



wwPDB X-ray Structure Validation Summary Report ⓘ

Jan 31, 2016 – 09:11 PM GMT

PDB ID : 1NUD
Title : Role of Calcium Ions in the Activation and Activity of the Transglutaminase
3 Enzyme (3 calciums, active form)
Authors : Ahvazi, B.
Deposited on : 2003-01-31
Resolution : 2.70 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) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

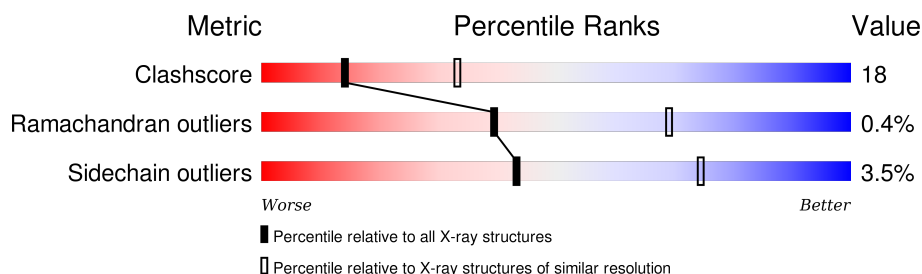
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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	102246	2422 (2.70-2.70)
Ramachandran outliers	100387	2382 (2.70-2.70)
Sidechain outliers	100360	2382 (2.70-2.70)

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	692	 66% 30% . .
1	B	692	 63% 32% . .

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 10921 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 Protein-glutamine glutamyltransferase E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	673	Total	C	N	O	S	0	0	0
			5250	3313	913	1001	23			
1	B	673	Total	C	N	O	S	0	0	0
			5250	3313	913	1001	23			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	250	ASP	ASN	SEE REMARK 999	UNP Q08188
A	264	LEU	PHE	ENGINEERED	UNP Q08188
A	561	ARG	LYS	SEE REMARK 999	UNP Q08188
A	653	ARG	GLY	SEE REMARK 999	UNP Q08188
B	250	ASP	ASN	SEE REMARK 999	UNP Q08188
B	264	LEU	PHE	ENGINEERED	UNP Q08188
B	561	ARG	LYS	SEE REMARK 999	UNP Q08188
B	653	ARG	GLY	SEE REMARK 999	UNP Q08188

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	3	Total	Ca	0	0
			3	3		
2	A	3	Total	Ca	0	0
			3	3		

- Molecule 3 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	4	Total	Cl	0	0
			4	4		
3	A	4	Total	Cl	0	0
			4	4		

- Molecule 4 is BROMIDE ION (three-letter code: BR) (formula: Br).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	5	Total 5	Br 5	0	0
4	A	4	Total 4	Br 4	0	0

- Molecule 5 is water.

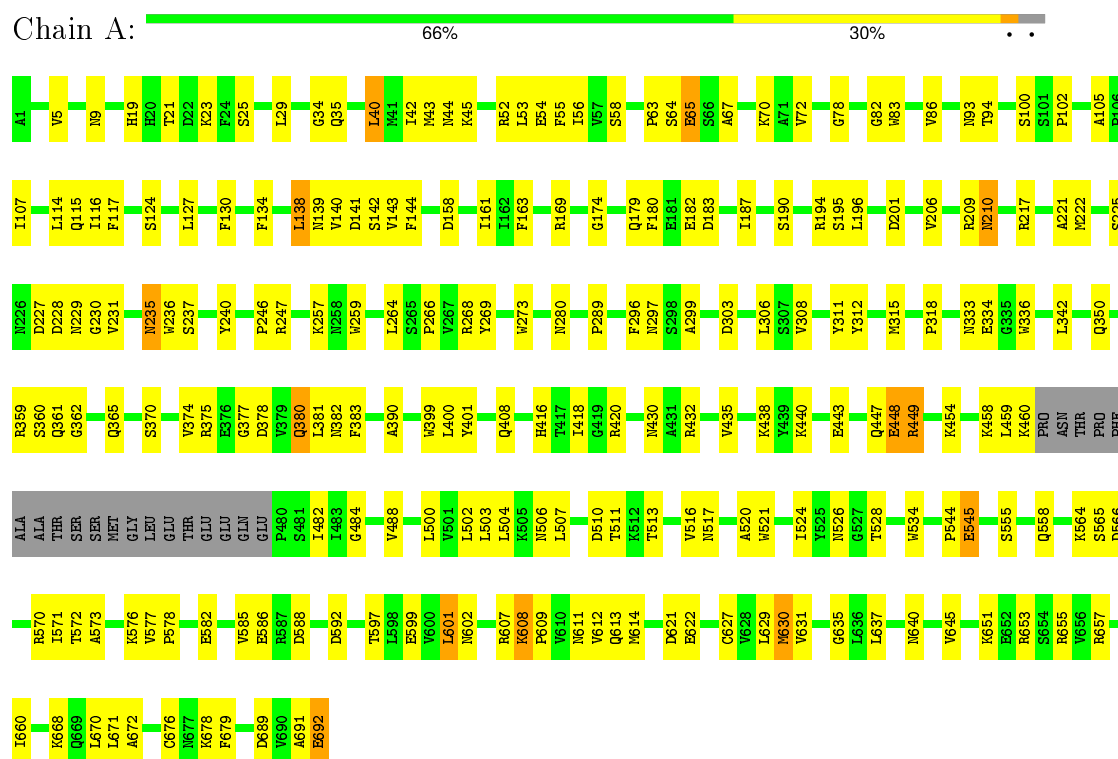
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	193	Total 193	O 193	0	0
5	B	205	Total 205	O 205	0	0

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 errors 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: Protein-glutamine glutamyltransferase E



L629	L542	ALA	R359
M630	L543	THR	G362
V631	P644	SER	V363
E632	E545	MET	F364
L637	E546	GLY	Q365
V645	E547	LEU	Q380
P646	A548	GLU	L381
G649	E549	THR	N382
P650	E560	GLU	F383
K651	R561	GLU	D384
L655	R562	GLN	N385
V656	L563	GLU	P386
P657	K564	P480	R396
I660	S565	I483	
S665	D566	G484	V399
K668	S567	V488	D402
D673	R570	M491	N403
K678	L571	L492	T404
F679	E580	K496	T405
I682	S581	E497	G406
K683	E582	V498	K407
A691	E586	N499	S415
E692	R587	L500	H416
	D588	W501	T417
	L589	L502	I418
	L590	L503	S423
	T597	R505	T424
	L598	N506	K425
	E599	L507	R432
	V600	S508	
	L601	R509	K440
	N602	D510	
	V606	T511	E443
	R607	K512	G444
	V610	T515	S445
	N611	T519	D446
	V612	A520	E448
	Q613	W521	R449
	N614		Q450
	L615	I524	V451
	F616	Y525	F452
	S617	N526	Q453
	N618	G527	
	P619	T528	K458
			L459
	E622	E532	K460
	P623	V533	P40
	V624	W534	ASN
	R625	K535	THR
	D626	D536	P40
	C627		PRE
	V633	T530	ALA

4 Data and refinement statistics

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

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	57.54Å 115.37Å 121.39Å 90.00° 92.66° 90.00°	Depositor
Resolution (Å)	20.00 – 2.70	Depositor
% Data completeness (in resolution range)	(Not available) (20.00-2.70)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.199 , 0.265	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	10921	wwPDB-VP
Average B, all atoms (Å ²)	20.0	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: CA, BR, CL

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	0.37	0/5360	0.62	0/7270
1	B	0.35	0/5360	0.62	0/7270
All	All	0.36	0/10720	0.62	0/14540

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	5250	0	5194	169	0
1	B	5250	0	5194	212	0
2	A	3	0	0	0	0
2	B	3	0	0	0	0
3	A	4	0	0	0	0
3	B	4	0	0	1	0
4	A	4	0	0	1	0
4	B	5	0	0	2	0
5	A	193	0	0	9	0
5	B	205	0	0	11	0
All	All	10921	0	10388	381	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 18.

The worst 5 of 381 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:576:LYS:HD3	1:A:582:GLU:HG3	1.35	1.08
1:B:448:GLU:HG3	1:B:449:ARG:HD2	1.47	0.94
1:A:611:ASN:HB3	1:A:657:ARG:NH2	1.82	0.92
1:B:611:ASN:HD22	1:B:657:ARG:HH22	1.21	0.89
1:A:82:GLY:HA2	1:A:102:PRO:HB3	1.54	0.88

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	669/692 (97%)	627 (94%)	39 (6%)	3 (0%)	39	69
1	B	669/692 (97%)	619 (92%)	47 (7%)	3 (0%)	39	69
All	All	1338/1384 (97%)	1246 (93%)	86 (6%)	6 (0%)	39	69

5 of 6 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	13	ALA
1	A	565	SER
1	B	201	ASP
1	A	201	ASP
1	B	227	ASP

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	579/595 (97%)	558 (96%)	21 (4%)	42	73
1	B	579/595 (97%)	559 (96%)	20 (4%)	43	74
All	All	1158/1190 (97%)	1117 (96%)	41 (4%)	43	74

5 of 41 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	630	MET
1	B	36	ASN
1	B	586	GLU
1	A	689	ASP
1	A	692	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 33 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	611	ASN
1	B	38	GLN
1	B	526	ASN
1	B	6	GLN
1	B	20	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 23 ligands modelled in this entry, 23 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 [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 will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates ⓘ

EDS was not executed - this section will therefore be empty.

6.4 Ligands ⓘ

EDS was not executed - this section will therefore be empty.

6.5 Other polymers ⓘ

EDS was not executed - this section will therefore be empty.