wwPDB X-ray Structure Validation Summary Report (i)

Jul 5, 2022 – 01:08 pm BST

PDB ID	:	7QSF
Title	:	Structure of E.coli Class 2 L-asparaginase EcAIII, mutant RDM1-12 (G206C, R207T, D210A, S211A)
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Deposited on	:	2022-01-13
Resolution	:	1.60 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:

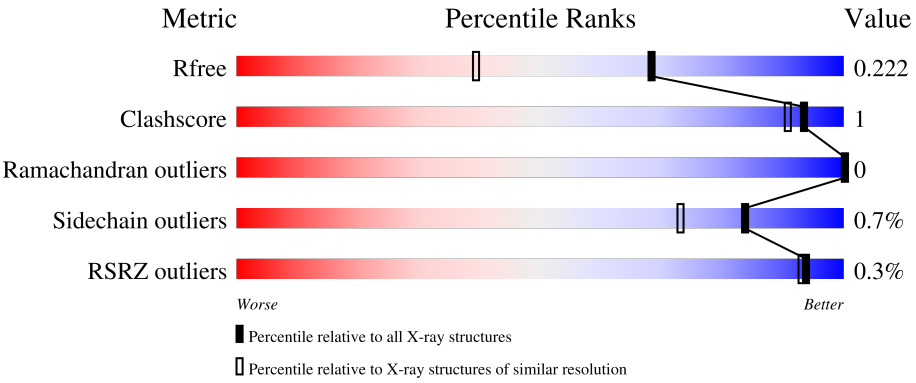
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.29
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0267
CCP4	:	7.1.010 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation 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 1.60 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	3398 (1.60-1.60)
Clashscore	141614	3665 (1.60-1.60)
Ramachandran outliers	138981	3564 (1.60-1.60)
Sidechain outliers	138945	3563 (1.60-1.60)
RSRZ outliers	127900	3321 (1.60-1.60)

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	87% · 11%
1	CCC	178	% 82% · 15%
2	BBB	143	% 93% · 6%
2	DDD	143	88% 6% 6%

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 4839 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	159	Total	C	N	O	S	0	2	0
			1199	748	214	228	9			
1	CCC	152	Total	C	N	O	S	0	2	0
			1147	720	200	218	9			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	BBB	134	Total	C	N	O	S	0	2	0
			947	594	157	188	8			
2	DDD	134	Total	C	N	O	S	0	2	0
			944	592	157	187	8			

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	THR	ARG	engineered mutation	UNP P37595
BBB	210	ALA	ASP	engineered mutation	UNP P37595
BBB	211	ALA	SER	engineered mutation	UNP P37595
DDD	206	CYS	GLY	engineered mutation	UNP P37595
DDD	207	THR	ARG	engineered mutation	UNP P37595
DDD	210	ALA	ASP	engineered mutation	UNP P37595
DDD	211	ALA	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	Na	0	0
			1	1		
3	CCC	1	Total	Na	0	0
			1	1		

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	CCC	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	201	Total O 202 202	0	1
5	BBB	105	Total O 105 105	0	0
5	CCC	169	Total O 169 169	0	0
5	DDD	122	Total O 122 122	0	0

3 Residue-property plots (i)

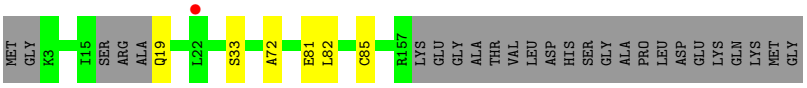
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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

Chain AAA:

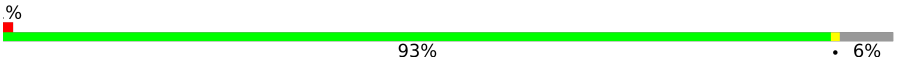
• Molecule 1: Isoaspartyl peptidase

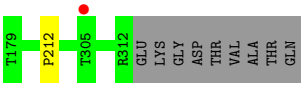
Chain CCC:



• Molecule 2: Isoaspartyl peptidase subunit beta

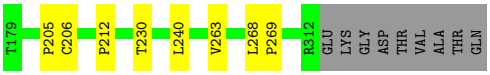
Chain BBB:





• Molecule 2: Isoaspartyl peptidase subunit beta

Chain DDD:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	51.62Å 75.05Å 149.14Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.05 – 1.60 19.05 – 1.60	Depositor EDS
% Data completeness (in resolution range)	90.2 (19.05-1.60) 90.2 (19.05-1.60)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.59 (at 1.60Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.174 , 0.211 0.185 , 0.222	Depositor DCC
R_{free} test set	1039 reflections (1.49%)	wwPDB-VP
Wilson B-factor (Å^2)	10.5	Xtriage
Anisotropy	0.136	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	(Not available) , (Not available)	EDS
L-test for twinning[2]	$< \|L\| > = 0.40$, $< L^2 > = 0.23$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	4839	wwPDB-VP
Average B, all atoms (Å^2)	18.0	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 20.62 % 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 8.3608e-03.*

[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

5.1 Standard geometry

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	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	AAA	0.84	0/1219	0.85	0/1642
1	CCC	0.83	0/1167	0.82	0/1574
2	BBB	0.87	0/968	0.88	0/1320
2	DDD	0.86	0/965	0.85	0/1316
All	All	0.85	0/4319	0.85	0/5852

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

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	1199	0	1215	4	0
1	CCC	1147	0	1160	4	0
2	BBB	947	0	933	1	0
2	DDD	944	0	932	6	0
3	AAA	1	0	0	0	0
3	CCC	1	0	0	0	0
4	CCC	1	0	0	0	0
4	DDD	1	0	0	0	0
5	AAA	202	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	BBB	105	0	0	0	0
5	CCC	169	0	0	1	0
5	DDD	122	0	0	1	0
All	All	4839	0	4240	12	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 1.

The worst 5 of 12 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:DDD:206:CYS:HB2	5:DDD:561:HOH:O	1.98	0.62
1:CCC:81:GLU:OE2	2:DDD:205:PRO:HB3	2.04	0.57
1:AAA:16:SER:HB3	1:AAA:19:GLN:HG3	1.92	0.51
1:AAA:85:CYS:HB2	2:BBB:212:PRO:HA	1.95	0.49
2:DDD:205:PRO:O	2:DDD:206:CYS:HB2	2.16	0.46

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	159/178 (89%)	157 (99%)	2 (1%)	0	100	100
1	CCC	150/178 (84%)	148 (99%)	2 (1%)	0	100	100
2	BBB	134/143 (94%)	129 (96%)	5 (4%)	0	100	100
2	DDD	134/143 (94%)	128 (96%)	6 (4%)	0	100	100
All	All	577/642 (90%)	562 (97%)	15 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains

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	119/136 (88%)	118 (99%)	1 (1%)	81 70
2	BBB	93/98 (95%)	93 (100%)	0	100 100
2	DDD	93/98 (95%)	91 (98%)	2 (2%)	52 27
All	All	428/468 (92%)	425 (99%)	3 (1%)	84 73

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	CCC	33	SER
2	DDD	230	THR
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

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

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

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, 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>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	AAA	159/178 (89%)	-0.31	0 100 100	11, 14, 32, 48	0
1	CCC	152/178 (85%)	-0.27	1 (0%) 87 87	11, 15, 36, 58	0
2	BBB	134/143 (93%)	-0.28	1 (0%) 87 87	11, 15, 27, 40	0
2	DDD	134/143 (93%)	-0.27	0 100 100	12, 14, 29, 44	0
All	All	579/642 (90%)	-0.28	2 (0%) 94 93	11, 14, 32, 58	0

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	CCC	22	LEU	2.5
2	BBB	305	THR	2.0

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, 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	B-factors(Å^2)	Q<0.9
3	NA	AAA	201	1/1	0.99	0.05	8,8,8,8	0
4	CL	CCC	202	1/1	0.99	0.04	17,17,17,17	0
3	NA	CCC	201	1/1	1.00	0.04	12,12,12,12	0
4	CL	DDD	401	1/1	1.00	0.03	16,16,16,16	0

6.5 Other polymers (i)

There are no such residues in this entry.