



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 01:59 AM UTC

PDB ID : 7QY6 / pdb_00007qy6
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 : 4-5-2 with Phenix2.0
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

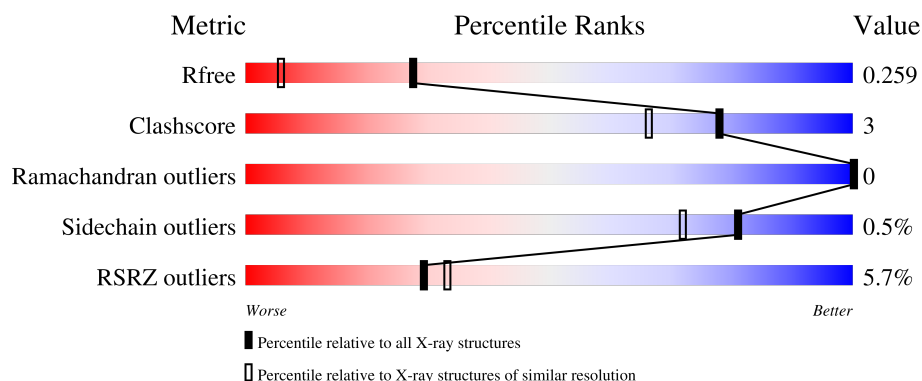
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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))
R_{free}	180053	2563 (1.66-1.66)
Clashscore	190562	2662 (1.66-1.66)
Ramachandran outliers	187476	2621 (1.66-1.66)
Sidechain outliers	187428	2621 (1.66-1.66)
RSRZ outliers	180081	2564 (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 $\leq 5\%$. 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	AAA	178	7% 79% 7% 13%
1	CCC	178	8% 81% 6% 13%
2	BBB	143	2% 86% 8% 6%
2	DDD	143	2% 85% 10% 6%

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
1	AAA	154	Total	C	N	O	S	0	2	0
			1156	722	201	223	10			
1	CCC	155	Total	C	N	O	S	0	1	0
			1165	727	206	222	10			

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

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

- Molecule 3 is SODIUM ION (CCD ID: 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 (CCD ID: 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

4 Data and refinement statistics

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 67.24 – 1.65	Depositor EDS
% Data completeness (in resolution range)	99.6 (67.24-1.65) 99.6 (67.24-1.65)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.95 (at 1.65Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.193 , 0.235 (Not available) , 0.259	Depositor DCC
R_{free} test set	814 reflections (1.18%)	wwPDB-VP
Wilson B-factor (Å ²)	23.4	Xtriage
Anisotropy	0.257	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 32.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	4649	wwPDB-VP
Average B, all atoms (Å ²)	30.0	wwPDB-VP

Xtriage'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	1.18	4/1176 (0.3%)	1.41	3/1588 (0.2%)
1	CCC	1.10	1/1182 (0.1%)	1.37	1/1594 (0.1%)
2	BBB	1.12	1/976 (0.1%)	1.25	0/1328
2	DDD	1.12	2/974 (0.2%)	1.26	3/1326 (0.2%)
All	All	1.13	8/4308 (0.2%)	1.33	7/5836 (0.1%)

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	CCC	9	HIS	CE1-NE2	6.54	1.39	1.32
2	DDD	242	ALA	C-O	5.75	1.30	1.24
1	AAA	9	HIS	CE1-NE2	5.52	1.38	1.32
2	BBB	212	PRO	C-O	-5.40	1.17	1.24
1	AAA	44[A]	GLU	C-O	5.32	1.30	1.24
1	AAA	44[B]	GLU	C-O	5.32	1.30	1.24
1	AAA	57	VAL	N-CA	5.15	1.52	1.46
2	DDD	229	CYS	C-O	5.04	1.30	1.23

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AAA	57	VAL	CA-C-O	-6.78	113.90	120.95
2	DDD	310	ILE	N-CA-C	-5.93	106.94	111.62
1	AAA	57	VAL	N-CA-C	5.88	116.62	110.62
2	DDD	245	ILE	N-CA-C	-5.86	104.62	110.30
1	AAA	53	VAL	CA-C-O	-5.55	114.63	120.57
2	DDD	281	ASP	CA-CB-CG	5.23	117.83	112.60
1	CCC	57	VAL	CA-C-O	-5.04	115.71	120.95

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	AAA	1156	0	1157	5	0
1	CCC	1165	0	1175	9	0
2	BBB	958	0	933	9	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
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	24	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 (24) 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:122[A]:MET:HE3	1:CCC:122[A]:MET:HB3	1.73	0.47
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:DDD:200:MET:SD	2:DDD:207:ARG:NH2	2.89	0.46
2:BBB:204:LEU:CD2	1:CCC:122[B]:MET:HE1	2.47	0.45
2:BBB:204:LEU:HD23	1:CCC:122[B]:MET:HE1	1.99	0.45
2:BBB:183:VAL:HG23	2:BBB:280:ILE:HD12	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AAA:122[A]:MET:HE3	1:AAA:122[A]:MET:HB3	1.81	0.42
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:BBB:239:ALA:O	2:BBB:240:LEU:C	2.64	0.40
2:DDD:263:VAL:O	2:DDD:268:LEU:HG	2.21	0.40

There are no symmetry-related clashes.

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	AAA	124/178 (70%)	123 (99%)	1 (1%)	0	100	100
1	CCC	154/178 (86%)	153 (99%)	1 (1%)	0	100	100
2	BBB	96/143 (67%)	94 (98%)	2 (2%)	0	100	100
2	DDD	134/143 (94%)	131 (98%)	3 (2%)	0	100	100
All	All	508/642 (79%)	501 (99%)	7 (1%)	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	AAA	119/136 (88%)	118 (99%)	1 (1%)	73	60
1	CCC	120/136 (88%)	119 (99%)	1 (1%)	73	60
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%)	81	72

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 ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

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

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	AAA	154/178 (86%)	0.59	13 (8%) 17 19	12, 25, 56, 73	2 (1%)
1	CCC	155/178 (87%)	0.69	14 (9%) 15 16	13, 29, 58, 67	1 (0%)
2	BBB	135/143 (94%)	0.47	3 (2%) 62 68	18, 26, 36, 59	1 (0%)
2	DDD	135/143 (94%)	0.56	3 (2%) 62 68	19, 27, 42, 64	1 (0%)
All	All	579/642 (90%)	0.58	33 (5%) 29 33	12, 27, 52, 73	5 (0%)

All (33) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	AAA	153	LEU	5.8
1	AAA	148	LEU	4.5
1	AAA	155	ALA	4.2
1	AAA	154	LEU	3.9
1	AAA	150	TYR	3.9
1	CCC	154	LEU	3.6
1	CCC	150	TYR	3.6
1	AAA	156	ALA	3.5
2	DDD	200	MET	3.5
1	AAA	18	ALA	3.3
1	CCC	148	LEU	3.3
1	CCC	15	ILE	3.2
1	CCC	14	ALA	2.9
1	CCC	155	ALA	2.9
1	AAA	16	SER	2.8
2	DDD	301	TYR	2.7
1	AAA	143	ILE	2.7
1	CCC	157	ARG	2.7
2	DDD	305	THR	2.5
1	CCC	3	LYS	2.5
1	AAA	14	ALA	2.5

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Mol	Chain	Res	Type	RSRZ
1	CCC	156	ALA	2.5
1	CCC	16	SER	2.4
2	BBB	200	MET	2.4
1	CCC	19	GLN	2.2
1	AAA	15	ILE	2.2
1	CCC	153	LEU	2.2
2	BBB	268	LEU	2.1
1	CCC	74	PHE	2.1
2	BBB	232	THR	2.1
1	AAA	142	GLU	2.1
1	AAA	147	SER	2.1
1	CCC	142	GLU	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 oligosaccharides 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($\text{\AA}^2$)	Q<0.9
3	NA	CCC	201	1/1	0.96	0.05	25,25,25,25	0
3	NA	AAA	201	1/1	0.97	0.05	23,23,23,23	0
4	CL	CCC	202	1/1	0.98	0.06	30,30,30,30	0
4	CL	AAA	202	1/1	0.99	0.04	29,29,29,29	0

6.5 Other polymers [i](#)

There are no such residues in this entry.