



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 14, 2016 – 04:42 AM EDT

PDB ID : 4XFQ
Title : Crystal Structure Basis for PEDV 3C Like Protease
Authors : Ye, G.; Fu, Z.F.; Peng, G.Q.
Deposited on : 2014-12-28
Resolution : 1.65 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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

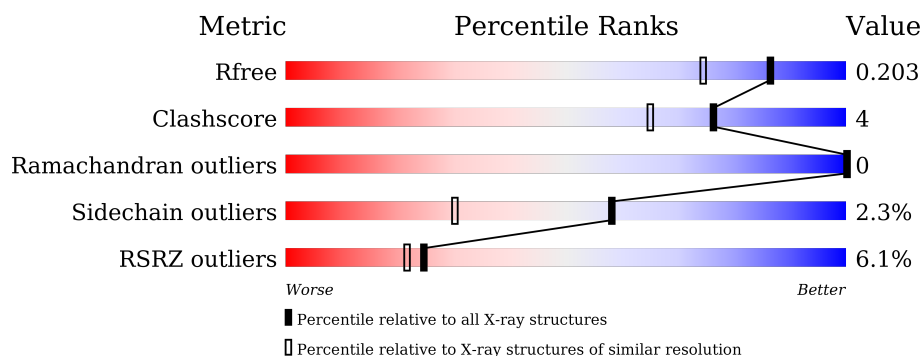
The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : unknown
Xtriage (Phenix) : 1.9-1692
EDS : rb-20027790
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20027790

i

X-RAY DIFFRACTION

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}	91344	1226 (1.66-1.66)
Clashscore	102246	1323 (1.66-1.66)
Ramachandran outliers	100387	1295 (1.66-1.66)
Sidechain outliers	100360	1295 (1.66-1.66)
RSRZ outliers	91569	1227 (1.66-1.66)

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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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	305	
1	B	305	

2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 4975 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 PEDV main protease.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	298	Total	C	N	O	S	0	0	0
			2270	1432	392	430	16			
1	B	294	Total	C	N	O	S	0	0	0
			2244	1418	388	422	16			

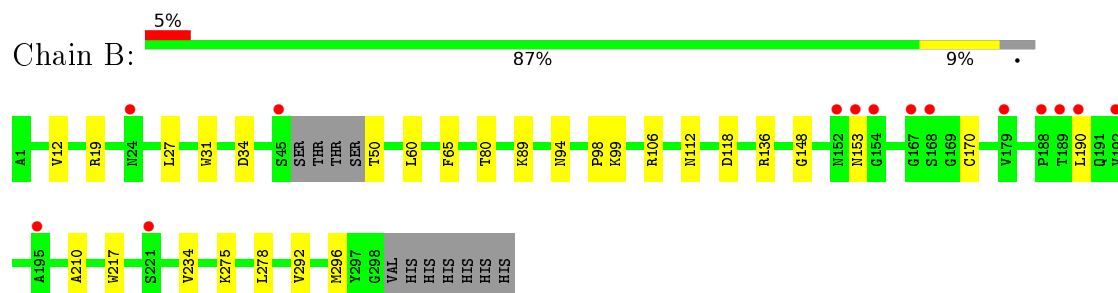
There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	299	VAL	-	expression tag	UNP K4L9I6
A	300	HIS	-	expression tag	UNP K4L9I6
A	301	HIS	-	expression tag	UNP K4L9I6
A	302	HIS	-	expression tag	UNP K4L9I6
A	303	HIS	-	expression tag	UNP K4L9I6
A	304	HIS	-	expression tag	UNP K4L9I6
A	305	HIS	-	expression tag	UNP K4L9I6
B	299	VAL	-	expression tag	UNP K4L9I6
B	300	HIS	-	expression tag	UNP K4L9I6
B	301	HIS	-	expression tag	UNP K4L9I6
B	302	HIS	-	expression tag	UNP K4L9I6
B	303	HIS	-	expression tag	UNP K4L9I6
B	304	HIS	-	expression tag	UNP K4L9I6
B	305	HIS	-	expression tag	UNP K4L9I6

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	225	Total	O	0	0
			225	225		
2	B	236	Total	O	0	0
			236	236		

- Molecule 1: PEDV main protease



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	56.64Å 91.06Å 57.98Å 90.00° 100.25° 90.00°	Depositor
Resolution (Å)	27.45 – 1.65 27.87 – 1.65	Depositor EDS
% Data completeness (in resolution range)	99.5 (27.45-1.65) 94.8 (27.87-1.65)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.11 (at 1.65Å)	Xtriage
Refinement program	phenix	Depositor
R, R_{free}	0.178 , 0.205 0.176 , 0.203	Depositor DCC
R_{free} test set	1910 reflections (2.90%)	DCC
Wilson B-factor (Å ²)	18.2	Xtriage
Anisotropy	0.760	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 51.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.019 for l,-k,h	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	4975	wwPDB-VP
Average B, all atoms (Å ²)	24.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.95% 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

5.1 Standard geometry

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	0.37	0/2316	0.57	0/3145
1	B	0.36	0/2289	0.56	0/3106
All	All	0.36	0/4605	0.56	0/6251

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

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	2270	0	2223	17	0
1	B	2244	0	2198	17	0
2	A	225	0	0	2	2
2	B	236	0	0	4	2
All	All	4975	0	4421	34	2

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 (34) 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:127:VAL:HB	1:A:136:ARG:HH21	1.34	0.92

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:136:ARG:HG3	1:A:136:ARG:HH11	1.53	0.73
1:A:224:ILE:HD11	1:A:228:ARG:HG3	1.76	0.68
1:A:128:ASN:H	1:A:136:ARG:NH2	1.95	0.65
1:A:128:ASN:O	1:A:136:ARG:NH2	2.32	0.63
1:A:223:ARG:NH2	1:A:257:ASP:OD2	2.31	0.62
1:A:136:ARG:HG3	1:A:136:ARG:NH1	2.14	0.61
1:B:19:ARG:HH11	1:B:118:ASP:HA	1.67	0.60
1:A:136:ARG:CZ	1:A:136:ARG:H	2.14	0.59
1:A:228:ARG:NH1	1:A:228:ARG:O	2.37	0.57
1:B:34:ASP:OD2	1:B:89:LYS:NZ	2.42	0.53
1:B:217:TRP:CD2	1:B:275:LYS:HD3	2.45	0.52
1:B:217:TRP:CE2	1:B:275:LYS:HD3	2.45	0.51
1:B:80:THR:HG23	2:B:483:HOH:O	2.11	0.51
1:B:50:THR:N	2:B:617:HOH:O	2.45	0.49
1:B:106:ARG:HG2	2:B:458:HOH:O	2.12	0.49
1:A:112:ASN:O	1:A:148:GLY:HA2	2.13	0.48
1:B:292:VAL:O	1:B:296:MET:HG2	2.13	0.48
1:B:112:ASN:O	1:B:148:GLY:HA2	2.14	0.47
1:A:157:GLU:HG3	2:A:605:HOH:O	2.14	0.46
1:B:170:CYS:HA	2:B:503:HOH:O	2.15	0.46
1:A:153:ASN:HB3	2:A:537:HOH:O	2.16	0.45
1:B:31:TRP:CE2	1:B:94:ASN:HB2	2.51	0.45
1:B:19:ARG:NH1	1:B:118:ASP:OD1	2.49	0.45
1:A:292:VAL:O	1:A:296:MET:HG2	2.17	0.45
1:B:210:ALA:HA	1:B:278:LEU:HD11	2.00	0.44
1:A:180:MET:CE	1:A:186:ASP:HB3	2.48	0.44
1:B:60:LEU:HD11	1:B:65:PHE:CE2	2.53	0.43
1:A:31:TRP:CE2	1:A:94:ASN:HB2	2.53	0.43
1:B:99:LYS:HB2	1:B:99:LYS:HE2	1.86	0.43
1:B:89:LYS:HG3	1:B:89:LYS:HZ2	1.66	0.42
1:A:15:LYS:HB3	1:A:15:LYS:HE3	1.82	0.42
1:A:45:SER:HA	1:A:46:SER:OG	2.21	0.41
1:B:12:VAL:CG2	1:B:98:PRO:HB3	2.51	0.41

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:438:HOH:O	2:B:430:HOH:O[1_554]	2.07	0.13
2:A:462:HOH:O	2:B:458:HOH:O[1_554]	2.09	0.11

5.3 Torsion angles

5.3.1 Protein backbone

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	296/305 (97%)	291 (98%)	5 (2%)	0	100	100
1	B	290/305 (95%)	285 (98%)	5 (2%)	0	100	100
All	All	586/610 (96%)	576 (98%)	10 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains

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	245/252 (97%)	239 (98%)	6 (2%)	57	28
1	B	241/252 (96%)	236 (98%)	5 (2%)	61	34
All	All	486/504 (96%)	475 (98%)	11 (2%)	58	30

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	27	LEU
1	A	45	SER
1	A	60	LEU
1	A	136	ARG
1	A	227	ASP
1	A	243	ASN
1	B	27	LEU
1	B	136	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	153	ASN
1	B	190	LEU
1	B	234	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	276	GLN

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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

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	298/305 (97%)	0.21	22 (7%) 17 15	12, 23, 44, 63	0
1	B	294/305 (96%)	0.09	14 (4%) 34 32	13, 21, 37, 48	1 (0%)
All	All	592/610 (97%)	0.15	36 (6%) 25 22	12, 22, 41, 63	1 (0%)

All (36) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	48	THR	7.8
1	A	47	THR	7.7
1	B	167	GLY	6.7
1	A	242	VAL	6.4
1	A	46	SER	6.2
1	A	167	GLY	4.5
1	B	192	VAL	4.3
1	B	190	LEU	4.2
1	A	271	ASN	3.8
1	A	190	LEU	3.7
1	A	195	ALA	3.6
1	B	24	ASN	3.6
1	A	45	SER	3.5
1	B	154	GLY	3.5
1	A	228	ARG	3.1
1	A	49	SER	3.1
1	B	195	ALA	3.1
1	A	63	HIS	3.0
1	A	168	SER	2.8
1	B	153	ASN	2.8
1	B	168	SER	2.7
1	A	188	PRO	2.7
1	A	73	PHE	2.7
1	A	194	GLY	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	243	ASN	2.6
1	A	153	ASN	2.3
1	A	50	THR	2.2
1	B	221	SER	2.2
1	B	189	THR	2.2
1	B	188	PRO	2.2
1	A	71	ASN	2.2
1	B	179	VAL	2.1
1	A	224	ILE	2.1
1	B	152	ASN	2.1
1	B	45	SER	2.0
1	A	152	ASN	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 carbohydrates in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.