



# wwPDB X-ray Structure Validation Summary Report ⓘ

Sep 4, 2017 – 09:30 AM EDT

PDB ID : 4P22  
Title : Crystal Structure of N-terminal Fragments of E1  
Authors : Xie, S.-T.  
Deposited on : unknown  
Resolution : 2.75 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](mailto: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.

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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)	:	1.9-1692
EDS	:	rb-20029824
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
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)	:	rb-20029824

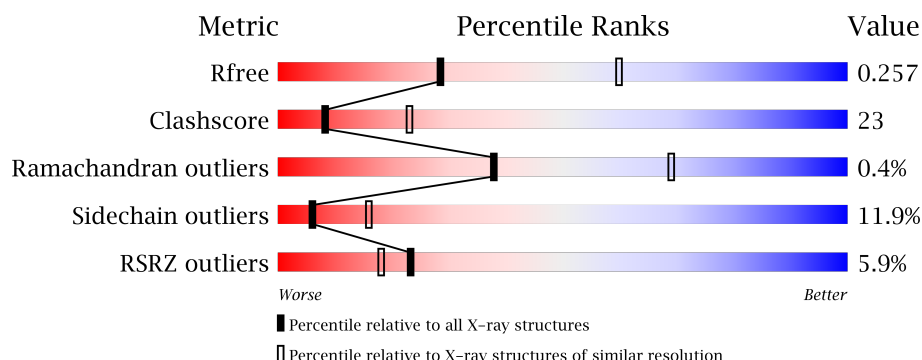
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.75 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))
$R_{free}$	100719	3666 (2.80-2.72)
Clashscore	112137	4174 (2.80-2.72)
Ramachandran outliers	110173	4103 (2.80-2.72)
Sidechain outliers	110143	4106 (2.80-2.72)
RSRZ outliers	101464	3697 (2.80-2.72)

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. 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	446	<div> <div>6%</div> <div> <div></div> <div>52%</div> <div>28%</div> <div>•</div> <div>17%</div> </div> </div>
1	B	446	<div> <div>4%</div> <div> <div></div> <div>58%</div> <div>21%</div> <div>5%</div> <div>16%</div> </div> </div>

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 5848 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 Ubiquitin-like modifier-activating enzyme 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	370	Total	C	N	O	S	0	0	0
			2851	1812	487	537	15			
1	B	375	Total	C	N	O	S	0	0	0
			2888	1834	492	546	16			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-6	GLY	-	expression tag	UNP P22314
A	-5	PRO	-	expression tag	UNP P22314
A	-4	HIS	-	expression tag	UNP P22314
A	-3	MET	-	expression tag	UNP P22314
A	-2	ALA	-	expression tag	UNP P22314
A	-1	ASP	-	expression tag	UNP P22314
A	0	LEU	-	expression tag	UNP P22314
A	352	ASP	GLU	engineered mutation	UNP P22314
B	-6	GLY	-	expression tag	UNP P22314
B	-5	PRO	-	expression tag	UNP P22314
B	-4	HIS	-	expression tag	UNP P22314
B	-3	MET	-	expression tag	UNP P22314
B	-2	ALA	-	expression tag	UNP P22314
B	-1	ASP	-	expression tag	UNP P22314
B	0	LEU	-	expression tag	UNP P22314
B	352	ASP	GLU	engineered mutation	UNP P22314

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	44	Total	O	0	0
			44	44		
2	B	65	Total	O	0	0
			65	65		



F417	M418	P419	I420	M421	Q422	W423	L424	Y425	F426	D427	A428	I429	E430	C431	LEU	PRO	GLU	ASP	LYS	GLU	VAL	LEU

## 4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	94.13Å 186.81Å 135.22Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.77 – 2.75 29.77 – 2.75	Depositor EDS
% Data completeness (in resolution range)	98.3 (29.77-2.75) 98.3 (29.77-2.75)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.72 (at 2.76Å)	Xtriage
Refinement program	PHENIX	Depositor
R, $R_{free}$	0.205 , 0.264 0.207 , 0.257	Depositor DCC
$R_{free}$ test set	1556 reflections (5.05%)	DCC
Wilson B-factor (Å <sup>2</sup> )	38.1	Xtriage
Anisotropy	0.620	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 56.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	5848	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.81% 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	0.45	1/2904 (0.0%)	0.63	0/3929
1	B	0.42	0/2943	0.63	0/3986
All	All	0.43	1/5847 (0.0%)	0.63	0/7915

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	60	TYR	CB-CG	-5.16	1.44	1.51

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	2851	0	2835	136	0
1	B	2888	0	2860	167	0
2	A	44	0	0	0	0
2	B	65	0	0	3	0
All	All	5848	0	5695	266	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 23.

The worst 5 of 266 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:B:80:LEU:CD2	1:B:128:ALA:HA	1.37	1.52
1:A:389:VAL:HG22	1:B:60:TYR:CE1	1.55	1.40
1:A:389:VAL:HG22	1:B:60:TYR:CZ	1.69	1.25
1:A:64:HIS:NE2	1:B:394:LEU:HA	1.57	1.19
1:B:80:LEU:HD22	1:B:128:ALA:CA	1.75	1.15

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	362/446 (81%)	341 (94%)	20 (6%)	1 (0%)	44	75
1	B	369/446 (83%)	352 (95%)	15 (4%)	2 (0%)	32	64
All	All	731/892 (82%)	693 (95%)	35 (5%)	3 (0%)	38	69

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	64	HIS
1	A	204	GLU
1	B	317	VAL

### 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	308/372 (83%)	276 (90%)	32 (10%)	8	21
1	B	312/372 (84%)	270 (86%)	42 (14%)	4	11
All	All	620/744 (83%)	546 (88%)	74 (12%)	6	16

5 of 74 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	54	LEU
1	B	115	GLN
1	B	378	LEU
1	B	57	ARG
1	B	74	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	422	GLN

### 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](#)

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 ⓘ

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, 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	370/446 (82%)	0.13	25 (6%) 18 13	16, 41, 107, 152	0
1	B	375/446 (84%)	-0.12	19 (5%) 29 23	15, 36, 78, 135	0
All	All	745/892 (83%)	0.00	44 (5%) 23 18	15, 38, 100, 152	0

The worst 5 of 44 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	204	GLU	5.8
1	A	216	PRO	5.6
1	B	60	TYR	5.1
1	B	318	THR	4.7
1	A	66	ALA	4.2

### 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](#)

There are no ligands in this entry.

### 6.5 Other polymers [i](#)

There are no such residues in this entry.