



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 26, 2026 – 06:18 AM UTC

PDB ID : 7MHQ / pdb_00007mhq
Title : Ensemble refinement structure of SARS-CoV-2 main protease (Mpro) at 310 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 : 1.96 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

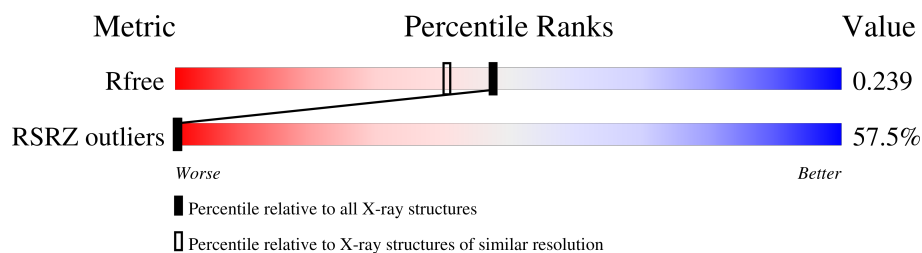
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.96 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	3494 (1.96-1.96)
RSRZ outliers	180081	3495 (1.96-1.96)

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	17-A	502	-	X	-	-
2	DMS	6-A	501	-	X	-	-
3	ZN	1-A	503	-	-	-	X

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 170649 atoms, of which 83700 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.

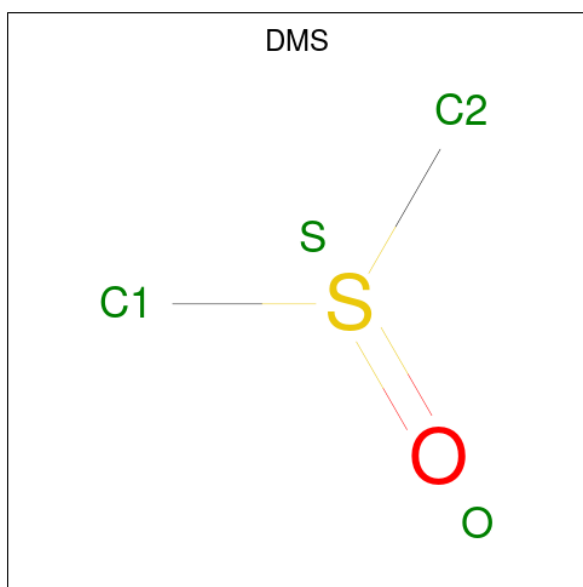
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	1-A	306	Total	C	H	N	O	S	0	0	0
			4680	1499	2313	402	444	22			
1	2-A	306	Total	C	H	N	O	S	0	0	0
			4680	1499	2313	402	444	22			
1	3-A	306	Total	C	H	N	O	S	0	0	0
			4680	1499	2313	402	444	22			
1	4-A	306	Total	C	H	N	O	S	0	0	0
			4680	1499	2313	402	444	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			

- 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 10	C 2	H 6	O 1	S 1	0	0
2	1-A	1	Total 10	C 2	H 6	O 1	S 1	0	0
2	2-A	1	Total 10	C 2	H 6	O 1	S 1	0	0
2	3-A	1	Total 10	C 2	H 6	O 1	S 1	0	0
2	4-A	1	Total 10	C 2	H 6	O 1	S 1	0	0
2	5-A	1	Total 10	C 2	H 6	O 1	S 1	0	0
2	6-A	1	Total 10	C 2	H 6	O 1	S 1	0	0
2	7-A	1	Total 10	C 2	H 6	O 1	S 1	0	0
2	8-A	1	Total 10	C 2	H 6	O 1	S 1	0	0
2	9-A	1	Total 10	C 2	H 6	O 1	S 1	0	0
2	10-A	1	Total 10	C 2	H 6	O 1	S 1	0	0
2	11-A	1	Total 10	C 2	H 6	O 1	S 1	0	0
2	12-A	1	Total 10	C 2	H 6	O 1	S 1	0	0
2	13-A	1	Total 10	C 2	H 6	O 1	S 1	0	0
2	14-A	1	Total 10	C 2	H 6	O 1	S 1	0	0
2	15-A	1	Total 10	C 2	H 6	O 1	S 1	0	0
2	16-A	1	Total 10	C 2	H 6	O 1	S 1	0	0
2	17-A	1	Total 10	C 2	H 6	O 1	S 1	0	0
2	18-A	1	Total 10	C 2	H 6	O 1	S 1	0	0
2	19-A	1	Total 10	C 2	H 6	O 1	S 1	0	0
2	20-A	1	Total 10	C 2	H 6	O 1	S 1	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
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		
2	36-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		

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

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
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
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

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	1-A	45	Total 45	O 45	0	0
4	2-A	45	Total 45	O 45	0	0
4	3-A	46	Total 46	O 46	0	0
4	4-A	37	Total 37	O 37	0	0
4	5-A	42	Total 42	O 42	0	0
4	6-A	43	Total 43	O 43	0	0
4	7-A	35	Total 35	O 35	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	8-A	33	Total 33	O 33	0	0
4	9-A	39	Total 39	O 39	0	0
4	10-A	37	Total 37	O 37	0	0
4	11-A	41	Total 41	O 41	0	0
4	12-A	42	Total 42	O 42	0	0
4	13-A	45	Total 45	O 45	0	0
4	14-A	43	Total 43	O 43	0	0
4	15-A	38	Total 38	O 38	0	0
4	16-A	30	Total 30	O 30	0	0
4	17-A	34	Total 34	O 34	0	0
4	18-A	46	Total 46	O 46	0	0
4	19-A	41	Total 41	O 41	0	0
4	20-A	38	Total 38	O 38	0	0
4	21-A	42	Total 42	O 42	0	0
4	22-A	44	Total 44	O 44	0	0
4	23-A	40	Total 40	O 40	0	0
4	24-A	33	Total 33	O 33	0	0
4	25-A	36	Total 36	O 36	0	0
4	26-A	41	Total 41	O 41	0	0
4	27-A	38	Total 38	O 38	0	0
4	28-A	39	Total 39	O 39	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	29-A	38	Total	O	0	0
			38	38		
4	30-A	37	Total	O	0	0
			37	37		
4	31-A	34	Total	O	0	0
			34	34		
4	32-A	34	Total	O	0	0
			34	34		
4	33-A	39	Total	O	0	0
			39	39		
4	34-A	48	Total	O	0	0
			48	48		
4	35-A	37	Total	O	0	0
			37	37		
4	36-A	33	Total	O	0	0
			33	33		

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	114.30Å 54.29Å 44.97Å 90.00° 102.12° 90.00°	Depositor
Resolution (Å)	43.97 – 1.96 43.97 – 1.96	Depositor EDS
% Data completeness (in resolution range)	99.8 (43.97-1.96) 56.7 (43.97-1.96)	Depositor EDS
R_{merge}	0.20	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.55 (at 1.97Å)	Xtriage
Refinement program	PHENIX (phenix.ensemble_refinement:1.19.2_4158)	Depositor
R, R_{free}	0.171 , 0.235 0.178 , 0.239	Depositor DCC
R_{free} test set	880 reflections (4.52%)	wwPDB-VP
Wilson B-factor (Å ²)	29.5	Xtriage
Anisotropy	0.246	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.01 , 47.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.87	EDS
Total number of atoms	170649	wwPDB-VP
Average B, all atoms (Å ²)	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.77% 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 108 ligands modelled in this entry, 36 are monoatomic - leaving 72 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	6-A	501	-	3,3,3	0.76	0	3,3,3	2.78	3 (100%)
2	DMS	32-A	501	-	3,3,3	0.91	0	3,3,3	0.99	0
2	DMS	29-A	501	-	3,3,3	0.81	0	3,3,3	1.35	1 (33%)
2	DMS	23-A	502	-	3,3,3	0.77	0	3,3,3	1.09	0
2	DMS	4-A	501	-	3,3,3	0.68	0	3,3,3	1.29	0
2	DMS	28-A	502	-	3,3,3	0.74	0	3,3,3	1.93	1 (33%)
2	DMS	21-A	502	-	3,3,3	0.76	0	3,3,3	2.02	2 (66%)
2	DMS	17-A	501	-	3,3,3	0.53	0	3,3,3	1.30	0
2	DMS	26-A	501	-	3,3,3	0.67	0	3,3,3	0.34	0
2	DMS	7-A	502	-	3,3,3	0.83	0	3,3,3	2.41	1 (33%)
2	DMS	25-A	501	-	3,3,3	0.77	0	3,3,3	1.79	1 (33%)
2	DMS	1-A	501	-	3,3,3	0.79	0	3,3,3	2.26	2 (66%)
2	DMS	34-A	502	-	3,3,3	0.86	0	3,3,3	1.86	1 (33%)
2	DMS	18-A	501	-	3,3,3	0.86	0	3,3,3	0.58	0
2	DMS	31-A	501	-	3,3,3	0.88	0	3,3,3	2.50	1 (33%)
2	DMS	14-A	501	-	3,3,3	0.57	0	3,3,3	0.81	0
2	DMS	35-A	501	-	3,3,3	0.73	0	3,3,3	0.51	0
2	DMS	2-A	502	-	3,3,3	0.82	0	3,3,3	0.55	0
2	DMS	11-A	502	-	3,3,3	0.81	0	3,3,3	0.25	0
2	DMS	12-A	502	-	3,3,3	0.77	0	3,3,3	1.38	1 (33%)
2	DMS	24-A	501	-	3,3,3	0.74	0	3,3,3	1.34	1 (33%)
2	DMS	15-A	502	-	3,3,3	0.72	0	3,3,3	2.01	1 (33%)
2	DMS	16-A	502	-	3,3,3	0.75	0	3,3,3	1.40	0
2	DMS	19-A	502	-	3,3,3	0.83	0	3,3,3	1.03	0
2	DMS	6-A	502	-	3,3,3	0.97	0	3,3,3	0.97	0
2	DMS	20-A	502	-	3,3,3	0.72	0	3,3,3	0.80	0
2	DMS	24-A	502	-	3,3,3	0.83	0	3,3,3	1.58	1 (33%)
2	DMS	10-A	501	-	3,3,3	0.75	0	3,3,3	1.10	0
2	DMS	9-A	502	-	3,3,3	0.59	0	3,3,3	1.37	1 (33%)
2	DMS	29-A	502	-	3,3,3	0.71	0	3,3,3	0.44	0
2	DMS	13-A	502	-	3,3,3	0.90	0	3,3,3	1.82	0
2	DMS	8-A	501	-	3,3,3	0.63	0	3,3,3	0.50	0
2	DMS	3-A	502	-	3,3,3	0.89	0	3,3,3	2.23	1 (33%)
2	DMS	9-A	501	-	3,3,3	0.61	0	3,3,3	1.40	1 (33%)
2	DMS	27-A	501	-	3,3,3	0.70	0	3,3,3	1.13	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	DMS	11-A	501	-	3,3,3	0.71	0	3,3,3	1.94	1 (33%)
2	DMS	28-A	501	-	3,3,3	0.93	0	3,3,3	1.19	0
2	DMS	31-A	502	-	3,3,3	0.57	0	3,3,3	2.01	1 (33%)
2	DMS	33-A	502	-	3,3,3	0.73	0	3,3,3	0.91	0
2	DMS	2-A	501	-	3,3,3	0.72	0	3,3,3	1.26	0
2	DMS	26-A	502	-	3,3,3	0.77	0	3,3,3	0.78	0
2	DMS	22-A	501	-	3,3,3	0.93	0	3,3,3	2.18	1 (33%)
2	DMS	5-A	501	-	3,3,3	0.63	0	3,3,3	1.24	0
2	DMS	32-A	502	-	3,3,3	0.88	0	3,3,3	1.99	2 (66%)
2	DMS	20-A	501	-	3,3,3	0.77	0	3,3,3	0.63	0
2	DMS	30-A	502	-	3,3,3	0.72	0	3,3,3	0.66	0
2	DMS	5-A	502	-	3,3,3	0.87	0	3,3,3	1.94	1 (33%)
2	DMS	36-A	501	-	3,3,3	0.75	0	3,3,3	1.20	0
2	DMS	4-A	502	-	3,3,3	0.77	0	3,3,3	0.79	0
2	DMS	34-A	501	-	3,3,3	0.61	0	3,3,3	1.27	1 (33%)
2	DMS	22-A	502	-	3,3,3	0.54	0	3,3,3	1.08	0
2	DMS	3-A	501	-	3,3,3	0.71	0	3,3,3	0.46	0
2	DMS	13-A	501	-	3,3,3	0.82	0	3,3,3	1.72	1 (33%)
2	DMS	16-A	501	-	3,3,3	0.86	0	3,3,3	1.25	0
2	DMS	19-A	501	-	3,3,3	0.60	0	3,3,3	1.42	0
2	DMS	8-A	502	-	3,3,3	0.81	0	3,3,3	1.14	0
2	DMS	1-A	502	-	3,3,3	0.85	0	3,3,3	0.90	0
2	DMS	12-A	501	-	3,3,3	0.64	0	3,3,3	0.88	0
2	DMS	25-A	502	-	3,3,3	0.92	0	3,3,3	0.77	0
2	DMS	27-A	502	-	3,3,3	0.94	0	3,3,3	0.47	0
2	DMS	14-A	502	-	3,3,3	0.81	0	3,3,3	2.14	1 (33%)
2	DMS	7-A	501	-	3,3,3	0.72	0	3,3,3	1.04	0
2	DMS	17-A	502	-	3,3,3	0.93	0	3,3,3	3.15	3 (100%)
2	DMS	18-A	502	-	3,3,3	0.73	0	3,3,3	1.51	1 (33%)
2	DMS	36-A	502	-	3,3,3	0.68	0	3,3,3	1.24	0
2	DMS	15-A	501	-	3,3,3	0.64	0	3,3,3	1.60	1 (33%)
2	DMS	23-A	501	-	3,3,3	0.85	0	3,3,3	2.09	1 (33%)
2	DMS	35-A	502	-	3,3,3	0.73	0	3,3,3	1.40	1 (33%)
2	DMS	33-A	501	-	3,3,3	0.73	0	3,3,3	1.09	0
2	DMS	30-A	501	-	3,3,3	0.79	0	3,3,3	1.01	0
2	DMS	21-A	501	-	3,3,3	0.67	0	3,3,3	0.92	0
2	DMS	10-A	502	-	3,3,3	0.84	0	3,3,3	1.18	0

There are no bond length outliers.

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	7-A	502	DMS	O-S-C2	4.16	127.30	106.49
2	17-A	502	DMS	O-S-C1	3.75	125.25	106.49
2	14-A	502	DMS	O-S-C1	3.61	124.55	106.49
2	31-A	501	DMS	O-S-C2	3.45	123.75	106.49
2	22-A	501	DMS	O-S-C1	3.40	123.53	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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	4-A	1
1	22-A	1
1	10-A	1
1	15-A	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
4	A	106:ILE	C	107:GLN	N	1.17
22	A	106:ILE	C	107:GLN	N	1.15
10	A	106:ILE	C	107:GLN	N	1.13
15	A	106:ILE	C	107:GLN	N	1.11

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%)	2.49	176 (57%) 0 0	1, 1, 1, 2	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	-	-	-	-
All	All	306/11016 (2%)	2.49	176 (57%) 0 0	1, 1, 1, 2	306 (100%)

The worst 5 of 176 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	1-A	300	CYS	8.9
1	1-A	304	THR	8.4
1	1-A	303	VAL	8.4
1	1-A	218	TRP	7.7
1	1-A	276	MET	7.4

5.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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(Å ²)	Q<0.9
2	DMS	1-A	502	4/4	0.49	0.35	40,41,41,41	10
2	DMS	2-A	501	4/4	-	-	38,39,39,39	10
2	DMS	3-A	501	4/4	-	-	38,39,39,39	10
2	DMS	4-A	501	4/4	-	-	38,39,39,39	10
2	DMS	5-A	501	4/4	-	-	38,39,39,39	10
2	DMS	6-A	501	4/4	-	-	38,39,39,39	10
2	DMS	7-A	501	4/4	-	-	38,39,39,39	10
2	DMS	8-A	501	4/4	-	-	38,39,39,39	10
2	DMS	9-A	501	4/4	-	-	38,39,39,39	10

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	DMS	10-A	501	4/4	-	-	38,39,39,39	10
2	DMS	11-A	501	4/4	-	-	38,39,39,39	10
2	DMS	12-A	501	4/4	-	-	38,39,39,39	10
2	DMS	13-A	501	4/4	-	-	38,39,39,39	10
2	DMS	14-A	501	4/4	-	-	38,39,39,39	10
2	DMS	15-A	501	4/4	-	-	38,39,39,39	10
2	DMS	16-A	501	4/4	-	-	38,39,39,39	10
2	DMS	17-A	501	4/4	-	-	38,39,39,39	10
2	DMS	18-A	501	4/4	-	-	38,39,39,39	10
2	DMS	19-A	501	4/4	-	-	38,39,39,39	10
2	DMS	20-A	501	4/4	-	-	38,39,39,39	10
2	DMS	21-A	501	4/4	-	-	38,39,39,39	10
2	DMS	22-A	501	4/4	-	-	38,39,39,39	10
2	DMS	23-A	501	4/4	-	-	38,39,39,39	10
2	DMS	24-A	501	4/4	-	-	38,39,39,39	10
2	DMS	25-A	501	4/4	-	-	38,39,39,39	10
2	DMS	26-A	501	4/4	-	-	38,39,39,39	10
2	DMS	27-A	501	4/4	-	-	38,39,39,39	10
2	DMS	28-A	501	4/4	-	-	38,39,39,39	10
2	DMS	29-A	501	4/4	-	-	38,39,39,39	10
2	DMS	30-A	501	4/4	-	-	38,39,39,39	10
2	DMS	31-A	501	4/4	-	-	38,39,39,39	10
2	DMS	32-A	501	4/4	-	-	38,39,39,39	10
2	DMS	33-A	501	4/4	-	-	38,39,39,39	10
2	DMS	34-A	501	4/4	-	-	38,39,39,39	10
2	DMS	35-A	501	4/4	-	-	38,39,39,39	10
2	DMS	36-A	501	4/4	-	-	38,39,39,39	10
3	ZN	1-A	503	1/1	0.69	0.62	41,41,41,41	1
2	DMS	2-A	502	4/4	-	-	40,41,41,41	10
2	DMS	3-A	502	4/4	-	-	40,41,41,41	10
2	DMS	4-A	502	4/4	-	-	40,41,41,41	10
2	DMS	5-A	502	4/4	-	-	40,41,41,41	10
2	DMS	6-A	502	4/4	-	-	40,41,41,41	10
2	DMS	7-A	502	4/4	-	-	40,41,41,41	10
2	DMS	8-A	502	4/4	-	-	40,41,41,41	10
2	DMS	9-A	502	4/4	-	-	40,41,41,41	10
2	DMS	10-A	502	4/4	-	-	40,41,41,41	10
2	DMS	11-A	502	4/4	-	-	40,41,41,41	10
2	DMS	12-A	502	4/4	-	-	40,41,41,41	10
2	DMS	13-A	502	4/4	-	-	40,41,41,41	10
2	DMS	14-A	502	4/4	-	-	40,41,41,41	10
2	DMS	15-A	502	4/4	-	-	40,41,41,41	10

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	DMS	16-A	502	4/4	-	-	40,41,41,41	10
2	DMS	17-A	502	4/4	-	-	40,41,41,41	10
2	DMS	18-A	502	4/4	-	-	40,41,41,41	10
2	DMS	19-A	502	4/4	-	-	40,41,41,41	10
2	DMS	20-A	502	4/4	-	-	40,41,41,41	10
2	DMS	21-A	502	4/4	-	-	40,41,41,41	10
2	DMS	22-A	502	4/4	-	-	40,41,41,41	10
2	DMS	23-A	502	4/4	-	-	40,41,41,41	10
2	DMS	24-A	502	4/4	-	-	40,41,41,41	10
2	DMS	25-A	502	4/4	-	-	40,41,41,41	10
2	DMS	26-A	502	4/4	-	-	40,41,41,41	10
2	DMS	27-A	502	4/4	-	-	40,41,41,41	10
2	DMS	28-A	502	4/4	-	-	40,41,41,41	10
2	DMS	29-A	502	4/4	-	-	40,41,41,41	10
2	DMS	30-A	502	4/4	-	-	40,41,41,41	10
2	DMS	31-A	502	4/4	-	-	40,41,41,41	10
2	DMS	32-A	502	4/4	-	-	40,41,41,41	10
2	DMS	33-A	502	4/4	-	-	40,41,41,41	10
2	DMS	34-A	502	4/4	-	-	40,41,41,41	10
2	DMS	35-A	502	4/4	-	-	40,41,41,41	10
2	DMS	36-A	502	4/4	-	-	40,41,41,41	10
2	DMS	1-A	501	4/4	0.92	0.13	38,39,39,39	10
3	ZN	2-A	503	1/1	-	-	41,41,41,41	1
3	ZN	3-A	503	1/1	-	-	41,41,41,41	1
3	ZN	4-A	503	1/1	-	-	41,41,41,41	1
3	ZN	5-A	503	1/1	-	-	41,41,41,41	1
3	ZN	6-A	503	1/1	-	-	41,41,41,41	1
3	ZN	7-A	503	1/1	-	-	41,41,41,41	1
3	ZN	8-A	503	1/1	-	-	41,41,41,41	1
3	ZN	9-A	503	1/1	-	-	41,41,41,41	1
3	ZN	10-A	503	1/1	-	-	41,41,41,41	1
3	ZN	11-A	503	1/1	-	-	41,41,41,41	1
3	ZN	12-A	503	1/1	-	-	41,41,41,41	1
3	ZN	13-A	503	1/1	-	-	41,41,41,41	1
3	ZN	14-A	503	1/1	-	-	41,41,41,41	1
3	ZN	15-A	503	1/1	-	-	41,41,41,41	1
3	ZN	16-A	503	1/1	-	-	41,41,41,41	1
3	ZN	17-A	503	1/1	-	-	41,41,41,41	1
3	ZN	18-A	503	1/1	-	-	41,41,41,41	1
3	ZN	19-A	503	1/1	-	-	41,41,41,41	1
3	ZN	20-A	503	1/1	-	-	41,41,41,41	1
3	ZN	21-A	503	1/1	-	-	41,41,41,41	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	ZN	22-A	503	1/1	-	-	41,41,41,41	1
3	ZN	23-A	503	1/1	-	-	41,41,41,41	1
3	ZN	24-A	503	1/1	-	-	41,41,41,41	1
3	ZN	25-A	503	1/1	-	-	41,41,41,41	1
3	ZN	26-A	503	1/1	-	-	41,41,41,41	1
3	ZN	27-A	503	1/1	-	-	41,41,41,41	1
3	ZN	28-A	503	1/1	-	-	41,41,41,41	1
3	ZN	29-A	503	1/1	-	-	41,41,41,41	1
3	ZN	30-A	503	1/1	-	-	41,41,41,41	1
3	ZN	31-A	503	1/1	-	-	41,41,41,41	1
3	ZN	32-A	503	1/1	-	-	41,41,41,41	1
3	ZN	33-A	503	1/1	-	-	41,41,41,41	1
3	ZN	34-A	503	1/1	-	-	41,41,41,41	1
3	ZN	35-A	503	1/1	-	-	41,41,41,41	1
3	ZN	36-A	503	1/1	-	-	41,41,41,41	1

5.5 Other polymers [i](#)

There are no such residues in this entry.