



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 07:18 AM UTC

PDB ID : 7QYM / pdb_00007qym
Title : Structure of E.coli Class 2 L-asparaginase EcAIII, mutant RDM1-18 (R207V, D210P, S211W)
Authors : Loch, J.I.; Klonecka, A.; Kadziolka, K.; Bonarek, P.; Barciszewski, J.; Imiolczyk, B.; Brzezinski, K.; Jaskolski, M.
Deposited on : 2022-01-28
Resolution : 1.20 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 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

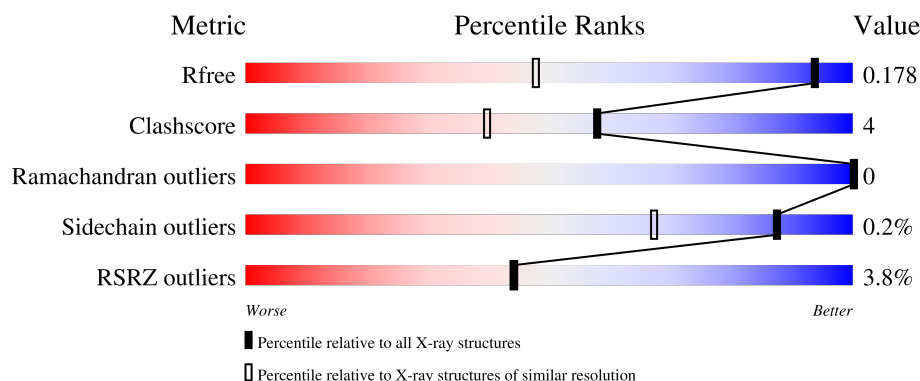
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.20 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}	180053	1216 (1.20-1.20)
Clashscore	190562	1265 (1.20-1.20)
Ramachandran outliers	187476	1226 (1.20-1.20)
Sidechain outliers	187428	1226 (1.20-1.20)
RSRZ outliers	180081	1214 (1.20-1.20)

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	AAA	178	7% 84% 12%
1	CCC	178	3% 87% 11%
2	BBB	143	% 86% 7% • 6%
2	DDD	143	2% 83% 9% • 6%

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 5073 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	156	Total	C	N	O	S	0	8	0
			1224	767	217	231	9			
1	CCC	159	Total	C	N	O	S	0	7	0
			1225	767	216	232	10			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	BBB	134	Total	C	N	O	S	0	4	0
			965	613	159	186	7			
2	DDD	134	Total	C	N	O	S	0	14	0
			1035	662	168	197	8			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
BBB	207	VAL	ARG	engineered mutation	UNP A0A066T6R7
BBB	210	PRO	ASP	engineered mutation	UNP A0A066T6R7
BBB	211	TRP	SER	engineered mutation	UNP A0A066T6R7
DDD	207	VAL	ARG	engineered mutation	UNP A0A066T6R7
DDD	210	PRO	ASP	engineered mutation	UNP A0A066T6R7
DDD	211	TRP	SER	engineered mutation	UNP A0A066T6R7

- 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	BBB	3	Total	Cl	0	0
			3	3		
4	DDD	2	Total	Cl	0	0
			2	2		

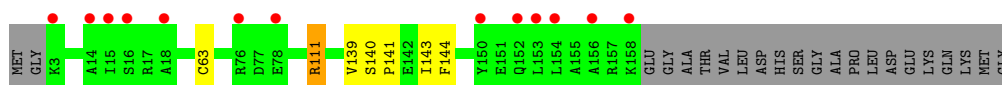
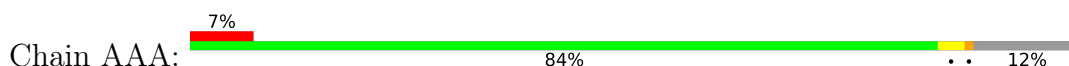
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	AAA	194	Total	O	0	1
			195	195		
5	BBB	107	Total	O	0	0
			107	107		
5	CCC	193	Total	O	0	1
			194	194		
5	DDD	120	Total	O	0	1
			121	121		

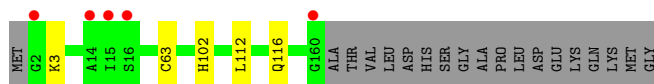
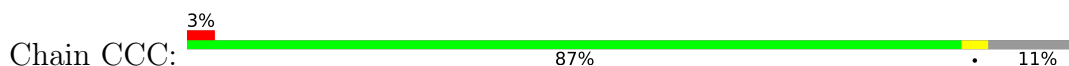
3 Residue-property plots [i](#)

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: Isoaspartyl peptidase



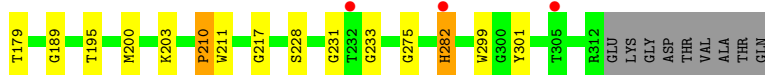
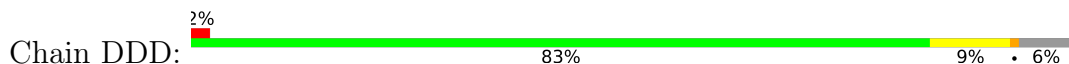
- Molecule 1: Isoaspartyl peptidase



- Molecule 2: Beta-aspartyl-peptidase



- Molecule 2: Beta-aspartyl-peptidase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	49.55Å 75.01Å 146.95Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	66.90 – 1.20 66.90 – 1.20	Depositor EDS
% Data completeness (in resolution range)	97.8 (66.90-1.20) 97.8 (66.90-1.20)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.54 (at 1.20Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.127 , 0.153 (Not available) , 0.178	Depositor DCC
R_{free} test set	1086 reflections (0.63%)	wwPDB-VP
Wilson B-factor (Å ²)	10.1	Xtriage
Anisotropy	1.472	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 49.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.98	EDS
Total number of atoms	5073	wwPDB-VP
Average B, all atoms (Å ²)	21.0	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 27.50 % 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 2.1732e-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	0.97	0/1248	1.09	1/1683 (0.1%)
1	CCC	0.94	0/1254	1.06	0/1689
2	BBB	0.92	0/995	1.06	3/1358 (0.2%)
2	DDD	0.92	2/1074 (0.2%)	0.98	0/1467
All	All	0.94	2/4571 (0.0%)	1.05	4/6197 (0.1%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	DDD	282	HIS	CG-ND1	5.99	1.44	1.38
2	DDD	210	PRO	C-O	-5.10	1.18	1.24

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	BBB	211	TRP	CA-CB-CG	-5.54	103.07	113.60
2	BBB	250	ASP	CA-CB-CG	5.47	118.07	112.60
2	BBB	212	PRO	N-CA-C	-5.11	108.84	114.92
1	AAA	111	ARG	CG-CD-NE	-5.03	100.93	112.00

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	1224	0	1251	5	0
1	CCC	1225	0	1253	7	0
2	BBB	965	0	965	9	0
2	DDD	1035	0	1039	21	0
3	AAA	1	0	0	0	0
3	CCC	1	0	0	0	0
4	BBB	3	0	0	0	0
4	DDD	2	0	0	0	0
5	AAA	195	0	0	1	0
5	BBB	107	0	0	3	0
5	CCC	194	0	0	3	0
5	DDD	121	0	0	1	0
All	All	5073	0	4508	40	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 (40) 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:63:CYS:SG	5:AAA:465:HOH:O	2.19	0.99
2:DDD:195[A]:THR:HG22	2:DDD:228:SER:OG	1.82	0.80
1:CCC:63:CYS:SG	5:CCC:462[A]:HOH:O	2.42	0.76
2:DDD:210:PRO:HG2	2:DDD:211[B]:TRP:CD2	2.23	0.73
1:AAA:139[B]:VAL:HG11	1:AAA:143[B]:ILE:HG21	1.72	0.72
1:CCC:63:CYS:SG	5:CCC:462[B]:HOH:O	2.49	0.70
2:DDD:195[A]:THR:HG22	2:DDD:228:SER:HG	1.59	0.65
2:DDD:189:GLY:O	2:DDD:282:HIS:HE1	1.82	0.63
2:DDD:203[A]:LYS:NZ	5:DDD:501:HOH:O	2.26	0.62
2:DDD:210:PRO:CD	2:DDD:233[A]:GLY:HA2	2.30	0.62
2:DDD:299:TRP:HZ3	2:DDD:301:TYR:CE2	2.19	0.61
2:DDD:210:PRO:HG2	2:DDD:211[B]:TRP:CE3	2.35	0.60
2:DDD:189:GLY:O	2:DDD:282:HIS:CE1	2.54	0.60
2:BBB:203[B]:LYS:CD	5:BBB:586:HOH:O	2.49	0.59
2:DDD:195[A]:THR:HG21	2:DDD:217:GLY:O	2.03	0.58
2:DDD:210:PRO:HG2	2:DDD:211[B]:TRP:CE2	2.39	0.58
2:DDD:210:PRO:CD	2:DDD:233[A]:GLY:CA	2.83	0.56
2:DDD:210:PRO:HD3	2:DDD:233[A]:GLY:CA	2.35	0.56
2:BBB:203[B]:LYS:HD3	5:BBB:586:HOH:O	2.06	0.54
1:AAA:139[B]:VAL:HG12	1:AAA:140[B]:SER:N	2.23	0.53
2:BBB:200:MET:HE2	2:BBB:211:TRP:CH2	2.43	0.53
1:CCC:102:HIS:HE1	5:CCC:441:HOH:O	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:DDD:200[B]:MET:HA	2:DDD:200[B]:MET:HE2	1.93	0.49
2:DDD:210:PRO:HD3	2:DDD:233[A]:GLY:C	2.39	0.48
1:CCC:112:LEU:HD12	1:CCC:116:GLN:NE2	2.29	0.47
2:BBB:268:LEU:HB2	2:BBB:269:PRO:HD3	1.97	0.47
1:AAA:139[B]:VAL:CG1	1:AAA:140[B]:SER:N	2.78	0.47
1:CCC:3:LYS:HG3	2:DDD:301:TYR:HD1	1.79	0.46
1:CCC:3:LYS:HG3	2:DDD:301:TYR:CD1	2.52	0.45
2:BBB:200:MET:HE3	5:BBB:578:HOH:O	2.18	0.44
1:CCC:112:LEU:CD1	1:CCC:116:GLN:NE2	2.81	0.44
2:BBB:299:TRP:HZ3	2:BBB:301:TYR:CE2	2.36	0.43
2:DDD:210:PRO:CG	2:DDD:233[A]:GLY:HA2	2.49	0.43
2:DDD:231[A]:GLY:HA3	2:DDD:275:GLY:HA3	2.02	0.42
2:DDD:179:THR:HG21	2:DDD:211[A]:TRP:CD1	2.55	0.42
1:AAA:141[B]:PRO:HA	1:AAA:144:PHE:CD2	2.55	0.41
2:BBB:195[A]:THR:HG21	2:BBB:211:TRP:O	2.20	0.41
2:BBB:200:MET:HE2	2:BBB:211:TRP:HH2	1.86	0.41
2:DDD:210:PRO:HD3	2:DDD:233[A]:GLY:O	2.21	0.40
2:BBB:235:VAL:HG12	2:BBB:268:LEU:HD22	2.04	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	162/178 (91%)	161 (99%)	1 (1%)	0	100	100
1	CCC	164/178 (92%)	163 (99%)	1 (1%)	0	100	100
2	BBB	136/143 (95%)	129 (95%)	7 (5%)	0	100	100
2	DDD	146/143 (102%)	140 (96%)	6 (4%)	0	100	100
All	All	608/642 (95%)	593 (98%)	15 (2%)	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	128/136 (94%)	127 (99%)	1 (1%)	73	44
1	CCC	128/136 (94%)	128 (100%)	0	100	100
2	BBB	96/99 (97%)	96 (100%)	0	100	100
2	DDD	104/99 (105%)	104 (100%)	0	100	100
All	All	456/470 (97%)	455 (100%)	1 (0%)	87	67

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	AAA	111	ARG

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 7 ligands modelled in this entry, 7 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 ⓘ

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	156/178 (87%)	0.17	13 (8%)	17 18	6, 17, 46, 63	8 (5%)
1	CCC	159/178 (89%)	-0.07	5 (3%)	51 51	7, 15, 30, 49	7 (4%)
2	BBB	134/143 (93%)	-0.12	1 (0%)	84 87	8, 16, 28, 47	4 (2%)
2	DDD	134/143 (93%)	-0.08	3 (2%)	62 63	7, 15, 27, 39	14 (10%)
All	All	583/642 (90%)	-0.02	22 (3%)	44 44	6, 16, 35, 63	33 (5%)

All (22) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	AAA	154	LEU	6.1
1	CCC	15[A]	ILE	5.5
1	AAA	153	LEU	5.0
1	AAA	15	ILE	4.0
1	CCC	2	GLY	3.5
1	CCC	160	GLY	3.3
2	DDD	305	THR	3.3
1	AAA	158	LYS	3.3
1	AAA	18	ALA	2.8
1	AAA	14	ALA	2.7
1	AAA	78	GLU	2.7
2	DDD	232[A]	THR	2.5
1	AAA	152	GLN	2.4
1	AAA	16	SER	2.4
1	AAA	3	LYS	2.4
1	AAA	76[A]	ARG	2.4
1	AAA	150	TYR	2.3
1	AAA	156	ALA	2.3
1	CCC	14	ALA	2.1
2	DDD	282	HIS	2.1
1	CCC	16[A]	SER	2.1
2	BBB	305	THR	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
4	CL	BBB	402	1/1	0.97	0.13	45,45,45,45	0
4	CL	DDD	402	1/1	0.98	0.11	32,32,32,32	0
4	CL	BBB	403	1/1	0.99	0.12	33,33,33,33	0
3	NA	AAA	201	1/1	0.99	0.05	14,14,14,14	0
4	CL	BBB	401	1/1	1.00	0.03	20,20,20,20	0
4	CL	DDD	401	1/1	1.00	0.03	20,20,20,20	0
3	NA	CCC	201	1/1	1.00	0.04	12,12,12,12	0

6.5 Other polymers [i](#)

There are no such residues in this entry.