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wwPDB X-ray Structure Validation Summary Report ⓘ

Jul 5, 2022 – 01:07 pm BST

PDB ID	:	7R5C
Title	:	Structure of E.coli Class 2 L-asparaginase EcAIII, mutant RDM1-29 (G206C, R207S, D210L, S211V)
Authors	:	Barciszewski, J.; Imiolczyk, B.; Loch, J.I.; Jaskolski, M.
Deposited on	:	2022-02-10
Resolution	:	2.20 Å(reported)

The following versions of software and data (see references ⓘ) were used in the production of this report:

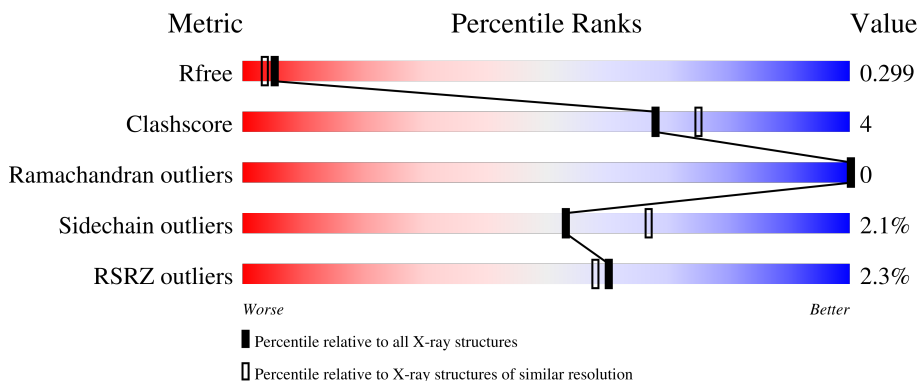|		
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.29
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0267
CCP4	:	7.1.010 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.29

1 Overall quality at a glance ⓘ

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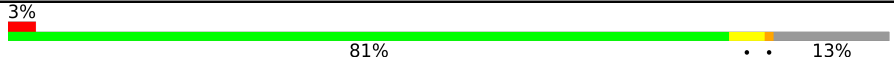*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.20 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	Percentile Ranks	Value
Rfree		0.299
Clashscore		4
Ramachandran outliers		0
Sidechain outliers		2.1%
RSRZ outliers		2.3%

Worse   *Better*

▮ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R$_{free}$	130704	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (2.20-2.20)

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 <=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% / 81% · · 13%
1	CCC	178	3% / 80% 7% 13%
2	BBB	143	% / 83% 10% · 6%
2	DDD	143	% / 83% 10% · 6%

2 Entry composition ⓘ

There are 6 unique types of molecules in this entry. The entry contains 4324 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	154	Total 1156	C 721	N 204	O 221	S 10	0	1	0
1	CCC	154	Total 1156	C 721	N 204	O 221	S 10	0	1	0

- Molecule 2 is a protein called Isoaspartyl peptidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	BBB	134	Total 941	C 590	N 157	O 186	S 8	0	0	0
2	DDD	135	Total 950	C 595	N 158	O 189	S 8	0	0	0

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
BBB	206	CYS	GLY	engineered mutation	UNP P37595
BBB	207	SER	ARG	engineered mutation	UNP P37595
BBB	210	LEU	ASP	engineered mutation	UNP P37595
BBB	211	VAL	SER	engineered mutation	UNP P37595
DDD	206	CYS	GLY	engineered mutation	UNP P37595
DDD	207	SER	ARG	engineered mutation	UNP P37595
DDD	210	LEU	ASP	engineered mutation	UNP P37595
DDD	211	VAL	SER	engineered mutation	UNP P37595

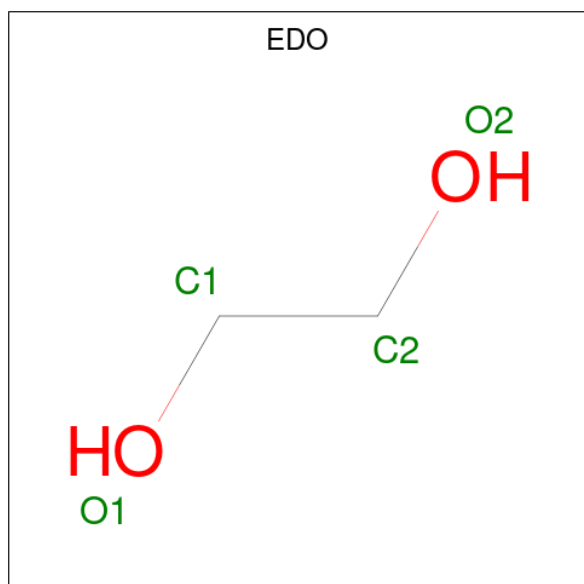- Molecule 3 is SODIUM ION (three-letter code: NA) (formula: Na).

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

- Molecule 4 is 2-AMINO-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (three-letter code: TRS) (formula: $C_4H_{12}NO_3$).
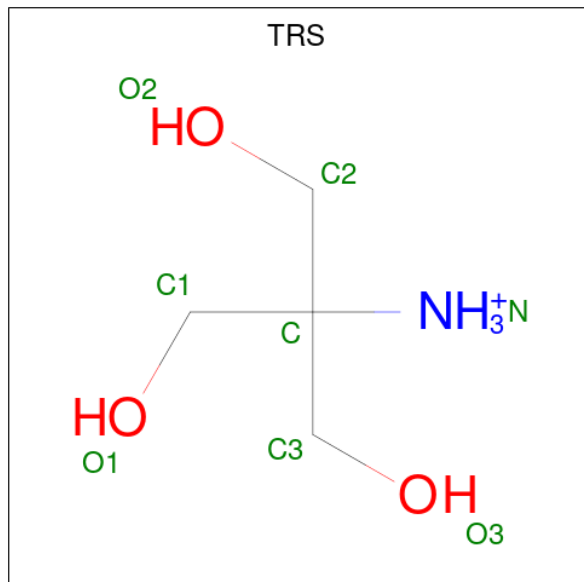
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	CCC	1	Total	C	N	O	0	0
			8	4	1	3		

- Molecule 5 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	DDD	1	Total	C	O	0	0
			4	2	2		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	AAA	26	Total 26	O 26	0	0
6	BBB	22	Total 22	O 22	0	0
6	CCC	36	Total 36	O 36	0	0
6	DDD	23	Total 23	O 23	0	0

3 Residue-property plots ⓘ

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.
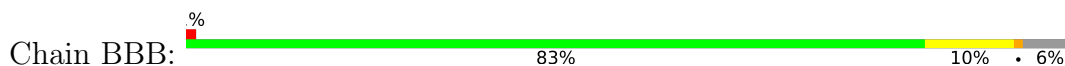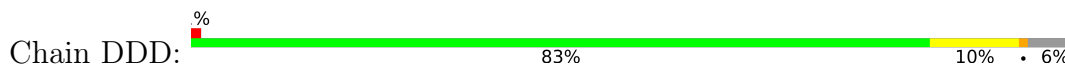
- Molecule 1: Isoaspartyl peptidase
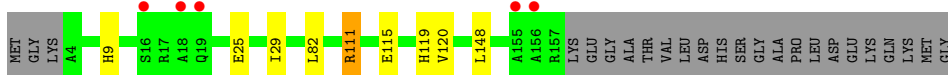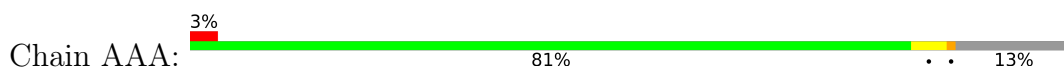
Chain AAA:

- Molecule 1: Isoaspartyl peptidase

Chain CCC:

- Molecule 2: Isoaspartyl peptidase

Chain BBB:

- Molecule 2: Isoaspartyl peptidase

Chain DDD:
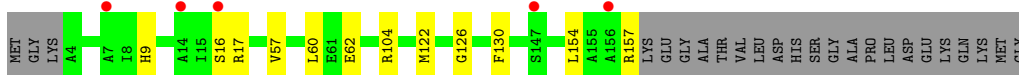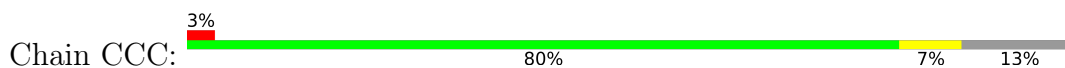
4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	51.79Å 77.86Å 148.36Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	21.48 – 2.20 21.48 – 2.20	Depositor EDS
% Data completeness (in resolution range)	97.0 (21.48-2.20) 97.2 (21.48-2.20)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.22 (at 2.19Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.249 , 0.301 0.255 , 0.299	Depositor DCC
R_{free} test set	1039 reflections (3.42%)	wwPDB-VP
Wilson B-factor (Å^2)	35.7	Xtriage
Anisotropy	0.194	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	(Not available) , (Not available)	EDS
L-test for twinning[2]	$< |L| > = 0.41$, $< L^2 > = 0.24$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	4324	wwPDB-VP
Average B, all atoms (Å^2)	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 15.15% of the height of the origin peak. No significant pseudotranslation is detected.*

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[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: TRS, NA, EDO

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	0.83	0/1173	0.88	0/1583
1	CCC	0.85	0/1173	0.92	0/1583
2	BBB	0.81	0/956	0.90	0/1303
2	DDD	0.78	0/965	0.93	0/1315
All	All	0.82	0/4267	0.91	0/5784

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	1156	0	1162	6	0
1	CCC	1156	0	1162	6	0
2	BBB	941	0	926	14	0
2	DDD	950	0	932	15	0
3	AAA	1	0	0	0	0
3	CCC	1	0	0	0	0
4	CCC	8	0	12	0	0
5	DDD	4	0	6	1	0
6	AAA	26	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	BBB	22	0	0	0	0
6	CCC	36	0	0	0	0
6	DDD	23	0	0	0	0
All	All	4324	0	4200	32	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.

The worst 5 of 32 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)
2:BBB:213:LEU:HD22	2:DDD:213:LEU:HD22	1.83	0.60
2:BBB:183:VAL:HG23	2:BBB:280:ILE:HD12	1.84	0.60
2:BBB:262:ARG:O	2:BBB:266:GLU:HB2	2.05	0.56
1:CCC:62:GLU:OE1	1:CCC:104:ARG:NH2	2.34	0.56
1:AAA:25:GLU:O	1:AAA:29:ILE:HG12	2.06	0.56

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	153/178 (86%)	148 (97%)	5 (3%)	0	100	100
1	CCC	153/178 (86%)	150 (98%)	3 (2%)	0	100	100
2	BBB	132/143 (92%)	126 (96%)	6 (4%)	0	100	100
2	DDD	133/143 (93%)	126 (95%)	7 (5%)	0	100	100
All	All	571/642 (89%)	550 (96%)	21 (4%)	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	119/136 (88%)	117 (98%)	2 (2%)	60	74
1	CCC	119/136 (88%)	115 (97%)	4 (3%)	37	47
2	BBB	93/100 (93%)	91 (98%)	2 (2%)	52	65
2	DDD	94/100 (94%)	93 (99%)	1 (1%)	73	85
All	All	425/472 (90%)	416 (98%)	9 (2%)	53	67

5 of 9 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	CCC	157	ARG
2	DDD	230	THR
2	BBB	312	ARG
1	CCC	16	SER
1	CCC	17	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 ⓘ

Of 4 ligands modelled in this entry, 2 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	$\#|Z| > 2$
4	TRS	CCC	201	-	7,7,7	0.37	0	9,9,9	0.63	0
5	EDO	DDD	401	-	3,3,3	0.19	0	2,2,2	0.37	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. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	TRS	CCC	201	-	-	0/9/9/9	-
5	EDO	DDD	401	-	-	0/1/1/1	-

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.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	DDD	401	EDO	1	0

5.7 Other polymers ⓘ

There are no such residues in this entry.

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5.8 Polymer linkage issues ⓘ

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	154/178 (86%)	0.18	5 (3%)	47	45	27, 37, 60, 72	0
1	CCC	154/178 (86%)	0.17	5 (3%)	47	45	20, 36, 61, 69	0
2	BBB	134/143 (93%)	0.26	2 (1%)	73	72	29, 39, 54, 66	0
2	DDD	135/143 (94%)	0.35	1 (0%)	87	86	26, 37, 54, 72	0
All	All	577/642 (89%)	0.23	13 (2%)	60	58	20, 37, 58, 72	0

The worst 5 of 13 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	CCC	14	ALA	5.3
1	CCC	156	ALA	3.7
1	AAA	155	ALA	3.2
2	BBB	305	THR	2.7
1	CCC	16	SER	2.6

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

There are no non-standard protein/DNA/RNA residues in this entry.

6.3   Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.4   Ligands ⓘ

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(Å^2)	Q<0.9
4	TRS	CCC	201	8/8	0.83	0.18	34,38,40,41	0
5	EDO	DDD	401	4/4	0.88	0.13	48,50,53,54	0
3	NA	AAA	201	1/1	0.97	0.11	37,37,37,37	0
3	NA	CCC	202	1/1	0.97	0.13	29,29,29,29	0

6.5 Other polymers ⓘ

There are no such residues in this entry.