



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 13, 2017 – 07:48 pm GMT

PDB ID : 1IHD
Title : Crystal Structure of Trigonal Form of D90E Mutant of Escherichia coli Asparaginase II
Authors : Borek, D.; Jaskolski, M.
Deposited on : 2001-04-19
Resolution : 2.65 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

<http://wwpdb.org/validation/2016/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)	:	1.9-1692
EDS	:	trunk28620
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	recalc28949

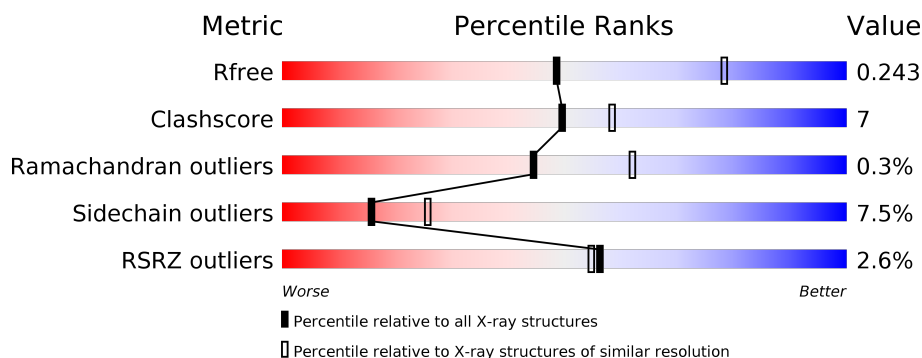
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.65 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}	100719	3491 (2.70-2.62)
Clashscore	112137	1026 (2.68-2.64)
Ramachandran outliers	110173	1010 (2.68-2.64)
Sidechain outliers	110143	1010 (2.68-2.64)
RSRZ outliers	101464	3511 (2.70-2.62)

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. 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	326	<div> <div>3%</div> <div> <div></div> <div>74%</div> <div>18%</div> <div>•• 6%</div> </div> </div>
1	C	326	<div> <div>2%</div> <div> <div></div> <div>75%</div> <div>17%</div> <div>•• 6%</div> </div> </div>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 4674 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 II.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	307	Total	C	N	O	S	0	1	0
			2306	1443	394	461	8			
1	C	308	Total	C	N	O	S	0	1	0
			2314	1447	396	463	8			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	90	GLU	ASP	ENGINEERED	UNP P00805
C	90	GLU	ASP	ENGINEERED	UNP P00805

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	26	Total	O	0	0
			26	26		
2	C	28	Total	O	0	0
			28	28		

4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α , β , γ	123.25Å 123.25Å 83.87Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	10.00 – 2.65 19.95 – 2.65	Depositor EDS
% Data completeness (in resolution range)	100.0 (10.00-2.65) 97.2 (19.95-2.65)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.21 (at 2.67Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.166 , 0.209 0.211 , 0.243	Depositor DCC
R_{free} test set	1079 reflections (5.13%)	DCC
Wilson B-factor (Å ²)	45.4	Xtriage
Anisotropy	0.017	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 23.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.034 for -h,-k,l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	4674	wwPDB-VP
Average B, all atoms (Å ²)	19.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.40% 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 [i](#)

5.1 Standard geometry [i](#)

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	0.66	1/2347 (0.0%)	0.91	11/3196 (0.3%)
1	C	0.68	2/2355 (0.1%)	0.95	13/3207 (0.4%)
All	All	0.67	3/4702 (0.1%)	0.93	24/6403 (0.4%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	93	GLU	CD-OE1	-6.16	1.18	1.25
1	A	93	GLU	CD-OE1	-5.36	1.19	1.25
1	C	93	GLU	CD-OE2	-5.33	1.19	1.25

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	60	ASP	CB-CG-OD2	7.65	125.18	118.30
1	C	93	GLU	OE1-CD-OE2	-7.63	114.14	123.30
1	C	286	ASP	CB-CG-OD2	7.05	124.65	118.30
1	A	93	GLU	OE1-CD-OE2	-6.83	115.10	123.30
1	C	285	ASP	CB-CG-OD2	6.65	124.29	118.30
1	A	233	ASP	CB-CG-OD2	6.60	124.24	118.30
1	C	106	ASP	CB-CG-OD2	6.24	123.92	118.30
1	A	78	ASP	CB-CG-OD2	6.18	123.87	118.30
1	A	285	ASP	CB-CG-OD2	6.18	123.86	118.30
1	A	106	ASP	CB-CG-OD2	6.15	123.84	118.30
1	A	60	ASP	CB-CG-OD2	5.97	123.68	118.30
1	A	138	ASP	CB-CG-OD2	5.96	123.67	118.30
1	C	188	ASP	CB-CG-OD2	5.96	123.66	118.30
1	C	159	ASP	CB-CG-OD2	5.89	123.61	118.30
1	A	188	ASP	CB-CG-OD2	5.75	123.47	118.30
1	C	138	ASP	CB-CG-OD2	5.66	123.39	118.30
1	A	159	ASP	CB-CG-OD2	5.53	123.28	118.30
1	C	233	ASP	CB-CG-OD2	5.53	123.28	118.30
1	C	315	ASP	CB-CG-OD2	5.34	123.11	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	225	ASP	CB-CG-OD2	5.23	123.01	118.30
1	A	255	ASP	CB-CG-OD2	5.20	122.98	118.30
1	C	156	ASP	CB-CG-OD2	5.17	122.95	118.30
1	C	255	ASP	CB-CG-OD2	5.10	122.89	118.30
1	A	286	ASP	CB-CG-OD2	5.02	122.82	118.30

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	2306	0	2303	32	0
1	C	2314	0	2309	36	0
2	A	26	0	0	0	0
2	C	28	0	0	0	0
All	All	4674	0	4612	62	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 7.

All (62) 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:163:THR:HB	1:A:170:THR:O	1.77	0.83
1:C:163:THR:HB	1:C:170:THR:O	1.79	0.83
1:C:267:VAL:HG21	1:C:291:PHE:CD1	2.18	0.78
1:C:175:ASN:HD21	1:C:276:GLY:H	1.33	0.76
1:C:164:ASN:HD22	1:C:167:ASP:H	1.33	0.75
1:A:267:VAL:CG2	1:A:291:PHE:CD1	2.69	0.75
1:C:267:VAL:CG2	1:C:291:PHE:CD1	2.70	0.75
1:A:267:VAL:HG21	1:A:291:PHE:CD1	2.23	0.73
1:C:175:ASN:ND2	1:C:276:GLY:H	1.89	0.70
1:A:300:GLN:HE21	1:C:272:ARG:CZ	2.05	0.69
1:C:73:ILE:HD11	1:C:85:ILE:HD11	1.74	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:117:PRO:HG2	1:C:120:SER:HB3	1.75	0.69
1:A:225:ASP:OD2	1:A:229:LYS:HE3	1.93	0.68
1:A:117:PRO:HG2	1:A:120:SER:HB3	1.75	0.68
1:A:73:ILE:HD11	1:A:85:ILE:HD11	1.77	0.67
1:A:267:VAL:HG21	1:A:291:PHE:CE1	2.33	0.63
1:C:267:VAL:HG21	1:C:291:PHE:CE1	2.33	0.63
1:A:106:ASP:OD1	1:A:106:ASP:N	2.23	0.61
1:A:53:VAL:HG23	1:A:54:VAL:HG13	1.83	0.61
1:A:198:THR:O	1:A:201:THR:HG23	2.01	0.60
1:C:53:VAL:HG23	1:C:54:VAL:HG13	1.85	0.59
1:C:106:ASP:OD1	1:C:106:ASP:N	2.27	0.58
1:A:76:ASP:O	1:A:79:LYS:HG3	2.03	0.58
1:C:267:VAL:HG23	1:C:267:VAL:O	2.03	0.58
1:A:300:GLN:NE2	1:C:272:ARG:HD2	2.20	0.57
1:C:225:ASP:OD2	1:C:229:LYS:HE3	2.06	0.56
1:C:198:THR:O	1:C:201:THR:HG23	2.06	0.55
1:C:268:VAL:HG23	1:C:306:LEU:HD22	1.90	0.54
1:C:298:ASN:HB2	1:C:299:PRO:CD	2.37	0.54
1:A:300:GLN:HE22	1:C:272:ARG:HD2	1.73	0.53
1:A:267:VAL:HG23	1:A:267:VAL:O	2.09	0.52
1:A:300:GLN:HE21	1:C:272:ARG:NE	2.11	0.48
1:A:298:ASN:HB2	1:A:299:PRO:CD	2.44	0.48
1:A:225:ASP:HB3	1:A:252:SER:HB3	1.95	0.48
1:C:112:VAL:HG22	1:C:113:GLY:N	2.30	0.47
1:C:261:ALA:HA	1:C:265:THR:O	2.15	0.47
1:C:69:LEU:HD23	1:C:69:LEU:HA	1.79	0.45
1:C:220:TYR:N	1:C:220:TYR:CD1	2.85	0.45
1:C:225:ASP:HB3	1:C:252:SER:HB3	1.99	0.45
1:C:125:GLY:N	1:C:126:PRO:CD	2.80	0.45
1:C:76:ASP:O	1:C:79:LYS:HG3	2.17	0.44
1:A:182:ILE:HG12	1:A:187:ILE:HG12	1.99	0.43
1:A:315:ASP:HA	1:A:316:PRO:HD3	1.90	0.43
1:A:226:LEU:HB2	1:A:227:PRO:HD3	2.00	0.43
1:A:107:LYS:HG2	1:A:107:LYS:H	1.51	0.43
1:C:225:ASP:CG	1:C:229:LYS:HE3	2.40	0.43
1:C:268:VAL:CG2	1:C:306:LEU:HD22	2.48	0.42
1:C:250:TYR:O	1:C:251:LYS:C	2.57	0.42
1:C:298:ASN:HB2	1:C:299:PRO:HD3	2.02	0.42
1:A:261:ALA:HA	1:A:265:THR:O	2.19	0.42
1:A:69:LEU:HD23	1:A:69:LEU:HA	1.69	0.42
1:A:2:PRO:HG2	1:A:137:ALA:HB1	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:248:ASN:OD1	1:A:249:LEU:N	2.50	0.41
1:C:315:ASP:HA	1:C:316:PRO:HD3	1.93	0.41
1:A:250:TYR:O	1:A:251:LYS:C	2.58	0.41
1:A:39:VAL:O	1:A:39:VAL:HG22	2.20	0.41
1:A:272:ARG:HD2	1:C:300:GLN:NE2	2.36	0.41
1:C:56:ILE:O	1:C:56:ILE:HG13	2.18	0.41
1:C:260:ALA:HB1	1:C:265:THR:HB	2.03	0.41
1:A:220:TYR:CE2	1:A:223:ALA:HA	2.56	0.40
1:A:158:ARG:CZ	1:A:297:LEU:HD21	2.52	0.40
1:A:272:ARG:NH1	1:C:300:GLN:HE21	2.20	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	A	304/326 (93%)	293 (96%)	10 (3%)	1 (0%)	44	62
1	C	305/326 (94%)	297 (97%)	7 (2%)	1 (0%)	44	62
All	All	609/652 (93%)	590 (97%)	17 (3%)	2 (0%)	44	62

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	251	LYS
1	C	251	LYS

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	A	253/266 (95%)	234 (92%)	19 (8%)	16	26
1	C	254/266 (96%)	235 (92%)	19 (8%)	16	26
All	All	507/532 (95%)	469 (92%)	38 (8%)	16	26

All (38) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	39	VAL
1	A	45	ILE
1	A	51	GLU
1	A	68	THR
1	A	79	LYS
1	A	86	THR
1	A	106	ASP
1	A	163	THR
1	A	179	LEU
1	A	201	THR
1	A	207	LYS
1	A	208	LEU
1	A	211	LEU
1	A	222	ASN
1	A	251	LYS
1	A	254	PHE
1	A	300	GLN
1	A	308	LEU
1	A	318	GLN
1	C	39	VAL
1	C	45	ILE
1	C	68	THR
1	C	79	LYS
1	C	86	THR
1	C	106	ASP
1	C	163	THR
1	C	179	LEU
1	C	186	LYS
1	C	201	THR
1	C	207	LYS
1	C	208	LEU
1	C	211	LEU
1	C	222	ASN

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Mol	Chain	Res	Type
1	C	251	LYS
1	C	254	PHE
1	C	300	GLN
1	C	308	LEU
1	C	318	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	52	GLN
1	A	64	ASN
1	A	131	ASN
1	A	190	GLN
1	C	52	GLN
1	C	131	ASN
1	C	164	ASN
1	C	175	ASN
1	C	190	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 ⓘ

There are no ligands in this entry.

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	307/326 (94%)	-0.22	9 (2%) 52 50	15, 19, 23, 26	0
1	C	308/326 (94%)	-0.22	7 (2%) 61 59	15, 19, 23, 26	0
All	All	615/652 (94%)	-0.22	16 (2%) 56 55	15, 19, 23, 26	0

All (16) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	37	ASN	3.7
1	A	119	THR	3.2
1	C	106	ASP	3.2
1	A	15	GLY	3.0
1	A	106	ASP	3.0
1	C	264	GLY	3.0
1	C	262	LYS	2.7
1	A	209	ASN	2.6
1	C	206	SER	2.5
1	C	281	ASP	2.5
1	A	78	ASP	2.5
1	C	207	LYS	2.3
1	C	209	ASN	2.3
1	A	14	ALA	2.1
1	A	139	LYS	2.1
1	A	262	LYS	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](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.