



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 29, 2026 – 12:17 AM UTC

PDB ID : 5W8T / pdb_00005w8t
Title : Crystal structure of MERS-CoV papain-like protease in complex with the C-terminal domain of human ISG15
Authors : Daczkowski, C.M.; Goodwin, O.Y.; Dzimianski, J.V.; Farhat, J.J.; Pegan, S.D.
Deposited on : 2017-06-22
Resolution : 2.76 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

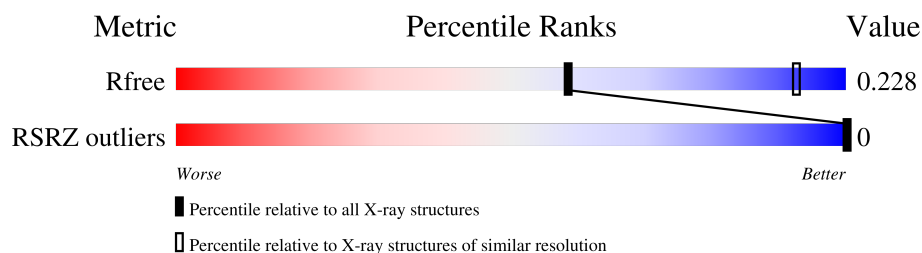
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.76 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	1009 (2.76-2.76)
RSRZ outliers	180081	1009 (2.76-2.76)

MolProbity failed to run properly - the sequence quality summary graphics cannot be shown.

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 6293 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 Ubiquitin-like protein ISG15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	77	Total	C	N	O	S	0	0	0
			615	392	107	115	1			
1	D	77	Total	C	N	O	S	0	0	0
			615	392	107	115	1			

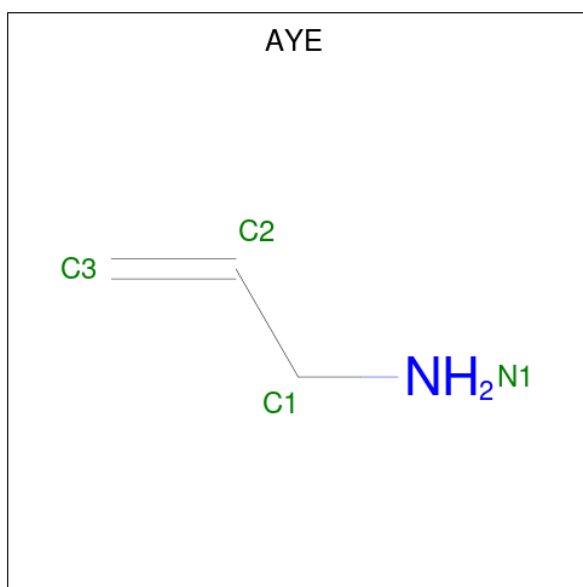
There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	79	MET	-	initiating methionine	UNP P05161
D	79	MET	-	initiating methionine	UNP P05161

- Molecule 2 is a protein called ORF1ab.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	A	319	Total	C	N	O	S	0	0	0
			2485	1583	425	458	19			
2	C	319	Total	C	N	O	S	0	0	0
			2485	1583	425	458	19			

- Molecule 3 is prop-2-en-1-amine (CCD ID: AYE) (formula: C₃H₇N).

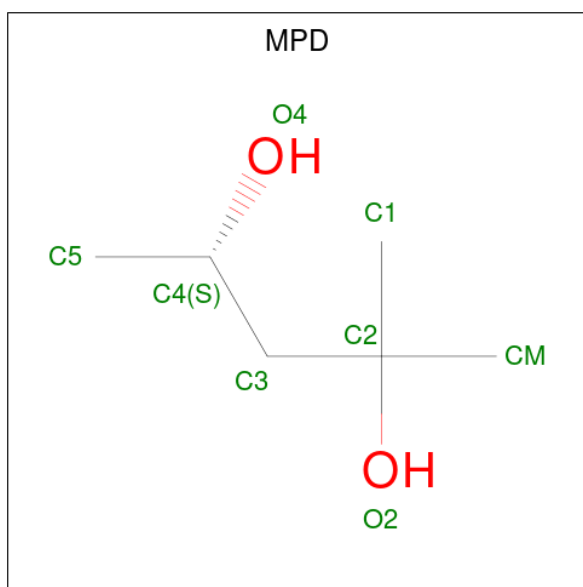


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	B	1	Total	C	N	0	0
			4	3	1		
3	D	1	Total	C	N	0	0
			4	3	1		

- Molecule 4 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	5	Total	Zn	0	0
			5	5		
4	C	1	Total	Zn	0	0
			1	1		

- Molecule 5 is (4S)-2-METHYL-2,4-PENTANEDIOL (CCD ID: MPD) (formula: C₆H₁₄O₂).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C O 8 6 2	0	0
5	A	1	Total C O 8 6 2	0	0
5	D	1	Total C O 8 6 2	0	0
5	D	1	Total C O 8 6 2	0	0
5	C	1	Total C O 8 6 2	0	0
5	C	1	Total C O 8 6 2	0	0

- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	B	2	Total O 2 2	0	0
6	A	11	Total O 11 11	0	0
6	D	6	Total O 6 6	0	0
6	C	12	Total O 12 12	0	0

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3 Data and refinement statistics

Property	Value	Source
Space group	P 43	Depositor
Cell constants a, b, c, α , β , γ	86.34Å 86.34Å 223.63Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	41.23 – 2.76 41.23 – 2.76	Depositor EDS
% Data completeness (in resolution range)	99.8 (41.23-2.76) 99.9 (41.23-2.76)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.14 (at 2.77Å)	Xtriage
Refinement program	PHENIX (1.11.1_2575: ???)	Depositor
R, R_{free}	0.187 , 0.224 0.194 , 0.228	Depositor DCC
R_{free} test set	2036 reflections (4.85%)	wwPDB-VP
Wilson B-factor (Å ²)	73.1	Xtriage
Anisotropy	0.419	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 39.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.478 for h,-k,-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	6293	wwPDB-VP
Average B, all atoms (Å ²)	84.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.12% 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](#)

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4.2 Too-close contacts [i](#)

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4.3 Torsion angles [i](#)

4.3.1 Protein backbone [i](#)

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4.3.2 Protein sidechains [i](#)

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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 14 ligands modelled in this entry, 6 are monoatomic - leaving 8 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	$\# Z > 2$
3	AYE	D	201	1,2	3,3,3	0.78	0	2,2,2	1.84	1 (50%)
5	MPD	C	403	-	7,7,7	0.70	0	9,10,10	0.37	0
5	MPD	D	202	-	7,7,7	0.74	0	9,10,10	0.39	0
3	AYE	B	201	1,2	3,3,3	0.76	0	2,2,2	1.85	1 (50%)
5	MPD	C	402	-	7,7,7	0.69	0	9,10,10	0.45	0
5	MPD	A	407	-	7,7,7	0.68	0	9,10,10	0.40	0
5	MPD	D	203	-	7,7,7	0.74	0	9,10,10	0.50	0
5	MPD	A	406	-	7,7,7	0.77	0	9,10,10	0.34	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	AYE	D	201	1,2	-	1/1/1/1	-
5	MPD	C	403	-	-	2/5/5/5	-
5	MPD	D	202	-	-	2/5/5/5	-
3	AYE	B	201	1,2	-	1/1/1/1	-
5	MPD	C	402	-	-	2/5/5/5	-
5	MPD	A	407	-	-	3/5/5/5	-
5	MPD	D	203	-	-	3/5/5/5	-
5	MPD	A	406	-	-	4/5/5/5	-

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	201	AYE	C1-C2-C3	-2.50	119.52	126.38
3	B	201	AYE	C1-C2-C3	-2.46	119.65	126.38

There are no chirality outliers.

All (18) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	407	MPD	O2-C2-C3-C4

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Mol	Chain	Res	Type	Atoms
5	A	407	MPD	CM-C2-C3-C4
5	D	202	MPD	C2-C3-C4-O4
5	D	202	MPD	C2-C3-C4-C5
5	C	403	MPD	C1-C2-C3-C4
3	B	201	AYE	N1-C1-C2-C3
3	D	201	AYE	N1-C1-C2-C3
5	A	407	MPD	C1-C2-C3-C4
5	D	203	MPD	C1-C2-C3-C4
5	C	402	MPD	CM-C2-C3-C4
5	A	406	MPD	C2-C3-C4-C5
5	A	406	MPD	O2-C2-C3-C4
5	A	406	MPD	C2-C3-C4-O4
5	D	203	MPD	C2-C3-C4-O4
5	A	406	MPD	CM-C2-C3-C4
5	D	203	MPD	CM-C2-C3-C4
5	C	402	MPD	C1-C2-C3-C4
5	C	403	MPD	CM-C2-C3-C4

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 [i](#)

5.1 Protein, DNA and RNA chains [i](#)

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	B	77/78 (98%)	-1.14	0 100 100	54, 74, 108, 121	0
1	D	77/78 (98%)	-1.15	0 100 100	54, 73, 105, 117	0
2	A	319/322 (99%)	-0.91	0 100 100	55, 84, 119, 154	0
2	C	319/322 (99%)	-0.92	0 100 100	53, 83, 119, 159	0
All	All	792/800 (99%)	-0.96	0 100 100	53, 82, 118, 159	0

There are no RSRZ outliers to report.

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

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

5.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	MPD	D	203	8/8	0.98	0.09	90,103,114,117	0
4	ZN	A	403	1/1	0.99	0.06	143,143,143,143	0
5	MPD	A	406	8/8	0.99	0.07	75,97,109,111	0
5	MPD	A	407	8/8	0.99	0.08	85,92,98,100	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	MPD	D	202	8/8	0.99	0.08	93,102,113,123	0
3	AYE	D	201	4/4	0.99	0.04	55,57,61,62	0
5	MPD	C	402	8/8	0.99	0.06	72,77,91,96	0
5	MPD	C	403	8/8	0.99	0.06	90,96,106,110	0
4	ZN	A	401	1/1	1.00	0.01	105,105,105,105	0
4	ZN	A	402	1/1	1.00	0.02	124,124,124,124	0
3	AYE	B	201	4/4	1.00	0.04	50,53,63,70	0
4	ZN	A	404	1/1	1.00	0.02	120,120,120,120	0
4	ZN	A	405	1/1	1.00	0.02	116,116,116,116	0
4	ZN	C	401	1/1	1.00	0.02	107,107,107,107	0

5.5 Other polymers [i](#)

There are no such residues in this entry.