



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 29, 2026 – 09:52 AM UTC

PDB ID : 4V51 / pdb_00004v51
Title : Structure of the *Thermus thermophilus* 70S ribosome complexed with mRNA, tRNA and paromomycin
Authors : Selmer, M.; Dunham, C.M.; Murphy, F.V.; Weixlbaumer, A.; Petry, S.; Weir, J.R.; Kelley, A.C.; Ramakrishnan, V.
Deposited on : 2006-07-31
Resolution : 2.80 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

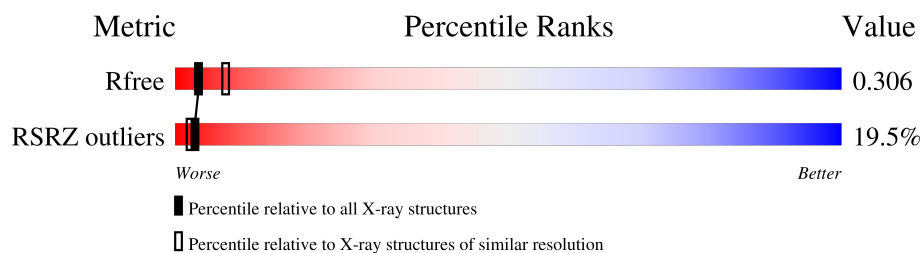
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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	3866 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

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

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
56	MG	AA	1697	-	-	-	X
56	MG	BA	3428	-	-	-	X
56	MG	CA	1673	-	-	-	X
56	MG	CA	1685	-	-	-	X
56	MG	CA	1719	-	-	-	X
56	MG	CX	102	-	-	-	X
56	MG	DA	3213	-	-	-	X
56	MG	DA	3219	-	-	-	X
56	MG	DA	3255	-	-	-	X
56	MG	DA	3261	-	-	-	X
56	MG	DA	3275	-	-	-	X

2 Entry composition

There are 58 unique types of molecules in this entry. The entry contains 291075 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a RNA chain called 16S ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	AA	1504	Total	C	N	O	P	0	0	0
			32329	14390	5992	10444	1503			
1	CA	1504	Total	C	N	O	P	0	0	0
			32329	14390	5992	10444	1503			

- Molecule 2 is a protein called 30S RIBOSOMAL PROTEIN S2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	AB	235	Total	C	N	O	S	0	0	1
			1901	1213	342	341	5			
2	CB	235	Total	C	N	O	S	0	0	1
			1901	1213	342	341	5			

- Molecule 3 is a protein called 30S RIBOSOMAL PROTEIN S3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	AC	207	Total	C	N	O	S	0	0	1
			1613	1016	315	281	1			
3	CC	207	Total	C	N	O	S	0	0	1
			1613	1016	315	281	1			

- Molecule 4 is a protein called 30S RIBOSOMAL PROTEIN S4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	AD	208	Total	C	N	O	S	0	0	0
			1703	1066	339	291	7			
4	CD	208	Total	C	N	O	S	0	0	0
			1703	1066	339	291	7			

- Molecule 5 is a protein called 30S RIBOSOMAL PROTEIN S5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	AE	151	Total	C	N	O	S	0	0	1
			1147	724	218	201	4			
5	CE	151	Total	C	N	O	S	0	0	1
			1147	724	218	201	4			

- Molecule 6 is a protein called 30S RIBOSOMAL PROTEIN S6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	AF	101	Total	C	N	O	S	0	0	0
			843	531	155	154	3			
6	CF	101	Total	C	N	O	S	0	0	0
			843	531	155	154	3			

- Molecule 7 is a protein called 30S RIBOSOMAL PROTEIN S7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	AG	155	Total	C	N	O	S	0	0	0
			1257	781	252	218	6			
7	CG	155	Total	C	N	O	S	0	0	0
			1257	781	252	218	6			

- Molecule 8 is a protein called 30S RIBOSOMAL PROTEIN S8.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	AH	138	Total	C	N	O	S	0	0	0
			1116	705	215	193	3			
8	CH	138	Total	C	N	O	S	0	0	0
			1116	705	215	193	3			

- Molecule 9 is a protein called 30S RIBOSOMAL PROTEIN S9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	AI	127	Total	C	N	O		0	0	0
			1011	639	198	174				
9	CI	127	Total	C	N	O		0	0	0
			1011	639	198	174				

- Molecule 10 is a protein called 30S RIBOSOMAL PROTEIN S10.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	AJ	99	Total	C	N	O	S	0	0	1
			795	499	157	138	1			

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	CJ	99	Total	C	N	O	S	0	0	1
			795	499	157	138	1			

- Molecule 11 is a protein called 30S RIBOSOMAL PROTEIN S11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	AK	119	Total	C	N	O	S	0	0	0
			885	549	168	165	3			
11	CK	119	Total	C	N	O	S	0	0	0
			885	549	168	165	3			

- Molecule 12 is a protein called 30S RIBOSOMAL PROTEIN S12.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	AL	125	Total	C	N	O	S	0	0	1
			971	611	196	163	1			
12	CL	125	Total	C	N	O	S	0	0	1
			971	611	196	163	1			

- Molecule 13 is a protein called 30S RIBOSOMAL PROTEIN S13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	AM	125	Total	C	N	O	S	0	0	1
			988	611	206	169	2			
13	CM	125	Total	C	N	O	S	0	0	1
			988	611	206	169	2			

- Molecule 14 is a protein called 30S RIBOSOMAL PROTEIN S14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	AN	60	Total	C	N	O	S	0	0	0
			492	312	104	72	4			
14	CN	60	Total	C	N	O	S	0	0	0
			492	312	104	72	4			

- Molecule 15 is a protein called 30S RIBOSOMAL PROTEIN S15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	AO	88	Total	C	N	O	S	0	0	0
			734	459	147	126	2			
15	CO	88	Total	C	N	O	S	0	0	0
			734	459	147	126	2			

- Molecule 16 is a protein called 30S RIBOSOMAL PROTEIN S16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	AP	84	Total	C	N	O	S	0	0	1
			701	443	140	117	1			
16	CP	84	Total	C	N	O	S	0	0	1
			701	443	140	117	1			

- Molecule 17 is a protein called 30S RIBOSOMAL PROTEIN S17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	AQ	100	Total	C	N	O	S	0	0	1
			824	528	152	142	2			
17	CQ	100	Total	C	N	O	S	0	0	1
			824	528	152	142	2			

- Molecule 18 is a protein called 30S RIBOSOMAL PROTEIN S18.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
18	AR	70	Total	C	N	O	0	0	0
			574	367	112	95			
18	CR	70	Total	C	N	O	0	0	0
			574	367	112	95			

- Molecule 19 is a protein called 30S RIBOSOMAL PROTEIN S19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	AS	79	Total	C	N	O	S	0	0	1
			630	403	115	110	2			
19	CS	79	Total	C	N	O	S	0	0	1
			630	403	115	110	2			

- Molecule 20 is a protein called 30S RIBOSOMAL PROTEIN S20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	AT	99	Total	C	N	O	S	0	0	0
			763	470	162	129	2			
20	CT	99	Total	C	N	O	S	0	0	0
			763	470	162	129	2			

- Molecule 21 is a protein called 30S RIBOSOMAL PROTEIN THX.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
21	AU	25	Total	C	N	O	0	0	1
			209	128	51	30			
21	CU	25	Total	C	N	O	0	0	1
			209	128	51	30			

- Molecule 22 is a RNA chain called P-SITE TRNA FMET (UNMODIFIED BASES EXCEPT FOR THYMINE 54).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	AV	77	Total	C	N	O	P	0	0	0
			1645	733	297	538	77			
22	CV	77	Total	C	N	O	P	0	0	0
			1645	733	297	538	77			

- Molecule 23 is a RNA chain called E-SITE TRNA PHE OR A-SITE TRNA PHE (UNMODIFIED BASES).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	AW	76	Total	C	N	O	P	0	0	0
			1623	723	290	534	76			
23	AY	19	Total	C	N	O	P	0	0	0
			407	183	78	128	18			
23	CW	76	Total	C	N	O	P	0	0	0
			1623	723	290	534	76			
23	CY	19	Total	C	N	O	P	0	0	0
			407	183	78	128	18			

- Molecule 24 is a RNA chain called MRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	AX	11	Total	C	N	O	P	0	0	0
			235	106	44	74	11			
24	CX	11	Total	C	N	O	P	0	0	0
			235	106	44	74	11			

- Molecule 25 is a protein called 50S RIBOSOMAL PROTEIN L27.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
25	B0	85	Total	C	N	O	S	0	0	0
			650	401	137	111	1			
25	D0	85	Total	C	N	O	S	0	0	0
			650	401	137	111	1			

- Molecule 26 is a protein called 50S RIBOSOMAL PROTEIN L28.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
26	B1	89	Total	C	N	O	0	0	1
			693	435	140	118			
26	D1	89	Total	C	N	O	0	0	1
			693	435	140	118			

- Molecule 27 is a protein called 50S RIBOSOMAL PROTEIN L29.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
27	B2	51	Total	C	N	O	S	0	0	1
			421	263	85	72	1			
27	D2	51	Total	C	N	O	S	0	0	1
			421	263	85	72	1			

- Molecule 28 is a protein called 50S RIBOSOMAL PROTEIN L30.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
28	B3	60	Total	C	N	O	S	0	0	1
			468	298	91	78	1			
28	D3	60	Total	C	N	O	S	0	0	1
			468	298	91	78	1			

- Molecule 29 is a protein called 50S RIBOSOMAL PROTEIN L31.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
29	B4	50	Total	C	N	O	0	0	1
			242	143	50	49			
29	D4	50	Total	C	N	O	0	0	1
			242	143	50	49			

- Molecule 30 is a protein called 50S RIBOSOMAL PROTEIN L32.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
30	B5	59	Total	C	N	O	S	0	0	0
			459	288	90	76	5			
30	D5	59	Total	C	N	O	S	0	0	0
			459	288	90	76	5			

- Molecule 31 is a protein called 50S RIBOSOMAL PROTEIN L33.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
31	B6	45	Total	C	N	O	S	0	0	1
			381	235	78	64	4			
31	D6	45	Total	C	N	O	S	0	0	1
			381	235	78	64	4			

- Molecule 32 is a protein called 50S RIBOSOMAL PROTEIN L34.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
32	B7	49	Total	C	N	O	S	0	0	1
			419	257	105	55	2			
32	D7	49	Total	C	N	O	S	0	0	1
			419	257	105	55	2			

- Molecule 33 is a protein called 50S RIBOSOMAL PROTEIN L35.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
33	B8	64	Total	C	N	O	S	0	0	1
			508	326	102	78	2			
33	D8	64	Total	C	N	O	S	0	0	1
			508	326	102	78	2			

- Molecule 34 is a RNA chain called 23S RIBOSOMAL RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
34	BA	2772	Total	C	N	O	P	0	0	0
			59708	26573	11171	19193	2771			
34	DA	2772	Total	C	N	O	P	0	0	0
			59708	26573	11171	19193	2771			

- Molecule 35 is a RNA chain called 5S RIBOSOMAL RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
35	BB	119	Total	C	N	O	P	0	0	0
			2551	1136	471	826	118			
35	DB	119	Total	C	N	O	P	0	0	0
			2551	1136	471	826	118			

- Molecule 36 is a protein called 50S RIBOSOMAL PROTEIN L1.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
36	BC	191	Total	C	N	O	0	0	1
			1142	691	221	230			

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
36	DC	191	Total	C	N	O	0	0	1
			1142	691	221	230			

- Molecule 37 is a protein called 50S RIBOSOMAL PROTEIN L2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
37	BD	272	Total	C	N	O	S	0	0	1
			2105	1329	417	356	3			
37	DD	272	Total	C	N	O	S	0	0	1
			2105	1329	417	356	3			

- Molecule 38 is a protein called 50S RIBOSOMAL PROTEIN L3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
38	BE	205	Total	C	N	O	S	0	0	1
			1564	988	300	270	6			
38	DE	205	Total	C	N	O	S	0	0	1
			1564	988	300	270	6			

- Molecule 39 is a protein called 50S RIBOSOMAL PROTEIN L4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
39	BF	208	Total	C	N	O	S	0	0	1
			1624	1035	304	282	3			
39	DF	208	Total	C	N	O	S	0	0	1
			1624	1035	304	282	3			

- Molecule 40 is a protein called 50S RIBOSOMAL PROTEIN L5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
40	BG	181	Total	C	N	O	S	0	0	0
			1474	942	268	260	4			
40	DG	181	Total	C	N	O	S	0	0	0
			1474	942	268	260	4			

- Molecule 41 is a protein called 50S RIBOSOMAL PROTEIN L6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
41	BH	160	Total	C	N	O	S	0	0	1
			1223	773	229	220	1			
41	DH	160	Total	C	N	O	S	0	0	1
			1223	773	229	220	1			

- Molecule 42 is a protein called 50S RIBOSOMAL PROTEIN L9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
42	BI	146	Total	C	N	O	S	0	0	1
			1132	723	201	207	1			
42	DI	146	Total	C	N	O	S	0	0	1
			1132	723	201	207	1			

- Molecule 43 is a protein called 50S RIBOSOMAL PROTEIN L13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
43	BN	139	Total	C	N	O	S	0	0	1
			1105	712	207	182	4			
43	DN	139	Total	C	N	O	S	0	0	1
			1105	712	207	182	4			

- Molecule 44 is a protein called 50S RIBOSOMAL PROTEIN L14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
44	BO	122	Total	C	N	O	S	0	0	0
			933	588	171	170	4			
44	DO	122	Total	C	N	O	S	0	0	0
			933	588	171	170	4			

- Molecule 45 is a protein called 50S RIBOSOMAL PROTEIN L15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
45	BP	146	Total	C	N	O	S	0	0	0
			1114	692	227	193	2			
45	DP	146	Total	C	N	O	S	0	0	0
			1114	692	227	193	2			

- Molecule 46 is a protein called 50S RIBOSOMAL PROTEIN L16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
46	BQ	136	Total	C	N	O	S	0	0	0
			1080	688	204	183	5			
46	DQ	136	Total	C	N	O	S	0	0	0
			1080	688	204	183	5			

- Molecule 47 is a protein called 50S RIBOSOMAL PROTEIN L17.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
47	BR	117	Total	C	N	O	0	0	0
			960	599	202	159			
47	DR	117	Total	C	N	O	0	0	0
			960	599	202	159			

- Molecule 48 is a protein called 50S RIBOSOMAL PROTEIN L18.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
48	BS	99	Total	C	N	O	0	0	1
			771	486	155	130			
48	DS	99	Total	C	N	O	0	0	1
			771	486	155	130			

- Molecule 49 is a protein called 50S RIBOSOMAL PROTEIN L19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
49	BT	138	Total	C	N	O	S	0	0	1
			1142	710	235	196	1			
49	DT	138	Total	C	N	O	S	0	0	1
			1142	710	235	196	1			

- Molecule 50 is a protein called 50S RIBOSOMAL PROTEIN L20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
50	BU	117	Total	C	N	O	S	0	0	0
			958	604	202	151	1			
50	DU	117	Total	C	N	O	S	0	0	0
			958	604	202	151	1			

- Molecule 51 is a protein called 50S RIBOSOMAL PROTEIN L21.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
51	BV	101	Total	C	N	O	S	0	0	0
			779	501	142	135	1			
51	DV	101	Total	C	N	O	S	0	0	0
			779	501	142	135	1			

- Molecule 52 is a protein called 50S RIBOSOMAL PROTEIN L22.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
52	BW	113	Total	C	N	O	S	0	0	0
			896	563	176	155	2			

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
52	DW	113	Total	C	N	O	S	0	0	0
			896	563	176	155	2			

- Molecule 53 is a protein called 50S RIBOSOMAL PROTEIN L23.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
53	BX	93	Total	C	N	O		0	0	1
			726	471	132	123				
53	DX	93	Total	C	N	O		0	0	1
			726	471	132	123				

- Molecule 54 is a protein called 50S RIBOSOMAL PROTEIN L24.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
54	BY	101	Total	C	N	O	S	0	0	1
			776	500	149	123	4			
54	DY	101	Total	C	N	O	S	0	0	1
			776	500	149	123	4			

- Molecule 55 is a protein called 50S RIBOSOMAL PROTEIN L25.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
55	BZ	177	Total	C	N	O	S	0	0	1
			1404	897	253	252	2			
55	DZ	177	Total	C	N	O	S	0	0	1
			1404	897	253	252	2			

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	AA	215	Total	Mg	0	0
			215	215		
56	AE	1	Total	Mg	0	0
			1	1		
56	AV	7	Total	Mg	0	0
			7	7		
56	AW	22	Total	Mg	0	0
			22	22		
56	AX	4	Total	Mg	0	0
			4	4		
56	AY	1	Total	Mg	0	0
			1	1		

Continued on next page...

Continued from previous page...

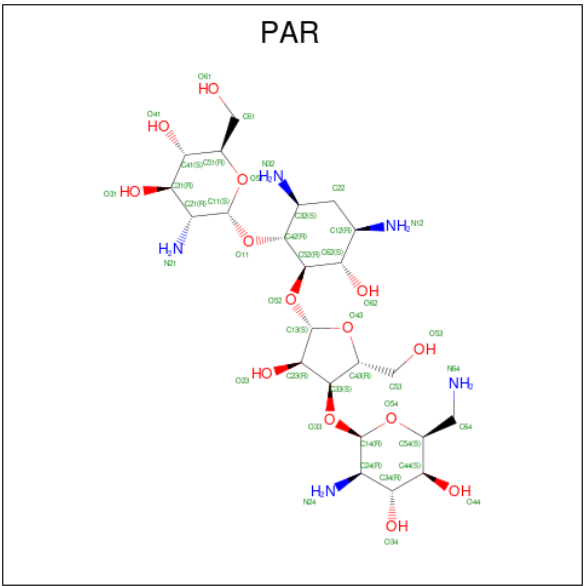
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	B1	1	Total 1	Mg 1	0	0
56	B2	5	Total 5	Mg 5	0	0
56	B3	1	Total 1	Mg 1	0	0
56	B5	2	Total 2	Mg 2	0	0
56	B7	2	Total 2	Mg 2	0	0
56	BA	454	Total 454	Mg 454	0	0
56	BB	19	Total 19	Mg 19	0	0
56	BE	1	Total 1	Mg 1	0	0
56	BF	2	Total 2	Mg 2	0	0
56	BN	1	Total 1	Mg 1	0	0
56	BO	1	Total 1	Mg 1	0	0
56	BV	1	Total 1	Mg 1	0	0
56	BX	1	Total 1	Mg 1	0	0
56	CA	189	Total 189	Mg 189	0	0
56	CF	1	Total 1	Mg 1	0	0
56	CJ	1	Total 1	Mg 1	0	0
56	CM	1	Total 1	Mg 1	0	0
56	CU	1	Total 1	Mg 1	0	0
56	CV	4	Total 4	Mg 4	0	0
56	CW	13	Total 13	Mg 13	0	0
56	CX	6	Total 6	Mg 6	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	D5	2	Total	Mg	0	0
			2	2		
56	DA	398	Total	Mg	0	0
			398	398		
56	DB	12	Total	Mg	0	0
			12	12		
56	DD	2	Total	Mg	0	0
			2	2		
56	DE	1	Total	Mg	0	0
			1	1		
56	DF	1	Total	Mg	0	0
			1	1		
56	DH	1	Total	Mg	0	0
			1	1		
56	DN	1	Total	Mg	0	0
			1	1		
56	DO	1	Total	Mg	0	0
			1	1		
56	DS	1	Total	Mg	0	0
			1	1		
56	DU	1	Total	Mg	0	0
			1	1		
56	DZ	1	Total	Mg	0	0
			1	1		

- Molecule 57 is PAROMOMYCIN (CCD ID: PAR) (formula: C₂₃H₄₅N₅O₁₄).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
57	AA	1	Total	C	N	O	0	0
			42	23	5	14		
57	CA	1	Total	C	N	O	0	0
			42	23	5	14		

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
58	AD	1	Total	Zn	0	0
			1	1		
58	AN	1	Total	Zn	0	0
			1	1		
58	CD	1	Total	Zn	0	0
			1	1		
58	CN	1	Total	Zn	0	0
			1	1		

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

3 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	213.32Å 452.95Å 631.36Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.80 50.00 – 2.80	Depositor EDS
% Data completeness (in resolution range)	90.7 (50.00-2.80) 90.7 (50.00-2.80)	Depositor EDS
R_{merge}	0.28	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.84 (at 2.81Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.272 , 0.313 0.266 , 0.306	Depositor DCC
R_{free} test set	64102 reflections (4.77%)	wwPDB-VP
Wilson B-factor (Å ²)	36.9	Xtriage
Anisotropy	0.160	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.21 , 86.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.35$, $\langle L^2 \rangle = 0.17$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.87	EDS
Total number of atoms	291075	wwPDB-VP
Average B, all atoms (Å ²)	58.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.24% 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](#)

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
22	5MU	CV	54	22	19,22,23	0.25	0	27,32,35	0.37	0
22	5MU	AV	54	22	19,22,23	0.24	0	27,32,35	0.37	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	5MU	CV	54	22	-	0/7/25/26	0/2/2/2
22	5MU	AV	54	22	-	0/7/25/26	0/2/2/2

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

4.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

4.6 Ligand geometry [i](#)

Of 1385 ligands modelled in this entry, 1383 are monoatomic - leaving 2 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
57	PAR	AA	1816	-	44,45,45	1.41	7 (15%)	63,67,67	1.16	4 (6%)
57	PAR	CA	1790	-	44,45,45	1.44	9 (20%)	63,67,67	1.28	6 (9%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
57	PAR	AA	1816	-	-	5/18/94/94	0/4/4/4
57	PAR	CA	1790	-	-	3/18/94/94	0/4/4/4

The worst 5 of 16 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
57	CA	1790	PAR	C34-C24	4.37	1.59	1.53
57	AA	1816	PAR	C52-C42	3.10	1.58	1.52
57	AA	1816	PAR	O54-C14	2.79	1.49	1.41
57	AA	1816	PAR	C11-C21	2.68	1.57	1.52
57	AA	1816	PAR	C14-C24	2.62	1.57	1.52

The worst 5 of 10 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
57	AA	1816	PAR	O33-C14-C24	5.13	116.47	108.08
57	CA	1790	PAR	O33-C14-C24	4.75	115.86	108.08
57	CA	1790	PAR	O54-C54-C64	3.70	113.18	106.07
57	CA	1790	PAR	C14-O54-C54	3.51	120.57	113.72
57	CA	1790	PAR	O52-C13-O43	-3.08	108.22	111.37

There are no chirality outliers.

5 of 8 torsion outliers are listed below:

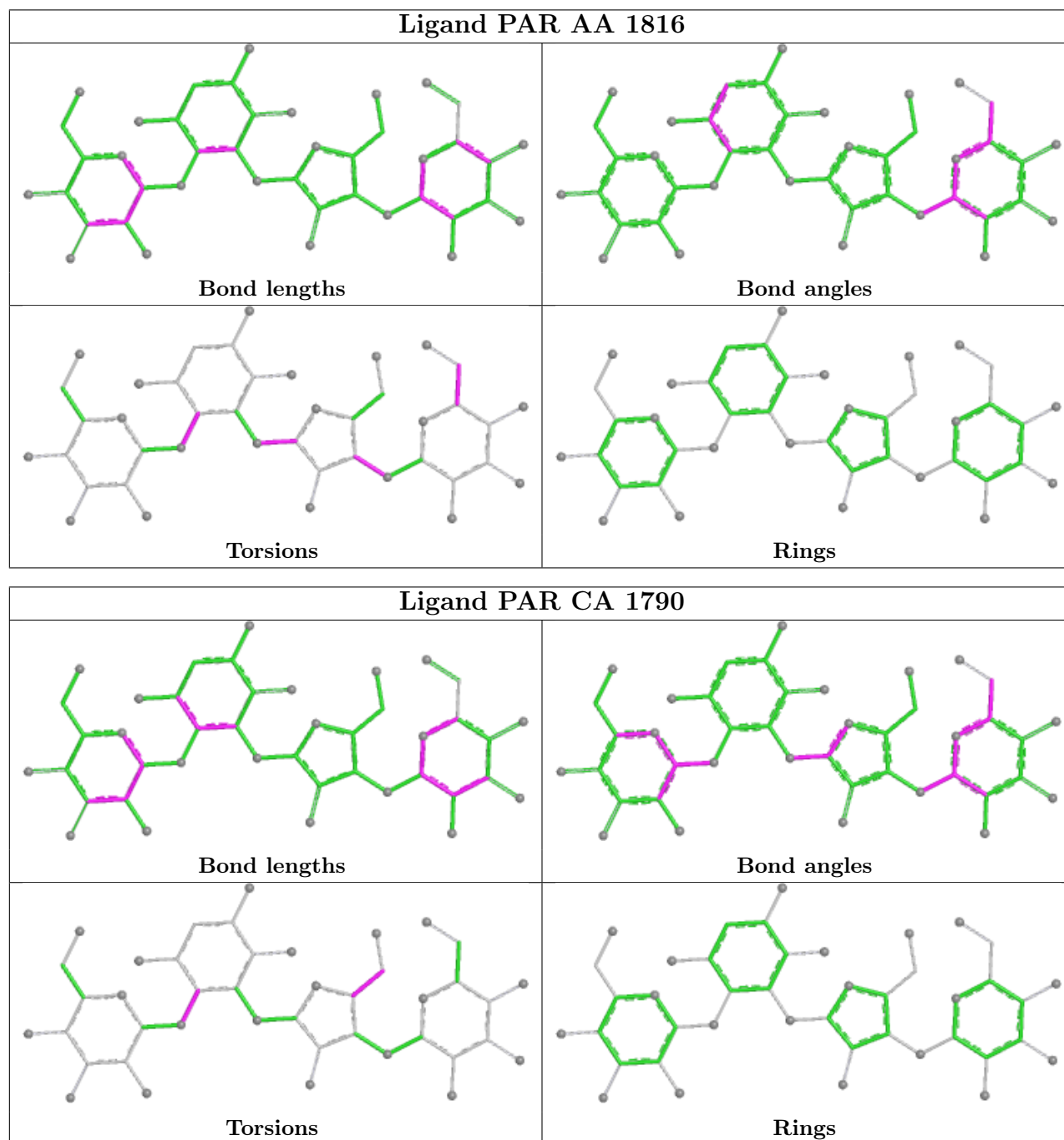
Mol	Chain	Res	Type	Atoms
57	CA	1790	PAR	O43-C43-C53-O53
57	CA	1790	PAR	C33-C43-C53-O53
57	AA	1816	PAR	O43-C13-O52-C52
57	AA	1816	PAR	C23-C13-O52-C52
57	AA	1816	PAR	O54-C54-C64-N64

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.



4.7 Other polymers ⓘ

There are no such residues in this entry.

4.8 Polymer linkage issues

The following chains have linkage breaks:

Mol	Chain	Number of breaks
13	AM	5
13	CM	5
9	CI	2
9	AI	2
31	B6	1
31	D6	1
40	BG	1
40	DG	1
51	BV	1
51	DV	1

The worst 5 of 20 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B6	46:HIS	C	47:THR	N	4.89
1	D6	46:HIS	C	47:THR	N	4.87
1	AM	69:GLU	C	70:LEU	N	4.66
1	CM	69:GLU	C	70:LEU	N	4.66
1	CI	53:VAL	C	54:ASP	N	4.02

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	AA	1504/1522 (98%)	0.17	124 (8%) 17 13	2, 42, 165, 200	0
1	CA	1504/1522 (98%)	0.40	132 (8%) 15 11	3, 50, 172, 200	0
2	AB	235/256 (91%)	1.44	68 (28%) 1 1	17, 94, 183, 200	0
2	CB	235/256 (91%)	1.94	101 (42%) 0 0	17, 104, 187, 200	0
3	AC	207/239 (86%)	1.24	56 (27%) 1 1	17, 70, 156, 200	0
3	CC	207/239 (86%)	1.43	58 (28%) 1 1	19, 84, 149, 190	0
4	AD	208/209 (99%)	0.62	34 (16%) 4 4	1, 43, 127, 198	0
4	CD	208/209 (99%)	0.97	39 (18%) 3 2	4, 51, 133, 182	0
5	AE	151/162 (93%)	0.75	18 (11%) 9 7	4, 51, 128, 177	0
5	CE	151/162 (93%)	0.77	23 (15%) 5 4	3, 56, 140, 185	0
6	AF	101/101 (100%)	0.63	12 (11%) 9 7	5, 48, 131, 156	0
6	CF	101/101 (100%)	0.58	13 (12%) 7 6	2, 54, 130, 151	0
7	AG	155/156 (99%)	1.46	52 (33%) 1 1	8, 68, 151, 184	0
7	CG	155/156 (99%)	1.97	67 (43%) 0 0	15, 87, 155, 190	0
8	AH	138/138 (100%)	0.84	19 (13%) 6 5	3, 52, 120, 173	0
8	CH	138/138 (100%)	0.90	23 (16%) 4 3	16, 58, 138, 152	0
9	AI	127/128 (99%)	1.92	51 (40%) 0 0	26, 97, 171, 200	0
9	CI	127/128 (99%)	2.33	67 (52%) 0 0	28, 111, 175, 200	0
10	AJ	99/105 (94%)	2.15	48 (48%) 0 0	17, 105, 178, 200	0
10	CJ	99/105 (94%)	2.43	52 (52%) 0 0	34, 123, 176, 197	0
11	AK	119/129 (92%)	0.91	17 (14%) 6 5	8, 46, 151, 192	0
11	CK	119/129 (92%)	1.13	24 (20%) 3 2	16, 61, 147, 200	0
12	AL	125/135 (92%)	0.84	23 (18%) 3 2	5, 38, 133, 200	0
12	CL	125/135 (92%)	0.92	28 (22%) 2 1	1, 38, 132, 200	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å ²)	Q<0.9
13	AM	125/126 (99%)	1.90	40 (32%)	1	1	13, 74, 159, 196	0
13	CM	125/126 (99%)	1.76	45 (36%)	1	0	19, 91, 160, 191	0
14	AN	60/61 (98%)	1.91	20 (33%)	1	1	14, 66, 161, 184	0
14	CN	60/61 (98%)	1.87	18 (30%)	1	1	19, 73, 143, 182	0
15	AO	88/89 (98%)	0.73	16 (18%)	3	2	2, 42, 129, 141	0
15	CO	88/89 (98%)	1.03	19 (21%)	2	2	2, 56, 124, 167	0
16	AP	84/88 (95%)	0.47	8 (9%)	14	10	6, 36, 104, 190	0
16	CP	84/88 (95%)	0.75	11 (13%)	7	6	6, 49, 121, 199	0
17	AQ	100/105 (95%)	0.59	13 (13%)	7	6	1, 45, 110, 193	0
17	CQ	100/105 (95%)	0.99	13 (13%)	7	6	18, 60, 105, 194	0
18	AR	70/88 (79%)	0.77	11 (15%)	5	4	10, 50, 140, 172	0
18	CR	70/88 (79%)	0.93	14 (20%)	3	2	7, 56, 144, 179	0
19	AS	79/93 (84%)	1.63	25 (31%)	1	1	22, 79, 186, 200	0
19	CS	79/93 (84%)	2.25	45 (56%)	0	0	25, 83, 175, 197	0
20	AT	99/106 (93%)	1.32	24 (24%)	2	1	5, 60, 152, 180	0
20	CT	99/106 (93%)	1.54	30 (30%)	1	1	17, 77, 141, 183	0
21	AU	25/27 (92%)	2.08	11 (44%)	0	0	27, 72, 128, 141	0
21	CU	25/27 (92%)	2.77	16 (64%)	0	0	40, 74, 127, 139	0
22	AV	76/77 (98%)	0.09	6 (7%)	18	13	14, 53, 143, 194	0
22	CV	76/77 (98%)	0.31	7 (9%)	14	10	21, 55, 146, 198	0
23	AW	76/76 (100%)	1.07	13 (17%)	4	3	30, 103, 164, 199	0
23	AY	19/76 (25%)	0.85	3 (15%)	5	4	23, 72, 190, 196	0
23	CW	76/76 (100%)	1.27	20 (26%)	1	1	35, 116, 165, 196	0
23	CY	19/76 (25%)	0.95	3 (15%)	5	4	26, 76, 186, 196	0
24	AX	11/24 (45%)	0.43	2 (18%)	3	2	12, 33, 170, 190	0
24	CX	11/24 (45%)	0.99	2 (18%)	3	2	14, 39, 167, 197	0
25	B0	85/85 (100%)	1.02	20 (23%)	2	1	8, 43, 138, 196	0
25	D0	85/85 (100%)	1.61	25 (29%)	1	1	18, 57, 137, 179	0
26	B1	89/98 (90%)	1.41	31 (34%)	1	0	1, 35, 143, 157	0
26	D1	89/98 (90%)	1.27	28 (31%)	1	1	1, 44, 145, 200	0
27	B2	51/72 (70%)	2.35	26 (50%)	0	0	5, 66, 145, 200	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å ²)	Q<0.9
27	D2	51/72 (70%)	2.46	26 (50%)	0	0	13, 79, 154, 200	0
28	B3	60/60 (100%)	0.94	13 (21%)	2	2	5, 57, 140, 190	0
28	D3	60/60 (100%)	1.61	22 (36%)	1	0	5, 58, 146, 198	0
29	B4	50/71 (70%)	1.82	18 (36%)	1	0	38, 90, 158, 173	0
29	D4	50/71 (70%)	2.53	26 (52%)	0	0	54, 117, 160, 198	0
30	B5	59/60 (98%)	1.55	23 (38%)	1	0	5, 51, 192, 200	0
30	D5	59/60 (98%)	1.11	11 (18%)	3	2	1, 65, 179, 200	0
31	B6	45/54 (83%)	2.62	26 (57%)	0	0	54, 103, 171, 180	0
31	D6	45/54 (83%)	3.24	31 (68%)	0	0	64, 139, 171, 189	0
32	B7	49/49 (100%)	0.24	7 (14%)	6	5	1, 19, 115, 165	0
32	D7	49/49 (100%)	0.32	6 (12%)	8	6	1, 19, 88, 174	0
33	B8	64/65 (98%)	1.51	18 (28%)	1	1	4, 44, 140, 195	0
33	D8	64/65 (98%)	1.73	22 (34%)	1	1	5, 52, 155, 192	0
34	BA	2772/2787 (99%)	-0.11	167 (6%)	27	21	1, 29, 145, 200	0
34	DA	2772/2787 (99%)	-0.03	189 (6%)	23	17	1, 30, 152, 200	0
35	BB	119/122 (97%)	0.34	5 (4%)	40	32	22, 64, 108, 197	0
35	DB	119/122 (97%)	0.86	11 (9%)	14	10	34, 76, 127, 188	0
36	BC	191/229 (83%)	2.38	108 (56%)	0	0	51, 144, 186, 200	0
36	DC	191/229 (83%)	2.49	108 (56%)	0	0	61, 146, 186, 200	0
37	BD	272/276 (98%)	0.10	21 (7%)	19	14	1, 19, 89, 196	0
37	DD	272/276 (98%)	0.12	17 (6%)	26	19	1, 21, 89, 200	0
38	BE	205/206 (99%)	1.04	51 (24%)	2	1	1, 46, 141, 193	0
38	DE	205/206 (99%)	1.03	45 (21%)	2	2	1, 43, 144, 199	0
39	BF	208/210 (99%)	0.74	38 (18%)	3	2	1, 44, 155, 200	0
39	DF	208/210 (99%)	0.92	45 (21%)	2	2	1, 44, 160, 200	0
40	BG	181/182 (99%)	1.11	45 (24%)	2	1	8, 65, 142, 188	0
40	DG	181/182 (99%)	1.63	62 (34%)	1	1	10, 82, 149, 195	0
41	BH	160/180 (88%)	2.38	86 (53%)	0	0	51, 124, 174, 200	0
41	DH	160/180 (88%)	1.98	63 (39%)	1	0	10, 102, 174, 194	0
42	BI	146/148 (98%)	1.48	43 (29%)	1	1	5, 78, 148, 187	0
42	DI	146/148 (98%)	3.08	91 (62%)	0	0	9, 124, 184, 200	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å ²)	Q<0.9
43	BN	139/140 (99%)	1.32	35 (25%)	1	1	10, 68, 144, 163	0
43	DN	139/140 (99%)	1.50	44 (31%)	1	1	15, 63, 141, 165	0
44	BO	122/122 (100%)	0.62	15 (12%)	8	6	3, 32, 103, 177	0
44	DO	122/122 (100%)	0.35	10 (8%)	17	13	1, 33, 102, 126	0
45	BP	146/150 (97%)	1.63	47 (32%)	1	1	1, 61, 159, 193	0
45	DP	146/150 (97%)	1.93	58 (39%)	1	0	2, 71, 165, 198	0
46	BQ	136/141 (96%)	1.47	40 (29%)	1	1	7, 58, 171, 200	0
46	DQ	136/141 (96%)	1.31	34 (25%)	2	1	7, 54, 164, 200	0
47	BR	117/118 (99%)	0.60	16 (13%)	6	5	3, 32, 132, 146	0
47	DR	117/118 (99%)	0.97	18 (15%)	5	4	3, 42, 126, 166	0
48	BS	99/112 (88%)	1.65	28 (28%)	1	1	21, 76, 134, 173	0
48	DS	99/112 (88%)	1.88	37 (37%)	1	0	24, 89, 143, 170	0
49	BT	138/146 (94%)	1.51	40 (28%)	1	1	3, 67, 169, 190	0
49	DT	138/146 (94%)	1.59	48 (34%)	1	0	7, 65, 171, 200	0
50	BU	117/118 (99%)	1.27	26 (22%)	2	1	5, 50, 142, 200	0
50	DU	117/118 (99%)	1.07	28 (23%)	2	1	1, 46, 145, 190	0
51	BV	101/101 (100%)	2.16	55 (54%)	0	0	14, 96, 174, 192	0
51	DV	101/101 (100%)	2.09	52 (51%)	0	0	11, 93, 172, 193	0
52	BW	113/113 (100%)	0.13	8 (7%)	22	16	1, 26, 121, 161	0
52	DW	113/113 (100%)	0.47	15 (13%)	7	5	3, 28, 126, 200	0
53	BX	93/96 (96%)	1.06	20 (21%)	2	2	1, 46, 137, 168	0
53	DX	93/96 (96%)	1.32	25 (26%)	1	1	8, 54, 138, 157	0
54	BY	101/110 (91%)	2.10	44 (43%)	0	0	1, 79, 170, 195	0
54	DY	101/110 (91%)	2.03	47 (46%)	0	0	1, 79, 177, 196	0
55	BZ	177/206 (85%)	1.74	67 (37%)	1	0	19, 96, 177, 200	0
55	DZ	177/206 (85%)	1.99	79 (44%)	0	0	18, 98, 178, 198	0
All	All	20972/21886 (95%)	0.80	4094 (19%)	3	2	1, 51, 163, 200	0

The worst 5 of 4094 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
42	DI	120	ILE	16.2
33	D8	65	GLU	15.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
42	DI	125	GLU	14.8
46	BQ	24	GLY	14.3
42	DI	88	ILE	13.9

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
22	5MU	AV	54	21/22	0.84	0.13	75,83,108,108	0
22	5MU	CV	54	21/22	0.89	0.10	64,75,79,79	0

5.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
56	MG	DA	3255	1/1	0.35	0.52	92,92,92,92	0
56	MG	AA	1633	1/1	0.41	0.37	90,90,90,90	0
56	MG	DA	3213	1/1	0.43	0.47	84,84,84,84	0
56	MG	DA	3261	1/1	0.55	0.61	94,94,94,94	0
56	MG	CA	1685	1/1	0.57	0.85	82,82,82,82	0
56	MG	DA	3275	1/1	0.63	0.53	75,75,75,75	0
56	MG	CA	1742	1/1	0.66	0.25	76,76,76,76	0
56	MG	BA	3296	1/1	0.68	0.30	75,75,75,75	0
56	MG	CA	1695	1/1	0.69	0.21	70,70,70,70	0
56	MG	BB	201	1/1	0.69	0.32	54,54,54,54	1
56	MG	DA	3330	1/1	0.69	0.26	81,81,81,81	0
56	MG	BA	3285	1/1	0.70	0.39	74,74,74,74	0
56	MG	CA	1673	1/1	0.70	0.43	80,80,80,80	1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	DB	202	1/1	0.70	0.12	57,57,57,57	0
56	MG	CA	1719	1/1	0.71	0.62	99,99,99,99	0
56	MG	BA	3376	1/1	0.71	0.22	47,47,47,47	0
56	MG	BB	213	1/1	0.72	0.21	71,71,71,71	0
56	MG	AA	1697	1/1	0.72	0.59	88,88,88,88	0
56	MG	DA	3217	1/1	0.73	0.24	62,62,62,62	0
56	MG	DA	3328	1/1	0.74	0.09	27,27,27,27	0
56	MG	CX	102	1/1	0.74	0.42	75,75,75,75	0
56	MG	CA	1697	1/1	0.74	0.32	49,49,49,49	0
56	MG	BB	205	1/1	0.75	0.38	35,35,35,35	1
56	MG	DA	3168	1/1	0.75	0.38	56,56,56,56	0
56	MG	BA	3233	1/1	0.75	0.24	77,77,77,77	0
56	MG	BA	3254	1/1	0.75	0.20	48,48,48,48	0
56	MG	BA	3214	1/1	0.75	0.31	44,44,44,44	0
56	MG	CA	1646	1/1	0.76	0.24	62,62,62,62	0
56	MG	CA	1758	1/1	0.76	0.12	44,44,44,44	0
56	MG	BA	3349	1/1	0.76	0.18	28,28,28,28	1
56	MG	CA	1706	1/1	0.77	0.18	54,54,54,54	0
56	MG	BA	3428	1/1	0.77	0.43	72,72,72,72	1
56	MG	CA	1725	1/1	0.77	0.19	56,56,56,56	0
56	MG	BA	3433	1/1	0.77	0.24	74,74,74,74	0
56	MG	AA	1782	1/1	0.77	0.20	68,68,68,68	0
56	MG	CW	107	1/1	0.77	0.13	63,63,63,63	1
56	MG	AW	113	1/1	0.77	0.15	46,46,46,46	1
56	MG	AA	1665	1/1	0.77	0.13	27,27,27,27	0
56	MG	BA	3413	1/1	0.78	0.22	63,63,63,63	0
56	MG	DA	3219	1/1	0.78	0.43	75,75,75,75	0
56	MG	CA	1722	1/1	0.78	0.36	70,70,70,70	0
56	MG	AA	1620	1/1	0.78	0.19	28,28,28,28	0
56	MG	DA	3137	1/1	0.78	0.29	62,62,62,62	0
56	MG	DA	3155	1/1	0.78	0.16	50,50,50,50	0
56	MG	CA	1734	1/1	0.78	0.11	59,59,59,59	0
56	MG	AA	1791	1/1	0.78	0.13	22,22,22,22	1
56	MG	DA	3310	1/1	0.79	0.10	50,50,50,50	0
56	MG	DA	3320	1/1	0.79	0.32	70,70,70,70	0
56	MG	BA	3408	1/1	0.79	0.07	46,46,46,46	0
56	MG	BA	3419	1/1	0.79	0.11	39,39,39,39	0
56	MG	DA	3334	1/1	0.79	0.14	34,34,34,34	1
56	MG	DA	3342	1/1	0.79	0.20	49,49,49,49	0
56	MG	CA	1752	1/1	0.79	0.26	83,83,83,83	0
56	MG	DA	3333	1/1	0.80	0.31	67,67,67,67	0
56	MG	AA	1745	1/1	0.80	0.17	56,56,56,56	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	DA	3248	1/1	0.80	0.45	82,82,82,82	0
56	MG	BB	203	1/1	0.80	0.11	52,52,52,52	0
56	MG	DB	204	1/1	0.80	0.14	48,48,48,48	0
56	MG	BA	3278	1/1	0.81	0.29	90,90,90,90	0
56	MG	BA	3154	1/1	0.81	0.08	28,28,28,28	1
56	MG	CA	1763	1/1	0.81	0.18	32,32,32,32	0
56	MG	DA	3250	1/1	0.81	0.15	57,57,57,57	0
56	MG	CW	104	1/1	0.81	0.18	46,46,46,46	0
56	MG	DA	3258	1/1	0.81	0.57	80,80,80,80	0
56	MG	AA	1750	1/1	0.81	0.18	57,57,57,57	0
56	MG	CA	1622	1/1	0.81	0.15	123,123,123,123	0
56	MG	AA	1808	1/1	0.81	0.12	33,33,33,33	0
56	MG	CA	1665	1/1	0.81	0.46	71,71,71,71	0
56	MG	BA	3375	1/1	0.81	0.21	42,42,42,42	1
56	MG	DA	3173	1/1	0.81	0.19	41,41,41,41	0
56	MG	DA	3187	1/1	0.81	0.46	86,86,86,86	0
56	MG	DA	3191	1/1	0.81	0.18	25,25,25,25	0
56	MG	DA	3203	1/1	0.81	0.18	58,58,58,58	0
56	MG	DA	3208	1/1	0.81	0.15	40,40,40,40	0
56	MG	AA	1648	1/1	0.81	0.28	86,86,86,86	0
56	MG	DB	205	1/1	0.81	0.19	51,51,51,51	0
56	MG	DA	3004	1/1	0.82	0.34	90,90,90,90	0
56	MG	CA	1711	1/1	0.82	0.22	63,63,63,63	0
56	MG	DA	3138	1/1	0.82	0.14	40,40,40,40	0
56	MG	CV	102	1/1	0.82	0.20	56,56,56,56	0
56	MG	DA	3167	1/1	0.82	0.27	101,101,101,101	0
56	MG	CV	103	1/1	0.82	0.22	56,56,56,56	0
56	MG	BA	3395	1/1	0.82	0.27	54,54,54,54	1
56	MG	CA	1637	1/1	0.82	0.56	81,81,81,81	0
56	MG	CW	109	1/1	0.82	0.12	81,81,81,81	0
56	MG	BA	3300	1/1	0.82	0.10	6,6,6,6	0
56	MG	BA	3323	1/1	0.83	0.13	79,79,79,79	0
56	MG	BA	3016	1/1	0.83	0.28	37,37,37,37	0
56	MG	BA	3258	1/1	0.83	0.23	70,70,70,70	0
56	MG	AA	1688	1/1	0.83	0.15	39,39,39,39	0
56	MG	BA	3157	1/1	0.83	0.32	39,39,39,39	0
56	MG	AA	1733	1/1	0.83	0.31	63,63,63,63	0
56	MG	AA	1738	1/1	0.83	0.23	49,49,49,49	0
56	MG	DA	3274	1/1	0.83	0.18	53,53,53,53	0
56	MG	DA	3163	1/1	0.83	0.29	51,51,51,51	0
56	MG	DA	3277	1/1	0.83	0.20	55,55,55,55	0
56	MG	BA	3158	1/1	0.84	0.26	44,44,44,44	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	AA	1661	1/1	0.84	0.24	60,60,60,60	0
56	MG	CX	104	1/1	0.84	0.12	31,31,31,31	1
56	MG	CA	1745	1/1	0.84	0.12	77,77,77,77	0
56	MG	AA	1716	1/1	0.84	0.63	73,73,73,73	0
56	MG	BA	3393	1/1	0.84	0.34	60,60,60,60	0
56	MG	AA	1799	1/1	0.84	0.20	71,71,71,71	0
56	MG	DA	3159	1/1	0.84	0.21	57,57,57,57	0
56	MG	CA	1652	1/1	0.84	0.23	52,52,52,52	0
56	MG	CA	1721	1/1	0.84	0.23	57,57,57,57	0
56	MG	DA	3358	1/1	0.84	0.38	54,54,54,54	0
56	MG	AA	1694	1/1	0.84	0.15	58,58,58,58	0
56	MG	BB	204	1/1	0.84	0.09	42,42,42,42	0
56	MG	DA	3268	1/1	0.84	0.25	51,51,51,51	0
56	MG	AA	1678	1/1	0.85	0.08	43,43,43,43	0
56	MG	BA	3346	1/1	0.85	0.19	60,60,60,60	0
56	MG	BB	212	1/1	0.85	0.07	18,18,18,18	1
56	MG	CA	1696	1/1	0.85	0.18	51,51,51,51	0
56	MG	DA	3122	1/1	0.85	0.30	43,43,43,43	0
56	MG	CA	1751	1/1	0.85	0.22	81,81,81,81	0
56	MG	BA	3415	1/1	0.85	0.18	38,38,38,38	0
56	MG	AE	201	1/1	0.85	0.12	47,47,47,47	0
56	MG	AW	106	1/1	0.85	0.09	26,26,26,26	0
56	MG	CA	1716	1/1	0.85	0.44	67,67,67,67	0
56	MG	BA	3213	1/1	0.85	0.08	19,19,19,19	0
56	MG	AA	1734	1/1	0.85	0.20	48,48,48,48	1
56	MG	AA	1735	1/1	0.85	0.50	84,84,84,84	0
56	MG	DA	3273	1/1	0.85	0.37	59,59,59,59	0
56	MG	AA	1698	1/1	0.86	0.23	38,38,38,38	0
56	MG	AA	1670	1/1	0.86	0.12	52,52,52,52	0
56	MG	DA	3007	1/1	0.86	0.27	39,39,39,39	0
56	MG	AW	120	1/1	0.86	0.08	52,52,52,52	0
56	MG	CA	1729	1/1	0.86	0.33	71,71,71,71	0
56	MG	DA	3270	1/1	0.86	0.13	47,47,47,47	0
56	MG	BA	3259	1/1	0.86	0.07	32,32,32,32	0
56	MG	CA	1739	1/1	0.86	0.28	66,66,66,66	0
56	MG	CA	1647	1/1	0.86	0.24	57,57,57,57	0
56	MG	CA	1744	1/1	0.86	0.14	64,64,64,64	0
56	MG	BA	3412	1/1	0.86	0.13	48,48,48,48	0
56	MG	DA	3312	1/1	0.86	0.11	44,44,44,44	0
56	MG	B2	101	1/1	0.86	0.12	36,36,36,36	0
56	MG	BA	3282	1/1	0.86	0.34	49,49,49,49	0
56	MG	AA	1776	1/1	0.86	0.07	30,30,30,30	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	BA	3064	1/1	0.86	0.19	30,30,30,30	0
56	MG	AA	1727	1/1	0.86	0.21	40,40,40,40	0
56	MG	AA	1603	1/1	0.86	0.21	47,47,47,47	0
56	MG	BA	3336	1/1	0.86	0.06	45,45,45,45	0
56	MG	AA	1626	1/1	0.86	0.17	50,50,50,50	0
56	MG	AA	1618	1/1	0.86	0.37	66,66,66,66	0
56	MG	AA	1667	1/1	0.86	0.23	50,50,50,50	0
56	MG	DO	201	1/1	0.86	0.20	67,67,67,67	0
56	MG	CA	1675	1/1	0.87	0.26	57,57,57,57	0
56	MG	BA	3230	1/1	0.87	0.09	36,36,36,36	0
56	MG	BA	3277	1/1	0.87	0.23	38,38,38,38	0
56	MG	CA	1634	1/1	0.87	0.15	17,17,17,17	0
56	MG	DA	3207	1/1	0.87	0.11	8,8,8,8	0
56	MG	B3	101	1/1	0.87	0.35	48,48,48,48	1
56	MG	CA	1644	1/1	0.87	0.14	59,59,59,59	0
56	MG	CA	1750	1/1	0.87	0.13	50,50,50,50	0
56	MG	DA	3218	1/1	0.87	0.13	27,27,27,27	0
56	MG	CA	1710	1/1	0.87	0.10	22,22,22,22	0
56	MG	BA	3279	1/1	0.87	0.16	55,55,55,55	0
56	MG	AW	109	1/1	0.87	0.11	34,34,34,34	1
56	MG	BA	3222	1/1	0.87	0.13	41,41,41,41	0
56	MG	DA	3369	1/1	0.87	0.11	46,46,46,46	0
56	MG	DA	3160	1/1	0.87	0.20	37,37,37,37	0
56	MG	BA	3361	1/1	0.87	0.07	53,53,53,53	0
56	MG	CA	1668	1/1	0.87	0.17	42,42,42,42	0
56	MG	DH	201	1/1	0.87	0.08	36,36,36,36	0
56	MG	BA	3374	1/1	0.87	0.11	48,48,48,48	0
56	MG	BF	302	1/1	0.88	0.12	46,46,46,46	0
56	MG	DA	3149	1/1	0.88	0.64	84,84,84,84	0
56	MG	DA	3151	1/1	0.88	0.11	46,46,46,46	0
56	MG	CA	1611	1/1	0.88	0.10	67,67,67,67	0
56	MG	AA	1651	1/1	0.88	0.23	35,35,35,35	0
56	MG	DA	3272	1/1	0.88	0.32	47,47,47,47	0
56	MG	AW	101	1/1	0.88	0.10	35,35,35,35	0
56	MG	BA	3353	1/1	0.88	0.23	42,42,42,42	1
56	MG	CA	1757	1/1	0.88	0.30	56,56,56,56	0
56	MG	CA	1638	1/1	0.88	0.17	42,42,42,42	0
56	MG	CA	1714	1/1	0.88	0.21	81,81,81,81	0
56	MG	B2	103	1/1	0.88	0.14	46,46,46,46	0
56	MG	BA	3429	1/1	0.88	0.15	41,41,41,41	0
56	MG	DA	3193	1/1	0.88	0.18	35,35,35,35	0
56	MG	AA	1792	1/1	0.88	0.23	74,74,74,74	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	DA	3206	1/1	0.88	0.08	47,47,47,47	0
56	MG	BA	3299	1/1	0.88	0.14	22,22,22,22	0
56	MG	CA	1723	1/1	0.88	0.42	65,65,65,65	0
56	MG	AA	1742	1/1	0.88	0.29	45,45,45,45	0
56	MG	BA	3221	1/1	0.88	0.30	49,49,49,49	0
56	MG	DA	3381	1/1	0.88	0.20	77,77,77,77	0
56	MG	BA	3332	1/1	0.88	0.19	53,53,53,53	1
56	MG	CA	1737	1/1	0.88	0.15	35,35,35,35	0
56	MG	DA	3240	1/1	0.88	0.21	43,43,43,43	0
56	MG	AA	1737	1/1	0.88	0.15	60,60,60,60	0
56	MG	BA	3345	1/1	0.88	0.07	59,59,59,59	0
56	MG	CA	1760	1/1	0.89	0.13	33,33,33,33	0
56	MG	CA	1762	1/1	0.89	0.18	39,39,39,39	0
56	MG	BA	3335	1/1	0.89	0.07	45,45,45,45	0
56	MG	DA	3209	1/1	0.89	0.24	31,31,31,31	0
56	MG	CA	1780	1/1	0.89	0.17	38,38,38,38	0
56	MG	DA	3214	1/1	0.89	0.14	32,32,32,32	0
56	MG	CA	1786	1/1	0.89	0.25	29,29,29,29	0
56	MG	AA	1810	1/1	0.89	0.25	47,47,47,47	0
56	MG	CA	1698	1/1	0.89	0.30	42,42,42,42	0
56	MG	DA	3231	1/1	0.89	0.33	72,72,72,72	0
56	MG	DA	3234	1/1	0.89	0.14	33,33,33,33	0
56	MG	AA	1814	1/1	0.89	0.16	25,25,25,25	0
56	MG	AA	1772	1/1	0.89	0.39	73,73,73,73	0
56	MG	BB	206	1/1	0.89	0.22	78,78,78,78	0
56	MG	DA	3253	1/1	0.89	0.29	71,71,71,71	0
56	MG	CW	111	1/1	0.89	0.21	77,77,77,77	0
56	MG	CA	1713	1/1	0.89	0.38	93,93,93,93	0
56	MG	BA	3103	1/1	0.89	0.09	55,55,55,55	0
56	MG	DA	3262	1/1	0.89	0.26	72,72,72,72	0
56	MG	CX	106	1/1	0.89	0.35	47,47,47,47	0
56	MG	BA	3109	1/1	0.89	0.15	34,34,34,34	0
56	MG	BA	3268	1/1	0.89	0.08	24,24,24,24	0
56	MG	DA	3022	1/1	0.89	0.16	37,37,37,37	0
56	MG	DA	3100	1/1	0.89	0.19	21,21,21,21	0
56	MG	BA	3367	1/1	0.89	0.13	50,50,50,50	0
56	MG	BA	3119	1/1	0.89	0.12	16,16,16,16	0
56	MG	BA	3125	1/1	0.89	0.25	18,18,18,18	0
56	MG	BA	3143	1/1	0.89	0.18	21,21,21,21	0
56	MG	BA	3377	1/1	0.89	0.10	43,43,43,43	0
56	MG	AA	1617	1/1	0.89	0.27	24,24,24,24	0
56	MG	AA	1681	1/1	0.89	0.08	21,21,21,21	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	AA	1647	1/1	0.89	0.24	71,71,71,71	0
56	MG	DA	3162	1/1	0.89	0.24	35,35,35,35	0
56	MG	CA	1650	1/1	0.89	0.16	68,68,68,68	0
56	MG	DA	3353	1/1	0.89	0.28	42,42,42,42	0
56	MG	AA	1677	1/1	0.89	0.18	41,41,41,41	0
56	MG	AA	1755	1/1	0.89	0.19	47,47,47,47	0
56	MG	BA	3305	1/1	0.89	0.14	30,30,30,30	0
56	MG	DA	3394	1/1	0.89	0.09	66,66,66,66	0
56	MG	BA	3314	1/1	0.89	0.25	47,47,47,47	1
56	MG	DA	3188	1/1	0.89	0.17	42,42,42,42	0
56	MG	AA	1807	1/1	0.89	0.10	19,19,19,19	1
56	MG	DB	207	1/1	0.89	0.13	52,52,52,52	1
56	MG	BA	3327	1/1	0.89	0.05	30,30,30,30	0
56	MG	AA	1763	1/1	0.89	0.69	58,58,58,58	1
56	MG	BA	3331	1/1	0.90	0.07	45,45,45,45	0
56	MG	CA	1642	1/1	0.90	0.25	56,56,56,56	0
56	MG	DA	3238	1/1	0.90	0.22	54,54,54,54	0
56	MG	BA	3166	1/1	0.90	0.07	39,39,39,39	0
56	MG	DA	3024	1/1	0.90	0.23	20,20,20,20	0
56	MG	DA	3036	1/1	0.90	0.14	43,43,43,43	0
56	MG	DA	3042	1/1	0.90	0.41	58,58,58,58	0
56	MG	DA	3069	1/1	0.90	0.22	45,45,45,45	0
56	MG	BA	3414	1/1	0.90	0.39	44,44,44,44	0
56	MG	DA	3116	1/1	0.90	0.07	10,10,10,10	0
56	MG	BA	3272	1/1	0.90	0.28	49,49,49,49	0
56	MG	BA	3181	1/1	0.90	0.13	36,36,36,36	0
56	MG	BA	3337	1/1	0.90	0.05	57,57,57,57	0
56	MG	CA	1661	1/1	0.90	0.16	13,13,13,13	0
56	MG	BA	3070	1/1	0.90	0.17	24,24,24,24	0
56	MG	AW	116	1/1	0.90	0.07	58,58,58,58	0
56	MG	CA	1671	1/1	0.90	0.08	42,42,42,42	0
56	MG	DA	3276	1/1	0.90	0.18	45,45,45,45	0
56	MG	BA	3216	1/1	0.90	0.10	50,50,50,50	0
56	MG	AA	1769	1/1	0.90	0.15	61,61,61,61	0
56	MG	CA	1676	1/1	0.90	0.41	46,46,46,46	0
56	MG	CA	1759	1/1	0.90	0.14	68,68,68,68	0
56	MG	AA	1748	1/1	0.90	0.18	59,59,59,59	0
56	MG	DA	3329	1/1	0.90	0.14	45,45,45,45	0
56	MG	AA	1606	1/1	0.90	0.32	53,53,53,53	0
56	MG	AA	1731	1/1	0.90	0.17	56,56,56,56	0
56	MG	CA	1776	1/1	0.90	0.36	44,44,44,44	0
56	MG	BB	207	1/1	0.90	0.10	23,23,23,23	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	AA	1809	1/1	0.90	0.23	40,40,40,40	1
56	MG	DA	3357	1/1	0.90	0.09	26,26,26,26	0
56	MG	BA	3043	1/1	0.90	0.38	82,82,82,82	0
56	MG	BB	218	1/1	0.90	0.07	36,36,36,36	1
56	MG	AA	1619	1/1	0.90	0.23	41,41,41,41	0
56	MG	DA	3391	1/1	0.90	0.14	62,62,62,62	1
56	MG	DA	3392	1/1	0.90	0.05	47,47,47,47	0
56	MG	DA	3393	1/1	0.90	0.06	80,80,80,80	0
56	MG	BA	3326	1/1	0.90	0.13	49,49,49,49	0
56	MG	CA	1615	1/1	0.90	0.14	61,61,61,61	0
56	MG	CW	110	1/1	0.90	0.08	38,38,38,38	0
56	MG	CA	1619	1/1	0.90	0.17	55,55,55,55	0
56	MG	BA	3261	1/1	0.90	0.10	24,24,24,24	0
56	MG	BA	3403	1/1	0.90	0.21	78,78,78,78	0
56	MG	BA	3330	1/1	0.90	0.06	33,33,33,33	0
56	MG	CA	1767	1/1	0.91	0.39	67,67,67,67	0
56	MG	CA	1768	1/1	0.91	0.15	37,37,37,37	0
56	MG	AA	1608	1/1	0.91	0.14	47,47,47,47	0
56	MG	CA	1674	1/1	0.91	0.10	58,58,58,58	0
56	MG	BA	3227	1/1	0.91	0.18	49,49,49,49	0
56	MG	CA	1787	1/1	0.91	0.21	39,39,39,39	1
56	MG	BA	3431	1/1	0.91	0.16	51,51,51,51	0
56	MG	CA	1680	1/1	0.91	0.14	51,51,51,51	0
56	MG	AA	1627	1/1	0.91	0.38	39,39,39,39	0
56	MG	CA	1691	1/1	0.91	0.19	56,56,56,56	0
56	MG	CA	1694	1/1	0.91	0.07	33,33,33,33	0
56	MG	BA	3452	1/1	0.91	0.21	39,39,39,39	0
56	MG	DA	3245	1/1	0.91	0.15	38,38,38,38	0
56	MG	AW	110	1/1	0.91	0.12	46,46,46,46	0
56	MG	BA	3253	1/1	0.91	0.18	38,38,38,38	0
56	MG	AA	1629	1/1	0.91	0.10	29,29,29,29	0
56	MG	BA	3255	1/1	0.91	0.16	28,28,28,28	0
56	MG	AA	1736	1/1	0.91	0.11	19,19,19,19	0
56	MG	BA	3147	1/1	0.91	0.07	20,20,20,20	0
56	MG	AA	1616	1/1	0.91	0.16	18,18,18,18	0
56	MG	AA	1721	1/1	0.91	0.13	28,28,28,28	0
56	MG	BB	215	1/1	0.91	0.09	40,40,40,40	0
56	MG	CA	1718	1/1	0.91	0.17	47,47,47,47	0
56	MG	AA	1686	1/1	0.91	0.20	52,52,52,52	0
56	MG	BA	3358	1/1	0.91	0.06	42,42,42,42	0
56	MG	DA	3106	1/1	0.91	0.11	15,15,15,15	0
56	MG	CA	1609	1/1	0.91	0.08	33,33,33,33	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	CA	1610	1/1	0.91	0.17	15,15,15,15	0
56	MG	DA	3279	1/1	0.91	0.12	15,15,15,15	0
56	MG	AA	1623	1/1	0.91	0.10	32,32,32,32	0
56	MG	BA	3178	1/1	0.91	0.31	54,54,54,54	0
56	MG	DA	3142	1/1	0.91	0.11	52,52,52,52	0
56	MG	BA	3373	1/1	0.91	0.09	39,39,39,39	0
56	MG	B5	102	1/1	0.91	0.14	24,24,24,24	0
56	MG	BA	3204	1/1	0.91	0.07	0,0,0,0	0
56	MG	BA	3212	1/1	0.91	0.21	47,47,47,47	0
56	MG	BA	3286	1/1	0.91	0.20	38,38,38,38	0
56	MG	DA	3339	1/1	0.91	0.06	17,17,17,17	0
56	MG	BA	3384	1/1	0.91	0.20	36,36,36,36	0
56	MG	BA	3293	1/1	0.91	0.13	51,51,51,51	0
56	MG	AA	1788	1/1	0.91	0.04	16,16,16,16	0
56	MG	AA	1790	1/1	0.91	0.08	65,65,65,65	0
56	MG	DA	3170	1/1	0.91	0.14	54,54,54,54	0
56	MG	DA	3379	1/1	0.91	0.14	31,31,31,31	0
56	MG	DA	3172	1/1	0.91	0.11	25,25,25,25	0
56	MG	DA	3389	1/1	0.91	0.16	22,22,22,22	0
56	MG	AW	103	1/1	0.91	0.08	51,51,51,51	0
56	MG	BA	3217	1/1	0.91	0.30	37,37,37,37	0
56	MG	BA	3308	1/1	0.91	0.08	25,25,25,25	0
56	MG	DA	3189	1/1	0.91	0.20	34,34,34,34	0
56	MG	BA	3218	1/1	0.91	0.23	56,56,56,56	0
56	MG	BA	3322	1/1	0.91	0.05	35,35,35,35	0
56	MG	DA	3200	1/1	0.91	0.11	26,26,26,26	0
56	MG	AW	105	1/1	0.91	0.08	64,64,64,64	0
56	MG	DA	3205	1/1	0.91	0.08	19,19,19,19	0
56	MG	DN	201	1/1	0.91	0.12	16,16,16,16	0
56	MG	CA	1765	1/1	0.91	0.11	38,38,38,38	0
56	MG	BA	3029	1/1	0.92	0.16	30,30,30,30	0
56	MG	DA	3177	1/1	0.92	0.16	22,22,22,22	0
56	MG	DA	3186	1/1	0.92	0.16	24,24,24,24	0
56	MG	CA	1601	1/1	0.92	0.06	26,26,26,26	0
56	MG	CA	1602	1/1	0.92	0.08	14,14,14,14	0
56	MG	CA	1604	1/1	0.92	0.27	45,45,45,45	0
56	MG	AA	1725	1/1	0.92	0.13	53,53,53,53	0
56	MG	AA	1749	1/1	0.92	0.25	38,38,38,38	0
56	MG	BA	3241	1/1	0.92	0.08	43,43,43,43	0
56	MG	AA	1685	1/1	0.92	0.06	38,38,38,38	0
56	MG	CA	1616	1/1	0.92	0.21	24,24,24,24	0
56	MG	CA	1617	1/1	0.92	0.08	25,25,25,25	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	BA	3088	1/1	0.92	0.26	35,35,35,35	0
56	MG	BA	3091	1/1	0.92	0.18	20,20,20,20	0
56	MG	AA	1730	1/1	0.92	0.32	82,82,82,82	0
56	MG	DA	3212	1/1	0.92	0.12	61,61,61,61	0
56	MG	AA	1812	1/1	0.92	0.15	50,50,50,50	0
56	MG	BA	3111	1/1	0.92	0.12	27,27,27,27	0
56	MG	CA	1639	1/1	0.92	0.24	71,71,71,71	0
56	MG	CA	1766	1/1	0.92	0.16	18,18,18,18	0
56	MG	AA	1758	1/1	0.92	0.17	62,62,62,62	0
56	MG	DA	3230	1/1	0.92	0.15	20,20,20,20	0
56	MG	CA	1643	1/1	0.92	0.29	48,48,48,48	0
56	MG	AA	1663	1/1	0.92	0.09	24,24,24,24	0
56	MG	BA	3275	1/1	0.92	0.07	19,19,19,19	0
56	MG	BA	3379	1/1	0.92	0.13	39,39,39,39	0
56	MG	BA	3128	1/1	0.92	0.26	18,18,18,18	0
56	MG	CJ	201	1/1	0.92	0.08	44,44,44,44	0
56	MG	BA	3142	1/1	0.92	0.22	66,66,66,66	0
56	MG	CA	1658	1/1	0.92	0.10	40,40,40,40	0
56	MG	CW	102	1/1	0.92	0.19	52,52,52,52	0
56	MG	AA	1767	1/1	0.92	0.18	48,48,48,48	0
56	MG	DA	3260	1/1	0.92	0.20	44,44,44,44	0
56	MG	CA	1663	1/1	0.92	0.10	32,32,32,32	0
56	MG	AA	1650	1/1	0.92	0.16	31,31,31,31	0
56	MG	BA	3148	1/1	0.92	0.12	37,37,37,37	0
56	MG	AA	1612	1/1	0.92	0.14	31,31,31,31	0
56	MG	CW	112	1/1	0.92	0.15	53,53,53,53	0
56	MG	AA	1775	1/1	0.92	0.18	29,29,29,29	0
56	MG	CX	103	1/1	0.92	0.07	40,40,40,40	0
56	MG	AA	1654	1/1	0.92	0.10	50,50,50,50	0
56	MG	AA	1657	1/1	0.92	0.20	50,50,50,50	0
56	MG	DA	3002	1/1	0.92	0.14	38,38,38,38	0
56	MG	BA	3168	1/1	0.92	0.15	22,22,22,22	0
56	MG	DA	3282	1/1	0.92	0.15	41,41,41,41	0
56	MG	DA	3285	1/1	0.92	0.18	15,15,15,15	0
56	MG	DA	3296	1/1	0.92	0.12	59,59,59,59	0
56	MG	BA	3422	1/1	0.92	0.24	39,39,39,39	0
56	MG	AA	1784	1/1	0.92	0.15	41,41,41,41	0
56	MG	DA	3318	1/1	0.92	0.13	45,45,45,45	0
56	MG	AA	1709	1/1	0.92	0.08	33,33,33,33	0
56	MG	DA	3324	1/1	0.92	0.37	56,56,56,56	0
56	MG	DA	3325	1/1	0.92	0.12	35,35,35,35	0
56	MG	BA	3430	1/1	0.92	0.17	30,30,30,30	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	BA	3309	1/1	0.92	0.12	14,14,14,14	0
56	MG	DA	3058	1/1	0.92	0.17	6,6,6,6	0
56	MG	AA	1715	1/1	0.92	0.07	24,24,24,24	0
56	MG	BA	3435	1/1	0.92	0.09	52,52,52,52	1
56	MG	DA	3101	1/1	0.92	0.18	38,38,38,38	0
56	MG	BA	3439	1/1	0.92	0.20	31,31,31,31	0
56	MG	DA	3346	1/1	0.92	0.12	29,29,29,29	0
56	MG	DA	3347	1/1	0.92	0.06	34,34,34,34	0
56	MG	BA	3446	1/1	0.92	0.18	43,43,43,43	0
56	MG	BA	3447	1/1	0.92	0.15	37,37,37,37	0
56	MG	BA	3320	1/1	0.92	0.09	37,37,37,37	0
56	MG	DA	3360	1/1	0.92	0.23	39,39,39,39	0
56	MG	AX	102	1/1	0.92	0.07	32,32,32,32	0
56	MG	DA	3371	1/1	0.92	0.23	40,40,40,40	0
56	MG	DA	3373	1/1	0.92	0.10	28,28,28,28	0
56	MG	AA	1660	1/1	0.92	0.20	61,61,61,61	0
56	MG	DA	3145	1/1	0.92	0.10	27,27,27,27	0
56	MG	DA	3384	1/1	0.92	0.07	25,25,25,25	0
56	MG	B2	102	1/1	0.92	0.10	44,44,44,44	0
56	MG	AA	1643	1/1	0.92	0.11	22,22,22,22	0
56	MG	BA	3329	1/1	0.92	0.07	34,34,34,34	0
56	MG	CA	1720	1/1	0.92	0.16	69,69,69,69	0
56	MG	AA	1794	1/1	0.92	0.26	56,56,56,56	0
56	MG	DA	3396	1/1	0.92	0.07	27,27,27,27	1
56	MG	AA	1795	1/1	0.92	0.25	30,30,30,30	0
56	MG	DB	203	1/1	0.92	0.13	33,33,33,33	0
56	MG	BA	3219	1/1	0.92	0.10	45,45,45,45	0
56	MG	AA	1747	1/1	0.92	0.07	37,37,37,37	0
56	MG	CA	1727	1/1	0.92	0.26	37,37,37,37	0
56	MG	DE	301	1/1	0.92	0.17	18,18,18,18	0
56	MG	DA	3169	1/1	0.92	0.13	27,27,27,27	0
56	MG	BA	3021	1/1	0.92	0.24	17,17,17,17	0
56	MG	CA	1730	1/1	0.92	0.22	56,56,56,56	0
56	MG	CA	1645	1/1	0.93	0.20	74,74,74,74	0
56	MG	BA	3436	1/1	0.93	0.11	39,39,39,39	1
56	MG	BA	3438	1/1	0.93	0.14	25,25,25,25	0
56	MG	DA	3112	1/1	0.93	0.04	0,0,0,0	0
56	MG	DA	3115	1/1	0.93	0.10	16,16,16,16	0
56	MG	CA	1648	1/1	0.93	0.07	34,34,34,34	0
56	MG	CA	1649	1/1	0.93	0.11	37,37,37,37	0
56	MG	DA	3263	1/1	0.93	0.19	30,30,30,30	0
56	MG	AY	101	1/1	0.93	0.20	56,56,56,56	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	BA	3107	1/1	0.93	0.25	53,53,53,53	0
56	MG	BA	3364	1/1	0.93	0.22	35,35,35,35	0
56	MG	DA	3144	1/1	0.93	0.16	31,31,31,31	0
56	MG	BA	3448	1/1	0.93	0.09	35,35,35,35	0
56	MG	AA	1679	1/1	0.93	0.08	5,5,5,5	1
56	MG	BA	3454	1/1	0.93	0.07	44,44,44,44	0
56	MG	DA	3152	1/1	0.93	0.07	17,17,17,17	0
56	MG	DA	3278	1/1	0.93	0.20	38,38,38,38	0
56	MG	DA	3153	1/1	0.93	0.22	40,40,40,40	0
56	MG	BA	3257	1/1	0.93	0.10	55,55,55,55	0
56	MG	DA	3283	1/1	0.93	0.17	35,35,35,35	0
56	MG	BA	3313	1/1	0.93	0.12	21,21,21,21	0
56	MG	AA	1703	1/1	0.93	0.22	23,23,23,23	0
56	MG	DA	3304	1/1	0.93	0.08	9,9,9,9	0
56	MG	BA	3315	1/1	0.93	0.11	43,43,43,43	0
56	MG	AW	102	1/1	0.93	0.08	51,51,51,51	0
56	MG	AA	1798	1/1	0.93	0.07	36,36,36,36	0
56	MG	BA	3215	1/1	0.93	0.16	30,30,30,30	0
56	MG	AA	1634	1/1	0.93	0.12	34,34,34,34	0
56	MG	AA	1802	1/1	0.93	0.08	44,44,44,44	0
56	MG	DA	3171	1/1	0.93	0.19	37,37,37,37	0
56	MG	BB	217	1/1	0.93	0.06	34,34,34,34	0
56	MG	CF	201	1/1	0.93	0.09	44,44,44,44	0
56	MG	BA	3401	1/1	0.93	0.13	48,48,48,48	0
56	MG	BA	3276	1/1	0.93	0.06	6,6,6,6	0
56	MG	BA	3407	1/1	0.93	0.05	40,40,40,40	0
56	MG	DA	3341	1/1	0.93	0.09	26,26,26,26	0
56	MG	AW	108	1/1	0.93	0.09	35,35,35,35	0
56	MG	DA	3344	1/1	0.93	0.16	32,32,32,32	0
56	MG	CA	1704	1/1	0.93	0.10	5,5,5,5	0
56	MG	BA	3409	1/1	0.93	0.12	53,53,53,53	0
56	MG	DA	3348	1/1	0.93	0.13	46,46,46,46	0
56	MG	DA	3352	1/1	0.93	0.09	9,9,9,9	0
56	MG	BA	3411	1/1	0.93	0.09	62,62,62,62	0
56	MG	AA	1690	1/1	0.93	0.16	48,48,48,48	0
56	MG	AA	1743	1/1	0.93	0.14	44,44,44,44	0
56	MG	AA	1789	1/1	0.93	0.06	18,18,18,18	0
56	MG	DA	3364	1/1	0.93	0.21	57,57,57,57	0
56	MG	BA	3069	1/1	0.93	0.10	36,36,36,36	0
56	MG	BA	3416	1/1	0.93	0.08	16,16,16,16	0
56	MG	AA	1684	1/1	0.93	0.13	17,17,17,17	0
56	MG	DA	3375	1/1	0.93	0.14	42,42,42,42	1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	BA	3343	1/1	0.93	0.10	34,34,34,34	0
56	MG	CA	1627	1/1	0.93	0.13	34,34,34,34	0
56	MG	CA	1631	1/1	0.93	0.29	48,48,48,48	0
56	MG	BA	3426	1/1	0.93	0.09	3,3,3,3	0
56	MG	BA	3344	1/1	0.93	0.05	17,17,17,17	0
56	MG	BA	3288	1/1	0.93	0.17	32,32,32,32	1
56	MG	DA	3029	1/1	0.93	0.16	36,36,36,36	0
56	MG	DA	3222	1/1	0.93	0.27	24,24,24,24	0
56	MG	DA	3395	1/1	0.93	0.08	45,45,45,45	0
56	MG	BA	3231	1/1	0.93	0.40	45,45,45,45	0
56	MG	BA	3347	1/1	0.93	0.06	22,22,22,22	1
56	MG	DA	3057	1/1	0.93	0.24	35,35,35,35	0
56	MG	DA	3237	1/1	0.93	0.11	15,15,15,15	0
56	MG	AA	1719	1/1	0.93	0.05	65,65,65,65	0
56	MG	AA	1615	1/1	0.93	0.16	33,33,33,33	0
56	MG	DB	211	1/1	0.93	0.08	45,45,45,45	0
56	MG	DA	3082	1/1	0.93	0.17	10,10,10,10	0
56	MG	DA	3246	1/1	0.93	0.14	38,38,38,38	0
56	MG	DA	3096	1/1	0.93	0.18	21,21,21,21	0
56	MG	DA	3249	1/1	0.93	0.55	57,57,57,57	0
56	MG	DZ	301	1/1	0.93	0.07	27,27,27,27	0
57	PAR	AA	1816	42/42	0.93	0.11	15,20,38,42	0
57	PAR	CA	1790	42/42	0.93	0.11	7,11,29,33	0
56	MG	BA	3291	1/1	0.94	0.08	12,12,12,12	0
56	MG	BA	3197	1/1	0.94	0.08	18,18,18,18	0
56	MG	AA	1602	1/1	0.94	0.10	39,39,39,39	0
56	MG	CA	1633	1/1	0.94	0.18	19,19,19,19	0
56	MG	BA	3406	1/1	0.94	0.22	18,18,18,18	0
56	MG	AV	106	1/1	0.94	0.17	40,40,40,40	0
56	MG	BA	3028	1/1	0.94	0.23	36,36,36,36	0
56	MG	CA	1772	1/1	0.94	0.12	37,37,37,37	0
56	MG	AV	107	1/1	0.94	0.09	25,25,25,25	0
56	MG	CA	1640	1/1	0.94	0.15	43,43,43,43	0
56	MG	BA	3410	1/1	0.94	0.06	41,41,41,41	0
56	MG	BA	3306	1/1	0.94	0.13	20,20,20,20	0
56	MG	CA	1789	1/1	0.94	0.21	33,33,33,33	0
56	MG	DA	3232	1/1	0.94	0.03	13,13,13,13	0
56	MG	AA	1751	1/1	0.94	0.07	19,19,19,19	0
56	MG	BA	3051	1/1	0.94	0.09	56,56,56,56	0
56	MG	AA	1753	1/1	0.94	0.16	26,26,26,26	0
56	MG	AA	1631	1/1	0.94	0.15	21,21,21,21	0
56	MG	AA	1701	1/1	0.94	0.05	18,18,18,18	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	BA	3417	1/1	0.94	0.20	29,29,29,29	0
56	MG	CW	105	1/1	0.94	0.09	30,30,30,30	0
56	MG	BA	3418	1/1	0.94	0.07	64,64,64,64	0
56	MG	CA	1651	1/1	0.94	0.19	31,31,31,31	0
56	MG	DA	3251	1/1	0.94	0.14	20,20,20,20	0
56	MG	BA	3316	1/1	0.94	0.20	49,49,49,49	0
56	MG	CA	1656	1/1	0.94	0.10	14,14,14,14	0
56	MG	DA	3256	1/1	0.94	0.07	22,22,22,22	0
56	MG	BA	3420	1/1	0.94	0.13	59,59,59,59	1
56	MG	BA	3317	1/1	0.94	0.14	50,50,50,50	0
56	MG	CA	1662	1/1	0.94	0.10	18,18,18,18	0
56	MG	BA	3425	1/1	0.94	0.06	61,61,61,61	0
56	MG	AA	1793	1/1	0.94	0.14	71,71,71,71	0
56	MG	AA	1760	1/1	0.94	0.09	48,48,48,48	0
56	MG	CA	1670	1/1	0.94	0.06	23,23,23,23	0
56	MG	AA	1604	1/1	0.94	0.14	52,52,52,52	0
56	MG	DA	3008	1/1	0.94	0.10	23,23,23,23	0
56	MG	DA	3010	1/1	0.94	0.11	44,44,44,44	0
56	MG	DA	3016	1/1	0.94	0.27	52,52,52,52	0
56	MG	BA	3229	1/1	0.94	0.12	36,36,36,36	0
56	MG	AA	1797	1/1	0.94	0.05	26,26,26,26	0
56	MG	AA	1739	1/1	0.94	0.12	23,23,23,23	0
56	MG	AA	1705	1/1	0.94	0.15	21,21,21,21	0
56	MG	DA	3280	1/1	0.94	0.06	16,16,16,16	0
56	MG	DA	3281	1/1	0.94	0.09	14,14,14,14	1
56	MG	DA	3037	1/1	0.94	0.19	4,4,4,4	0
56	MG	BA	3237	1/1	0.94	0.32	35,35,35,35	0
56	MG	DA	3048	1/1	0.94	0.10	53,53,53,53	0
56	MG	DA	3291	1/1	0.94	0.07	0,0,0,0	0
56	MG	AW	118	1/1	0.94	0.11	46,46,46,46	0
56	MG	DA	3297	1/1	0.94	0.17	23,23,23,23	0
56	MG	BA	3245	1/1	0.94	0.09	9,9,9,9	0
56	MG	DA	3061	1/1	0.94	0.20	0,0,0,0	0
56	MG	DA	3067	1/1	0.94	0.11	26,26,26,26	0
56	MG	DA	3316	1/1	0.94	0.14	7,7,7,7	0
56	MG	DA	3068	1/1	0.94	0.10	14,14,14,14	0
56	MG	BA	3441	1/1	0.94	0.11	33,33,33,33	0
56	MG	DA	3321	1/1	0.94	0.07	45,45,45,45	1
56	MG	DA	3071	1/1	0.94	0.10	18,18,18,18	0
56	MG	BA	3442	1/1	0.94	0.14	29,29,29,29	0
56	MG	AA	1729	1/1	0.94	0.09	45,45,45,45	0
56	MG	DA	3098	1/1	0.94	0.13	19,19,19,19	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	AW	122	1/1	0.94	0.06	37,37,37,37	0
56	MG	DA	3332	1/1	0.94	0.06	45,45,45,45	0
56	MG	BA	3341	1/1	0.94	0.12	21,21,21,21	0
56	MG	BA	3450	1/1	0.94	0.15	55,55,55,55	0
56	MG	BA	3129	1/1	0.94	0.06	21,21,21,21	0
56	MG	DA	3340	1/1	0.94	0.09	30,30,30,30	0
56	MG	BA	3256	1/1	0.94	0.10	22,22,22,22	0
56	MG	AA	1773	1/1	0.94	0.11	41,41,41,41	0
56	MG	AA	1708	1/1	0.94	0.15	41,41,41,41	0
56	MG	AA	1653	1/1	0.94	0.13	39,39,39,39	0
56	MG	AA	1781	1/1	0.94	0.16	27,27,27,27	0
56	MG	BA	3150	1/1	0.94	0.13	35,35,35,35	0
56	MG	DA	3350	1/1	0.94	0.09	37,37,37,37	0
56	MG	BA	3354	1/1	0.94	0.06	35,35,35,35	0
56	MG	BB	209	1/1	0.94	0.12	49,49,49,49	0
56	MG	DA	3148	1/1	0.94	0.12	5,5,5,5	0
56	MG	BA	3269	1/1	0.94	0.41	43,43,43,43	0
56	MG	BA	3360	1/1	0.94	0.11	25,25,25,25	0
56	MG	BB	214	1/1	0.94	0.14	46,46,46,46	0
56	MG	DA	3367	1/1	0.94	0.04	19,19,19,19	0
56	MG	DA	3368	1/1	0.94	0.36	71,71,71,71	0
56	MG	CA	1724	1/1	0.94	0.10	38,38,38,38	0
56	MG	BA	3153	1/1	0.94	0.07	37,37,37,37	0
56	MG	AA	1713	1/1	0.94	0.11	7,7,7,7	0
56	MG	DA	3374	1/1	0.94	0.11	50,50,50,50	0
56	MG	AA	1813	1/1	0.94	0.07	25,25,25,25	0
56	MG	DA	3376	1/1	0.94	0.15	25,25,25,25	0
56	MG	BA	3372	1/1	0.94	0.10	43,43,43,43	1
56	MG	DA	3380	1/1	0.94	0.26	55,55,55,55	0
56	MG	CA	1732	1/1	0.94	0.16	43,43,43,43	0
56	MG	DA	3165	1/1	0.94	0.11	38,38,38,38	0
56	MG	AA	1673	1/1	0.94	0.12	26,26,26,26	0
56	MG	CA	1735	1/1	0.94	0.16	17,17,17,17	0
56	MG	BA	3002	1/1	0.94	0.13	21,21,21,21	0
56	MG	CA	1738	1/1	0.94	0.05	23,23,23,23	0
56	MG	CA	1603	1/1	0.94	0.06	25,25,25,25	0
56	MG	CA	1741	1/1	0.94	0.24	40,40,40,40	0
56	MG	BA	3167	1/1	0.94	0.14	33,33,33,33	0
56	MG	BA	3004	1/1	0.94	0.42	77,77,77,77	0
56	MG	DA	3183	1/1	0.94	0.05	0,0,0,0	0
56	MG	DA	3185	1/1	0.94	0.12	8,8,8,8	1
56	MG	BA	3172	1/1	0.94	0.20	22,22,22,22	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	BA	3005	1/1	0.94	0.09	26,26,26,26	0
56	MG	BA	3380	1/1	0.94	0.38	77,77,77,77	0
56	MG	BA	3012	1/1	0.94	0.08	20,20,20,20	0
56	MG	CA	1755	1/1	0.94	0.10	26,26,26,26	1
56	MG	CA	1756	1/1	0.94	0.06	41,41,41,41	0
56	MG	DA	3199	1/1	0.94	0.07	26,26,26,26	0
56	MG	BA	3390	1/1	0.94	0.06	20,20,20,20	1
56	MG	BA	3289	1/1	0.94	0.14	41,41,41,41	0
56	MG	CA	1620	1/1	0.94	0.24	32,32,32,32	0
56	MG	BA	3194	1/1	0.95	0.20	30,30,30,30	0
56	MG	DA	3236	1/1	0.95	0.15	54,54,54,54	0
56	MG	AA	1712	1/1	0.95	0.06	22,22,22,22	0
56	MG	DA	3001	1/1	0.95	0.15	20,20,20,20	0
56	MG	BA	3369	1/1	0.95	0.05	30,30,30,30	0
56	MG	BA	3203	1/1	0.95	0.17	14,14,14,14	0
56	MG	BA	3112	1/1	0.95	0.05	31,31,31,31	0
56	MG	BA	3114	1/1	0.95	0.17	0,0,0,0	0
56	MG	BA	3287	1/1	0.95	0.14	46,46,46,46	0
56	MG	DA	3012	1/1	0.95	0.12	27,27,27,27	0
56	MG	AW	117	1/1	0.95	0.07	24,24,24,24	0
56	MG	DA	3020	1/1	0.95	0.17	1,1,1,1	0
56	MG	BB	210	1/1	0.95	0.08	33,33,33,33	1
56	MG	BA	3120	1/1	0.95	0.04	23,23,23,23	0
56	MG	DA	3028	1/1	0.95	0.13	0,0,0,0	0
56	MG	BA	3018	1/1	0.95	0.19	22,22,22,22	0
56	MG	DA	3032	1/1	0.95	0.21	59,59,59,59	0
56	MG	AA	1638	1/1	0.95	0.18	24,24,24,24	0
56	MG	BA	3383	1/1	0.95	0.05	37,37,37,37	0
56	MG	DA	3038	1/1	0.95	0.10	17,17,17,17	0
56	MG	AV	102	1/1	0.95	0.07	28,28,28,28	0
56	MG	BA	3298	1/1	0.95	0.17	25,25,25,25	0
56	MG	BA	3135	1/1	0.95	0.07	18,18,18,18	0
56	MG	BN	201	1/1	0.95	0.05	25,25,25,25	0
56	MG	BA	3137	1/1	0.95	0.15	6,6,6,6	0
56	MG	DA	3062	1/1	0.95	0.23	13,13,13,13	0
56	MG	BA	3396	1/1	0.95	0.06	15,15,15,15	0
56	MG	BA	3397	1/1	0.95	0.12	32,32,32,32	0
56	MG	BA	3400	1/1	0.95	0.13	46,46,46,46	0
56	MG	CA	1606	1/1	0.95	0.16	16,16,16,16	0
56	MG	CA	1726	1/1	0.95	0.13	29,29,29,29	0
56	MG	DA	3084	1/1	0.95	0.13	29,29,29,29	0
56	MG	DA	3093	1/1	0.95	0.10	16,16,16,16	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	BA	3302	1/1	0.95	0.13	14,14,14,14	0
56	MG	CA	1728	1/1	0.95	0.17	42,42,42,42	0
56	MG	DA	3292	1/1	0.95	0.07	5,5,5,5	0
56	MG	BA	3138	1/1	0.95	0.15	12,12,12,12	0
56	MG	BA	3141	1/1	0.95	0.07	20,20,20,20	0
56	MG	DA	3298	1/1	0.95	0.12	5,5,5,5	0
56	MG	CA	1731	1/1	0.95	0.09	32,32,32,32	0
56	MG	DA	3305	1/1	0.95	0.06	28,28,28,28	0
56	MG	DA	3307	1/1	0.95	0.06	34,34,34,34	1
56	MG	DA	3111	1/1	0.95	0.15	1,1,1,1	0
56	MG	BA	3223	1/1	0.95	0.08	8,8,8,8	0
56	MG	DA	3314	1/1	0.95	0.09	16,16,16,16	0
56	MG	CA	1733	1/1	0.95	0.06	31,31,31,31	0
56	MG	BA	3226	1/1	0.95	0.15	20,20,20,20	0
56	MG	DA	3319	1/1	0.95	0.05	52,52,52,52	0
56	MG	AA	1777	1/1	0.95	0.22	55,55,55,55	0
56	MG	DA	3123	1/1	0.95	0.08	20,20,20,20	0
56	MG	DA	3128	1/1	0.95	0.12	0,0,0,0	0
56	MG	BA	3033	1/1	0.95	0.24	30,30,30,30	0
56	MG	BA	3036	1/1	0.95	0.12	25,25,25,25	0
56	MG	AA	1671	1/1	0.95	0.15	19,19,19,19	0
56	MG	BA	3044	1/1	0.95	0.16	5,5,5,5	0
56	MG	BA	3234	1/1	0.95	0.27	29,29,29,29	0
56	MG	BA	3152	1/1	0.95	0.22	45,45,45,45	0
56	MG	BA	3239	1/1	0.95	0.20	12,12,12,12	0
56	MG	DA	3150	1/1	0.95	0.17	40,40,40,40	0
56	MG	CA	1635	1/1	0.95	0.21	19,19,19,19	0
56	MG	BA	3325	1/1	0.95	0.04	28,28,28,28	0
56	MG	BA	3240	1/1	0.95	0.13	15,15,15,15	0
56	MG	AA	1624	1/1	0.95	0.11	33,33,33,33	0
56	MG	AA	1783	1/1	0.95	0.22	46,46,46,46	0
56	MG	CA	1641	1/1	0.95	0.09	13,13,13,13	0
56	MG	DA	3161	1/1	0.95	0.14	39,39,39,39	0
56	MG	DA	3349	1/1	0.95	0.12	27,27,27,27	0
56	MG	BA	3251	1/1	0.95	0.13	11,11,11,11	0
56	MG	DA	3351	1/1	0.95	0.06	16,16,16,16	0
56	MG	BA	3424	1/1	0.95	0.14	38,38,38,38	0
56	MG	BA	3155	1/1	0.95	0.47	66,66,66,66	0
56	MG	BA	3156	1/1	0.95	0.11	28,28,28,28	0
56	MG	BA	3333	1/1	0.95	0.06	41,41,41,41	0
56	MG	CA	1764	1/1	0.95	0.09	15,15,15,15	0
56	MG	AA	1766	1/1	0.95	0.09	23,23,23,23	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	DA	3365	1/1	0.95	0.14	29,29,29,29	0
56	MG	AA	1786	1/1	0.95	0.19	31,31,31,31	0
56	MG	BA	3072	1/1	0.95	0.21	13,13,13,13	0
56	MG	BA	3432	1/1	0.95	0.06	15,15,15,15	0
56	MG	CA	1769	1/1	0.95	0.05	18,18,18,18	0
56	MG	AA	1668	1/1	0.95	0.10	23,23,23,23	0
56	MG	CA	1775	1/1	0.95	0.16	35,35,35,35	0
56	MG	BA	3434	1/1	0.95	0.06	28,28,28,28	0
56	MG	AA	1768	1/1	0.95	0.04	14,14,14,14	1
56	MG	DA	3377	1/1	0.95	0.04	6,6,6,6	1
56	MG	CA	1781	1/1	0.95	0.17	29,29,29,29	0
56	MG	AA	1710	1/1	0.95	0.09	29,29,29,29	0
56	MG	CA	1660	1/1	0.95	0.17	22,22,22,22	0
56	MG	DA	3382	1/1	0.95	0.04	6,6,6,6	0
56	MG	CA	1788	1/1	0.95	0.11	42,42,42,42	1
56	MG	DA	3387	1/1	0.95	0.06	11,11,11,11	0
56	MG	BA	3265	1/1	0.95	0.29	37,37,37,37	0
56	MG	BA	3266	1/1	0.95	0.17	28,28,28,28	0
56	MG	BA	3174	1/1	0.95	0.08	0,0,0,0	0
56	MG	CU	101	1/1	0.95	0.03	38,38,38,38	0
56	MG	CV	101	1/1	0.95	0.13	32,32,32,32	0
56	MG	BA	3177	1/1	0.95	0.12	7,7,7,7	0
56	MG	CA	1667	1/1	0.95	0.15	41,41,41,41	0
56	MG	DB	201	1/1	0.95	0.05	19,19,19,19	0
56	MG	CV	104	1/1	0.95	0.19	36,36,36,36	0
56	MG	BA	3445	1/1	0.95	0.13	52,52,52,52	0
56	MG	BA	3271	1/1	0.95	0.16	33,33,33,33	0
56	MG	AA	1752	1/1	0.95	0.16	25,25,25,25	0
56	MG	CA	1672	1/1	0.95	0.09	32,32,32,32	0
56	MG	AA	1723	1/1	0.95	0.04	9,9,9,9	0
56	MG	DD	302	1/1	0.95	0.06	7,7,7,7	0
56	MG	BA	3449	1/1	0.95	0.12	27,27,27,27	0
56	MG	DA	3221	1/1	0.95	0.07	11,11,11,11	0
56	MG	BA	3184	1/1	0.95	0.15	1,1,1,1	0
56	MG	DA	3229	1/1	0.95	0.16	1,1,1,1	0
56	MG	DS	201	1/1	0.95	0.12	14,14,14,14	1
56	MG	DU	201	1/1	0.95	0.08	45,45,45,45	0
56	MG	BA	3451	1/1	0.95	0.10	43,43,43,43	0
56	MG	CA	1677	1/1	0.95	0.06	28,28,28,28	0
56	MG	BA	3190	1/1	0.95	0.15	49,49,49,49	0
56	MG	AA	1714	1/1	0.96	0.05	28,28,28,28	0
56	MG	BA	3022	1/1	0.96	0.12	25,25,25,25	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	DA	3195	1/1	0.96	0.05	0,0,0,0	1
56	MG	BA	3023	1/1	0.96	0.18	0,0,0,0	0
56	MG	BA	3378	1/1	0.96	0.05	54,54,54,54	1
56	MG	DA	3202	1/1	0.96	0.14	37,37,37,37	0
56	MG	AA	1762	1/1	0.96	0.03	18,18,18,18	0
56	MG	DA	3204	1/1	0.96	0.11	8,8,8,8	0
56	MG	CA	1618	1/1	0.96	0.08	25,25,25,25	0
56	MG	AA	1692	1/1	0.96	0.18	0,0,0,0	0
56	MG	BA	3382	1/1	0.96	0.14	63,63,63,63	0
56	MG	BA	3032	1/1	0.96	0.06	17,17,17,17	0
56	MG	CA	1625	1/1	0.96	0.12	19,19,19,19	0
56	MG	CA	1626	1/1	0.96	0.19	11,11,11,11	0
56	MG	CA	1779	1/1	0.96	0.19	31,31,31,31	0
56	MG	BA	3270	1/1	0.96	0.06	0,0,0,0	0
56	MG	DA	3215	1/1	0.96	0.04	31,31,31,31	0
56	MG	CA	1629	1/1	0.96	0.08	10,10,10,10	0
56	MG	CA	1782	1/1	0.96	0.14	29,29,29,29	0
56	MG	BA	3387	1/1	0.96	0.05	38,38,38,38	0
56	MG	BA	3388	1/1	0.96	0.17	22,22,22,22	0
56	MG	BA	3160	1/1	0.96	0.14	17,17,17,17	0
56	MG	DA	3225	1/1	0.96	0.13	22,22,22,22	0
56	MG	DA	3227	1/1	0.96	0.12	8,8,8,8	0
56	MG	BA	3391	1/1	0.96	0.07	26,26,26,26	0
56	MG	CA	1636	1/1	0.96	0.15	36,36,36,36	0
56	MG	BA	3392	1/1	0.96	0.03	8,8,8,8	0
56	MG	BA	3162	1/1	0.96	0.07	12,12,12,12	0
56	MG	BA	3394	1/1	0.96	0.10	26,26,26,26	0
56	MG	DA	3235	1/1	0.96	0.20	39,39,39,39	0
56	MG	BA	3273	1/1	0.96	0.11	20,20,20,20	0
56	MG	BA	3164	1/1	0.96	0.06	9,9,9,9	0
56	MG	AA	1764	1/1	0.96	0.08	6,6,6,6	0
56	MG	CW	101	1/1	0.96	0.10	36,36,36,36	0
56	MG	DA	3244	1/1	0.96	0.22	0,0,0,0	0
56	MG	AA	1693	1/1	0.96	0.34	43,43,43,43	0
56	MG	CW	103	1/1	0.96	0.10	45,45,45,45	0
56	MG	BA	3037	1/1	0.96	0.22	0,0,0,0	0
56	MG	BA	3402	1/1	0.96	0.07	19,19,19,19	0
56	MG	CW	106	1/1	0.96	0.06	50,50,50,50	1
56	MG	BA	3170	1/1	0.96	0.14	0,0,0,0	0
56	MG	BA	3405	1/1	0.96	0.05	11,11,11,11	0
56	MG	DA	3254	1/1	0.96	0.04	1,1,1,1	0
56	MG	AA	1741	1/1	0.96	0.04	38,38,38,38	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	BA	3283	1/1	0.96	0.08	36,36,36,36	0
56	MG	AA	1621	1/1	0.96	0.07	14,14,14,14	0
56	MG	BA	3176	1/1	0.96	0.13	11,11,11,11	0
56	MG	BA	3046	1/1	0.96	0.18	0,0,0,0	0
56	MG	BA	3049	1/1	0.96	0.27	36,36,36,36	0
56	MG	BA	3179	1/1	0.96	0.12	28,28,28,28	0
56	MG	DA	3267	1/1	0.96	0.08	13,13,13,13	0
56	MG	AA	1632	1/1	0.96	0.20	24,24,24,24	0
56	MG	DA	3269	1/1	0.96	0.23	33,33,33,33	0
56	MG	BA	3183	1/1	0.96	0.09	18,18,18,18	0
56	MG	DA	3271	1/1	0.96	0.16	7,7,7,7	0
56	MG	BA	3294	1/1	0.96	0.06	6,6,6,6	0
56	MG	DA	3006	1/1	0.96	0.19	41,41,41,41	0
56	MG	BA	3057	1/1	0.96	0.19	17,17,17,17	0
56	MG	CA	1664	1/1	0.96	0.19	28,28,28,28	0
56	MG	DA	3009	1/1	0.96	0.16	3,3,3,3	0
56	MG	BA	3185	1/1	0.96	0.09	9,9,9,9	0
56	MG	BA	3188	1/1	0.96	0.18	13,13,13,13	0
56	MG	BA	3058	1/1	0.96	0.20	0,0,0,0	0
56	MG	BA	3191	1/1	0.96	0.19	23,23,23,23	0
56	MG	BA	3421	1/1	0.96	0.07	44,44,44,44	0
56	MG	BA	3303	1/1	0.96	0.11	15,15,15,15	0
56	MG	DA	3027	1/1	0.96	0.25	39,39,39,39	0
56	MG	AW	112	1/1	0.96	0.04	29,29,29,29	0
56	MG	DA	3288	1/1	0.96	0.07	25,25,25,25	1
56	MG	AA	1744	1/1	0.96	0.12	18,18,18,18	0
56	MG	BA	3199	1/1	0.96	0.14	9,9,9,9	0
56	MG	AA	1666	1/1	0.96	0.14	1,1,1,1	0
56	MG	BA	3312	1/1	0.96	0.19	0,0,0,0	0
56	MG	AA	1801	1/1	0.96	0.10	34,34,34,34	0
56	MG	DA	3300	1/1	0.96	0.17	13,13,13,13	0
56	MG	DA	3302	1/1	0.96	0.16	11,11,11,11	0
56	MG	DA	3040	1/1	0.96	0.08	45,45,45,45	0
56	MG	DA	3041	1/1	0.96	0.15	8,8,8,8	0
56	MG	CA	1684	1/1	0.96	0.19	30,30,30,30	0
56	MG	DA	3309	1/1	0.96	0.05	6,6,6,6	0
56	MG	BA	3205	1/1	0.96	0.10	0,0,0,0	0
56	MG	DA	3311	1/1	0.96	0.17	53,53,53,53	0
56	MG	DA	3050	1/1	0.96	0.26	0,0,0,0	0
56	MG	DA	3313	1/1	0.96	0.12	35,35,35,35	1
56	MG	DA	3051	1/1	0.96	0.16	0,0,0,0	0
56	MG	CA	1688	1/1	0.96	0.22	46,46,46,46	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	BA	3207	1/1	0.96	0.05	0,0,0,0	0
56	MG	CA	1692	1/1	0.96	0.08	19,19,19,19	0
56	MG	AA	1680	1/1	0.96	0.05	30,30,30,30	0
56	MG	AA	1803	1/1	0.96	0.08	48,48,48,48	0
56	MG	DA	3322	1/1	0.96	0.08	27,27,27,27	0
56	MG	BA	3318	1/1	0.96	0.12	30,30,30,30	0
56	MG	BA	3102	1/1	0.96	0.05	15,15,15,15	0
56	MG	DA	3326	1/1	0.96	0.25	25,25,25,25	0
56	MG	DA	3070	1/1	0.96	0.19	0,0,0,0	0
56	MG	BA	3437	1/1	0.96	0.04	4,4,4,4	0
56	MG	CA	1700	1/1	0.96	0.11	20,20,20,20	0
56	MG	CA	1703	1/1	0.96	0.10	19,19,19,19	0
56	MG	DA	3086	1/1	0.96	0.14	0,0,0,0	0
56	MG	AW	121	1/1	0.96	0.04	36,36,36,36	0
56	MG	DA	3337	1/1	0.96	0.05	4,4,4,4	0
56	MG	AA	1804	1/1	0.96	0.11	31,31,31,31	0
56	MG	CA	1708	1/1	0.96	0.11	43,43,43,43	0
56	MG	DA	3099	1/1	0.96	0.10	10,10,10,10	0
56	MG	CA	1709	1/1	0.96	0.07	9,9,9,9	0
56	MG	AA	1805	1/1	0.96	0.04	0,0,0,0	0
56	MG	AX	104	1/1	0.96	0.10	44,44,44,44	0
56	MG	BA	3443	1/1	0.96	0.07	20,20,20,20	0
56	MG	AA	1645	1/1	0.96	0.21	25,25,25,25	0
56	MG	CA	1715	1/1	0.96	0.09	55,55,55,55	0
56	MG	BA	3220	1/1	0.96	0.14	29,29,29,29	0
56	MG	AA	1601	1/1	0.96	0.07	35,35,35,35	0
56	MG	AA	1779	1/1	0.96	0.19	46,46,46,46	0
56	MG	AA	1706	1/1	0.96	0.06	10,10,10,10	0
56	MG	DA	3129	1/1	0.96	0.05	6,6,6,6	0
56	MG	DA	3132	1/1	0.96	0.06	13,13,13,13	0
56	MG	DA	3359	1/1	0.96	0.14	15,15,15,15	0
56	MG	DA	3133	1/1	0.96	0.09	39,39,39,39	0
56	MG	DA	3361	1/1	0.96	0.14	5,5,5,5	0
56	MG	DA	3363	1/1	0.96	0.13	30,30,30,30	0
56	MG	DA	3135	1/1	0.96	0.22	7,7,7,7	0
56	MG	BA	3224	1/1	0.96	0.16	2,2,2,2	0
56	MG	BA	3124	1/1	0.96	0.13	17,17,17,17	0
56	MG	AA	1811	1/1	0.96	0.07	16,16,16,16	0
56	MG	BA	3453	1/1	0.96	0.05	49,49,49,49	0
56	MG	B5	101	1/1	0.96	0.12	6,6,6,6	0
56	MG	DA	3147	1/1	0.96	0.13	19,19,19,19	0
56	MG	AA	1614	1/1	0.96	0.07	19,19,19,19	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	BA	3001	1/1	0.96	0.20	38,38,38,38	0
56	MG	BA	3136	1/1	0.96	0.13	8,8,8,8	0
56	MG	AA	1636	1/1	0.96	0.12	27,27,27,27	1
56	MG	AA	1662	1/1	0.96	0.11	31,31,31,31	0
56	MG	BA	3139	1/1	0.96	0.06	9,9,9,9	0
56	MG	DA	3154	1/1	0.96	0.17	31,31,31,31	0
56	MG	BB	208	1/1	0.96	0.04	27,27,27,27	0
56	MG	DA	3383	1/1	0.96	0.09	32,32,32,32	0
56	MG	DA	3156	1/1	0.96	0.14	36,36,36,36	0
56	MG	DA	3157	1/1	0.96	0.18	34,34,34,34	0
56	MG	DA	3388	1/1	0.96	0.13	15,15,15,15	0
56	MG	BA	3348	1/1	0.96	0.06	26,26,26,26	0
56	MG	AA	1785	1/1	0.96	0.10	32,32,32,32	0
56	MG	BB	211	1/1	0.96	0.09	40,40,40,40	1
56	MG	CA	1736	1/1	0.96	0.04	30,30,30,30	0
56	MG	BA	3006	1/1	0.96	0.18	24,24,24,24	0
56	MG	BA	3244	1/1	0.96	0.05	19,19,19,19	0
56	MG	BA	3009	1/1	0.96	0.16	20,20,20,20	0
56	MG	BA	3359	1/1	0.96	0.04	75,75,75,75	0
56	MG	BB	216	1/1	0.96	0.07	11,11,11,11	1
56	MG	BA	3250	1/1	0.96	0.09	22,22,22,22	1
56	MG	BA	3144	1/1	0.96	0.13	8,8,8,8	0
56	MG	BA	3362	1/1	0.96	0.12	58,58,58,58	0
56	MG	BA	3146	1/1	0.96	0.22	0,0,0,0	0
56	MG	DB	208	1/1	0.96	0.10	9,9,9,9	0
56	MG	DB	210	1/1	0.96	0.04	15,15,15,15	0
56	MG	DA	3176	1/1	0.96	0.17	13,13,13,13	0
56	MG	DB	212	1/1	0.96	0.04	27,27,27,27	0
56	MG	BX	101	1/1	0.96	0.10	26,26,26,26	0
56	MG	DA	3178	1/1	0.96	0.12	19,19,19,19	0
56	MG	DA	3181	1/1	0.96	0.06	17,17,17,17	0
56	MG	BA	3366	1/1	0.96	0.10	27,27,27,27	0
56	MG	DA	3184	1/1	0.96	0.12	10,10,10,10	0
56	MG	AA	1689	1/1	0.96	0.21	50,50,50,50	0
56	MG	BA	3014	1/1	0.96	0.17	7,7,7,7	0
56	MG	BA	3149	1/1	0.96	0.07	10,10,10,10	0
56	MG	AA	1787	1/1	0.96	0.05	15,15,15,15	0
56	MG	AA	1674	1/1	0.96	0.18	33,33,33,33	0
56	MG	BA	3371	1/1	0.97	0.06	15,15,15,15	0
56	MG	DA	3197	1/1	0.97	0.12	13,13,13,13	0
56	MG	AA	1642	1/1	0.97	0.14	8,8,8,8	0
56	MG	BA	3008	1/1	0.97	0.20	22,22,22,22	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	CA	1621	1/1	0.97	0.16	0,0,0,0	0
56	MG	BA	3242	1/1	0.97	0.10	4,4,4,4	0
56	MG	BA	3131	1/1	0.97	0.20	0,0,0,0	0
56	MG	AA	1691	1/1	0.97	0.06	11,11,11,11	0
56	MG	BA	3249	1/1	0.97	0.07	11,11,11,11	0
56	MG	CA	1628	1/1	0.97	0.05	35,35,35,35	0
56	MG	AA	1761	1/1	0.97	0.12	16,16,16,16	0
56	MG	AA	1609	1/1	0.97	0.25	44,44,44,44	0
56	MG	DA	3211	1/1	0.97	0.07	1,1,1,1	0
56	MG	BA	3252	1/1	0.97	0.19	25,25,25,25	0
56	MG	BA	3381	1/1	0.97	0.07	21,21,21,21	0
56	MG	AA	1644	1/1	0.97	0.05	17,17,17,17	0
56	MG	BA	3017	1/1	0.97	0.05	19,19,19,19	0
56	MG	BA	3140	1/1	0.97	0.04	10,10,10,10	0
56	MG	BA	3386	1/1	0.97	0.07	85,85,85,85	0
56	MG	AA	1655	1/1	0.97	0.08	32,32,32,32	0
56	MG	DA	3220	1/1	0.97	0.15	3,3,3,3	0
56	MG	BA	3020	1/1	0.97	0.14	1,1,1,1	0
56	MG	AA	1765	1/1	0.97	0.06	43,43,43,43	0
56	MG	DA	3224	1/1	0.97	0.20	2,2,2,2	0
56	MG	AW	107	1/1	0.97	0.04	28,28,28,28	0
56	MG	DA	3226	1/1	0.97	0.06	5,5,5,5	0
56	MG	AA	1695	1/1	0.97	0.26	13,13,13,13	1
56	MG	DA	3228	1/1	0.97	0.12	19,19,19,19	0
56	MG	BA	3262	1/1	0.97	0.08	20,20,20,20	0
56	MG	BA	3263	1/1	0.97	0.07	4,4,4,4	0
56	MG	AA	1740	1/1	0.97	0.07	40,40,40,40	0
56	MG	AA	1717	1/1	0.97	0.04	21,21,21,21	0
56	MG	DA	3233	1/1	0.97	0.07	0,0,0,0	0
56	MG	AA	1718	1/1	0.97	0.11	0,0,0,0	0
56	MG	BA	3399	1/1	0.97	0.29	27,27,27,27	0
56	MG	AA	1800	1/1	0.97	0.04	36,36,36,36	0
56	MG	BA	3035	1/1	0.97	0.18	10,10,10,10	0
56	MG	AW	115	1/1	0.97	0.03	42,42,42,42	0
56	MG	DA	3239	1/1	0.97	0.15	39,39,39,39	0
56	MG	CW	113	1/1	0.97	0.07	24,24,24,24	0
56	MG	DA	3243	1/1	0.97	0.05	3,3,3,3	0
56	MG	AA	1770	1/1	0.97	0.06	16,16,16,16	0
56	MG	CA	1657	1/1	0.97	0.18	24,24,24,24	0
56	MG	BA	3039	1/1	0.97	0.17	31,31,31,31	0
56	MG	DA	3247	1/1	0.97	0.14	18,18,18,18	0
56	MG	CX	105	1/1	0.97	0.04	41,41,41,41	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	CA	1659	1/1	0.97	0.04	9,9,9,9	0
56	MG	BA	3042	1/1	0.97	0.05	13,13,13,13	0
56	MG	AA	1635	1/1	0.97	0.13	16,16,16,16	0
56	MG	DA	3003	1/1	0.97	0.10	26,26,26,26	0
56	MG	AA	1683	1/1	0.97	0.04	17,17,17,17	0
56	MG	AA	1669	1/1	0.97	0.32	38,38,38,38	0
56	MG	BA	3161	1/1	0.97	0.06	11,11,11,11	0
56	MG	BA	3280	1/1	0.97	0.10	10,10,10,10	0
56	MG	CA	1666	1/1	0.97	0.07	41,41,41,41	0
56	MG	BA	3047	1/1	0.97	0.22	0,0,0,0	0
56	MG	DA	3011	1/1	0.97	0.16	11,11,11,11	0
56	MG	AA	1724	1/1	0.97	0.02	0,0,0,0	0
56	MG	DA	3265	1/1	0.97	0.05	0,0,0,0	0
56	MG	CA	1669	1/1	0.97	0.08	0,0,0,0	0
56	MG	DA	3017	1/1	0.97	0.12	6,6,6,6	0
56	MG	DA	3019	1/1	0.97	0.15	0,0,0,0	0
56	MG	BA	3050	1/1	0.97	0.13	0,0,0,0	0
56	MG	AA	1806	1/1	0.97	0.24	24,24,24,24	0
56	MG	DA	3023	1/1	0.97	0.18	0,0,0,0	0
56	MG	BA	3053	1/1	0.97	0.13	0,0,0,0	0
56	MG	DA	3025	1/1	0.97	0.11	6,6,6,6	0
56	MG	BA	3054	1/1	0.97	0.11	0,0,0,0	0
56	MG	BA	3055	1/1	0.97	0.03	0,0,0,0	0
56	MG	BA	3173	1/1	0.97	0.14	14,14,14,14	0
56	MG	AX	101	1/1	0.97	0.07	0,0,0,0	0
56	MG	DA	3034	1/1	0.97	0.09	7,7,7,7	0
56	MG	AA	1702	1/1	0.97	0.15	23,23,23,23	0
56	MG	BA	3059	1/1	0.97	0.11	16,16,16,16	0
56	MG	CA	1683	1/1	0.97	0.03	2,2,2,2	0
56	MG	BA	3061	1/1	0.97	0.12	0,0,0,0	0
56	MG	DA	3284	1/1	0.97	0.11	12,12,12,12	0
56	MG	BA	3062	1/1	0.97	0.19	0,0,0,0	0
56	MG	DA	3287	1/1	0.97	0.19	17,17,17,17	0
56	MG	CA	1686	1/1	0.97	0.07	57,57,57,57	0
56	MG	AX	103	1/1	0.97	0.04	29,29,29,29	0
56	MG	DA	3049	1/1	0.97	0.14	0,0,0,0	0
56	MG	CA	1689	1/1	0.97	0.06	0,0,0,0	0
56	MG	CA	1690	1/1	0.97	0.06	19,19,19,19	0
56	MG	BA	3182	1/1	0.97	0.15	16,16,16,16	0
56	MG	DA	3299	1/1	0.97	0.07	0,0,0,0	0
56	MG	BA	3067	1/1	0.97	0.09	5,5,5,5	0
56	MG	DA	3301	1/1	0.97	0.14	18,18,18,18	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	DA	3060	1/1	0.97	0.23	0,0,0,0	0
56	MG	CA	1693	1/1	0.97	0.09	18,18,18,18	1
56	MG	AA	1658	1/1	0.97	0.09	37,37,37,37	0
56	MG	DA	3065	1/1	0.97	0.14	0,0,0,0	0
56	MG	AA	1780	1/1	0.97	0.16	60,60,60,60	0
56	MG	BA	3186	1/1	0.97	0.15	25,25,25,25	0
56	MG	BA	3187	1/1	0.97	0.14	2,2,2,2	0
56	MG	BA	3071	1/1	0.97	0.15	20,20,20,20	0
56	MG	CA	1699	1/1	0.97	0.12	0,0,0,0	0
56	MG	DA	3074	1/1	0.97	0.15	11,11,11,11	0
56	MG	DA	3075	1/1	0.97	0.18	0,0,0,0	0
56	MG	DA	3081	1/1	0.97	0.14	4,4,4,4	0
56	MG	BA	3189	1/1	0.97	0.10	3,3,3,3	0
56	MG	DA	3083	1/1	0.97	0.14	13,13,13,13	0
56	MG	CA	1701	1/1	0.97	0.10	16,16,16,16	0
56	MG	CA	1702	1/1	0.97	0.07	36,36,36,36	0
56	MG	DA	3323	1/1	0.97	0.21	31,31,31,31	0
56	MG	DA	3087	1/1	0.97	0.22	23,23,23,23	0
56	MG	DA	3089	1/1	0.97	0.11	4,4,4,4	0
56	MG	AA	1628	1/1	0.97	0.10	2,2,2,2	0
56	MG	BA	3073	1/1	0.97	0.12	4,4,4,4	0
56	MG	CA	1705	1/1	0.97	0.16	22,22,22,22	0
56	MG	BA	3076	1/1	0.97	0.13	4,4,4,4	0
56	MG	CA	1707	1/1	0.97	0.12	6,6,6,6	0
56	MG	BA	3077	1/1	0.97	0.12	6,6,6,6	0
56	MG	BA	3080	1/1	0.97	0.11	0,0,0,0	0
56	MG	DA	3336	1/1	0.97	0.05	3,3,3,3	1
56	MG	DA	3109	1/1	0.97	0.17	0,0,0,0	0
56	MG	DA	3338	1/1	0.97	0.07	53,53,53,53	0
56	MG	BA	3319	1/1	0.97	0.09	0,0,0,0	0
56	MG	BA	3201	1/1	0.97	0.14	21,21,21,21	0
56	MG	CA	1712	1/1	0.97	0.14	19,19,19,19	0
56	MG	BA	3202	1/1	0.97	0.06	0,0,0,0	0
56	MG	DA	3120	1/1	0.97	0.14	25,25,25,25	0
56	MG	BA	3082	1/1	0.97	0.08	22,22,22,22	0
56	MG	BA	3324	1/1	0.97	0.05	18,18,18,18	1
56	MG	DA	3124	1/1	0.97	0.14	0,0,0,0	0
56	MG	BA	3087	1/1	0.97	0.13	16,16,16,16	0
56	MG	CA	1717	1/1	0.97	0.05	16,16,16,16	0
56	MG	DA	3130	1/1	0.97	0.06	14,14,14,14	0
56	MG	DA	3131	1/1	0.97	0.15	0,0,0,0	0
56	MG	AA	1687	1/1	0.97	0.09	10,10,10,10	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	DA	3355	1/1	0.97	0.05	7,7,7,7	0
56	MG	BA	3206	1/1	0.97	0.07	25,25,25,25	0
56	MG	DA	3134	1/1	0.97	0.14	4,4,4,4	0
56	MG	BA	3328	1/1	0.97	0.04	30,30,30,30	0
56	MG	DA	3136	1/1	0.97	0.17	3,3,3,3	0
56	MG	BA	3089	1/1	0.97	0.17	6,6,6,6	0
56	MG	DA	3362	1/1	0.97	0.14	10,10,10,10	1
56	MG	BA	3208	1/1	0.97	0.06	8,8,8,8	0
56	MG	DA	3139	1/1	0.97	0.08	28,28,28,28	0
56	MG	BA	3211	1/1	0.97	0.19	42,42,42,42	0
56	MG	DA	3366	1/1	0.97	0.08	3,3,3,3	0
56	MG	BA	3090	1/1	0.97	0.09	0,0,0,0	0
56	MG	BB	202	1/1	0.97	0.03	14,14,14,14	0
56	MG	DA	3146	1/1	0.97	0.14	22,22,22,22	0
56	MG	AA	1610	1/1	0.97	0.16	0,0,0,0	0
56	MG	BA	3334	1/1	0.97	0.05	40,40,40,40	0
56	MG	BA	3094	1/1	0.97	0.18	0,0,0,0	0
56	MG	BA	3100	1/1	0.97	0.14	3,3,3,3	0
56	MG	B2	104	1/1	0.97	0.06	34,34,34,34	0
56	MG	BA	3338	1/1	0.97	0.08	22,22,22,22	1
56	MG	BA	3340	1/1	0.97	0.06	28,28,28,28	0
56	MG	AA	1732	1/1	0.97	0.07	3,3,3,3	0
56	MG	BA	3342	1/1	0.97	0.13	52,52,52,52	1
56	MG	BA	3104	1/1	0.97	0.14	12,12,12,12	0
56	MG	BA	3105	1/1	0.97	0.14	13,13,13,13	0
56	MG	BA	3106	1/1	0.97	0.13	0,0,0,0	0
56	MG	DA	3385	1/1	0.97	0.04	29,29,29,29	0
56	MG	AA	1754	1/1	0.97	0.10	16,16,16,16	0
56	MG	AA	1639	1/1	0.97	0.17	30,30,30,30	0
56	MG	CA	1740	1/1	0.97	0.11	19,19,19,19	0
56	MG	DA	3390	1/1	0.97	0.10	73,73,73,73	0
56	MG	BA	3110	1/1	0.97	0.11	0,0,0,0	0
56	MG	DA	3164	1/1	0.97	0.04	8,8,8,8	0
56	MG	B7	101	1/1	0.97	0.10	7,7,7,7	0
56	MG	BF	301	1/1	0.97	0.14	17,17,17,17	0
56	MG	BA	3351	1/1	0.97	0.15	78,78,78,78	0
56	MG	CA	1746	1/1	0.97	0.18	18,18,18,18	0
56	MG	DA	3397	1/1	0.97	0.06	31,31,31,31	0
56	MG	CA	1748	1/1	0.97	0.10	7,7,7,7	0
56	MG	B7	102	1/1	0.97	0.08	11,11,11,11	1
56	MG	BV	201	1/1	0.97	0.15	23,23,23,23	0
56	MG	BA	3113	1/1	0.97	0.14	14,14,14,14	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	DA	3174	1/1	0.97	0.15	26,26,26,26	0
56	MG	CA	1753	1/1	0.97	0.09	33,33,33,33	0
56	MG	BA	3228	1/1	0.97	0.14	46,46,46,46	0
56	MG	DB	209	1/1	0.97	0.08	20,20,20,20	0
56	MG	AA	1756	1/1	0.97	0.12	15,15,15,15	0
56	MG	DA	3180	1/1	0.97	0.18	0,0,0,0	0
56	MG	BA	3116	1/1	0.97	0.15	12,12,12,12	0
56	MG	AV	103	1/1	0.97	0.13	28,28,28,28	0
56	MG	BA	3232	1/1	0.97	0.15	23,23,23,23	0
56	MG	DF	301	1/1	0.97	0.13	29,29,29,29	0
56	MG	BA	3003	1/1	0.97	0.12	28,28,28,28	0
56	MG	BA	3365	1/1	0.97	0.24	60,60,60,60	0
56	MG	BA	3122	1/1	0.97	0.09	8,8,8,8	0
56	MG	CA	1612	1/1	0.97	0.07	17,17,17,17	0
56	MG	AV	104	1/1	0.97	0.08	27,27,27,27	0
56	MG	AV	105	1/1	0.97	0.14	12,12,12,12	0
56	MG	DA	3192	1/1	0.97	0.17	17,17,17,17	0
56	MG	BA	3370	1/1	0.97	0.12	28,28,28,28	1
56	MG	BA	3127	1/1	0.98	0.13	8,8,8,8	0
56	MG	BA	3274	1/1	0.98	0.09	0,0,0,0	0
56	MG	BA	3195	1/1	0.98	0.16	16,16,16,16	0
56	MG	AA	1771	1/1	0.98	0.07	6,6,6,6	0
56	MG	DA	3223	1/1	0.98	0.17	11,11,11,11	0
56	MG	BA	3198	1/1	0.98	0.10	0,0,0,0	0
56	MG	DA	3030	1/1	0.98	0.12	0,0,0,0	0
56	MG	BB	219	1/1	0.98	0.09	24,24,24,24	0
56	MG	BE	301	1/1	0.98	0.12	8,8,8,8	0
56	MG	DA	3035	1/1	0.98	0.10	0,0,0,0	0
56	MG	AA	1637	1/1	0.98	0.12	0,0,0,0	0
56	MG	BA	3200	1/1	0.98	0.02	5,5,5,5	1
56	MG	BA	3065	1/1	0.98	0.09	1,1,1,1	0
56	MG	DA	3039	1/1	0.98	0.08	10,10,10,10	0
56	MG	BO	201	1/1	0.98	0.16	13,13,13,13	0
56	MG	BA	3134	1/1	0.98	0.09	1,1,1,1	0
56	MG	AA	1625	1/1	0.98	0.10	3,3,3,3	0
56	MG	DA	3043	1/1	0.98	0.14	2,2,2,2	0
56	MG	DA	3044	1/1	0.98	0.07	15,15,15,15	0
56	MG	DA	3045	1/1	0.98	0.09	1,1,1,1	0
56	MG	DA	3047	1/1	0.98	0.14	0,0,0,0	0
56	MG	BA	3068	1/1	0.98	0.12	0,0,0,0	0
56	MG	DA	3241	1/1	0.98	0.14	12,12,12,12	0
56	MG	DA	3242	1/1	0.98	0.18	9,9,9,9	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	AA	1796	1/1	0.98	0.05	10,10,10,10	1
56	MG	AA	1649	1/1	0.98	0.13	0,0,0,0	0
56	MG	AA	1605	1/1	0.98	0.02	16,16,16,16	0
56	MG	DA	3052	1/1	0.98	0.17	0,0,0,0	0
56	MG	DA	3054	1/1	0.98	0.09	5,5,5,5	0
56	MG	DA	3055	1/1	0.98	0.15	0,0,0,0	0
56	MG	DA	3056	1/1	0.98	0.14	9,9,9,9	0
56	MG	BA	3024	1/1	0.98	0.15	0,0,0,0	0
56	MG	CA	1607	1/1	0.98	0.17	15,15,15,15	0
56	MG	DA	3059	1/1	0.98	0.17	0,0,0,0	0
56	MG	BA	3290	1/1	0.98	0.06	2,2,2,2	0
56	MG	BA	3210	1/1	0.98	0.10	11,11,11,11	0
56	MG	BA	3292	1/1	0.98	0.07	14,14,14,14	0
56	MG	DA	3257	1/1	0.98	0.12	27,27,27,27	0
56	MG	DA	3063	1/1	0.98	0.13	0,0,0,0	0
56	MG	BA	3026	1/1	0.98	0.17	0,0,0,0	0
56	MG	DA	3066	1/1	0.98	0.15	0,0,0,0	0
56	MG	CA	1613	1/1	0.98	0.20	4,4,4,4	0
56	MG	CA	1614	1/1	0.98	0.10	20,20,20,20	0
56	MG	DA	3264	1/1	0.98	0.08	11,11,11,11	0
56	MG	BA	3389	1/1	0.98	0.07	0,0,0,0	0
56	MG	DA	3266	1/1	0.98	0.06	11,11,11,11	0
56	MG	BA	3075	1/1	0.98	0.15	0,0,0,0	0
56	MG	BA	3295	1/1	0.98	0.13	16,16,16,16	0
56	MG	BA	3027	1/1	0.98	0.06	8,8,8,8	0
56	MG	BA	3297	1/1	0.98	0.16	7,7,7,7	0
56	MG	DA	3079	1/1	0.98	0.12	13,13,13,13	0
56	MG	AA	1682	1/1	0.98	0.13	17,17,17,17	0
56	MG	BA	3145	1/1	0.98	0.20	0,0,0,0	0
56	MG	BA	3078	1/1	0.98	0.17	11,11,11,11	0
56	MG	CA	1623	1/1	0.98	0.05	9,9,9,9	0
56	MG	CA	1624	1/1	0.98	0.03	16,16,16,16	0
56	MG	BA	3301	1/1	0.98	0.11	19,19,19,19	0
56	MG	DA	3088	1/1	0.98	0.13	4,4,4,4	0
56	MG	AA	1778	1/1	0.98	0.09	0,0,0,0	0
56	MG	DA	3090	1/1	0.98	0.09	0,0,0,0	0
56	MG	DA	3091	1/1	0.98	0.12	0,0,0,0	0
56	MG	BA	3030	1/1	0.98	0.10	0,0,0,0	0
56	MG	DA	3094	1/1	0.98	0.09	10,10,10,10	0
56	MG	DA	3095	1/1	0.98	0.20	0,0,0,0	0
56	MG	CA	1743	1/1	0.98	0.13	1,1,1,1	0
56	MG	DA	3097	1/1	0.98	0.11	12,12,12,12	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	BA	3304	1/1	0.98	0.06	35,35,35,35	0
56	MG	DA	3289	1/1	0.98	0.10	18,18,18,18	0
56	MG	DA	3290	1/1	0.98	0.06	0,0,0,0	0
56	MG	BA	3083	1/1	0.98	0.12	20,20,20,20	0
56	MG	BA	3085	1/1	0.98	0.14	0,0,0,0	0
56	MG	DA	3295	1/1	0.98	0.03	6,6,6,6	0
56	MG	CA	1747	1/1	0.98	0.07	28,28,28,28	0
56	MG	DA	3103	1/1	0.98	0.14	9,9,9,9	0
56	MG	DA	3104	1/1	0.98	0.09	9,9,9,9	0
56	MG	DA	3105	1/1	0.98	0.12	6,6,6,6	0
56	MG	CA	1632	1/1	0.98	0.03	11,11,11,11	0
56	MG	CA	1749	1/1	0.98	0.04	7,7,7,7	0
56	MG	DA	3110	1/1	0.98	0.14	1,1,1,1	0
56	MG	DA	3303	1/1	0.98	0.07	11,11,11,11	0
56	MG	BA	3404	1/1	0.98	0.20	17,17,17,17	0
56	MG	AA	1640	1/1	0.98	0.18	18,18,18,18	0
56	MG	DA	3114	1/1	0.98	0.05	8,8,8,8	0
56	MG	DA	3308	1/1	0.98	0.03	20,20,20,20	0
56	MG	AA	1641	1/1	0.98	0.08	0,0,0,0	0
56	MG	BA	3310	1/1	0.98	0.18	22,22,22,22	0
56	MG	DA	3117	1/1	0.98	0.07	1,1,1,1	0
56	MG	DA	3119	1/1	0.98	0.09	7,7,7,7	0
56	MG	CA	1754	1/1	0.98	0.11	6,6,6,6	0
56	MG	DA	3121	1/1	0.98	0.07	12,12,12,12	0
56	MG	DA	3315	1/1	0.98	0.06	4,4,4,4	0
56	MG	BA	3311	1/1	0.98	0.05	2,2,2,2	0
56	MG	DA	3317	1/1	0.98	0.03	11,11,11,11	1
56	MG	AW	104	1/1	0.98	0.07	28,28,28,28	0
56	MG	AA	1759	1/1	0.98	0.07	5,5,5,5	1
56	MG	DA	3125	1/1	0.98	0.12	0,0,0,0	0
56	MG	DA	3126	1/1	0.98	0.09	29,29,29,29	0
56	MG	BA	3225	1/1	0.98	0.14	0,0,0,0	0
56	MG	AA	1722	1/1	0.98	0.12	20,20,20,20	0
56	MG	BA	3092	1/1	0.98	0.12	0,0,0,0	0
56	MG	CA	1761	1/1	0.98	0.26	26,26,26,26	0
56	MG	AA	1622	1/1	0.98	0.09	8,8,8,8	0
56	MG	BA	3159	1/1	0.98	0.12	12,12,12,12	0
56	MG	BA	3098	1/1	0.98	0.07	5,5,5,5	0
56	MG	BA	3099	1/1	0.98	0.18	1,1,1,1	0
56	MG	DA	3331	1/1	0.98	0.15	42,42,42,42	0
56	MG	BA	3040	1/1	0.98	0.07	22,22,22,22	0
56	MG	BA	3163	1/1	0.98	0.03	17,17,17,17	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	BA	3101	1/1	0.98	0.07	3,3,3,3	0
56	MG	BA	3235	1/1	0.98	0.10	7,7,7,7	0
56	MG	DA	3140	1/1	0.98	0.12	22,22,22,22	0
56	MG	DA	3141	1/1	0.98	0.10	0,0,0,0	0
56	MG	CA	1770	1/1	0.98	0.11	14,14,14,14	0
56	MG	DA	3143	1/1	0.98	0.18	36,36,36,36	0
56	MG	CA	1771	1/1	0.98	0.10	28,28,28,28	0
56	MG	BA	3236	1/1	0.98	0.05	3,3,3,3	0
56	MG	DA	3343	1/1	0.98	0.12	4,4,4,4	0
56	MG	CA	1773	1/1	0.98	0.05	13,13,13,13	0
56	MG	DA	3345	1/1	0.98	0.20	17,17,17,17	0
56	MG	CA	1774	1/1	0.98	0.18	21,21,21,21	0
56	MG	BA	3423	1/1	0.98	0.07	21,21,21,21	0
56	MG	CA	1653	1/1	0.98	0.08	60,60,60,60	0
56	MG	CA	1777	1/1	0.98	0.14	0,0,0,0	0
56	MG	CA	1778	1/1	0.98	0.10	3,3,3,3	0
56	MG	CA	1654	1/1	0.98	0.14	41,41,41,41	0
56	MG	CA	1655	1/1	0.98	0.14	0,0,0,0	0
56	MG	BA	3165	1/1	0.98	0.16	0,0,0,0	0
56	MG	BA	3041	1/1	0.98	0.12	0,0,0,0	0
56	MG	DA	3356	1/1	0.98	0.05	12,12,12,12	0
56	MG	CA	1783	1/1	0.98	0.18	13,13,13,13	0
56	MG	CA	1784	1/1	0.98	0.06	15,15,15,15	0
56	MG	DA	3158	1/1	0.98	0.12	5,5,5,5	0
56	MG	CA	1785	1/1	0.98	0.11	44,44,44,44	0
56	MG	AA	1613	1/1	0.98	0.17	2,2,2,2	0
56	MG	BA	3427	1/1	0.98	0.04	12,12,12,12	0
56	MG	AA	1656	1/1	0.98	0.09	12,12,12,12	0
56	MG	AA	1726	1/1	0.98	0.13	12,12,12,12	0
56	MG	BA	3243	1/1	0.98	0.23	18,18,18,18	0
56	MG	BA	3171	1/1	0.98	0.10	0,0,0,0	1
56	MG	DA	3166	1/1	0.98	0.03	0,0,0,0	0
56	MG	AW	111	1/1	0.98	0.04	32,32,32,32	1
56	MG	BA	3246	1/1	0.98	0.04	15,15,15,15	0
56	MG	DA	3370	1/1	0.98	0.11	22,22,22,22	0
56	MG	BA	3247	1/1	0.98	0.09	0,0,0,0	0
56	MG	BA	3248	1/1	0.98	0.14	33,33,33,33	0
56	MG	AA	1611	1/1	0.98	0.10	18,18,18,18	0
56	MG	BA	3339	1/1	0.98	0.03	0,0,0,0	1
56	MG	BA	3108	1/1	0.98	0.03	0,0,0,0	0
56	MG	BA	3175	1/1	0.98	0.12	0,0,0,0	0
56	MG	DA	3378	1/1	0.98	0.12	8,8,8,8	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	DA	3175	1/1	0.98	0.15	30,30,30,30	0
56	MG	BA	3440	1/1	0.98	0.04	33,33,33,33	0
56	MG	AA	1746	1/1	0.98	0.03	11,11,11,11	0
56	MG	AW	114	1/1	0.98	0.03	25,25,25,25	1
56	MG	DA	3179	1/1	0.98	0.09	10,10,10,10	0
56	MG	AA	1630	1/1	0.98	0.07	13,13,13,13	0
56	MG	BA	3444	1/1	0.98	0.06	7,7,7,7	0
56	MG	BA	3052	1/1	0.98	0.23	0,0,0,0	0
56	MG	CA	1678	1/1	0.98	0.10	0,0,0,0	0
56	MG	CA	1679	1/1	0.98	0.06	4,4,4,4	0
56	MG	BA	3180	1/1	0.98	0.13	33,33,33,33	0
56	MG	CA	1681	1/1	0.98	0.06	40,40,40,40	0
56	MG	AA	1659	1/1	0.98	0.04	14,14,14,14	1
56	MG	AA	1676	1/1	0.98	0.03	7,7,7,7	0
56	MG	DA	3190	1/1	0.98	0.03	2,2,2,2	0
56	MG	BA	3115	1/1	0.98	0.10	0,0,0,0	0
56	MG	BA	3350	1/1	0.98	0.11	32,32,32,32	0
56	MG	D5	101	1/1	0.98	0.09	7,7,7,7	0
56	MG	DA	3398	1/1	0.98	0.13	7,7,7,7	0
56	MG	BA	3010	1/1	0.98	0.05	30,30,30,30	0
56	MG	DA	3196	1/1	0.98	0.17	18,18,18,18	0
56	MG	BA	3352	1/1	0.98	0.05	30,30,30,30	1
56	MG	BA	3117	1/1	0.98	0.16	3,3,3,3	0
56	MG	BA	3011	1/1	0.98	0.13	0,0,0,0	0
56	MG	DB	206	1/1	0.98	0.06	0,0,0,0	1
56	MG	DA	3201	1/1	0.98	0.14	7,7,7,7	0
56	MG	BA	3355	1/1	0.98	0.14	20,20,20,20	0
56	MG	BA	3356	1/1	0.98	0.05	37,37,37,37	0
56	MG	BA	3357	1/1	0.98	0.04	19,19,19,19	0
56	MG	BA	3264	1/1	0.98	0.18	0,0,0,0	0
56	MG	AA	1646	1/1	0.98	0.17	3,3,3,3	0
56	MG	DD	301	1/1	0.98	0.12	1,1,1,1	0
56	MG	AW	119	1/1	0.98	0.02	19,19,19,19	0
56	MG	BA	3267	1/1	0.98	0.07	43,43,43,43	0
56	MG	BA	3060	1/1	0.98	0.18	0,0,0,0	0
56	MG	AA	1815	1/1	0.98	0.14	36,36,36,36	0
56	MG	DA	3018	1/1	0.98	0.11	3,3,3,3	0
56	MG	BA	3126	1/1	0.98	0.04	1,1,1,1	0
56	MG	BA	3192	1/1	0.98	0.11	0,0,0,0	0
56	MG	DA	3021	1/1	0.98	0.16	0,0,0,0	0
56	MG	DA	3216	1/1	0.98	0.21	34,34,34,34	0
56	MG	BA	3193	1/1	0.98	0.12	8,8,8,8	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	BA	3368	1/1	0.98	0.10	32,32,32,32	0
58	ZN	AD	301	1/1	0.98	0.11	21,21,21,21	0
56	MG	D5	102	1/1	0.99	0.02	6,6,6,6	1
56	MG	BA	3034	1/1	0.99	0.11	0,0,0,0	0
56	MG	DA	3072	1/1	0.99	0.06	0,0,0,0	0
56	MG	DA	3073	1/1	0.99	0.09	0,0,0,0	0
56	MG	B2	105	1/1	0.99	0.05	0,0,0,0	0
56	MG	BA	3063	1/1	0.99	0.17	0,0,0,0	0
56	MG	DA	3076	1/1	0.99	0.13	0,0,0,0	0
56	MG	DA	3077	1/1	0.99	0.11	0,0,0,0	0
56	MG	DA	3078	1/1	0.99	0.15	2,2,2,2	0
56	MG	BA	3321	1/1	0.99	0.06	4,4,4,4	0
56	MG	DA	3080	1/1	0.99	0.14	0,0,0,0	0
56	MG	DA	3005	1/1	0.99	0.04	13,13,13,13	0
56	MG	BA	3013	1/1	0.99	0.08	0,0,0,0	0
56	MG	AA	1774	1/1	0.99	0.02	9,9,9,9	0
56	MG	BA	3066	1/1	0.99	0.07	0,0,0,0	0
56	MG	DA	3252	1/1	0.99	0.02	0,0,0,0	1
56	MG	DA	3085	1/1	0.99	0.15	0,0,0,0	0
56	MG	BA	3038	1/1	0.99	0.15	10,10,10,10	0
56	MG	BA	3015	1/1	0.99	0.08	0,0,0,0	0
56	MG	AA	1728	1/1	0.99	0.05	2,2,2,2	0
56	MG	AA	1699	1/1	0.99	0.10	0,0,0,0	0
56	MG	DA	3013	1/1	0.99	0.09	1,1,1,1	0
56	MG	DA	3259	1/1	0.99	0.07	14,14,14,14	0
56	MG	DA	3014	1/1	0.99	0.16	4,4,4,4	0
56	MG	AA	1700	1/1	0.99	0.06	31,31,31,31	0
56	MG	BA	3281	1/1	0.99	0.09	0,0,0,0	0
56	MG	CA	1605	1/1	0.99	0.09	10,10,10,10	0
56	MG	BA	3019	1/1	0.99	0.16	0,0,0,0	0
56	MG	BA	3151	1/1	0.99	0.07	2,2,2,2	0
56	MG	BA	3284	1/1	0.99	0.13	14,14,14,14	0
56	MG	BA	3238	1/1	0.99	0.14	0,0,0,0	0
56	MG	BA	3385	1/1	0.99	0.04	12,12,12,12	0
56	MG	DA	3182	1/1	0.99	0.08	5,5,5,5	0
56	MG	AV	101	1/1	0.99	0.03	5,5,5,5	0
56	MG	DA	3102	1/1	0.99	0.16	0,0,0,0	0
56	MG	AA	1720	1/1	0.99	0.12	29,29,29,29	0
56	MG	DA	3026	1/1	0.99	0.19	0,0,0,0	0
56	MG	AA	1607	1/1	0.99	0.04	12,12,12,12	0
56	MG	BA	3048	1/1	0.99	0.13	0,0,0,0	0
56	MG	DA	3107	1/1	0.99	0.15	12,12,12,12	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	DA	3108	1/1	0.99	0.14	0,0,0,0	0
56	MG	DA	3372	1/1	0.99	0.02	12,12,12,12	0
56	MG	AA	1664	1/1	0.99	0.11	0,0,0,0	0
56	MG	AA	1675	1/1	0.99	0.13	4,4,4,4	0
56	MG	BA	3081	1/1	0.99	0.08	10,10,10,10	0
56	MG	DA	3194	1/1	0.99	0.06	0,0,0,0	1
56	MG	DA	3033	1/1	0.99	0.05	17,17,17,17	1
56	MG	DA	3113	1/1	0.99	0.12	11,11,11,11	0
56	MG	BA	3025	1/1	0.99	0.11	0,0,0,0	0
56	MG	DA	3198	1/1	0.99	0.09	10,10,10,10	0
56	MG	DA	3286	1/1	0.99	0.03	0,0,0,0	0
56	MG	BA	3118	1/1	0.99	0.08	0,0,0,0	0
56	MG	AA	1757	1/1	0.99	0.05	0,0,0,0	0
56	MG	BA	3084	1/1	0.99	0.14	0,0,0,0	0
56	MG	DA	3118	1/1	0.99	0.09	6,6,6,6	0
56	MG	DA	3386	1/1	0.99	0.24	0,0,0,0	0
56	MG	B1	101	1/1	0.99	0.07	0,0,0,0	0
56	MG	BA	3398	1/1	0.99	0.06	9,9,9,9	1
56	MG	DA	3293	1/1	0.99	0.05	2,2,2,2	0
56	MG	DA	3294	1/1	0.99	0.15	0,0,0,0	0
56	MG	BA	3123	1/1	0.99	0.11	6,6,6,6	0
56	MG	CM	201	1/1	0.99	0.05	21,21,21,21	0
56	MG	BA	3086	1/1	0.99	0.09	2,2,2,2	0
56	MG	BA	3209	1/1	0.99	0.08	15,15,15,15	0
56	MG	CA	1682	1/1	0.99	0.05	32,32,32,32	0
56	MG	DA	3210	1/1	0.99	0.09	0,0,0,0	0
56	MG	BA	3007	1/1	0.99	0.27	0,0,0,0	0
56	MG	DA	3127	1/1	0.99	0.07	0,0,0,0	0
56	MG	DA	3046	1/1	0.99	0.21	0,0,0,0	0
56	MG	AA	1704	1/1	0.99	0.03	0,0,0,0	0
56	MG	CA	1630	1/1	0.99	0.09	0,0,0,0	0
56	MG	BA	3056	1/1	0.99	0.15	0,0,0,0	0
56	MG	CA	1687	1/1	0.99	0.02	0,0,0,0	0
56	MG	BA	3169	1/1	0.99	0.10	8,8,8,8	0
56	MG	AA	1652	1/1	0.99	0.04	7,7,7,7	0
56	MG	DA	3053	1/1	0.99	0.04	24,24,24,24	0
56	MG	BA	3031	1/1	0.99	0.12	11,11,11,11	0
56	MG	BA	3307	1/1	0.99	0.05	7,7,7,7	0
56	MG	CW	108	1/1	0.99	0.06	10,10,10,10	1
56	MG	BA	3260	1/1	0.99	0.02	23,23,23,23	0
56	MG	BA	3130	1/1	0.99	0.06	4,4,4,4	0
56	MG	AA	1672	1/1	0.99	0.11	0,0,0,0	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	BA	3132	1/1	0.99	0.11	2,2,2,2	0
56	MG	BA	3133	1/1	0.99	0.07	11,11,11,11	0
56	MG	CX	101	1/1	0.99	0.07	3,3,3,3	0
56	MG	BA	3093	1/1	0.99	0.11	15,15,15,15	0
56	MG	DA	3064	1/1	0.99	0.13	0,0,0,0	0
56	MG	BA	3363	1/1	0.99	0.07	8,8,8,8	0
56	MG	AA	1707	1/1	0.99	0.08	2,2,2,2	0
56	MG	BA	3095	1/1	0.99	0.10	0,0,0,0	0
56	MG	BA	3096	1/1	0.99	0.09	0,0,0,0	0
56	MG	DA	3327	1/1	0.99	0.03	6,6,6,6	0
56	MG	BA	3097	1/1	0.99	0.09	2,2,2,2	0
58	ZN	AN	101	1/1	0.99	0.04	50,50,50,50	0
58	ZN	CD	301	1/1	0.99	0.12	24,24,24,24	0
56	MG	BA	3045	1/1	1.00	0.07	0,0,0,0	0
56	MG	DA	3306	1/1	1.00	0.05	6,6,6,6	0
56	MG	AA	1696	1/1	1.00	0.08	0,0,0,0	0
56	MG	BA	3196	1/1	1.00	0.02	0,0,0,0	0
56	MG	BA	3074	1/1	1.00	0.12	10,10,10,10	0
56	MG	BA	3079	1/1	1.00	0.09	0,0,0,0	0
56	MG	DA	3335	1/1	1.00	0.03	10,10,10,10	0
56	MG	AA	1711	1/1	1.00	0.04	8,8,8,8	0
56	MG	DA	3031	1/1	1.00	0.04	0,0,0,0	0
56	MG	DA	3092	1/1	1.00	0.05	4,4,4,4	0
56	MG	BA	3121	1/1	1.00	0.09	2,2,2,2	0
56	MG	CA	1608	1/1	1.00	0.06	0,0,0,0	0
56	MG	DA	3354	1/1	1.00	0.02	2,2,2,2	0
56	MG	DA	3015	1/1	1.00	0.07	0,0,0,0	0
58	ZN	CN	101	1/1	1.00	0.01	53,53,53,53	0

5.5 Other polymers ⓘ

There are no such residues in this entry.