MG	CM	1833	1/1	0.88	0.24	54,54,54,54	0
83	MG	1	3452	1/1	0.88	0.20	34,34,34,34	0
83	MG	CM	1835	1/1	0.88	0.24	62,62,62,62	0
83	MG	AS	3529	1/1	0.88	0.23	41,41,41,41	0
83	MG	1	3476	1/1	0.88	0.16	31,31,31,31	0
83	MG	AS	3637	1/1	0.88	0.18	51,51,51,51	0
83	MG	CM	1849	1/1	0.88	0.34	48,48,48,48	0
83	MG	1	3502	1/1	0.88	0.10	35,35,35,35	0
83	MG	1	3442	1/1	0.88	0.32	48,48,48,48	0
83	MG	B	1930	1/1	0.88	0.17	75,75,75,75	0
83	MG	1	3660	1/1	0.88	0.19	37,37,37,37	0
83	MG	1	3913	1/1	0.88	0.10	56,56,56,56	0
83	MG	AS	3541	1/1	0.88	0.20	40,40,40,40	0
83	MG	1	3914	1/1	0.88	0.11	49,49,49,49	0
83	MG	1	3665	1/1	0.88	0.22	40,40,40,40	0
83	MG	CM	1871	1/1	0.88	0.23	33,33,33,33	0
83	MG	4	208	1/1	0.88	0.21	45,45,45,45	0
83	MG	AS	3550	1/1	0.88	0.19	43,43,43,43	0
83	MG	AS	3553	1/1	0.88	0.24	37,37,37,37	0
83	MG	1	3407	1/1	0.88	0.32	32,32,32,32	0
83	MG	1	3562	1/1	0.88	0.23	58,58,58,58	0
83	MG	AS	3562	1/1	0.88	0.25	39,39,39,39	0
83	MG	j	303	1/1	0.88	0.21	23,23,23,23	0
83	MG	AS	3566	1/1	0.88	0.18	37,37,37,37	0
83	MG	AS	3462	1/1	0.88	0.28	43,43,43,43	0
83	MG	CM	1889	1/1	0.88	0.30	37,37,37,37	0
83	MG	AS	3464	1/1	0.88	0.26	30,30,30,30	0
83	MG	AS	3572	1/1	0.88	0.17	65,65,65,65	0
83	MG	1	3699	1/1	0.88	0.20	39,39,39,39	0
83	MG	1	3510	1/1	0.88	0.17	47,47,47,47	0
83	MG	B	1816	1/1	0.88	0.31	63,63,63,63	0
83	MG	1	3792	1/1	0.88	0.38	37,37,37,37	0
83	MG	AS	3473	1/1	0.88	0.23	45,45,45,45	0
83	MG	B	1888	1/1	0.88	0.20	47,47,47,47	0
83	MG	1	3739	1/1	0.88	0.26	28,28,28,28	0
83	MG	o	303	1/1	0.88	0.08	52,52,52,52	0
83	MG	DB	201	1/1	0.88	0.13	56,56,56,56	0
83	MG	1	3630	1/1	0.88	0.23	46,46,46,46	0
83	MG	1	3467	1/1	0.88	0.26	62,62,62,62	0
83	MG	1	3425	1/1	0.88	0.16	39,39,39,39	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
83	MG	1	3888	1/1	0.88	0.07	65,65,65,65	0
83	MG	1	3927	1/1	0.88	0.25	46,46,46,46	0
83	MG	w	303	1/1	0.88	0.09	46,46,46,46	0
83	MG	BJ	302	1/1	0.88	0.15	61,61,61,61	0
83	MG	x	203	1/1	0.88	0.12	62,62,62,62	0
83	MG	BV	201	1/1	0.88	0.26	39,39,39,39	0
83	MG	AS	3485	1/1	0.89	0.26	30,30,30,30	0
83	MG	B	1883	1/1	0.89	0.08	92,92,92,92	0
83	MG	AS	3489	1/1	0.89	0.30	43,43,43,43	0
83	MG	1	3456	1/1	0.89	0.17	32,32,32,32	0
83	MG	B	1810	1/1	0.89	0.25	59,59,59,59	0
83	MG	CL	303	1/1	0.89	0.12	66,66,66,66	0
83	MG	CM	1801	1/1	0.89	0.17	31,31,31,31	0
83	MG	B	1886	1/1	0.89	0.17	77,77,77,77	0
83	MG	AS	3605	1/1	0.89	0.10	46,46,46,46	0
83	MG	B	1812	1/1	0.89	0.22	39,39,39,39	0
83	MG	B	1813	1/1	0.89	0.21	62,62,62,62	0
83	MG	1	3662	1/1	0.89	0.12	61,61,61,61	0
83	MG	1	3406	1/1	0.89	0.29	33,33,33,33	0
83	MG	CM	1811	1/1	0.89	0.14	44,44,44,44	0
83	MG	1	3834	1/1	0.89	0.20	36,36,36,36	0
83	MG	1	3459	1/1	0.89	0.10	39,39,39,39	0
83	MG	AS	3619	1/1	0.89	0.23	50,50,50,50	0
83	MG	1	3427	1/1	0.89	0.28	30,30,30,30	0
83	MG	Y	202	1/1	0.89	0.20	85,85,85,85	0
83	MG	1	3698	1/1	0.89	0.09	34,34,34,34	0
83	MG	1	3670	1/1	0.89	0.19	40,40,40,40	0
83	MG	1	3741	1/1	0.89	0.16	58,58,58,58	0
83	MG	AS	3627	1/1	0.89	0.19	56,56,56,56	0
83	MG	1	3885	1/1	0.89	0.22	45,45,45,45	0
83	MG	AS	3405	1/1	0.89	0.24	30,30,30,30	0
83	MG	AS	3408	1/1	0.89	0.12	38,38,38,38	0
83	MG	x	201	1/1	0.89	0.29	28,28,28,28	0
83	MG	1	3590	1/1	0.89	0.18	38,38,38,38	0
83	MG	CM	1842	1/1	0.89	0.34	55,55,55,55	0
83	MG	1	3672	1/1	0.89	0.07	28,28,28,28	0
83	MG	AS	3415	1/1	0.89	0.26	33,33,33,33	0
83	MG	AS	3638	1/1	0.89	0.12	60,60,60,60	0
83	MG	1	3519	1/1	0.89	0.20	50,50,50,50	0
83	MG	1	3845	1/1	0.89	0.14	63,63,63,63	0
83	MG	AS	3531	1/1	0.89	0.18	47,47,47,47	0
83	MG	1	3608	1/1	0.89	0.28	60,60,60,60	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
83	MG	1	3437	1/1	0.89	0.31	29,29,29,29	0
83	MG	3	204	1/1	0.89	0.24	57,57,57,57	0
83	MG	8	201	1/1	0.89	0.16	45,45,45,45	0
83	MG	1	3850	1/1	0.89	0.14	54,54,54,54	0
83	MG	9	201	1/1	0.89	0.30	58,58,58,58	0
83	MG	1	3851	1/1	0.89	0.08	49,49,49,49	0
83	MG	1	3649	1/1	0.89	0.09	38,38,38,38	0
83	MG	AS	3658	1/1	0.89	0.13	59,59,59,59	0
83	MG	AS	3440	1/1	0.89	0.23	47,47,47,47	0
83	MG	B	1925	1/1	0.89	0.09	53,53,53,53	0
83	MG	AS	3551	1/1	0.89	0.26	34,34,34,34	0
83	MG	1	3431	1/1	0.89	0.18	42,42,42,42	0
83	MG	AS	3444	1/1	0.89	0.15	40,40,40,40	0
83	MG	AS	3449	1/1	0.89	0.18	42,42,42,42	0
83	MG	CM	1890	1/1	0.89	0.33	38,38,38,38	0
83	MG	B	1856	1/1	0.89	0.13	53,53,53,53	0
83	MG	1	3682	1/1	0.89	0.07	61,61,61,61	0
83	MG	AS	3565	1/1	0.89	0.17	46,46,46,46	0
83	MG	1	3761	1/1	0.89	0.31	27,27,27,27	0
83	MG	CM	1898	1/1	0.89	0.31	44,44,44,44	0
83	MG	1	3616	1/1	0.89	0.27	30,30,30,30	0
83	MG	CM	1902	1/1	0.89	0.18	40,40,40,40	0
83	MG	1	3466	1/1	0.89	0.25	36,36,36,36	0
83	MG	AT	208	1/1	0.89	0.15	53,53,53,53	0
83	MG	B	1862	1/1	0.89	0.15	61,61,61,61	0
83	MG	1	3906	1/1	0.89	0.14	32,32,32,32	0
83	MG	1	3726	1/1	0.89	0.17	53,53,53,53	0
83	MG	AH	202	1/1	0.89	0.10	65,65,65,65	0
83	MG	1	3654	1/1	0.89	0.14	64,64,64,64	0
83	MG	B	1874	1/1	0.89	0.23	54,54,54,54	0
84	3K5	AS	3401	57/57	0.89	0.16	52,66,85,87	0
83	MG	1	3769	1/1	0.89	0.15	35,35,35,35	0
83	MG	1	3655	1/1	0.89	0.12	52,52,52,52	0
83	MG	1	3656	1/1	0.89	0.19	49,49,49,49	0
83	MG	1	3777	1/1	0.89	0.14	44,44,44,44	0
83	MG	B	1950	1/1	0.89	0.16	67,67,67,67	0
83	MG	AS	3594	1/1	0.89	0.09	46,46,46,46	0
83	MG	1	3659	1/1	0.89	0.16	37,37,37,37	0
83	MG	AS	3439	1/1	0.90	0.21	29,29,29,29	0
83	MG	1	3490	1/1	0.90	0.30	36,36,36,36	0
83	MG	1	3813	1/1	0.90	0.09	64,64,64,64	0
83	MG	v	302	1/1	0.90	0.17	33,33,33,33	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
83	MG	1	3421	1/1	0.90	0.18	10,10,10,10	0
83	MG	AS	3448	1/1	0.90	0.15	45,45,45,45	0
83	MG	1	3597	1/1	0.90	0.24	56,56,56,56	0
83	MG	1	3855	1/1	0.90	0.22	36,36,36,36	0
83	MG	B	1818	1/1	0.90	0.30	39,39,39,39	0
83	MG	1	3895	1/1	0.90	0.14	44,44,44,44	0
83	MG	AS	3456	1/1	0.90	0.22	42,42,42,42	0
83	MG	1	3536	1/1	0.90	0.23	28,28,28,28	0
83	MG	1	3552	1/1	0.90	0.19	47,47,47,47	0
83	MG	1	3648	1/1	0.90	0.06	54,54,54,54	0
83	MG	1	3509	1/1	0.90	0.19	30,30,30,30	0
83	MG	CM	1832	1/1	0.90	0.28	32,32,32,32	0
83	MG	B	1889	1/1	0.90	0.14	44,44,44,44	0
83	MG	1	3789	1/1	0.90	0.18	42,42,42,42	0
83	MG	1	3695	1/1	0.90	0.09	42,42,42,42	0
83	MG	CM	1836	1/1	0.90	0.22	55,55,55,55	0
83	MG	CM	1837	1/1	0.90	0.27	56,56,56,56	0
83	MG	1	3501	1/1	0.90	0.20	39,39,39,39	0
83	MG	AS	3561	1/1	0.90	0.21	38,38,38,38	0
83	MG	B	1834	1/1	0.90	0.21	27,27,27,27	0
83	MG	1	3828	1/1	0.90	0.19	49,49,49,49	0
83	MG	AS	3474	1/1	0.90	0.26	52,52,52,52	0
83	MG	AS	3654	1/1	0.90	0.16	34,34,34,34	0
83	MG	AS	3479	1/1	0.90	0.12	32,32,32,32	0
83	MG	1	3793	1/1	0.90	0.14	33,33,33,33	0
83	MG	CM	1859	1/1	0.90	0.11	43,43,43,43	0
83	MG	B	1899	1/1	0.90	0.23	60,60,60,60	0
83	MG	1	3571	1/1	0.90	0.28	40,40,40,40	0
83	MG	1	3795	1/1	0.90	0.15	45,45,45,45	0
83	MG	AS	3578	1/1	0.90	0.26	34,34,34,34	0
83	MG	AS	3668	1/1	0.90	0.09	46,46,46,46	0
83	MG	1	3910	1/1	0.90	0.10	62,62,62,62	0
83	MG	1	3912	1/1	0.90	0.05	60,60,60,60	0
83	MG	AS	3487	1/1	0.90	0.37	39,39,39,39	0
83	MG	AC	101	1/1	0.90	0.12	50,50,50,50	0
83	MG	B	1908	1/1	0.90	0.25	49,49,49,49	0
83	MG	AT	201	1/1	0.90	0.25	21,21,21,21	0
83	MG	AT	202	1/1	0.90	0.21	30,30,30,30	0
83	MG	1	3572	1/1	0.90	0.10	29,29,29,29	0
83	MG	1	3517	1/1	0.90	0.19	33,33,33,33	0
83	MG	AS	3495	1/1	0.90	0.15	38,38,38,38	0
83	MG	B	1845	1/1	0.90	0.24	55,55,55,55	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
83	MG	1	3587	1/1	0.90	0.14	52,52,52,52	0
83	MG	1	3404	1/1	0.90	0.18	49,49,49,49	0
83	MG	B	1854	1/1	0.90	0.09	62,62,62,62	0
83	MG	1	3802	1/1	0.90	0.14	74,74,74,74	0
83	MG	1	3560	1/1	0.90	0.13	42,42,42,42	0
83	MG	BB	301	1/1	0.90	0.29	44,44,44,44	0
83	MG	j	304	1/1	0.90	0.15	55,55,55,55	0
83	MG	AS	3507	1/1	0.90	0.18	68,68,68,68	0
83	MG	BE	302	1/1	0.90	0.18	33,33,33,33	0
83	MG	k	402	1/1	0.90	0.15	63,63,63,63	0
83	MG	AS	3511	1/1	0.90	0.18	41,41,41,41	0
83	MG	1	3704	1/1	0.90	0.22	63,63,63,63	0
83	MG	AS	3608	1/1	0.90	0.18	44,44,44,44	0
83	MG	AP	202	1/1	0.90	0.22	34,34,34,34	0
83	MG	1	3529	1/1	0.90	0.19	47,47,47,47	0
83	MG	1	3711	1/1	0.90	0.14	38,38,38,38	0
83	MG	AS	3612	1/1	0.90	0.13	52,52,52,52	0
83	MG	AS	3614	1/1	0.90	0.17	56,56,56,56	0
83	MG	AS	3615	1/1	0.90	0.17	41,41,41,41	0
83	MG	B	1865	1/1	0.90	0.21	53,53,53,53	0
83	MG	1	3779	1/1	0.90	0.17	40,40,40,40	0
83	MG	1	3887	1/1	0.90	0.07	32,32,32,32	0
83	MG	CM	1803	1/1	0.90	0.23	33,33,33,33	0
83	MG	1	3848	1/1	0.90	0.17	37,37,37,37	0
86	GET	B	1801	34/34	0.90	0.14	103,112,118,123	0
83	MG	CM	1824	1/1	0.91	0.09	35,35,35,35	0
83	MG	AS	3451	1/1	0.91	0.27	38,38,38,38	0
83	MG	CM	1827	1/1	0.91	0.21	47,47,47,47	0
83	MG	1	3827	1/1	0.91	0.18	33,33,33,33	0
83	MG	CM	1830	1/1	0.91	0.20	38,38,38,38	0
83	MG	1	3430	1/1	0.91	0.11	33,33,33,33	0
83	MG	1	3710	1/1	0.91	0.14	31,31,31,31	0
83	MG	B	1815	1/1	0.91	0.30	51,51,51,51	0
83	MG	AS	3671	1/1	0.91	0.18	58,58,58,58	0
83	MG	1	3401	1/1	0.91	0.36	28,28,28,28	0
83	MG	1	3712	1/1	0.91	0.15	31,31,31,31	0
83	MG	1	3588	1/1	0.91	0.15	40,40,40,40	0
83	MG	AS	3463	1/1	0.91	0.18	31,31,31,31	0
83	MG	B	1820	1/1	0.91	0.20	45,45,45,45	0
83	MG	CM	1843	1/1	0.91	0.15	44,44,44,44	0
83	MG	CM	1844	1/1	0.91	0.13	18,18,18,18	0
83	MG	AS	3465	1/1	0.91	0.18	39,39,39,39	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
83	MG	B	1821	1/1	0.91	0.24	37,37,37,37	0
83	MG	AT	206	1/1	0.91	0.24	36,36,36,36	0
83	MG	B	1868	1/1	0.91	0.18	67,67,67,67	0
83	MG	CM	1855	1/1	0.91	0.27	53,53,53,53	0
83	MG	1	3589	1/1	0.91	0.23	31,31,31,31	0
83	MG	AS	3537	1/1	0.91	0.19	40,40,40,40	0
83	MG	1	3674	1/1	0.91	0.09	42,42,42,42	0
83	MG	1	3415	1/1	0.91	0.40	29,29,29,29	0
83	MG	1	3677	1/1	0.91	0.14	57,57,57,57	0
83	MG	AW	301	1/1	0.91	0.15	35,35,35,35	0
83	MG	B	1924	1/1	0.91	0.15	50,50,50,50	0
83	MG	AW	304	1/1	0.91	0.11	66,66,66,66	0
83	MG	1	3811	1/1	0.91	0.06	56,56,56,56	0
83	MG	1	3749	1/1	0.91	0.18	48,48,48,48	0
83	MG	1	3723	1/1	0.91	0.07	34,34,34,34	0
83	MG	1	3639	1/1	0.91	0.21	24,24,24,24	0
83	MG	1	3514	1/1	0.91	0.23	50,50,50,50	0
83	MG	1	3477	1/1	0.91	0.19	34,34,34,34	0
83	MG	1	3879	1/1	0.91	0.19	48,48,48,48	0
83	MG	3	207	1/1	0.91	0.07	42,42,42,42	0
83	MG	AS	3426	1/1	0.91	0.21	27,27,27,27	0
83	MG	1	3880	1/1	0.91	0.14	56,56,56,56	0
83	MG	1	3756	1/1	0.91	0.17	42,42,42,42	0
83	MG	AS	3429	1/1	0.91	0.22	28,28,28,28	0
83	MG	AM	102	1/1	0.91	0.08	58,58,58,58	0
83	MG	B	1890	1/1	0.91	0.16	60,60,60,60	0
83	MG	CK	103	1/1	0.91	0.20	45,45,45,45	0
83	MG	AS	3639	1/1	0.91	0.16	46,46,46,46	0
83	MG	3	210	1/1	0.91	0.29	54,54,54,54	0
83	MG	1	3469	1/1	0.91	0.20	46,46,46,46	0
83	MG	1	3495	1/1	0.91	0.14	44,44,44,44	0
83	MG	AS	3580	1/1	0.91	0.26	44,44,44,44	0
83	MG	AS	3582	1/1	0.91	0.14	47,47,47,47	0
83	MG	x	202	1/1	0.91	0.08	41,41,41,41	0
83	MG	1	3615	1/1	0.91	0.11	46,46,46,46	0
83	MG	B	1849	1/1	0.91	0.16	52,52,52,52	0
83	MG	AS	3508	1/1	0.91	0.20	55,55,55,55	0
83	MG	1	3685	1/1	0.91	0.13	89,89,89,89	0
83	MG	DQ	101	1/1	0.91	0.09	60,60,60,60	0
83	MG	CM	1812	1/1	0.91	0.19	47,47,47,47	0
83	MG	AS	3653	1/1	0.91	0.27	35,35,35,35	0
83	MG	AS	3445	1/1	0.91	0.24	30,30,30,30	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
83	MG	B	1852	1/1	0.91	0.18	79,79,79,79	0
83	MG	1	3568	1/1	0.91	0.14	38,38,38,38	0
83	MG	AS	3660	1/1	0.91	0.25	68,68,68,68	0
83	MG	CM	1821	1/1	0.91	0.24	46,46,46,46	0
83	MG	B	1811	1/1	0.91	0.22	26,26,26,26	0
83	MG	AS	3595	1/1	0.91	0.34	49,49,49,49	0
83	MG	AS	3626	1/1	0.92	0.08	52,52,52,52	0
83	MG	1	3482	1/1	0.92	0.21	39,39,39,39	0
83	MG	B	1931	1/1	0.92	0.18	51,51,51,51	0
83	MG	B	1867	1/1	0.92	0.18	87,87,87,87	0
83	MG	u	201	1/1	0.92	0.06	34,34,34,34	0
83	MG	AS	3632	1/1	0.92	0.09	50,50,50,50	0
83	MG	1	3760	1/1	0.92	0.19	41,41,41,41	0
83	MG	1	3884	1/1	0.92	0.22	45,45,45,45	0
83	MG	AS	3635	1/1	0.92	0.11	48,48,48,48	0
83	MG	CM	1815	1/1	0.92	0.16	28,28,28,28	0
83	MG	1	3661	1/1	0.92	0.07	40,40,40,40	0
83	MG	AS	3539	1/1	0.92	0.18	43,43,43,43	0
83	MG	1	3605	1/1	0.92	0.14	46,46,46,46	0
83	MG	1	3692	1/1	0.92	0.19	49,49,49,49	0
83	MG	AS	3453	1/1	0.92	0.11	40,40,40,40	0
83	MG	1	3403	1/1	0.92	0.20	27,27,27,27	0
83	MG	1	3807	1/1	0.92	0.29	41,41,41,41	0
83	MG	1	3632	1/1	0.92	0.12	40,40,40,40	0
83	MG	1	3522	1/1	0.92	0.16	35,35,35,35	0
83	MG	CM	1828	1/1	0.92	0.39	41,41,41,41	0
83	MG	AS	3552	1/1	0.92	0.20	29,29,29,29	0
83	MG	1	3772	1/1	0.92	0.06	34,34,34,34	0
83	MG	AS	3556	1/1	0.92	0.14	38,38,38,38	0
83	MG	B	1947	1/1	0.92	0.10	72,72,72,72	0
83	MG	AS	3558	1/1	0.92	0.20	47,47,47,47	0
83	MG	AS	3652	1/1	0.92	0.10	46,46,46,46	0
83	MG	1	3447	1/1	0.92	0.25	28,28,28,28	0
83	MG	1	3610	1/1	0.92	0.19	37,37,37,37	0
83	MG	B	1827	1/1	0.92	0.18	44,44,44,44	0
83	MG	AS	3656	1/1	0.92	0.09	42,42,42,42	0
83	MG	AS	3657	1/1	0.92	0.14	60,60,60,60	0
83	MG	1	3854	1/1	0.92	0.10	41,41,41,41	0
83	MG	B	1829	1/1	0.92	0.17	45,45,45,45	0
83	MG	CM	1847	1/1	0.92	0.19	37,37,37,37	0
83	MG	1	3612	1/1	0.92	0.15	38,38,38,38	0
83	MG	1	3472	1/1	0.92	0.26	22,22,22,22	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
83	MG	CM	1850	1/1	0.92	0.11	79,79,79,79	0
83	MG	1	3489	1/1	0.92	0.15	58,58,58,58	0
83	MG	AS	3472	1/1	0.92	0.10	35,35,35,35	0
83	MG	1	3436	1/1	0.92	0.08	30,30,30,30	0
83	MG	1	3528	1/1	0.92	0.12	45,45,45,45	0
83	MG	AS	3477	1/1	0.92	0.15	40,40,40,40	0
83	MG	1	3820	1/1	0.92	0.14	45,45,45,45	0
83	MG	1	3428	1/1	0.92	0.23	36,36,36,36	0
83	MG	1	3705	1/1	0.92	0.36	47,47,47,47	0
83	MG	CM	1865	1/1	0.92	0.11	71,71,71,71	0
83	MG	1	3823	1/1	0.92	0.08	34,34,34,34	0
83	MG	B	1901	1/1	0.92	0.13	50,50,50,50	0
83	MG	1	3511	1/1	0.92	0.24	29,29,29,29	0
83	MG	Z	201	1/1	0.92	0.16	51,51,51,51	0
83	MG	CM	1874	1/1	0.92	0.21	62,62,62,62	0
83	MG	Z	202	1/1	0.92	0.22	48,48,48,48	0
83	MG	AT	205	1/1	0.92	0.15	50,50,50,50	0
83	MG	Z	203	1/1	0.92	0.20	74,74,74,74	0
83	MG	1	3911	1/1	0.92	0.07	83,83,83,83	0
83	MG	AS	3491	1/1	0.92	0.16	34,34,34,34	0
83	MG	B	1905	1/1	0.92	0.18	37,37,37,37	0
83	MG	1	3709	1/1	0.92	0.23	34,34,34,34	0
83	MG	4	210	1/1	0.92	0.10	42,42,42,42	0
83	MG	CM	1888	1/1	0.92	0.11	46,46,46,46	0
83	MG	1	3444	1/1	0.92	0.18	43,43,43,43	0
83	MG	AS	3410	1/1	0.92	0.27	31,31,31,31	0
83	MG	1	3748	1/1	0.92	0.23	32,32,32,32	0
83	MG	CM	1894	1/1	0.92	0.24	42,42,42,42	0
83	MG	B	1910	1/1	0.92	0.25	58,58,58,58	0
83	MG	1	3830	1/1	0.92	0.10	43,43,43,43	0
83	MG	BB	302	1/1	0.92	0.23	32,32,32,32	0
83	MG	1	3916	1/1	0.92	0.10	49,49,49,49	0
83	MG	AS	3417	1/1	0.92	0.20	26,26,26,26	0
83	MG	BE	301	1/1	0.92	0.19	33,33,33,33	0
83	MG	AS	3607	1/1	0.92	0.20	46,46,46,46	0
83	MG	1	3596	1/1	0.92	0.19	30,30,30,30	0
83	MG	B	1853	1/1	0.92	0.18	46,46,46,46	0
83	MG	1	3534	1/1	0.92	0.08	34,34,34,34	0
83	MG	1	3535	1/1	0.92	0.20	26,26,26,26	0
83	MG	B	1802	1/1	0.92	0.16	41,41,41,41	0
83	MG	AS	3613	1/1	0.92	0.07	40,40,40,40	0
83	MG	B	1803	1/1	0.92	0.28	34,34,34,34	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
83	MG	1	3515	1/1	0.92	0.16	38,38,38,38	0
83	MG	1	3478	1/1	0.92	0.19	31,31,31,31	0
83	MG	AS	3430	1/1	0.92	0.25	33,33,33,33	0
83	MG	o	302	1/1	0.92	0.09	24,24,24,24	0
83	MG	CL	301	1/1	0.92	0.15	39,39,39,39	0
83	MG	B	1808	1/1	0.92	0.07	88,88,88,88	0
83	MG	AS	3435	1/1	0.92	0.19	33,33,33,33	0
83	MG	1	3838	1/1	0.92	0.20	34,34,34,34	0
83	MG	1	3429	1/1	0.92	0.26	27,27,27,27	0
85	ZN	DS	201	1/1	0.92	0.12	192,192,192,192	0
83	MG	B	1929	1/1	0.92	0.21	62,62,62,62	0
86	GET	CM	1904	34/34	0.92	0.22	98,107,112,116	0
83	MG	B	1893	1/1	0.93	0.15	55,55,55,55	0
83	MG	1	3707	1/1	0.93	0.17	43,43,43,43	0
83	MG	j	301	1/1	0.93	0.08	28,28,28,28	0
83	MG	1	3487	1/1	0.93	0.29	27,27,27,27	0
83	MG	AS	3526	1/1	0.93	0.14	53,53,53,53	0
83	MG	1	3791	1/1	0.93	0.15	35,35,35,35	0
83	MG	1	3413	1/1	0.93	0.23	36,36,36,36	0
83	MG	B	1843	1/1	0.93	0.19	35,35,35,35	0
83	MG	k	401	1/1	0.93	0.11	66,66,66,66	0
83	MG	1	3538	1/1	0.93	0.16	54,54,54,54	0
83	MG	AS	3460	1/1	0.93	0.25	34,34,34,34	0
83	MG	Q	201	1/1	0.93	0.09	40,40,40,40	0
83	MG	1	3600	1/1	0.93	0.16	44,44,44,44	0
83	MG	AS	3616	1/1	0.93	0.25	44,44,44,44	0
83	MG	B	1847	1/1	0.93	0.30	51,51,51,51	0
83	MG	AP	203	1/1	0.93	0.16	67,67,67,67	0
83	MG	1	3716	1/1	0.93	0.13	31,31,31,31	0
83	MG	CM	1856	1/1	0.93	0.19	31,31,31,31	0
83	MG	CM	1857	1/1	0.93	0.17	49,49,49,49	0
83	MG	1	3520	1/1	0.93	0.12	26,26,26,26	0
83	MG	1	3625	1/1	0.93	0.22	38,38,38,38	0
83	MG	CM	1860	1/1	0.93	0.18	52,52,52,52	0
83	MG	1	3414	1/1	0.93	0.36	43,43,43,43	0
83	MG	AS	3549	1/1	0.93	0.22	43,43,43,43	0
83	MG	AS	3624	1/1	0.93	0.10	40,40,40,40	0
83	MG	1	3479	1/1	0.93	0.23	26,26,26,26	0
83	MG	1	3506	1/1	0.93	0.19	26,26,26,26	0
83	MG	CM	1868	1/1	0.93	0.14	86,86,86,86	0
83	MG	CM	1869	1/1	0.93	0.18	58,58,58,58	0
83	MG	f	102	1/1	0.93	0.09	59,59,59,59	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
83	MG	1	3606	1/1	0.93	0.08	61,61,61,61	0
83	MG	1	3762	1/1	0.93	0.14	38,38,38,38	0
83	MG	1	3492	1/1	0.93	0.16	35,35,35,35	0
83	MG	1	3663	1/1	0.93	0.18	48,48,48,48	0
83	MG	1	3546	1/1	0.93	0.23	42,42,42,42	0
83	MG	AS	3560	1/1	0.93	0.26	46,46,46,46	0
83	MG	w	301	1/1	0.93	0.17	36,36,36,36	0
83	MG	1	3666	1/1	0.93	0.10	40,40,40,40	0
83	MG	1	3810	1/1	0.93	0.13	34,34,34,34	0
83	MG	CK	102	1/1	0.93	0.25	57,57,57,57	0
83	MG	1	3420	1/1	0.93	0.39	39,39,39,39	0
83	MG	1	3549	1/1	0.93	0.16	24,24,24,24	0
83	MG	1	3611	1/1	0.93	0.27	34,34,34,34	0
83	MG	B	1870	1/1	0.93	0.18	74,74,74,74	0
83	MG	CM	1891	1/1	0.93	0.10	49,49,49,49	0
83	MG	1	3732	1/1	0.93	0.13	49,49,49,49	0
83	MG	B	1873	1/1	0.93	0.18	41,41,41,41	0
83	MG	AS	3576	1/1	0.93	0.17	49,49,49,49	0
83	MG	CM	1805	1/1	0.93	0.14	23,23,23,23	0
83	MG	1	3775	1/1	0.93	0.11	31,31,31,31	0
83	MG	1	3816	1/1	0.93	0.18	45,45,45,45	0
83	MG	1	3474	1/1	0.93	0.26	17,17,17,17	0
83	MG	1	3902	1/1	0.93	0.08	41,41,41,41	0
83	MG	AS	3650	1/1	0.93	0.13	39,39,39,39	0
83	MG	1	3613	1/1	0.93	0.23	37,37,37,37	0
83	MG	AS	3431	1/1	0.93	0.21	35,35,35,35	0
83	MG	AS	3585	1/1	0.93	0.23	36,36,36,36	0
83	MG	1	3859	1/1	0.93	0.07	58,58,58,58	0
83	MG	1	3513	1/1	0.93	0.15	33,33,33,33	0
83	MG	CM	1816	1/1	0.93	0.28	32,32,32,32	0
83	MG	1	3410	1/1	0.93	0.22	23,23,23,23	0
83	MG	AS	3590	1/1	0.93	0.10	44,44,44,44	0
84	3K5	1	3402	57/57	0.93	0.13	42,54,71,76	0
83	MG	1	3675	1/1	0.93	0.17	47,47,47,47	0
83	MG	1	3411	1/1	0.93	0.29	23,23,23,23	0
83	MG	1	3740	1/1	0.93	0.23	30,30,30,30	0
83	MG	B	1833	1/1	0.93	0.20	43,43,43,43	0
83	MG	AS	3664	1/1	0.93	0.06	87,87,87,87	0
83	MG	4	206	1/1	0.93	0.24	32,32,32,32	0
83	MG	1	3824	1/1	0.93	0.30	43,43,43,43	0
83	MG	B	1948	1/1	0.93	0.11	70,70,70,70	0
83	MG	1	3516	1/1	0.93	0.19	25,25,25,25	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
83	MG	AS	3446	1/1	0.93	0.26	48,48,48,48	0
83	MG	1	3485	1/1	0.93	0.20	28,28,28,28	0
83	MG	1	3434	1/1	0.94	0.23	37,37,37,37	0
83	MG	B	1848	1/1	0.94	0.14	45,45,45,45	0
83	MG	1	3657	1/1	0.94	0.22	41,41,41,41	0
83	MG	B	1938	1/1	0.94	0.15	42,42,42,42	0
83	MG	1	3678	1/1	0.94	0.12	43,43,43,43	0
83	MG	B	1851	1/1	0.94	0.10	71,71,71,71	0
83	MG	1	3744	1/1	0.94	0.19	28,28,28,28	0
83	MG	6	202	1/1	0.94	0.17	45,45,45,45	0
83	MG	1	3831	1/1	0.94	0.12	39,39,39,39	0
83	MG	AS	3604	1/1	0.94	0.12	35,35,35,35	0
83	MG	AS	3542	1/1	0.94	0.23	33,33,33,33	0
83	MG	AS	3659	1/1	0.94	0.21	42,42,42,42	0
83	MG	1	3491	1/1	0.94	0.14	49,49,49,49	0
83	MG	1	3561	1/1	0.94	0.16	30,30,30,30	0
83	MG	B	1819	1/1	0.94	0.24	47,47,47,47	0
83	MG	AS	3663	1/1	0.94	0.05	87,87,87,87	0
83	MG	AS	3546	1/1	0.94	0.22	41,41,41,41	0
83	MG	1	3448	1/1	0.94	0.20	26,26,26,26	0
83	MG	1	3780	1/1	0.94	0.15	43,43,43,43	0
83	MG	B	1904	1/1	0.94	0.22	57,57,57,57	0
83	MG	1	3898	1/1	0.94	0.15	38,38,38,38	0
83	MG	CM	1880	1/1	0.94	0.16	45,45,45,45	0
83	MG	1	3866	1/1	0.94	0.17	46,46,46,46	0
83	MG	1	3725	1/1	0.94	0.21	29,29,29,29	0
83	MG	1	3542	1/1	0.94	0.20	36,36,36,36	0
83	MG	CM	1886	1/1	0.94	0.13	52,52,52,52	0
83	MG	1	3645	1/1	0.94	0.14	31,31,31,31	0
83	MG	3	201	1/1	0.94	0.19	25,25,25,25	0
83	MG	1	3752	1/1	0.94	0.15	38,38,38,38	0
83	MG	1	3486	1/1	0.94	0.10	37,37,37,37	0
83	MG	1	3554	1/1	0.94	0.06	55,55,55,55	0
83	MG	AS	3502	1/1	0.94	0.24	52,52,52,52	0
83	MG	3	206	1/1	0.94	0.18	63,63,63,63	0
83	MG	1	3500	1/1	0.94	0.20	35,35,35,35	0
83	MG	CM	1826	1/1	0.94	0.19	36,36,36,36	0
83	MG	1	3508	1/1	0.94	0.23	41,41,41,41	0
83	MG	CM	1900	1/1	0.94	0.20	41,41,41,41	0
83	MG	AS	3570	1/1	0.94	0.16	38,38,38,38	0
83	MG	B	1917	1/1	0.94	0.10	45,45,45,45	0
83	MG	1	3759	1/1	0.94	0.17	49,49,49,49	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
83	MG	CM	1831	1/1	0.94	0.11	45,45,45,45	0
83	MG	1	3617	1/1	0.94	0.19	41,41,41,41	0
83	MG	B	1920	1/1	0.94	0.06	90,90,90,90	0
83	MG	AS	3577	1/1	0.94	0.14	52,52,52,52	0
83	MG	B	1921	1/1	0.94	0.10	41,41,41,41	0
83	MG	1	3651	1/1	0.94	0.15	42,42,42,42	0
83	MG	1	3557	1/1	0.94	0.18	47,47,47,47	0
83	MG	1	3593	1/1	0.94	0.14	48,48,48,48	0
83	MG	1	3714	1/1	0.94	0.17	27,27,27,27	0
83	MG	B	1926	1/1	0.94	0.15	46,46,46,46	0
83	MG	AS	3519	1/1	0.94	0.16	31,31,31,31	0
83	MG	1	3537	1/1	0.94	0.14	37,37,37,37	0
83	MG	1	3798	1/1	0.94	0.12	34,34,34,34	0
83	MG	B	1807	1/1	0.94	0.20	44,44,44,44	0
83	MG	1	3886	1/1	0.94	0.18	54,54,54,54	0
83	MG	1	3635	1/1	0.94	0.11	37,37,37,37	0
83	MG	CM	1852	1/1	0.94	0.13	41,41,41,41	0
83	MG	BK	201	1/1	0.94	0.24	35,35,35,35	0
83	MG	AS	3467	1/1	0.94	0.10	46,46,46,46	0
83	MG	0	202	1/1	0.94	0.16	39,39,39,39	0
83	MG	AS	3416	1/1	0.95	0.08	63,63,63,63	0
83	MG	1	3664	1/1	0.95	0.07	51,51,51,51	0
83	MG	AS	3418	1/1	0.95	0.27	26,26,26,26	0
83	MG	3	205	1/1	0.95	0.21	40,40,40,40	0
83	MG	CM	1851	1/1	0.95	0.17	44,44,44,44	0
83	MG	1	3865	1/1	0.95	0.19	39,39,39,39	0
83	MG	1	3644	1/1	0.95	0.13	36,36,36,36	0
83	MG	AS	3424	1/1	0.95	0.20	22,22,22,22	0
83	MG	1	3833	1/1	0.95	0.12	34,34,34,34	0
83	MG	1	3426	1/1	0.95	0.14	27,27,27,27	0
83	MG	AS	3629	1/1	0.95	0.09	43,43,43,43	0
83	MG	1	3689	1/1	0.95	0.08	49,49,49,49	0
83	MG	B	1894	1/1	0.95	0.16	50,50,50,50	0
83	MG	1	3458	1/1	0.95	0.19	28,28,28,28	0
83	MG	BJ	301	1/1	0.95	0.09	40,40,40,40	0
83	MG	1	3424	1/1	0.95	0.24	25,25,25,25	0
83	MG	1	3806	1/1	0.95	0.06	32,32,32,32	0
83	MG	AS	3432	1/1	0.95	0.35	30,30,30,30	0
83	MG	1	3416	1/1	0.95	0.25	37,37,37,37	0
83	MG	CM	1867	1/1	0.95	0.18	43,43,43,43	0
83	MG	AS	3568	1/1	0.95	0.20	26,26,26,26	0
83	MG	1	3743	1/1	0.95	0.17	34,34,34,34	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
83	MG	1	3719	1/1	0.95	0.23	43,43,43,43	0
83	MG	0	204	1/1	0.95	0.31	54,54,54,54	0
83	MG	1	3778	1/1	0.95	0.16	33,33,33,33	0
83	MG	CM	1873	1/1	0.95	0.22	40,40,40,40	0
83	MG	1	3461	1/1	0.95	0.20	21,21,21,21	0
83	MG	1	3746	1/1	0.95	0.30	31,31,31,31	0
83	MG	6	201	1/1	0.95	0.14	40,40,40,40	0
83	MG	AS	3506	1/1	0.95	0.08	61,61,61,61	0
83	MG	AS	3442	1/1	0.95	0.26	33,33,33,33	0
83	MG	B	1859	1/1	0.95	0.10	78,78,78,78	0
83	MG	1	3532	1/1	0.95	0.25	32,32,32,32	0
83	MG	7	201	1/1	0.95	0.09	26,26,26,26	0
83	MG	1	3471	1/1	0.95	0.22	33,33,33,33	0
83	MG	B	1863	1/1	0.95	0.08	89,89,89,89	0
83	MG	B	1822	1/1	0.95	0.20	38,38,38,38	0
83	MG	CM	1887	1/1	0.95	0.17	66,66,66,66	0
83	MG	AS	3515	1/1	0.95	0.12	35,35,35,35	0
83	MG	1	3435	1/1	0.95	0.14	21,21,21,21	0
83	MG	1	3849	1/1	0.95	0.12	44,44,44,44	0
83	MG	1	3507	1/1	0.95	0.23	37,37,37,37	0
83	MG	CM	1892	1/1	0.95	0.18	48,48,48,48	0
83	MG	1	3473	1/1	0.95	0.28	24,24,24,24	0
83	MG	1	3634	1/1	0.95	0.07	27,27,27,27	0
83	MG	1	3464	1/1	0.95	0.19	27,27,27,27	0
83	MG	AS	3457	1/1	0.95	0.30	28,28,28,28	0
83	MG	AS	3523	1/1	0.95	0.14	39,39,39,39	0
83	MG	B	1871	1/1	0.95	0.14	56,56,56,56	0
83	MG	CM	1899	1/1	0.95	0.10	38,38,38,38	0
83	MG	1	3890	1/1	0.95	0.20	36,36,36,36	0
83	MG	1	3636	1/1	0.95	0.14	34,34,34,34	0
83	MG	AS	3666	1/1	0.95	0.16	32,32,32,32	0
83	MG	1	3658	1/1	0.95	0.18	32,32,32,32	0
83	MG	B	1875	1/1	0.95	0.12	65,65,65,65	0
83	MG	AS	3603	1/1	0.95	0.12	35,35,35,35	0
83	MG	AS	3532	1/1	0.95	0.18	31,31,31,31	0
83	MG	1	3757	1/1	0.95	0.21	53,53,53,53	0
83	MG	1	3441	1/1	0.95	0.16	30,30,30,30	0
83	MG	AS	3673	1/1	0.95	0.15	31,31,31,31	0
83	MG	AS	3403	1/1	0.95	0.23	18,18,18,18	0
83	MG	1	3604	1/1	0.95	0.22	39,39,39,39	0
83	MG	1	3498	1/1	0.95	0.26	30,30,30,30	0
83	MG	AS	3468	1/1	0.95	0.24	37,37,37,37	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
83	MG	1	3733	1/1	0.95	0.17	35,35,35,35	0
83	MG	r	302	1/1	0.95	0.25	32,32,32,32	0
83	MG	1	3541	1/1	0.95	0.11	34,34,34,34	0
83	MG	1	3512	1/1	0.95	0.18	23,23,23,23	0
83	MG	1	3764	1/1	0.95	0.24	52,52,52,52	0
83	MG	B	1933	1/1	0.95	0.12	75,75,75,75	0
83	MG	CM	1841	1/1	0.95	0.22	36,36,36,36	0
83	MG	AS	3476	1/1	0.95	0.20	26,26,26,26	0
83	MG	AS	3547	1/1	0.95	0.19	31,31,31,31	0
83	MG	AS	3548	1/1	0.95	0.17	34,34,34,34	0
83	MG	AS	3406	1/1	0.96	0.42	32,32,32,32	0
83	MG	AS	3538	1/1	0.96	0.09	45,45,45,45	0
83	MG	CM	1882	1/1	0.96	0.18	38,38,38,38	0
83	MG	1	3843	1/1	0.96	0.06	45,45,45,45	0
83	MG	BZ	201	1/1	0.96	0.07	38,38,38,38	0
83	MG	AS	3581	1/1	0.96	0.13	44,44,44,44	0
83	MG	1	3493	1/1	0.96	0.23	26,26,26,26	0
83	MG	1	3642	1/1	0.96	0.18	27,27,27,27	0
83	MG	AS	3412	1/1	0.96	0.06	28,28,28,28	0
83	MG	B	1932	1/1	0.96	0.09	25,25,25,25	0
83	MG	1	3708	1/1	0.96	0.17	33,33,33,33	0
83	MG	1	3829	1/1	0.96	0.14	44,44,44,44	0
83	MG	AS	3588	1/1	0.96	0.17	36,36,36,36	0
83	MG	r	301	1/1	0.96	0.21	34,34,34,34	0
83	MG	1	3643	1/1	0.96	0.29	34,34,34,34	0
83	MG	CM	1802	1/1	0.96	0.37	33,33,33,33	0
83	MG	AS	3447	1/1	0.96	0.13	35,35,35,35	0
83	MG	AS	3478	1/1	0.96	0.18	37,37,37,37	0
83	MG	1	3867	1/1	0.96	0.09	45,45,45,45	0
83	MG	1	3533	1/1	0.96	0.18	30,30,30,30	0
83	MG	1	3553	1/1	0.96	0.04	46,46,46,46	0
83	MG	AS	3482	1/1	0.96	0.17	28,28,28,28	0
83	MG	1	3783	1/1	0.96	0.17	40,40,40,40	0
83	MG	AS	3423	1/1	0.96	0.16	37,37,37,37	0
83	MG	1	3523	1/1	0.96	0.12	29,29,29,29	0
83	MG	v	303	1/1	0.96	0.09	28,28,28,28	0
83	MG	1	3667	1/1	0.96	0.11	42,42,42,42	0
83	MG	1	3715	1/1	0.96	0.16	45,45,45,45	0
83	MG	1	3770	1/1	0.96	0.14	36,36,36,36	0
83	MG	AS	3563	1/1	0.96	0.13	48,48,48,48	0
83	MG	AS	3525	1/1	0.96	0.18	45,45,45,45	0
83	MG	1	3771	1/1	0.96	0.04	34,34,34,34	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
83	MG	AS	3527	1/1	0.96	0.19	33,33,33,33	0
83	MG	1	3877	1/1	0.96	0.12	43,43,43,43	0
83	MG	1	3547	1/1	0.96	0.17	46,46,46,46	0
83	MG	AS	3569	1/1	0.96	0.17	33,33,33,33	0
83	MG	AS	3494	1/1	0.96	0.24	43,43,43,43	0
83	MG	AR	402	1/1	0.96	0.14	61,61,61,61	0
83	MG	1	3412	1/1	0.96	0.25	29,29,29,29	0
83	MG	AS	3573	1/1	0.96	0.22	41,41,41,41	0
83	MG	AS	3574	1/1	0.96	0.27	44,44,44,44	0
83	MG	1	3480	1/1	0.96	0.20	20,20,20,20	0
83	MG	AS	3499	1/1	0.96	0.15	39,39,39,39	0
83	MG	1	3505	1/1	0.96	0.11	37,37,37,37	0
83	MG	AS	3528	1/1	0.97	0.13	66,66,66,66	0
83	MG	1	3776	1/1	0.97	0.13	33,33,33,33	0
83	MG	1	3701	1/1	0.97	0.13	25,25,25,25	0
83	MG	AS	3497	1/1	0.97	0.13	34,34,34,34	0
83	MG	1	3796	1/1	0.97	0.15	51,51,51,51	0
83	MG	1	3440	1/1	0.97	0.35	25,25,25,25	0
83	MG	1	3768	1/1	0.97	0.17	26,26,26,26	0
83	MG	CM	1881	1/1	0.97	0.13	38,38,38,38	0
83	MG	AS	3420	1/1	0.97	0.20	26,26,26,26	0
83	MG	AS	3409	1/1	0.97	0.23	19,19,19,19	0
83	MG	AS	3554	1/1	0.97	0.15	23,23,23,23	0
83	MG	AW	302	1/1	0.97	0.20	40,40,40,40	0
83	MG	AS	3555	1/1	0.97	0.09	36,36,36,36	0
83	MG	B	1877	1/1	0.97	0.21	46,46,46,46	0
83	MG	CM	1838	1/1	0.97	0.15	29,29,29,29	0
83	MG	AS	3488	1/1	0.97	0.13	40,40,40,40	0
83	MG	CM	1818	1/1	0.97	0.07	27,27,27,27	0
83	MG	1	3713	1/1	0.97	0.17	36,36,36,36	0
83	MG	AS	3475	1/1	0.97	0.24	32,32,32,32	0
83	MG	Q	202	1/1	0.97	0.12	71,71,71,71	0
83	MG	1	3753	1/1	0.97	0.14	29,29,29,29	0
83	MG	CM	1845	1/1	0.97	0.15	39,39,39,39	0
83	MG	CM	1846	1/1	0.97	0.12	37,37,37,37	0
83	MG	1	3907	1/1	0.97	0.06	30,30,30,30	0
83	MG	AS	3452	1/1	0.97	0.14	23,23,23,23	0
83	MG	AS	3640	1/1	0.98	0.06	40,40,40,40	0
83	MG	AS	3510	1/1	0.98	0.18	27,27,27,27	0
83	MG	1	3409	1/1	0.98	0.14	30,30,30,30	0
85	ZN	c	201	1/1	0.98	0.04	77,77,77,77	0
83	MG	AS	3402	1/1	0.98	0.07	43,43,43,43	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
85	ZN	f	101	1/1	0.98	0.05	82,82,82,82	0
83	MG	1	3578	1/1	0.98	0.24	30,30,30,30	0
83	MG	1	3462	1/1	0.98	0.15	20,20,20,20	0
83	MG	1	3868	1/1	0.98	0.05	48,48,48,48	0
85	ZN	CK	101	1/1	0.98	0.03	100,100,100,100	0
83	MG	4	209	1/1	0.98	0.10	46,46,46,46	0
85	ZN	DQ	102	1/1	0.98	0.12	55,55,55,55	0
83	MG	AS	3407	1/1	0.98	0.14	23,23,23,23	0
83	MG	B	1880	1/1	0.98	0.08	70,70,70,70	0
83	MG	1	3567	1/1	0.98	0.12	22,22,22,22	0
85	ZN	CH	101	1/1	0.99	0.11	109,109,109,109	0
85	ZN	AQ	101	1/1	0.99	0.04	69,69,69,69	0
83	MG	CM	1862	1/1	0.99	0.08	37,37,37,37	0
85	ZN	DN	201	1/1	0.99	0.02	58,58,58,58	0
83	MG	1	3408	1/1	0.99	0.04	49,49,49,49	0
85	ZN	AK	101	1/1	0.99	0.05	53,53,53,53	0
85	ZN	AN	101	1/1	0.99	0.08	103,103,103,103	0
83	MG	AS	3438	1/1	0.99	0.08	24,24,24,24	0
85	ZN	CE	101	1/1	0.99	0.02	63,63,63,63	0

5.5 Other polymers

There are no such residues in this entry.