



Full wwPDB X-ray Structure Validation Report ⓘ

Jul 5, 2022 – 01:07 pm BST

PDB ID : 7QY6
Title : Structure of E.coli Class 2 L-asparaginase EcAIII, wild type (WT EcAIII)
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Deposited on : 2022-01-27
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

<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 : 4.02b-467
Xtrriage (Phenix) : 1.13
EDS : **FAILED**
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.29

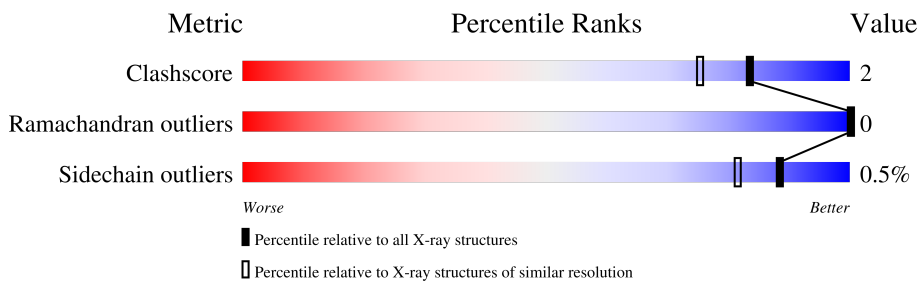
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.65 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))
Clashscore	141614	1931 (1.66-1.66)
Ramachandran outliers	138981	1891 (1.66-1.66)
Sidechain outliers	138945	1891 (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 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 $\leq 5\%$.

Note EDS failed to run properly.

Mol	Chain	Length	Quality of chain
1	AAA	178	
1	CCC	178	
2	BBB	143	
2	DDD	143	

2 Entry composition i

There are 5 unique types of molecules in this entry. The entry contains 4649 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 Isoaspartyl peptidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	AAA	154	1156	722	201	223	10	0	2	0
1	CCC	155	1165	727	206	222	10	0	1	0

- Molecule 2 is a protein called Beta-aspartyl-peptidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	BBB	135	958	597	161	193	7	0	1	0
2	DDD	135	956	597	161	191	7	0	1	0

- Molecule 3 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	AAA	1	Total	Na	0	0
			1	1		
3	CCC	1	Total	Na	0	0
			1	1		

- Molecule 4 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	AAA	1	Total	Cl	0	0
			1	1		
4	CCC	1	Total	Cl	0	0
			1	1		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	AAA	126	Total 126	O 126	0	0
5	BBB	88	Total 88	O 88	0	0
5	CCC	128	Total 128	O 128	0	0
5	DDD	68	Total 68	O 68	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. 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. 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.


Note EDS failed to run properly.

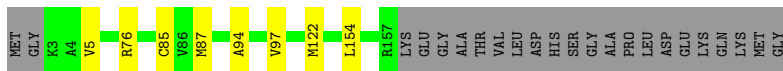
- Molecule 1: Isoaspartyl peptidase

Chain AAA:  82% 13%



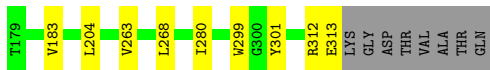
- Molecule 1: Isoaspartyl peptidase

Chain CCC:  83% 13%



- Molecule 2: Beta-aspartyl-peptidase

Chain BBB:  88% 6% 6%



- Molecule 2: Beta-aspartyl-peptidase

Chain DDD:  88% 6% 6%



4 Data and refinement statistics

EDS failed to run properly - this section is therefore incomplete.

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	50.48Å 75.35Å 147.99Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	67.24 – 1.65	Depositor
% Data completeness (in resolution range)	99.6 (67.24-1.65)	Depositor
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.95 (at 1.65Å)	Xtrriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.193 , 0.235	Depositor
Wilson B-factor (Å ²)	23.4	Xtrriage
Anisotropy	0.257	Xtrriage
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
Total number of atoms	4649	wwPDB-VP
Average B, all atoms (Å ²)	30.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 28.07 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.9658e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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: CL, 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	AAA	0.83	0/1176	0.93	0/1588
1	CCC	0.75	0/1182	0.88	0/1594
2	BBB	0.76	0/976	0.89	0/1328
2	DDD	0.75	0/974	0.89	0/1326
All	All	0.77	0/4308	0.90	0/5836

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	AAA	1156	0	1157	4	0
1	CCC	1165	0	1175	7	0
2	BBB	958	0	933	7	0
2	DDD	956	0	936	7	0
3	AAA	1	0	0	0	0
3	CCC	1	0	0	0	0
4	AAA	1	0	0	0	0
4	CCC	1	0	0	0	0
5	AAA	126	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	BBB	88	0	0	0	0
5	CCC	128	0	0	0	0
5	DDD	68	0	0	2	0
All	All	4649	0	4201	20	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 2.

All (20) 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:AAA:87:MET:HG3	1:AAA:94:ALA:HB2	1.66	0.77
1:CCC:87:MET:HG3	1:CCC:94:ALA:HB2	1.78	0.64
2:DDD:203:LYS:HA	5:DDD:423:HOH:O	2.03	0.59
1:CCC:5:VAL:HB	2:DDD:301:TYR:CD1	2.45	0.52
2:BBB:312:ARG:O	2:BBB:313:GLU:HB3	2.12	0.48
1:CCC:76:ARG:HA	2:DDD:202:ASN:OD1	2.15	0.46
2:BBB:204:LEU:HD23	1:CCC:122[B]:MET:CE	2.46	0.46
2:BBB:204:LEU:HD23	1:CCC:122[B]:MET:HE3	1.97	0.46
2:DDD:200:MET:SD	2:DDD:207:ARG:NH2	2.89	0.46
2:BBB:183:VAL:HG23	2:BBB:280:ILE:HD12	2.00	0.43
1:CCC:85:CYS:HB2	2:DDD:212:PRO:HA	2.00	0.42
2:BBB:299:TRP:HZ3	2:BBB:301:TYR:CE2	2.38	0.42
1:AAA:95:GLY:O	1:AAA:110:ALA:HB1	2.20	0.41
2:DDD:312:ARG:HG3	5:DDD:417:HOH:O	2.20	0.41
2:BBB:263:VAL:O	2:BBB:268:LEU:HG	2.20	0.41
2:BBB:183:VAL:HG23	2:BBB:280:ILE:CD1	2.51	0.41
1:AAA:43:LEU:CD2	1:AAA:52:VAL:HG21	2.51	0.41
2:DDD:263:VAL:O	2:DDD:268:LEU:HG	2.21	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	AAA	154/178 (86%)	153 (99%)	1 (1%)	0	100	100
1	CCC	154/178 (86%)	153 (99%)	1 (1%)	0	100	100
2	BBB	134/143 (94%)	131 (98%)	3 (2%)	0	100	100
2	DDD	134/143 (94%)	131 (98%)	3 (2%)	0	100	100
All	All	576/642 (90%)	568 (99%)	8 (1%)	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	AAA	119/136 (88%)	118 (99%)	1 (1%)	81	70
1	CCC	120/136 (88%)	119 (99%)	1 (1%)	81	70
2	BBB	94/99 (95%)	94 (100%)	0	100	100
2	DDD	94/99 (95%)	94 (100%)	0	100	100
All	All	427/470 (91%)	425 (100%)	2 (0%)	88	81

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	AAA	64	PRO
1	CCC	154	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 4 ligands modelled in this entry, 4 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 [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

EDS failed to run properly - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains

EDS failed to run properly - this section is therefore empty.

6.3 Carbohydrates

EDS failed to run properly - this section is therefore empty.

6.4 Ligands

EDS failed to run properly - this section is therefore empty.

6.5 Other polymers

EDS failed to run properly - this section is therefore empty.