



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 23, 2026 – 11:28 AM UTC

PDB ID : 6BY1 / pdb_00006by1
Title : E. coli pH03H9 complex
Authors : Amiri, H.; Noller, H.F.
Deposited on : 2017-12-19
Resolution : 3.94 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
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

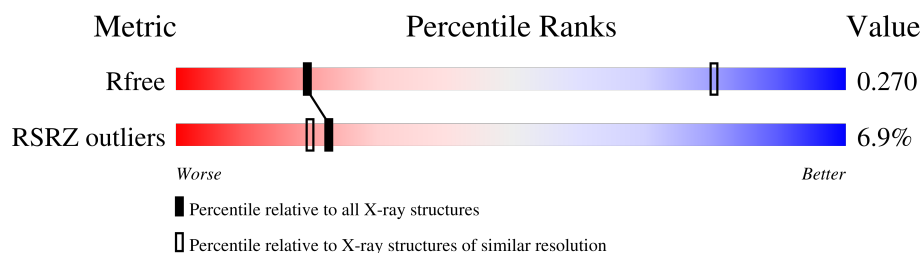
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.94 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	1022 (4.12-3.76)
RSRZ outliers	180081	1022 (4.12-3.76)

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	1609	-	-	-	X
56	MG	AA	1629	-	-	-	X
56	MG	BA	1607	-	-	-	X
56	MG	BA	1620	-	-	-	X
56	MG	BA	1628	-	-	-	X
56	MG	BA	1636	-	-	-	X
56	MG	CA	3166	-	-	-	X
56	MG	DA	3037	-	-	-	X
56	MG	DA	3060	-	-	-	X
56	MG	DA	3076	-	-	-	X
56	MG	DA	3083	-	-	-	X

2 Entry composition [i](#)

There are 58 unique types of molecules in this entry. The entry contains 296390 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	1540	Total	C	N	O	P	0	1	0
			33037	14735	6057	10705	1540			
1	BA	1541	Total	C	N	O	P	0	0	0
			33057	14744	6059	10713	1541			

- Molecule 2 is a RNA chain called 23S ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	CA	2867	Total	C	N	O	P	0	0	0
			61550	27457	11328	19898	2867			
2	DA	2869	Total	C	N	O	P	0	0	0
			61593	27477	11339	19908	2869			

- Molecule 3 is a RNA chain called 5S ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	CB	118	Total	C	N	O	P	0	0	0
			2529	1126	464	821	118			
3	DB	118	Total	C	N	O	P	0	0	0
			2529	1126	464	821	118			

- Molecule 4 is a RNA chain called Valine-specific transfer RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	AV	76	Total	C	N	O	P	0	0	0
			1623	723	292	532	76			
4	AY	76	Total	C	N	O	P	0	0	0
			1623	723	292	532	76			
4	AW	76	Total	C	N	O	P	0	0	0
			1623	723	292	532	76			
4	BV	76	Total	C	N	O	P	0	0	0
			1623	723	292	532	76			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	BW	76	Total	C	N	O	P	0	0	0
			1623	723	292	532	76			

- Molecule 5 is a protein called 50S ribosomal protein L2.

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

- Molecule 6 is a protein called 50S ribosomal protein L3.

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

- Molecule 7 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	CE	181	Total	C	N	O	S	0	0	0
			1404	881	261	258	4			
7	DE	180	Total	C	N	O	S	0	0	0
			1393	875	257	257	4			

- Molecule 8 is a protein called 50S ribosomal protein L5.

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

- Molecule 9 is a protein called 50S ribosomal protein L6.

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

- Molecule 10 is a protein called 50S ribosomal protein L9.

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

- Molecule 11 is a protein called 50S ribosomal protein L10.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	C5	109	Total	C	N	O	S	0	0	0
			825	521	149	151	4			

- Molecule 12 is a protein called 50S ribosomal protein L11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	CI	71	Total	C	N	O	S	0	0	0
			511	313	93	102	3			
12	DI	72	Total	C	N	O	S	0	0	0
			518	317	94	104	3			

- Molecule 13 is a protein called 50S ribosomal protein L13.

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

- Molecule 14 is a protein called 50S ribosomal protein L14.

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

- Molecule 15 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	CL	143	Total	C	N	O	S	0	0	0
			1045	649	206	189	1			

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

- Molecule 16 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	CM	135	Total	C	N	O	S	0	0	0
			1065	681	204	175	5			
16	DM	136	Total	C	N	O	S	0	0	0
			1074	686	205	177	6			

- Molecule 17 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	CN	121	Total	C	N	O	S	0	0	0
			969	599	198	167	5			
17	DN	121	Total	C	N	O	S	0	0	0
			969	599	198	167	5			

- Molecule 18 is a protein called 50S ribosomal protein L18.

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

- Molecule 19 is a protein called 50S ribosomal protein L19.

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

- Molecule 20 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	CQ	117	Total	C	N	O		0	0	0
			947	604	192	151				
20	DQ	117	Total	C	N	O		0	0	0
			947	604	192	151				

- Molecule 21 is a protein called 50S ribosomal protein L21.

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

- Molecule 22 is a protein called 50S ribosomal protein L22.

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

- Molecule 23 is a protein called 50S ribosomal protein L23.

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

- Molecule 24 is a protein called 50S ribosomal protein L24.

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

- Molecule 25 is a protein called 50S ribosomal protein L25.

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

- Molecule 26 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	CW	75	Total	C	N	O	S	0	0	0
			574	356	116	101	1			
26	DW	75	Total	C	N	O	S	0	0	0
			574	356	116	101	1			

- Molecule 27 is a protein called 50S ribosomal protein L28.

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

- Molecule 28 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
28	CY	61	Total	C	N	O	S	0	0	0
			499	308	97	92	2			
28	DY	63	Total	C	N	O	S	0	0	0
			509	313	99	95	2			

- Molecule 29 is a protein called 50S ribosomal protein L30.

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

- Molecule 30 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
30	C0	39	Total	C	N	O	S	0	0	0
			293	179	52	57	5			
30	D0	39	Total	C	N	O	S	0	0	0
			293	179	52	57	5			

- Molecule 31 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
31	C1	56	Total	C	N	O	S	0	0	0
			444	269	94	80	1			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
31	D1	56	Total	C	N	O	S	0	0	0
			444	269	94	80	1			

- Molecule 32 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
32	C2	50	Total	C	N	O		0	0	0
			410	263	75	72				
32	D2	50	Total	C	N	O		0	0	0
			410	263	75	72				

- Molecule 33 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
33	C3	46	Total	C	N	O	S	0	0	0
			377	228	90	57	2			
33	D3	46	Total	C	N	O	S	0	0	0
			377	228	90	57	2			

- Molecule 34 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
34	C4	61	Total	C	N	O	S	0	0	0
			479	306	102	69	2			
34	D4	62	Total	C	N	O	S	0	0	0
			486	311	103	70	2			

- Molecule 35 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
35	C6	38	Total	C	N	O	S	0	0	0
			302	185	65	48	4			
35	D6	38	Total	C	N	O	S	0	0	0
			302	185	65	48	4			

- Molecule 36 is a RNA chain called Messenger RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
36	AX	30	Total	C	N	O	P	0	0	0
			653	293	130	200	30			
36	BX	30	Total	C	N	O	P	0	0	0
			653	293	130	200	30			

- Molecule 37 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
37	AB	225	Total	C	N	O	S	0	0	0
			1757	1111	315	323	8			
37	BB	225	Total	C	N	O	S	0	0	0
			1757	1111	315	323	8			

- Molecule 38 is a protein called 30S ribosomal protein S3.

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

- Molecule 39 is a protein called 30S ribosomal protein S4.

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

- Molecule 40 is a protein called 30S ribosomal protein S5.

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

- Molecule 41 is a protein called 30S ribosomal protein S6.

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

- Molecule 42 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
42	AG	135	Total	C	N	O	S	0	0	0
			1058	659	203	192	4			
42	BG	132	Total	C	N	O	S	0	0	0
			1035	644	200	187	4			

- Molecule 43 is a protein called 30S ribosomal protein S8.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
43	AH	128	Total	C	N	O	S	0	0	0
			973	613	172	182	6			
43	BH	129	Total	C	N	O	S	0	0	0
			979	616	173	184	6			

- Molecule 44 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
44	AI	124	Total	C	N	O	S	0	0	0
			995	619	199	174	3			
44	BI	127	Total	C	N	O	S	0	0	0
			1022	634	206	179	3			

- Molecule 45 is a protein called 30S ribosomal protein S10.

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

- Molecule 46 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
46	AK	116	Total	C	N	O	S	0	0	0
			869	535	173	158	3			
46	BK	117	Total	C	N	O	S	0	0	0
			877	540	174	160	3			

- Molecule 47 is a protein called 30S ribosomal protein S12.

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

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
47	BL	123	Total	C	N	O	S	0	0	0
			955	590	196	165	4			

- Molecule 48 is a protein called 30S ribosomal protein S13.

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

- Molecule 49 is a protein called 30S ribosomal protein S14.

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

- Molecule 50 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
50	AO	88	Total	C	N	O	S	0	0	0
			714	439	144	130	1			
50	BO	88	Total	C	N	O	S	0	0	0
			714	439	144	130	1			

- Molecule 51 is a protein called 30S ribosomal protein S16.

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

- Molecule 52 is a protein called 30S ribosomal protein S17.

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

- Molecule 53 is a protein called 30S ribosomal protein S18.

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

- Molecule 54 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
54	AS	79	Total	C	N	O	S	0	0	0
			638	408	120	108	2			
54	BS	79	Total	C	N	O	S	0	0	0
			638	408	120	108	2			

- Molecule 55 is a protein called 30S ribosomal protein S20.

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

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	AA	50	Total	Mg	0	0
			50	50		
56	CA	167	Total	Mg	0	0
			167	167		
56	CB	3	Total	Mg	0	0
			3	3		
56	CC	1	Total	Mg	0	0
			1	1		
56	CN	2	Total	Mg	0	0
			2	2		
56	CQ	1	Total	Mg	0	0
			1	1		
56	C4	1	Total	Mg	0	0
			1	1		
56	BA	49	Total	Mg	0	0
			49	49		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	DA	166	Total 166	Mg 166	0	0
56	DB	3	Total 3	Mg 3	0	0
56	DN	1	Total 1	Mg 1	0	0
56	DQ	1	Total 1	Mg 1	0	0

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	C0	1	Total 1	Zn 1	0	0
57	C6	1	Total 1	Zn 1	0	0
57	D0	1	Total 1	Zn 1	0	0
57	D6	1	Total 1	Zn 1	0	0

- Molecule 58 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
58	AA	481	Total 481	O 481	0	0
58	CA	1106	Total 1106	O 1106	0	0
58	CB	49	Total 49	O 49	0	0
58	AV	28	Total 28	O 28	0	0
58	AY	5	Total 5	O 5	0	0
58	CC	13	Total 13	O 13	0	0
58	CD	10	Total 10	O 10	0	0
58	CE	16	Total 16	O 16	0	0
58	CF	14	Total 14	O 14	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
58	CG	18	Total	O	0	0
			18	18		
58	CH	8	Total	O	0	0
			8	8		
58	C5	7	Total	O	0	0
			7	7		
58	CI	4	Total	O	0	0
			4	4		
58	CJ	9	Total	O	0	0
			9	9		
58	CK	7	Total	O	0	0
			7	7		
58	CL	8	Total	O	0	0
			8	8		
58	CM	4	Total	O	0	0
			4	4		
58	CN	6	Total	O	0	0
			6	6		
58	CO	8	Total	O	0	0
			8	8		
58	CP	8	Total	O	0	0
			8	8		
58	CQ	2	Total	O	0	0
			2	2		
58	CR	7	Total	O	0	0
			7	7		
58	CS	3	Total	O	0	0
			3	3		
58	CT	7	Total	O	0	0
			7	7		
58	CU	13	Total	O	0	0
			13	13		
58	CV	10	Total	O	0	0
			10	10		
58	CW	4	Total	O	0	0
			4	4		
58	CX	3	Total	O	0	0
			3	3		
58	CY	3	Total	O	0	0
			3	3		
58	CZ	1	Total	O	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
58	C1	5	Total	O	0	0
			5	5		
58	C2	1	Total	O	0	0
			1	1		
58	C3	2	Total	O	0	0
			2	2		
58	C4	2	Total	O	0	0
			2	2		
58	C6	3	Total	O	0	0
			3	3		
58	AX	4	Total	O	0	0
			4	4		
58	AW	32	Total	O	0	0
			32	32		
58	AB	7	Total	O	0	0
			7	7		
58	AC	15	Total	O	0	0
			15	15		
58	AD	10	Total	O	0	0
			10	10		
58	AE	12	Total	O	0	0
			12	12		
58	AF	6	Total	O	0	0
			6	6		
58	AG	5	Total	O	0	0
			5	5		
58	AH	7	Total	O	0	0
			7	7		
58	AI	6	Total	O	0	0
			6	6		
58	AJ	4	Total	O	0	0
			4	4		
58	AK	10	Total	O	0	0
			10	10		
58	AL	9	Total	O	0	0
			9	9		
58	AM	6	Total	O	0	0
			6	6		
58	AN	3	Total	O	0	0
			3	3		
58	AO	7	Total	O	0	0
			7	7		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
58	AP	4	Total 4	O 4	0	0
58	AQ	8	Total 8	O 8	0	0
58	AR	1	Total 1	O 1	0	0
58	AS	4	Total 4	O 4	0	0
58	AT	4	Total 4	O 4	0	0
58	BA	461	Total 461	O 461	0	0
58	DA	1005	Total 1005	O 1005	0	0
58	DB	32	Total 32	O 32	0	0
58	BV	13	Total 13	O 13	0	0
58	DC	28	Total 28	O 28	0	0
58	DD	15	Total 15	O 15	0	0
58	DE	12	Total 12	O 12	0	0
58	DF	4	Total 4	O 4	0	0
58	DG	6	Total 6	O 6	0	0
58	DH	4	Total 4	O 4	0	0
58	DJ	3	Total 3	O 3	0	0
58	DK	5	Total 5	O 5	0	0
58	DL	10	Total 10	O 10	0	0
58	DM	6	Total 6	O 6	0	0
58	DN	6	Total 6	O 6	0	0
58	DO	4	Total 4	O 4	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
58	DP	6	Total	O	0	0
			6	6		
58	DQ	5	Total	O	0	0
			5	5		
58	DR	13	Total	O	0	0
			13	13		
58	DS	9	Total	O	0	0
			9	9		
58	DT	10	Total	O	0	0
			10	10		
58	DU	14	Total	O	0	0
			14	14		
58	DV	7	Total	O	0	0
			7	7		
58	DW	3	Total	O	0	0
			3	3		
58	DX	3	Total	O	0	0
			3	3		
58	DY	7	Total	O	0	0
			7	7		
58	DZ	2	Total	O	0	0
			2	2		
58	D0	2	Total	O	0	0
			2	2		
58	D1	11	Total	O	0	0
			11	11		
58	D2	2	Total	O	0	0
			2	2		
58	D3	2	Total	O	0	0
			2	2		
58	D6	1	Total	O	0	0
			1	1		
58	BX	5	Total	O	0	0
			5	5		
58	BW	23	Total	O	0	0
			23	23		
58	BB	2	Total	O	0	0
			2	2		
58	BC	8	Total	O	0	0
			8	8		
58	BD	24	Total	O	0	0
			24	24		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
58	BE	18	Total	O	0	0
			18	18		
58	BF	6	Total	O	0	0
			6	6		
58	BG	4	Total	O	0	0
			4	4		
58	BH	12	Total	O	0	0
			12	12		
58	BI	9	Total	O	0	0
			9	9		
58	BJ	8	Total	O	0	0
			8	8		
58	BK	5	Total	O	0	0
			5	5		
58	BL	8	Total	O	0	0
			8	8		
58	BM	6	Total	O	0	0
			6	6		
58	BN	5	Total	O	0	0
			5	5		
58	BO	2	Total	O	0	0
			2	2		
58	BP	5	Total	O	0	0
			5	5		
58	BQ	10	Total	O	0	0
			10	10		
58	BR	1	Total	O	0	0
			1	1		
58	BS	3	Total	O	0	0
			3	3		
58	BT	2	Total	O	0	0
			2	2		

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3 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	211.66Å 433.91Å 623.53Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	59.99 – 3.94 59.99 – 3.94	Depositor EDS
% Data completeness (in resolution range)	99.9 (59.99-3.94) 99.9 (59.99-3.94)	Depositor EDS
R_{merge}	0.57	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.21 (at 3.88Å)	Xtriage
Refinement program	PHENIX 1.12_2829	Depositor
R, R_{free}	0.249 , 0.269 0.250 , 0.270	Depositor DCC
R_{free} test set	10092 reflections (2.01%)	wwPDB-VP
Wilson B-factor (Å ²)	137.5	Xtriage
Anisotropy	0.118	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.17 , 40.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.37$, $\langle L^2 \rangle = 0.20$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	296390	wwPDB-VP
Average B, all atoms (Å ²)	136.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.47% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

4 Model quality [i](#)

4.1 Standard geometry [i](#)

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

4.2 Too-close contacts [i](#)

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

4.3 Torsion angles [i](#)

4.3.1 Protein backbone [i](#)

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

4.3.2 Protein sidechains [i](#)

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

4.3.3 RNA [i](#)

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

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

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

4.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

4.6 Ligand geometry [i](#)

Of 449 ligands modelled in this entry, 449 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

4.7 Other polymers [i](#)

There are no such residues in this entry.

4.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
2	DA	9
1	BA	4
1	AA	1

The worst 5 of 14 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	DA	2105:U	O3'	2118:U	P	30.28
1	DA	2185:U	O3'	2186:G	P	7.24
1	DA	2103:C	O3'	2104:C	P	6.01
1	DA	1887:C	O3'	1888:G	P	5.11
1	DA	2140:G	O3'	2141:G	P	3.75

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	1540/1541 (99%)	0.38	68 (4%)	39	29	95, 154, 226, 359	2 (0%)
1	BA	1541/1541 (100%)	0.35	72 (4%)	36	28	110, 157, 207, 259	3 (0%)
2	CA	2867/2904 (98%)	0.02	57 (1%)	65	46	69, 94, 175, 296	33 (1%)
2	DA	2869/2904 (98%)	0.17	68 (2%)	59	43	86, 126, 215, 320	26 (0%)
3	CB	118/118 (100%)	-0.14	0	100	100	81, 108, 131, 159	0
3	DB	118/118 (100%)	0.05	3 (2%)	58	41	133, 191, 210, 222	0
4	AV	76/76 (100%)	0.39	7 (9%)	14	16	125, 166, 186, 201	0
4	AW	76/76 (100%)	0.45	6 (7%)	18	18	119, 157, 180, 196	0
4	AY	76/76 (100%)	2.04	28 (36%)	1	2	94, 177, 187, 190	76 (100%)
4	BV	76/76 (100%)	0.65	7 (9%)	14	16	138, 193, 215, 225	0
4	BW	76/76 (100%)	0.28	2 (2%)	57	40	142, 195, 208, 221	0
5	CC	271/271 (100%)	0.57	19 (7%)	22	20	71, 99, 117, 127	0
5	DC	271/271 (100%)	0.83	34 (12%)	8	11	98, 122, 143, 158	0
6	CD	209/209 (100%)	0.53	11 (5%)	32	26	70, 90, 110, 165	0
6	DD	209/209 (100%)	0.34	10 (4%)	35	28	89, 113, 130, 143	0
7	CE	181/181 (100%)	0.41	16 (8%)	15	16	68, 95, 111, 133	0
7	DE	180/181 (99%)	0.49	13 (7%)	21	19	92, 128, 142, 151	0
8	CF	177/177 (100%)	0.49	13 (7%)	21	19	113, 134, 158, 170	0
8	DF	177/177 (100%)	0.79	20 (11%)	10	13	136, 191, 224, 239	0
9	CG	176/176 (100%)	0.27	9 (5%)	33	26	88, 105, 120, 148	0
9	DG	176/176 (100%)	0.37	10 (5%)	29	24	132, 150, 165, 176	0
10	CH	149/149 (100%)	0.15	3 (2%)	65	46	101, 151, 164, 168	0
10	DH	149/149 (100%)	0.52	5 (3%)	48	34	139, 210, 238, 243	0
11	C5	109/109 (100%)	0.37	5 (4%)	37	29	131, 173, 190, 197	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
12	CI	71/72 (98%)	1.33	20 (28%) 1 3	168, 186, 196, 198	71 (100%)
12	DI	72/72 (100%)	0.80	4 (5%) 30 24	262, 278, 291, 295	0
13	CJ	142/142 (100%)	0.23	4 (2%) 55 39	68, 86, 104, 121	0
13	DJ	142/142 (100%)	0.81	17 (11%) 9 12	97, 114, 129, 147	0
14	CK	122/122 (100%)	0.34	5 (4%) 41 31	77, 92, 114, 125	0
14	DK	122/122 (100%)	0.62	14 (11%) 9 12	97, 114, 129, 139	0
15	CL	143/143 (100%)	0.86	18 (12%) 8 11	74, 99, 116, 130	0
15	DL	143/143 (100%)	0.97	18 (12%) 8 11	98, 150, 167, 182	0
16	CM	135/136 (99%)	0.45	8 (5%) 28 24	78, 94, 113, 127	0
16	DM	136/136 (100%)	0.65	13 (9%) 13 15	117, 138, 151, 164	0
17	CN	121/121 (100%)	0.51	8 (6%) 24 21	72, 87, 99, 100	0
17	DN	121/121 (100%)	0.86	17 (14%) 6 9	89, 106, 122, 146	0
18	CO	116/116 (100%)	0.39	6 (5%) 33 26	93, 111, 126, 131	0
18	DO	116/116 (100%)	0.84	14 (12%) 8 12	169, 188, 201, 208	0
19	CP	114/114 (100%)	0.59	15 (13%) 7 10	76, 96, 125, 135	0
19	DP	114/114 (100%)	0.38	3 (2%) 57 40	108, 121, 142, 154	0
20	CQ	117/117 (100%)	0.51	6 (5%) 33 26	68, 80, 97, 112	0
20	DQ	117/117 (100%)	0.53	8 (6%) 23 21	84, 108, 120, 127	0
21	CR	103/103 (100%)	0.20	6 (5%) 29 24	70, 94, 109, 118	0
21	DR	103/103 (100%)	0.45	5 (4%) 35 27	99, 116, 130, 141	0
22	CS	110/110 (100%)	0.64	10 (9%) 15 16	69, 87, 102, 121	0
22	DS	110/110 (100%)	0.52	5 (4%) 38 29	84, 104, 119, 131	0
23	CT	93/93 (100%)	0.50	4 (4%) 40 30	78, 97, 123, 138	0
23	DT	93/93 (100%)	1.10	15 (16%) 4 8	107, 127, 150, 166	0
24	CU	102/102 (100%)	0.31	4 (3%) 43 31	77, 96, 118, 137	0
24	DU	102/102 (100%)	0.58	5 (4%) 35 27	97, 123, 149, 165	0
25	CV	94/94 (100%)	0.19	1 (1%) 78 58	78, 101, 116, 119	0
25	DV	94/94 (100%)	-0.21	0 100 100	132, 146, 157, 161	0
26	CW	75/75 (100%)	0.78	9 (12%) 9 12	82, 95, 110, 155	0
26	DW	75/75 (100%)	0.70	10 (13%) 7 10	129, 148, 161, 172	0
27	CX	77/77 (100%)	0.87	10 (12%) 7 10	83, 98, 117, 123	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
27	DX	77/77 (100%)	0.81	8 (10%) 11 13	118, 135, 151, 156	0
28	CY	61/63 (96%)	0.47	4 (6%) 24 21	94, 109, 122, 145	0
28	DY	63/63 (100%)	0.39	5 (7%) 18 18	118, 133, 150, 154	0
29	CZ	58/58 (100%)	0.72	6 (10%) 12 13	74, 88, 108, 128	0
29	DZ	58/58 (100%)	0.73	4 (6%) 23 20	121, 137, 146, 152	0
30	C0	39/39 (100%)	1.55	12 (30%) 1 3	112, 125, 133, 136	39 (100%)
30	D0	39/39 (100%)	2.18	19 (48%) 0 1	134, 146, 153, 154	39 (100%)
31	C1	56/56 (100%)	0.36	5 (8%) 15 16	67, 91, 115, 127	0
31	D1	56/56 (100%)	0.51	3 (5%) 31 25	89, 110, 123, 135	0
32	C2	50/50 (100%)	0.63	4 (8%) 18 18	128, 140, 154, 158	0
32	D2	50/50 (100%)	2.93	36 (72%) 0 0	122, 134, 139, 142	50 (100%)
33	C3	46/46 (100%)	0.75	4 (8%) 16 17	68, 87, 102, 108	0
33	D3	46/46 (100%)	0.82	3 (6%) 25 21	101, 110, 120, 140	0
34	C4	61/62 (98%)	0.91	8 (13%) 7 10	79, 108, 121, 123	0
34	D4	62/62 (100%)	1.81	21 (33%) 1 2	135, 160, 171, 175	0
35	C6	38/38 (100%)	0.65	0 100 100	88, 103, 122, 149	0
35	D6	38/38 (100%)	1.16	7 (18%) 3 6	126, 137, 150, 178	0
36	AX	30/46 (65%)	2.66	17 (56%) 0 1	123, 192, 227, 257	1 (3%)
36	BX	30/46 (65%)	3.00	20 (66%) 0 0	140, 182, 233, 239	1 (3%)
37	AB	225/225 (100%)	0.34	8 (3%) 46 33	161, 181, 193, 207	0
37	BB	225/225 (100%)	0.34	8 (3%) 46 33	168, 197, 211, 218	0
38	AC	206/206 (100%)	0.47	17 (8%) 17 18	147, 163, 176, 198	0
38	BC	206/206 (100%)	0.57	27 (13%) 7 10	140, 159, 171, 180	0
39	AD	205/205 (100%)	1.13	36 (17%) 4 6	138, 166, 180, 185	0
39	BD	205/205 (100%)	0.74	25 (12%) 8 11	126, 144, 156, 172	0
40	AE	150/150 (100%)	1.01	30 (20%) 3 5	121, 145, 160, 165	0
40	BE	150/150 (100%)	0.47	7 (4%) 36 28	126, 149, 161, 171	0
41	AF	100/100 (100%)	0.14	2 (2%) 65 46	113, 136, 153, 159	0
41	BF	100/100 (100%)	0.65	8 (8%) 18 18	145, 158, 171, 178	0
42	AG	135/179 (75%)	0.57	11 (8%) 18 18	149, 173, 188, 200	0
42	BG	132/179 (73%)	0.62	6 (4%) 38 29	169, 196, 215, 225	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
43	AH	128/129 (99%)	0.63	11 (8%) 16 17	135, 146, 164, 171	0
43	BH	129/129 (100%)	0.59	11 (8%) 16 17	141, 154, 164, 172	0
44	AI	124/130 (95%)	1.12	21 (16%) 4 7	146, 178, 189, 200	0
44	BI	127/130 (97%)	0.83	14 (11%) 10 13	161, 193, 206, 210	0
45	AJ	98/98 (100%)	1.22	20 (20%) 3 5	149, 182, 197, 200	0
45	BJ	98/98 (100%)	1.33	20 (20%) 3 5	151, 176, 189, 193	0
46	AK	116/117 (99%)	0.31	5 (4%) 40 30	96, 131, 147, 161	0
46	BK	117/117 (100%)	0.46	10 (8%) 16 17	142, 170, 187, 192	0
47	AL	123/123 (100%)	1.03	17 (13%) 6 10	116, 134, 148, 176	0
47	BL	123/123 (100%)	0.75	11 (8%) 15 16	111, 128, 142, 153	0
48	AM	114/114 (100%)	0.56	6 (5%) 32 26	135, 168, 206, 227	0
48	BM	114/114 (100%)	0.64	10 (8%) 15 16	164, 190, 212, 243	0
49	AN	96/101 (95%)	1.29	22 (22%) 2 4	147, 168, 180, 189	0
49	BN	96/101 (95%)	1.51	28 (29%) 1 3	153, 166, 177, 185	0
50	AO	88/89 (98%)	0.36	4 (4%) 38 29	112, 131, 150, 159	0
50	BO	88/89 (98%)	0.59	6 (6%) 23 21	135, 153, 167, 172	0
51	AP	82/82 (100%)	1.37	20 (24%) 2 4	147, 169, 179, 195	0
51	BP	82/82 (100%)	1.27	17 (20%) 2 4	122, 148, 174, 189	0
52	AQ	80/80 (100%)	0.72	6 (7%) 20 19	126, 151, 163, 170	0
52	BQ	80/80 (100%)	0.96	14 (17%) 4 6	131, 150, 161, 173	0
53	AR	55/55 (100%)	0.34	2 (3%) 46 33	126, 139, 157, 161	0
53	BR	55/55 (100%)	0.45	3 (5%) 30 25	152, 162, 183, 200	0
54	AS	79/79 (100%)	0.29	2 (2%) 58 41	156, 170, 179, 184	0
54	BS	79/79 (100%)	0.58	5 (6%) 26 22	165, 179, 188, 193	0
55	AT	85/85 (100%)	0.98	13 (15%) 5 8	134, 154, 166, 176	0
55	BT	85/85 (100%)	0.71	5 (5%) 28 24	131, 151, 163, 170	0
All	All	20800/21025 (98%)	0.45	1442 (6%) 23 20	67, 135, 201, 359	341 (1%)

The worst 5 of 1442 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	BA	387	U	8.5
44	BI	107	ALA	8.4

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Mol	Chain	Res	Type	RSRZ
45	BJ	62	ARG	8.3
10	DH	23	ALA	8.2
30	D0	22	MET	8.1

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

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

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	AA	1640	1/1	-0.21	0.28	127,127,127,127	0
56	MG	BA	1645	1/1	-0.00	0.23	144,144,144,144	0
56	MG	DA	3060	1/1	0.00	0.51	73,73,73,73	1
56	MG	BA	1641	1/1	0.03	0.23	134,134,134,134	0
56	MG	AA	1611	1/1	0.05	0.17	165,165,165,165	1
56	MG	BA	1628	1/1	0.12	0.41	120,120,120,120	0
56	MG	AA	1642	1/1	0.24	0.29	122,122,122,122	0
56	MG	AA	1641	1/1	0.25	0.28	171,171,171,171	0
56	MG	AA	1644	1/1	0.29	0.22	164,164,164,164	0
56	MG	DA	3165	1/1	0.32	0.37	60,60,60,60	0
56	MG	BA	1648	1/1	0.33	0.34	109,109,109,109	0
56	MG	AA	1633	1/1	0.36	0.14	108,108,108,108	1
56	MG	BA	1620	1/1	0.36	0.57	104,104,104,104	0
56	MG	AA	1629	1/1	0.39	0.44	127,127,127,127	0
56	MG	BA	1612	1/1	0.40	0.29	116,116,116,116	0
56	MG	BA	1607	1/1	0.44	0.40	87,87,87,87	0
56	MG	AA	1609	1/1	0.46	0.43	127,127,127,127	1
56	MG	DB	203	1/1	0.48	0.22	131,131,131,131	0
56	MG	CA	3007	1/1	0.50	0.23	88,88,88,88	0
56	MG	CA	3068	1/1	0.52	0.22	101,101,101,101	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	AA	1646	1/1	0.53	0.28	132,132,132,132	0
56	MG	DA	3090	1/1	0.54	0.19	60,60,60,60	0
56	MG	DA	3018	1/1	0.56	0.33	95,95,95,95	0
56	MG	AA	1604	1/1	0.57	0.08	182,182,182,182	1
56	MG	AA	1647	1/1	0.57	0.27	105,105,105,105	0
56	MG	DA	3160	1/1	0.58	0.28	78,78,78,78	0
56	MG	DA	3083	1/1	0.58	0.45	73,73,73,73	0
56	MG	BA	1642	1/1	0.58	0.33	107,107,107,107	0
56	MG	CA	3091	1/1	0.59	0.24	98,98,98,98	0
56	MG	DA	3087	1/1	0.59	0.26	104,104,104,104	0
56	MG	BA	1605	1/1	0.59	0.22	104,104,104,104	0
56	MG	BA	1626	1/1	0.60	0.23	114,114,114,114	0
56	MG	BA	1629	1/1	0.61	0.16	161,161,161,161	0
56	MG	DA	3069	1/1	0.61	0.16	166,166,166,166	0
56	MG	DA	3051	1/1	0.62	0.28	99,99,99,99	1
56	MG	CA	3147	1/1	0.63	0.27	93,93,93,93	0
56	MG	BA	1611	1/1	0.64	0.19	130,130,130,130	0
56	MG	CA	3164	1/1	0.64	0.31	60,60,60,60	0
56	MG	DA	3130	1/1	0.65	0.39	100,100,100,100	0
56	MG	BA	1627	1/1	0.66	0.16	132,132,132,132	0
56	MG	AA	1627	1/1	0.66	0.16	128,128,128,128	0
56	MG	AA	1648	1/1	0.67	0.17	149,149,149,149	0
56	MG	DA	3094	1/1	0.67	0.21	77,77,77,77	0
56	MG	CA	3153	1/1	0.67	0.32	73,73,73,73	1
56	MG	AA	1613	1/1	0.68	0.24	104,104,104,104	0
56	MG	CA	3005	1/1	0.68	0.21	90,90,90,90	1
56	MG	AA	1610	1/1	0.68	0.22	114,114,114,114	0
56	MG	DA	3112	1/1	0.69	0.16	101,101,101,101	0
56	MG	DA	3037	1/1	0.69	0.42	83,83,83,83	0
56	MG	DA	3134	1/1	0.69	0.28	67,67,67,67	0
56	MG	BA	1644	1/1	0.69	0.27	78,78,78,78	0
56	MG	BA	1638	1/1	0.69	0.17	154,154,154,154	0
56	MG	DA	3036	1/1	0.69	0.17	102,102,102,102	0
56	MG	CA	3088	1/1	0.70	0.26	83,83,83,83	1
56	MG	CA	3054	1/1	0.70	0.29	65,65,65,65	0
56	MG	CA	3040	1/1	0.70	0.23	88,88,88,88	1
56	MG	BA	1622	1/1	0.71	0.28	105,105,105,105	0
56	MG	CA	3138	1/1	0.71	0.15	102,102,102,102	0
56	MG	DA	3159	1/1	0.71	0.11	95,95,95,95	0
56	MG	CA	3151	1/1	0.72	0.24	75,75,75,75	0
56	MG	DA	3141	1/1	0.72	0.10	151,151,151,151	1
56	MG	DA	3097	1/1	0.72	0.31	78,78,78,78	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	DA	3100	1/1	0.72	0.34	76,76,76,76	0
56	MG	DA	3164	1/1	0.72	0.15	60,60,60,60	0
56	MG	CA	3166	1/1	0.72	0.45	60,60,60,60	0
56	MG	DA	3166	1/1	0.72	0.17	137,137,137,137	0
56	MG	CA	3026	1/1	0.72	0.15	70,70,70,70	1
56	MG	BA	1636	1/1	0.73	0.57	99,99,99,99	0
56	MG	DA	3007	1/1	0.73	0.20	72,72,72,72	0
56	MG	BA	1623	1/1	0.73	0.11	139,139,139,139	0
56	MG	DN	201	1/1	0.73	0.22	84,84,84,84	1
56	MG	DA	3149	1/1	0.74	0.20	68,68,68,68	0
56	MG	DA	3029	1/1	0.75	0.39	72,72,72,72	1
56	MG	AA	1645	1/1	0.75	0.20	148,148,148,148	0
56	MG	CA	3146	1/1	0.75	0.24	78,78,78,78	0
56	MG	BA	1646	1/1	0.75	0.27	81,81,81,81	0
56	MG	DA	3076	1/1	0.76	0.61	76,76,76,76	1
56	MG	DA	3088	1/1	0.76	0.20	88,88,88,88	1
56	MG	AA	1605	1/1	0.76	0.07	155,155,155,155	1
56	MG	CA	3090	1/1	0.77	0.30	83,83,83,83	0
56	MG	DA	3158	1/1	0.77	0.31	64,64,64,64	0
56	MG	AA	1650	1/1	0.77	0.28	86,86,86,86	0
56	MG	AA	1630	1/1	0.78	0.12	158,158,158,158	0
56	MG	CA	3155	1/1	0.78	0.22	81,81,81,81	1
56	MG	DA	3068	1/1	0.78	0.23	84,84,84,84	0
56	MG	BA	1608	1/1	0.78	0.28	127,127,127,127	0
56	MG	AA	1606	1/1	0.78	0.13	110,110,110,110	0
56	MG	DA	3157	1/1	0.78	0.29	83,83,83,83	0
56	MG	AA	1619	1/1	0.78	0.12	124,124,124,124	0
56	MG	BA	1631	1/1	0.79	0.13	155,155,155,155	0
56	MG	CA	3127	1/1	0.79	0.31	42,42,42,42	0
56	MG	DA	3066	1/1	0.79	0.24	81,81,81,81	0
56	MG	DA	3052	1/1	0.80	0.40	54,54,54,54	0
56	MG	AA	1632	1/1	0.80	0.15	151,151,151,151	0
56	MG	C4	101	1/1	0.80	0.26	73,73,73,73	0
56	MG	BA	1639	1/1	0.80	0.14	155,155,155,155	1
56	MG	CA	3149	1/1	0.80	0.25	95,95,95,95	1
56	MG	DA	3075	1/1	0.80	0.14	90,90,90,90	0
56	MG	BA	1633	1/1	0.80	0.16	102,102,102,102	0
56	MG	DA	3146	1/1	0.81	0.17	96,96,96,96	0
56	MG	DA	3127	1/1	0.81	0.46	43,43,43,43	0
56	MG	DA	3154	1/1	0.81	0.33	68,68,68,68	0
56	MG	CA	3165	1/1	0.81	0.35	60,60,60,60	0
56	MG	DA	3092	1/1	0.81	0.20	102,102,102,102	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	BA	1609	1/1	0.81	0.14	110,110,110,110	0
56	MG	DA	3122	1/1	0.82	0.13	103,103,103,103	0
56	MG	DA	3135	1/1	0.82	0.30	92,92,92,92	0
56	MG	DA	3040	1/1	0.82	0.16	90,90,90,90	1
56	MG	CA	3070	1/1	0.82	0.18	76,76,76,76	0
56	MG	DA	3132	1/1	0.82	0.16	105,105,105,105	0
56	MG	DA	3013	1/1	0.83	0.35	51,51,51,51	0
56	MG	CA	3137	1/1	0.83	0.18	67,67,67,67	1
56	MG	DA	3025	1/1	0.83	0.35	88,88,88,88	0
56	MG	DA	3072	1/1	0.83	0.18	79,79,79,79	0
56	MG	DA	3073	1/1	0.83	0.21	93,93,93,93	1
56	MG	BA	1635	1/1	0.83	0.12	141,141,141,141	0
56	MG	AA	1643	1/1	0.83	0.16	85,85,85,85	0
56	MG	DA	3140	1/1	0.84	0.20	98,98,98,98	1
56	MG	BA	1643	1/1	0.84	0.18	114,114,114,114	1
56	MG	DA	3015	1/1	0.84	0.30	73,73,73,73	0
56	MG	DA	3056	1/1	0.84	0.19	84,84,84,84	0
56	MG	BA	1610	1/1	0.84	0.07	147,147,147,147	0
56	MG	AA	1608	1/1	0.84	0.18	106,106,106,106	0
56	MG	DA	3118	1/1	0.84	0.18	103,103,103,103	0
56	MG	CA	3113	1/1	0.85	0.19	81,81,81,81	0
56	MG	DA	3062	1/1	0.85	0.14	95,95,95,95	1
56	MG	DA	3063	1/1	0.85	0.15	105,105,105,105	0
56	MG	CA	3150	1/1	0.85	0.16	91,91,91,91	0
56	MG	BA	1624	1/1	0.85	0.11	119,119,119,119	0
56	MG	DA	3161	1/1	0.85	0.21	92,92,92,92	0
56	MG	DA	3162	1/1	0.85	0.42	77,77,77,77	0
56	MG	CA	3143	1/1	0.85	0.27	63,63,63,63	0
56	MG	AA	1616	1/1	0.85	0.14	92,92,92,92	0
56	MG	AA	1638	1/1	0.85	0.14	55,55,55,55	0
56	MG	DB	202	1/1	0.85	0.17	95,95,95,95	0
56	MG	CA	3162	1/1	0.85	0.32	56,56,56,56	1
56	MG	BA	1621	1/1	0.85	0.22	91,91,91,91	0
56	MG	DA	3021	1/1	0.86	0.11	92,92,92,92	1
56	MG	CA	3019	1/1	0.86	0.15	78,78,78,78	1
56	MG	DA	3028	1/1	0.86	0.19	76,76,76,76	0
56	MG	BA	1618	1/1	0.86	0.13	144,144,144,144	0
56	MG	DA	3151	1/1	0.86	0.47	88,88,88,88	0
56	MG	DA	3137	1/1	0.86	0.29	68,68,68,68	0
56	MG	CA	3060	1/1	0.87	0.36	48,48,48,48	0
56	MG	DA	3098	1/1	0.87	0.18	84,84,84,84	0
56	MG	DA	3136	1/1	0.87	0.36	78,78,78,78	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	DA	3082	1/1	0.87	0.21	106,106,106,106	0
56	MG	DA	3110	1/1	0.87	0.10	108,108,108,108	0
56	MG	AA	1631	1/1	0.87	0.07	148,148,148,148	1
56	MG	BA	1649	1/1	0.87	0.11	72,72,72,72	0
56	MG	CA	3015	1/1	0.87	0.30	87,87,87,87	0
56	MG	BA	1617	1/1	0.87	0.11	124,124,124,124	0
56	MG	DA	3035	1/1	0.87	0.12	96,96,96,96	0
56	MG	CA	3079	1/1	0.87	0.28	64,64,64,64	0
57	ZN	D0	101	1/1	0.87	0.09	210,210,210,210	1
56	MG	CA	3043	1/1	0.88	0.18	59,59,59,59	0
56	MG	CA	3141	1/1	0.88	0.13	67,67,67,67	1
56	MG	CA	3093	1/1	0.88	0.15	100,100,100,100	0
56	MG	CA	3020	1/1	0.88	0.43	45,45,45,45	1
56	MG	BA	1632	1/1	0.88	0.07	191,191,191,191	0
56	MG	DA	3131	1/1	0.88	0.23	78,78,78,78	0
56	MG	CA	3118	1/1	0.88	0.16	82,82,82,82	1
56	MG	CA	3024	1/1	0.88	0.22	59,59,59,59	0
56	MG	CA	3041	1/1	0.88	0.11	67,67,67,67	1
56	MG	CB	201	1/1	0.88	0.18	113,113,113,113	1
56	MG	DA	3155	1/1	0.89	0.12	79,79,79,79	0
56	MG	CA	3087	1/1	0.89	0.46	74,74,74,74	0
56	MG	CA	3052	1/1	0.89	0.25	76,76,76,76	1
56	MG	CA	3144	1/1	0.89	0.29	57,57,57,57	0
56	MG	CA	3035	1/1	0.89	0.21	37,37,37,37	0
56	MG	CA	3133	1/1	0.89	0.31	47,47,47,47	0
56	MG	DA	3139	1/1	0.89	0.09	99,99,99,99	0
56	MG	DA	3058	1/1	0.89	0.20	83,83,83,83	0
56	MG	DA	3027	1/1	0.89	0.16	92,92,92,92	0
56	MG	DA	3145	1/1	0.89	0.17	30,30,30,30	1
56	MG	CA	3148	1/1	0.89	0.33	98,98,98,98	0
56	MG	CA	3001	1/1	0.89	0.14	62,62,62,62	1
56	MG	CA	3084	1/1	0.89	0.31	85,85,85,85	0
56	MG	BA	1613	1/1	0.89	0.16	88,88,88,88	0
56	MG	DA	3081	1/1	0.90	0.39	55,55,55,55	0
56	MG	CB	202	1/1	0.90	0.13	80,80,80,80	0
56	MG	CA	3159	1/1	0.90	0.11	93,93,93,93	0
56	MG	DA	3163	1/1	0.90	0.11	60,60,60,60	0
56	MG	DA	3084	1/1	0.90	0.26	85,85,85,85	0
56	MG	CA	3083	1/1	0.90	0.21	81,81,81,81	1
56	MG	CA	3011	1/1	0.90	0.25	52,52,52,52	0
56	MG	DA	3156	1/1	0.90	0.14	109,109,109,109	0
56	MG	CA	3152	1/1	0.90	0.20	57,57,57,57	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	AA	1622	1/1	0.90	0.20	92,92,92,92	0
56	MG	CA	3050	1/1	0.90	0.23	56,56,56,56	0
56	MG	DA	3117	1/1	0.91	0.11	95,95,95,95	0
56	MG	DA	3152	1/1	0.91	0.09	103,103,103,103	0
56	MG	CA	3013	1/1	0.91	0.32	55,55,55,55	0
56	MG	CA	3129	1/1	0.91	0.12	80,80,80,80	0
56	MG	DA	3061	1/1	0.91	0.17	73,73,73,73	0
56	MG	DA	3128	1/1	0.91	0.07	121,121,121,121	1
56	MG	BA	1634	1/1	0.91	0.09	129,129,129,129	0
56	MG	BA	1647	1/1	0.91	0.15	104,104,104,104	0
56	MG	DA	3089	1/1	0.91	0.07	115,115,115,115	0
56	MG	DA	3032	1/1	0.91	0.26	93,93,93,93	0
56	MG	AA	1639	1/1	0.91	0.14	137,137,137,137	1
56	MG	AA	1624	1/1	0.91	0.12	130,130,130,130	0
56	MG	CN	202	1/1	0.91	0.15	64,64,64,64	0
56	MG	CA	3069	1/1	0.91	0.12	69,69,69,69	0
56	MG	AA	1615	1/1	0.91	0.18	103,103,103,103	0
56	MG	DA	3109	1/1	0.91	0.14	123,123,123,123	0
56	MG	BA	1606	1/1	0.91	0.14	100,100,100,100	0
56	MG	CA	3142	1/1	0.91	0.15	57,57,57,57	0
56	MG	DA	3113	1/1	0.91	0.29	85,85,85,85	0
56	MG	AA	1601	1/1	0.92	0.11	102,102,102,102	0
56	MG	CA	3126	1/1	0.92	0.16	67,67,67,67	0
56	MG	CA	3075	1/1	0.92	0.22	78,78,78,78	1
56	MG	AA	1602	1/1	0.92	0.27	177,177,177,177	0
56	MG	DA	3133	1/1	0.92	0.34	77,77,77,77	0
56	MG	DA	3001	1/1	0.92	0.17	71,71,71,71	1
56	MG	DA	3103	1/1	0.92	0.08	95,95,95,95	1
56	MG	CA	3082	1/1	0.92	0.09	84,84,84,84	0
56	MG	CA	3135	1/1	0.92	0.23	55,55,55,55	0
56	MG	AA	1649	1/1	0.92	0.17	140,140,140,140	0
56	MG	DA	3067	1/1	0.92	0.15	129,129,129,129	0
56	MG	DA	3116	1/1	0.92	0.22	93,93,93,93	1
56	MG	DA	3144	1/1	0.92	0.16	112,112,112,112	0
56	MG	CA	3102	1/1	0.92	0.18	55,55,55,55	0
56	MG	AA	1617	1/1	0.92	0.14	107,107,107,107	0
56	MG	DA	3070	1/1	0.92	0.15	69,69,69,69	0
56	MG	DA	3150	1/1	0.92	0.21	28,28,28,28	1
56	MG	DQ	801	1/1	0.92	0.45	60,60,60,60	0
56	MG	DA	3091	1/1	0.92	0.10	132,132,132,132	1
56	MG	BA	1625	1/1	0.93	0.16	171,171,171,171	0
56	MG	DA	3022	1/1	0.93	0.13	86,86,86,86	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	BA	1615	1/1	0.93	0.05	115,115,115,115	0
56	MG	CA	3100	1/1	0.93	0.34	66,66,66,66	0
56	MG	AA	1628	1/1	0.93	0.10	143,143,143,143	0
56	MG	AA	1607	1/1	0.93	0.10	98,98,98,98	0
56	MG	DA	3002	1/1	0.93	0.15	89,89,89,89	0
56	MG	DA	3101	1/1	0.93	0.13	125,125,125,125	1
56	MG	CA	3008	1/1	0.93	0.11	69,69,69,69	0
56	MG	DA	3107	1/1	0.93	0.11	112,112,112,112	0
56	MG	BA	1604	1/1	0.93	0.07	147,147,147,147	0
56	MG	CA	3119	1/1	0.93	0.12	81,81,81,81	1
56	MG	CA	3010	1/1	0.93	0.14	89,89,89,89	1
56	MG	DA	3050	1/1	0.93	0.16	79,79,79,79	0
56	MG	CA	3025	1/1	0.94	0.23	66,66,66,66	1
56	MG	DA	3012	1/1	0.94	0.10	81,81,81,81	0
56	MG	DA	3043	1/1	0.94	0.11	104,104,104,104	0
56	MG	DA	3099	1/1	0.94	0.12	114,114,114,114	1
56	MG	DA	3048	1/1	0.94	0.07	93,93,93,93	1
56	MG	CA	3110	1/1	0.94	0.07	86,86,86,86	1
56	MG	CA	3154	1/1	0.94	0.16	78,78,78,78	1
56	MG	CA	3132	1/1	0.94	0.20	67,67,67,67	0
56	MG	BA	1630	1/1	0.94	0.05	160,160,160,160	0
56	MG	CA	3156	1/1	0.94	0.09	84,84,84,84	0
56	MG	CA	3077	1/1	0.94	0.12	101,101,101,101	0
56	MG	CA	3037	1/1	0.94	0.21	40,40,40,40	0
56	MG	CA	3136	1/1	0.94	0.11	66,66,66,66	0
56	MG	CA	3002	1/1	0.94	0.19	67,67,67,67	1
56	MG	CA	3122	1/1	0.94	0.12	77,77,77,77	1
56	MG	CA	3101	1/1	0.94	0.07	84,84,84,84	0
56	MG	DA	3005	1/1	0.94	0.10	120,120,120,120	0
57	ZN	C0	101	1/1	0.94	0.09	177,177,177,177	1
56	MG	DA	3093	1/1	0.94	0.13	76,76,76,76	0
56	MG	BA	1616	1/1	0.95	0.12	136,136,136,136	0
56	MG	CA	3053	1/1	0.95	0.09	72,72,72,72	1
56	MG	BA	1640	1/1	0.95	0.08	145,145,145,145	0
56	MG	CA	3117	1/1	0.95	0.15	49,49,49,49	0
56	MG	BA	1619	1/1	0.95	0.05	133,133,133,133	0
56	MG	AA	1635	1/1	0.95	0.06	133,133,133,133	1
56	MG	CA	3036	1/1	0.95	0.08	80,80,80,80	1
56	MG	AA	1636	1/1	0.95	0.21	104,104,104,104	1
56	MG	AA	1637	1/1	0.95	0.18	186,186,186,186	0
56	MG	DA	3045	1/1	0.95	0.08	102,102,102,102	0
56	MG	AA	1626	1/1	0.95	0.29	107,107,107,107	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	CA	3072	1/1	0.95	0.09	73,73,73,73	1
56	MG	CA	3131	1/1	0.95	0.13	53,53,53,53	0
56	MG	CA	3096	1/1	0.95	0.17	68,68,68,68	1
56	MG	AA	1620	1/1	0.95	0.04	160,160,160,160	1
56	MG	DA	3057	1/1	0.95	0.12	101,101,101,101	0
56	MG	DA	3004	1/1	0.95	0.07	122,122,122,122	0
56	MG	DA	3059	1/1	0.95	0.17	94,94,94,94	1
56	MG	CA	3134	1/1	0.95	0.11	75,75,75,75	0
56	MG	DA	3006	1/1	0.95	0.07	114,114,114,114	1
56	MG	CA	3044	1/1	0.95	0.11	86,86,86,86	1
56	MG	DA	3010	1/1	0.95	0.09	97,97,97,97	0
56	MG	AA	1634	1/1	0.95	0.09	122,122,122,122	1
56	MG	CA	3104	1/1	0.95	0.13	85,85,85,85	1
56	MG	CA	3033	1/1	0.95	0.10	65,65,65,65	0
56	MG	DA	3016	1/1	0.95	0.22	90,90,90,90	0
56	MG	CA	3160	1/1	0.95	0.12	68,68,68,68	0
56	MG	DA	3071	1/1	0.95	0.11	101,101,101,101	1
56	MG	BA	1614	1/1	0.95	0.05	128,128,128,128	1
56	MG	CA	3139	1/1	0.95	0.11	88,88,88,88	0
56	MG	BA	1637	1/1	0.95	0.05	150,150,150,150	0
56	MG	DA	3026	1/1	0.95	0.07	102,102,102,102	0
56	MG	DA	3078	1/1	0.95	0.06	151,151,151,151	0
56	MG	DA	3079	1/1	0.96	0.09	144,144,144,144	0
56	MG	DA	3080	1/1	0.96	0.15	98,98,98,98	1
56	MG	DA	3039	1/1	0.96	0.10	74,74,74,74	0
56	MG	CA	3073	1/1	0.96	0.12	73,73,73,73	1
56	MG	DA	3042	1/1	0.96	0.06	97,97,97,97	0
56	MG	CA	3111	1/1	0.96	0.06	74,74,74,74	0
56	MG	CA	3021	1/1	0.96	0.13	78,78,78,78	0
56	MG	DA	3138	1/1	0.96	0.26	58,58,58,58	0
56	MG	DA	3047	1/1	0.96	0.10	122,122,122,122	0
56	MG	CA	3028	1/1	0.96	0.09	58,58,58,58	0
56	MG	CA	3065	1/1	0.96	0.09	76,76,76,76	1
56	MG	DA	3142	1/1	0.96	0.14	100,100,100,100	0
56	MG	CA	3047	1/1	0.96	0.12	94,94,94,94	0
56	MG	CA	3157	1/1	0.96	0.13	52,52,52,52	0
56	MG	DA	3011	1/1	0.96	0.12	80,80,80,80	0
56	MG	DA	3147	1/1	0.96	0.08	100,100,100,100	1
56	MG	CA	3120	1/1	0.96	0.07	71,71,71,71	1
56	MG	DA	3096	1/1	0.96	0.08	78,78,78,78	1
56	MG	CA	3097	1/1	0.96	0.15	67,67,67,67	1
56	MG	DA	3014	1/1	0.96	0.07	95,95,95,95	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	DA	3153	1/1	0.96	0.11	93,93,93,93	0
56	MG	AA	1614	1/1	0.96	0.16	103,103,103,103	0
56	MG	AA	1625	1/1	0.96	0.07	100,100,100,100	1
56	MG	CA	3145	1/1	0.96	0.07	69,69,69,69	0
56	MG	CA	3128	1/1	0.96	0.08	56,56,56,56	0
56	MG	CA	3085	1/1	0.96	0.08	71,71,71,71	0
56	MG	CA	3042	1/1	0.96	0.07	77,77,77,77	1
56	MG	CB	203	1/1	0.96	0.10	77,77,77,77	0
56	MG	CC	301	1/1	0.96	0.10	74,74,74,74	0
56	MG	CN	201	1/1	0.96	0.06	86,86,86,86	1
56	MG	DA	3114	1/1	0.96	0.10	98,98,98,98	1
56	MG	CA	3106	1/1	0.96	0.08	82,82,82,82	0
56	MG	DA	3030	1/1	0.96	0.07	132,132,132,132	1
56	MG	CQ	801	1/1	0.96	0.11	56,56,56,56	0
56	MG	DB	201	1/1	0.96	0.03	204,204,204,204	1
56	MG	DA	3119	1/1	0.96	0.07	92,92,92,92	0
56	MG	DA	3074	1/1	0.96	0.10	92,92,92,92	0
56	MG	DA	3126	1/1	0.96	0.04	93,93,93,93	0
56	MG	CA	3109	1/1	0.96	0.07	90,90,90,90	1
56	MG	BA	1601	1/1	0.96	0.12	115,115,115,115	0
57	ZN	C6	101	1/1	0.96	0.07	98,98,98,98	0
56	MG	BA	1602	1/1	0.96	0.10	132,132,132,132	0
56	MG	DA	3019	1/1	0.97	0.09	102,102,102,102	1
56	MG	DA	3108	1/1	0.97	0.08	97,97,97,97	0
56	MG	DA	3049	1/1	0.97	0.08	96,96,96,96	0
56	MG	CA	3061	1/1	0.97	0.13	95,95,95,95	1
56	MG	CA	3098	1/1	0.97	0.07	98,98,98,98	0
56	MG	DA	3024	1/1	0.97	0.12	98,98,98,98	0
56	MG	DA	3054	1/1	0.97	0.08	70,70,70,70	0
56	MG	DA	3115	1/1	0.97	0.07	139,139,139,139	0
56	MG	CA	3062	1/1	0.97	0.06	90,90,90,90	1
56	MG	CA	3140	1/1	0.97	0.11	61,61,61,61	0
56	MG	CA	3064	1/1	0.97	0.07	70,70,70,70	0
56	MG	DA	3086	1/1	0.97	0.07	125,125,125,125	1
56	MG	DA	3120	1/1	0.97	0.07	98,98,98,98	0
56	MG	DA	3121	1/1	0.97	0.06	100,100,100,100	1
56	MG	CA	3038	1/1	0.97	0.10	67,67,67,67	0
56	MG	DA	3125	1/1	0.97	0.10	92,92,92,92	1
56	MG	AA	1603	1/1	0.97	0.04	148,148,148,148	1
56	MG	BA	1603	1/1	0.97	0.06	121,121,121,121	0
56	MG	CA	3022	1/1	0.97	0.08	75,75,75,75	1
56	MG	DA	3034	1/1	0.97	0.04	99,99,99,99	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	DA	3065	1/1	0.97	0.07	85,85,85,85	0
56	MG	CA	3161	1/1	0.97	0.08	97,97,97,97	0
56	MG	CA	3130	1/1	0.97	0.10	62,62,62,62	1
56	MG	AA	1618	1/1	0.97	0.11	106,106,106,106	1
56	MG	AA	1612	1/1	0.97	0.05	128,128,128,128	0
56	MG	CA	3056	1/1	0.97	0.09	73,73,73,73	0
56	MG	CA	3059	1/1	0.97	0.14	60,60,60,60	0
56	MG	CA	3094	1/1	0.97	0.25	74,74,74,74	0
56	MG	DA	3017	1/1	0.97	0.15	73,73,73,73	0
56	MG	CA	3012	1/1	0.97	0.10	67,67,67,67	1
56	MG	DA	3106	1/1	0.97	0.07	90,90,90,90	1
56	MG	CA	3125	1/1	0.98	0.05	82,82,82,82	1
56	MG	CA	3095	1/1	0.98	0.06	86,86,86,86	1
56	MG	CA	3049	1/1	0.98	0.08	73,73,73,73	0
56	MG	DA	3064	1/1	0.98	0.06	95,95,95,95	0
56	MG	CA	3034	1/1	0.98	0.08	68,68,68,68	0
56	MG	DA	3143	1/1	0.98	0.10	53,53,53,53	0
56	MG	AA	1621	1/1	0.98	0.12	90,90,90,90	0
56	MG	CA	3003	1/1	0.98	0.10	82,82,82,82	0
56	MG	DA	3031	1/1	0.98	0.06	116,116,116,116	0
56	MG	CA	3014	1/1	0.98	0.13	72,72,72,72	1
56	MG	DA	3148	1/1	0.98	0.04	88,88,88,88	0
56	MG	DA	3003	1/1	0.98	0.04	121,121,121,121	0
56	MG	CA	3055	1/1	0.98	0.14	71,71,71,71	0
56	MG	AA	1623	1/1	0.98	0.10	104,104,104,104	1
56	MG	CA	3105	1/1	0.98	0.10	85,85,85,85	1
56	MG	CA	3058	1/1	0.98	0.07	74,74,74,74	1
56	MG	DA	3009	1/1	0.98	0.07	106,106,106,106	0
56	MG	DA	3041	1/1	0.98	0.07	100,100,100,100	0
56	MG	DA	3077	1/1	0.98	0.09	90,90,90,90	0
56	MG	CA	3158	1/1	0.98	0.08	73,73,73,73	0
56	MG	CA	3108	1/1	0.98	0.10	71,71,71,71	0
56	MG	DA	3044	1/1	0.98	0.03	125,125,125,125	0
56	MG	CA	3039	1/1	0.98	0.09	62,62,62,62	0
56	MG	CA	3016	1/1	0.98	0.32	20,20,20,20	0
56	MG	CA	3017	1/1	0.98	0.08	64,64,64,64	0
56	MG	CA	3018	1/1	0.98	0.06	90,90,90,90	1
56	MG	CA	3116	1/1	0.98	0.07	83,83,83,83	1
56	MG	CA	3089	1/1	0.98	0.07	92,92,92,92	1
56	MG	DA	3129	1/1	0.98	0.08	92,92,92,92	1
56	MG	CA	3167	1/1	0.98	0.05	102,102,102,102	0
56	MG	CA	3029	1/1	0.98	0.12	57,57,57,57	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	DA	3055	1/1	0.98	0.08	85,85,85,85	0
56	MG	DA	3020	1/1	0.98	0.11	77,77,77,77	0
56	MG	CA	3031	1/1	0.98	0.09	66,66,66,66	1
56	MG	CA	3006	1/1	0.98	0.06	90,90,90,90	1
56	MG	DA	3023	1/1	0.98	0.06	100,100,100,100	1
56	MG	CA	3048	1/1	0.98	0.12	80,80,80,80	1
56	MG	CA	3027	1/1	0.99	0.09	74,74,74,74	1
56	MG	CA	3057	1/1	0.99	0.03	78,78,78,78	1
56	MG	DA	3095	1/1	0.99	0.04	76,76,76,76	0
56	MG	CA	3112	1/1	0.99	0.04	73,73,73,73	1
56	MG	CA	3071	1/1	0.99	0.04	77,77,77,77	0
56	MG	CA	3114	1/1	0.99	0.06	73,73,73,73	1
56	MG	CA	3115	1/1	0.99	0.04	70,70,70,70	1
56	MG	CA	3009	1/1	0.99	0.04	69,69,69,69	0
56	MG	DA	3033	1/1	0.99	0.07	104,104,104,104	0
56	MG	DA	3102	1/1	0.99	0.03	98,98,98,98	1
56	MG	CA	3092	1/1	0.99	0.05	85,85,85,85	0
56	MG	DA	3104	1/1	0.99	0.09	101,101,101,101	0
56	MG	DA	3105	1/1	0.99	0.06	92,92,92,92	0
56	MG	CA	3004	1/1	0.99	0.09	78,78,78,78	0
56	MG	CA	3074	1/1	0.99	0.04	70,70,70,70	0
56	MG	CA	3030	1/1	0.99	0.03	84,84,84,84	1
56	MG	DA	3038	1/1	0.99	0.06	75,75,75,75	1
56	MG	DA	3008	1/1	0.99	0.05	103,103,103,103	1
56	MG	DA	3111	1/1	0.99	0.02	108,108,108,108	1
56	MG	CA	3121	1/1	0.99	0.10	86,86,86,86	1
56	MG	CA	3051	1/1	0.99	0.05	82,82,82,82	1
56	MG	CA	3123	1/1	0.99	0.13	83,83,83,83	1
56	MG	CA	3124	1/1	0.99	0.09	75,75,75,75	1
56	MG	CA	3078	1/1	0.99	0.04	102,102,102,102	1
56	MG	CA	3023	1/1	0.99	0.04	80,80,80,80	1
56	MG	DA	3046	1/1	0.99	0.04	111,111,111,111	1
56	MG	CA	3099	1/1	0.99	0.04	84,84,84,84	1
56	MG	CA	3080	1/1	0.99	0.04	62,62,62,62	1
56	MG	CA	3081	1/1	0.99	0.05	73,73,73,73	1
56	MG	CA	3032	1/1	0.99	0.12	79,79,79,79	0
56	MG	DA	3123	1/1	0.99	0.03	120,120,120,120	1
56	MG	DA	3124	1/1	0.99	0.05	104,104,104,104	0
56	MG	CA	3103	1/1	0.99	0.09	80,80,80,80	1
56	MG	DA	3085	1/1	0.99	0.04	112,112,112,112	0
56	MG	CA	3045	1/1	0.99	0.03	83,83,83,83	1
56	MG	DA	3053	1/1	0.99	0.03	98,98,98,98	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	CA	3066	1/1	0.99	0.05	80,80,80,80	1
56	MG	CA	3067	1/1	0.99	0.07	68,68,68,68	1
56	MG	CA	3086	1/1	0.99	0.08	93,93,93,93	1
56	MG	CA	3163	1/1	0.99	0.17	81,81,81,81	1
56	MG	CA	3046	1/1	0.99	0.08	77,77,77,77	1
57	ZN	D6	101	1/1	0.99	0.03	128,128,128,128	0
56	MG	CA	3076	1/1	1.00	0.02	68,68,68,68	0
56	MG	CA	3107	1/1	1.00	0.06	83,83,83,83	1
56	MG	CA	3063	1/1	1.00	0.04	94,94,94,94	1

5.5 Other polymers [i](#)

There are no such residues in this entry.