



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 12, 2021 – 02:07 PM JST

PDB ID : 7F0U
Title : porcine epidemic diarrhea virus papain-like protease 2 C44S mutant in complex with mono ubiquitin
Authors : Chu, H.F.; Lin, T.H.
Deposited on : 2021-06-07
Resolution : 2.20 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Xtriage (Phenix) : 1.13
EDS : 2.23.2
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.23.2

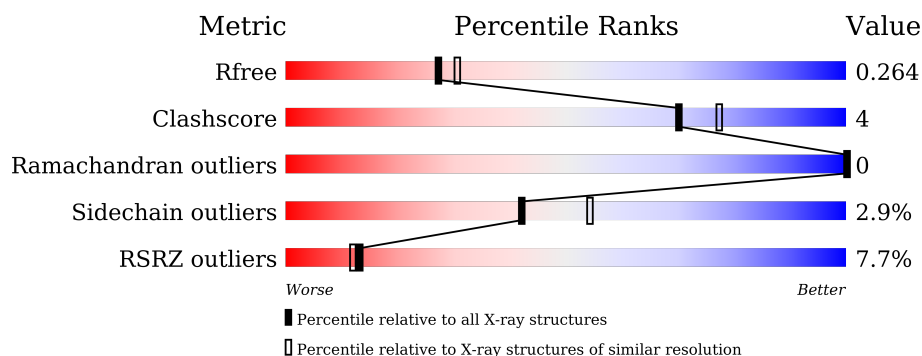
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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}	130704	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (2.20-2.20)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	237	<div> <div>6%</div> <div>84%</div> <div>7%</div> <div>8%</div> </div>
1	B	237	<div> <div>8%</div> <div>80%</div> <div>11%</div> <div>8%</div> </div>
2	C	76	<div> <div>92%</div> <div>8%</div> </div>
2	D	76	<div> <div>14%</div> <div>89%</div> <div>9%</div> </div>

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	ZN	A	301	-	-	X	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 4727 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 papain-like protease 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	217	Total	C	N	O	S	0	2	0
			1677	1073	283	310	11			
1	B	217	Total	C	N	O	S	0	3	0
			1642	1043	279	309	11			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	44	SER	CYS	engineered mutation	UNP A0A0U2C377
B	44	SER	CYS	engineered mutation	UNP A0A0U2C377

- Molecule 2 is a protein called Ubiquitin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	76	Total	C	N	O	S	0	0	0
			602	378	105	118	1			
2	D	76	Total	C	N	O		0	0	0
			557	345	102	110				

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Zn	0	0
			1	1		
3	B	1	Total	Zn	0	0
			1	1		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	123	Total	O	0	0
			123	123		

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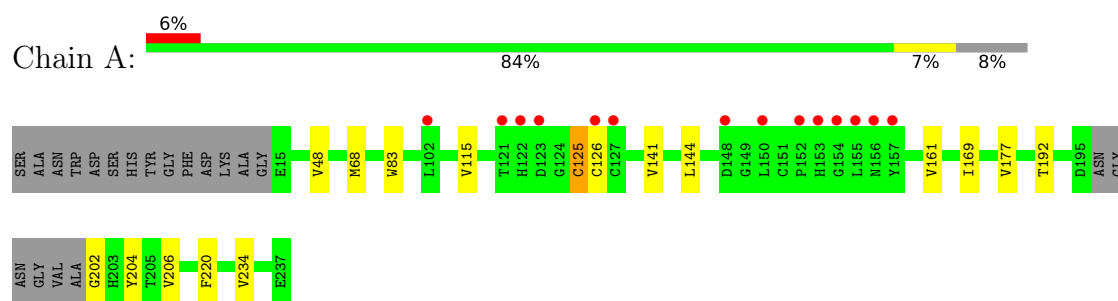
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	53	Total 53	O 53	0	0
4	C	41	Total 41	O 41	0	0
4	D	30	Total 30	O 30	0	0

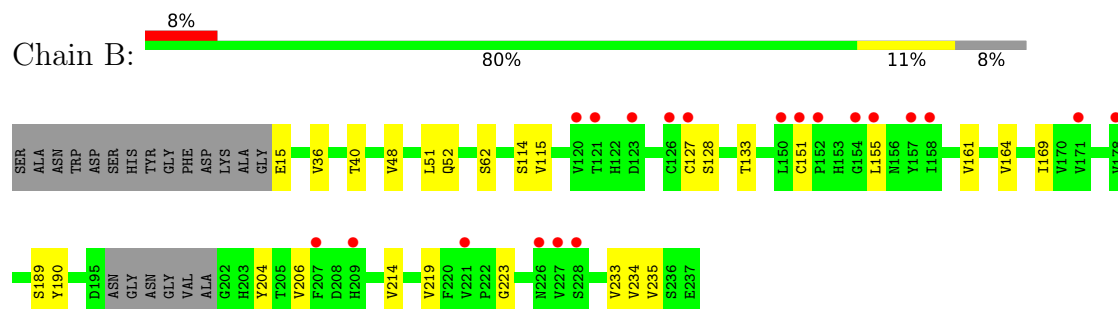
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

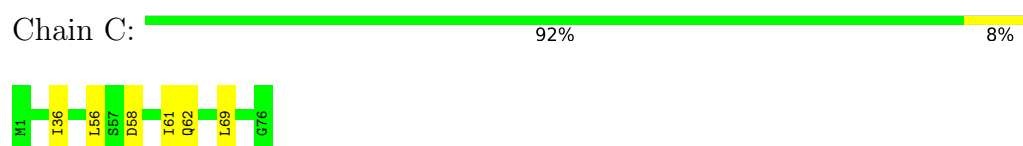
- Molecule 1: papain-like protease 2



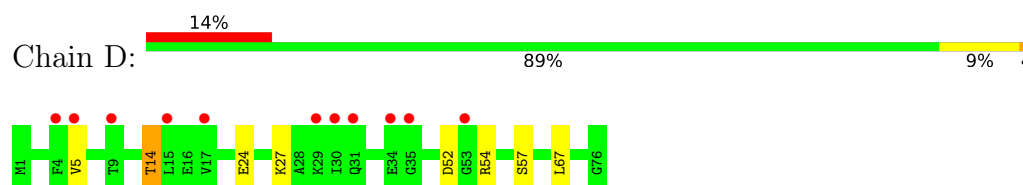
- Molecule 1: papain-like protease 2



- Molecule 2: Ubiquitin



- Molecule 2: Ubiquitin



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	37.13Å 86.45Å 90.70Å 90.00° 91.79° 90.00°	Depositor
Resolution (Å)	29.18 – 2.20 29.16 – 2.20	Depositor EDS
% Data completeness (in resolution range)	99.2 (29.18-2.20) 99.3 (29.16-2.20)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.99 (at 2.20Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.226 , 0.260 0.229 , 0.264	Depositor DCC
R_{free} test set	1647 reflections (5.66%)	wwPDB-VP
Wilson B-factor (Å ²)	29.1	Xtriage
Anisotropy	0.046	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 42.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.034 for h,-k,-l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	4727	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 5.75% 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.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: ZN

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 $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.64	0/1721	0.75	0/2347
1	B	0.69	0/1681	0.75	0/2294
2	C	0.66	0/608	0.78	0/816
2	D	0.69	0/562	0.79	0/760
All	All	0.67	0/4572	0.76	0/6217

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1677	0	1641	12	0
1	B	1642	0	1581	13	0
2	C	602	0	629	3	0
2	D	557	0	538	4	0
3	A	1	0	0	2	0
3	B	1	0	0	0	0
4	A	123	0	0	2	0
4	B	53	0	0	2	0
4	C	41	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	D	30	0	0	1	0
All	All	4727	0	4389	32	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

All (32) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:126:CYS:HG	3:A:301:ZN:ZN	0.80	0.95
1:A:126:CYS:SG	3:A:301:ZN:ZN	1.71	0.77
1:B:115:VAL:HG13	1:B:161:VAL:HG13	1.82	0.60
1:B:164:VAL:HG21	1:B:235:VAL:HG11	1.84	0.59
1:A:141:VAL:CG2	1:A:177[A]:VAL:HG21	2.32	0.58
2:D:14:THR:HG23	4:D:117:HOH:O	2.08	0.54
1:B:48:VAL:HG11	1:B:204:TYR:HB3	1.92	0.52
1:A:48:VAL:HG11	1:A:204:TYR:HB3	1.93	0.51
1:A:68:MET:HE1	1:A:83:TRP:HB2	1.95	0.49
1:A:125:CYS:SG	1:A:126:CYS:N	2.86	0.48
2:D:27:LYS:NZ	2:D:52:ASP:OD1	2.44	0.48
1:B:15:GLU:N	4:B:406:HOH:O	2.46	0.48
2:C:58:ASP:OD1	4:C:101:HOH:O	2.20	0.47
1:B:169:ILE:HG12	1:B:234:VAL:HG22	1.98	0.46
2:D:24:GLU:OE2	2:D:24:GLU:N	2.45	0.46
2:D:5:VAL:HA	2:D:67:LEU:O	2.16	0.45
1:B:214:VAL:HG23	1:B:223:GLY:HA3	1.97	0.45
1:A:115:VAL:HG13	1:A:161:VAL:HG13	1.98	0.44
1:A:144:LEU:HD23	4:A:449:HOH:O	2.17	0.44
1:B:164:VAL:HG11	1:B:235:VAL:HG12	2.00	0.44
2:C:36:ILE:HD13	2:C:69:LEU:HD21	1.99	0.43
1:B:40:THR:HG22	4:B:407:HOH:O	2.19	0.43
1:A:125:CYS:SG	1:A:126:CYS:SG	3.14	0.42
1:B:36:VAL:HG12	1:B:51:LEU:HD21	2.02	0.42
1:B:114:SER:HB3	1:B:133:THR:HG22	2.00	0.42
1:B:190:TYR:CD2	1:B:233[B]:VAL:HG22	2.54	0.42
1:A:48:VAL:HG12	1:A:206:VAL:HG23	2.02	0.42
1:B:52:GLN:HA	1:B:52:GLN:OE1	2.19	0.42
1:A:169:ILE:HG12	1:A:234:VAL:HG22	2.02	0.42
1:B:48:VAL:HG12	1:B:206:VAL:HG23	2.02	0.41
1:A:202:GLY:N	4:A:410:HOH:O	2.52	0.41
2:C:56:LEU:HD22	2:C:61:ILE:HG21	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	215/237 (91%)	211 (98%)	4 (2%)	0	100	100
1	B	216/237 (91%)	210 (97%)	6 (3%)	0	100	100
2	C	74/76 (97%)	74 (100%)	0	0	100	100
2	D	74/76 (97%)	69 (93%)	5 (7%)	0	100	100
All	All	579/626 (92%)	564 (97%)	15 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	189/202 (94%)	186 (98%)	3 (2%)	62	76
1	B	180/202 (89%)	173 (96%)	7 (4%)	32	41
2	C	68/68 (100%)	67 (98%)	1 (2%)	65	78
2	D	55/68 (81%)	52 (94%)	3 (6%)	21	26
All	All	492/540 (91%)	478 (97%)	14 (3%)	42	56

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	125	CYS
1	A	192	THR
1	A	220	PHE
1	B	62	SER
1	B	127	CYS
1	B	128	SER
1	B	151	CYS
1	B	155	LEU
1	B	189	SER
1	B	219	VAL
2	C	62	GLN
2	D	14	THR
2	D	54	ARG
2	D	57	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	103	ASN
1	A	122	HIS
1	A	138	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 2 ligands modelled in this entry, 2 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.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 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	A	217/237 (91%)	0.20	14 (6%) 18 17	16, 26, 73, 99	0
1	B	217/237 (91%)	0.59	20 (9%) 9 7	18, 43, 68, 84	0
2	C	76/76 (100%)	-0.15	0 100 100	18, 31, 43, 53	0
2	D	76/76 (100%)	1.00	11 (14%) 2 2	23, 54, 72, 78	0
All	All	586/626 (93%)	0.40	45 (7%) 13 12	16, 35, 69, 99	0

All (45) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	152	PRO	7.1
1	A	155	LEU	5.4
1	A	153	HIS	5.0
1	A	156	ASN	5.0
1	B	227	VAL	5.0
1	B	154	GLY	4.7
1	A	150	LEU	4.4
2	D	17	VAL	4.3
2	D	34	GLU	4.1
2	D	35	GLY	4.0
1	A	154	GLY	4.0
1	A	123	ASP	3.9
1	A	148	ASP	3.8
1	A	122	HIS	3.8
1	B	151	CYS	3.6
1	B	155	LEU	3.5
1	B	158	ILE	3.4
2	D	30	ILE	3.4
1	B	209	HIS	3.4
1	B	150	LEU	3.3
1	A	127	CYS	3.2

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Mol	Chain	Res	Type	RSRZ
2	D	5	VAL	3.0
1	B	126	CYS	2.9
1	A	126	CYS	2.8
1	B	120	VAL	2.7
1	B	207	PHE	2.7
1	B	123	ASP	2.7
2	D	15	LEU	2.7
1	B	152	PRO	2.6
1	B	157	TYR	2.6
1	A	121	THR	2.6
2	D	31	GLN	2.4
1	B	228	SER	2.4
1	B	221	VAL	2.4
1	B	171	VAL	2.3
2	D	4	PHE	2.2
1	A	157	TYR	2.2
1	A	102	LEU	2.2
1	B	121	THR	2.1
1	B	178	VAL	2.1
2	D	9	THR	2.1
2	D	53	GLY	2.1
1	B	127	CYS	2.1
1	B	226	ASN	2.0
2	D	29	LYS	2.0

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

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

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 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(\AA^2)	Q<0.9
3	ZN	A	301	1/1	0.94	0.07	78,78,78,78	0
3	ZN	B	301	1/1	0.96	0.06	72,72,72,72	0

6.5 Other polymers [i](#)

There are no such residues in this entry.