WORLDWIDE PDB PROTEIN DATA BANK

wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 14, 2017 – 09:07 am GMT

PDB ID	:	1NBE
Title	:	ASPARTATE TRANSCARBAMOYLASE REGULATORY CHAIN MUTANT (T82A)
Authors	:	Williams, M.K.; Stec, B.; Kantrowitz, E.R.
Deposited on	:	1998-04-25
Resolution	:	2.60 Å(reported)

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

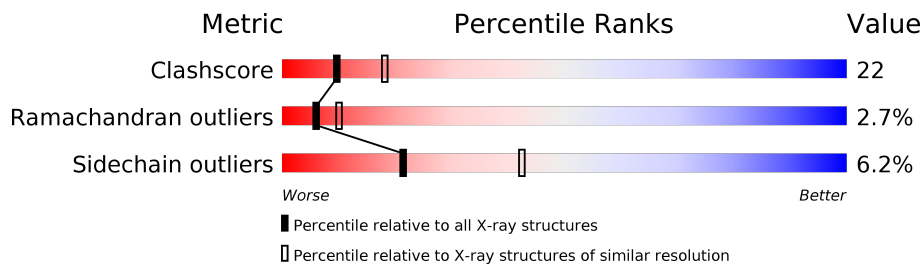|		
MolProbity	:	4.02b-467
Mogul	:	1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	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 2.60 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	Percentile Ranks	Value
Clashscore		22
Ramachandran outliers		2.7%
Sidechain outliers		6.2%

Worse — *Better*

■ Percentile relative to all X-ray structures
▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	112137	2895 (2.60-2.60)
Ramachandran outliers	110173	2848 (2.60-2.60)
Sidechain outliers	110143	2848 (2.60-2.60)

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 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 <=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	64% 32% ・ ・
1	C	310	65% 33% ・
2	B	153	59% 33% 7% ・
2	D	153	56% 40% ・ ・

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
4	MLT	A	311	X	-	-	-
4	MLT	A	312	X	-	-	-
4	MLT	C	311	X	-	-	-
4	MLT	C	312	X	-	-	-

2 Entry composition ⓘ

There are 5 unique types of molecules in this entry. The entry contains 7816 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 2415	C 1527	N 423	O 456	S 9	0	0	0
1	C	310	Total 2415	C 1527	N 423	O 456	S 9	0	0	0

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	60	GLN	GLU	CONFLICT	UNP P0A786
A	147	GLN	GLU	CONFLICT	UNP P0A786
A	149	GLU	GLN	CONFLICT	UNP P0A786
A	196	GLU	GLN	CONFLICT	UNP P0A786
C	60	GLN	GLU	CONFLICT	UNP P0A786
C	147	GLN	GLU	CONFLICT	UNP P0A786
C	149	GLU	GLN	CONFLICT	UNP P0A786
C	196	GLU	GLN	CONFLICT	UNP P0A786

- Molecule 2 is a protein called ASPARTATE TRANSCARBAMOYLASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	153	Total 1199	C 751	N 213	O 229	S 6	0	0	0
2	D	153	Total 1199	C 751	N 213	O 229	S 6	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	82	ALA	THR	ENGINEERED	UNP P0A7F3
D	82	ALA	THR	ENGINEERED	UNP P0A7F3

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

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

- Molecule 4 is MALATE ION (three-letter code: MLT) (formula: $C_4H_6O_5$).
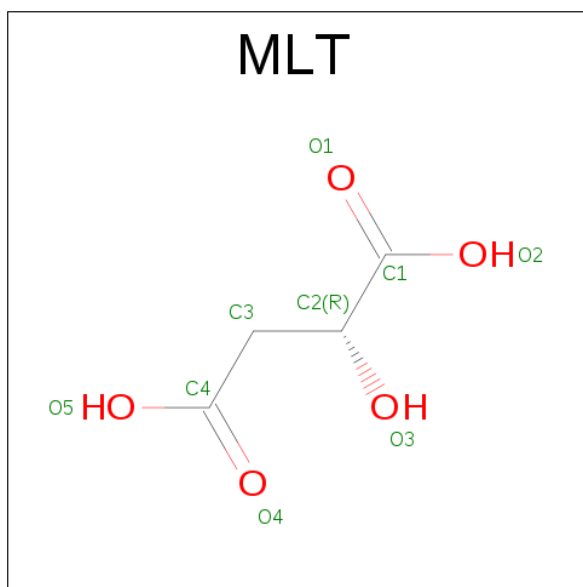
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total 9	C 4	O 5	0	0
4	A	1	Total 9	C 4	O 5	0	0
4	C	1	Total 9	C 4	O 5	0	0
4	C	1	Total 9	C 4	O 5	0	0

- Molecule 5 is water.

| Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	145	Total 145	O 145	0	0
5	B	90	Total 90	O 90	0	0
5	C	222	Total 222	O 222	0	0
5	D	93	Total 93	O 93	0	0

3 Residue-property plots ⓘ

These plots are drawn for all protein, RNA and DNA 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.
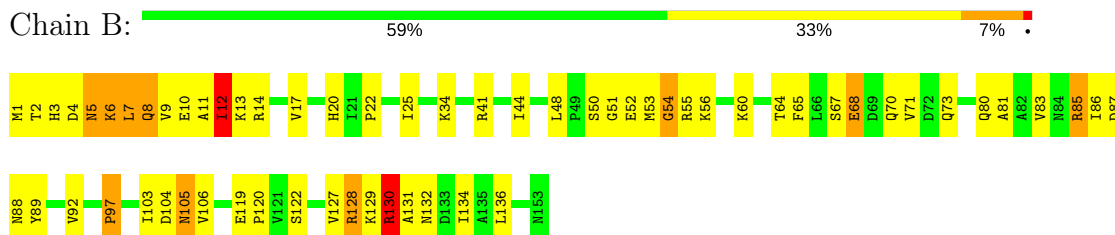
Note EDS was not executed.

• Molecule 1: ASPARTATE TRANSCARBAMOYLASE
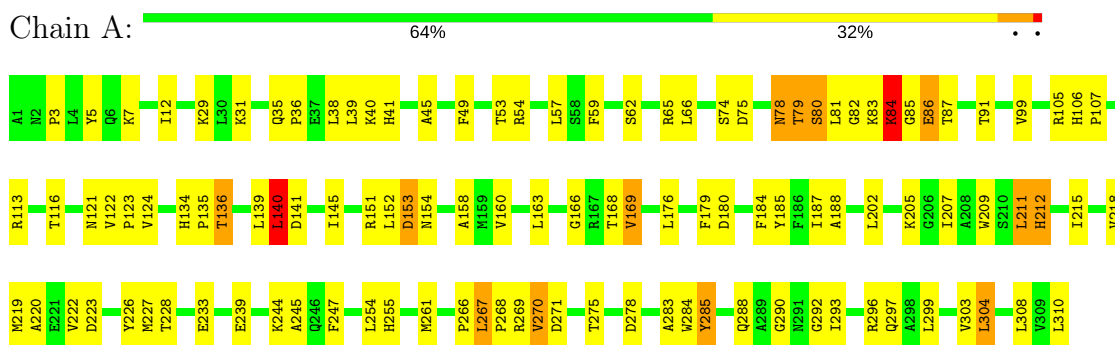
• Molecule 1: ASPARTATE TRANSCARBAMOYLASE
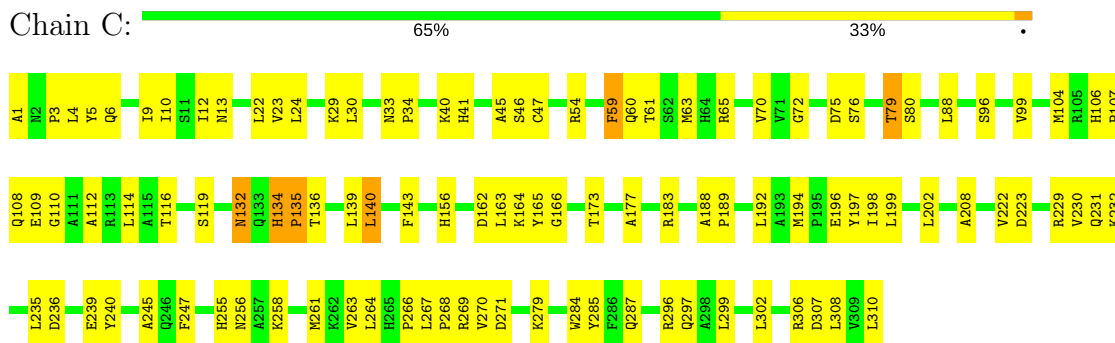
• Molecule 2: ASPARTATE TRANSCARBAMOYLASE

• Molecule 2: ASPARTATE TRANSCARBAMOYLASE

Chain D:

56%   40%

M1 N5 K6 L7 Q8 V9 E10 A11 I12 K13 R14 G15 T16 V17 H20 I21 P22 G26 F27 K28 L29 L30 T38 I42 T43 I44 S50 G51 E52 M53 K56 D57 K60 I61 T64 F65 L66 S67 E68 D69 Q70 V71 Y77 Q80 A81 A82 V83 N84 R85

K94 S95 R96 P97 S98 L99 P100 E101 D104 N105 V106 C109 P110 N111 S112 N113 H117 A126 V127 R128 K129 R130 A131 N132 D133 I134 A135 L136 K139 Y140 S146 V150 N153
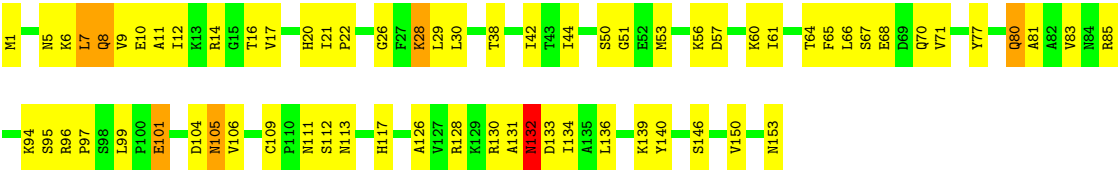
4 Data and refinement statistics (i)

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

Property	Value	Source
Space group	P 3 2 1	Depositor
Cell constants a, b, c, α, β, γ	122.47Å 122.47Å 142.77Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	10.00 – 2.60	Depositor
% Data completeness (in resolution range)	85.0 (10.00-2.60)	Depositor
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR 3.1	Depositor
R, R_{free}	0.177 , 0.237	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	7816	wwPDB-VP
Average B, all atoms (Å^2)	22.0	wwPDB-VP

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, MLT

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	0.69	0/2461	0.95	7/3339 (0.2%)
1	C	0.71	0/2461	0.87	2/3339 (0.1%)
2	B	0.65	0/1217	1.01	5/1644 (0.3%)
2	D	0.64	0/1217	0.89	3/1644 (0.2%)
All	All	0.69	0/7356	0.92	17/9966 (0.2%)

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	0	2

There are no bond length outliers.

The worst 5 of 17 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	84	LYS	CB-CA-C	11.25	132.90	110.40
1	A	140	LEU	CA-CB-CG	9.21	136.48	115.30
1	C	140	LEU	CA-CB-CG	8.60	135.07	115.30
2	B	130	ARG	NE-CZ-NH2	8.12	124.36	120.30
2	D	28	LYS	N-CA-CB	-7.74	96.67	110.60

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	5	TYR	Sidechain

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Mol	Chain	Res	Type	Group
1	A	84	LYS	Mainchain

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	2415	0	2422	102	0
1	C	2415	0	2422	77	0
2	B	1199	0	1216	80	0
2	D	1199	0	1217	80	0
3	B	1	0	0	0	0
3	D	1	0	0	0	0
4	A	18	0	8	0	0
4	C	18	0	8	0	0
5	A	145	0	0	8	0
5	B	90	0	0	6	0
5	C	222	0	0	7	0
5	D	93	0	0	11	0
All	All	7816	0	7293	313	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 22.

The worst 5 of 313 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:B:8:GLN:CB	2:D:8:GLN:HE21	1.42	1.30
2:B:8:GLN:HB3	2:D:8:GLN:NE2	1.49	1.24
2:D:6:LYS:HB3	5:D:155:HOH:O	1.44	1.14
1:A:79:THR:HG22	1:A:81:LEU:HB3	1.26	1.10
2:B:129:LYS:HE3	2:B:132:ASN:HA	1.35	1.07

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%)	281 (91%)	17 (6%)	10 (3%)	5	7
1	C	308/310 (99%)	274 (89%)	28 (9%)	6 (2%)	9	18
2	B	151/153 (99%)	126 (83%)	20 (13%)	5 (3%)	4	7
2	D	151/153 (99%)	130 (86%)	17 (11%)	4 (3%)	6	10
All	All	918/926 (99%)	811 (88%)	82 (9%)	25 (3%)	6	10

5 of 25 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	244	LYS
1	A	270	VAL
2	B	51	GLY
2	B	105	ASN
2	D	105	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	261/261 (100%)	244 (94%)	17 (6%)	20	39
1	C	261/261 (100%)	252 (97%)	9 (3%)	42	69
2	B	136/136 (100%)	127 (93%)	9 (7%)	19	38
2	D	136/136 (100%)	122 (90%)	14 (10%)	8	15
All	All	794/794 (100%)	745 (94%)	49 (6%)	21	42

5 of 49 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	68	GLU
1	C	13	ASN
2	D	132	ASN
2	B	97	PRO
1	C	59	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 22 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	13	ASN
1	C	137	GLN
2	D	113	ASN
1	C	21	ASN
1	C	78	ASN

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 6 ligands modelled in this entry, 2 are monoatomic - leaving 4 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#$\|Z\|>2$	Counts	RMSZ	#$\|Z\|>2$
4	MLT	A	311	-	2,8,8	0.40	0	4,10,10	0.59	0
4	MLT	A	312	-	2,8,8	0.94	0	4,10,10	0.53	0
4	MLT	C	311	-	2,8,8	1.04	0	4,10,10	0.68	0
4	MLT	C	312	-	2,8,8	0.66	0	4,10,10	0.74	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	MLT	A	311	-	1/1/3/3	0/2/8/8	0/0/0/0
4	MLT	A	312	-	1/1/3/3	0/2/8/8	0/0/0/0
4	MLT	C	311	-	1/1/3/3	0/2/8/8	0/0/0/0
4	MLT	C	312	-	1/1/3/3	0/2/8/8	0/0/0/0

There are no bond length outliers.

There are no bond angle outliers.

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	C	311	MLT	C2
4	A	312	MLT	C2
4	C	312	MLT	C2
4	A	311	MLT	C2

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 ⓘ

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.