



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2018 – 09:45 AM EST

PDB ID : 9ATC
Title : ATCASE Y165F MUTANT
Authors : Ha, Y.; Allewell, N.M.
Deposited on : 1998-06-26
Resolution : 2.40 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) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20030736

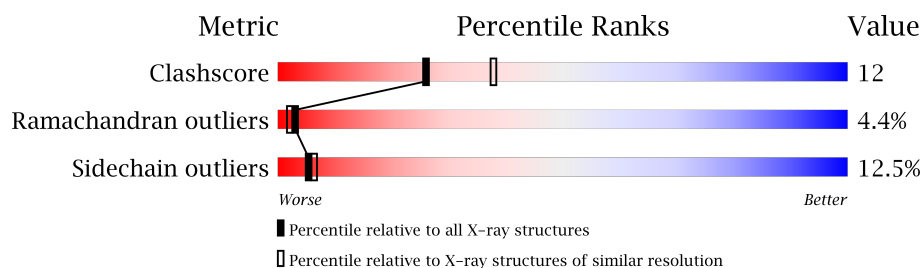
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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	112137	3674 (2.40-2.40)
Ramachandran outliers	110173	3616 (2.40-2.40)
Sidechain outliers	110143	3617 (2.40-2.40)

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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	310	
2	B	146	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 3409 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 ASPARTATE TRANSCARBAMOYLASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	310	Total	C	N	O	S	0	0	0
			2378	1509	415	445	9			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	165	PHE	TYR	ENGINEERED MUTATION	UNP P0A786

- Molecule 2 is a protein called ASPARTATE TRANSCARBAMOYLASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	146	Total	C	N	O	S	0	0	0
			1030	647	182	197	4			

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Zn	0	0
			1	1		

Note EDS was not executed.

Chain A: 67% 29% 4%



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	R 3 2	Depositor
Cell constants a, b, c, α , β , γ	100.60 Å 100.60 Å 100.60 Å 81.40° 81.40° 81.40°	Depositor
Resolution (Å)	10.00 – 2.40	Depositor
% Data completeness (in resolution range)	83.0 (10.00-2.40)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
Refinement program	X-PLOR 3.8	Depositor
R, R_{free}	0.252 , 0.344	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	3409	wwPDB-VP
Average B, all atoms (Å ²)	23.0	wwPDB-VP

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: ZN

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	0.74	0/2424	1.40	16/3293 (0.5%)
2	B	0.73	0/1046	1.52	8/1427 (0.6%)
All	All	0.74	0/3470	1.43	24/4720 (0.5%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	B	0	2

There are no bond length outliers.

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	284	TRP	CE2-CD2-CG	-8.03	100.88	107.30
1	A	284	TRP	CD1-CG-CD2	7.75	112.50	106.30
2	B	99	LEU	CA-CB-CG	7.53	132.61	115.30
1	A	17	ARG	NE-CZ-NH2	-7.50	116.55	120.30
1	A	209	TRP	CE2-CD2-CG	-7.42	101.36	107.30
1	A	209	TRP	CD1-CG-CD2	7.21	112.07	106.30
2	B	14	ARG	NE-CZ-NH2	-7.17	116.72	120.30
1	A	284	TRP	CG-CD2-CE3	6.80	140.02	133.90
1	A	209	TRP	CG-CD2-CE3	6.45	139.71	133.90
1	A	285	TYR	CB-CG-CD1	-6.37	117.18	121.00
1	A	81	LEU	CA-CB-CG	6.18	129.52	115.30
1	A	113	ARG	NE-CZ-NH1	6.11	123.35	120.30
1	A	183	ARG	NE-CZ-NH2	-5.98	117.31	120.30
1	A	54	ARG	NE-CZ-NH1	5.65	123.12	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	96	ARG	NE-CZ-NH1	5.59	123.09	120.30
2	B	144	GLU	CA-CB-CG	5.57	125.66	113.40
1	A	209	TRP	CB-CG-CD1	-5.49	119.86	127.00
1	A	284	TRP	CB-CG-CD1	-5.46	119.90	127.00
2	B	14	ARG	NE-CZ-NH1	5.40	123.00	120.30
1	A	222	VAL	N-CA-CB	-5.22	100.02	111.50
2	B	149	VAL	CA-CB-CG2	-5.20	103.10	110.90
2	B	66	LEU	CA-CB-CG	5.15	127.14	115.30
1	A	54	ARG	NE-CZ-NH2	-5.09	117.75	120.30
2	B	83	VAL	N-CA-C	-5.04	97.41	111.00

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	119	GLU	Peptide
2	B	78	ALA	Peptide

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	2378	0	2362	50	0
2	B	1030	0	950	29	0
3	B	1	0	0	0	0
All	All	3409	0	3312	79	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 12.

All (79) 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:9:ILE:HD11	1:A:125:LEU:HG	1.54	0.88
2:B:105:ASN:HD22	2:B:106:VAL:H	1.29	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:129:LYS:NZ	2:B:132:ASN:HD22	1.84	0.75
1:A:2:ASN:HD22	1:A:4:LEU:H	1.40	0.69
1:A:251:ALA:HA	1:A:254:LEU:HD23	1.75	0.68
1:A:9:ILE:H	1:A:9:ILE:HD13	1.61	0.64
2:B:129:LYS:HE2	2:B:132:ASN:HB3	1.82	0.62
2:B:23:ALA:HB1	2:B:24:GLN:NE2	2.14	0.61
1:A:136:THR:HB	1:A:296:ARG:NH1	2.15	0.61
1:A:13:ASN:HD21	1:A:174:GLN:HB3	1.66	0.61
1:A:154:ASN:HD22	1:A:181:GLY:HA3	1.66	0.60
1:A:227:MET:HG3	1:A:273:ILE:HD11	1.82	0.60
2:B:129:LYS:HB3	2:B:134:ILE:HA	1.83	0.60
1:A:194:MET:SD	1:A:195:PRO:HD2	2.42	0.60
2:B:105:ASN:ND2	2:B:106:VAL:H	2.01	0.57
1:A:91:THR:O	1:A:95:ILE:HG12	2.05	0.56
1:A:236:ASP:HB3	1:A:239:GLU:HB3	1.87	0.56
1:A:243:VAL:HG22	1:A:247:PHE:HE2	1.71	0.56
2:B:129:LYS:HZ2	2:B:132:ASN:HD22	1.54	0.55
1:A:19:ASP:O	1:A:23:VAL:HG23	2.07	0.55
1:A:269:ARG:HH11	1:A:273:ILE:HG22	1.71	0.55
2:B:21:ILE:HD12	2:B:21:ILE:H	1.72	0.55
1:A:163:LEU:HD12	1:A:188:ALA:HB2	1.90	0.54
2:B:105:ASN:HD22	2:B:106:VAL:N	2.04	0.54
1:A:232:LYS:NZ	1:A:237:PRO:HA	2.23	0.54
1:A:141:ASP:O	1:A:145:ILE:HG23	2.08	0.53
1:A:154:ASN:HA	1:A:182:ASN:H	1.74	0.53
1:A:305:ASN:HD22	1:A:308:LEU:HD12	1.75	0.52
2:B:119:GLU:HB3	2:B:121:VAL:HG22	1.92	0.51
1:A:95:ILE:O	1:A:99:VAL:HG22	2.11	0.51
1:A:269:ARG:NH1	1:A:273:ILE:HG22	2.25	0.51
1:A:192:LEU:HD21	1:A:234:ARG:HB3	1.92	0.51
1:A:145:ILE:HG22	1:A:264:LEU:HD11	1.93	0.51
2:B:13:LYS:HA	2:B:86:ILE:HD11	1.94	0.50
2:B:129:LYS:HZ3	2:B:132:ASN:HD22	1.59	0.50
2:B:18:ILE:HG22	2:B:21:ILE:HD11	1.92	0.50
2:B:40:GLN:O	2:B:42:ILE:HG13	2.12	0.49
2:B:67:SER:HB3	2:B:70:GLN:HG3	1.95	0.48
2:B:14:ARG:H	2:B:86:ILE:HG12	1.79	0.47
1:A:235:LEU:O	1:A:236:ASP:HB2	2.14	0.47
2:B:129:LYS:CE	2:B:132:ASN:HB3	2.45	0.46
1:A:128:GLY:HA2	1:A:133:GLN:O	2.15	0.46
1:A:59:PHE:CZ	1:A:136:THR:HG21	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:232:LYS:HZ2	1:A:237:PRO:HA	1.81	0.45
2:B:85:ARG:HD2	2:B:87:ASP:CB	2.46	0.45
1:A:154:ASN:ND2	1:A:181:GLY:HA3	2.32	0.45
1:A:4:LEU:HD23	1:A:302:LEU:HD23	1.99	0.44
1:A:187:ILE:HG22	1:A:247:PHE:CE1	2.52	0.44
2:B:85:ARG:O	2:B:91:VAL:HA	2.17	0.44
2:B:99:LEU:HD21	2:B:130:ARG:HA	2.00	0.44
1:A:166:GLY:O	1:A:169:VAL:HG22	2.17	0.43
1:A:240:TYR:O	1:A:244:LYS:HB2	2.18	0.43
1:A:9:ILE:HD12	1:A:303:VAL:HG21	2.00	0.43
2:B:14:ARG:HA	2:B:86:ILE:HG23	2.00	0.43
1:A:122:VAL:HA	1:A:123:PRO:HD2	1.94	0.42
1:A:38:LEU:HD11	1:A:305:ASN:HD21	1.83	0.42
2:B:119:GLU:HA	2:B:120:PRO:HD2	1.88	0.42
2:B:86:ILE:HG13	2:B:90:GLU:HA	2.00	0.42
1:A:12:ILE:HD12	1:A:12:ILE:HA	1.93	0.42
1:A:261:MET:C	1:A:261:MET:SD	2.98	0.42
1:A:45:ALA:HB2	1:A:99:VAL:HG11	2.01	0.42
2:B:129:LYS:HG3	2:B:131:ALA:H	1.84	0.42
1:A:260:ASN:ND2	1:A:260:ASN:H	2.17	0.42
1:A:146:GLN:HG3	1:A:147:GLU:N	2.35	0.42
1:A:223:ASP:O	1:A:261:MET:HA	2.19	0.42
2:B:42:ILE:O	2:B:44:ILE:HG13	2.20	0.41
2:B:21:ILE:CG2	2:B:25:ILE:HB	2.50	0.41
1:A:20:LEU:HD12	1:A:139:LEU:HD21	2.01	0.41
1:A:8:HIS:ND1	1:A:123:PRO:HA	2.35	0.41
1:A:9:ILE:N	1:A:9:ILE:HD13	2.32	0.41
2:B:147:HIS:O	2:B:151:LEU:HB2	2.21	0.41
2:B:65:PHE:CZ	2:B:85:ARG:HD3	2.55	0.41
2:B:15:GLY:H	2:B:86:ILE:HG23	1.84	0.41
1:A:298:ALA:O	1:A:302:LEU:HD13	2.21	0.41
1:A:137:GLN:O	1:A:140:LEU:HG	2.21	0.40
1:A:30:LEU:HD13	1:A:297:GLN:HE21	1.85	0.40
1:A:156:HIS:HB3	1:A:185:TYR:HE2	1.86	0.40
1:A:227:MET:O	1:A:266:PRO:HD2	2.22	0.40
1:A:164:LYS:HA	1:A:195:PRO:HD3	2.02	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	308/310 (99%)	278 (90%)	24 (8%)	6 (2%)	9	11
2	B	144/146 (99%)	102 (71%)	28 (19%)	14 (10%)	1	0
All	All	452/456 (99%)	380 (84%)	52 (12%)	20 (4%)	3	2

All (20) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	182	ASN
1	A	236	ASP
2	B	40	GLN
2	B	55	ARG
2	B	79	PRO
2	B	91	VAL
2	B	133	ASP
1	A	77	ALA
2	B	25	ILE
2	B	14	ARG
2	B	46	LEU
2	B	105	ASN
2	B	129	LYS
1	A	129	ASP
2	B	120	PRO
1	A	85	GLY
2	B	88	ASN
2	B	43	THR
2	B	93	GLY
1	A	309	VAL

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	251/261 (96%)	222 (88%)	29 (12%)	6	8
2	B	100/130 (77%)	85 (85%)	15 (15%)	3	4
All	All	351/391 (90%)	307 (88%)	44 (12%)	5	6

All (44) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	ASN
1	A	4	LEU
1	A	9	ILE
1	A	14	ASP
1	A	15	LEU
1	A	17	ARG
1	A	21	ASN
1	A	24	LEU
1	A	29	LYS
1	A	35	GLN
1	A	46	SER
1	A	59	PHE
1	A	83	LYS
1	A	87	THR
1	A	108	GLN
1	A	129	ASP
1	A	136	THR
1	A	146	GLN
1	A	159	MET
1	A	201	MET
1	A	204	GLU
1	A	228	THR
1	A	260	ASN
1	A	261	MET
1	A	280	THR
1	A	285	TYR
1	A	299	LEU
1	A	304	LEU
1	A	310	LEU
2	B	24	GLN
2	B	32	LEU

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Mol	Chain	Res	Type
2	B	48	LEU
2	B	57	ASP
2	B	64	THR
2	B	65	PHE
2	B	69	ASP
2	B	82	THR
2	B	95	SER
2	B	104	ASP
2	B	105	ASN
2	B	116	SER
2	B	119	GLU
2	B	144	GLU
2	B	153	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	2	ASN
1	A	13	ASN
1	A	108	GLN
1	A	154	ASN
1	A	255	HIS
1	A	297	GLN
1	A	305	ASN
2	B	24	GLN
2	B	105	ASN
2	B	113	ASN
2	B	132	ASN
2	B	147	HIS

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 [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 1 ligands modelled in this entry, 1 is 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 ⓘ

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates ⓘ

EDS was not executed - this section is therefore empty.

6.4 Ligands ⓘ

EDS was not executed - this section is therefore empty.

6.5 Other polymers ⓘ

EDS was not executed - this section is therefore empty.