



Full wwPDB X-ray Structure Validation Report ⓘ

May 29, 2020 – 04:41 am BST

PDB ID : 4ET0
Title : Crystal structure of circularly permuted human asparaginase-like protein 1
Authors : Li, W.Z.; Yogesha, S.D.; Zhang, Y.
Deposited on : 2012-04-23
Resolution : 3.30 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 ⓘ symbol.

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

MolProbity : 4.02b-467
Xtriage (Phenix) : 1.13
EDS : 2.11
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

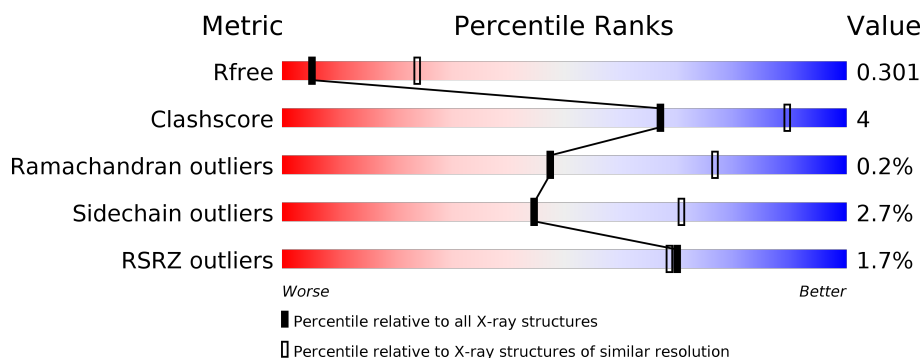
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.30 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	1149 (3.34-3.26)
Clashscore	141614	1205 (3.34-3.26)
Ramachandran outliers	138981	1183 (3.34-3.26)
Sidechain outliers	138945	1182 (3.34-3.26)
RSRZ outliers	127900	1115 (3.34-3.26)

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 on 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 $\leq 5\%$. 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	A	327	<div> <div> <div></div> <div>81%</div> <div>9%</div> <div>10%</div> </div> <div> <div></div> <div>9%</div> </div> </div>
1	B	327	<div> <div> <div></div> <div>81%</div> <div>9%</div> <div>9%</div> </div> <div> <div></div> <div>9%</div> </div> </div>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 4304 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 L-asparaginase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	295	Total	C	N	O	S	0	0	0
			2142	1331	377	421	13			
1	B	298	Total	C	N	O	S	0	0	0
			2160	1342	381	424	13			

There are 40 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	GLY	-	LINKER	UNP Q7L266
A	167A	HIS	-	EXPRESSION TAG	UNP Q7L266
A	167B	HIS	-	EXPRESSION TAG	UNP Q7L266
A	167C	HIS	-	EXPRESSION TAG	UNP Q7L266
A	167D	HIS	-	EXPRESSION TAG	UNP Q7L266
A	167E	HIS	-	EXPRESSION TAG	UNP Q7L266
A	167F	HIS	-	EXPRESSION TAG	UNP Q7L266
A	167G	MET	-	SEE REMARK 999	UNP Q7L266
A	309	GLY	-	LINKER	UNP Q7L266
A	310	ALA	-	LINKER	UNP Q7L266
A	311	GLY	-	LINKER	UNP Q7L266
A	312	SER	-	LINKER	UNP Q7L266
A	313	GLY	-	LINKER	UNP Q7L266
A	314	ALA	-	LINKER	UNP Q7L266
A	315	GLY	-	LINKER	UNP Q7L266
A	316	SER	-	LINKER	UNP Q7L266
A	317	GLY	-	LINKER	UNP Q7L266
A	318	ALA	-	LINKER	UNP Q7L266
A	319	GLY	-	LINKER	UNP Q7L266
A	320	GLY	-	LINKER	UNP Q7L266
B	1	GLY	-	LINKER	UNP Q7L266
B	167A	HIS	-	EXPRESSION TAG	UNP Q7L266
B	167B	HIS	-	EXPRESSION TAG	UNP Q7L266
B	167C	HIS	-	EXPRESSION TAG	UNP Q7L266
B	167D	HIS	-	EXPRESSION TAG	UNP Q7L266

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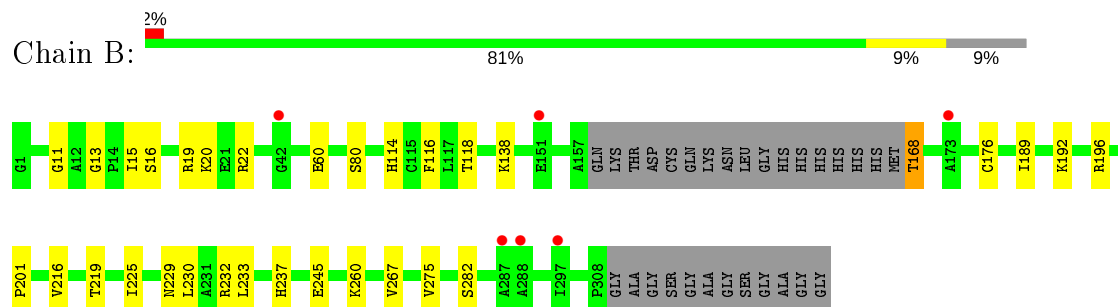
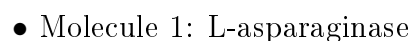
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Chain	Residue	Modelled	Actual	Comment	Reference
B	167E	HIS	-	EXPRESSION TAG	UNP Q7L266
B	167F	HIS	-	EXPRESSION TAG	UNP Q7L266
B	167G	MET	-	SEE REMARK 999	UNP Q7L266
B	309	GLY	-	LINKER	UNP Q7L266
B	310	ALA	-	LINKER	UNP Q7L266
B	311	GLY	-	LINKER	UNP Q7L266
B	312	SER	-	LINKER	UNP Q7L266
B	313	GLY	-	LINKER	UNP Q7L266
B	314	ALA	-	LINKER	UNP Q7L266
B	315	GLY	-	LINKER	UNP Q7L266
B	316	SER	-	LINKER	UNP Q7L266
B	317	GLY	-	LINKER	UNP Q7L266
B	318	ALA	-	LINKER	UNP Q7L266
B	319	GLY	-	LINKER	UNP Q7L266
B	320	GLY	-	LINKER	UNP Q7L266

- Molecule 2 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	1	Total Na 1 1	0	0
2	A	1	Total Na 1 1	0	0

- Molecule 1: L-asparaginase



4 Data and refinement statistics

Property	Value	Source
Space group	P 65 2 2	Depositor
Cell constants a, b, c, α , β , γ	108.64Å 108.64Å 275.14Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	47.50 – 3.30 46.74 – 3.30	Depositor EDS
% Data completeness (in resolution range)	97.4 (47.50-3.30) 97.4 (46.74-3.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.66 (at 3.32Å)	Xtriage
Refinement program	BUSTER 2.10.0	Depositor
R, R_{free}	0.214 , 0.249 0.261 , 0.301	Depositor DCC
R_{free} test set	746 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	67.6	Xtriage
Anisotropy	1.157	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 42.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.40$, $\langle L^2 \rangle = 0.23$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	4304	wwPDB-VP
Average B, all atoms (Å ²)	127.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.16% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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.

5 Model quality

5.1 Standard geometry

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	A	0.51	0/2173	0.72	0/2938
1	B	0.50	0/2191	0.72	0/2961
All	All	0.51	0/4364	0.72	0/5899

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	A	2142	0	2147	18	0
1	B	2160	0	2168	23	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
All	All	4304	0	4315	34	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.

All (34) 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:A:118:THR:OG1	1:B:118:THR:HG21	1.64	0.97
1:B:15:ILE:HG23	1:B:20:LYS:HG3	1.47	0.95
1:A:229:ASN:HD21	1:B:229:ASN:HD21	0.95	0.91
1:A:229:ASN:ND2	1:B:229:ASN:HD21	1.71	0.87
1:B:15:ILE:HD11	1:B:19:ARG:HB3	1.56	0.86
1:A:229:ASN:HD21	1:B:229:ASN:ND2	1.74	0.85
1:A:168:THR:N	1:A:186:THR:HB	2.08	0.68
1:B:233:LEU:HG	1:B:237:HIS:HE1	1.63	0.64
1:B:15:ILE:HG23	1:B:20:LYS:CG	2.27	0.59
1:B:11:GLY:HA2	1:B:282:SER:O	2.07	0.55
1:A:11:GLY:HA2	1:A:282:SER:O	2.09	0.53
1:B:80:SER:HB3	1:B:201:PRO:HA	1.92	0.52
1:A:111:LYS:HG3	1:A:129:MET:HE1	1.93	0.51
1:B:168:THR:HB	1:B:219:THR:OG1	2.10	0.51
1:A:80:SER:HB3	1:A:201:PRO:HA	1.92	0.50
1:A:62:ASN:ND2	1:A:168:THR:OG1	2.45	0.50
1:B:245:GLU:HG3	1:B:275:VAL:HG21	1.93	0.49
1:B:216:VAL:HG22	1:B:267:VAL:HG13	1.95	0.48
1:B:225:ILE:HG23	1:B:230:LEU:HB3	1.96	0.47
1:A:225:ILE:HG23	1:A:230:LEU:HB3	1.95	0.47
1:A:216:VAL:HG22	1:A:267:VAL:HG13	1.96	0.47
1:A:197:VAL:HG21	1:B:118:THR:OG1	2.14	0.47
1:B:189:ILE:HG13	1:B:192:LYS:HB3	1.96	0.47
1:B:233:LEU:O	1:B:237:HIS:ND1	2.50	0.44
1:A:28:VAL:HG22	1:A:293:LEU:HD21	1.98	0.44
1:A:196:ARG:HG3	1:B:114:HIS:CG	2.54	0.43
1:A:298:ASP:HB2	1:A:301:ASP:OD1	2.19	0.43
1:A:114:HIS:CG	1:B:196:ARG:HG3	2.54	0.42
1:B:138:LYS:HD3	1:B:138:LYS:HA	1.91	0.42
1:B:15:ILE:CG2	1:B:20:LYS:HG3	2.34	0.42
1:B:229:ASN:ND2	1:B:232:ARG:HB3	2.34	0.41
1:B:22:ARG:HB3	1:B:60:GLU:HG3	2.02	0.41
1:A:229:ASN:ND2	1:A:232:ARG:HB3	2.37	0.40
1:A:147:ARG:NE	1:A:190:VAL:HG21	2.37	0.40

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	A	291/327 (89%)	282 (97%)	9 (3%)	0	100	100
1	B	294/327 (90%)	283 (96%)	10 (3%)	1 (0%)	41	71
All	All	585/654 (89%)	565 (97%)	19 (3%)	1 (0%)	47	77

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	13	GLY

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	A	223/242 (92%)	216 (97%)	7 (3%)	40	67
1	B	224/242 (93%)	219 (98%)	5 (2%)	52	74
All	All	447/484 (92%)	435 (97%)	12 (3%)	44	71

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	16	SER
1	A	111	LYS
1	A	116	PHE
1	A	182	TYR
1	A	260	LYS

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Mol	Chain	Res	Type
1	A	301	ASP
1	A	307	LEU
1	B	16	SER
1	B	116	PHE
1	B	168	THR
1	B	176	CYS
1	B	260	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	62	ASN
1	A	229	ASN
1	B	120	GLN

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 carbohydrates in this entry.

5.6 Ligand geometry ⓘ

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

There are no such residues in this entry.

5.8 Polymer linkage issues

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, 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	A	295/327 (90%)	0.33	4 (1%) 75 75	80, 124, 154, 165	0
1	B	298/327 (91%)	0.33	6 (2%) 65 64	87, 128, 156, 189	0
All	All	593/654 (90%)	0.33	10 (1%) 70 68	80, 126, 154, 189	0

All (10) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	14	PRO	3.4
1	B	42	GLY	3.0
1	A	15	ILE	2.8
1	B	287	ALA	2.7
1	B	297	ILE	2.5
1	B	151	GLU	2.3
1	B	288	ALA	2.3
1	B	173	ALA	2.2
1	A	69	LEU	2.1
1	A	153	HIS	2.1

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 carbohydrates 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, 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
2	NA	B	401	1/1	0.41	0.26	25,25,25,25	0
2	NA	A	401	1/1	0.95	0.21	49,49,49,49	0

6.5 Other polymers [i](#)

There are no such residues in this entry.