



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 27, 2023 – 07:32 pm BST

PDB ID : 8BQO
Title : Structure of E.coli Class 2 L-asparaginase EcAIII, mutant M200I
Authors : Sciuk, A.; Ruszkowski, M.; Jaskolski, M.; Loch, J.I.
Deposited on : 2022-11-21
Resolution : 2.10 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
Mogul : 1.8.4, CSD as541be (2020)
Xtrriage (Phenix) : 1.13
EDS : 2.32.2
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) : 2.32.2

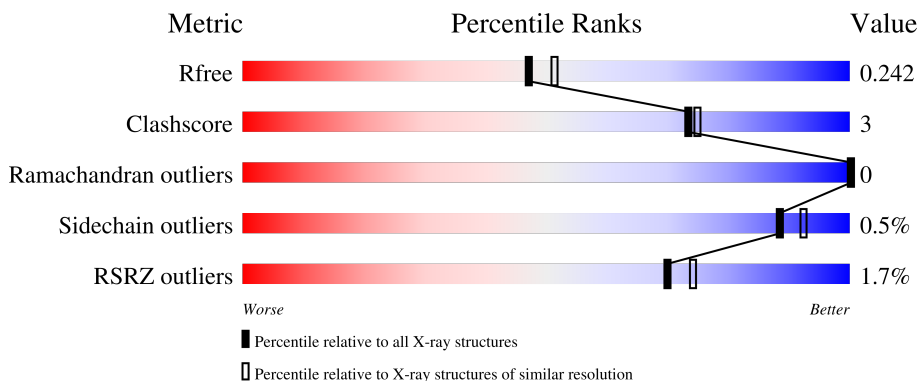
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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 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	 2% 85% 5% 10%
1	CCC	178	 3% 79% 8% 13%
2	BBB	143	 89% 5% 6%
2	DDD	143	 84% 9% 6%

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 4517 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 subunit alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	AAA	161	1203	749	213	231	10	0	1	0
1	CCC	155	1171	730	207	224	10	0	2	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AAA	1	MET	-	initiating methionine	UNP P37595
CCC	1	MET	-	initiating methionine	UNP P37595

- Molecule 2 is a protein called Isoaspartyl peptidase subunit beta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	BBB	134	947	593	160	188	6	0	1	0
2	DDD	134	947	593	160	188	6	0	1	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
BBB	200	ILE	MET	engineered mutation	UNP P37595
DDD	200	ILE	MET	engineered mutation	UNP P37595

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	AAA	1	Total C O 6 3 3	0	0
3	BBB	1	Total C O 6 3 3	0	0

- Molecule 4 is SODIUM ION (three-letter code: NA) (formula: Na).

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

- Molecule 5 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	BBB	1	Total Cl 1 1	0	0

- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	AAA	82	Total O 82 82	0	0
6	BBB	56	Total O 56 56	0	0

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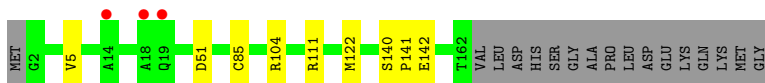
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	CCC	63	Total 63	O 63	0	0
6	DDD	33	Total 33	O 33	0	0

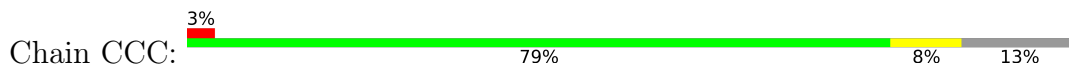
3 Residue-property plots [i](#)

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 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.

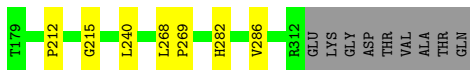
- Molecule 1: Isoaspartyl peptidase subunit alpha



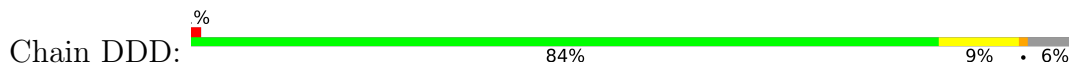
- Molecule 1: Isoaspartyl peptidase subunit alpha



- Molecule 2: Isoaspartyl peptidase subunit beta



- Molecule 2: Isoaspartyl peptidase subunit beta



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	52.92Å 77.67Å 148.28Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	17.21 – 2.10 17.20 – 2.10	Depositor EDS
% Data completeness (in resolution range)	97.5 (17.21-2.10) 97.7 (17.20-2.10)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.51 (at 2.11Å)	Xtrriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.182 , 0.232 0.192 , 0.242	Depositor DCC
R_{free} test set	1064 reflections (2.99%)	wwPDB-VP
Wilson B-factor (Å ²)	16.3	Xtrriage
Anisotropy	0.096	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.42 , 57.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	4517	wwPDB-VP
Average B, all atoms (Å ²)	19.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.35% 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 [i](#)

5.1 Standard geometry [i](#)

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

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	0.73	0/1220	0.86	0/1644
1	CCC	0.73	0/1188	0.82	0/1602
2	BBB	0.74	0/965	0.87	0/1315
2	DDD	0.72	0/965	0.85	0/1315
All	All	0.73	0/4338	0.85	0/5876

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	1203	0	1212	7	0
1	CCC	1171	0	1179	9	0
2	BBB	947	0	932	10	0
2	DDD	947	0	932	13	0
3	AAA	6	0	8	0	0
3	BBB	6	0	8	0	0
4	AAA	1	0	0	0	0
4	CCC	1	0	0	0	0
5	BBB	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	AAA	82	0	0	2	0
6	BBB	56	0	0	1	0
6	CCC	63	0	0	0	0
6	DDD	33	0	0	1	0
All	All	4517	0	4271	28	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 (28) 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:140:SER:HB3	1:AAA:142:GLU:OE1	1.76	0.85
2:BBB:240:LEU:HD11	2:DDD:215:GLY:HA3	1.67	0.75
2:BBB:240:LEU:HD12	2:DDD:243:TYR:CG	2.23	0.74
2:BBB:240:LEU:HD13	2:DDD:240:LEU:HD23	1.83	0.59
1:AAA:5:VAL:HG21	2:BBB:286[B]:VAL:HG21	1.85	0.58
2:DDD:304:ASP:OD1	2:DDD:305:THR:N	2.37	0.50
1:CCC:25:GLU:O	1:CCC:29:ILE:HG12	2.13	0.49
2:BBB:240:LEU:HD13	2:DDD:240:LEU:CD2	2.43	0.49
1:CCC:3:LYS:HE2	6:DDD:401:HOH:O	2.11	0.49
1:CCC:23:GLN:O	1:CCC:27:ARG:HG2	2.13	0.48
1:AAA:85:CYS:HB2	2:BBB:212:PRO:HA	1.97	0.46
1:AAA:51:ASP:OD1	1:AAA:111:ARG:NH2	2.41	0.45
2:BBB:215:GLY:HA3	2:DDD:240:LEU:HD21	1.99	0.45
1:AAA:141:PRO:CB	6:AAA:349:HOH:O	2.64	0.45
1:CCC:112:LEU:HD21	1:CCC:134:ARG:HB2	1.99	0.45
1:AAA:104:ARG:HD2	6:AAA:358:HOH:O	2.17	0.44
2:BBB:240:LEU:HD12	2:DDD:243:TYR:CB	2.47	0.44
1:AAA:122[B]:MET:HA	2:DDD:206:GLY:O	2.18	0.44
2:BBB:268:LEU:HB2	2:BBB:269:PRO:HD3	2.00	0.44
1:CCC:5:VAL:HG21	2:DDD:286[B]:VAL:HG21	2.01	0.43
2:DDD:226:ALA:O	2:DDD:279:ALA:HA	2.19	0.42
1:CCC:22:LEU:O	1:CCC:26:LEU:HG	2.19	0.42
2:DDD:260:CYS:HB3	2:DDD:289:PRO:HG3	2.01	0.42
2:BBB:282:HIS:HE1	6:BBB:553:HOH:O	2.01	0.42
1:CCC:98:ALA:HB3	1:CCC:123:ILE:HG22	2.03	0.41
2:DDD:268:LEU:HB2	2:DDD:269:PRO:HD3	2.02	0.40
1:CCC:85:CYS:HB2	2:DDD:212:PRO:HA	2.04	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	160/178 (90%)	157 (98%)	3 (2%)	0	100	100
1	CCC	155/178 (87%)	151 (97%)	4 (3%)	0	100	100
2	BBB	133/143 (93%)	128 (96%)	5 (4%)	0	100	100
2	DDD	133/143 (93%)	128 (96%)	5 (4%)	0	100	100
All	All	581/642 (90%)	564 (97%)	17 (3%)	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	123/136 (90%)	123 (100%)	0	100	100
1	CCC	121/136 (89%)	120 (99%)	1 (1%)	81	86
2	BBB	93/99 (94%)	93 (100%)	0	100	100
2	DDD	93/99 (94%)	92 (99%)	1 (1%)	73	79
All	All	430/470 (92%)	428 (100%)	2 (0%)	88	92

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

Mol	Chain	Res	Type
1	CCC	106	PRO
2	DDD	240	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 5 ligands modelled in this entry, 3 are monoatomic - leaving 2 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	GOL	AAA	201	-	5,5,5	0.10	0	5,5,5	0.28	0
3	GOL	BBB	401	-	5,5,5	0.10	0	5,5,5	0.33	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '2' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GOL	AAA	201	-	-	2/4/4/4	-
3	GOL	BBB	401	-	-	2/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	AAA	201	GOL	C1-C2-C3-O3
3	BBB	401	GOL	O1-C1-C2-O2
3	BBB	401	GOL	O1-C1-C2-C3
3	AAA	201	GOL	O2-C2-C3-O3

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	161/178 (90%)	-0.07	3 (1%) 66 71	9, 15, 35, 54	0
1	CCC	155/178 (87%)	0.16	5 (3%) 47 54	10, 20, 40, 50	0
2	BBB	134/143 (93%)	-0.24	0 100 100	8, 15, 26, 32	0
2	DDD	134/143 (93%)	-0.06	2 (1%) 73 77	11, 19, 33, 45	0
All	All	584/642 (90%)	-0.05	10 (1%) 70 74	8, 17, 35, 54	0

All (10) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	AAA	18	ALA	4.6
1	CCC	18	ALA	3.3
1	AAA	19	GLN	3.3
1	CCC	14	ALA	3.2
1	CCC	156	ALA	3.1
1	CCC	148	LEU	3.1
2	DDD	305	THR	2.7
1	CCC	6	ILE	2.5
1	AAA	14	ALA	2.3
2	DDD	303	GLY	2.1

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
3	GOL	AAA	201	6/6	0.86	0.22	29,39,43,46	0
3	GOL	BBB	401	6/6	0.88	0.20	49,50,51,53	0
4	NA	AAA	202	1/1	0.98	0.06	15,15,15,15	0
4	NA	CCC	201	1/1	0.98	0.07	13,13,13,13	0
5	CL	BBB	402	1/1	0.99	0.03	19,19,19,19	0

6.5 Other polymers [i](#)

There are no such residues in this entry.