

wwPDB X-ray Structure Validation Summary Report (i)

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PDB ID	:	7QYM
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.; Imiol-
		czyk, B.; Brzezinski, K.; Jaskolski, M.
Deposited on		
Resolution	:	1.20 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:

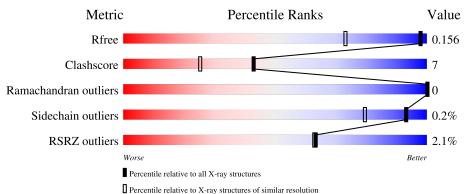
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.29
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0267
CCP4	:	7.1.010 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)		
Validation Pipeline (wwPDB-VP)	:	2.29

1 Overall quality at a glance (i)

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

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	$\begin{array}{c} \textbf{Whole archive} \\ \textbf{(\#Entries)} \end{array}$	${f Similar\ resolution}\ (\#{ m Entries,\ resolution\ range}({ m \AA}))$
R_{free}	130704	1223 (1.22-1.18)
Clashscore	141614	1286 (1.22-1.18)
Ramachandran outliers	138981	1240 (1.22-1.18)
Sidechain outliers	138945	1239 (1.22-1.18)
RSRZ outliers	127900	1200 (1.22-1.18)

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	3% 84%	•• 12%
1	CCC	178	2% 85%	• 11%
2	BBB	143	.% 8 7%	6% • 6%
2	DDD	143	% 83 %	11% 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	ААА	156	Total	С	Ν	0	\mathbf{S}	0	8	0
L		100	1224	767	217	231	9	0		
1	CCC	159	Total	С	Ν	0	\mathbf{S}	0	7	0
1		159	1225	767	216	232	10	0		

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

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace		
9	BBB	134	Total	С	Ν	0	S	0	4	0
	DDD	104	965	613	159	186	7	0		
0	DDD	134	Total	С	Ν	0	S	0	14	0
	עעע	104	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 (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	3	Total Cl 3 3	0	0
4	DDD	2	Total Cl 2 2	0	0

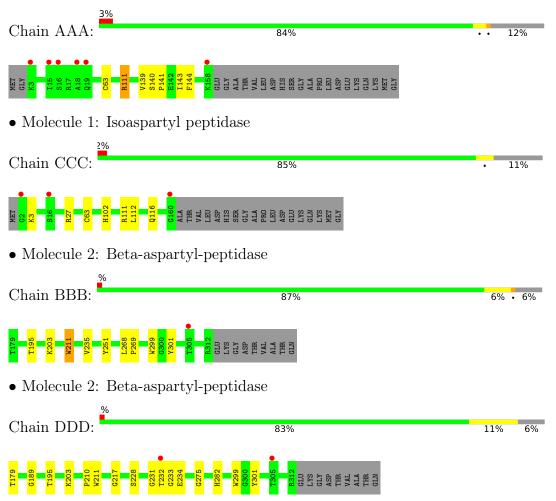
• Molecule 5 is water.

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



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



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants	49.55Å 75.01Å 146.95Å	Depositor
a, b, c, α , β , γ	90.00° 90.00° 90.00°	Depositor
Resolution (Å)	66.90 - 1.20	Depositor
Resolution (A)	66.81 - 1.20	EDS
% Data completeness	97.8 (66.90-1.20)	Depositor
(in resolution range)	97.8(66.81-1.20)	EDS
R _{merge}	0.09	Depositor
R _{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	$1.54 (at 1.20 \text{\AA})$	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
D D.	0.127 , 0.153	Depositor
R, R_{free}	0.127 , 0.156	DCC
R_{free} test set	1086 reflections (0.65%)	wwPDB-VP
Wilson B-factor $(Å^2)$	10.1	Xtriage
Anisotropy	1.472	Xtriage
Bulk solvent $k_{sol}(e/Å^3), B_{sol}(Å^2)$	(Not available), (Not available)	EDS
L-test for twinning ²	$ L > = 0.48, < L^2 > = 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.

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.



¹Intensities 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: NA, CL

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		
	Unam	RMSZ	# Z > 5	RMSZ	# Z > 5	
1	AAA	0.69	0/1248	0.82	1/1683~(0.1%)	
1	CCC	0.69	0/1254	0.85	1/1689~(0.1%)	
2	BBB	0.65	0/995	0.87	2/1358~(0.1%)	
2	DDD	0.67	0/1074	0.87	0/1467	
All	All	0.68	0/4571	0.85	4/6197~(0.1%)	

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Ζ	$\mathbf{Observed}(^{o})$	$\operatorname{Ideal}(^{o})$
2	BBB	251	TYR	CB-CG-CD1	6.30	124.78	121.00
1	CCC	111	ARG	NE-CZ-NH1	-5.81	117.39	120.30
2	BBB	211	TRP	CA-CB-CG	-5.60	103.07	113.70
1	AAA	111	ARG	CG-CD-NE	-5.18	100.93	111.80

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	9	0
1	CCC	1225	0	1253	8	0
2	BBB	965	0	965	11	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	DDD	1035	0	1039	35	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	5	0
5	BBB	107	0	0	7	0
5	CCC	194	0	0	6	0
5	DDD	121	0	0	14	0
All	All	5073	0	4508	61	0

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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 7.

The worst 5 of 61 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:141[A]:PRO:HD3	5:AAA:324:HOH:O	1.20	1.27
5:CCC:430:HOH:O	2:DDD:232[B]:THR:HG23	1.33	1.23
2:DDD:203[A]:LYS:CD	5:DDD:557:HOH:O	2.00	1.09
2:BBB:203[A]:LYS:CD	5:BBB:553:HOH:O	2.03	1.04
2:DDD:203[A]:LYS:HD3	5:DDD:557:HOH:O	1.54	1.00

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	entiles
1	AAA	162/178~(91%)	161 (99%)	1 (1%)	0	100	100
1	CCC	164/178~(92%)	163 (99%)	1 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
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

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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%)	81 55
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%)	93 79

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 monosaccharides 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 (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	$\langle RSRZ \rangle$	#RSRZ>2	$OWAB(Å^2)$	Q < 0.9
1	AAA	156/178~(87%)	-0.27	6 (3%) 40 40	11, 18, 46, 63	0
1	CCC	159/178~(89%)	-0.39	3 (1%) 66 67	10, 15, 31, 49	0
2	BBB	134/143~(93%)	-0.48	1 (0%) 87 87	11, 16, 28, 47	0
2	DDD	134/143~(93%)	-0.38	2 (1%) 73 74	10, 16, 27, 39	0
All	All	583/642~(90%)	-0.38	12 (2%) 63 63	10, 16, 37, 63	0

The worst 5 of 12 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	AAA	15	ILE	3.7
1	CCC	2	GLY	3.7
1	AAA	16	SER	3.4
1	AAA	18	ALA	3.4
1	AAA	19	GLN	3.1

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, 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	$\mathbf{B} ext{-factors}(\mathbf{A}^2)$	Q < 0.9
4	CL	BBB	402	1/1	0.95	0.15	$45,\!45,\!45,\!45$	0
4	CL	BBB	403	1/1	0.99	0.10	33,33,33,33	0
4	CL	DDD	402	1/1	0.99	0.06	32,32,32,32	0
3	NA	AAA	201	1/1	1.00	0.05	14,14,14,14	0
3	NA	CCC	201	1/1	1.00	0.03	12,12,12,12	0
4	CL	DDD	401	1/1	1.00	0.03	20,20,20,20	0
4	CL	BBB	401	1/1	1.00	0.02	20,20,20,20	0

6.5 Other polymers (i)

There are no such residues in this entry.

