



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 29, 2020 – 03:13 PM BST

PDB ID : 5ZBI
Title : Crystal structure of asparaginyl endopeptidases from *Viola Canadensis*
Authors : Wong, Y.H.; Lescar, J.
Deposited on : 2018-02-12
Resolution : 2.09 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	:	2.13
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)	:	2.13

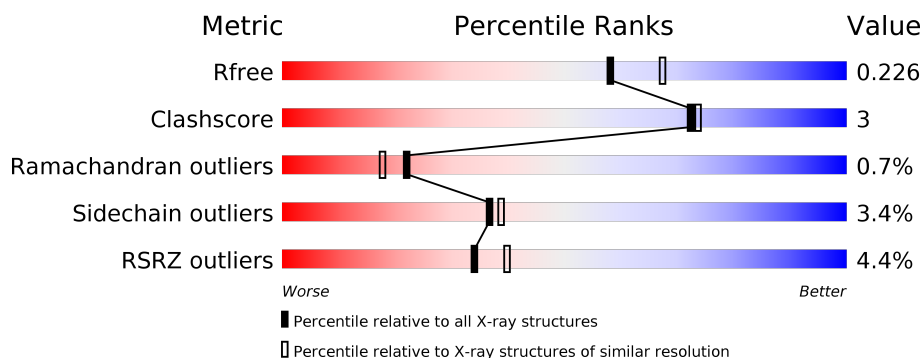
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.09 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	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (2.10-2.10)

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 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	532	<div> <div>3%</div> <div> <div></div> <div>72%</div> <div>6%</div> <div>21%</div> </div> </div>
1	B	532	<div> <div>4%</div> <div> <div></div> <div>70%</div> <div>7%</div> <div>22%</div> </div> </div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 7056 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 Peptide asparaginyl ligase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	420	Total	C	N	O	S	0	0	0
			3296	2090	552	635	19			
1	B	415	Total	C	N	O	S	0	0	0
			3261	2068	546	628	19			

- Molecule 2 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Na	0	0
			1	1		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	291	Total	O	0	0
			291	291		
3	B	207	Total	O	0	0
			207	207		

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.

- Chain A:
-
- Sequence logo for Chain A. The y-axis represents information content in bits. The x-axis shows positions 1 to 100. The sequence is: MET, ALA, HIS, HIS, HIS, HIS, HIS, MET, GLN, ILE, PHE, VAL, LYS, THR, THR, LEU, LEU, GLY, THR, THR, THR, THR, LEU, LEU, GLU, VAL, GLU, PRO, SER, ASP, THR, ILE, GLU, ASN, VAL, LYS, ALA, LYS, ILE, GLN, ASP, LYS, GLU, GLY, ILE, PRO, ASP, PRO, ASP, GLN, GLN, ARG, LEU, ILE, PHE, ALA, GLY, LYS, GLN, LEU, GLU.

- [illegible]

4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	184.47Å 62.08Å 82.91Å 90.00° 106.81° 90.00°	Depositor
Resolution (Å)	44.42 – 2.09 44.15 – 2.09	Depositor EDS
% Data completeness (in resolution range)	99.4 (44.42-2.09) 99.7 (44.15-2.09)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.05 (at 2.10Å)	Xtriage
Refinement program	BUSTER 2.10.3	Depositor
R, R_{free}	0.189 , 0.225 0.188 , 0.226	Depositor DCC
R_{free} test set	2661 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	27.2	Xtriage
Anisotropy	0.567	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 58.4	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	0.96	EDS
Total number of atoms	7056	wwPDB-VP
Average B, all atoms (Å ²)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.36% 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

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

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	0.53	1/3377 (0.0%)	0.64	0/4579
1	B	0.49	0/3340	0.65	0/4527
All	All	0.51	1/6717 (0.0%)	0.64	0/9106

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	174	MET	SD-CE	-5.19	1.48	1.77

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	3296	0	3176	21	0
1	B	3261	0	3146	21	0
2	A	1	0	0	0	0
3	A	291	0	0	2	0
3	B	207	0	0	1	0
All	All	7056	0	6322	42	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 3.

All (42) 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:165:ASP:CG	1:A:166:HIS:H	1.56	1.05
1:A:56:SER:HB3	1:A:165:ASP:OD1	1.62	0.99
1:B:165:ASP:CG	1:B:166:HIS:H	1.58	0.98
1:B:56:SER:HB3	1:B:165:ASP:OD1	1.63	0.96
1:A:165:ASP:CG	1:A:166:HIS:N	2.35	0.81
1:B:165:ASP:CG	1:B:166:HIS:N	2.36	0.72
1:A:331:SER:H	1:A:332:PRO:HD3	1.58	0.69
1:B:337:VAL:HG21	1:B:345:HIS:CE1	2.27	0.69
1:B:111:LYS:HD3	1:B:249:PRO:HG2	1.78	0.65
1:A:345:HIS:CD2	3:A:682:HOH:O	2.53	0.62
1:A:167:GLY:HA3	1:A:207:ALA:HB1	1.87	0.56
1:B:277:THR:HA	1:B:307:SER:HA	1.90	0.54
1:A:445:ILE:HG23	1:A:450:ILE:HB	1.90	0.54
1:B:400:MET:O	1:B:440:ARG:HD2	2.09	0.53
1:A:345:HIS:HD2	3:A:682:HOH:O	1.89	0.52
1:B:445:ILE:HG23	1:B:450:ILE:HB	1.91	0.52
1:B:416:CYS:HG	1:B:446:CYS:CB	2.22	0.51
1:B:245:GLU:CB	1:B:246:PRO:HD3	2.42	0.50
1:A:277:THR:HA	1:A:307:SER:HA	1.94	0.48
1:B:398:GLU:O	1:B:402:THR:HB	2.14	0.47
1:B:242:PRO:HB3	1:B:250:ALA:HA	1.97	0.47
1:B:395:LYS:HE3	1:B:395:LYS:HB2	1.81	0.46
1:A:331:SER:N	1:A:332:PRO:HD3	2.27	0.45
1:B:245:GLU:HB3	1:B:246:PRO:HD3	1.98	0.45
1:A:331:SER:N	1:A:332:PRO:CD	2.80	0.45
1:A:127:VAL:HG12	1:A:174:MET:HE3	1.97	0.45
1:B:167:GLY:HA3	1:B:207:ALA:HB1	1.99	0.45
1:B:276:GLN:HG3	1:B:323:TYR:CD2	2.52	0.45
1:A:342:ALA:O	1:A:345:HIS:HB2	2.17	0.44
1:A:209:GLU:HG3	1:A:232:ALA:HA	2.00	0.44
1:B:278:LEU:HB2	1:B:304:SER:HA	2.00	0.43
1:A:276:GLN:HG3	1:A:323:TYR:CD2	2.54	0.43
1:A:278:LEU:HB2	1:A:304:SER:HA	2.01	0.42
1:A:89:MET:O	1:A:123:THR:HA	2.19	0.42
1:A:64:HIS:CG	1:A:165:ASP:HA	2.55	0.42
1:B:280:GLN:HG2	1:B:326:GLU:HA	2.01	0.41
1:A:331:SER:H	1:A:332:PRO:CD	2.31	0.41
1:B:166:HIS:HA	3:B:634:HOH:O	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:201:LEU:HB3	1:B:224:ILE:HG12	2.03	0.41
1:A:238:VAL:HG21	1:A:342:ALA:HB2	2.03	0.40
1:B:240:TYR:HB3	1:B:248:VAL:HG21	2.02	0.40
1:A:50:ALA:HA	1:A:160:PHE:O	2.22	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	416/532 (78%)	404 (97%)	9 (2%)	3 (1%)	22	18
1	B	411/532 (77%)	395 (96%)	13 (3%)	3 (1%)	22	18
All	All	827/1064 (78%)	799 (97%)	22 (3%)	6 (1%)	22	18

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	165	ASP
1	B	165	ASP
1	B	245	GLU
1	B	432	SER
1	A	245	GLU
1	A	331	SER

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	355/454 (78%)	345 (97%)	10 (3%)	43	47
1	B	350/454 (77%)	336 (96%)	14 (4%)	31	32
All	All	705/908 (78%)	681 (97%)	24 (3%)	37	39

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	108	SER
1	A	203	PHE
1	A	209	GLU
1	A	321	ARG
1	A	331	SER
1	A	333	HIS
1	A	352	GLN
1	A	359	ARG
1	A	454	LYS
1	A	465	ASN
1	B	60	GLN
1	B	108	SER
1	B	177	GLU
1	B	203	PHE
1	B	244	GLN
1	B	300	ASP
1	B	321	ARG
1	B	326	GLU
1	B	350	LYS
1	B	359	ARG
1	B	367	GLN
1	B	395	LYS
1	B	402	THR
1	B	432	SER

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

Mol	Chain	Res	Type
1	A	377	HIS
1	B	107	ASN
1	B	244	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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 1 ligands modelled in this entry, 1 is 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 [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	420/532 (78%)	0.00	14 (3%) 46 53	17, 27, 54, 93	0
1	B	415/532 (78%)	0.30	23 (5%) 25 31	20, 38, 69, 109	0
All	All	835/1064 (78%)	0.15	37 (4%) 34 40	17, 32, 63, 109	0

All (37) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	329	SER	10.2
1	A	466	PHE	9.8
1	A	331	SER	8.8
1	B	45	ALA	7.0
1	B	394	ALA	6.8
1	A	45	ALA	6.2
1	A	465	ASN	6.0
1	A	330	SER	5.3
1	A	467	PRO	4.4
1	B	244	GLN	4.3
1	B	247	PRO	4.3
1	B	392	SER	3.9
1	B	326	GLU	3.8
1	B	325	ASP	3.5
1	A	324	GLU	3.5
1	B	245	GLU	3.4
1	A	245	GLU	3.3
1	B	432	SER	3.3
1	A	332	PRO	3.1
1	B	243	SER	3.1
1	B	402	THR	2.9
1	B	324	GLU	2.8
1	B	429	GLY	2.7
1	B	309	PHE	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	325	ASP	2.6
1	B	464	LEU	2.6
1	B	427	HIS	2.5
1	B	322	GLN	2.4
1	B	46	GLY	2.2
1	A	464	LEU	2.2
1	B	141	THR	2.2
1	B	275	THR	2.2
1	A	321	ARG	2.2
1	B	109	PRO	2.1
1	B	139	ASN	2.1
1	B	456	GLY	2.0
1	A	322	GLN	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
2	NA	A	501	1/1	0.68	0.29	51,51,51,51	0

6.5 Other polymers [i](#)

There are no such residues in this entry.