



wwPDB X-ray Structure Validation Summary Report ⓘ

Jan 31, 2016 – 07:40 PM GMT

PDB ID : 1GQ3
Title : STRUCTURE OF THE R105A MUTANT CATALYTIC TRIMER OF
ESCHERICHIA COLI ASPARTATE TRANSCARBAMOYLASE AT 2.0-Å
RESOLUTION
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Deposited on : 2001-11-19
Resolution : 2.01 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
<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
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
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) : trunk26865

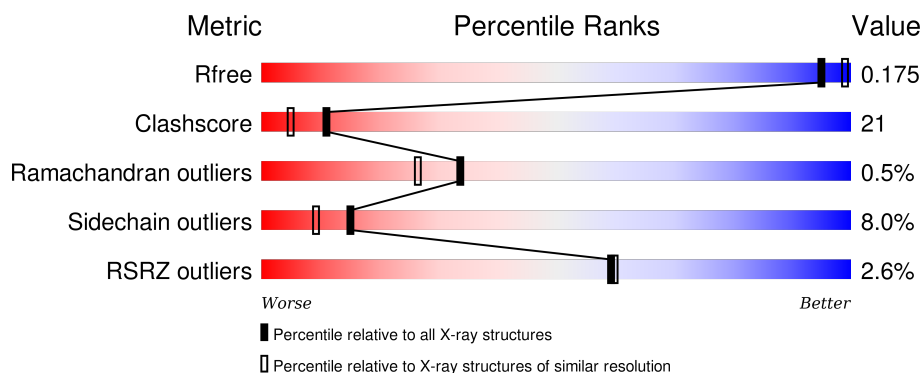
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.01 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}	91344	6249 (2.00-2.00)
Clashscore	102246	7340 (2.00-2.00)
Ramachandran outliers	100387	7248 (2.00-2.00)
Sidechain outliers	100360	7247 (2.00-2.00)
RSRZ outliers	91569	6262 (2.00-2.00)

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	310	<div> <div>2%</div> <div>58% 29% 7% 5%</div> </div>
1	B	310	<div> <div>4%</div> <div>49% 35% 7% 9%</div> </div>
1	C	310	<div> <div>%</div> <div>64% 31% 5%</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	CA	C	1310	-	-	-	X

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 7331 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 CARBAMOYLTRANSFERASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	294	Total	C	N	O	S	0	0	0
			2294	1455	399	431	9			
1	B	283	Total	C	N	O	S	0	0	0
			2184	1383	381	411	9			
1	C	308	Total	C	N	O	S	0	0	0
			2395	1515	418	453	9			

There are 3 discrepancies between the modelled and reference sequences:

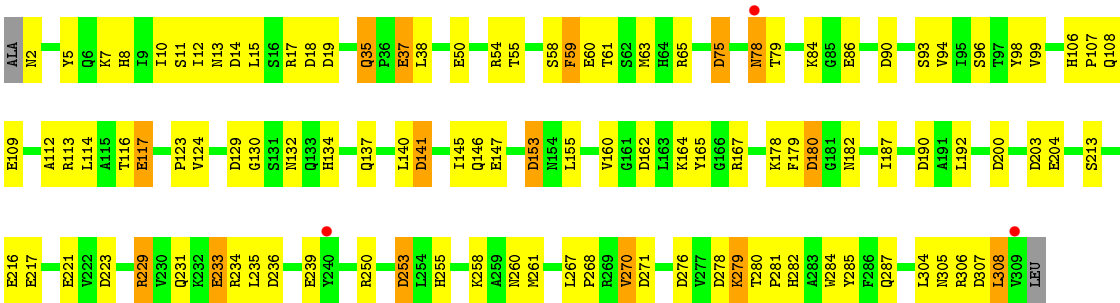
Chain	Residue	Modelled	Actual	Comment	Reference
A	105	ALA	ARG	ENGINEERED	UNP P00479
B	105	ALA	ARG	ENGINEERED	UNP P00479
C	105	ALA	ARG	ENGINEERED	UNP P00479

- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	C	1	Total	Ca	0	0
			1	1		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	128	Total	O	0	0
			128	128		
3	B	125	Total	O	0	0
			125	125		
3	C	204	Total	O	0	0
			204	204		



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	56.03Å 81.10Å 211.65Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	18.29 – 2.01 18.29 – 2.01	Depositor EDS
% Data completeness (in resolution range)	89.8 (18.29-2.01) 88.8 (18.29-2.01)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	55.12 (at 2.00Å)	Xtriage
Refinement program	TNT 5F	Depositor
R, R_{free}	0.195 , 0.281 0.192 , 0.175	Depositor DCC
R_{free} test set	149 reflections (0.26%)	DCC
Wilson B-factor (Å ²)	21.6	Xtriage
Anisotropy	0.678	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 112.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	0 of 57660 reflections	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	7331	wwPDB-VP
Average B, all atoms (Å ²)	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.03% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: CA

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	0.80	13/2338 (0.6%)	1.15	36/3173 (1.1%)
1	B	0.74	6/2225 (0.3%)	1.10	35/3023 (1.2%)
1	C	0.79	11/2441 (0.5%)	1.14	39/3314 (1.2%)
All	All	0.78	30/7004 (0.4%)	1.13	110/9510 (1.2%)

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
1	A	1	0

The worst 5 of 30 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	217	GLU	CD-OE2	6.24	1.32	1.25
1	B	50	GLU	CD-OE2	6.24	1.32	1.25
1	A	272	GLU	CD-OE2	6.19	1.32	1.25
1	A	86	GLU	CD-OE2	6.10	1.32	1.25
1	C	221	GLU	CD-OE2	5.96	1.32	1.25

The worst 5 of 110 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	253	ASP	CB-CG-OD2	-12.01	107.49	118.30
1	B	153	ASP	CB-CG-OD1	8.92	126.33	118.30
1	C	307	ASP	CB-CG-OD2	-7.39	111.64	118.30
1	C	236	ASP	CB-CG-OD2	-7.29	111.74	118.30
1	B	17	ARG	NE-CZ-NH1	7.22	123.91	120.30

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	168	THR	CB

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	2294	0	2292	104	0
1	B	2184	0	2171	107	0
1	C	2395	0	2395	80	0
2	C	1	0	0	0	0
3	A	128	0	0	5	0
3	B	125	0	0	8	0
3	C	204	0	0	15	0
All	All	7331	0	6858	287	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 21.

The worst 5 of 287 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:280:THR:HG22	1:A:282:HIS:H	1.21	1.04
1:B:8:HIS:HD2	1:B:124:VAL:H	1.06	1.00
1:A:250:ARG:HH11	1:A:250:ARG:HG3	1.32	0.92
1:A:219:MET:HB3	1:A:256:ASN:HD21	1.35	0.92
1:A:280:THR:HG23	1:A:281:PRO:HD2	1.54	0.87

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	288/310 (93%)	268 (93%)	20 (7%)	0	100	100
1	B	277/310 (89%)	256 (92%)	19 (7%)	2 (1%)	26	19
1	C	306/310 (99%)	294 (96%)	10 (3%)	2 (1%)	26	19
All	All	871/930 (94%)	818 (94%)	49 (6%)	4 (0%)	34	26

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	270	VAL
1	C	270	VAL
1	B	167	ARG
1	C	132	ASN

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	247/260 (95%)	224 (91%)	23 (9%)	11	6
1	B	235/260 (90%)	210 (89%)	25 (11%)	8	4
1	C	259/260 (100%)	248 (96%)	11 (4%)	36	31
All	All	741/780 (95%)	682 (92%)	59 (8%)	15	9

5 of 59 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	24	LEU
1	B	140	LEU
1	C	146	GLN
1	B	29	LYS
1	B	59	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 31 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	132	ASN
1	B	291	ASN
1	C	260	ASN
1	B	146	GLN
1	C	8	HIS

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 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 [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	294/310 (94%)	0.02	7 (2%) 62 63	15, 29, 63, 84	0
1	B	283/310 (91%)	0.04	13 (4%) 36 38	15, 30, 63, 82	0
1	C	308/310 (99%)	-0.32	3 (0%) 84 84	13, 23, 48, 70	0
All	All	885/930 (95%)	-0.09	23 (2%) 59 60	13, 27, 59, 84	0

The worst 5 of 23 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	306	ARG	3.7
1	A	237	PRO	3.7
1	B	78	ASN	3.6
1	B	191	ALA	3.5
1	B	255	HIS	3.2

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(\AA^2)	Q<0.9
2	CA	C	1310	1/1	0.97	0.25	5.93	1,1,1,1	0

6.5 Other polymers [i](#)

There are no such residues in this entry.