

# wwPDB X-ray Structure Validation Summary Report (i)

Jul 5, 2022 – 01:08 pm BST

PDB ID : 7QQ8

Title: Structure of E.coli Class 2 L-asparaginase EcAIII, mutant RDM1-8 (G206Y,

R207Q, D210P, S211T)

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Deposited on : 2022-01-06

Resolution : 1.80 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 (i) 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 (1)) were used in the production of this report:

MolProbity : 4.02b-467 Xtriage (Phenix) : 1.13

EDS: 2.29

Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)

Refmac: 5.8.0267

CCP4 : 7.1.010 (Gargrove)

Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)

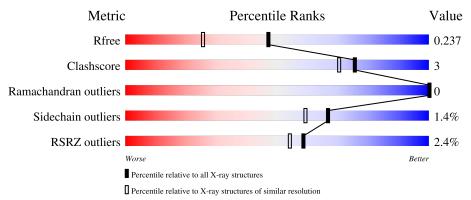
Validation Pipeline (wwPDB-VP) : 2.29

# 1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: X- $RAY\ DIFFRACTION$ 

The reported resolution of this entry is 1.80 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 $(\# \mathrm{Entries})$	$\begin{array}{c} {\rm Similar\ resolution} \\ (\#{\rm Entries},{\rm resolution\ range}({\rm \AA})) \end{array}$
$R_{free}$	130704	5950 (1.80-1.80)
Clashscore	141614	6793 (1.80-1.80)
Ramachandran outliers	138981	6697 (1.80-1.80)
Sidechain outliers	138945	6696 (1.80-1.80)
RSRZ outliers	127900	5850 (1.80-1.80)

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 <=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	83%	•• 13%
1	CCC	178	82%	5% 13%
2	BBB	143	84%	10% 6%
2	DDD	143	84%	10% • 6%



# 2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 4672 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 Beta-aspartyl-peptidase.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace		
1	AAA	154	Total	С	N	О	S	0	1	0
1	11111	104	1168	729	205	224	10		4	0
1	CCC	155	Total	С	N	О	S	0	1	0
1		199	1163	725	206	223	9	U	1	U

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

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace		
2	BBB	134	Total 953	C 600	N 158	O 188	S 7	0	1	0
2	DDD	135	Total 970	C 610	N 162	O 191	S 7	0	2	0

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
BBB	206	TYR	GLY	engineered mutation	UNP J7QNS8
BBB	207	GLN	ARG	engineered mutation	UNP J7QNS8
BBB	210	PRO	ASP	engineered mutation	UNP J7QNS8
BBB	211	THR	SER	engineered mutation	UNP J7QNS8
DDD	206	TYR	GLY	engineered mutation	UNP J7QNS8
DDD	207	GLN	ARG	engineered mutation	UNP J7QNS8
DDD	210	PRO	ASP	engineered mutation	UNP J7QNS8
DDD	211	THR	SER	engineered mutation	UNP J7QNS8

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

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



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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	BBB	1	Total Cl 1 1	0	0
4	DDD	1	Total Cl 1 1	0	0

• Molecule 5 is water.

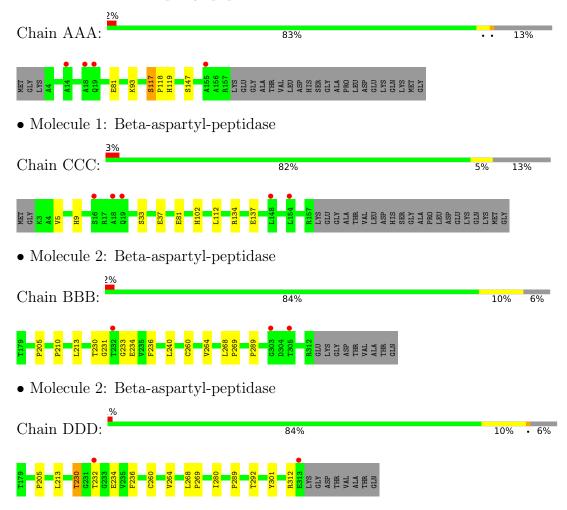
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	AAA	121	Total O 122 122	0	1
5	BBB	84	Total O 85 85	0	1
5	CCC	119	Total O 119 119	0	0
5	DDD	88	Total O 88 88	0	0



# 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: Beta-aspartyl-peptidase





# 4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants	50.01Å 74.89Å 147.84Å	Depositor
a, b, c, $\alpha$ , $\beta$ , $\gamma$	90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.16 - 1.80	Depositor
resolution (A)	19.16 - 1.80	EDS
% Data completeness	93.4 (19.16-1.80)	Depositor
(in resolution range)	93.5 (19.16-1.80)	EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$< I/\sigma(I) > 1$	1.62 (at 1.80Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
P.P.	0.196 , 0.236	Depositor
$R, R_{free}$	0.203 , $0.237$	DCC
$R_{free}$ test set	1001 reflections $(2.05\%)$	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	14.6	Xtriage
Anisotropy	0.336	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$ , $B_{sol}(Å^2)$	(Not available), (Not available)	EDS
L-test for twinning <sup>2</sup>	$  <  L  > = 0.46, < L^2 > = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	4672	wwPDB-VP
Average B, all atoms $(Å^2)$	19.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 17.33% of the height of the origin peak. No significant pseudotranslation is detected.

<sup>&</sup>lt;sup>2</sup>Theoretical values of <|L|>,  $<L^2>$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.



 $<sup>^1 {\</sup>rm Intensities}$  estimated from amplitudes.

# 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		
IVIOI	Chain	RMSZ	# Z  > 5	RMSZ	# Z  > 5	
1	AAA	0.74	0/1194	0.83	0/1611	
1	CCC	0.82	0/1180	0.89	0/1592	
2	BBB	0.74	0/973	0.91	0/1328	
2	DDD	0.72	0/993	0.92	0/1354	
All	All	0.76	0/4340	0.88	0/5885	

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)	$\mathbf{H}(\mathbf{added})$	Clashes	Symm-Clashes
1	AAA	1168	0	1180	5	0
1	CCC	1163	0	1171	7	0
2	BBB	953	0	936	7	0
2	DDD	970	0	955	13	0
3	AAA	1	0	0	0	0
3	CCC	1	0	0	0	0
4	BBB	1	0	0	0	0
4	DDD	1	0	0	0	0
5	AAA	122	0	0	2	0

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	Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
	5	BBB	85	0	0	0	0
ſ	5	CCC	119	0	0	3	0
	5	DDD	88	0	0	1	0
	All	All	4672	0	4242	26	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.

The worst 5 of 26 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	$\begin{array}{c} {\rm Interatomic} \\ {\rm distance} \ ({\rm \AA}) \end{array}$	Clash overlap (Å)	
1:AAA:118:PRO:O	2:DDD:234:GLU:HG2	1.60	1.00	
2:DDD:232:THR:O	2:DDD:236:PHE:HD1	1.88	0.56	
2:DDD:264:VAL:HA	2:DDD:268:LEU:HD12	1.89	0.55	
1:AAA:93:LYS:CE	5:AAA:407:HOH:O	2.54	0.55	
1:AAA:93:LYS:HE2	5:AAA:407:HOH:O	2.07	0.54	

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	Perce	ntiles
1	AAA	156/178 (88%)	151 (97%)	5 (3%)	0	100	100
1	CCC	154/178 (86%)	151 (98%)	3 (2%)	0	100	100
2	BBB	133/143 (93%)	128 (96%)	5 (4%)	0	100	100
2	DDD	135/143 (94%)	129 (96%)	6 (4%)	0	100	100
All	All	578/642 (90%)	559 (97%)	19 (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	Perce	ntiles
1	AAA	122/136~(90%)	120 (98%)	2 (2%)	62	54
1	CCC	120/136 (88%)	120 (100%)	0	100	100
2	BBB	94/100 (94%)	91 (97%)	3 (3%)	39	25
2	DDD	96/100 (96%)	95 (99%)	1 (1%)	76	71
All	All	432/472 (92%)	426 (99%)	6 (1%)	67	59

5 of 6 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	BBB	234	GLU
2	BBB	240	LEU
2	DDD	230	THR
1	AAA	147	SER
1	AAA	117	SER

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 (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,  $95^{th}$  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 $>$	$\# \mathrm{RSRZ}{>}2$	$OWAB(Å^2)$	Q < 0.9
1	AAA	154/178~(86%)	-0.07	4 (2%) 56 51	10, 17, 43, 59	0
1	CCC	155/178 (87%)	-0.12	5 (3%) 47 41	6, 14, 39, 50	0
2	BBB	134/143 (93%)	-0.17	3 (2%) 62 57	9, 17, 32, 41	0
2	DDD	135/143 (94%)	-0.21	2 (1%) 73 70	5, 15, 32, 48	0
All	All	578/642 (90%)	-0.14	14 (2%) 59 54	5, 16, 37, 59	0

The worst 5 of 14 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	CCC	16	SER	3.7
2	DDD	232	THR	3.7
1	AAA	19	GLN	3.4
1	AAA	18	ALA	3.3
2	BBB	232	THR	3.0

#### 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,  $95^{th}$  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	$\mathbf{B} ext{-}\mathbf{factors}(\mathbf{\mathring{A}}^2)$	Q<0.9
3	NA	AAA	201	1/1	0.99	0.04	11,11,11,11	0
3	NA	CCC	201	1/1	0.99	0.05	12,12,12,12	0
4	CL	BBB	401	1/1	0.99	0.03	19,19,19,19	0
4	CL	DDD	401	1/1	0.99	0.03	18,18,18,18	0

# 6.5 Other polymers (i)

There are no such residues in this entry.

