Full wwPDB X-ray Structure Validation Report (i)

Jul 5, 2022 – 01:06 pm BST

PDB ID	:	7QTC
Title	:	Structure of E.coli Class 2 L-asparaginase EcAIII, mutant RDM1-3 (G206H, R207T, D210P, S211Q)
Authors	:	Loch, J.I.; Kadziolka, K.; Jaskolski, M.
Deposited on	:	2022-01-14
Resolution	:	2.55 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 (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 (i)) were used in the production of this report:

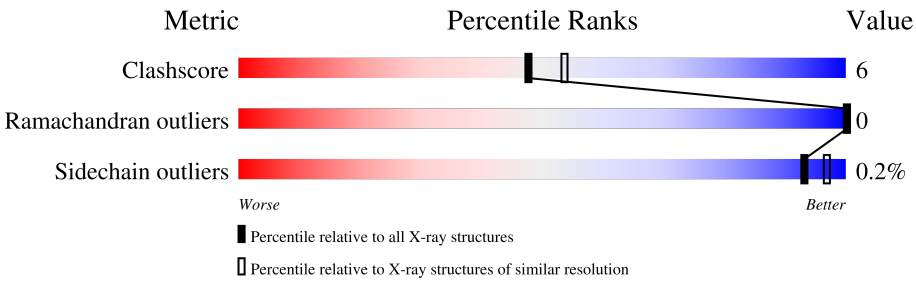
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	FAILED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.29

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 2.55 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))
Clashscore	141614	1332 (2.56-2.52)
Ramachandran outliers	138981	1315 (2.56-2.52)
Sidechain outliers	138945	1315 (2.56-2.52)

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%

Note EDS failed to run properly.

Mol	Chain	Length	Quality of chain
1	AAA	178	71% 10% • 19%
1	CCC	178	69% 11% 20%
2	BBB	143	77% 17% 6%
2	DDD	143	80% 13% 6%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 4174 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
			Total	C	N	O	S			
1	AAA	144	1065	663	188	205	9	0	0	0
1	CCC	142	1052	655	185	203	9	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	BBB	135	960	602	161	190	7	0	1	0
2	DDD	134	953	598	160	188	7	0	1	0

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
BBB	206	HIS	GLY	engineered mutation	UNP P37595
BBB	207	THR	ARG	engineered mutation	UNP P37595
BBB	210	PRO	ASP	engineered mutation	UNP P37595
BBB	211	GLN	SER	engineered mutation	UNP P37595
DDD	206	HIS	GLY	engineered mutation	UNP P37595
DDD	207	THR	ARG	engineered mutation	UNP P37595
DDD	210	PRO	ASP	engineered mutation	UNP P37595
DDD	211	GLN	SER	engineered mutation	UNP P37595

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

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

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	AAA	46	46	46	0	0
			Total	O		
4	BBB	25	25	25	0	0
			Total	O		
4	CCC	50	50	50	0	0
			Total	O		
4	DDD	21	21	21	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. 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. 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.

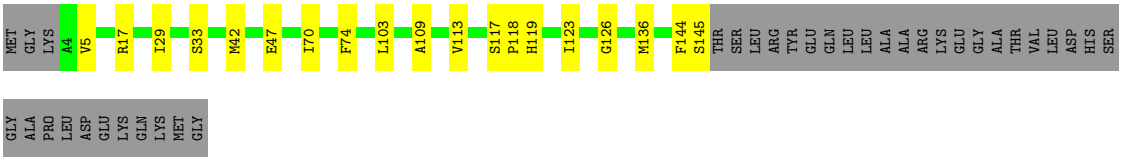
Note EDS failed to run properly.

• Molecule 1: Isoaspartyl peptidase

Chain AAA:

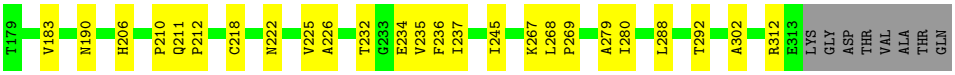
• Molecule 1: Isoaspartyl peptidase

Chain CCC:



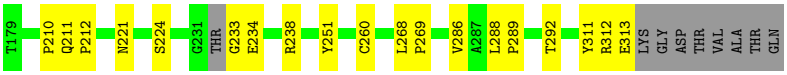
• Molecule 2: Isoaspartyl peptidase subunit beta

Chain BBB:



• Molecule 2: Isoaspartyl peptidase subunit beta

Chain DDD:



4 Data and refinement statistics (i)

EDS failed to run properly - this section is therefore incomplete.

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	51.35Å 75.04Å 149.03Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.36 – 2.55	Depositor
% Data completeness (in resolution range)	92.0 (20.36-2.55)	Depositor
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.29 (at 2.56Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.202 , 0.248	Depositor
Wilson B-factor (Å^2)	30.5	Xtriage
Anisotropy	0.219	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	4174	wwPDB-VP
Average B, all atoms (Å^2)	35.0	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 20.39 % 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 8.7878e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[1]Intensities estimated from amplitudes.

[2]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.

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

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	0.77	0/1078	0.88	0/1454
1	CCC	0.75	0/1065	0.89	0/1438
2	BBB	0.80	0/980	0.92	0/1337
2	DDD	0.74	0/972	0.90	0/1324
All	All	0.77	0/4095	0.90	0/5553

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	1065	0	1065	15	0
1	CCC	1052	0	1049	14	0
2	BBB	960	0	940	16	0
2	DDD	953	0	932	12	0
3	AAA	1	0	0	0	0
3	CCC	1	0	0	0	0
4	AAA	46	0	0	1	0
4	BBB	25	0	0	1	0
4	CCC	50	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	DDD	21	0	0	0	0
All	All	4174	0	3986	49	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 6.

All (49) 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:23:GLN:HE21	1:AAA:27:ARG:HH22	1.35	0.72
2:BBB:267:LYS:NZ	2:DDD:251:TYR:OH	2.28	0.66
2:DDD:234:GLU:HG2	2:DDD:238:ARG:HH11	1.61	0.65
1:AAA:123:ILE:HD12	1:CCC:123:ILE:HG21	1.80	0.62
2:DDD:210:PRO:HD3	2:DDD:233:GLY:HA3	1.81	0.61
2:BBB:234:GLU:HG3	2:BBB:235:VAL:N	2.18	0.59
1:CCC:113:VAL:O	1:CCC:117:SER:HB3	2.03	0.58
2:DDD:292:THR:O	2:DDD:312:ARG:NH1	2.38	0.56
1:CCC:17:ARG:HD3	2:DDD:311:TYR:CE2	2.41	0.56
1:AAA:113:VAL:O	1:AAA:117:SER:HB3	2.06	0.56
1:AAA:5:VAL:HG13	2:BBB:280:ILE:HD13	1.88	0.55
2:BBB:292:THR:O	2:BBB:312:ARG:NH1	2.39	0.55
2:BBB:268:LEU:HB2	2:BBB:269:PRO:HD3	1.88	0.54
2:DDD:221:ASN:HB3	2:DDD:224:SER:OG	2.08	0.53
1:CCC:103:LEU:HD22	1:CCC:136:MET:HE2	1.93	0.51
1:AAA:123:ILE:HD12	1:CCC:123:ILE:CG2	2.41	0.51
1:AAA:44:GLU:HB2	2:BBB:302:ALA:HB1	1.92	0.50
1:AAA:98:ALA:HB3	1:AAA:123:ILE:HG22	1.94	0.49
2:DDD:260:CYS:HB3	2:DDD:289:PRO:HG3	1.95	0.49
2:BBB:183:VAL:HG23	2:BBB:280:ILE:HG13	1.95	0.48
2:BBB:226:ALA:O	2:BBB:279:ALA:HA	2.13	0.48
1:CCC:103:LEU:HD22	1:CCC:136:MET:CE	2.43	0.48
1:AAA:23:GLN:NE2	1:AAA:27:ARG:HH22	2.09	0.47
2:BBB:210:PRO:HB3	2:BBB:237:ILE:HG13	1.96	0.47
2:BBB:225:VAL:HG11	2:BBB:245:ILE:HG22	1.96	0.47
2:DDD:288:LEU:HD12	2:DDD:288:LEU:N	2.29	0.46
2:DDD:268:LEU:HB2	2:DDD:269:PRO:HD3	1.98	0.46
2:BBB:288:LEU:N	2:BBB:288:LEU:HD12	2.31	0.46
1:AAA:86:VAL:HG11	1:AAA:111:ARG:HG2	1.98	0.46
1:CCC:5:VAL:HG21	2:DDD:286[B]:VAL:HG21	1.98	0.46
1:CCC:42:MET:O	1:CCC:47:GLU:HG2	2.16	0.45
1:CCC:118:PRO:HG2	1:CCC:119:HIS:CD2	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AAA:33:SER:HA	1:AAA:36:VAL:HG12	1.98	0.45
1:AAA:22:LEU:O	1:AAA:26:LEU:HG	2.16	0.45
1:CCC:74:PHE:HZ	1:CCC:145:SER:HG	1.64	0.44
2:DDD:312:ARG:O	2:DDD:313:GLU:HB2	2.17	0.44
1:AAA:41:LYS:HB3	1:AAA:41:LYS:HE3	1.75	0.43
2:BBB:232:THR:O	2:BBB:236:PHE:HD1	2.01	0.43
1:CCC:29:ILE:O	1:CCC:33:SER:HB2	2.18	0.43
2:BBB:190:ASN:HA	2:BBB:222:ASN:HD21	1.83	0.43
2:DDD:211:GLN:N	2:DDD:212:PRO:HD2	2.33	0.43
1:CCC:109:ALA:O	1:CCC:113:VAL:HG23	2.19	0.42
2:BBB:211:GLN:N	2:BBB:212:PRO:HD2	2.35	0.42
2:BBB:218:CYS:HB3	4:BBB:404:HOH:O	2.20	0.41
1:CCC:70:ILE:HA	1:CCC:144:PHE:HA	2.01	0.41
1:AAA:97:VAL:HA	1:AAA:122:MET:O	2.21	0.41
2:BBB:206:HIS:CB	1:CCC:126:GLY:HA3	2.50	0.41
1:AAA:23:GLN:HE21	1:AAA:27:ARG:NH2	2.10	0.41
1:AAA:99:GLY:HA3	4:AAA:333:HOH:O	2.21	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	142/178 (80%)	141 (99%)	1 (1%)	0	100	100
1	CCC	140/178 (79%)	139 (99%)	1 (1%)	0	100	100
2	BBB	134/143 (94%)	126 (94%)	8 (6%)	0	100	100
2	DDD	131/143 (92%)	125 (95%)	6 (5%)	0	100	100
All	All	547/642 (85%)	531 (97%)	16 (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	109/136 (80%)	108 (99%)	1 (1%)	78	86
1	CCC	108/136 (79%)	108 (100%)	0	100	100
2	BBB	95/100 (95%)	95 (100%)	0	100	100
2	DDD	94/100 (94%)	94 (100%)	0	100	100
All	All	406/472 (86%)	405 (100%)	1 (0%)	93	97

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

Mol	Chain	Res	Type
1	AAA	41	LYS

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 2 ligands modelled in this entry, 2 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)

EDS failed to run properly - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains (i)

EDS failed to run properly - this section is therefore empty.

6.3 Carbohydrates (i)

EDS failed to run properly - this section is therefore empty.

6.4 Ligands (i)

EDS failed to run properly - this section is therefore empty.

6.5 Other polymers (i)

EDS failed to run properly - this section is therefore empty.