



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 29, 2026 – 07:20 AM UTC

PDB ID : 4V5B / pdb_00004v5b
Title : Structure of PDF binding helix in complex with the ribosome.
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Maier, T.; Schaffitzel, C.; Wiedmann, B.; Bukau, B.; Ban, N.
Deposited on : 2007-11-22
Resolution : 3.74 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
Xtrriage (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

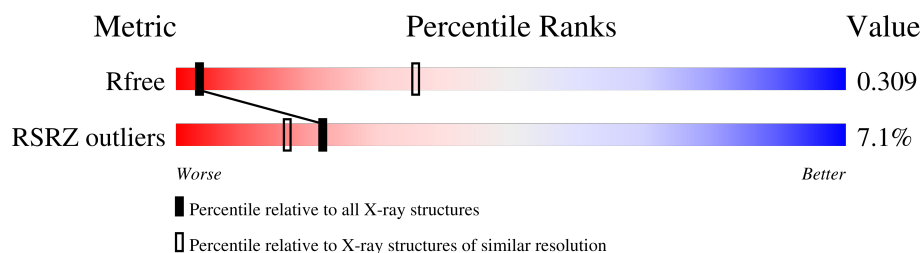
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.74 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	1234 (3.88-3.60)
RSRZ outliers	180081	1233 (3.88-3.60)

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	MG	AB	4092	-	-	-	X
54	MG	BA	4021	-	-	-	X

2 Entry composition

There are 55 unique types of molecules in this entry. The entry contains 284264 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 protein called 50S RIBOSOMAL PROTEIN L32.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A0	56	Total	C	N	O	S	0	0	0
			444	269	94	80	1			
1	C0	56	Total	C	N	O	S	0	0	0
			444	269	94	80	1			

- Molecule 2 is a protein called 50S RIBOSOMAL PROTEIN L33.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	A1	54	Total	C	N	O	0	0	0
			441	284	81	76			
2	C1	54	Total	C	N	O	0	0	0
			441	284	81	76			

- Molecule 3 is a protein called 50S RIBOSOMAL PROTEIN L34.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	A2	46	Total	C	N	O	S	0	0	0
			377	228	90	57	2			
3	C2	46	Total	C	N	O	S	0	0	0
			377	228	90	57	2			

- Molecule 4 is a protein called 50S RIBOSOMAL PROTEIN L35.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	A3	64	Total	C	N	O	S	0	0	0
			504	323	105	74	2			
4	C3	64	Total	C	N	O	S	0	0	0
			504	323	105	74	2			

- Molecule 5 is a protein called 50S RIBOSOMAL PROTEIN L36.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	A4	38	Total	C	N	O	S	0	0	0
			302	185	65	48	4			
5	C4	38	Total	C	N	O	S	0	0	0
			302	185	65	48	4			

- Molecule 6 is a protein called C-TERM HELIX PDF.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
6	A5	16	Total	C	N	O	0	0	0
			134	84	28	22			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A5	146	ALA	LEU	engineered mutation	UNP P0A6K3

- Molecule 7 is a RNA chain called 5S RIBOSOMAL RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	AA	117	Total	C	N	O	P	0	0	0
			2507	1116	459	815	117			
7	CA	117	Total	C	N	O	P	0	0	0
			2507	1116	459	815	117			

- Molecule 8 is a RNA chain called 23S RIBOSOMAL RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	AB	2841	Total	C	N	O	P	0	0	0
			60995	27210	11229	19715	2841			
8	CB	2841	Total	C	N	O	P	0	0	0
			60995	27210	11229	19715	2841			

- Molecule 9 is a protein called 50S RIBOSOMAL PROTEIN L2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	AC	268	Total	C	N	O	S	0	0	1
			2054	1271	417	359	7			
9	CC	268	Total	C	N	O	S	0	0	1
			2054	1271	417	359	7			

- Molecule 10 is a protein called 50S RIBOSOMAL PROTEIN L3.

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

- Molecule 11 is a protein called 50S RIBOSOMAL PROTEIN L4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	AE	201	Total	C	N	O	S	0	0	0
			1552	974	283	290	5			
11	CE	201	Total	C	N	O	S	0	0	0
			1552	974	283	290	5			

- Molecule 12 is a protein called 50S RIBOSOMAL PROTEIN L5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	AF	178	Total	C	N	O	S	0	0	0
			1420	905	251	258	6			
12	CF	178	Total	C	N	O	S	0	0	0
			1420	905	251	258	6			

- Molecule 13 is a protein called 50S RIBOSOMAL PROTEIN L6.

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

- Molecule 14 is a protein called 50S RIBOSOMAL PROTEIN L9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	AH	149	Total	C	N	O	S	0	0	0
			1111	699	197	214	1			
14	CH	149	Total	C	N	O	S	0	0	0
			1111	699	197	214	1			

- Molecule 15 is a protein called 50S RIBOSOMAL PROTEIN L11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	AI	141	Total	C	N	O	S	0	0	0
			1032	651	179	196	6			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	CI	141	Total	C	N	O	S	0	0	0
			1032	651	179	196	6			

- Molecule 16 is a protein called 50S RIBOSOMAL PROTEIN L13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	AJ	141	Total	C	N	O	S	0	0	1
			1113	704	211	194	4			
16	CJ	141	Total	C	N	O	S	0	0	1
			1113	704	211	194	4			

- Molecule 17 is a protein called 50S RIBOSOMAL PROTEIN L14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	AK	122	Total	C	N	O	S	0	0	1
			931	582	180	164	5			
17	CK	122	Total	C	N	O	S	0	0	1
			931	582	180	164	5			

- Molecule 18 is a protein called 50S RIBOSOMAL PROTEIN L15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
18	AL	144	Total	C	N	O	S	0	0	0
			1053	654	207	190	2			
18	CL	144	Total	C	N	O	S	0	0	0
			1053	654	207	190	2			

- Molecule 19 is a protein called 50S RIBOSOMAL PROTEIN L16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	AM	136	Total	C	N	O	S	0	0	0
			1074	686	205	177	6			
19	CM	136	Total	C	N	O	S	0	0	0
			1074	686	205	177	6			

- Molecule 20 is a protein called 50S RIBOSOMAL PROTEIN L17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	AN	127	Total	C	N	O	S	0	0	0
			1008	621	204	178	5			
20	CN	127	Total	C	N	O	S	0	0	0
			1008	621	204	178	5			

- Molecule 21 is a protein called 50S RIBOSOMAL PROTEIN L18.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
21	AO	117	Total	C	N	O	S	0	0	0
			900	557	179	163	1			
21	CO	117	Total	C	N	O	S	0	0	0
			900	557	179	163	1			

- Molecule 22 is a protein called 50S RIBOSOMAL PROTEIN L19.

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

- Molecule 23 is a protein called 50S RIBOSOMAL PROTEIN L20.

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

- Molecule 24 is a protein called 50S RIBOSOMAL PROTEIN L21.

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

- Molecule 25 is a protein called 50S RIBOSOMAL PROTEIN L22.

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

- Molecule 26 is a protein called 50S RIBOSOMAL PROTEIN L23.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	AT	100	Total	C	N	O	S	0	0	1
			778	491	146	139	2			
26	CT	100	Total	C	N	O	S	0	0	1
			778	491	146	139	2			

- Molecule 27 is a protein called 50S RIBOSOMAL PROTEIN L24.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
27	AU	103	Total	C	N	O	S	0	0	1
			780	492	147	141				
27	CU	103	Total	C	N	O	S	0	0	1
			780	492	147	141				

- Molecule 28 is a protein called 50S RIBOSOMAL PROTEIN L25.

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

- Molecule 29 is a protein called 50S RIBOSOMAL PROTEIN L27.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
29	AW	84	Total	C	N	O	S	0	0	0
			634	391	129	113	1			
29	CW	84	Total	C	N	O	S	0	0	0
			634	391	129	113	1			

- Molecule 30 is a protein called 50S RIBOSOMAL PROTEIN L29.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
30	AX	63	Total	C	N	O	S	0	0	0
			509	313	99	95	2			
30	CX	63	Total	C	N	O	S	0	0	0
			509	313	99	95	2			

- Molecule 31 is a protein called 50S RIBOSOMAL PROTEIN L30.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
31	AY	58	Total	C	N	O	S	0	0	0
			449	281	87	79	2			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
31	CY	58	Total	C	N	O	S	0	0	0
			449	281	87	79	2			

- Molecule 32 is a protein called 50S RIBOSOMAL PROTEIN L31.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
32	AZ	70	Total	C	N	O	S	0	0	0
			549	339	104	100	6			
32	CZ	70	Total	C	N	O	S	0	0	0
			549	339	104	100	6			

- Molecule 33 is a RNA chain called 16S RIBOSOMAL RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
33	BA	1530	Total	C	N	O	P	0	0	0
			32831	14642	6024	10635	1530			
33	DA	1530	Total	C	N	O	P	0	0	0
			32831	14642	6024	10635	1530			

- Molecule 34 is a protein called 30S RIBOSOMAL PROTEIN S2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
34	BB	219	Total	C	N	O	S	0	0	1
			1705	1081	306	311	7			
34	DB	219	Total	C	N	O	S	0	0	1
			1705	1081	306	311	7			

- Molecule 35 is a protein called 30S RIBOSOMAL PROTEIN S3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
35	BC	207	Total	C	N	O	S	0	0	1
			1625	1028	306	288	3			
35	DC	207	Total	C	N	O	S	0	0	1
			1625	1028	306	288	3			

- Molecule 36 is a protein called 30S RIBOSOMAL PROTEIN S4.

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

- Molecule 37 is a protein called 30S RIBOSOMAL PROTEIN S5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
37	BE	151	Total	C	N	O	S	0	0	1
			1106	687	212	201	6			
37	DE	151	Total	C	N	O	S	0	0	1
			1106	687	212	201	6			

- Molecule 38 is a protein called 30S RIBOSOMAL PROTEIN S6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
38	BF	101	Total	C	N	O	S	0	0	1
			818	515	149	148	6			
38	DF	101	Total	C	N	O	S	0	0	1
			818	515	149	148	6			

- Molecule 39 is a protein called 30S RIBOSOMAL PROTEIN S7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
39	BG	151	Total	C	N	O	S	0	0	1
			1175	730	227	214	4			
39	DG	153	Total	C	N	O	S	0	0	1
			1197	745	231	217	4			

- Molecule 40 is a protein called 30S RIBOSOMAL PROTEIN S8.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
40	BH	129	Total	C	N	O	S	0	0	0
			979	616	173	184	6			
40	DH	129	Total	C	N	O	S	0	0	0
			979	616	173	184	6			

- Molecule 41 is a protein called 30S RIBOSOMAL PROTEIN S9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
41	BI	127	Total	C	N	O	S	0	0	0
			1022	634	206	179	3			
41	DI	127	Total	C	N	O	S	0	0	0
			1022	634	206	179	3			

- Molecule 42 is a protein called 30S RIBOSOMAL PROTEIN S10.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
42	BJ	99	Total	C	N	O	S	0	0	1
			787	493	151	142	1			
42	DJ	99	Total	C	N	O	S	0	0	1
			787	493	151	142	1			

- Molecule 43 is a protein called 30S RIBOSOMAL PROTEIN S11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
43	BK	117	Total	C	N	O	S	0	0	0
			877	540	174	160	3			
43	DK	117	Total	C	N	O	S	0	0	0
			877	540	174	160	3			

- Molecule 44 is a protein called 30S RIBOSOMAL PROTEIN S12.

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

- Molecule 45 is a protein called 30S RIBOSOMAL PROTEIN S13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
45	BM	115	Total	C	N	O	S	0	0	1
			884	546	179	156	3			
45	DM	114	Total	C	N	O	S	0	0	1
			877	541	178	155	3			

- Molecule 46 is a protein called 30S RIBOSOMAL PROTEIN S14.

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

- Molecule 47 is a protein called 30S RIBOSOMAL PROTEIN S15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
47	BO	88	Total	C	N	O	S	0	0	0
			716	440	146	129	1			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
47	DO	88	Total	C	N	O	S	0	0	0
			716	440	146	129	1			

- Molecule 48 is a protein called 30S RIBOSOMAL PROTEIN S16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
48	BP	82	Total	C	N	O	S	0	0	0
			649	406	128	114	1			
48	DP	81	Total	C	N	O	S	0	0	1
			639	400	127	111	1			

- Molecule 49 is a protein called 30S RIBOSOMAL PROTEIN S17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
49	BQ	81	Total	C	N	O	S	0	0	1
			649	411	122	113	3			
49	DQ	81	Total	C	N	O	S	0	0	0
			657	417	122	115	3			

- Molecule 50 is a protein called 30S RIBOSOMAL PROTEIN S18.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
50	BR	56	Total	C	N	O	0	0	1
			456	288	87	81			
50	DR	56	Total	C	N	O	0	0	1
			456	288	87	81			

- Molecule 51 is a protein called 30S RIBOSOMAL PROTEIN S19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
51	BS	80	Total	C	N	O	S	0	0	1
			638	408	121	107	2			
51	DS	81	Total	C	N	O	S	0	0	1
			645	413	122	108	2			

- Molecule 52 is a protein called 30S RIBOSOMAL PROTEIN S20.

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

- Molecule 53 is a protein called 30S RIBOSOMAL PROTEIN S21.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
53	BU	52	Total	C	N	O	S	0	0	1
			426	265	87	73	1			
53	DU	52	Total	C	N	O	S	0	0	1
			426	265	87	73	1			

- Molecule 54 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
54	AB	109	Total	Mg	0	0
			109	109		
54	AE	1	Total	Mg	0	0
			1	1		
54	BA	58	Total	Mg	0	0
			58	58		
54	BN	1	Total	Mg	0	0
			1	1		
54	BT	1	Total	Mg	0	0
			1	1		
54	CB	109	Total	Mg	0	0
			109	109		
54	CC	1	Total	Mg	0	0
			1	1		
54	CL	1	Total	Mg	0	0
			1	1		
54	DA	61	Total	Mg	0	0
			61	61		
54	DN	1	Total	Mg	0	0
			1	1		

- Molecule 55 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
55	A2	2	Total	O	0	0
			2	2		
55	AB	489	Total	O	0	0
			489	489		
55	AC	3	Total	O	0	0
			3	3		
55	AD	1	Total	O	0	0
			1	1		
55	AE	3	Total	O	0	0
			3	3		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
55	AJ	2	Total O 2 2	0	0
55	AL	3	Total O 3 3	0	0
55	BA	284	Total O 284 284	0	0
55	BE	3	Total O 3 3	0	0
55	BI	2	Total O 2 2	0	0
55	BK	1	Total O 1 1	0	0
55	BL	2	Total O 2 2	0	0
55	BN	3	Total O 3 3	0	0
55	BP	1	Total O 1 1	0	0
55	BT	2	Total O 2 2	0	0
55	C0	1	Total O 1 1	0	0
55	C2	2	Total O 2 2	0	0
55	CB	485	Total O 485 485	0	0
55	CC	3	Total O 3 3	0	0
55	CD	1	Total O 1 1	0	0
55	CE	1	Total O 1 1	0	0
55	CJ	2	Total O 2 2	0	0
55	CK	1	Total O 1 1	0	0
55	CL	5	Total O 5 5	0	0
55	CN	3	Total O 3 3	0	0
55	CP	1	Total O 1 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
55	CQ	1	Total 1	O 1	0	0
55	CT	2	Total 2	O 2	0	0
55	CU	1	Total 1	O 1	0	0
55	DA	293	Total 293	O 293	0	0
55	DD	1	Total 1	O 1	0	0
55	DE	2	Total 2	O 2	0	0
55	DG	1	Total 1	O 1	0	0
55	DL	4	Total 4	O 4	0	0
55	DN	2	Total 2	O 2	0	0
55	DP	1	Total 1	O 1	0	0
55	DT	3	Total 3	O 3	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	208.18Å 380.08Å 736.70Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 3.74 50.00 – 3.74	Depositor EDS
% Data completeness (in resolution range)	91.5 (50.00-3.74) 91.5 (50.00-3.74)	Depositor EDS
R_{merge}	0.18	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.52 (at 3.77Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.259 , 0.323 0.251 , 0.309	Depositor DCC
R_{free} test set	5544 reflections (1.01%)	wwPDB-VP
Wilson B-factor (Å ²)	90.4	Xtriage
Anisotropy	0.290	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.19 , 71.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.34$, $\langle L^2 \rangle = 0.17$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	284264	wwPDB-VP
Average B, all atoms (Å ²)	129.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.64% 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 343 ligands modelled in this entry, 343 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
33	BA	1
15	CI	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	BA	1045:C	O3'	1046:A	P	4.69
1	CI	72:THR	C	73:PRO	N	4.33

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	A0	56/56 (100%)	0.74	7 (12%) 8 10	109, 149, 271, 317	0
1	C0	56/56 (100%)	1.16	11 (19%) 3 4	97, 120, 190, 244	0
2	A1	54/54 (100%)	0.88	10 (18%) 3 4	124, 143, 239, 296	0
2	C1	54/54 (100%)	0.71	3 (5%) 30 20	92, 113, 223, 254	0
3	A2	46/46 (100%)	1.08	12 (26%) 1 2	74, 92, 165, 271	0
3	C2	46/46 (100%)	1.03	9 (19%) 3 4	68, 103, 198, 264	0
4	A3	64/64 (100%)	1.73	23 (35%) 1 1	80, 106, 228, 309	0
4	C3	64/64 (100%)	1.73	22 (34%) 1 1	69, 99, 174, 229	0
5	A4	38/38 (100%)	1.71	15 (39%) 1 1	115, 135, 250, 284	0
5	C4	38/38 (100%)	2.61	22 (57%) 0 0	124, 144, 238, 298	0
6	A5	16/16 (100%)	-0.41	0 100 100	73, 108, 197, 216	0
7	AA	117/120 (97%)	-0.11	2 (1%) 69 44	78, 127, 174, 316	0
7	CA	117/120 (97%)	-0.00	4 (3%) 48 31	71, 126, 170, 285	0
8	AB	2841/2904 (97%)	0.07	80 (2%) 55 35	57, 105, 213, 373	0
8	CB	2841/2904 (97%)	-0.05	58 (2%) 65 42	41, 89, 202, 421	0
9	AC	268/273 (98%)	0.79	38 (14%) 6 8	71, 107, 196, 257	0
9	CC	268/273 (98%)	0.80	37 (13%) 6 8	63, 91, 165, 248	0
10	AD	209/209 (100%)	0.83	28 (13%) 7 9	12, 127, 226, 325	0
10	CD	209/209 (100%)	0.68	21 (10%) 12 13	11, 94, 186, 271	0
11	AE	201/201 (100%)	0.57	19 (9%) 14 13	92, 120, 206, 299	0
11	CE	201/201 (100%)	0.95	31 (15%) 5 7	88, 117, 224, 290	0
12	AF	178/178 (100%)	0.38	10 (5%) 30 20	121, 170, 253, 334	0
12	CF	178/178 (100%)	0.30	8 (4%) 38 25	92, 155, 224, 286	0
13	AG	176/176 (100%)	-0.07	4 (2%) 61 39	100, 137, 207, 246	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å ²)	Q<0.9
13	CG	176/176 (100%)	0.51	15 (8%)	16 14	88, 138, 222, 271	0
14	AH	149/149 (100%)	0.33	6 (4%)	42 28	71, 314, 427, 456	0
14	CH	149/149 (100%)	0.12	7 (4%)	36 24	107, 147, 233, 274	0
15	AI	141/141 (100%)	0.76	20 (14%)	6 8	155, 233, 307, 356	0
15	CI	141/141 (100%)	0.97	23 (16%)	4 6	219, 343, 422, 470	0
16	AJ	141/142 (99%)	0.85	23 (16%)	4 6	105, 130, 217, 267	0
16	CJ	141/142 (99%)	1.10	29 (20%)	2 3	104, 121, 207, 250	0
17	AK	122/123 (99%)	0.46	7 (5%)	29 20	81, 109, 162, 234	0
17	CK	122/123 (99%)	0.39	4 (3%)	49 31	80, 94, 127, 208	0
18	AL	144/144 (100%)	1.69	44 (30%)	1 2	94, 138, 281, 363	0
18	CL	144/144 (100%)	1.33	37 (25%)	1 2	83, 128, 275, 315	0
19	AM	136/136 (100%)	0.91	22 (16%)	4 6	105, 126, 222, 268	0
19	CM	136/136 (100%)	0.75	17 (12%)	8 10	77, 108, 223, 279	0
20	AN	127/127 (100%)	0.78	19 (14%)	5 7	96, 114, 200, 251	0
20	CN	127/127 (100%)	0.34	4 (3%)	51 32	58, 78, 155, 257	0
21	AO	117/117 (100%)	0.72	16 (13%)	6 8	107, 162, 236, 299	0
21	CO	117/117 (100%)	0.58	16 (13%)	6 8	52, 118, 211, 255	0
22	AP	114/114 (100%)	0.53	9 (7%)	18 15	85, 123, 219, 281	0
22	CP	114/114 (100%)	0.39	11 (9%)	13 13	77, 96, 196, 257	0
23	AQ	117/117 (100%)	0.65	10 (8%)	16 14	70, 106, 152, 203	0
23	CQ	117/117 (100%)	0.63	10 (8%)	16 14	70, 93, 148, 225	0
24	AR	103/103 (100%)	0.92	21 (20%)	3 4	105, 145, 250, 346	0
24	CR	103/103 (100%)	0.76	16 (15%)	5 7	87, 132, 229, 286	0
25	AS	110/110 (100%)	0.59	10 (9%)	15 13	77, 106, 167, 279	0
25	CS	110/110 (100%)	0.38	5 (4%)	38 25	49, 85, 152, 211	0
26	AT	100/100 (100%)	0.65	12 (12%)	9 10	94, 130, 222, 250	0
26	CT	100/100 (100%)	0.80	7 (7%)	22 17	85, 120, 248, 278	0
27	AU	103/103 (100%)	1.34	29 (28%)	1 2	90, 140, 235, 264	0
27	CU	103/103 (100%)	1.01	22 (21%)	2 3	118, 162, 256, 281	0
28	AV	94/94 (100%)	0.19	6 (6%)	25 18	86, 136, 209, 234	0
28	CV	94/94 (100%)	0.18	5 (5%)	32 22	87, 124, 194, 215	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
29	AW	84/84 (100%)	0.99	18 (21%) 2 3	116, 147, 244, 330	0
29	CW	84/84 (100%)	1.27	17 (20%) 3 3	111, 136, 238, 275	0
30	AX	63/63 (100%)	0.34	2 (3%) 50 32	84, 130, 208, 247	0
30	CX	63/63 (100%)	0.55	6 (9%) 14 13	86, 150, 233, 320	0
31	AY	58/58 (100%)	0.87	9 (15%) 5 7	116, 143, 272, 279	0
31	CY	58/58 (100%)	1.01	11 (18%) 3 4	126, 138, 240, 249	0
32	AZ	70/70 (100%)	0.51	7 (10%) 12 13	66, 104, 170, 258	0
32	CZ	70/70 (100%)	0.98	12 (17%) 4 6	70, 91, 169, 255	0
33	BA	1530/1542 (99%)	0.09	38 (2%) 58 37	70, 137, 279, 497	0
33	DA	1530/1542 (99%)	-0.11	25 (1%) 70 45	45, 111, 224, 368	0
34	BB	219/240 (91%)	0.07	5 (2%) 61 39	94, 175, 269, 316	0
34	DB	219/240 (91%)	-0.03	2 (0%) 81 58	108, 159, 243, 292	0
35	BC	207/232 (89%)	0.05	9 (4%) 40 26	87, 169, 255, 315	0
35	DC	207/232 (89%)	-0.03	7 (3%) 48 31	113, 140, 207, 226	0
36	BD	205/205 (100%)	0.50	16 (7%) 19 15	61, 139, 230, 325	0
36	DD	205/205 (100%)	-0.02	4 (1%) 65 42	71, 102, 169, 227	0
37	BE	151/166 (90%)	0.37	13 (8%) 16 14	75, 156, 254, 336	0
37	DE	151/166 (90%)	-0.10	5 (3%) 49 31	56, 99, 174, 250	0
38	BF	101/135 (74%)	0.21	6 (5%) 28 20	57, 140, 224, 279	0
38	DF	101/135 (74%)	0.25	5 (4%) 34 23	110, 137, 200, 247	0
39	BG	151/178 (84%)	0.50	15 (9%) 13 13	94, 206, 288, 333	0
39	DG	153/178 (85%)	0.02	4 (2%) 57 36	44, 144, 206, 228	0
40	BH	129/129 (100%)	0.45	9 (6%) 22 17	76, 157, 231, 297	0
40	DH	129/129 (100%)	0.02	4 (3%) 51 32	70, 98, 166, 216	0
41	BI	127/129 (98%)	0.76	19 (14%) 5 7	90, 194, 271, 307	0
41	DI	127/129 (98%)	0.51	16 (12%) 8 10	103, 165, 231, 281	0
42	BJ	99/103 (96%)	1.19	23 (23%) 2 3	131, 254, 373, 423	0
42	DJ	99/103 (96%)	0.78	11 (11%) 10 11	130, 173, 223, 237	0
43	BK	117/128 (91%)	0.31	6 (5%) 33 23	54, 128, 245, 290	0
43	DK	117/128 (91%)	0.20	8 (6%) 23 17	69, 100, 165, 222	0
44	BL	123/123 (100%)	0.68	14 (11%) 10 11	50, 138, 215, 332	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
44	DL	123/123 (100%)	0.44	10 (8%) 18 14	64, 95, 150, 211	0
45	BM	115/117 (98%)	0.50	5 (4%) 40 26	144, 252, 315, 344	0
45	DM	114/117 (97%)	0.24	7 (6%) 27 19	113, 171, 221, 288	0
46	BN	96/100 (96%)	0.95	17 (17%) 4 5	85, 188, 308, 367	0
46	DN	96/100 (96%)	0.88	16 (16%) 4 6	105, 153, 250, 295	0
47	BO	88/89 (98%)	0.17	3 (3%) 48 31	67, 133, 213, 255	0
47	DO	88/89 (98%)	0.20	4 (4%) 38 25	73, 105, 170, 201	0
48	BP	82/82 (100%)	0.70	8 (9%) 13 13	90, 168, 269, 347	0
48	DP	81/82 (98%)	0.33	5 (6%) 26 19	69, 93, 145, 202	0
49	BQ	81/83 (97%)	0.81	15 (18%) 3 4	101, 180, 266, 301	0
49	DQ	81/83 (97%)	0.19	5 (6%) 26 19	65, 109, 172, 212	0
50	BR	56/74 (75%)	0.19	1 (1%) 67 43	66, 117, 216, 283	0
50	DR	56/74 (75%)	0.23	2 (3%) 46 30	74, 103, 172, 253	0
51	BS	80/91 (87%)	0.78	12 (15%) 5 7	152, 267, 315, 366	0
51	DS	81/91 (89%)	0.46	9 (11%) 10 11	122, 182, 230, 249	0
52	BT	85/86 (98%)	0.60	9 (10%) 11 12	76, 155, 224, 256	0
52	DT	85/86 (98%)	0.47	13 (15%) 5 7	79, 97, 185, 219	0
53	BU	52/71 (73%)	0.37	3 (5%) 29 20	91, 171, 256, 300	0
53	DU	52/71 (73%)	0.71	8 (15%) 5 7	95, 140, 201, 249	0
All	All	20487/21050 (97%)	0.32	1454 (7%) 22 16	11, 121, 254, 497	0

The worst 5 of 1454 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
5	C4	31	PRO	10.8
26	CT	72	GLN	9.3
27	AU	56	GLY	9.0
13	CG	172	GLU	9.0
15	CI	83	ALA	8.8

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 ⓘ

There are no oligosaccharides in this entry.

5.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	AB	4092	1/1	0.65	0.63	27,27,27,27	1
54	MG	BA	4021	1/1	0.75	0.51	28,28,28,28	1
54	MG	DA	1626	1/1	0.79	0.14	11,11,11,11	1
54	MG	CB	3108	1/1	0.81	0.41	53,53,53,53	1
54	MG	AB	4031	1/1	0.81	0.08	56,56,56,56	0
54	MG	BA	4053	1/1	0.82	0.14	109,109,109,109	0
54	MG	AB	4022	1/1	0.82	0.20	11,11,11,11	0
54	MG	BA	4023	1/1	0.82	0.76	63,63,63,63	1
54	MG	DA	1610	1/1	0.83	0.07	48,48,48,48	0
54	MG	AB	4013	1/1	0.83	0.08	46,46,46,46	0
54	MG	BA	4018	1/1	0.84	0.08	64,64,64,64	0
54	MG	DA	1644	1/1	0.84	0.29	53,53,53,53	0
54	MG	DA	1612	1/1	0.85	0.13	81,81,81,81	0
54	MG	AB	4099	1/1	0.86	0.11	12,12,12,12	1
54	MG	BA	4028	1/1	0.86	0.12	61,61,61,61	0
54	MG	BA	4013	1/1	0.87	0.11	73,73,73,73	0
54	MG	BA	4056	1/1	0.87	0.30	81,81,81,81	0
54	MG	DA	1613	1/1	0.87	0.10	62,62,62,62	0
54	MG	CB	3080	1/1	0.87	2.20	55,55,55,55	1
54	MG	BA	4042	1/1	0.87	0.23	69,69,69,69	0
54	MG	DA	1632	1/1	0.88	0.20	90,90,90,90	0
54	MG	BA	4054	1/1	0.88	0.23	90,90,90,90	0
54	MG	DA	1628	1/1	0.89	0.22	33,33,33,33	1
54	MG	DA	1625	1/1	0.89	0.76	37,37,37,37	1
54	MG	BA	4044	1/1	0.89	0.14	86,86,86,86	0
54	MG	DA	1651	1/1	0.89	0.10	56,56,56,56	0
54	MG	AB	4026	1/1	0.90	0.14	78,78,78,78	0
54	MG	BN	201	1/1	0.90	0.17	61,61,61,61	0
54	MG	DA	1608	1/1	0.90	0.11	41,41,41,41	0
54	MG	CB	3063	1/1	0.90	0.15	11,11,11,11	0
54	MG	BA	4043	1/1	0.91	0.14	25,25,25,25	0
54	MG	AB	4096	1/1	0.91	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
54	MG	BA	4035	1/1	0.91	0.28	30,30,30,30	0
54	MG	AB	4047	1/1	0.91	0.06	48,48,48,48	0
54	MG	CB	3099	1/1	0.91	0.12	43,43,43,43	0
54	MG	DA	1624	1/1	0.91	0.20	57,57,57,57	0
54	MG	AB	4050	1/1	0.92	0.14	49,49,49,49	0
54	MG	AB	4045	1/1	0.92	0.08	51,51,51,51	0
54	MG	BA	4022	1/1	0.92	0.19	14,14,14,14	0
54	MG	CB	3090	1/1	0.92	0.09	67,67,67,67	0
54	MG	CB	3094	1/1	0.92	0.13	16,16,16,16	0
54	MG	BA	4012	1/1	0.92	0.10	54,54,54,54	0
54	MG	BA	4025	1/1	0.92	0.07	37,37,37,37	0
54	MG	DA	1634	1/1	0.92	0.11	110,110,110,110	0
54	MG	BA	4026	1/1	0.92	0.10	75,75,75,75	0
54	MG	AB	4095	1/1	0.92	0.09	47,47,47,47	0
54	MG	CB	3104	1/1	0.93	0.20	6,6,6,6	0
54	MG	AB	4082	1/1	0.93	0.17	50,50,50,50	0
54	MG	AB	4025	1/1	0.93	0.17	129,129,129,129	0
54	MG	AB	4004	1/1	0.93	0.11	41,41,41,41	0
54	MG	BA	4031	1/1	0.93	0.36	40,40,40,40	0
54	MG	CB	3040	1/1	0.93	0.14	46,46,46,46	0
54	MG	DA	1619	1/1	0.93	0.08	64,64,64,64	0
54	MG	CB	3052	1/1	0.93	0.20	43,43,43,43	0
54	MG	BA	4032	1/1	0.93	0.13	27,27,27,27	0
54	MG	CB	3077	1/1	0.93	0.05	76,76,76,76	0
54	MG	CB	3079	1/1	0.93	0.05	54,54,54,54	0
54	MG	BA	4020	1/1	0.93	0.13	77,77,77,77	0
54	MG	AB	4007	1/1	0.93	0.14	37,37,37,37	0
54	MG	DA	1637	1/1	0.93	0.06	109,109,109,109	0
54	MG	AB	4075	1/1	0.93	0.12	41,41,41,41	0
54	MG	BA	4002	1/1	0.93	0.07	86,86,86,86	0
54	MG	CB	3106	1/1	0.94	0.07	20,20,20,20	0
54	MG	CB	3007	1/1	0.94	0.07	25,25,25,25	0
54	MG	DA	1607	1/1	0.94	0.08	54,54,54,54	0
54	MG	CB	3014	1/1	0.94	0.08	33,33,33,33	0
54	MG	CB	3036	1/1	0.94	0.16	19,19,19,19	0
54	MG	BA	4038	1/1	0.94	0.10	50,50,50,50	0
54	MG	CB	3043	1/1	0.94	0.11	69,69,69,69	0
54	MG	AB	4101	1/1	0.94	0.07	25,25,25,25	0
54	MG	AB	4003	1/1	0.94	0.05	26,26,26,26	0
54	MG	BA	4027	1/1	0.94	0.09	68,68,68,68	0
54	MG	BA	4047	1/1	0.94	0.04	29,29,29,29	0
54	MG	BA	4005	1/1	0.94	0.15	59,59,59,59	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	DA	1629	1/1	0.94	0.29	52,52,52,52	0
54	MG	CB	3087	1/1	0.94	0.23	25,25,25,25	0
54	MG	AB	4098	1/1	0.94	0.23	37,37,37,37	0
54	MG	AB	4023	1/1	0.94	0.18	66,66,66,66	0
54	MG	BA	4024	1/1	0.94	0.08	32,32,32,32	1
54	MG	DA	1648	1/1	0.94	0.06	43,43,43,43	0
54	MG	DA	1649	1/1	0.94	0.06	45,45,45,45	0
54	MG	BT	101	1/1	0.94	0.08	27,27,27,27	0
54	MG	CB	3029	1/1	0.95	0.08	39,39,39,39	0
54	MG	CL	201	1/1	0.95	0.05	43,43,43,43	0
54	MG	AB	4053	1/1	0.95	0.07	14,14,14,14	0
54	MG	CB	3037	1/1	0.95	0.13	10,10,10,10	0
54	MG	DA	1609	1/1	0.95	0.06	56,56,56,56	0
54	MG	AB	4064	1/1	0.95	0.05	43,43,43,43	0
54	MG	BA	4015	1/1	0.95	0.05	59,59,59,59	0
54	MG	CB	3048	1/1	0.95	0.17	4,4,4,4	0
54	MG	DA	1614	1/1	0.95	0.13	25,25,25,25	0
54	MG	DA	1618	1/1	0.95	0.06	30,30,30,30	0
54	MG	CB	3050	1/1	0.95	0.03	45,45,45,45	0
54	MG	DA	1623	1/1	0.95	0.15	20,20,20,20	0
54	MG	CB	3051	1/1	0.95	0.15	12,12,12,12	0
54	MG	BA	4048	1/1	0.95	0.05	73,73,73,73	0
54	MG	BA	4049	1/1	0.95	0.19	100,100,100,100	0
54	MG	AB	4065	1/1	0.95	0.09	20,20,20,20	0
54	MG	BA	4030	1/1	0.95	0.21	34,34,34,34	0
54	MG	AB	4011	1/1	0.95	0.13	45,45,45,45	0
54	MG	AB	4048	1/1	0.95	0.17	22,22,22,22	0
54	MG	BA	4001	1/1	0.95	0.07	69,69,69,69	0
54	MG	AB	4091	1/1	0.95	0.06	34,34,34,34	0
54	MG	DA	1647	1/1	0.95	0.07	30,30,30,30	0
54	MG	CB	3010	1/1	0.95	0.07	30,30,30,30	0
54	MG	AB	4017	1/1	0.95	0.19	10,10,10,10	0
54	MG	CB	3020	1/1	0.95	0.18	8,8,8,8	0
54	MG	DA	1659	1/1	0.95	0.08	85,85,85,85	0
54	MG	CB	3101	1/1	0.96	0.17	8,8,8,8	0
54	MG	BA	4033	1/1	0.96	0.06	90,90,90,90	0
54	MG	AB	4043	1/1	0.96	0.17	16,16,16,16	0
54	MG	AB	4055	1/1	0.96	0.04	68,68,68,68	0
54	MG	CB	3032	1/1	0.96	0.05	52,52,52,52	0
54	MG	DA	1605	1/1	0.96	0.07	76,76,76,76	0
54	MG	BA	4019	1/1	0.96	0.13	11,11,11,11	0
54	MG	AB	4063	1/1	0.96	0.12	16,16,16,16	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	CB	3038	1/1	0.96	0.07	58,58,58,58	0
54	MG	AB	4008	1/1	0.96	0.07	38,38,38,38	0
54	MG	BA	4046	1/1	0.96	0.11	62,62,62,62	0
54	MG	AB	4097	1/1	0.96	0.13	17,17,17,17	0
54	MG	CB	3049	1/1	0.96	0.11	30,30,30,30	1
54	MG	AB	4015	1/1	0.96	0.11	3,3,3,3	0
54	MG	AB	4069	1/1	0.96	0.09	51,51,51,51	0
54	MG	DA	1622	1/1	0.96	0.12	27,27,27,27	0
54	MG	BA	4051	1/1	0.96	0.12	79,79,79,79	0
54	MG	AB	4033	1/1	0.96	0.04	52,52,52,52	0
54	MG	CB	3065	1/1	0.96	0.09	26,26,26,26	0
54	MG	CB	3071	1/1	0.96	0.12	52,52,52,52	0
54	MG	CB	3072	1/1	0.96	0.16	42,42,42,42	0
54	MG	CB	3074	1/1	0.96	0.05	33,33,33,33	0
54	MG	AB	4108	1/1	0.96	0.09	9,9,9,9	0
54	MG	AB	4078	1/1	0.96	0.05	35,35,35,35	0
54	MG	AB	4034	1/1	0.96	0.09	51,51,51,51	0
54	MG	DA	1641	1/1	0.96	0.15	63,63,63,63	0
54	MG	AB	4085	1/1	0.96	0.13	53,53,53,53	0
54	MG	DA	1645	1/1	0.96	0.06	56,56,56,56	0
54	MG	CB	3005	1/1	0.96	0.05	26,26,26,26	0
54	MG	CB	3093	1/1	0.96	0.10	3,3,3,3	0
54	MG	AB	4088	1/1	0.96	0.10	24,24,24,24	0
54	MG	CB	3096	1/1	0.96	0.10	38,38,38,38	0
54	MG	DA	1653	1/1	0.96	0.07	21,21,21,21	0
54	MG	DA	1657	1/1	0.96	0.40	63,63,63,63	0
54	MG	AB	4090	1/1	0.96	0.14	37,37,37,37	0
54	MG	CB	3027	1/1	0.97	0.10	40,40,40,40	0
54	MG	AB	4074	1/1	0.97	0.11	50,50,50,50	0
54	MG	CB	3030	1/1	0.97	0.14	17,17,17,17	0
54	MG	CB	3102	1/1	0.97	0.08	17,17,17,17	0
54	MG	AB	4057	1/1	0.97	0.14	49,49,49,49	0
54	MG	CB	3105	1/1	0.97	0.12	20,20,20,20	0
54	MG	BA	4007	1/1	0.97	0.09	81,81,81,81	0
54	MG	AB	4061	1/1	0.97	0.10	35,35,35,35	0
54	MG	AB	4080	1/1	0.97	0.09	17,17,17,17	0
54	MG	DA	1603	1/1	0.97	0.05	22,22,22,22	0
54	MG	BA	4014	1/1	0.97	0.05	44,44,44,44	0
54	MG	CB	3041	1/1	0.97	0.04	19,19,19,19	0
54	MG	CB	3042	1/1	0.97	0.11	18,18,18,18	0
54	MG	BA	4029	1/1	0.97	0.05	44,44,44,44	0
54	MG	AB	4029	1/1	0.97	0.05	55,55,55,55	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	DA	1611	1/1	0.97	0.05	51,51,51,51	0
54	MG	BA	4017	1/1	0.97	0.04	42,42,42,42	0
54	MG	BA	4055	1/1	0.97	0.10	27,27,27,27	0
54	MG	AB	4040	1/1	0.97	0.10	77,77,77,77	0
54	MG	BA	4057	1/1	0.97	0.04	29,29,29,29	0
54	MG	CB	3058	1/1	0.97	0.06	31,31,31,31	0
54	MG	CB	3061	1/1	0.97	0.04	31,31,31,31	0
54	MG	AB	4046	1/1	0.97	0.06	26,26,26,26	0
54	MG	BA	4034	1/1	0.97	0.13	48,48,48,48	0
54	MG	CB	3070	1/1	0.97	0.16	33,33,33,33	0
54	MG	CB	3001	1/1	0.97	0.12	9,9,9,9	0
54	MG	DA	1627	1/1	0.97	0.05	51,51,51,51	0
54	MG	AB	4103	1/1	0.97	0.06	13,13,13,13	0
54	MG	BA	4037	1/1	0.97	0.06	58,58,58,58	0
54	MG	CB	3075	1/1	0.97	0.05	61,61,61,61	0
54	MG	CB	3076	1/1	0.97	0.13	15,15,15,15	0
54	MG	DA	1635	1/1	0.97	0.06	41,41,41,41	0
54	MG	AB	4068	1/1	0.97	0.09	21,21,21,21	0
54	MG	CB	3078	1/1	0.97	0.06	57,57,57,57	0
54	MG	CB	3011	1/1	0.97	0.04	33,33,33,33	0
54	MG	BA	4041	1/1	0.97	0.05	54,54,54,54	0
54	MG	CB	3084	1/1	0.97	0.05	24,24,24,24	0
54	MG	CB	3017	1/1	0.97	0.05	13,13,13,13	0
54	MG	CB	3088	1/1	0.97	0.04	52,52,52,52	0
54	MG	CB	3019	1/1	0.97	0.07	11,11,11,11	0
54	MG	CB	3091	1/1	0.97	0.06	42,42,42,42	0
54	MG	AB	4042	1/1	0.97	0.04	90,90,90,90	0
54	MG	CB	3026	1/1	0.97	0.10	10,10,10,10	0
54	MG	BA	4011	1/1	0.98	0.04	56,56,56,56	0
54	MG	AB	4049	1/1	0.98	0.13	21,21,21,21	0
54	MG	CB	3031	1/1	0.98	0.06	55,55,55,55	0
54	MG	CB	3097	1/1	0.98	0.05	9,9,9,9	0
54	MG	AB	4032	1/1	0.98	0.08	35,35,35,35	0
54	MG	CB	3100	1/1	0.98	0.06	43,43,43,43	0
54	MG	CB	3033	1/1	0.98	0.04	33,33,33,33	0
54	MG	AB	4052	1/1	0.98	0.06	25,25,25,25	0
54	MG	BA	4045	1/1	0.98	0.08	59,59,59,59	0
54	MG	AB	4083	1/1	0.98	0.04	29,29,29,29	0
54	MG	CB	3039	1/1	0.98	0.11	27,27,27,27	0
54	MG	CB	3107	1/1	0.98	0.03	22,22,22,22	0
54	MG	BA	4016	1/1	0.98	0.03	47,47,47,47	0
54	MG	CC	301	1/1	0.98	0.08	89,89,89,89	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	AB	4020	1/1	0.98	0.07	67,67,67,67	0
54	MG	DA	1602	1/1	0.98	0.04	13,13,13,13	0
54	MG	AB	4087	1/1	0.98	0.09	38,38,38,38	0
54	MG	AB	4021	1/1	0.98	0.06	33,33,33,33	0
54	MG	CB	3044	1/1	0.98	0.14	83,83,83,83	0
54	MG	CB	3046	1/1	0.98	0.07	29,29,29,29	0
54	MG	AB	4056	1/1	0.98	0.07	9,9,9,9	0
54	MG	AB	4036	1/1	0.98	0.05	12,12,12,12	0
54	MG	AB	4059	1/1	0.98	0.07	55,55,55,55	0
54	MG	AB	4060	1/1	0.98	0.07	36,36,36,36	0
54	MG	AB	4039	1/1	0.98	0.06	25,25,25,25	0
54	MG	CB	3057	1/1	0.98	0.04	7,7,7,7	0
54	MG	AB	4062	1/1	0.98	0.08	30,30,30,30	0
54	MG	AB	4012	1/1	0.98	0.04	44,44,44,44	0
54	MG	AB	4006	1/1	0.98	0.11	12,12,12,12	0
54	MG	CB	3002	1/1	0.98	0.13	54,54,54,54	0
54	MG	CB	3066	1/1	0.98	0.07	45,45,45,45	0
54	MG	CB	3067	1/1	0.98	0.05	9,9,9,9	0
54	MG	CB	3068	1/1	0.98	0.07	59,59,59,59	0
54	MG	CB	3004	1/1	0.98	0.04	9,9,9,9	0
54	MG	AB	4100	1/1	0.98	0.08	25,25,25,25	0
54	MG	CB	3006	1/1	0.98	0.07	19,19,19,19	0
54	MG	CB	3073	1/1	0.98	0.07	14,14,14,14	0
54	MG	AB	4014	1/1	0.98	0.09	18,18,18,18	0
54	MG	CB	3008	1/1	0.98	0.04	16,16,16,16	0
54	MG	AB	4067	1/1	0.98	0.04	31,31,31,31	0
54	MG	DA	1638	1/1	0.98	0.08	12,12,12,12	0
54	MG	DA	1639	1/1	0.98	0.04	79,79,79,79	0
54	MG	DA	1640	1/1	0.98	0.07	17,17,17,17	0
54	MG	AB	4009	1/1	0.98	0.04	58,58,58,58	0
54	MG	AB	4016	1/1	0.98	0.15	68,68,68,68	0
54	MG	AB	4030	1/1	0.98	0.05	34,34,34,34	0
54	MG	DA	1646	1/1	0.98	0.08	50,50,50,50	0
54	MG	CB	3018	1/1	0.98	0.10	25,25,25,25	0
54	MG	BA	4004	1/1	0.98	0.04	34,34,34,34	0
54	MG	AB	4001	1/1	0.98	0.05	5,5,5,5	0
54	MG	DA	1650	1/1	0.98	0.08	48,48,48,48	0
54	MG	CB	3024	1/1	0.98	0.04	21,21,21,21	0
54	MG	AB	4077	1/1	0.98	0.08	28,28,28,28	0
54	MG	DA	1654	1/1	0.98	0.05	13,13,13,13	0
54	MG	BA	4008	1/1	0.98	0.05	21,21,21,21	0
54	MG	DA	1658	1/1	0.98	0.17	47,47,47,47	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	CB	3092	1/1	0.98	0.06	7,7,7,7	0
54	MG	DA	1661	1/1	0.98	0.04	13,13,13,13	0
54	MG	DN	201	1/1	0.98	0.10	48,48,48,48	0
54	MG	BA	4039	1/1	0.99	0.07	31,31,31,31	0
54	MG	CB	3028	1/1	0.99	0.12	46,46,46,46	0
54	MG	BA	4040	1/1	0.99	0.03	49,49,49,49	0
54	MG	CB	3095	1/1	0.99	0.06	22,22,22,22	0
54	MG	AB	4081	1/1	0.99	0.07	60,60,60,60	0
54	MG	BA	4006	1/1	0.99	0.07	42,42,42,42	0
54	MG	CB	3098	1/1	0.99	0.04	7,7,7,7	0
54	MG	AB	4027	1/1	0.99	0.04	22,22,22,22	0
54	MG	AB	4035	1/1	0.99	0.05	39,39,39,39	0
54	MG	CB	3034	1/1	0.99	0.07	7,7,7,7	0
54	MG	CB	3035	1/1	0.99	0.07	20,20,20,20	0
54	MG	CB	3103	1/1	0.99	0.09	10,10,10,10	0
54	MG	BA	4009	1/1	0.99	0.04	34,34,34,34	0
54	MG	BA	4010	1/1	0.99	0.07	17,17,17,17	0
54	MG	AB	4028	1/1	0.99	0.04	16,16,16,16	0
54	MG	AB	4086	1/1	0.99	0.04	39,39,39,39	0
54	MG	AB	4037	1/1	0.99	0.03	25,25,25,25	0
54	MG	CB	3109	1/1	0.99	0.05	16,16,16,16	0
54	MG	BA	4050	1/1	0.99	0.09	51,51,51,51	0
54	MG	AB	4038	1/1	0.99	0.06	30,30,30,30	0
54	MG	DA	1601	1/1	0.99	0.07	28,28,28,28	0
54	MG	BA	4052	1/1	0.99	0.03	33,33,33,33	0
54	MG	AB	4089	1/1	0.99	0.02	31,31,31,31	0
54	MG	DA	1604	1/1	0.99	0.07	35,35,35,35	0
54	MG	CB	3045	1/1	0.99	0.12	67,67,67,67	0
54	MG	DA	1606	1/1	0.99	0.04	18,18,18,18	0
54	MG	AB	4066	1/1	0.99	0.05	33,33,33,33	0
54	MG	AB	4018	1/1	0.99	0.03	32,32,32,32	0
54	MG	AB	4019	1/1	0.99	0.04	29,29,29,29	0
54	MG	AB	4094	1/1	0.99	0.07	15,15,15,15	0
54	MG	BA	4058	1/1	0.99	0.03	78,78,78,78	0
54	MG	AB	4041	1/1	0.99	0.04	11,11,11,11	0
54	MG	CB	3053	1/1	0.99	0.03	5,5,5,5	0
54	MG	CB	3054	1/1	0.99	0.03	13,13,13,13	0
54	MG	DA	1615	1/1	0.99	0.06	95,95,95,95	0
54	MG	DA	1616	1/1	0.99	0.05	21,21,21,21	0
54	MG	DA	1617	1/1	0.99	0.04	10,10,10,10	0
54	MG	CB	3056	1/1	0.99	0.07	8,8,8,8	0
54	MG	AB	4070	1/1	0.99	0.02	20,20,20,20	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	DA	1621	1/1	0.99	0.07	18,18,18,18	0
54	MG	AB	4071	1/1	0.99	0.09	29,29,29,29	0
54	MG	CB	3059	1/1	0.99	0.04	12,12,12,12	0
54	MG	CB	3060	1/1	0.99	0.08	78,78,78,78	0
54	MG	AB	4072	1/1	0.99	0.07	44,44,44,44	0
54	MG	CB	3003	1/1	0.99	0.04	8,8,8,8	0
54	MG	CB	3064	1/1	0.99	0.11	63,63,63,63	0
54	MG	AB	4073	1/1	0.99	0.06	21,21,21,21	0
54	MG	AB	4024	1/1	0.99	0.07	54,54,54,54	0
54	MG	DA	1630	1/1	0.99	0.03	29,29,29,29	0
54	MG	DA	1631	1/1	0.99	0.03	22,22,22,22	0
54	MG	AB	4010	1/1	0.99	0.04	32,32,32,32	0
54	MG	AB	4102	1/1	0.99	0.05	63,63,63,63	0
54	MG	AB	4076	1/1	0.99	0.08	23,23,23,23	0
54	MG	DA	1636	1/1	0.99	0.03	43,43,43,43	0
54	MG	CB	3009	1/1	0.99	0.03	13,13,13,13	0
54	MG	AB	4104	1/1	0.99	0.04	26,26,26,26	0
54	MG	AB	4105	1/1	0.99	0.04	33,33,33,33	0
54	MG	CB	3012	1/1	0.99	0.04	10,10,10,10	0
54	MG	CB	3013	1/1	0.99	0.04	14,14,14,14	0
54	MG	DA	1643	1/1	0.99	0.05	70,70,70,70	0
54	MG	AB	4106	1/1	0.99	0.03	9,9,9,9	0
54	MG	CB	3015	1/1	0.99	0.11	9,9,9,9	0
54	MG	CB	3016	1/1	0.99	0.07	18,18,18,18	0
54	MG	AB	4058	1/1	0.99	0.05	20,20,20,20	0
54	MG	AB	4109	1/1	0.99	0.03	34,34,34,34	0
54	MG	CB	3082	1/1	0.99	0.03	17,17,17,17	0
54	MG	CB	3083	1/1	0.99	0.03	9,9,9,9	0
54	MG	AE	301	1/1	0.99	0.02	10,10,10,10	0
54	MG	CB	3085	1/1	0.99	0.10	16,16,16,16	0
54	MG	CB	3086	1/1	0.99	0.04	17,17,17,17	0
54	MG	DA	1655	1/1	0.99	0.02	12,12,12,12	0
54	MG	AB	4044	1/1	0.99	0.05	17,17,17,17	0
54	MG	CB	3021	1/1	0.99	0.02	22,22,22,22	0
54	MG	CB	3089	1/1	0.99	0.07	38,38,38,38	0
54	MG	DA	1660	1/1	0.99	0.06	14,14,14,14	0
54	MG	AB	4079	1/1	0.99	0.10	43,43,43,43	0
54	MG	AB	4002	1/1	0.99	0.04	27,27,27,27	0
54	MG	DA	1642	1/1	1.00	0.02	31,31,31,31	0
54	MG	CB	3055	1/1	1.00	0.03	5,5,5,5	0
54	MG	AB	4084	1/1	1.00	0.02	21,21,21,21	0
54	MG	CB	3022	1/1	1.00	0.04	21,21,21,21	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	CB	3023	1/1	1.00	0.04	7,7,7,7	0
54	MG	AB	4093	1/1	1.00	0.04	4,4,4,4	0
54	MG	CB	3047	1/1	1.00	0.03	10,10,10,10	0
54	MG	CB	3025	1/1	1.00	0.04	27,27,27,27	0
54	MG	CB	3062	1/1	1.00	0.01	7,7,7,7	0
54	MG	AB	4054	1/1	1.00	0.09	10,10,10,10	0
54	MG	DA	1652	1/1	1.00	0.03	21,21,21,21	0
54	MG	DA	1633	1/1	1.00	0.03	3,3,3,3	0
54	MG	BA	4036	1/1	1.00	0.02	5,5,5,5	0
54	MG	AB	4005	1/1	1.00	0.03	11,11,11,11	0
54	MG	DA	1656	1/1	1.00	0.03	15,15,15,15	0
54	MG	CB	3081	1/1	1.00	0.05	10,10,10,10	0
54	MG	AB	4051	1/1	1.00	0.04	7,7,7,7	0
54	MG	DA	1620	1/1	1.00	0.01	19,19,19,19	0
54	MG	BA	4003	1/1	1.00	0.12	29,29,29,29	0
54	MG	AB	4107	1/1	1.00	0.03	6,6,6,6	0
54	MG	CB	3069	1/1	1.00	0.06	10,10,10,10	0

5.5 Other polymers [i](#)

There are no such residues in this entry.