

Full wwPDB X-ray Structure Validation Report (i)

Oct 2, 2023 – 01:47 PM EDT

PDB ID : 6NSV

Title : Crystal structure of the human CHIP TPR domain in complex with a 5mer

acetylated optimized peptide

Authors: Basu, K.; Ravalin, M.; Bohn, M.-F.; Craik, C.S.; Gestwicki, J.E.

Deposited on : 2019-01-25

Resolution : 1.30 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.orgA user guide is available at

https://www.wwpdb.org/validation/2017/XrayValidationReportHelp with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at http://www.wwpdb.org/validation/2017/FAQs#types.

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

MolProbity : FAILED

Mogul : 1.8.5 (274361), CSD as541be (2020)

Xtriage (Phenix) : 1.13

EDS : FAILED

Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)

Ideal geometry (proteins) : Engh & Huber (2001) Ideal geometry (DNA, RNA) : Parkinson et al. (1996)

Validation Pipeline (wwPDB-VP) : 2.35.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: X-RAY DIFFRACTION

The reported resolution of this entry is 1.30 Å.

There are no overall percentile quality scores available for this entry.

MolProbity and EDS failed to run properly - the sequence quality summary graphics cannot be shown.



2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 4562 atoms, of which 2115 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 E3 ubiquitin-protein ligase CHIP.

Mol	Chain	Residues			Aton	ıs			ZeroOcc	AltConf	Trace
1	A	128	Total 2012	C 642		N 187	O 188	S 6	0	1	0
1	В	130	Total 2061	C 654		N 189	O 196	S 6	0	1	0

• Molecule 2 is a protein called ACE-LEU-TRP-TRP-PRO-ASP.

Mol	Chain	Residues		Ato	oms			ZeroOcc	AltConf	Trace
9	C	6	Total	С	Н	N	О	0	0	0
		0	88	39	33	7	9	U	U	0
9	D	6	Total	С	Н	N	О	0	0	0
2	ש	0	88	39	33	7	9	U	U	

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

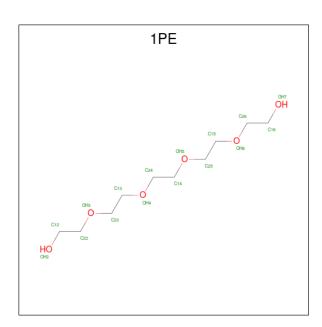
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Cl 1 1	0	0

• Molecule 4 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total Na 1 1	0	0
4	В	1	Total Na 1 1	0	0

• Molecule 5 is PENTAETHYLENE GLYCOL (three-letter code: 1PE) (formula: C₁₀H₂₂O₆).





Mol	Chain	Residues	A	A ton	ns		ZeroOcc	AltConf
5	٨	1	Total	С	Н	О	0	0
5	А	1	38	10	22	6	0	0
5	D	1	Total	С	Н	О	0	0
3	Б	1	38	10	22	6	0	U

• Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	117	Total O 117 117	0	0
6	В	108	Total O 108 108	0	0
6	С	4	Total O 4 4	0	0
6	D	5	Total O 5 5	0	0

MolProbity and EDS failed to run properly - this section is therefore empty.



3 Data and refinement statistics (i)

EDS failed to run properly - this section is therefore incomplete.

Property	Value	Source	
Space group	P 2 21 21	Depositor	
Cell constants	46.22Å 71.92Å 77.79Å	Depositor	
a, b, c, α , β , γ	90.00° 90.00° 90.00°	Depositor	
Resolution (Å)	39.73 - 1.30	Depositor	
% Data completeness	94.7 (39.73-1.30)	Depositor	
(in resolution range)	,	1	
R_{merge}	(Not available)	Depositor	
R_{sym}	(Not available)	Depositor	
$< I/\sigma(I) > 1$	1.84 (at 1.31Å)	Xtriage	
Refinement program	PHENIX (1.14_3260: ???)	Depositor	
R, R_{free}	0.214 , 0.243	Depositor	
Wilson B-factor (\mathring{A}^2)	12.3	Xtriage	
Anisotropy	0.637	Xtriage	
L-test for twinning ²	$ < L > = 0.47, < L^2> = 0.30$	Xtriage	
Estimated twinning fraction	No twinning to report.	Xtriage	
Total number of atoms	4562	wwPDB-VP	
Average B, all atoms (\mathring{A}^2)	27.0	wwPDB-VP	

Xtriage's analysis on translational NCS is as follows: The analyses of the Patterson function reveals a significant off-origin peak that is 39.60 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 3.0987e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.

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



¹Intensities estimated from amplitudes.

4 Model quality (i)

4.1 Standard geometry (i)

MolProbity failed to run properly - this section is therefore empty.

4.2 Too-close contacts (i)

MolProbity failed to run properly - this section is therefore empty.

4.3 Torsion angles (i)

4.3.1 Protein backbone (i)

MolProbity failed to run properly - this section is therefore empty.

4.3.2 Protein sidechains (i)

MolProbity failed to run properly - this section is therefore empty.

4.3.3 RNA (i)

MolProbity failed to run properly - this section is therefore empty.

4.4 Non-standard residues in protein, DNA, RNA chains (i)

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

4.5 Carbohydrates (i)

There are no monosaccharides in this entry.

4.6 Ligand geometry (i)

Of 5 ligands modelled in this entry, 3 are monoatomic - leaving 2 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	Link Bond lengths			В	ond ang	les
MIOI	туре	Chain	nes	LIIIK	Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	1PE	A	203	-	15,15,15	0.39	0	14,14,14	1.06	1 (7%)
5	1PE	В	202	-	15,15,15	0.54	0	14,14,14	0.94	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
5	1PE	A	203	-	-	8/13/13/13	-
5	1PE	В	202	-	-	9/13/13/13	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$\mathbf{Observed}(^o)$	$\operatorname{Ideal}({}^{o})$
5	A	203	1PE	OH3-C23-C13	2.49	121.62	110.39

There are no chirality outliers.

All (17) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	В	202	1PE	OH6-C15-C25-OH5
5	В	202	1PE	OH5-C14-C24-OH4
5	A	203	1PE	ОН4-С13-С23-ОН3
5	A	203	1PE	C23-C13-OH4-C24
5	A	203	1PE	OH7-C16-C26-OH6
5	A	203	1PE	C12-C22-OH3-C23
5	В	202	1PE	C16-C26-OH6-C15
5	A	203	1PE	C16-C26-OH6-C15
5	В	202	1PE	OH7-C16-C26-OH6
5	A	203	1PE	OH5-C14-C24-OH4
5	В	202	1PE	ОН4-С13-С23-ОН3
5	В	202	1PE	OH2-C12-C22-OH3
5	В	202	1PE	C14-C24-OH4-C13
5	В	202	1PE	C15-C25-OH5-C14
5	A	203	1PE	OH6-C15-C25-OH5

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Mol	Chain	Res	Type	Atoms
5	A	203	1PE	C25-C15-OH6-C26
5	В	202	1PE	C23-C13-OH4-C24

There are no ring outliers.

No monomer is involved in short contacts.

4.7 Other polymers (i)

There are no such residues in this entry.

4.8 Polymer linkage issues (i)

There are no chain breaks in this entry.



5 Fit of model and data (i)

5.1 Protein, DNA and RNA chains (i)

EDS failed to run properly - this section is therefore empty.

5.2 Non-standard residues in protein, DNA, RNA chains (i)

EDS failed to run properly - this section is therefore empty.

5.3 Carbohydrates (i)

EDS failed to run properly - this section is therefore empty.

5.4 Ligands (i)

EDS failed to run properly - this section is therefore empty.

5.5 Other polymers (i)

EDS failed to run properly - this section is therefore empty.

