



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 26, 2026 – 06:50 AM UTC

PDB ID : 7MHO / pdb_00007mho
Title : Ensemble refinement structure of SARS-CoV-2 main protease (Mpro) at 298 K
Authors : Ebrahim, A.; Riley, B.T.; Kumaran, D.; Andi, B.; Fuchs, M.R.; McSweeney, S.; Keedy, D.A.
Deposited on : 2021-04-15
Resolution : 1.88 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	FAILED
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
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

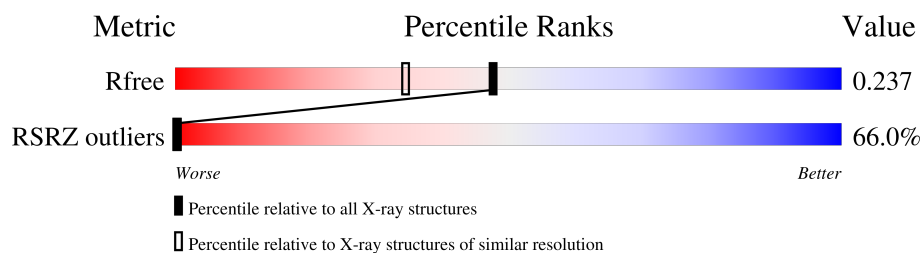
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.88 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	1220 (1.88-1.88)
RSRZ outliers	180081	1220 (1.88-1.88)

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
2	DMS	1-A	401	-	-	-	X
2	DMS	34-A	401	-	X	-	-
2	DMS	58-A	401	-	X	-	-
2	DMS	70-A	402	-	X	-	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 355880 atoms, of which 174375 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 3C-like proteinase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	1-A	306	Total	C	H	N	O	S	0	0	0
			4680	1499	2313	402	444	22			
1	2-A	306	Total	C	H	N	O	S	0	0	0
			4680	1499	2313	402	444	22			
1	3-A	306	Total	C	H	N	O	S	0	0	0
			4680	1499	2313	402	444	22			
1	4-A	306	Total	C	H	N	O	S	0	0	0
			4680	1499	2313	402	444	22			
1	5-A	306	Total	C	H	N	O	S	0	0	0
			4680	1499	2313	402	444	22			
1	6-A	306	Total	C	H	N	O	S	0	0	0
			4680	1499	2313	402	444	22			
1	7-A	306	Total	C	H	N	O	S	0	0	0
			4680	1499	2313	402	444	22			
1	8-A	306	Total	C	H	N	O	S	0	0	0
			4680	1499	2313	402	444	22			
1	9-A	306	Total	C	H	N	O	S	0	0	0
			4680	1499	2313	402	444	22			
1	10-A	306	Total	C	H	N	O	S	0	0	0
			4680	1499	2313	402	444	22			
1	11-A	306	Total	C	H	N	O	S	0	0	0
			4680	1499	2313	402	444	22			
1	12-A	306	Total	C	H	N	O	S	0	0	0
			4680	1499	2313	402	444	22			
1	13-A	306	Total	C	H	N	O	S	0	0	0
			4680	1499	2313	402	444	22			
1	14-A	306	Total	C	H	N	O	S	0	0	0
			4680	1499	2313	402	444	22			
1	15-A	306	Total	C	H	N	O	S	0	0	0
			4680	1499	2313	402	444	22			
1	16-A	306	Total	C	H	N	O	S	0	0	0
			4680	1499	2313	402	444	22			

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Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	17-A	306	Total	C	H	N	O	S	0	0	0
			4680	1499	2313	402	444	22			
1	18-A	306	Total	C	H	N	O	S	0	0	0
			4680	1499	2313	402	444	22			
1	19-A	306	Total	C	H	N	O	S	0	0	0
			4680	1499	2313	402	444	22			
1	20-A	306	Total	C	H	N	O	S	0	0	0
			4680	1499	2313	402	444	22			
1	21-A	306	Total	C	H	N	O	S	0	0	0
			4680	1499	2313	402	444	22			
1	22-A	306	Total	C	H	N	O	S	0	0	0
			4680	1499	2313	402	444	22			
1	23-A	306	Total	C	H	N	O	S	0	0	0
			4680	1499	2313	402	444	22			
1	24-A	306	Total	C	H	N	O	S	0	0	0
			4680	1499	2313	402	444	22			
1	25-A	306	Total	C	H	N	O	S	0	0	0
			4680	1499	2313	402	444	22			
1	26-A	306	Total	C	H	N	O	S	0	0	0
			4680	1499	2313	402	444	22			
1	27-A	306	Total	C	H	N	O	S	0	0	0
			4680	1499	2313	402	444	22			
1	28-A	306	Total	C	H	N	O	S	0	0	0
			4680	1499	2313	402	444	22			
1	29-A	306	Total	C	H	N	O	S	0	0	0
			4680	1499	2313	402	444	22			
1	30-A	306	Total	C	H	N	O	S	0	0	0
			4680	1499	2313	402	444	22			
1	31-A	306	Total	C	H	N	O	S	0	0	0
			4680	1499	2313	402	444	22			
1	32-A	306	Total	C	H	N	O	S	0	0	0
			4680	1499	2313	402	444	22			
1	33-A	306	Total	C	H	N	O	S	0	0	0
			4680	1499	2313	402	444	22			
1	34-A	306	Total	C	H	N	O	S	0	0	0
			4680	1499	2313	402	444	22			
1	35-A	306	Total	C	H	N	O	S	0	0	0
			4680	1499	2313	402	444	22			
1	36-A	306	Total	C	H	N	O	S	0	0	0
			4680	1499	2313	402	444	22			
1	37-A	306	Total	C	H	N	O	S	0	0	0
			4680	1499	2313	402	444	22			

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Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	38-A	306	Total	C	H	N	O	S	0	0	0
			4680	1499	2313	402	444	22			
1	39-A	306	Total	C	H	N	O	S	0	0	0
			4680	1499	2313	402	444	22			
1	40-A	306	Total	C	H	N	O	S	0	0	0
			4680	1499	2313	402	444	22			
1	41-A	306	Total	C	H	N	O	S	0	0	0
			4680	1499	2313	402	444	22			
1	42-A	306	Total	C	H	N	O	S	0	0	0
			4680	1499	2313	402	444	22			
1	43-A	306	Total	C	H	N	O	S	0	0	0
			4680	1499	2313	402	444	22			
1	44-A	306	Total	C	H	N	O	S	0	0	0
			4680	1499	2313	402	444	22			
1	45-A	306	Total	C	H	N	O	S	0	0	0
			4680	1499	2313	402	444	22			
1	46-A	306	Total	C	H	N	O	S	0	0	0
			4680	1499	2313	402	444	22			
1	47-A	306	Total	C	H	N	O	S	0	0	0
			4680	1499	2313	402	444	22			
1	48-A	306	Total	C	H	N	O	S	0	0	0
			4680	1499	2313	402	444	22			
1	49-A	306	Total	C	H	N	O	S	0	0	0
			4680	1499	2313	402	444	22			
1	50-A	306	Total	C	H	N	O	S	0	0	0
			4680	1499	2313	402	444	22			
1	51-A	306	Total	C	H	N	O	S	0	0	0
			4680	1499	2313	402	444	22			
1	52-A	306	Total	C	H	N	O	S	0	0	0
			4680	1499	2313	402	444	22			
1	53-A	306	Total	C	H	N	O	S	0	0	0
			4680	1499	2313	402	444	22			
1	54-A	306	Total	C	H	N	O	S	0	0	0
			4680	1499	2313	402	444	22			
1	55-A	306	Total	C	H	N	O	S	0	0	0
			4680	1499	2313	402	444	22			
1	56-A	306	Total	C	H	N	O	S	0	0	0
			4680	1499	2313	402	444	22			
1	57-A	306	Total	C	H	N	O	S	0	0	0
			4680	1499	2313	402	444	22			
1	58-A	306	Total	C	H	N	O	S	0	0	0
			4680	1499	2313	402	444	22			

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Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	59-A	306	Total	C	H	N	O	S	0	0	0
			4680	1499	2313	402	444	22			
1	60-A	306	Total	C	H	N	O	S	0	0	0
			4680	1499	2313	402	444	22			
1	61-A	306	Total	C	H	N	O	S	0	0	0
			4680	1499	2313	402	444	22			
1	62-A	306	Total	C	H	N	O	S	0	0	0
			4680	1499	2313	402	444	22			
1	63-A	306	Total	C	H	N	O	S	0	0	0
			4680	1499	2313	402	444	22			
1	64-A	306	Total	C	H	N	O	S	0	0	0
			4680	1499	2313	402	444	22			
1	65-A	306	Total	C	H	N	O	S	0	0	0
			4680	1499	2313	402	444	22			
1	66-A	306	Total	C	H	N	O	S	0	0	0
			4680	1499	2313	402	444	22			
1	67-A	306	Total	C	H	N	O	S	0	0	0
			4680	1499	2313	402	444	22			
1	68-A	306	Total	C	H	N	O	S	0	0	0
			4680	1499	2313	402	444	22			
1	69-A	306	Total	C	H	N	O	S	0	0	0
			4680	1499	2313	402	444	22			
1	70-A	306	Total	C	H	N	O	S	0	0	0
			4680	1499	2313	402	444	22			
1	71-A	306	Total	C	H	N	O	S	0	0	0
			4680	1499	2313	402	444	22			
1	72-A	306	Total	C	H	N	O	S	0	0	0
			4680	1499	2313	402	444	22			
1	73-A	306	Total	C	H	N	O	S	0	0	0
			4680	1499	2313	402	444	22			
1	74-A	306	Total	C	H	N	O	S	0	0	0
			4680	1499	2313	402	444	22			
1	75-A	306	Total	C	H	N	O	S	0	0	0
			4680	1499	2313	402	444	22			

- Molecule 2 is DIMETHYL SULFOXIDE (CCD ID: DMS) (formula: C₂H₆OS).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	1-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	2-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	3-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	4-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	5-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	6-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	7-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	8-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	9-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	10-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	11-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	12-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	13-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	14-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	15-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	16-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	17-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	18-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	19-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	20-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	21-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	22-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	23-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	24-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	25-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	26-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	27-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	28-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	29-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	30-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	31-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	32-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	33-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	34-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	35-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	36-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	37-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	38-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	39-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	40-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	41-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	42-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	43-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	44-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	45-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	46-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	47-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	48-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	49-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	50-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	51-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	52-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	53-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	54-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	55-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	56-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	57-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	58-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	59-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	60-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	61-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	62-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	63-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	64-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	65-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	66-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	67-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	68-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	69-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	70-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	71-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	72-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	73-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	74-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	75-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	1-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	2-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	3-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	4-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	5-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	6-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	7-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	8-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	9-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	10-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	11-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	12-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	13-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	14-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	15-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	16-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	17-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	18-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	19-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	20-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	21-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	22-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	23-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	24-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	25-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	26-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	27-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	28-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	29-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	30-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	31-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	32-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	33-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	34-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	35-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	36-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	37-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	38-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	39-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	40-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	41-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	42-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	43-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	44-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	45-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	46-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	47-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	48-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	49-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	50-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	51-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	52-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	53-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	54-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	55-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	56-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	57-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	58-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	59-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	60-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	61-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	62-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	63-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	64-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	65-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	66-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	67-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	68-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	69-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	70-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	71-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	72-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	73-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	74-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	75-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		

- Molecule 3 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	1-A	1	Total	Zn	0	0
			1	1		
3	2-A	1	Total	Zn	0	0
			1	1		
3	3-A	1	Total	Zn	0	0
			1	1		
3	4-A	1	Total	Zn	0	0
			1	1		
3	5-A	1	Total	Zn	0	0
			1	1		
3	6-A	1	Total	Zn	0	0
			1	1		
3	7-A	1	Total	Zn	0	0
			1	1		
3	8-A	1	Total	Zn	0	0
			1	1		
3	9-A	1	Total	Zn	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	10-A	1	Total 1	Zn 1	0	0
3	11-A	1	Total 1	Zn 1	0	0
3	12-A	1	Total 1	Zn 1	0	0
3	13-A	1	Total 1	Zn 1	0	0
3	14-A	1	Total 1	Zn 1	0	0
3	15-A	1	Total 1	Zn 1	0	0
3	16-A	1	Total 1	Zn 1	0	0
3	17-A	1	Total 1	Zn 1	0	0
3	18-A	1	Total 1	Zn 1	0	0
3	19-A	1	Total 1	Zn 1	0	0
3	20-A	1	Total 1	Zn 1	0	0
3	21-A	1	Total 1	Zn 1	0	0
3	22-A	1	Total 1	Zn 1	0	0
3	23-A	1	Total 1	Zn 1	0	0
3	24-A	1	Total 1	Zn 1	0	0
3	25-A	1	Total 1	Zn 1	0	0
3	26-A	1	Total 1	Zn 1	0	0
3	27-A	1	Total 1	Zn 1	0	0
3	28-A	1	Total 1	Zn 1	0	0
3	29-A	1	Total 1	Zn 1	0	0
3	30-A	1	Total 1	Zn 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	31-A	1	Total 1	Zn 1	0	0
3	32-A	1	Total 1	Zn 1	0	0
3	33-A	1	Total 1	Zn 1	0	0
3	34-A	1	Total 1	Zn 1	0	0
3	35-A	1	Total 1	Zn 1	0	0
3	36-A	1	Total 1	Zn 1	0	0
3	37-A	1	Total 1	Zn 1	0	0
3	38-A	1	Total 1	Zn 1	0	0
3	39-A	1	Total 1	Zn 1	0	0
3	40-A	1	Total 1	Zn 1	0	0
3	41-A	1	Total 1	Zn 1	0	0
3	42-A	1	Total 1	Zn 1	0	0
3	43-A	1	Total 1	Zn 1	0	0
3	44-A	1	Total 1	Zn 1	0	0
3	45-A	1	Total 1	Zn 1	0	0
3	46-A	1	Total 1	Zn 1	0	0
3	47-A	1	Total 1	Zn 1	0	0
3	48-A	1	Total 1	Zn 1	0	0
3	49-A	1	Total 1	Zn 1	0	0
3	50-A	1	Total 1	Zn 1	0	0
3	51-A	1	Total 1	Zn 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	52-A	1	Total 1	Zn 1	0	0
3	53-A	1	Total 1	Zn 1	0	0
3	54-A	1	Total 1	Zn 1	0	0
3	55-A	1	Total 1	Zn 1	0	0
3	56-A	1	Total 1	Zn 1	0	0
3	57-A	1	Total 1	Zn 1	0	0
3	58-A	1	Total 1	Zn 1	0	0
3	59-A	1	Total 1	Zn 1	0	0
3	60-A	1	Total 1	Zn 1	0	0
3	61-A	1	Total 1	Zn 1	0	0
3	62-A	1	Total 1	Zn 1	0	0
3	63-A	1	Total 1	Zn 1	0	0
3	64-A	1	Total 1	Zn 1	0	0
3	65-A	1	Total 1	Zn 1	0	0
3	66-A	1	Total 1	Zn 1	0	0
3	67-A	1	Total 1	Zn 1	0	0
3	68-A	1	Total 1	Zn 1	0	0
3	69-A	1	Total 1	Zn 1	0	0
3	70-A	1	Total 1	Zn 1	0	0
3	71-A	1	Total 1	Zn 1	0	0
3	72-A	1	Total 1	Zn 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	73-A	1	Total 1	Zn 1	0	0
3	74-A	1	Total 1	Zn 1	0	0
3	75-A	1	Total 1	Zn 1	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	1-A	40	Total 40	O 40	0	0
4	2-A	38	Total 38	O 38	0	0
4	3-A	50	Total 50	O 50	0	0
4	4-A	44	Total 44	O 44	0	0
4	5-A	37	Total 37	O 37	0	0
4	6-A	41	Total 41	O 41	0	0
4	7-A	37	Total 37	O 37	0	0
4	8-A	33	Total 33	O 33	0	0
4	9-A	38	Total 38	O 38	0	0
4	10-A	38	Total 38	O 38	0	0
4	11-A	43	Total 43	O 43	0	0
4	12-A	48	Total 48	O 48	0	0
4	13-A	48	Total 48	O 48	0	0
4	14-A	49	Total 49	O 49	0	0
4	15-A	47	Total 47	O 47	0	0
4	16-A	49	Total 49	O 49	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	17-A	39	Total 39	O 39	0	0
4	18-A	43	Total 43	O 43	0	0
4	19-A	39	Total 39	O 39	0	0
4	20-A	48	Total 48	O 48	0	0
4	21-A	45	Total 45	O 45	0	0
4	22-A	49	Total 49	O 49	0	0
4	23-A	44	Total 44	O 44	0	0
4	24-A	51	Total 51	O 51	0	0
4	25-A	52	Total 52	O 52	0	0
4	26-A	48	Total 48	O 48	0	0
4	27-A	43	Total 43	O 43	0	0
4	28-A	41	Total 41	O 41	0	0
4	29-A	43	Total 43	O 43	0	0
4	30-A	43	Total 43	O 43	0	0
4	31-A	44	Total 44	O 44	0	0
4	32-A	46	Total 46	O 46	0	0
4	33-A	47	Total 47	O 47	0	0
4	34-A	39	Total 39	O 39	0	0
4	35-A	41	Total 41	O 41	0	0
4	36-A	41	Total 41	O 41	0	0
4	37-A	43	Total 43	O 43	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	38-A	44	Total O 44 44	0	0
4	39-A	45	Total O 45 45	0	0
4	40-A	41	Total O 41 41	0	0
4	41-A	43	Total O 43 43	0	0
4	42-A	39	Total O 39 39	0	0
4	43-A	49	Total O 49 49	0	0
4	44-A	47	Total O 47 47	0	0
4	45-A	51	Total O 51 51	0	0
4	46-A	54	Total O 54 54	0	0
4	47-A	47	Total O 47 47	0	0
4	48-A	44	Total O 44 44	0	0
4	49-A	39	Total O 39 39	0	0
4	50-A	46	Total O 46 46	0	0
4	51-A	41	Total O 41 41	0	0
4	52-A	43	Total O 43 43	0	0
4	53-A	42	Total O 42 42	0	0
4	54-A	56	Total O 56 56	0	0
4	55-A	52	Total O 52 52	0	0
4	56-A	46	Total O 46 46	0	0
4	57-A	46	Total O 46 46	0	0
4	58-A	39	Total O 39 39	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	59-A	39	Total 39	O 39	0	0
4	60-A	37	Total 37	O 37	0	0
4	61-A	41	Total 41	O 41	0	0
4	62-A	44	Total 44	O 44	0	0
4	63-A	40	Total 40	O 40	0	0
4	64-A	43	Total 43	O 43	0	0
4	65-A	37	Total 37	O 37	0	0
4	66-A	44	Total 44	O 44	0	0
4	67-A	44	Total 44	O 44	0	0
4	68-A	42	Total 42	O 42	0	0
4	69-A	44	Total 44	O 44	0	0
4	70-A	45	Total 45	O 45	0	0
4	71-A	50	Total 50	O 50	0	0
4	72-A	50	Total 50	O 50	0	0
4	73-A	50	Total 50	O 50	0	0
4	74-A	48	Total 48	O 48	0	0
4	75-A	44	Total 44	O 44	0	0

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

3 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	114.97Å 54.62Å 45.19Å 90.00° 101.67° 90.00°	Depositor
Resolution (Å)	49.14 – 1.88 49.14 – 1.88	Depositor EDS
% Data completeness (in resolution range)	99.2 (49.14-1.88) 90.6 (49.14-1.88)	Depositor EDS
R_{merge}	0.18	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.38 (at 1.88Å)	Xtriage
Refinement program	PHENIX (phenix.ensemble_refinement:1.19.2_4158)	Depositor
R, R_{free}	0.150 , 0.208 0.179 , 0.237	Depositor DCC
R_{free} test set	1107 reflections (4.93%)	wwPDB-VP
Wilson B-factor (Å ²)	29.6	Xtriage
Anisotropy	0.174	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.00 , 45.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	355880	wwPDB-VP
Average B, all atoms (Å ²)	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.28% 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 225 ligands modelled in this entry, 75 are monoatomic - leaving 150 for Mogul analysis.

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	DMS	32-A	402	-	3,3,3	0.67	0	3,3,3	0.55	0
2	DMS	75-A	402	-	3,3,3	0.60	0	3,3,3	0.26	0
2	DMS	61-A	402	-	3,3,3	0.68	0	3,3,3	1.61	1 (33%)
2	DMS	52-A	402	-	3,3,3	0.66	0	3,3,3	2.07	1 (33%)
2	DMS	52-A	401	-	3,3,3	0.92	0	3,3,3	1.62	1 (33%)
2	DMS	4-A	402	-	3,3,3	0.76	0	3,3,3	1.16	0
2	DMS	42-A	402	-	3,3,3	0.69	0	3,3,3	0.52	0
2	DMS	41-A	402	-	3,3,3	0.78	0	3,3,3	1.51	1 (33%)
2	DMS	14-A	401	-	3,3,3	0.96	0	3,3,3	0.74	0
2	DMS	73-A	401	-	3,3,3	0.73	0	3,3,3	1.00	0
2	DMS	22-A	402	-	3,3,3	0.81	0	3,3,3	2.58	2 (66%)
2	DMS	22-A	401	-	3,3,3	0.77	0	3,3,3	1.90	2 (66%)
2	DMS	19-A	402	-	3,3,3	0.83	0	3,3,3	1.10	0
2	DMS	61-A	401	-	3,3,3	0.75	0	3,3,3	1.21	0
2	DMS	2-A	401	-	3,3,3	0.85	0	3,3,3	0.90	0
2	DMS	14-A	402	-	3,3,3	0.68	0	3,3,3	0.91	0
2	DMS	30-A	402	-	3,3,3	0.78	0	3,3,3	1.21	0
2	DMS	73-A	402	-	3,3,3	0.90	0	3,3,3	0.34	0
2	DMS	19-A	401	-	3,3,3	0.85	0	3,3,3	0.70	0
2	DMS	27-A	401	-	3,3,3	0.74	0	3,3,3	1.09	0
2	DMS	62-A	402	-	3,3,3	0.81	0	3,3,3	1.07	0
2	DMS	2-A	402	-	3,3,3	0.75	0	3,3,3	1.53	1 (33%)
2	DMS	62-A	401	-	3,3,3	0.73	0	3,3,3	0.79	0
2	DMS	56-A	401	-	3,3,3	0.98	0	3,3,3	0.63	0
2	DMS	31-A	402	-	3,3,3	0.71	0	3,3,3	1.14	0
2	DMS	41-A	401	-	3,3,3	0.79	0	3,3,3	1.41	0
2	DMS	28-A	401	-	3,3,3	0.74	0	3,3,3	0.85	0
2	DMS	34-A	402	-	3,3,3	0.93	0	3,3,3	1.76	1 (33%)
2	DMS	63-A	402	-	3,3,3	0.75	0	3,3,3	0.82	0
2	DMS	51-A	402	-	3,3,3	0.87	0	3,3,3	0.99	0
2	DMS	36-A	401	-	3,3,3	0.77	0	3,3,3	0.60	0
2	DMS	1-A	402	-	3,3,3	0.76	0	3,3,3	1.84	1 (33%)
2	DMS	58-A	401	-	3,3,3	0.86	0	3,3,3	3.12	3 (100%)
2	DMS	45-A	402	-	3,3,3	0.84	0	3,3,3	1.28	1 (33%)
2	DMS	39-A	401	-	3,3,3	0.86	0	3,3,3	1.60	1 (33%)
2	DMS	36-A	402	-	3,3,3	0.93	0	3,3,3	2.11	1 (33%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	DMS	57-A	401	-	3,3,3	0.71	0	3,3,3	1.19	0
2	DMS	59-A	401	-	3,3,3	0.79	0	3,3,3	0.56	0
2	DMS	63-A	401	-	3,3,3	0.68	0	3,3,3	0.88	0
2	DMS	64-A	402	-	3,3,3	0.85	0	3,3,3	2.10	1 (33%)
2	DMS	39-A	402	-	3,3,3	0.83	0	3,3,3	0.93	0
2	DMS	65-A	402	-	3,3,3	0.61	0	3,3,3	0.45	0
2	DMS	46-A	401	-	3,3,3	0.94	0	3,3,3	1.33	1 (33%)
2	DMS	60-A	401	-	3,3,3	0.78	0	3,3,3	0.82	0
2	DMS	24-A	402	-	3,3,3	0.79	0	3,3,3	0.76	0
2	DMS	51-A	401	-	3,3,3	0.81	0	3,3,3	3.12	2 (66%)
2	DMS	24-A	401	-	3,3,3	0.81	0	3,3,3	0.94	0
2	DMS	71-A	402	-	3,3,3	0.72	0	3,3,3	0.71	0
2	DMS	46-A	402	-	3,3,3	1.00	0	3,3,3	2.02	1 (33%)
2	DMS	47-A	401	-	3,3,3	0.79	0	3,3,3	0.48	0
2	DMS	37-A	402	-	3,3,3	0.89	0	3,3,3	1.51	1 (33%)
2	DMS	55-A	402	-	3,3,3	0.55	0	3,3,3	1.32	0
2	DMS	43-A	402	-	3,3,3	0.67	0	3,3,3	1.36	0
2	DMS	74-A	401	-	3,3,3	0.86	0	3,3,3	0.78	0
2	DMS	7-A	402	-	3,3,3	0.93	0	3,3,3	1.26	0
2	DMS	45-A	401	-	3,3,3	1.01	0	3,3,3	0.53	0
2	DMS	71-A	401	-	3,3,3	0.86	0	3,3,3	0.95	0
2	DMS	35-A	401	-	3,3,3	0.72	0	3,3,3	1.20	0
2	DMS	8-A	401	-	3,3,3	0.99	0	3,3,3	0.83	0
2	DMS	13-A	402	-	3,3,3	0.89	0	3,3,3	0.67	0
2	DMS	25-A	401	-	3,3,3	0.86	0	3,3,3	0.75	0
2	DMS	55-A	401	-	3,3,3	0.85	0	3,3,3	1.69	1 (33%)
2	DMS	8-A	402	-	3,3,3	0.75	0	3,3,3	1.69	1 (33%)
2	DMS	72-A	401	-	3,3,3	0.78	0	3,3,3	0.57	0
2	DMS	40-A	401	-	3,3,3	0.97	0	3,3,3	0.61	0
2	DMS	27-A	402	-	3,3,3	0.74	0	3,3,3	0.85	0
2	DMS	9-A	401	-	3,3,3	0.98	0	3,3,3	0.93	0
2	DMS	32-A	401	-	3,3,3	0.74	0	3,3,3	2.62	2 (66%)
2	DMS	29-A	402	-	3,3,3	0.89	0	3,3,3	2.93	2 (66%)
2	DMS	26-A	402	-	3,3,3	0.85	0	3,3,3	0.39	0
2	DMS	48-A	402	-	3,3,3	0.83	0	3,3,3	1.38	0
2	DMS	49-A	402	-	3,3,3	0.74	0	3,3,3	1.33	0
2	DMS	15-A	402	-	3,3,3	0.67	0	3,3,3	1.31	0
2	DMS	49-A	401	-	3,3,3	0.63	0	3,3,3	1.02	0
2	DMS	16-A	401	-	3,3,3	0.92	0	3,3,3	1.73	1 (33%)
2	DMS	60-A	402	-	3,3,3	0.91	0	3,3,3	1.68	1 (33%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	DMS	21-A	401	-	3,3,3	0.78	0	3,3,3	1.79	0
2	DMS	16-A	402	-	3,3,3	0.70	0	3,3,3	0.77	0
2	DMS	13-A	401	-	3,3,3	0.95	0	3,3,3	2.26	2 (66%)
2	DMS	17-A	402	-	3,3,3	1.17	0	3,3,3	1.63	0
2	DMS	47-A	402	-	3,3,3	0.95	0	3,3,3	1.48	1 (33%)
2	DMS	35-A	402	-	3,3,3	0.75	0	3,3,3	0.97	0
2	DMS	43-A	401	-	3,3,3	0.67	0	3,3,3	1.71	1 (33%)
2	DMS	53-A	401	-	3,3,3	0.87	0	3,3,3	1.22	0
2	DMS	74-A	402	-	3,3,3	0.80	0	3,3,3	1.15	0
2	DMS	69-A	401	-	3,3,3	0.90	0	3,3,3	1.15	0
2	DMS	33-A	401	-	3,3,3	0.72	0	3,3,3	1.32	0
2	DMS	75-A	401	-	3,3,3	0.79	0	3,3,3	1.15	0
2	DMS	56-A	402	-	3,3,3	0.71	0	3,3,3	0.55	0
2	DMS	53-A	402	-	3,3,3	0.86	0	3,3,3	0.68	0
2	DMS	20-A	401	-	3,3,3	0.65	0	3,3,3	1.16	0
2	DMS	68-A	401	-	3,3,3	0.78	0	3,3,3	1.38	1 (33%)
2	DMS	10-A	402	-	3,3,3	0.78	0	3,3,3	1.19	0
2	DMS	26-A	401	-	3,3,3	0.82	0	3,3,3	0.73	0
2	DMS	7-A	401	-	3,3,3	0.69	0	3,3,3	1.89	1 (33%)
2	DMS	69-A	402	-	3,3,3	0.80	0	3,3,3	1.59	1 (33%)
2	DMS	23-A	402	-	3,3,3	0.76	0	3,3,3	0.44	0
2	DMS	12-A	401	-	3,3,3	0.60	0	3,3,3	1.44	0
2	DMS	17-A	401	-	3,3,3	0.86	0	3,3,3	0.58	0
2	DMS	54-A	401	-	3,3,3	0.91	0	3,3,3	0.52	0
2	DMS	58-A	402	-	3,3,3	0.78	0	3,3,3	1.93	2 (66%)
2	DMS	70-A	401	-	3,3,3	0.63	0	3,3,3	0.12	0
2	DMS	64-A	401	-	3,3,3	0.80	0	3,3,3	1.85	1 (33%)
2	DMS	72-A	402	-	3,3,3	0.63	0	3,3,3	1.02	0
2	DMS	42-A	401	-	3,3,3	0.81	0	3,3,3	0.62	0
2	DMS	40-A	402	-	3,3,3	0.75	0	3,3,3	0.99	0
2	DMS	12-A	402	-	3,3,3	0.84	0	3,3,3	1.09	0
2	DMS	54-A	402	-	3,3,3	0.86	0	3,3,3	0.67	0
2	DMS	9-A	402	-	3,3,3	0.82	0	3,3,3	2.11	1 (33%)
2	DMS	18-A	401	-	3,3,3	0.92	0	3,3,3	1.44	0
2	DMS	65-A	401	-	3,3,3	0.82	0	3,3,3	1.09	0
2	DMS	5-A	402	-	3,3,3	0.70	0	3,3,3	2.01	1 (33%)
2	DMS	4-A	401	-	3,3,3	1.00	0	3,3,3	0.49	0
2	DMS	5-A	401	-	3,3,3	0.97	0	3,3,3	0.40	0
2	DMS	30-A	401	-	3,3,3	0.58	0	3,3,3	1.96	1 (33%)
2	DMS	37-A	401	-	3,3,3	0.72	0	3,3,3	1.39	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	DMS	11-A	402	-	3,3,3	0.85	0	3,3,3	0.88	0
2	DMS	15-A	401	-	3,3,3	1.04	0	3,3,3	2.15	2 (66%)
2	DMS	48-A	401	-	3,3,3	0.77	0	3,3,3	1.19	0
2	DMS	6-A	402	-	3,3,3	0.63	0	3,3,3	1.29	0
2	DMS	29-A	401	-	3,3,3	0.88	0	3,3,3	1.06	0
2	DMS	66-A	401	-	3,3,3	0.76	0	3,3,3	0.85	0
2	DMS	20-A	402	-	3,3,3	0.87	0	3,3,3	1.03	0
2	DMS	67-A	401	-	3,3,3	0.85	0	3,3,3	1.14	0
2	DMS	38-A	401	-	3,3,3	0.84	0	3,3,3	0.97	0
2	DMS	66-A	402	-	3,3,3	0.62	0	3,3,3	1.58	1 (33%)
2	DMS	34-A	401	-	3,3,3	0.78	0	3,3,3	3.22	3 (100%)
2	DMS	67-A	402	-	3,3,3	0.70	0	3,3,3	0.49	0
2	DMS	11-A	401	-	3,3,3	0.80	0	3,3,3	1.06	0
2	DMS	44-A	401	-	3,3,3	0.95	0	3,3,3	0.68	0
2	DMS	31-A	401	-	3,3,3	0.82	0	3,3,3	0.62	0
2	DMS	1-A	401	-	3,3,3	0.84	0	3,3,3	1.88	1 (33%)
2	DMS	6-A	401	-	3,3,3	0.55	0	3,3,3	0.94	0
2	DMS	38-A	402	-	3,3,3	0.90	0	3,3,3	1.05	0
2	DMS	57-A	402	-	3,3,3	0.88	0	3,3,3	1.07	0
2	DMS	59-A	402	-	3,3,3	0.80	0	3,3,3	1.06	0
2	DMS	44-A	402	-	3,3,3	0.71	0	3,3,3	1.23	0
2	DMS	3-A	401	-	3,3,3	0.58	0	3,3,3	1.96	1 (33%)
2	DMS	21-A	402	-	3,3,3	0.93	0	3,3,3	1.27	0
2	DMS	33-A	402	-	3,3,3	0.75	0	3,3,3	1.29	1 (33%)
2	DMS	10-A	401	-	3,3,3	0.92	0	3,3,3	0.61	0
2	DMS	25-A	402	-	3,3,3	1.05	0	3,3,3	1.05	0
2	DMS	23-A	401	-	3,3,3	0.90	0	3,3,3	0.45	0
2	DMS	28-A	402	-	3,3,3	0.75	0	3,3,3	0.38	0
2	DMS	50-A	402	-	3,3,3	0.90	0	3,3,3	1.53	0
2	DMS	18-A	402	-	3,3,3	0.62	0	3,3,3	1.95	1 (33%)
2	DMS	3-A	402	-	3,3,3	0.77	0	3,3,3	0.81	0
2	DMS	50-A	401	-	3,3,3	0.85	0	3,3,3	1.22	0
2	DMS	68-A	402	-	3,3,3	0.78	0	3,3,3	1.30	0
2	DMS	70-A	402	-	3,3,3	0.76	0	3,3,3	2.83	3 (100%)

There are no bond length outliers.

All (57) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	29-A	402	DMS	O-S-C2	3.77	125.38	106.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	34-A	401	DMS	O-S-C2	3.72	125.09	106.49
2	32-A	401	DMS	O-S-C1	3.69	124.95	106.49
2	51-A	401	DMS	O-S-C2	3.68	124.91	106.49
2	22-A	402	DMS	O-S-C2	3.52	124.13	106.49
2	58-A	401	DMS	O-S-C2	3.51	124.05	106.49
2	51-A	401	DMS	C2-S-C1	3.48	116.25	98.42
2	70-A	402	DMS	O-S-C2	3.43	123.66	106.49
2	3-A	401	DMS	O-S-C1	3.30	122.99	106.49
2	36-A	402	DMS	O-S-C2	3.23	122.67	106.49
2	58-A	401	DMS	O-S-C1	3.18	122.43	106.49
2	7-A	401	DMS	O-S-C2	-3.16	90.67	106.49
2	9-A	402	DMS	O-S-C1	3.10	122.02	106.49
2	29-A	402	DMS	O-S-C1	3.10	122.02	106.49
2	52-A	402	DMS	O-S-C2	3.10	122.02	106.49
2	34-A	401	DMS	O-S-C1	3.07	121.84	106.49
2	5-A	402	DMS	O-S-C1	3.03	121.64	106.49
2	13-A	401	DMS	C2-S-C1	2.99	113.72	98.42
2	64-A	402	DMS	O-S-C1	2.98	121.40	106.49
2	16-A	401	DMS	C2-S-C1	2.90	113.27	98.42
2	15-A	401	DMS	O-S-C1	2.88	120.93	106.49
2	34-A	401	DMS	C2-S-C1	2.81	112.84	98.42
2	8-A	402	DMS	O-S-C1	2.79	120.48	106.49
2	18-A	402	DMS	O-S-C1	2.68	119.93	106.49
2	64-A	401	DMS	O-S-C1	2.68	119.90	106.49
2	70-A	402	DMS	O-S-C1	2.66	119.81	106.49
2	1-A	402	DMS	O-S-C2	-2.60	93.47	106.49
2	32-A	401	DMS	O-S-C2	2.59	119.46	106.49
2	58-A	401	DMS	C2-S-C1	2.59	111.69	98.42
2	1-A	401	DMS	C2-S-C1	-2.56	85.31	98.42
2	55-A	401	DMS	C2-S-C1	2.53	111.39	98.42
2	22-A	402	DMS	O-S-C1	2.50	119.02	106.49
2	47-A	402	DMS	O-S-C1	2.47	118.86	106.49
2	68-A	401	DMS	O-S-C2	2.38	118.41	106.49
2	46-A	402	DMS	O-S-C1	2.38	118.39	106.49
2	22-A	401	DMS	O-S-C2	2.34	118.21	106.49
2	34-A	402	DMS	O-S-C1	2.32	118.11	106.49
2	52-A	401	DMS	O-S-C2	2.31	118.08	106.49
2	37-A	402	DMS	O-S-C2	2.28	117.91	106.49
2	70-A	402	DMS	C2-S-C1	2.26	110.00	98.42
2	69-A	402	DMS	O-S-C2	2.22	117.61	106.49
2	30-A	401	DMS	C2-S-C1	2.19	109.64	98.42
2	46-A	401	DMS	O-S-C2	2.18	117.38	106.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	58-A	402	DMS	O-S-C2	2.17	117.38	106.49
2	15-A	401	DMS	O-S-C2	2.17	117.34	106.49
2	41-A	402	DMS	O-S-C1	2.16	117.31	106.49
2	58-A	402	DMS	O-S-C1	2.15	117.25	106.49
2	66-A	402	DMS	O-S-C1	2.15	117.24	106.49
2	13-A	401	DMS	O-S-C1	2.14	117.19	106.49
2	43-A	401	DMS	C2-S-C1	2.13	109.35	98.42
2	33-A	402	DMS	C2-S-C1	-2.11	87.61	98.42
2	45-A	402	DMS	O-S-C1	2.11	117.05	106.49
2	61-A	402	DMS	O-S-C1	2.11	117.05	106.49
2	39-A	401	DMS	O-S-C2	2.04	116.68	106.49
2	2-A	402	DMS	C2-S-C1	2.02	108.79	98.42
2	22-A	401	DMS	C2-S-C1	2.02	108.77	98.42
2	60-A	402	DMS	O-S-C1	2.02	116.59	106.49

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](#)

There are no chain breaks in this entry.

5 Fit of model and data ⓘ

5.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	1-A	306/306 (100%)	2.82	202 (66%) 0 0	0, 0, 0, 0	306 (100%)
1	2-A	0/306	-	-	-	-
1	3-A	0/306	-	-	-	-
1	4-A	0/306	-	-	-	-
1	5-A	0/306	-	-	-	-
1	6-A	0/306	-	-	-	-
1	7-A	0/306	-	-	-	-
1	8-A	0/306	-	-	-	-
1	9-A	0/306	-	-	-	-
1	10-A	0/306	-	-	-	-
1	11-A	0/306	-	-	-	-
1	12-A	0/306	-	-	-	-
1	13-A	0/306	-	-	-	-
1	14-A	0/306	-	-	-	-
1	15-A	0/306	-	-	-	-
1	16-A	0/306	-	-	-	-
1	17-A	0/306	-	-	-	-
1	18-A	0/306	-	-	-	-
1	19-A	0/306	-	-	-	-
1	20-A	0/306	-	-	-	-
1	21-A	0/306	-	-	-	-
1	22-A	0/306	-	-	-	-
1	23-A	0/306	-	-	-	-
1	24-A	0/306	-	-	-	-
1	25-A	0/306	-	-	-	-
1	26-A	0/306	-	-	-	-
1	27-A	0/306	-	-	-	-
1	28-A	0/306	-	-	-	-
1	29-A	0/306	-	-	-	-
1	30-A	0/306	-	-	-	-
1	31-A	0/306	-	-	-	-
1	32-A	0/306	-	-	-	-

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	33-A	0/306	-	-	-	-
1	34-A	0/306	-	-	-	-
1	35-A	0/306	-	-	-	-
1	36-A	0/306	-	-	-	-
1	37-A	0/306	-	-	-	-
1	38-A	0/306	-	-	-	-
1	39-A	0/306	-	-	-	-
1	40-A	0/306	-	-	-	-
1	41-A	0/306	-	-	-	-
1	42-A	0/306	-	-	-	-
1	43-A	0/306	-	-	-	-
1	44-A	0/306	-	-	-	-
1	45-A	0/306	-	-	-	-
1	46-A	0/306	-	-	-	-
1	47-A	0/306	-	-	-	-
1	48-A	0/306	-	-	-	-
1	49-A	0/306	-	-	-	-
1	50-A	0/306	-	-	-	-
1	51-A	0/306	-	-	-	-
1	52-A	0/306	-	-	-	-
1	53-A	0/306	-	-	-	-
1	54-A	0/306	-	-	-	-
1	55-A	0/306	-	-	-	-
1	56-A	0/306	-	-	-	-
1	57-A	0/306	-	-	-	-
1	58-A	0/306	-	-	-	-
1	59-A	0/306	-	-	-	-
1	60-A	0/306	-	-	-	-
1	61-A	0/306	-	-	-	-
1	62-A	0/306	-	-	-	-
1	63-A	0/306	-	-	-	-
1	64-A	0/306	-	-	-	-
1	65-A	0/306	-	-	-	-
1	66-A	0/306	-	-	-	-
1	67-A	0/306	-	-	-	-
1	68-A	0/306	-	-	-	-
1	69-A	0/306	-	-	-	-
1	70-A	0/306	-	-	-	-
1	71-A	0/306	-	-	-	-
1	72-A	0/306	-	-	-	-
1	73-A	0/306	-	-	-	-
1	74-A	0/306	-	-	-	-

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	75-A	0/306	-	-	-	-
All	All	306/22950 (1%)	2.82	202 (66%) 0 0	0, 0, 0, 0	306 (100%)

All (202) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	1-A	301	SER	12.0
1	1-A	153	ASP	11.9
1	1-A	302	GLY	8.4
1	1-A	93	THR	7.4
1	1-A	249	ILE	7.0
1	1-A	18	VAL	6.9
1	1-A	242	LEU	6.6
1	1-A	165	MET	6.5
1	1-A	303	VAL	6.3
1	1-A	156	CYS	6.2
1	1-A	304	THR	6.0
1	1-A	155	ASP	5.8
1	1-A	243	THR	5.7
1	1-A	59	ILE	5.6
1	1-A	75	LEU	5.5
1	1-A	300	CYS	5.5
1	1-A	91	VAL	5.3
1	1-A	49	MET	5.3
1	1-A	294	PHE	5.3
1	1-A	68	VAL	5.2
1	1-A	275	GLY	5.2
1	1-A	276	MET	5.2
1	1-A	221	ASN	5.2
1	1-A	79	GLY	4.9
1	1-A	76	ARG	4.9
1	1-A	273	GLN	4.9
1	1-A	106	ILE	4.8
1	1-A	6	MET	4.8
1	1-A	99	PRO	4.8
1	1-A	274	ASN	4.8
1	1-A	22	CYS	4.8
1	1-A	236	LYS	4.7
1	1-A	62	SER	4.6
1	1-A	81	SER	4.5
1	1-A	305	PHE	4.5
1	1-A	86	VAL	4.5

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Mol	Chain	Res	Type	RSRZ
1	1-A	77	VAL	4.5
1	1-A	130	MET	4.4
1	1-A	235	MET	4.4
1	1-A	154	TYR	4.3
1	1-A	230	PHE	4.3
1	1-A	74	GLN	4.3
1	1-A	47	GLU	4.3
1	1-A	67	LEU	4.3
1	1-A	306	GLN	4.2
1	1-A	188	ARG	4.2
1	1-A	190	THR	4.2
1	1-A	232	LEU	4.2
1	1-A	96	PRO	4.2
1	1-A	157	VAL	4.1
1	1-A	73	VAL	4.1
1	1-A	101	TYR	4.1
1	1-A	267	SER	4.1
1	1-A	286	LEU	4.1
1	1-A	70	ALA	4.0
1	1-A	278	GLY	4.0
1	1-A	61	LYS	4.0
1	1-A	98	THR	4.0
1	1-A	58	LEU	4.0
1	1-A	191	ALA	4.0
1	1-A	223	PHE	4.0
1	1-A	169	THR	3.9
1	1-A	95	ASN	3.9
1	1-A	136	ILE	3.9
1	1-A	299	GLN	3.9
1	1-A	134	PHE	3.9
1	1-A	266	ALA	3.8
1	1-A	253	LEU	3.8
1	1-A	222	ARG	3.8
1	1-A	283	GLY	3.7
1	1-A	71	GLY	3.7
1	1-A	45	THR	3.7
1	1-A	72	ASN	3.7
1	1-A	217	ARG	3.7
1	1-A	1	SER	3.7
1	1-A	194	ALA	3.6
1	1-A	51	ASN	3.6
1	1-A	19	GLN	3.6

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Mol	Chain	Res	Type	RSRZ
1	1-A	43	ILE	3.5
1	1-A	123	SER	3.5
1	1-A	239	TYR	3.5
1	1-A	87	LEU	3.5
1	1-A	102	LYS	3.4
1	1-A	46	SER	3.4
1	1-A	196	THR	3.4
1	1-A	20	VAL	3.4
1	1-A	171	VAL	3.4
1	1-A	36	VAL	3.3
1	1-A	213	ILE	3.3
1	1-A	57	LEU	3.3
1	1-A	112	PHE	3.3
1	1-A	277	ASN	3.3
1	1-A	26	THR	3.3
1	1-A	110	GLN	3.2
1	1-A	24	THR	3.2
1	1-A	42	VAL	3.2
1	1-A	205	LEU	3.2
1	1-A	121	SER	3.2
1	1-A	237	TYR	3.2
1	1-A	297	VAL	3.2
1	1-A	279	ARG	3.2
1	1-A	94	ALA	3.1
1	1-A	90	LYS	3.1
1	1-A	202	VAL	3.0
1	1-A	60	ARG	3.0
1	1-A	270	GLU	3.0
1	1-A	37	TYR	3.0
1	1-A	238	ASN	3.0
1	1-A	225	THR	3.0
1	1-A	29	GLY	3.0
1	1-A	259	ILE	3.0
1	1-A	63	ASN	2.9
1	1-A	215	GLY	2.9
1	1-A	103	PHE	2.9
1	1-A	210	ALA	2.9
1	1-A	152	ILE	2.9
1	1-A	193	ALA	2.9
1	1-A	220	LEU	2.9
1	1-A	227	LEU	2.9
1	1-A	3	PHE	2.8

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Mol	Chain	Res	Type	RSRZ
1	1-A	262	LEU	2.8
1	1-A	272	LEU	2.8
1	1-A	298	ARG	2.8
1	1-A	35	VAL	2.8
1	1-A	212	VAL	2.8
1	1-A	66	PHE	2.8
1	1-A	89	LEU	2.8
1	1-A	54	TYR	2.7
1	1-A	170	GLY	2.7
1	1-A	50	LEU	2.7
1	1-A	122	PRO	2.7
1	1-A	184	PRO	2.7
1	1-A	284	SER	2.7
1	1-A	218	TRP	2.7
1	1-A	228	ASN	2.7
1	1-A	260	ALA	2.7
1	1-A	8	PHE	2.7
1	1-A	280	THR	2.7
1	1-A	269	LYS	2.7
1	1-A	34	ASP	2.6
1	1-A	208	LEU	2.6
1	1-A	116	ALA	2.6
1	1-A	185	PHE	2.6
1	1-A	30	LEU	2.6
1	1-A	268	LEU	2.6
1	1-A	281	ILE	2.6
1	1-A	92	ASP	2.6
1	1-A	203	ASN	2.6
1	1-A	168	PRO	2.6
1	1-A	207	TRP	2.6
1	1-A	107	GLN	2.6
1	1-A	53	ASN	2.6
1	1-A	27	LEU	2.5
1	1-A	31	TRP	2.5
1	1-A	25	THR	2.5
1	1-A	150	PHE	2.5
1	1-A	78	ILE	2.5
1	1-A	105	ARG	2.4
1	1-A	100	LYS	2.4
1	1-A	233	VAL	2.4
1	1-A	246	HIS	2.4
1	1-A	250	LEU	2.4

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Mol	Chain	Res	Type	RSRZ
1	1-A	181	PHE	2.4
1	1-A	293	PRO	2.4
1	1-A	56	ASP	2.4
1	1-A	14	GLU	2.4
1	1-A	287	LEU	2.3
1	1-A	201	THR	2.3
1	1-A	290	GLU	2.3
1	1-A	23	GLY	2.3
1	1-A	186	VAL	2.3
1	1-A	44	CYS	2.3
1	1-A	141	LEU	2.3
1	1-A	198	THR	2.3
1	1-A	214	ASN	2.3
1	1-A	206	ALA	2.3
1	1-A	211	ALA	2.3
1	1-A	114	VAL	2.3
1	1-A	288	GLU	2.3
1	1-A	226	THR	2.3
1	1-A	271	LEU	2.3
1	1-A	118	TYR	2.2
1	1-A	183	GLY	2.2
1	1-A	189	GLN	2.2
1	1-A	261	VAL	2.2
1	1-A	167	LEU	2.2
1	1-A	182	TYR	2.2
1	1-A	142	ASN	2.2
1	1-A	9	PRO	2.2
1	1-A	125	VAL	2.1
1	1-A	195	GLY	2.1
1	1-A	224	THR	2.1
1	1-A	38	CYS	2.1
1	1-A	41	HIS	2.1
1	1-A	180	ASN	2.1
1	1-A	209	TYR	2.1
1	1-A	69	GLN	2.1
1	1-A	252	PRO	2.1
1	1-A	28	ASN	2.0
1	1-A	16	CYS	2.0
1	1-A	240	GLU	2.0
1	1-A	80	HIS	2.0

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($\text{\AA}^2$)	Q<0.9
2	DMS	1-A	401	4/4	0.21	0.48	32,33,33,34	10
2	DMS	2-A	401	4/4	-	-	32,33,33,34	10
2	DMS	3-A	401	4/4	-	-	32,33,33,34	10
2	DMS	4-A	401	4/4	-	-	32,33,33,34	10
2	DMS	5-A	401	4/4	-	-	32,33,33,34	10
2	DMS	6-A	401	4/4	-	-	32,33,33,34	10
2	DMS	7-A	401	4/4	-	-	32,33,33,34	10
2	DMS	8-A	401	4/4	-	-	32,33,33,34	10
2	DMS	9-A	401	4/4	-	-	32,33,33,34	10
2	DMS	10-A	401	4/4	-	-	32,33,33,34	10
2	DMS	11-A	401	4/4	-	-	32,33,33,34	10
2	DMS	12-A	401	4/4	-	-	32,33,33,34	10
2	DMS	13-A	401	4/4	-	-	32,33,33,34	10
2	DMS	14-A	401	4/4	-	-	32,33,33,34	10
2	DMS	15-A	401	4/4	-	-	32,33,33,34	10
2	DMS	16-A	401	4/4	-	-	32,33,33,34	10
2	DMS	17-A	401	4/4	-	-	32,33,33,34	10
2	DMS	18-A	401	4/4	-	-	32,33,33,34	10
2	DMS	19-A	401	4/4	-	-	32,33,33,34	10
2	DMS	20-A	401	4/4	-	-	32,33,33,34	10
2	DMS	21-A	401	4/4	-	-	32,33,33,34	10
2	DMS	22-A	401	4/4	-	-	32,33,33,34	10
2	DMS	23-A	401	4/4	-	-	32,33,33,34	10
2	DMS	24-A	401	4/4	-	-	32,33,33,34	10
2	DMS	25-A	401	4/4	-	-	32,33,33,34	10
2	DMS	26-A	401	4/4	-	-	32,33,33,34	10
2	DMS	27-A	401	4/4	-	-	32,33,33,34	10

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	DMS	28-A	401	4/4	-	-	32,33,33,34	10
2	DMS	29-A	401	4/4	-	-	32,33,33,34	10
2	DMS	30-A	401	4/4	-	-	32,33,33,34	10
2	DMS	31-A	401	4/4	-	-	32,33,33,34	10
2	DMS	32-A	401	4/4	-	-	32,33,33,34	10
2	DMS	33-A	401	4/4	-	-	32,33,33,34	10
2	DMS	34-A	401	4/4	-	-	32,33,33,34	10
2	DMS	35-A	401	4/4	-	-	32,33,33,34	10
2	DMS	36-A	401	4/4	-	-	32,33,33,34	10
2	DMS	37-A	401	4/4	-	-	32,33,33,34	10
2	DMS	38-A	401	4/4	-	-	32,33,33,34	10
2	DMS	39-A	401	4/4	-	-	32,33,33,34	10
2	DMS	40-A	401	4/4	-	-	32,33,33,34	10
2	DMS	41-A	401	4/4	-	-	32,33,33,34	10
2	DMS	42-A	401	4/4	-	-	32,33,33,34	10
2	DMS	43-A	401	4/4	-	-	32,33,33,34	10
2	DMS	44-A	401	4/4	-	-	32,33,33,34	10
2	DMS	45-A	401	4/4	-	-	32,33,33,34	10
2	DMS	46-A	401	4/4	-	-	32,33,33,34	10
2	DMS	47-A	401	4/4	-	-	32,33,33,34	10
2	DMS	48-A	401	4/4	-	-	32,33,33,34	10
2	DMS	49-A	401	4/4	-	-	32,33,33,34	10
2	DMS	50-A	401	4/4	-	-	32,33,33,34	10
2	DMS	51-A	401	4/4	-	-	32,33,33,34	10
2	DMS	52-A	401	4/4	-	-	32,33,33,34	10
2	DMS	53-A	401	4/4	-	-	32,33,33,34	10
2	DMS	54-A	401	4/4	-	-	32,33,33,34	10
2	DMS	55-A	401	4/4	-	-	32,33,33,34	10
2	DMS	56-A	401	4/4	-	-	32,33,33,34	10
2	DMS	57-A	401	4/4	-	-	32,33,33,34	10
2	DMS	58-A	401	4/4	-	-	32,33,33,34	10
2	DMS	59-A	401	4/4	-	-	32,33,33,34	10
2	DMS	60-A	401	4/4	-	-	32,33,33,34	10
2	DMS	61-A	401	4/4	-	-	32,33,33,34	10
2	DMS	62-A	401	4/4	-	-	32,33,33,34	10
2	DMS	63-A	401	4/4	-	-	32,33,33,34	10
2	DMS	64-A	401	4/4	-	-	32,33,33,34	10
2	DMS	65-A	401	4/4	-	-	32,33,33,34	10
2	DMS	66-A	401	4/4	-	-	32,33,33,34	10
2	DMS	67-A	401	4/4	-	-	32,33,33,34	10
2	DMS	68-A	401	4/4	-	-	32,33,33,34	10
2	DMS	69-A	401	4/4	-	-	32,33,33,34	10

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	DMS	70-A	401	4/4	-	-	32,33,33,34	10
2	DMS	71-A	401	4/4	-	-	32,33,33,34	10
2	DMS	72-A	401	4/4	-	-	32,33,33,34	10
2	DMS	73-A	401	4/4	-	-	32,33,33,34	10
2	DMS	74-A	401	4/4	-	-	32,33,33,34	10
2	DMS	75-A	401	4/4	-	-	32,33,33,34	10
2	DMS	1-A	402	4/4	0.64	0.34	34,35,35,35	10
2	DMS	2-A	402	4/4	-	-	34,35,35,35	10
2	DMS	3-A	402	4/4	-	-	34,35,35,35	10
2	DMS	4-A	402	4/4	-	-	34,35,35,35	10
2	DMS	5-A	402	4/4	-	-	34,35,35,35	10
2	DMS	6-A	402	4/4	-	-	34,35,35,35	10
2	DMS	7-A	402	4/4	-	-	34,35,35,35	10
2	DMS	8-A	402	4/4	-	-	34,35,35,35	10
2	DMS	9-A	402	4/4	-	-	34,35,35,35	10
2	DMS	10-A	402	4/4	-	-	34,35,35,35	10
2	DMS	11-A	402	4/4	-	-	34,35,35,35	10
2	DMS	12-A	402	4/4	-	-	34,35,35,35	10
2	DMS	13-A	402	4/4	-	-	34,35,35,35	10
2	DMS	14-A	402	4/4	-	-	34,35,35,35	10
2	DMS	15-A	402	4/4	-	-	34,35,35,35	10
2	DMS	16-A	402	4/4	-	-	34,35,35,35	10
2	DMS	17-A	402	4/4	-	-	34,35,35,35	10
2	DMS	18-A	402	4/4	-	-	34,35,35,35	10
2	DMS	19-A	402	4/4	-	-	34,35,35,35	10
2	DMS	20-A	402	4/4	-	-	34,35,35,35	10
2	DMS	21-A	402	4/4	-	-	34,35,35,35	10
2	DMS	22-A	402	4/4	-	-	34,35,35,35	10
2	DMS	23-A	402	4/4	-	-	34,35,35,35	10
2	DMS	24-A	402	4/4	-	-	34,35,35,35	10
2	DMS	25-A	402	4/4	-	-	34,35,35,35	10
2	DMS	26-A	402	4/4	-	-	34,35,35,35	10
2	DMS	27-A	402	4/4	-	-	34,35,35,35	10
2	DMS	28-A	402	4/4	-	-	34,35,35,35	10
2	DMS	29-A	402	4/4	-	-	34,35,35,35	10
2	DMS	30-A	402	4/4	-	-	34,35,35,35	10
2	DMS	31-A	402	4/4	-	-	34,35,35,35	10
2	DMS	32-A	402	4/4	-	-	34,35,35,35	10
2	DMS	33-A	402	4/4	-	-	34,35,35,35	10
2	DMS	34-A	402	4/4	-	-	34,35,35,35	10
2	DMS	35-A	402	4/4	-	-	34,35,35,35	10
2	DMS	36-A	402	4/4	-	-	34,35,35,35	10

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	DMS	37-A	402	4/4	-	-	34,35,35,35	10
2	DMS	38-A	402	4/4	-	-	34,35,35,35	10
2	DMS	39-A	402	4/4	-	-	34,35,35,35	10
2	DMS	40-A	402	4/4	-	-	34,35,35,35	10
2	DMS	41-A	402	4/4	-	-	34,35,35,35	10
2	DMS	42-A	402	4/4	-	-	34,35,35,35	10
2	DMS	43-A	402	4/4	-	-	34,35,35,35	10
2	DMS	44-A	402	4/4	-	-	34,35,35,35	10
2	DMS	45-A	402	4/4	-	-	34,35,35,35	10
2	DMS	46-A	402	4/4	-	-	34,35,35,35	10
2	DMS	47-A	402	4/4	-	-	34,35,35,35	10
2	DMS	48-A	402	4/4	-	-	34,35,35,35	10
2	DMS	49-A	402	4/4	-	-	34,35,35,35	10
2	DMS	50-A	402	4/4	-	-	34,35,35,35	10
2	DMS	51-A	402	4/4	-	-	34,35,35,35	10
2	DMS	52-A	402	4/4	-	-	34,35,35,35	10
2	DMS	53-A	402	4/4	-	-	34,35,35,35	10
2	DMS	54-A	402	4/4	-	-	34,35,35,35	10
2	DMS	55-A	402	4/4	-	-	34,35,35,35	10
2	DMS	56-A	402	4/4	-	-	34,35,35,35	10
2	DMS	57-A	402	4/4	-	-	34,35,35,35	10
2	DMS	58-A	402	4/4	-	-	34,35,35,35	10
2	DMS	59-A	402	4/4	-	-	34,35,35,35	10
2	DMS	60-A	402	4/4	-	-	34,35,35,35	10
2	DMS	61-A	402	4/4	-	-	34,35,35,35	10
2	DMS	62-A	402	4/4	-	-	34,35,35,35	10
2	DMS	63-A	402	4/4	-	-	34,35,35,35	10
2	DMS	64-A	402	4/4	-	-	34,35,35,35	10
2	DMS	65-A	402	4/4	-	-	34,35,35,35	10
2	DMS	66-A	402	4/4	-	-	34,35,35,35	10
2	DMS	67-A	402	4/4	-	-	34,35,35,35	10
2	DMS	68-A	402	4/4	-	-	34,35,35,35	10
2	DMS	69-A	402	4/4	-	-	34,35,35,35	10
2	DMS	70-A	402	4/4	-	-	34,35,35,35	10
2	DMS	71-A	402	4/4	-	-	34,35,35,35	10
2	DMS	72-A	402	4/4	-	-	34,35,35,35	10
2	DMS	73-A	402	4/4	-	-	34,35,35,35	10
2	DMS	74-A	402	4/4	-	-	34,35,35,35	10
2	DMS	75-A	402	4/4	-	-	34,35,35,35	10
3	ZN	1-A	403	1/1	0.85	0.44	35,35,35,35	1
3	ZN	2-A	403	1/1	-	-	35,35,35,35	1
3	ZN	3-A	403	1/1	-	-	35,35,35,35	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	ZN	4-A	403	1/1	-	-	35,35,35,35	1
3	ZN	5-A	403	1/1	-	-	35,35,35,35	1
3	ZN	6-A	403	1/1	-	-	35,35,35,35	1
3	ZN	7-A	403	1/1	-	-	35,35,35,35	1
3	ZN	8-A	403	1/1	-	-	35,35,35,35	1
3	ZN	9-A	403	1/1	-	-	35,35,35,35	1
3	ZN	10-A	403	1/1	-	-	35,35,35,35	1
3	ZN	11-A	403	1/1	-	-	35,35,35,35	1
3	ZN	12-A	403	1/1	-	-	35,35,35,35	1
3	ZN	13-A	403	1/1	-	-	35,35,35,35	1
3	ZN	14-A	403	1/1	-	-	35,35,35,35	1
3	ZN	15-A	403	1/1	-	-	35,35,35,35	1
3	ZN	16-A	403	1/1	-	-	35,35,35,35	1
3	ZN	17-A	403	1/1	-	-	35,35,35,35	1
3	ZN	18-A	403	1/1	-	-	35,35,35,35	1
3	ZN	19-A	403	1/1	-	-	35,35,35,35	1
3	ZN	20-A	403	1/1	-	-	35,35,35,35	1
3	ZN	21-A	403	1/1	-	-	35,35,35,35	1
3	ZN	22-A	403	1/1	-	-	35,35,35,35	1
3	ZN	23-A	403	1/1	-	-	35,35,35,35	1
3	ZN	24-A	403	1/1	-	-	35,35,35,35	1
3	ZN	25-A	403	1/1	-	-	35,35,35,35	1
3	ZN	26-A	403	1/1	-	-	35,35,35,35	1
3	ZN	27-A	403	1/1	-	-	35,35,35,35	1
3	ZN	28-A	403	1/1	-	-	35,35,35,35	1
3	ZN	29-A	403	1/1	-	-	35,35,35,35	1
3	ZN	30-A	403	1/1	-	-	35,35,35,35	1
3	ZN	31-A	403	1/1	-	-	35,35,35,35	1
3	ZN	32-A	403	1/1	-	-	35,35,35,35	1
3	ZN	33-A	403	1/1	-	-	35,35,35,35	1
3	ZN	34-A	403	1/1	-	-	35,35,35,35	1
3	ZN	35-A	403	1/1	-	-	35,35,35,35	1
3	ZN	36-A	403	1/1	-	-	35,35,35,35	1
3	ZN	37-A	403	1/1	-	-	35,35,35,35	1
3	ZN	38-A	403	1/1	-	-	35,35,35,35	1
3	ZN	39-A	403	1/1	-	-	35,35,35,35	1
3	ZN	40-A	403	1/1	-	-	35,35,35,35	1
3	ZN	41-A	403	1/1	-	-	35,35,35,35	1
3	ZN	42-A	403	1/1	-	-	35,35,35,35	1
3	ZN	43-A	403	1/1	-	-	35,35,35,35	1
3	ZN	44-A	403	1/1	-	-	35,35,35,35	1
3	ZN	45-A	403	1/1	-	-	35,35,35,35	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	ZN	46-A	403	1/1	-	-	35,35,35,35	1
3	ZN	47-A	403	1/1	-	-	35,35,35,35	1
3	ZN	48-A	403	1/1	-	-	35,35,35,35	1
3	ZN	49-A	403	1/1	-	-	35,35,35,35	1
3	ZN	50-A	403	1/1	-	-	35,35,35,35	1
3	ZN	51-A	403	1/1	-	-	35,35,35,35	1
3	ZN	52-A	403	1/1	-	-	35,35,35,35	1
3	ZN	53-A	403	1/1	-	-	35,35,35,35	1
3	ZN	54-A	403	1/1	-	-	35,35,35,35	1
3	ZN	55-A	403	1/1	-	-	35,35,35,35	1
3	ZN	56-A	403	1/1	-	-	35,35,35,35	1
3	ZN	57-A	403	1/1	-	-	35,35,35,35	1
3	ZN	58-A	403	1/1	-	-	35,35,35,35	1
3	ZN	59-A	403	1/1	-	-	35,35,35,35	1
3	ZN	60-A	403	1/1	-	-	35,35,35,35	1
3	ZN	61-A	403	1/1	-	-	35,35,35,35	1
3	ZN	62-A	403	1/1	-	-	35,35,35,35	1
3	ZN	63-A	403	1/1	-	-	35,35,35,35	1
3	ZN	64-A	403	1/1	-	-	35,35,35,35	1
3	ZN	65-A	403	1/1	-	-	35,35,35,35	1
3	ZN	66-A	403	1/1	-	-	35,35,35,35	1
3	ZN	67-A	403	1/1	-	-	35,35,35,35	1
3	ZN	68-A	403	1/1	-	-	35,35,35,35	1
3	ZN	69-A	403	1/1	-	-	35,35,35,35	1
3	ZN	70-A	403	1/1	-	-	35,35,35,35	1
3	ZN	71-A	403	1/1	-	-	35,35,35,35	1
3	ZN	72-A	403	1/1	-	-	35,35,35,35	1
3	ZN	73-A	403	1/1	-	-	35,35,35,35	1
3	ZN	74-A	403	1/1	-	-	35,35,35,35	1
3	ZN	75-A	403	1/1	-	-	35,35,35,35	1

5.5 Other polymers ⓘ

There are no such residues in this entry.