



# wwPDB X-ray Structure Validation Summary Report

Feb 28, 2014 – 01:44 AM GMT

PDB ID : 2C8H  
Title : STRUCTURE OF THE PN LOOP Q182A MUTANT C3BOT1 EXOENZYME (NAD-BOUND STATE, CRYSTAL FORM I)  
Authors : Stura, E.A.; Menetrey, J.; Flatau, G.; Boquet, P.; Menez, A.  
Deposited on : 2005-12-03  
Resolution : 1.65 Å(reported)

This is a wwPDB validation summary report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

---

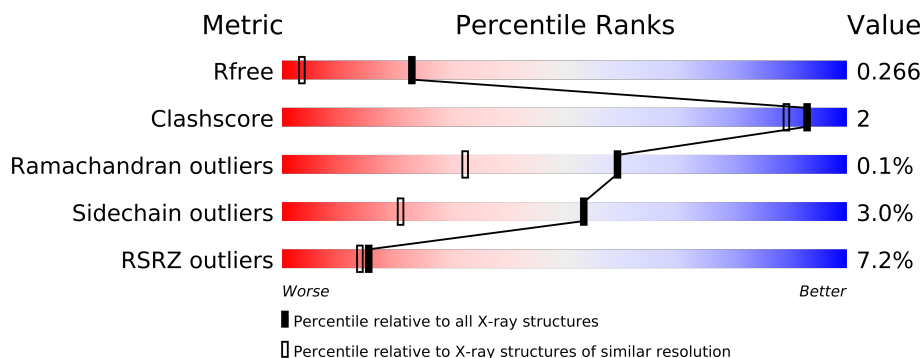
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.15 2013
Xtriage (Phenix)	:	dev-1323
EDS	:	stable22639
Percentile statistics	:	21963
Refmac	:	5.8.0049
CCP4	:	6.3.0 (Settle)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	stable22683

# 1 Overall quality at a glance

The reported resolution of this entry is 1.65 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))
$R_{free}$	66092	1404 (1.68-1.64)
Clashscore	79885	1001 (1.66-1.66)
Ramachandran outliers	78287	1581 (1.68-1.64)
Sidechain outliers	78261	1580 (1.68-1.64)
RSRZ outliers	66119	1404 (1.68-1.64)

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	211	
1	B	211	
1	C	211	
1	D	211	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
2	NAD	B	1250	-	X
3	SO4	D	1248	-	X
3	SO4	D	1249	-	X

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 7257 atoms, of which 0 are hydrogen and 0 are deuterium.

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 MONO-ADP-RIBOSYLTRANSFERASEC3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	204	Total	C	N	O	S	4	0	0
			1598	1015	272	304	7			
1	B	205	Total	C	N	O	S	24	0	0
			1606	1021	273	305	7			
1	C	208	Total	C	N	O	S	9	0	0
			1626	1034	277	308	7			
1	D	204	Total	C	N	O	S	10	0	0
			1595	1014	271	303	7			

There are 4 discrepancies between the modelled and reference sequences:

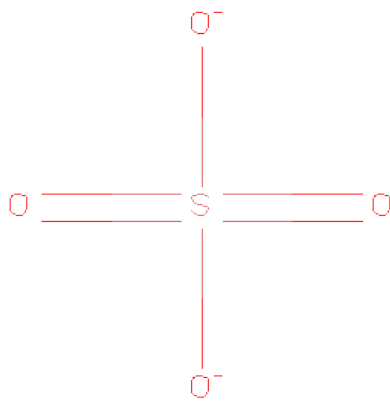
Chain	Residue	Modelled	Actual	Comment	Reference
A	182	ALA	GLN	ENGINEERED MUTATION	UNP P15879
B	182	ALA	GLN	ENGINEERED MUTATION	UNP P15879
C	182	ALA	GLN	ENGINEERED MUTATION	UNP P15879
D	182	ALA	GLN	ENGINEERED MUTATION	UNP P15879

- Molecule 2 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (three-letter code: NAD) (formula:  $C_{21}H_{27}N_7O_{14}P_2$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	B	1	Total	C	N	O	P	0	0
			44	21	7	14	2		

- Molecule 3 is SULFATE ION (three-letter code: SO<sub>4</sub>) (formula: O<sub>4</sub>S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		

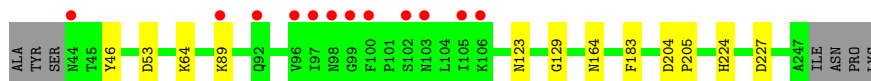
Continued on next page...

*Continued from previous page...*

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	B	1	Total	O	S	0	0
			5	4	1		
3	C	1	Total	O	S	0	0
			5	4	1		
3	D	1	Total	O	S	0	0
			5	4	1		
3	D	1	Total	O	S	0	0
			5	4	1		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	230	Total	O	0	0
			230	230		
4	B	147	Total	O	0	0
			147	147		
4	C	157	Total	O	0	0
			157	157		
4	D	180	Total	O	0	0
			180	180		



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	105.39Å 75.61Å 120.78Å 90.00° 102.75° 90.00°	Depositor
Resolution (Å)	31.78 – 1.65 31.79 – 1.65	Depositor EDS
% Data completeness (in resolution range)	100.0 (31.78-1.65) 96.7 (31.79-1.65)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.64 (at 1.65Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, $R_{free}$	0.216 , 0.259 0.223 , 0.266	Depositor DCC
$R_{free}$ test set	5365 reflections (5.25%)	DCC
Wilson B-factor (Å <sup>2</sup> )	24.9	Xtriage
Anisotropy	0.297	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 44.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 107532 reflections	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	7257	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.29% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: SO4, NAD

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	0.33	0/1626	0.62	3/2184 (0.1%)
1	B	0.41	1/1634 (0.1%)	0.65	4/2195 (0.2%)
1	C	0.36	0/1655	0.65	2/2224 (0.1%)
1	D	0.32	0/1623	0.63	2/2180 (0.1%)
All	All	0.36	1/6538 (0.0%)	0.64	11/8783 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	85	GLU	CB-CG	-9.30	1.34	1.52

The worst 5 of 11 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	233	ASP	CB-CG-OD2	6.71	124.33	118.30
1	D	227	ASP	CB-CG-OD2	6.56	124.20	118.30
1	B	227	ASP	CB-CG-OD2	5.61	123.35	118.30
1	B	85	GLU	CA-CB-CG	5.43	125.35	113.40
1	A	227	ASP	CB-CG-OD2	5.29	123.06	118.30

There are no chirality outliers.

There are no planarity outliers.

### 5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the



chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1598	0	1618	4	0
1	B	1606	0	1629	8	0
1	C	1626	0	1646	5	0
1	D	1595	0	1614	5	0
2	A	44	0	26	0	0
2	B	44	0	26	0	0
3	A	10	0	0	0	0
3	B	5	0	0	0	0
3	C	5	0	0	0	0
3	D	10	0	0	0	0
4	A	230	0	0	1	0
4	B	147	0	0	0	0
4	C	157	0	0	0	0
4	D	180	0	0	0	0
All	All	7257	0	6559	22	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 2.

The worst 5 of 22 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:51:ASN:HD21	1:C:54:GLN:HE21	1.25	0.83
1:C:51:ASN:HD21	1:C:54:GLN:NE2	1.97	0.63
1:D:129:GLY:HA3	1:D:183:PHE:HB2	1.81	0.62
1:B:93:ASN:O	1:B:96:VAL:HG22	2.02	0.60
1:A:133:ALA:HB2	1:A:140:GLN:NE2	2.18	0.58

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	202/211 (96%)	200 (99%)	2 (1%)	0	100	100
1	B	203/211 (96%)	200 (98%)	3 (2%)	0	100	100
1	C	206/211 (98%)	200 (97%)	5 (2%)	1 (0%)	38	13
1	D	202/211 (96%)	201 (100%)	1 (0%)	0	100	100
All	All	813/844 (96%)	801 (98%)	11 (1%)	1 (0%)	59	32

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	147	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	172/178 (97%)	171 (99%)	1 (1%)	92	83
1	B	173/178 (97%)	164 (95%)	9 (5%)	32	7
1	C	174/178 (98%)	165 (95%)	9 (5%)	32	7
1	D	171/178 (96%)	169 (99%)	2 (1%)	82	63
All	All	690/712 (97%)	669 (97%)	21 (3%)	53	21

5 of 21 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	107	GLN
1	C	93	ASN
1	C	142	THR
1	B	106	LYS
1	C	227	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 13 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	54	GLN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	C	93	ASN
1	C	236	GLN
1	B	224	HIS
1	C	224	HIS

### 5.3.3 RNA ⓘ

There are no RNA chains 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 ⓘ

8 ligands are modelled in this entry.

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	$\# Z  > 2$
2	NAD	A	1248	-	48,48,48	1.28	3 (6%)	73,73,73	1.68	7 (9%)
3	SO4	A	1249	-	4,4,4	0.35	0	6,6,6	0.16	0
3	SO4	A	1250	-	4,4,4	0.25	0	6,6,6	0.07	0
2	NAD	B	1250	-	48,48,48	1.36	4 (8%)	73,73,73	1.81	11 (15%)
3	SO4	B	1251	-	4,4,4	0.33	0	6,6,6	0.20	0
3	SO4	C	1252	-	4,4,4	0.27	0	6,6,6	0.07	0
3	SO4	D	1248	-	4,4,4	0.24	0	6,6,6	0.19	0
3	SO4	D	1249	-	4,4,4	0.31	0	6,6,6	0.07	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
2	NAD	A	1248	-	-	0/30/62/62	0/3/5/5
3	SO4	A	1249	-	-	0/0/0/0	0/0/0/0
3	SO4	A	1250	-	-	0/0/0/0	0/0/0/0
2	NAD	B	1250	-	-	0/30/62/62	0/3/5/5
3	SO4	B	1251	-	-	0/0/0/0	0/0/0/0
3	SO4	C	1252	-	-	0/0/0/0	0/0/0/0
3	SO4	D	1248	-	-	0/0/0/0	0/0/0/0
3	SO4	D	1249	-	-	0/0/0/0	0/0/0/0

The worst 5 of 7 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1250	NAD	O7N-C7N	7.03	1.40	1.24
2	A	1248	NAD	O7N-C7N	6.46	1.39	1.24
2	A	1248	NAD	C2A-N3A	3.39	1.38	1.32
2	B	1250	NAD	C2A-N3A	3.33	1.38	1.32
2	B	1250	NAD	C2A-N1A	2.49	1.38	1.33

The worst 5 of 18 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1250	NAD	N3A-C2A-N1A	-10.14	120.23	128.71
2	A	1248	NAD	N3A-C2A-N1A	-9.84	120.48	128.71
2	A	1248	NAD	C3N-C7N-N7N	4.78	123.22	117.77
2	B	1250	NAD	C3N-C7N-N7N	4.49	122.88	117.77
2	B	1250	NAD	O4D-C1D-N1N	4.15	112.19	107.95

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 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 ⓘ

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	204/211 (96%)	0.09	5 (2%) 54 56	17, 25, 33, 35	1 (0%)
1	B	205/211 (97%)	0.59	17 (8%) 11 9	21, 29, 55, 65	5 (2%)
1	C	208/211 (98%)	0.56	26 (12%) 5 3	16, 27, 53, 59	2 (0%)
1	D	204/211 (96%)	0.37	12 (5%) 22 20	18, 28, 44, 51	2 (0%)
All	All	821/844 (97%)	0.40	60 (7%) 15 13	16, 27, 48, 65	10 (1%)

The worst 5 of 60 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	100	PHE	6.0
1	D	100	PHE	5.2
1	C	148	GLY	5.0
1	A	247	ALA	4.9
1	B	101	PRO	4.9

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

There are no non-standard protein/DNA/RNA residues in this entry.

### 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

### 6.4 Ligands ⓘ

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, 95<sup>th</sup> 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	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
3	SO4	D	1249	5/5	0.18	4.33	29,30,30,31	5
3	SO4	D	1248	5/5	0.22	3.27	34,34,35,35	5
2	NAD	B	1250	44/44	0.20	2.79	33,38,44,45	44
3	SO4	C	1252	5/5	0.19	1.86	39,39,39,39	5
3	SO4	A	1250	5/5	0.15	1.39	35,35,36,37	5
2	NAD	A	1248	44/44	0.11	0.39	21,24,27,29	0
3	SO4	A	1249	5/5	0.09	-0.31	30,31,32,32	5
3	SO4	B	1251	5/5	0.10	-0.42	30,30,32,32	5

## 6.5 Other polymers ⓘ

There are no such residues in this entry.