



# Full wwPDB X-ray Structure Validation Report ⓘ

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PDB ID : 8G33  
Title : Activated form of a CDCL long protein  
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Deposited on : 2023-02-06  
Resolution : 2.49 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](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4.02b-467  
Xtriage (Phenix) : 1.13  
EDS : 2.36  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.36

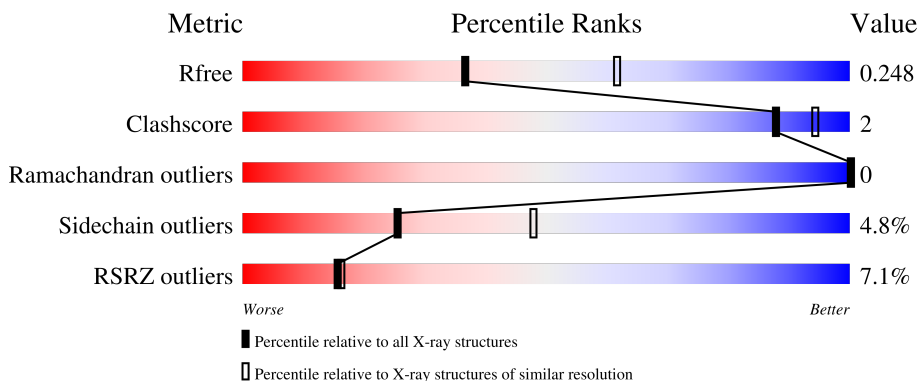
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.49 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))
$R_{free}$	130704	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

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 of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. 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	497	

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 6973 atoms, of which 3436 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 Hemolysin.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
1	A	436	6928	2231	3436	576	679	6	0	0	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	20	GLY	-	expression tag	UNP A0A1T3IZT7
A	21	SER	-	expression tag	UNP A0A1T3IZT7
A	22	HIS	-	expression tag	UNP A0A1T3IZT7
A	23	MET	-	expression tag	UNP A0A1T3IZT7

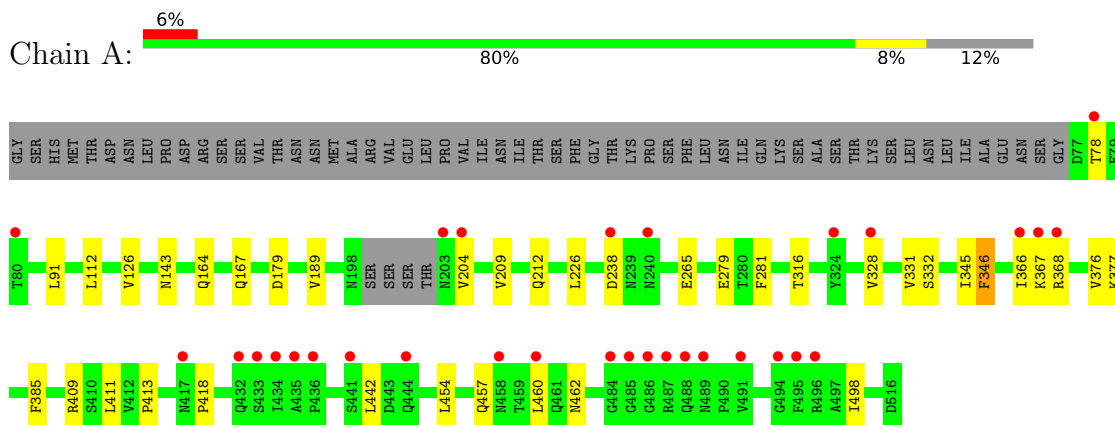
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	45	Total	O	0	0
			45	45		

### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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.

- Molecule 1: Hemolysin



## 4 Data and refinement statistics

Property	Value	Source
Space group	I 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	61.73Å 24.45Å 300.19Å 90.00° 93.19° 90.00°	Depositor
Resolution (Å)	44.22 – 2.49 44.22 – 2.49	Depositor EDS
% Data completeness (in resolution range)	99.1 (44.22-2.49) 99.1 (44.22-2.49)	Depositor EDS
$R_{merge}$	0.17	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.26 (at 2.48Å)	Xtrriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, $R_{free}$	0.207 , 0.248 0.210 , 0.248	Depositor DCC
$R_{free}$ test set	816 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	36.3	Xtrriage
Anisotropy	0.380	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.46 , 52.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	6973	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	48.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.33% of the height of the origin peak. No significant pseudotranslation is detected.*

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

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

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	0.26	0/3567	0.47	0/4825

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 [i](#)

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	3492	3436	3434	14	0
2	A	45	0	0	0	0
All	All	3537	3436	3434	14	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 2.

All (14) 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:204:VAL:HG21	1:A:367:LYS:CB	2.28	0.63
1:A:204:VAL:HG21	1:A:367:LYS:HB3	1.83	0.60
1:A:212:GLN:NE2	1:A:413:PRO:O	2.43	0.52
1:A:442:LEU:CD2	1:A:498:ILE:HD13	2.42	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:204:VAL:HG21	1:A:367:LYS:HB2	1.92	0.49
1:A:78:THR:HG22	1:A:367:LYS:HA	1.93	0.49
1:A:418:PRO:HA	1:A:460:LEU:HD21	1.95	0.48
1:A:112:LEU:HD22	1:A:112:LEU:N	2.29	0.47
1:A:345:ILE:HD12	1:A:346:PHE:CE1	2.51	0.45
1:A:126:VAL:HG21	1:A:226:LEU:HB3	1.97	0.45
1:A:91:LEU:HD11	1:A:189:VAL:HG21	1.98	0.45
1:A:331:VAL:O	1:A:331:VAL:HG12	2.19	0.43
1:A:209:VAL:HG13	1:A:265:GLU:HG2	2.02	0.40
1:A:179:ASP:HB2	1:A:366:ILE:CD1	2.52	0.40

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	432/497 (87%)	416 (96%)	16 (4%)	0	<b>100</b>   <b>100</b>

There are no Ramachandran outliers to report.

### 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	392/447 (88%)	373 (95%)	19 (5%)	25   48

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	143	ASN
1	A	164	GLN
1	A	167	GLN
1	A	238	ASP
1	A	279	GLU
1	A	281	PHE
1	A	316	THR
1	A	328	VAL
1	A	332	SER
1	A	346	PHE
1	A	368	ARG
1	A	376	VAL
1	A	377	LYS
1	A	385	PHE
1	A	409	ARG
1	A	411	LEU
1	A	454	LEU
1	A	457	GLN
1	A	462	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 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 monosaccharides in this entry.

### 5.6 Ligand geometry [i](#)

There are no ligands in this entry.



## 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

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	436/497 (87%)	0.52	31 (7%) <b>16</b> <b>16</b>	20, 40, 75, 104	0

All (31) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	488	GLN	5.1
1	A	489	ASN	4.7
1	A	494	GLY	4.6
1	A	460	LEU	4.4
1	A	487	ARG	4.1
1	A	204	VAL	4.0
1	A	238	ASP	3.9
1	A	435	ALA	3.9
1	A	434	ILE	3.8
1	A	417	ASN	3.7
1	A	368	ARG	3.6
1	A	441	SER	3.5
1	A	203	ASN	3.5
1	A	486	GLY	3.2
1	A	491	VAL	3.0
1	A	495	PHE	2.9
1	A	484	GLY	2.8
1	A	78	THR	2.8
1	A	328	VAL	2.7
1	A	436	PRO	2.6
1	A	444	GLN	2.5
1	A	485	GLY	2.4
1	A	458	ASN	2.4
1	A	367	LYS	2.4
1	A	496	ARG	2.3
1	A	324	TYR	2.3
1	A	433	SER	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	80	THR	2.1
1	A	366	ILE	2.1
1	A	240	ASN	2.1
1	A	432	GLN	2.1

## 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 monosaccharides in this entry.

## 6.4 Ligands [i](#)

There are no ligands in this entry.

## 6.5 Other polymers [i](#)

There are no such residues in this entry.