



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 17, 2026 – 01:41 AM UTC

PDB ID : 4U27 / pdb_00004u27
Title : Crystal structure of the E. coli ribosome bound to flopristin and linopristin.
Authors : Noeske, J.; Huang, J.; Olivier, N.B.; Giacobbe, R.A.; Zambrowski, M.; Cate, J.H.D.
Deposited on : 2014-07-16
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 : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
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) : 2.48.1

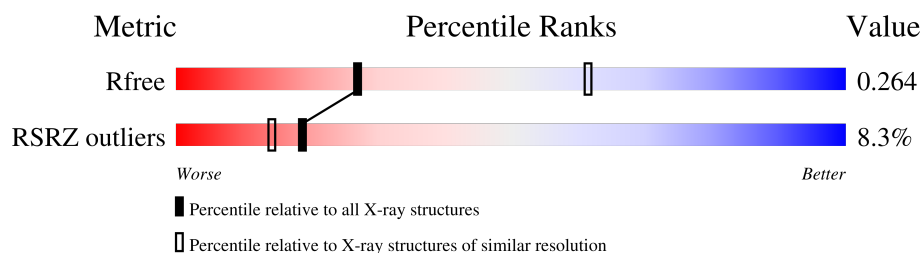
1 Overall quality at a glance

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}	164625	3657 (2.80-2.80)
RSRZ outliers	164620	3659 (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
54	MHW	B6	1	-	X	-	-
54	MHW	D6	1	-	X	-	-
55	MG	BA	3137	-	-	-	X
55	MG	DA	3027	-	-	-	X
55	MG	DA	3062	-	-	-	X

2 Entry composition

There are 58 unique types of molecules in this entry. The entry contains 288396 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 rRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	AA	1538	Total	C	N	O	P	0	0	0
			32995	14716	6050	10691	1538			
1	CA	1539	Total	C	N	O	P	0	0	0
			33015	14725	6052	10699	1539			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	AB	218	Total	C	N	O	S	0	0	0
			1705	1081	305	312	7			
2	CB	218	Total	C	N	O	S	0	0	0
			1705	1081	305	312	7			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	AC	206	Total	C	N	O	S	0	0	0
			1625	1028	305	289	3			
3	CC	206	Total	C	N	O	S	0	0	0
			1625	1028	305	289	3			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	AD	205	Total	C	N	O	S	0	0	0
			1643	1026	315	298	4			
4	CD	205	Total	C	N	O	S	0	0	0
			1643	1026	315	298	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	AE	150	Total	C	N	O	S	0	0	0
			1106	687	211	202	6			
5	CE	150	Total	C	N	O	S	0	0	0
			1106	687	211	202	6			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	AF	100	Total	C	N	O	S	0	0	0
			818	515	148	149	6			
6	CF	100	Total	C	N	O	S	0	0	0
			818	515	148	149	6			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	AG	151	Total	C	N	O	S	0	0	0
			1182	735	227	216	4			
7	CG	151	Total	C	N	O	S	0	0	0
			1182	735	227	216	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	AH	129	Total	C	N	O	S	0	0	0
			979	616	173	184	6			
8	CH	129	Total	C	N	O	S	0	0	0
			979	616	173	184	6			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	AI	127	Total	C	N	O	S	0	0	0
			1022	634	206	179	3			
9	CI	127	Total	C	N	O	S	0	0	0
			1022	634	206	179	3			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	AJ	98	Total	C	N	O	S	0	0	0
			787	493	150	143	1			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	CJ	98	Total	C	N	O	S	0	0	0
			787	493	150	143	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	AK	117	Total	C	N	O	S	0	0	0
			877	540	174	160	3			
11	CK	117	Total	C	N	O	S	0	0	0
			877	540	174	160	3			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	AL	123	Total	C	N	O	S	0	0	0
			955	590	196	165	4			
12	CL	123	Total	C	N	O	S	0	0	0
			955	590	196	165	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	AM	114	Total	C	N	O	S	0	0	0
			884	546	178	157	3			
13	CM	114	Total	C	N	O	S	0	0	0
			884	546	178	157	3			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	AN	96	Total	C	N	O	S	0	0	0
			774	483	160	128	3			
14	CN	96	Total	C	N	O	S	0	0	0
			774	483	160	128	3			

- 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
			710	437	143	129	1			
15	CO	88	Total	C	N	O	S	0	0	0
			710	437	143	129	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	AP	82	Total	C	N	O	S	0	0	0
			649	406	128	114	1			
16	CP	82	Total	C	N	O	S	0	0	0
			649	406	128	114	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	AQ	80	Total	C	N	O	S	0	0	0
			649	411	121	114	3			
17	CQ	80	Total	C	N	O	S	0	0	0
			649	411	121	114	3			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
18	AR	55	Total	C	N	O	0	0	0
			456	288	86	82			
18	CR	55	Total	C	N	O	0	0	0
			456	288	86	82			

- 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	0
			638	408	120	108	2			
19	CS	79	Total	C	N	O	S	0	0	0
			638	408	120	108	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	AT	85	Total	C	N	O	S	0	0	0
			665	411	137	114	3			
20	CT	85	Total	C	N	O	S	0	0	0
			665	411	137	114	3			

- Molecule 21 is a protein called 30S ribosomal protein S21.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
21	AU	51	Total	C	N	O	S	0	0	0
			426	265	86	74	1			
21	CU	51	Total	C	N	O	S	0	0	0
			426	265	86	74	1			

- Molecule 22 is a RNA chain called 23S rRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	BA	2897	Total	C	N	O	P	0	0	0
			62195	27745	11446	20107	2897			
22	DA	2897	Total	C	N	O	P	0	0	0
			62195	27745	11446	20107	2897			

- Molecule 23 is a RNA chain called 5S rRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	BB	119	Total	C	N	O	P	0	0	0
			2549	1135	466	829	119			
23	DB	118	Total	C	N	O	P	0	0	0
			2529	1126	464	821	118			

- Molecule 24 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	BC	271	Total	C	N	O	S	0	0	0
			2083	1288	423	365	7			
24	DC	271	Total	C	N	O	S	0	0	0
			2083	1288	423	365	7			

- Molecule 25 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
25	BD	209	Total	C	N	O	S	0	0	0
			1565	979	288	294	4			
25	DD	209	Total	C	N	O	S	0	0	0
			1565	979	288	294	4			

- Molecule 26 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	BE	201	Total	C	N	O	S	0	0	0
			1552	974	283	290	5			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	DE	201	Total	C	N	O	S	0	0	0
			1552	974	283	290	5			

- Molecule 27 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
27	BF	177	Total	C	N	O	S	0	0	0
			1411	899	249	257	6			
27	DF	177	Total	C	N	O	S	0	0	0
			1411	899	249	257	6			

- Molecule 28 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
28	BG	176	Total	C	N	O	S	0	0	0
			1323	832	243	246	2			
28	DG	176	Total	C	N	O	S	0	0	0
			1323	832	243	246	2			

- Molecule 29 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
29	BH	149	Total	C	N	O	S	0	0	0
			1110	699	197	213	1			
29	DH	149	Total	C	N	O	S	0	0	0
			1110	699	197	213	1			

- Molecule 30 is a protein called 50S ribosomal protein L11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
30	BI	141	Total	C	N	O	S	0	0	0
			1032	651	179	196	6			
30	DI	141	Total	C	N	O	S	0	0	0
			1032	651	179	196	6			

- Molecule 31 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
31	BJ	142	Total	C	N	O	S	0	0	0
			1129	714	212	199	4			
31	DJ	142	Total	C	N	O	S	0	0	0
			1129	714	212	199	4			

- Molecule 32 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
32	BK	122	Total	C	N	O	S	0	0	0
			939	587	180	166	6			
32	DK	122	Total	C	N	O	S	0	0	0
			939	587	180	166	6			

- Molecule 33 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
33	BL	143	Total	C	N	O	S	0	0	0
			1045	649	206	189	1			
33	DL	143	Total	C	N	O	S	0	0	0
			1045	649	206	189	1			

- Molecule 34 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
34	BM	136	Total	C	N	O	S	0	0	0
			1074	686	205	177	6			
34	DM	136	Total	C	N	O	S	0	0	0
			1074	686	205	177	6			

- Molecule 35 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
35	BN	120	Total	C	N	O	S	0	0	0
			961	593	196	167	5			
35	DN	120	Total	C	N	O	S	0	0	0
			961	593	196	167	5			

- Molecule 36 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
36	BO	116	Total	C	N	O	0	0	0
			892	552	178	162			
36	DO	116	Total	C	N	O	0	0	0
			892	552	178	162			

- Molecule 37 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
37	BP	114	Total	C	N	O	S	0	0	0
			917	574	179	163	1			
37	DP	114	Total	C	N	O	S	0	0	0
			917	574	179	163	1			

- Molecule 38 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
38	BQ	117	Total	C	N	O	S	0	0	0
			947	604	192	151				
38	DQ	117	Total	C	N	O	S	0	0	0
			947	604	192	151				

- Molecule 39 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
39	BR	103	Total	C	N	O	S	0	0	0
			816	516	153	145	2			
39	DR	103	Total	C	N	O	S	0	0	0
			816	516	153	145	2			

- Molecule 40 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
40	BS	110	Total	C	N	O	S	0	0	0
			857	532	166	156	3			
40	DS	110	Total	C	N	O	S	0	0	0
			857	532	166	156	3			

- Molecule 41 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
41	BT	93	Total	C	N	O	S	0	0	0
			739	466	139	132	2			
41	DT	93	Total	C	N	O	S	0	0	0
			739	466	139	132	2			

- Molecule 42 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
42	BU	102	Total	C	N	O	S	0	0	0
			780	492	146	142				

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
42	DU	102	Total	C	N	O			
			780	492	146	142	0	0	0

- Molecule 43 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
43	BV	94	Total	C	N	O	S		
			753	479	137	134	3	0	0
43	DV	94	Total	C	N	O	S		
			753	479	137	134	3	0	0

- Molecule 44 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
44	BW	76	Total	C	N	O	S		
			580	359	117	103	1	0	0
44	DW	75	Total	C	N	O	S		
			569	353	113	102	1	0	0

- Molecule 45 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
45	BX	77	Total	C	N	O	S		
			625	388	129	106	2	0	0
45	DX	77	Total	C	N	O	S		
			625	388	129	106	2	0	0

- Molecule 46 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
46	BY	63	Total	C	N	O	S		
			509	313	99	95	2	0	0
46	DY	63	Total	C	N	O	S		
			509	313	99	95	2	0	0

- Molecule 47 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
47	BZ	58	Total	C	N	O	S		
			449	281	87	79	2	0	0
47	DZ	58	Total	C	N	O	S		
			449	281	87	79	2	0	0

- Molecule 48 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
48	B0	56	Total	C	N	O	S	0	0	0
			444	269	94	80	1			
48	D0	56	Total	C	N	O	S	0	0	0
			444	269	94	80	1			

- Molecule 49 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
49	B1	50	Total	C	N	O	0	0	0
			410	263	75	72			
49	D1	50	Total	C	N	O	0	0	0
			410	263	75	72			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
50	B2	46	Total	C	N	O	S	0	0	0
			377	228	90	57	2			
50	D2	46	Total	C	N	O	S	0	0	0
			377	228	90	57	2			

- Molecule 51 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
51	B3	64	Total	C	N	O	S	0	0	0
			504	323	105	74	2			
51	D3	64	Total	C	N	O	S	0	0	0
			504	323	105	74	2			

- Molecule 52 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
52	B4	38	Total	C	N	O	S	0	0	0
			302	185	65	48	4			
52	D4	38	Total	C	N	O	S	0	0	0
			302	185	65	48	4			

- Molecule 53 is a protein called 50S ribosomal protein L1.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
53	B5	191	Total	C	N	O	0	0	1
			1142	691	221	230			

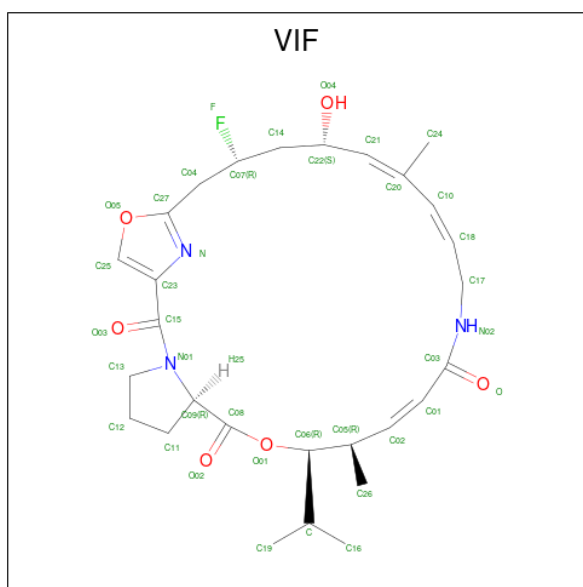
- Molecule 54 is a protein called Linopristin.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
54	B6	7	Total	C	N	O	0	0	0
			69	50	9	10			
54	D6	7	Total	C	N	O	0	0	0
			69	50	9	10			

- Molecule 55 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
55	AA	72	Total	Mg	0	0
			72	72		
55	BA	193	Total	Mg	0	0
			193	193		
55	BB	4	Total	Mg	0	0
			4	4		
55	BD	1	Total	Mg	0	0
			1	1		
55	BQ	1	Total	Mg	0	0
			1	1		
55	CA	56	Total	Mg	0	0
			56	56		
55	DA	167	Total	Mg	0	0
			167	167		
55	DB	3	Total	Mg	0	0
			3	3		
55	D2	1	Total	Mg	0	0
			1	1		

- Molecule 56 is Flopristin (CCD ID: VIF) (formula: C₂₈H₃₈FN₃O₆).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
56	BA	1	Total	C	F	N	O	0
			38	28	1	3	6	
56	DA	1	Total	C	F	N	O	0
			38	28	1	3	6	

- Molecule 57 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	B4	1	Total	Zn	0	0
			1	1		
57	D4	1	Total	Zn	0	0
			1	1		

- Molecule 58 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
58	AA	193	Total	O	0	0
			193	193		
58	AL	2	Total	O	0	0
			2	2		
58	AN	5	Total	O	0	0
			5	5		
58	AT	2	Total	O	0	0
			2	2		
58	AU	1	Total	O	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
58	BA	623	Total 623	O 623	0	0
58	BB	14	Total 14	O 14	0	0
58	BC	6	Total 6	O 6	0	0
58	BD	3	Total 3	O 3	0	0
58	BE	4	Total 4	O 4	0	0
58	BF	1	Total 1	O 1	0	0
58	BG	1	Total 1	O 1	0	0
58	BL	4	Total 4	O 4	0	0
58	BN	3	Total 3	O 3	0	0
58	BS	1	Total 1	O 1	0	0
58	BT	1	Total 1	O 1	0	0
58	B2	1	Total 1	O 1	0	0
58	B3	2	Total 2	O 2	0	0
58	B4	2	Total 2	O 2	0	0
58	CA	192	Total 192	O 192	0	0
58	CL	1	Total 1	O 1	0	0
58	CN	3	Total 3	O 3	0	0
58	CT	1	Total 1	O 1	0	0
58	CU	1	Total 1	O 1	0	0
58	DA	608	Total 608	O 608	0	0
58	DB	13	Total 13	O 13	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
58	DC	11	Total 11	O 11	0	0
58	DD	4	Total 4	O 4	0	0
58	DE	5	Total 5	O 5	0	0
58	DJ	1	Total 1	O 1	0	0
58	DL	4	Total 4	O 4	0	0
58	DN	2	Total 2	O 2	0	0
58	DT	1	Total 1	O 1	0	0
58	DU	1	Total 1	O 1	0	0
58	DV	1	Total 1	O 1	0	0
58	D0	1	Total 1	O 1	0	0
58	D2	1	Total 1	O 1	0	0
58	D3	2	Total 2	O 2	0	0
58	D4	1	Total 1	O 1	0	0

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

3 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	211.97Å 434.65Å 623.91Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	69.36 – 2.80 69.36 – 2.80	Depositor EDS
% Data completeness (in resolution range)	89.2 (69.36-2.80) 89.2 (69.36-2.80)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.37 (at 2.81Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.1_1168)	Depositor
R, R_{free}	0.215 , 0.260 0.220 , 0.264	Depositor DCC
R_{free} test set	5006 reflections (0.40%)	wwPDB-VP
Wilson B-factor (Å ²)	51.2	Xtriage
Anisotropy	0.182	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 48.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	288396	wwPDB-VP
Average B, all atoms (Å ²)	60.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.01% 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](#)

10 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	$\# Z > 2$
54	MHW	B6	1	54	9,9,10	3.61	4 (44%)	10,11,13	2.83	6 (60%)
54	004	B6	7	54	9,10,11	4.39	7 (77%)	9,12,14	1.38	1 (11%)
54	04X	D6	6	54	14,16,17	1.19	1 (7%)	11,20,22	4.89	7 (63%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
54	04X	B6	6	54	14,16,17	1.48	1 (7%)	11,20,22	4.75	6 (54%)
54	MHU	D6	5	54	14,15,16	2.99	7 (50%)	18,19,21	2.56	2 (11%)
54	DBB	D6	3	54	4,5,6	0.67	0	1,5,7	1.85	0
54	MHU	B6	5	54	14,15,16	3.05	8 (57%)	18,19,21	2.92	5 (27%)
54	004	D6	7	54	9,10,11	3.71	7 (77%)	9,12,14	1.78	3 (33%)
54	MHW	D6	1	54	9,9,10	3.58	4 (44%)	10,11,13	2.58	6 (60%)
54	DBB	B6	3	54	4,5,6	0.38	0	1,5,7	1.34	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
54	MHW	B6	1	54	-	0/2/2/4	0/1/1/1
54	004	B6	7	54	-	0/4/6/8	0/1/1/1
54	04X	D6	6	54	-	3/5/24/26	0/2/2/2
54	04X	B6	6	54	-	2/5/24/26	0/2/2/2
54	MHU	D6	5	54	-	2/9/12/14	0/1/1/1
54	DBB	D6	3	54	-	1/3/4/6	-
54	MHU	B6	5	54	-	0/9/12/14	0/1/1/1
54	004	D6	7	54	-	1/4/6/8	0/1/1/1
54	MHW	D6	1	54	-	0/2/2/4	0/1/1/1
54	DBB	B6	3	54	-	0/3/4/6	-

The worst 5 of 39 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
54	B6	7	004	CB-CA	-9.04	1.43	1.52
54	B6	1	MHW	CA-N	-7.11	1.27	1.35
54	D6	1	MHW	CA-N	-6.91	1.27	1.35
54	B6	5	MHU	CE1-CD1	6.48	1.49	1.38
54	D6	5	MHU	CE1-CD1	6.35	1.49	1.38

The worst 5 of 36 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	D6	6	04X	C0-N1-C1	13.70	132.45	111.14
54	B6	6	04X	C0-N1-C1	13.26	131.77	111.14
54	B6	5	MHU	CB-CA-N	8.24	122.61	110.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	D6	5	MHU	CB-CA-N	8.00	122.26	110.48
54	B6	5	MHU	O-C-CA	-7.21	106.23	124.77

There are no chirality outliers.

5 of 9 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
54	D6	3	DBB	O-C-CA-CB
54	B6	6	04X	CD-C0-N1-C1
54	D6	6	04X	CD-C0-N1-C1
54	D6	6	04X	N1-C0-CD-CG
54	D6	5	MHU	CA-CB-CG-CD2

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 502 ligands modelled in this entry, 500 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
56	VIF	DA	3001	-	35,40,40	2.38	14 (40%)	43,55,55	2.32	13 (30%)
56	VIF	BA	3001	-	35,40,40	2.37	15 (42%)	43,55,55	2.16	14 (32%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns.

'-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
56	VIF	DA	3001	-	-	5/42/58/58	0/2/3/3
56	VIF	BA	3001	-	-	3/42/58/58	0/2/3/3

The worst 5 of 29 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
56	BA	3001	VIF	O01-C06	-4.81	1.37	1.44
56	DA	3001	VIF	O04-C22	-4.66	1.35	1.43
56	DA	3001	VIF	O01-C06	-4.56	1.38	1.44
56	BA	3001	VIF	O01-C08	-4.50	1.24	1.34
56	DA	3001	VIF	O01-C08	-4.43	1.24	1.34

The worst 5 of 27 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
56	BA	3001	VIF	C02-C01-C03	-6.79	106.72	122.67
56	DA	3001	VIF	C02-C01-C03	-6.36	107.71	122.67
56	DA	3001	VIF	C14-C07-C04	-6.23	105.13	113.89
56	DA	3001	VIF	C18-C10-C20	-6.01	116.82	125.89
56	BA	3001	VIF	O01-C08-C09	4.61	120.38	110.80

There are no chirality outliers.

5 of 8 torsion outliers are listed below:

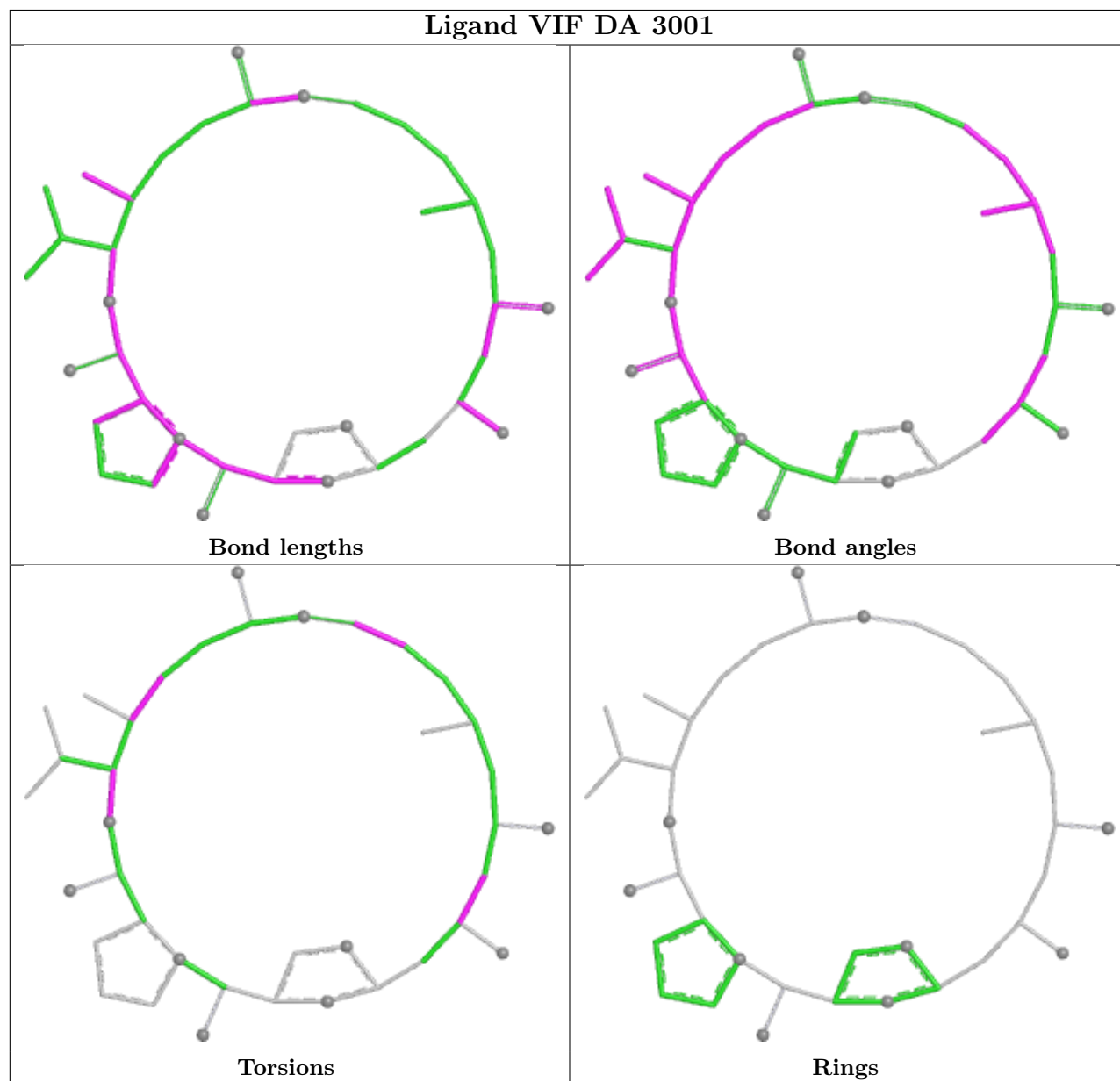
Mol	Chain	Res	Type	Atoms
56	DA	3001	VIF	F-C07-C14-C22
56	BA	3001	VIF	C02-C01-C03-O
56	BA	3001	VIF	C02-C01-C03-N02
56	DA	3001	VIF	C05-C06-O01-C08
56	DA	3001	VIF	C-C06-O01-C08

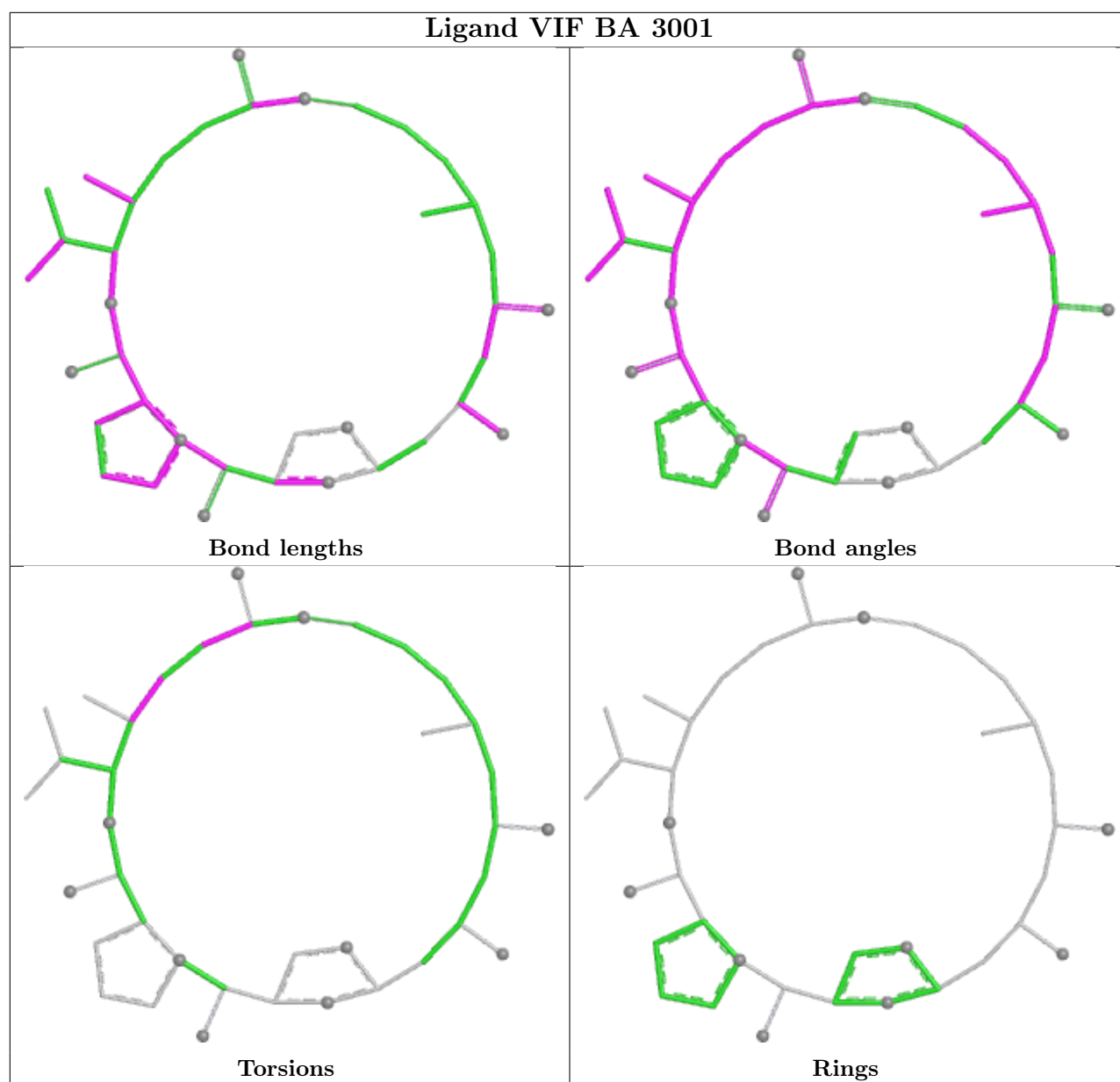
There are no ring outliers.

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 [i](#)

There are no such residues in this entry.

4.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

5 Fit of model and data ⓘ

5.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	AA	1538/1539 (99%)	-0.14	32 (2%) 63 55	13, 50, 135, 180	0
1	CA	1539/1539 (100%)	0.36	67 (4%) 39 32	27, 70, 145, 177	0
2	AB	218/218 (100%)	0.51	12 (5%) 32 25	38, 73, 99, 121	0
2	CB	218/218 (100%)	0.92	25 (11%) 11 9	61, 87, 107, 125	0
3	AC	206/206 (100%)	-0.03	5 (2%) 59 51	33, 57, 78, 93	0
3	CC	206/206 (100%)	0.54	10 (4%) 36 28	48, 78, 95, 105	0
4	AD	205/205 (100%)	0.20	9 (4%) 39 32	32, 55, 79, 105	0
4	CD	205/205 (100%)	-0.03	10 (4%) 36 28	18, 38, 64, 88	0
5	AE	150/150 (100%)	0.08	5 (3%) 49 41	30, 48, 79, 102	0
5	CE	150/150 (100%)	0.35	8 (5%) 33 26	32, 56, 82, 104	0
6	AF	100/100 (100%)	0.10	2 (2%) 64 56	34, 58, 73, 86	0
6	CF	100/100 (100%)	0.43	6 (6%) 29 22	44, 74, 93, 105	0
7	AG	151/151 (100%)	0.34	7 (4%) 38 30	54, 77, 96, 102	0
7	CG	151/151 (100%)	1.57	42 (27%) 2 2	81, 100, 109, 114	0
8	AH	129/129 (100%)	-0.13	2 (1%) 70 63	27, 48, 66, 76	0
8	CH	129/129 (100%)	0.27	4 (3%) 51 43	49, 65, 80, 90	0
9	AI	127/127 (100%)	0.75	14 (11%) 12 9	43, 73, 96, 109	0
9	CI	127/127 (100%)	1.27	23 (18%) 4 4	71, 93, 110, 122	0
10	AJ	98/98 (100%)	0.73	10 (10%) 13 10	40, 64, 92, 122	0
10	CJ	98/98 (100%)	1.38	25 (25%) 2 2	72, 93, 111, 125	0
11	AK	117/117 (100%)	0.37	4 (3%) 48 40	27, 65, 91, 115	0
11	CK	117/117 (100%)	0.07	3 (2%) 57 49	39, 66, 79, 93	0
12	AL	123/123 (100%)	-0.03	6 (4%) 36 28	18, 35, 64, 96	0
12	CL	123/123 (100%)	0.45	8 (6%) 26 20	38, 52, 78, 98	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	AM	114/114 (100%)	0.23	3 (2%) 57 49	45, 68, 92, 102	0
13	CM	114/114 (100%)	1.95	54 (47%) 0 1	96, 108, 116, 119	0
14	AN	96/100 (96%)	0.70	12 (12%) 9 8	37, 58, 94, 103	0
14	CN	96/100 (96%)	1.36	25 (26%) 2 2	69, 94, 111, 120	0
15	AO	88/88 (100%)	0.18	2 (2%) 61 52	28, 51, 65, 90	0
15	CO	88/88 (100%)	0.13	1 (1%) 77 71	40, 62, 80, 98	0
16	AP	82/82 (100%)	0.33	7 (8%) 18 14	31, 47, 85, 101	0
16	CP	82/82 (100%)	0.64	3 (3%) 45 37	44, 61, 87, 105	0
17	AQ	80/80 (100%)	0.36	4 (5%) 35 28	27, 49, 77, 122	0
17	CQ	80/80 (100%)	0.93	9 (11%) 11 9	44, 75, 97, 102	0
18	AR	55/55 (100%)	-0.06	1 (1%) 67 60	39, 52, 78, 108	0
18	CR	55/55 (100%)	0.23	3 (5%) 32 25	42, 55, 79, 111	0
19	AS	79/79 (100%)	0.54	7 (8%) 17 13	52, 68, 89, 102	0
19	CS	79/79 (100%)	2.10	41 (51%) 0 0	89, 108, 118, 124	0
20	AT	85/85 (100%)	0.22	5 (5%) 29 22	34, 48, 70, 103	0
20	CT	85/85 (100%)	0.99	11 (12%) 9 7	55, 73, 91, 97	0
21	AU	51/51 (100%)	1.51	14 (27%) 2 2	48, 74, 95, 106	0
21	CU	51/51 (100%)	1.28	12 (23%) 2 3	45, 71, 96, 105	0
22	BA	2897/2903 (99%)	-0.60	131 (4%) 39 31	0, 13, 130, 195	0
22	DA	2897/2903 (99%)	0.76	160 (5%) 32 25	40, 82, 145, 181	0
23	BB	119/119 (100%)	-0.80	1 (0%) 82 77	2, 23, 49, 85	0
23	DB	118/119 (99%)	0.77	3 (2%) 58 49	66, 112, 133, 143	0
24	BC	271/271 (100%)	-0.56	3 (1%) 77 71	3, 19, 36, 51	0
24	DC	271/271 (100%)	0.71	28 (10%) 13 10	43, 61, 77, 89	0
25	BD	209/209 (100%)	-0.85	0 100 100	0, 10, 34, 68	0
25	DD	209/209 (100%)	0.91	28 (13%) 8 7	49, 68, 83, 96	0
26	BE	201/201 (100%)	-0.60	1 (0%) 87 83	1, 23, 54, 90	0
26	DE	201/201 (100%)	1.36	43 (21%) 3 3	42, 84, 100, 108	0
27	BF	177/177 (100%)	-0.16	1 (0%) 85 81	20, 41, 78, 90	0
27	DF	177/177 (100%)	1.21	24 (13%) 8 7	90, 107, 119, 125	0
28	BG	176/176 (100%)	-0.37	1 (0%) 85 81	17, 37, 62, 84	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
28	DG	176/176 (100%)	1.11	27 (15%) 6 5	72, 93, 105, 114	0
29	BH	149/149 (100%)	2.32	81 (54%) 0 0	25, 102, 121, 129	0
29	DH	149/149 (100%)	1.41	34 (22%) 2 3	25, 92, 107, 115	0
30	BI	141/141 (100%)	1.89	61 (43%) 1 1	90, 111, 122, 133	0
30	DI	141/141 (100%)	2.56	82 (58%) 0 0	101, 117, 127, 130	0
31	BJ	142/142 (100%)	-0.84	0 100 100	1, 6, 22, 36	0
31	DJ	142/142 (100%)	0.70	20 (14%) 7 6	50, 66, 79, 96	0
32	BK	122/122 (100%)	-0.75	2 (1%) 70 63	4, 12, 32, 67	0
32	DK	122/122 (100%)	0.53	10 (8%) 19 14	46, 63, 82, 97	0
33	BL	143/143 (100%)	-0.49	1 (0%) 84 79	1, 18, 43, 74	0
33	DL	143/143 (100%)	1.33	32 (22%) 3 3	46, 79, 94, 113	0
34	BM	136/136 (100%)	-0.81	1 (0%) 84 79	1, 9, 29, 84	0
34	DM	136/136 (100%)	0.53	6 (4%) 39 32	45, 69, 82, 101	0
35	BN	120/120 (100%)	-0.86	0 100 100	2, 7, 16, 52	0
35	DN	120/120 (100%)	1.28	19 (15%) 6 5	56, 75, 88, 114	0
36	BO	116/116 (100%)	-0.53	0 100 100	13, 24, 42, 50	0
36	DO	116/116 (100%)	0.92	12 (10%) 13 10	80, 94, 105, 114	0
37	BP	114/114 (100%)	-0.66	0 100 100	6, 18, 42, 64	0
37	DP	114/114 (100%)	0.68	4 (3%) 47 39	57, 69, 86, 91	0
38	BQ	117/117 (100%)	-0.84	0 100 100	1, 4, 13, 31	0
38	DQ	117/117 (100%)	0.94	19 (16%) 5 5	52, 67, 78, 82	0
39	BR	103/103 (100%)	-0.63	1 (0%) 79 73	0, 11, 33, 66	0
39	DR	103/103 (100%)	1.00	12 (11%) 10 9	51, 77, 88, 99	0
40	BS	110/110 (100%)	-0.82	1 (0%) 81 75	1, 4, 21, 80	0
40	DS	110/110 (100%)	1.21	23 (20%) 3 3	57, 74, 89, 100	0
41	BT	93/93 (100%)	-0.30	6 (6%) 26 20	8, 26, 75, 103	0
41	DT	93/93 (100%)	1.82	37 (39%) 1 1	66, 85, 103, 117	0
42	BU	102/102 (100%)	-0.45	0 100 100	12, 28, 63, 92	0
42	DU	102/102 (100%)	1.99	44 (43%) 1 1	75, 90, 109, 118	0
43	BV	94/94 (100%)	-0.79	0 100 100	5, 19, 41, 53	0
43	DV	94/94 (100%)	0.59	4 (4%) 40 32	69, 84, 95, 104	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
44	BW	76/76 (100%)	-0.68	1 (1%) 74 67	4, 12, 27, 54	0
44	DW	75/76 (98%)	1.05	11 (14%) 7 6	60, 80, 90, 105	0
45	BX	77/77 (100%)	-0.40	1 (1%) 74 67	6, 24, 51, 73	0
45	DX	77/77 (100%)	1.24	16 (20%) 3 3	51, 71, 84, 87	0
46	BY	63/63 (100%)	0.03	3 (4%) 36 29	20, 40, 73, 93	0
46	DY	63/63 (100%)	1.42	15 (23%) 2 3	78, 94, 100, 105	0
47	BZ	58/58 (100%)	-0.77	0 100 100	2, 6, 23, 42	0
47	DZ	58/58 (100%)	0.84	6 (10%) 13 10	58, 71, 81, 94	0
48	B0	56/56 (100%)	-0.78	0 100 100	0, 9, 36, 68	0
48	D0	56/56 (100%)	1.13	9 (16%) 5 5	56, 78, 92, 102	0
49	B1	50/50 (100%)	-0.50	1 (2%) 64 56	17, 29, 49, 77	0
49	D1	50/50 (100%)	1.19	9 (18%) 4 4	69, 84, 93, 103	0
50	B2	46/46 (100%)	-0.69	1 (2%) 62 53	3, 9, 16, 88	0
50	D2	46/46 (100%)	1.50	13 (28%) 1 2	56, 68, 79, 102	0
51	B3	64/64 (100%)	-0.77	0 100 100	4, 9, 16, 31	0
51	D3	64/64 (100%)	1.56	20 (31%) 1 1	57, 71, 80, 81	0
52	B4	38/38 (100%)	-0.69	0 100 100	8, 16, 35, 52	0
52	D4	38/38 (100%)	1.39	9 (23%) 2 3	58, 75, 87, 101	0
53	B5	191/228 (83%)	2.16	95 (49%) 0 1	99, 115, 127, 135	0
54	B6	2/7 (28%)	-0.92	0 100 100	1, 1, 1, 1	0
54	D6	2/7 (28%)	0.91	1 (50%) 0 1	47, 47, 47, 57	0
All	All	20738/20808 (99%)	0.31	1727 (8%) 19 14	0, 62, 120, 195	0

The worst 5 of 1727 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
30	BI	53	LEU	11.3
29	BH	146	VAL	8.8
42	DU	58	ILE	8.6
9	CI	128	SER	8.4
30	DI	10	LYS	7.4

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($\text{\AA}^2$)	Q<0.9
54	MHU	D6	5	15/16	0.83	0.20	45,56,65,65	0
54	04X	D6	6	15/16	0.83	0.15	46,56,70,73	0
54	004	D6	7	10/11	0.86	0.12	40,51,56,56	0
54	DBB	D6	3	6/7	0.89	0.20	45,52,56,63	0
54	MHW	D6	1	9/10	0.90	0.12	36,47,54,54	0
54	04X	B6	6	15/16	0.95	0.09	1,3,15,15	0
54	004	B6	7	10/11	0.96	0.09	0,0,1,2	0
54	MHU	B6	5	15/16	0.96	0.09	0,1,3,6	0
54	DBB	B6	3	6/7	0.97	0.08	0,1,1,4	0
54	MHW	B6	1	9/10	0.97	0.06	0,1,2,9	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($\text{\AA}^2$)	Q<0.9
55	MG	DA	3027	1/1	-0.34	0.47	96,96,96,96	0
55	MG	BA	3137	1/1	0.13	0.53	66,66,66,66	0
55	MG	DA	3134	1/1	0.15	0.37	100,100,100,100	0
55	MG	DA	3127	1/1	0.25	0.15	86,86,86,86	0
55	MG	BA	3016	1/1	0.48	0.34	59,59,59,59	0
55	MG	DA	3114	1/1	0.48	0.15	80,80,80,80	0
55	MG	CA	1649	1/1	0.59	0.33	71,71,71,71	0
55	MG	DA	3103	1/1	0.60	0.16	83,83,83,83	0
55	MG	DA	3042	1/1	0.60	0.22	68,68,68,68	0
55	MG	BA	3062	1/1	0.65	0.32	57,57,57,57	0
55	MG	DA	3101	1/1	0.65	0.21	78,78,78,78	0
55	MG	DA	3132	1/1	0.66	0.26	89,89,89,89	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	CA	1630	1/1	0.66	0.17	105,105,105,105	0
55	MG	DA	3154	1/1	0.66	0.33	70,70,70,70	0
55	MG	DA	3116	1/1	0.67	0.17	96,96,96,96	0
55	MG	DA	3041	1/1	0.70	0.14	92,92,92,92	0
55	MG	DA	3113	1/1	0.70	0.35	77,77,77,77	0
55	MG	DA	3063	1/1	0.71	0.24	93,93,93,93	0
55	MG	DA	3062	1/1	0.73	0.59	104,104,104,104	0
55	MG	AA	1668	1/1	0.74	0.21	58,58,58,58	0
55	MG	DA	3120	1/1	0.74	0.24	97,97,97,97	0
55	MG	DA	3057	1/1	0.75	0.22	88,88,88,88	0
55	MG	AA	1658	1/1	0.76	0.18	72,72,72,72	0
55	MG	DA	3110	1/1	0.76	0.18	48,48,48,48	0
55	MG	DA	3094	1/1	0.77	0.12	93,93,93,93	0
55	MG	DA	3033	1/1	0.78	0.17	71,71,71,71	0
55	MG	DA	3014	1/1	0.78	0.15	80,80,80,80	0
55	MG	DA	3028	1/1	0.78	0.11	83,83,83,83	0
55	MG	BA	3099	1/1	0.79	0.22	64,64,64,64	0
55	MG	DA	3121	1/1	0.79	0.21	78,78,78,78	0
55	MG	DA	3061	1/1	0.80	0.21	80,80,80,80	0
55	MG	BA	3041	1/1	0.80	0.33	2,2,2,2	0
55	MG	CA	1636	1/1	0.80	0.15	113,113,113,113	0
55	MG	DA	3074	1/1	0.80	0.17	68,68,68,68	0
55	MG	DA	3093	1/1	0.80	0.20	101,101,101,101	0
55	MG	DA	3138	1/1	0.80	0.25	52,52,52,52	0
55	MG	DA	3020	1/1	0.80	0.15	83,83,83,83	0
55	MG	CA	1635	1/1	0.81	0.10	120,120,120,120	0
55	MG	DA	3036	1/1	0.81	0.11	70,70,70,70	0
55	MG	DA	3007	1/1	0.81	0.13	101,101,101,101	0
55	MG	CA	1646	1/1	0.81	0.21	65,65,65,65	0
55	MG	DA	3045	1/1	0.81	0.14	95,95,95,95	0
55	MG	AA	1665	1/1	0.82	0.09	48,48,48,48	0
55	MG	DA	3136	1/1	0.82	0.17	84,84,84,84	0
55	MG	BA	3058	1/1	0.82	0.32	45,45,45,45	0
55	MG	DA	3149	1/1	0.82	0.22	54,54,54,54	0
55	MG	CA	1656	1/1	0.82	0.15	53,53,53,53	0
55	MG	DA	3100	1/1	0.83	0.18	81,81,81,81	0
55	MG	CA	1643	1/1	0.83	0.28	56,56,56,56	0
55	MG	CA	1633	1/1	0.83	0.16	78,78,78,78	0
55	MG	CA	1641	1/1	0.83	0.24	67,67,67,67	0
55	MG	DA	3163	1/1	0.83	0.07	71,71,71,71	0
55	MG	DA	3166	1/1	0.83	0.20	57,57,57,57	0
55	MG	AA	1659	1/1	0.84	0.10	61,61,61,61	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	AA	1660	1/1	0.84	0.38	70,70,70,70	0
55	MG	DA	3148	1/1	0.84	0.15	58,58,58,58	0
55	MG	DA	3108	1/1	0.84	0.11	72,72,72,72	0
55	MG	DA	3150	1/1	0.84	0.21	61,61,61,61	0
55	MG	AA	1649	1/1	0.84	0.09	46,46,46,46	0
55	MG	DA	3095	1/1	0.84	0.09	80,80,80,80	0
55	MG	BA	3134	1/1	0.84	0.28	47,47,47,47	0
55	MG	DA	3139	1/1	0.85	0.26	49,49,49,49	0
55	MG	DA	3146	1/1	0.85	0.15	84,84,84,84	0
55	MG	BA	3048	1/1	0.85	0.12	53,53,53,53	0
55	MG	CA	1645	1/1	0.85	0.12	40,40,40,40	0
55	MG	BA	3084	1/1	0.85	0.19	49,49,49,49	0
55	MG	CA	1625	1/1	0.85	0.10	43,43,43,43	0
55	MG	DA	3072	1/1	0.85	0.12	80,80,80,80	0
55	MG	BA	3037	1/1	0.85	0.22	35,35,35,35	0
55	MG	BA	3088	1/1	0.86	0.21	37,37,37,37	0
55	MG	DA	3025	1/1	0.86	0.21	56,56,56,56	0
55	MG	DA	3009	1/1	0.86	0.19	81,81,81,81	0
55	MG	DA	3157	1/1	0.86	0.27	63,63,63,63	0
55	MG	DA	3076	1/1	0.86	0.12	70,70,70,70	0
55	MG	CA	1628	1/1	0.86	0.14	98,98,98,98	0
55	MG	BA	3083	1/1	0.87	0.15	20,20,20,20	0
55	MG	CA	1647	1/1	0.87	0.08	45,45,45,45	0
55	MG	CA	1605	1/1	0.87	0.10	88,88,88,88	0
55	MG	DA	3147	1/1	0.87	0.09	60,60,60,60	0
55	MG	DA	3073	1/1	0.87	0.16	72,72,72,72	0
55	MG	DA	3124	1/1	0.87	0.09	51,51,51,51	0
55	MG	DA	3125	1/1	0.87	0.13	92,92,92,92	0
55	MG	DA	3049	1/1	0.87	0.09	109,109,109,109	0
55	MG	DA	3016	1/1	0.87	0.21	78,78,78,78	0
55	MG	DA	3079	1/1	0.87	0.10	92,92,92,92	0
55	MG	CA	1638	1/1	0.87	0.09	84,84,84,84	0
55	MG	DA	3145	1/1	0.88	0.18	67,67,67,67	0
55	MG	BA	3081	1/1	0.88	0.08	16,16,16,16	0
55	MG	DA	3109	1/1	0.88	0.13	50,50,50,50	0
55	MG	BA	3147	1/1	0.88	0.20	39,39,39,39	0
55	MG	BA	3159	1/1	0.88	0.14	21,21,21,21	0
55	MG	BA	3173	1/1	0.88	0.10	32,32,32,32	0
55	MG	DA	3153	1/1	0.88	0.25	62,62,62,62	0
55	MG	BA	3193	1/1	0.88	0.13	42,42,42,42	0
55	MG	AA	1655	1/1	0.88	0.24	45,45,45,45	0
55	MG	AA	1670	1/1	0.88	0.14	56,56,56,56	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	DA	3144	1/1	0.88	0.15	30,30,30,30	0
55	MG	CA	1614	1/1	0.89	0.08	49,49,49,49	0
55	MG	AA	1653	1/1	0.89	0.24	51,51,51,51	0
55	MG	BA	3056	1/1	0.89	0.13	29,29,29,29	0
55	MG	DA	3047	1/1	0.89	0.09	80,80,80,80	0
55	MG	DA	3005	1/1	0.89	0.18	94,94,94,94	0
55	MG	BA	3191	1/1	0.89	0.23	20,20,20,20	0
55	MG	DA	3030	1/1	0.89	0.14	72,72,72,72	0
55	MG	AA	1647	1/1	0.89	0.15	58,58,58,58	0
55	MG	DA	3117	1/1	0.89	0.19	73,73,73,73	0
55	MG	DA	3141	1/1	0.89	0.22	41,41,41,41	0
55	MG	BA	3003	1/1	0.89	0.09	23,23,23,23	0
55	MG	DA	3126	1/1	0.90	0.09	59,59,59,59	0
55	MG	AA	1644	1/1	0.90	0.17	58,58,58,58	0
55	MG	DA	3058	1/1	0.90	0.13	73,73,73,73	0
55	MG	BA	3136	1/1	0.90	0.13	34,34,34,34	0
55	MG	AA	1662	1/1	0.90	0.11	47,47,47,47	0
55	MG	AA	1645	1/1	0.90	0.08	53,53,53,53	0
55	MG	CA	1655	1/1	0.90	0.15	51,51,51,51	0
55	MG	CA	1642	1/1	0.90	0.26	29,29,29,29	0
55	MG	DA	3161	1/1	0.90	0.13	49,49,49,49	0
55	MG	DA	3003	1/1	0.90	0.19	92,92,92,92	0
55	MG	BA	3154	1/1	0.90	0.12	34,34,34,34	0
55	MG	DA	3082	1/1	0.91	0.08	66,66,66,66	0
55	MG	DA	3143	1/1	0.91	0.12	39,39,39,39	0
55	MG	AA	1635	1/1	0.91	0.13	65,65,65,65	0
55	MG	AA	1652	1/1	0.91	0.35	56,56,56,56	0
55	MG	DA	3059	1/1	0.91	0.21	70,70,70,70	0
55	MG	BA	3174	1/1	0.91	0.07	27,27,27,27	0
55	MG	CA	1631	1/1	0.91	0.10	92,92,92,92	0
55	MG	BA	3089	1/1	0.91	0.11	22,22,22,22	0
55	MG	DA	3107	1/1	0.91	0.08	48,48,48,48	0
55	MG	DA	3011	1/1	0.91	0.11	60,60,60,60	0
55	MG	AA	1632	1/1	0.91	0.09	54,54,54,54	0
55	MG	BA	3148	1/1	0.91	0.09	24,24,24,24	0
55	MG	DA	3158	1/1	0.91	0.16	49,49,49,49	0
55	MG	CA	1654	1/1	0.91	0.06	58,58,58,58	0
55	MG	BA	3132	1/1	0.91	0.21	50,50,50,50	0
55	MG	DA	3165	1/1	0.91	0.09	68,68,68,68	0
55	MG	DA	3140	1/1	0.91	0.17	28,28,28,28	0
55	MG	BA	3060	1/1	0.92	0.12	9,9,9,9	0
55	MG	CA	1652	1/1	0.92	0.07	62,62,62,62	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	DA	3050	1/1	0.92	0.10	83,83,83,83	0
55	MG	DA	3089	1/1	0.92	0.06	78,78,78,78	0
55	MG	DA	3092	1/1	0.92	0.07	77,77,77,77	0
55	MG	DA	3055	1/1	0.92	0.12	41,41,41,41	0
55	MG	BA	3047	1/1	0.92	0.07	9,9,9,9	0
55	MG	BA	3079	1/1	0.92	0.06	37,37,37,37	0
55	MG	BA	3149	1/1	0.92	0.14	27,27,27,27	0
55	MG	CA	1615	1/1	0.92	0.11	55,55,55,55	0
55	MG	DA	3156	1/1	0.92	0.18	42,42,42,42	0
55	MG	BA	3102	1/1	0.92	0.08	10,10,10,10	0
55	MG	AA	1672	1/1	0.92	0.28	49,49,49,49	0
55	MG	DA	3070	1/1	0.92	0.15	86,86,86,86	0
55	MG	CA	1629	1/1	0.92	0.07	80,80,80,80	0
55	MG	AA	1666	1/1	0.92	0.21	41,41,41,41	0
55	MG	BA	3005	1/1	0.92	0.09	42,42,42,42	0
55	MG	DA	3167	1/1	0.92	0.27	43,43,43,43	0
55	MG	AA	1650	1/1	0.93	0.08	37,37,37,37	0
55	MG	BA	3015	1/1	0.93	0.08	6,6,6,6	0
55	MG	CA	1601	1/1	0.93	0.07	45,45,45,45	0
55	MG	DA	3133	1/1	0.93	0.19	53,53,53,53	0
55	MG	AA	1663	1/1	0.93	0.07	41,41,41,41	0
55	MG	DA	3087	1/1	0.93	0.07	69,69,69,69	0
55	MG	CA	1606	1/1	0.93	0.09	70,70,70,70	0
55	MG	DA	3090	1/1	0.93	0.09	80,80,80,80	0
55	MG	BA	3026	1/1	0.93	0.15	36,36,36,36	0
55	MG	CA	1651	1/1	0.93	0.07	50,50,50,50	0
55	MG	BA	3061	1/1	0.93	0.20	28,28,28,28	0
55	MG	DA	3043	1/1	0.93	0.09	82,82,82,82	0
55	MG	CA	1617	1/1	0.93	0.08	40,40,40,40	0
55	MG	BA	3151	1/1	0.93	0.14	49,49,49,49	0
55	MG	BA	3153	1/1	0.93	0.13	11,11,11,11	0
55	MG	DA	3104	1/1	0.93	0.13	67,67,67,67	0
55	MG	AA	1609	1/1	0.93	0.07	35,35,35,35	0
55	MG	BA	3157	1/1	0.93	0.20	27,27,27,27	0
55	MG	DA	3151	1/1	0.93	0.31	49,49,49,49	0
55	MG	DA	3006	1/1	0.93	0.06	98,98,98,98	0
55	MG	BA	3158	1/1	0.93	0.10	15,15,15,15	0
55	MG	DA	3008	1/1	0.93	0.16	100,100,100,100	0
55	MG	BA	3103	1/1	0.93	0.16	13,13,13,13	0
55	MG	BA	3002	1/1	0.93	0.09	15,15,15,15	0
55	MG	DA	3159	1/1	0.93	0.17	61,61,61,61	0
55	MG	AA	1657	1/1	0.93	0.10	46,46,46,46	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	BA	3187	1/1	0.93	0.12	25,25,25,25	0
55	MG	DA	3071	1/1	0.93	0.05	96,96,96,96	0
55	MG	DA	3017	1/1	0.93	0.09	84,84,84,84	0
55	MG	BA	3190	1/1	0.93	0.17	39,39,39,39	0
56	VIF	DA	3001	38/38	0.93	0.13	34,47,57,61	0
55	MG	BA	3035	1/1	0.94	0.19	47,47,47,47	0
55	MG	AA	1654	1/1	0.94	0.14	30,30,30,30	0
55	MG	DA	3065	1/1	0.94	0.11	43,43,43,43	0
55	MG	DA	3142	1/1	0.94	0.20	40,40,40,40	0
55	MG	DA	3029	1/1	0.94	0.11	65,65,65,65	0
55	MG	BA	3072	1/1	0.94	0.12	23,23,23,23	0
55	MG	AA	1614	1/1	0.94	0.16	55,55,55,55	0
55	MG	AA	1661	1/1	0.94	0.11	53,53,53,53	0
55	MG	DA	3111	1/1	0.94	0.07	43,43,43,43	0
55	MG	DA	3112	1/1	0.94	0.08	70,70,70,70	0
55	MG	AA	1669	1/1	0.94	0.14	51,51,51,51	0
55	MG	AA	1616	1/1	0.94	0.07	50,50,50,50	0
55	MG	BA	3138	1/1	0.94	0.20	4,4,4,4	0
55	MG	DA	3080	1/1	0.94	0.05	101,101,101,101	0
55	MG	BA	3184	1/1	0.94	0.09	10,10,10,10	0
55	MG	DA	3155	1/1	0.94	0.14	45,45,45,45	0
55	MG	DA	3012	1/1	0.94	0.17	74,74,74,74	0
55	MG	CA	1648	1/1	0.94	0.18	30,30,30,30	0
55	MG	AA	1630	1/1	0.94	0.14	63,63,63,63	0
55	MG	BA	3189	1/1	0.94	0.11	44,44,44,44	0
55	MG	DA	3160	1/1	0.94	0.10	74,74,74,74	0
55	MG	DA	3019	1/1	0.94	0.09	85,85,85,85	0
55	MG	BA	3028	1/1	0.94	0.15	15,15,15,15	0
55	MG	BA	3091	1/1	0.94	0.04	23,23,23,23	0
55	MG	DA	3098	1/1	0.94	0.10	73,73,73,73	0
55	MG	DA	3099	1/1	0.94	0.10	50,50,50,50	0
55	MG	DA	3168	1/1	0.94	0.11	47,47,47,47	0
55	MG	D2	101	1/1	0.94	0.08	77,77,77,77	0
55	MG	DA	3026	1/1	0.94	0.12	67,67,67,67	0
55	MG	AA	1627	1/1	0.95	0.11	58,58,58,58	0
55	MG	BA	3020	1/1	0.95	0.07	8,8,8,8	0
55	MG	AA	1651	1/1	0.95	0.20	40,40,40,40	0
55	MG	DA	3128	1/1	0.95	0.07	71,71,71,71	0
55	MG	DA	3078	1/1	0.95	0.11	83,83,83,83	0
55	MG	CA	1644	1/1	0.95	0.06	55,55,55,55	0
55	MG	BA	3150	1/1	0.95	0.14	45,45,45,45	0
55	MG	DA	3081	1/1	0.95	0.10	84,84,84,84	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	DA	3137	1/1	0.95	0.11	88,88,88,88	0
55	MG	BA	3074	1/1	0.95	0.06	14,14,14,14	0
55	MG	DA	3084	1/1	0.95	0.12	72,72,72,72	0
55	MG	DA	3085	1/1	0.95	0.06	78,78,78,78	0
55	MG	BA	3075	1/1	0.95	0.11	29,29,29,29	0
55	MG	BA	3112	1/1	0.95	0.07	8,8,8,8	0
55	MG	CA	1608	1/1	0.95	0.10	63,63,63,63	0
55	MG	CA	1650	1/1	0.95	0.16	44,44,44,44	0
55	MG	CA	1611	1/1	0.95	0.13	82,82,82,82	0
55	MG	BA	3113	1/1	0.95	0.05	13,13,13,13	0
55	MG	BA	3125	1/1	0.95	0.17	20,20,20,20	0
55	MG	BA	3049	1/1	0.95	0.09	13,13,13,13	0
55	MG	DA	3046	1/1	0.95	0.05	77,77,77,77	0
55	MG	CA	1622	1/1	0.95	0.10	51,51,51,51	0
55	MG	DA	3002	1/1	0.95	0.06	65,65,65,65	0
55	MG	BA	3166	1/1	0.95	0.17	36,36,36,36	0
55	MG	DA	3052	1/1	0.95	0.05	49,49,49,49	0
55	MG	DA	3053	1/1	0.95	0.06	45,45,45,45	0
55	MG	DA	3054	1/1	0.95	0.07	41,41,41,41	0
55	MG	CA	1627	1/1	0.95	0.14	76,76,76,76	0
55	MG	BA	3055	1/1	0.95	0.08	6,6,6,6	0
55	MG	AA	1612	1/1	0.95	0.06	37,37,37,37	0
55	MG	BA	3175	1/1	0.95	0.13	33,33,33,33	0
55	MG	BA	3177	1/1	0.95	0.17	29,29,29,29	0
55	MG	DA	3162	1/1	0.95	0.08	35,35,35,35	0
55	MG	DA	3010	1/1	0.95	0.05	68,68,68,68	0
55	MG	DA	3164	1/1	0.95	0.17	57,57,57,57	0
55	MG	DA	3115	1/1	0.95	0.05	51,51,51,51	0
55	MG	BA	3178	1/1	0.95	0.10	13,13,13,13	0
55	MG	AA	1656	1/1	0.95	0.10	36,36,36,36	0
55	MG	BA	3185	1/1	0.95	0.23	25,25,25,25	0
55	MG	CA	1637	1/1	0.95	0.12	64,64,64,64	0
55	MG	AA	1671	1/1	0.95	0.39	47,47,47,47	0
55	MG	BA	3122	1/1	0.96	0.09	39,39,39,39	0
55	MG	DA	3056	1/1	0.96	0.09	66,66,66,66	0
55	MG	CA	1613	1/1	0.96	0.05	24,24,24,24	0
55	MG	AA	1619	1/1	0.96	0.16	37,37,37,37	0
55	MG	BA	3165	1/1	0.96	0.10	5,5,5,5	0
55	MG	AA	1631	1/1	0.96	0.12	48,48,48,48	0
55	MG	CA	1619	1/1	0.96	0.06	40,40,40,40	0
55	MG	CA	1621	1/1	0.96	0.07	71,71,71,71	0
55	MG	DA	3064	1/1	0.96	0.08	48,48,48,48	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	BA	3170	1/1	0.96	0.06	33,33,33,33	0
55	MG	DA	3066	1/1	0.96	0.06	39,39,39,39	0
55	MG	BA	3171	1/1	0.96	0.07	24,24,24,24	0
55	MG	AA	1626	1/1	0.96	0.06	19,19,19,19	0
55	MG	AA	1634	1/1	0.96	0.05	42,42,42,42	0
55	MG	AA	1664	1/1	0.96	0.07	42,42,42,42	0
55	MG	BA	3176	1/1	0.96	0.09	13,13,13,13	0
55	MG	DA	3075	1/1	0.96	0.07	63,63,63,63	0
55	MG	AA	1617	1/1	0.96	0.08	51,51,51,51	0
55	MG	DA	3077	1/1	0.96	0.07	65,65,65,65	0
55	MG	BA	3141	1/1	0.96	0.14	26,26,26,26	0
55	MG	BA	3180	1/1	0.96	0.22	40,40,40,40	0
55	MG	BA	3182	1/1	0.96	0.09	20,20,20,20	0
55	MG	BA	3183	1/1	0.96	0.14	24,24,24,24	0
55	MG	BA	3142	1/1	0.96	0.24	5,5,5,5	0
55	MG	CA	1639	1/1	0.96	0.05	49,49,49,49	0
55	MG	BA	3145	1/1	0.96	0.09	41,41,41,41	0
55	MG	DA	3086	1/1	0.96	0.09	72,72,72,72	0
55	MG	BA	3186	1/1	0.96	0.08	32,32,32,32	0
55	MG	DA	3032	1/1	0.96	0.05	63,63,63,63	0
55	MG	BA	3146	1/1	0.96	0.11	15,15,15,15	0
55	MG	DA	3091	1/1	0.96	0.09	76,76,76,76	0
55	MG	DA	3034	1/1	0.96	0.06	62,62,62,62	0
55	MG	BA	3100	1/1	0.96	0.07	14,14,14,14	0
55	MG	DA	3038	1/1	0.96	0.05	75,75,75,75	0
55	MG	DA	3040	1/1	0.96	0.07	60,60,60,60	0
55	MG	AA	1637	1/1	0.96	0.05	16,16,16,16	0
55	MG	BA	3006	1/1	0.96	0.06	51,51,51,51	0
55	MG	BA	3192	1/1	0.96	0.08	34,34,34,34	0
55	MG	BA	3105	1/1	0.96	0.13	0,0,0,0	0
55	MG	AA	1667	1/1	0.96	0.11	54,54,54,54	0
55	MG	CA	1604	1/1	0.96	0.05	89,89,89,89	0
55	MG	DA	3105	1/1	0.96	0.06	67,67,67,67	0
55	MG	DA	3106	1/1	0.96	0.12	72,72,72,72	0
55	MG	DA	3048	1/1	0.96	0.09	53,53,53,53	0
55	MG	AA	1638	1/1	0.96	0.05	77,77,77,77	0
55	MG	BA	3115	1/1	0.96	0.06	17,17,17,17	0
55	MG	CA	1653	1/1	0.96	0.11	42,42,42,42	0
55	MG	DB	203	1/1	0.96	0.05	83,83,83,83	0
55	MG	BA	3116	1/1	0.96	0.15	50,50,50,50	0
55	MG	CA	1609	1/1	0.96	0.07	77,77,77,77	0
55	MG	BA	3024	1/1	0.97	0.06	4,4,4,4	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	AA	1643	1/1	0.97	0.15	25,25,25,25	0
55	MG	CA	1624	1/1	0.97	0.05	47,47,47,47	0
55	MG	BA	3077	1/1	0.97	0.12	61,61,61,61	0
55	MG	BA	3181	1/1	0.97	0.11	19,19,19,19	0
55	MG	DA	3119	1/1	0.97	0.08	46,46,46,46	0
55	MG	BA	3078	1/1	0.97	0.04	31,31,31,31	0
55	MG	DA	3015	1/1	0.97	0.06	44,44,44,44	0
55	MG	BA	3111	1/1	0.97	0.07	24,24,24,24	0
55	MG	DA	3068	1/1	0.97	0.04	47,47,47,47	0
55	MG	DA	3069	1/1	0.97	0.05	60,60,60,60	0
55	MG	AA	1624	1/1	0.97	0.05	35,35,35,35	0
55	MG	BA	3080	1/1	0.97	0.07	17,17,17,17	0
55	MG	DA	3129	1/1	0.97	0.09	75,75,75,75	0
55	MG	CA	1632	1/1	0.97	0.08	74,74,74,74	0
55	MG	DA	3021	1/1	0.97	0.04	64,64,64,64	0
55	MG	DA	3022	1/1	0.97	0.07	62,62,62,62	0
55	MG	DA	3135	1/1	0.97	0.07	53,53,53,53	0
55	MG	DA	3023	1/1	0.97	0.09	42,42,42,42	0
55	MG	AA	1603	1/1	0.97	0.14	48,48,48,48	0
55	MG	AA	1610	1/1	0.97	0.11	63,63,63,63	0
55	MG	BA	3117	1/1	0.97	0.06	3,3,3,3	0
55	MG	BA	3119	1/1	0.97	0.05	14,14,14,14	0
55	MG	BA	3120	1/1	0.97	0.19	32,32,32,32	0
55	MG	BA	3121	1/1	0.97	0.06	7,7,7,7	0
55	MG	DA	3031	1/1	0.97	0.06	57,57,57,57	0
55	MG	AA	1636	1/1	0.97	0.08	42,42,42,42	0
55	MG	BA	3194	1/1	0.97	0.08	32,32,32,32	0
55	MG	BB	204	1/1	0.97	0.26	21,21,21,21	0
55	MG	DA	3035	1/1	0.97	0.04	41,41,41,41	0
55	MG	BD	301	1/1	0.97	0.07	27,27,27,27	0
55	MG	DA	3037	1/1	0.97	0.04	54,54,54,54	0
55	MG	BA	3160	1/1	0.97	0.07	29,29,29,29	0
55	MG	DA	3039	1/1	0.97	0.08	63,63,63,63	0
55	MG	CA	1602	1/1	0.97	0.10	69,69,69,69	0
55	MG	BA	3085	1/1	0.97	0.14	16,16,16,16	0
55	MG	BA	3086	1/1	0.97	0.05	5,5,5,5	0
55	MG	DA	3096	1/1	0.97	0.07	75,75,75,75	0
55	MG	BA	3167	1/1	0.97	0.04	21,21,21,21	0
55	MG	CA	1607	1/1	0.97	0.07	47,47,47,47	0
55	MG	BA	3169	1/1	0.97	0.12	34,34,34,34	0
55	MG	BA	3133	1/1	0.97	0.10	37,37,37,37	0
55	MG	DA	3102	1/1	0.97	0.05	58,58,58,58	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	CA	1610	1/1	0.97	0.07	64,64,64,64	0
55	MG	AA	1605	1/1	0.97	0.06	33,33,33,33	0
55	MG	CA	1612	1/1	0.97	0.05	44,44,44,44	0
55	MG	DA	3051	1/1	0.97	0.05	54,54,54,54	0
55	MG	BA	3172	1/1	0.97	0.05	32,32,32,32	0
55	MG	BA	3063	1/1	0.97	0.04	6,6,6,6	0
55	MG	BA	3070	1/1	0.97	0.07	50,50,50,50	0
55	MG	DB	201	1/1	0.97	0.05	97,97,97,97	0
55	MG	AA	1613	1/1	0.97	0.04	30,30,30,30	0
55	MG	CA	1618	1/1	0.97	0.05	45,45,45,45	0
56	VIF	BA	3001	38/38	0.97	0.07	0,2,7,10	0
55	MG	BA	3140	1/1	0.97	0.12	3,3,3,3	0
55	MG	DA	3004	1/1	0.98	0.04	65,65,65,65	0
55	MG	BA	3032	1/1	0.98	0.09	5,5,5,5	0
55	MG	BA	3162	1/1	0.98	0.16	37,37,37,37	0
55	MG	BA	3163	1/1	0.98	0.09	31,31,31,31	0
55	MG	DA	3118	1/1	0.98	0.05	66,66,66,66	0
55	MG	BA	3164	1/1	0.98	0.21	19,19,19,19	0
55	MG	AA	1608	1/1	0.98	0.04	16,16,16,16	0
55	MG	AA	1601	1/1	0.98	0.03	41,41,41,41	0
55	MG	BA	3040	1/1	0.98	0.04	3,3,3,3	0
55	MG	BA	3168	1/1	0.98	0.09	35,35,35,35	0
55	MG	CA	1616	1/1	0.98	0.03	33,33,33,33	0
55	MG	AA	1628	1/1	0.98	0.04	35,35,35,35	0
55	MG	BA	3044	1/1	0.98	0.07	19,19,19,19	0
55	MG	BA	3045	1/1	0.98	0.04	21,21,21,21	0
55	MG	DA	3018	1/1	0.98	0.05	51,51,51,51	0
55	MG	CA	1620	1/1	0.98	0.04	65,65,65,65	0
55	MG	BA	3124	1/1	0.98	0.07	5,5,5,5	0
55	MG	BA	3004	1/1	0.98	0.04	25,25,25,25	0
55	MG	CA	1623	1/1	0.98	0.09	35,35,35,35	0
55	MG	BA	3126	1/1	0.98	0.05	4,4,4,4	0
55	MG	AA	1639	1/1	0.98	0.05	60,60,60,60	0
55	MG	CA	1626	1/1	0.98	0.05	43,43,43,43	0
55	MG	AA	1640	1/1	0.98	0.04	45,45,45,45	0
55	MG	BA	3052	1/1	0.98	0.04	3,3,3,3	0
55	MG	DA	3083	1/1	0.98	0.04	49,49,49,49	0
55	MG	BA	3053	1/1	0.98	0.04	6,6,6,6	0
55	MG	BA	3179	1/1	0.98	0.10	34,34,34,34	0
55	MG	BA	3013	1/1	0.98	0.05	0,0,0,0	0
55	MG	AA	1602	1/1	0.98	0.11	46,46,46,46	0
55	MG	DA	3088	1/1	0.98	0.03	52,52,52,52	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	BA	3139	1/1	0.98	0.18	0,0,0,0	0
55	MG	BA	3092	1/1	0.98	0.04	55,55,55,55	0
55	MG	BA	3094	1/1	0.98	0.04	30,30,30,30	0
55	MG	BA	3095	1/1	0.98	0.04	20,20,20,20	0
55	MG	DA	3152	1/1	0.98	0.10	47,47,47,47	0
55	MG	BA	3143	1/1	0.98	0.20	14,14,14,14	0
55	MG	BA	3096	1/1	0.98	0.10	10,10,10,10	0
55	MG	BA	3188	1/1	0.98	0.05	16,16,16,16	0
55	MG	AA	1606	1/1	0.98	0.04	41,41,41,41	0
55	MG	DA	3097	1/1	0.98	0.05	51,51,51,51	0
55	MG	AA	1621	1/1	0.98	0.04	35,35,35,35	0
55	MG	AA	1646	1/1	0.98	0.14	55,55,55,55	0
55	MG	BA	3025	1/1	0.98	0.02	0,0,0,0	0
55	MG	BA	3104	1/1	0.98	0.04	18,18,18,18	0
55	MG	AA	1607	1/1	0.98	0.04	41,41,41,41	0
55	MG	BB	203	1/1	0.98	0.04	15,15,15,15	0
55	MG	BA	3152	1/1	0.98	0.04	18,18,18,18	0
55	MG	BA	3108	1/1	0.98	0.05	9,9,9,9	0
55	MG	BQ	201	1/1	0.98	0.10	1,1,1,1	0
55	MG	BA	3110	1/1	0.98	0.12	0,0,0,0	0
55	MG	BA	3155	1/1	0.98	0.04	26,26,26,26	0
55	MG	CA	1603	1/1	0.98	0.04	36,36,36,36	0
55	MG	DB	202	1/1	0.98	0.05	65,65,65,65	0
55	MG	BA	3156	1/1	0.98	0.10	23,23,23,23	0
55	MG	BA	3069	1/1	0.98	0.05	0,0,0,0	0
55	MG	AA	1625	1/1	0.98	0.04	33,33,33,33	0
55	MG	BA	3030	1/1	0.98	0.10	12,12,12,12	0
55	MG	BA	3093	1/1	0.99	0.06	38,38,38,38	0
55	MG	BA	3050	1/1	0.99	0.04	6,6,6,6	0
55	MG	BA	3051	1/1	0.99	0.03	5,5,5,5	0
55	MG	AA	1615	1/1	0.99	0.05	50,50,50,50	0
55	MG	BA	3098	1/1	0.99	0.03	2,2,2,2	0
55	MG	DA	3060	1/1	0.99	0.04	43,43,43,43	0
55	MG	BA	3021	1/1	0.99	0.06	2,2,2,2	0
55	MG	BA	3054	1/1	0.99	0.05	2,2,2,2	0
55	MG	BA	3022	1/1	0.99	0.03	0,0,0,0	0
55	MG	DA	3122	1/1	0.99	0.03	44,44,44,44	0
55	MG	BA	3023	1/1	0.99	0.05	0,0,0,0	0
55	MG	BA	3057	1/1	0.99	0.05	3,3,3,3	0
55	MG	AA	1622	1/1	0.99	0.10	17,17,17,17	0
55	MG	DA	3067	1/1	0.99	0.03	42,42,42,42	0
55	MG	BA	3106	1/1	0.99	0.14	0,0,0,0	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	BA	3161	1/1	0.99	0.03	13,13,13,13	0
55	MG	DA	3130	1/1	0.99	0.07	39,39,39,39	0
55	MG	DA	3131	1/1	0.99	0.03	67,67,67,67	0
55	MG	AA	1633	1/1	0.99	0.03	41,41,41,41	0
55	MG	DA	3013	1/1	0.99	0.04	34,34,34,34	0
55	MG	BA	3109	1/1	0.99	0.10	1,1,1,1	0
55	MG	AA	1648	1/1	0.99	0.03	57,57,57,57	0
55	MG	BA	3027	1/1	0.99	0.04	4,4,4,4	0
55	MG	AA	1604	1/1	0.99	0.02	58,58,58,58	0
55	MG	BA	3064	1/1	0.99	0.08	0,0,0,0	0
55	MG	BA	3114	1/1	0.99	0.07	0,0,0,0	0
55	MG	BA	3065	1/1	0.99	0.10	0,0,0,0	0
55	MG	BA	3067	1/1	0.99	0.06	1,1,1,1	0
55	MG	BA	3068	1/1	0.99	0.07	0,0,0,0	0
55	MG	BA	3118	1/1	0.99	0.03	1,1,1,1	0
55	MG	DA	3024	1/1	0.99	0.03	61,61,61,61	0
55	MG	BA	3029	1/1	0.99	0.03	2,2,2,2	0
55	MG	AA	1641	1/1	0.99	0.05	15,15,15,15	0
55	MG	BA	3071	1/1	0.99	0.04	5,5,5,5	0
55	MG	BA	3007	1/1	0.99	0.02	17,17,17,17	0
55	MG	BA	3123	1/1	0.99	0.06	0,0,0,0	0
55	MG	BA	3034	1/1	0.99	0.16	0,0,0,0	0
55	MG	BA	3008	1/1	0.99	0.04	22,22,22,22	0
55	MG	BA	3076	1/1	0.99	0.04	4,4,4,4	0
55	MG	BA	3127	1/1	0.99	0.07	6,6,6,6	0
55	MG	CA	1634	1/1	0.99	0.03	52,52,52,52	0
55	MG	BA	3129	1/1	0.99	0.04	5,5,5,5	0
55	MG	BA	3036	1/1	0.99	0.03	0,0,0,0	0
55	MG	BA	3009	1/1	0.99	0.02	5,5,5,5	0
55	MG	BA	3038	1/1	0.99	0.10	0,0,0,0	0
55	MG	BA	3135	1/1	0.99	0.04	2,2,2,2	0
55	MG	CA	1640	1/1	0.99	0.04	31,31,31,31	0
55	MG	BA	3039	1/1	0.99	0.02	0,0,0,0	0
55	MG	BA	3011	1/1	0.99	0.06	1,1,1,1	0
55	MG	BA	3012	1/1	0.99	0.03	25,25,25,25	0
55	MG	DA	3044	1/1	0.99	0.06	47,47,47,47	0
55	MG	BA	3043	1/1	0.99	0.04	11,11,11,11	0
55	MG	AA	1642	1/1	0.99	0.04	15,15,15,15	0
55	MG	BA	3014	1/1	0.99	0.04	0,0,0,0	0
55	MG	BA	3087	1/1	0.99	0.09	1,1,1,1	0
55	MG	BA	3046	1/1	0.99	0.03	2,2,2,2	0
55	MG	BB	201	1/1	0.99	0.02	29,29,29,29	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	AA	1629	1/1	0.99	0.04	54,54,54,54	0
55	MG	BA	3090	1/1	0.99	0.04	1,1,1,1	0
55	MG	AA	1620	1/1	0.99	0.03	59,59,59,59	0
55	MG	BA	3018	1/1	0.99	0.07	0,0,0,0	0
55	MG	BB	202	1/1	1.00	0.02	2,2,2,2	0
55	MG	BA	3101	1/1	1.00	0.02	2,2,2,2	0
55	MG	BA	3010	1/1	1.00	0.02	0,0,0,0	0
55	MG	AA	1611	1/1	1.00	0.01	19,19,19,19	0
55	MG	AA	1618	1/1	1.00	0.01	41,41,41,41	0
55	MG	BA	3017	1/1	1.00	0.07	1,1,1,1	0
55	MG	BA	3066	1/1	1.00	0.04	1,1,1,1	0
55	MG	BA	3107	1/1	1.00	0.12	0,0,0,0	0
55	MG	AA	1623	1/1	1.00	0.04	46,46,46,46	0
55	MG	BA	3144	1/1	1.00	0.11	8,8,8,8	0
55	MG	BA	3031	1/1	1.00	0.04	2,2,2,2	0
55	MG	BA	3019	1/1	1.00	0.05	12,12,12,12	0
55	MG	BA	3082	1/1	1.00	0.04	0,0,0,0	0
55	MG	BA	3128	1/1	1.00	0.01	0,0,0,0	0
55	MG	DA	3123	1/1	1.00	0.07	37,37,37,37	0
55	MG	BA	3059	1/1	1.00	0.06	13,13,13,13	0
55	MG	BA	3130	1/1	1.00	0.02	0,0,0,0	0
55	MG	BA	3131	1/1	1.00	0.06	0,0,0,0	0
55	MG	BA	3097	1/1	1.00	0.04	5,5,5,5	0
55	MG	BA	3033	1/1	1.00	0.03	4,4,4,4	0
55	MG	BA	3042	1/1	1.00	0.05	11,11,11,11	0
55	MG	BA	3073	1/1	1.00	0.04	2,2,2,2	0
57	ZN	B4	101	1/1	1.00	0.02	24,24,24,24	0
57	ZN	D4	101	1/1	1.00	0.02	86,86,86,86	0

5.5 Other polymers

There are no such residues in this entry.