



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 10, 2020 – 03:19 AM BST

PDB ID : 5OWN
Title : Structure of TgPLP1 MACPF domain
Authors : Ni, T.; Gilbert, R.J.C.
Deposited on : 2017-09-01
Resolution : 3.11 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

A user guide is available at

<https://www.wwpdb.org/validation/2017/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 : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.13.1
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) : 2.13.1

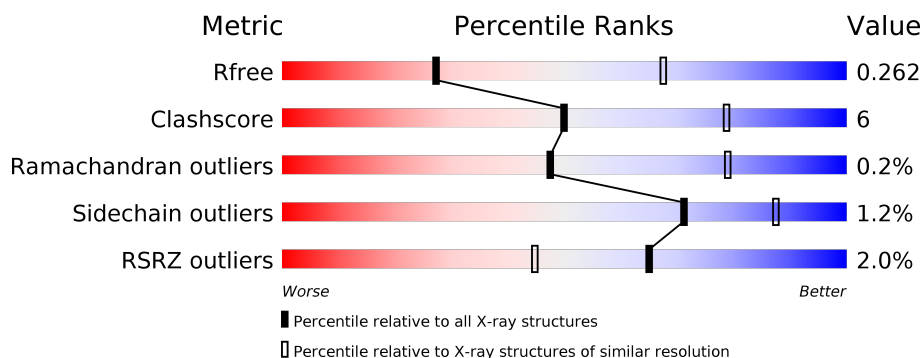
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.11 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	1292 (3.14-3.10)
Clashscore	141614	1389 (3.14-3.10)
Ramachandran outliers	138981	1337 (3.14-3.10)
Sidechain outliers	138945	1337 (3.14-3.10)
RSRZ outliers	127900	1260 (3.14-3.10)

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 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	356	<div> <div>2%</div> <div> <div></div> <div>69%</div> <div>13%</div> <div>17%</div> </div> </div>
1	B	356	<div> <div>%</div> <div> <div></div> <div>68%</div> <div>13%</div> <div>18%</div> </div> </div>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 4566 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 Perforin-like protein 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	295	Total	C	N	O	S	0	0	0
			2291	1452	392	433	14			
1	B	291	Total	C	N	O	S	0	0	0
			2261	1433	387	427	14			

There are 28 discrepancies between the modelled and reference sequences:

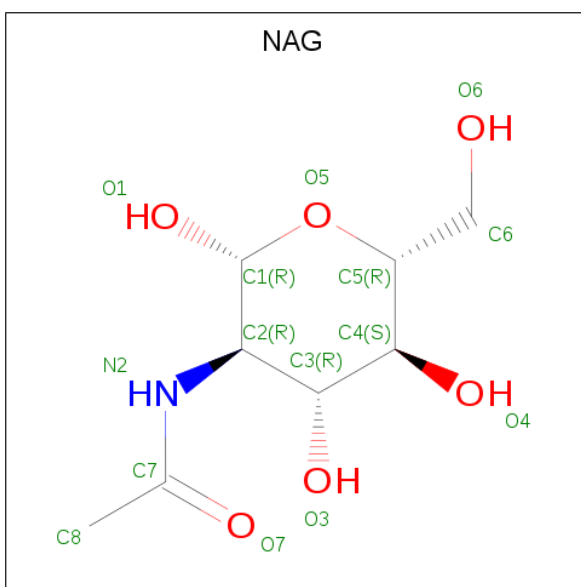
Chain	Residue	Modelled	Actual	Comment	Reference
A	459	GLU	-	expression tag	UNP G3G7T1
A	460	THR	-	expression tag	UNP G3G7T1
A	461	GLY	-	expression tag	UNP G3G7T1
A	720	GLN	ASN	conflict	UNP G3G7T1
A	744	GLN	ASN	conflict	UNP G3G7T1
A	806	GLY	-	expression tag	UNP G3G7T1
A	807	THR	-	expression tag	UNP G3G7T1
A	808	LYS	-	expression tag	UNP G3G7T1
A	809	HIS	-	expression tag	UNP G3G7T1
A	810	HIS	-	expression tag	UNP G3G7T1
A	811	HIS	-	expression tag	UNP G3G7T1
A	812	HIS	-	expression tag	UNP G3G7T1
A	813	HIS	-	expression tag	UNP G3G7T1
A	814	HIS	-	expression tag	UNP G3G7T1
B	459	GLU	-	expression tag	UNP G3G7T1
B	460	THR	-	expression tag	UNP G3G7T1
B	461	GLY	-	expression tag	UNP G3G7T1
B	720	GLN	ASN	conflict	UNP G3G7T1
B	744	GLN	ASN	conflict	UNP G3G7T1
B	806	GLY	-	expression tag	UNP G3G7T1
B	807	THR	-	expression tag	UNP G3G7T1
B	808	LYS	-	expression tag	UNP G3G7T1
B	809	HIS	-	expression tag	UNP G3G7T1
B	810	HIS	-	expression tag	UNP G3G7T1
B	811	HIS	-	expression tag	UNP G3G7T1

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Chain	Residue	Modelled	Actual	Comment	Reference
B	812	HIS	-	expression tag	UNP G3G7T1
B	813	HIS	-	expression tag	UNP G3G7T1
B	814	HIS	-	expression tag	UNP G3G7T1

- Molecule 2 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			14	8	1	5		

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.

Chain A:

69% 13% 17%

2%

GLU THR GLY THR VAL PRO A465 A471 G482 S485 D489 P490 G491 I492 R493 P494 P495 T500 T501 ALA GLN ASN ASP GLY VAL SER ASP LEU THR V514 C528 R529 Q530 S531 E532 T533 I534 L537 E546 K580 D581 T582 R583 T584 Y585 M586 L587 K588 H589 Y590 A599 G600 SER ASN HIS PHE W606 W607 V622 F623 D624 A625 A631 C632 S633 A634 E635 Q636 K637 R638 A645 C646 M650 A671 T676 V679 T680 A681 R691 Q694 K697 K701 L704 GLY GLY VAL SER GLY GLY ALA GLN GLY THR SER

Chain B:

4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	95.23 Å 206.58 Å 82.74 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	55.80 – 3.11 59.79 – 3.11	Depositor EDS
% Data completeness (in resolution range)	99.9 (55.80-3.11) 99.9 (59.79-3.11)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.47 (at 3.13 Å)	Xtriage
Refinement program	PHENIX (1.12_2829: ???)	Depositor
R, R_{free}	0.235 , 0.262 0.234 , 0.262	Depositor DCC
R_{free} test set	753 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	87.3	Xtriage
Anisotropy	0.678	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 71.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	4566	wwPDB-VP
Average B, all atoms (Å ²)	103.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.26% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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](#)

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

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	0/2341	0.45	0/3173
1	B	0.27	0/2311	0.48	1/3129 (0.0%)
All	All	0.26	0/4652	0.47	1/6302 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	527	ALA	CB-CA-C	-5.50	101.85	110.10

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	2291	0	2244	26	0
1	B	2261	0	2211	28	0
2	A	14	0	13	1	0
All	All	4566	0	4468	52	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 6.

All (52) 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:524:GLN:HE21	1:B:593:ARG:HH22	1.35	0.74
1:A:471:ALA:HA	1:A:495:PRO:HA	1.70	0.74
1:A:738:GLY:O	1:A:754:TRP:NE1	2.24	0.69
1:B:482:GLY:HA2	1:B:737:ILE:HD11	1.82	0.62
1:B:530:GLN:HA	1:B:590:TYR:O	2.00	0.60
1:B:471:ALA:HA	1:B:495:PRO:HA	1.84	0.60
1:A:482:GLY:HA2	1:A:737:ILE:HD11	1.86	0.58
1:A:494:PRO:HD3	1:B:614:ALA:HB1	1.85	0.58
1:A:631:ALA:HB1	1:A:645:ALA:HB1	1.86	0.57
1:A:588:LYS:HG2	1:A:676:THR:HG22	1.86	0.57
1:A:530:GLN:HA	1:A:590:TYR:O	2.05	0.57
1:B:479:ASN:ND2	1:B:482:GLY:O	2.38	0.57
1:B:532:GLU:HA	1:B:588:LYS:O	2.04	0.56
1:B:550:ASP:OD2	1:B:674:LYS:NZ	2.35	0.56
1:B:480:PRO:O	1:B:674:LYS:NZ	2.38	0.54
1:A:632:CYS:HB2	1:A:646:CYS:HA	1.90	0.53
1:A:681:ALA:HB2	1:A:730:VAL:HG12	1.91	0.53
1:A:676:THR:OG1	1:A:735:LEU:HB2	2.10	0.51
1:A:633:SER:H	1:A:636:GLN:HB3	1.76	0.51
1:A:635:GLU:HA	1:A:638:ARG:HG2	1.92	0.50
1:A:485:SER:HB3	1:B:498:ARG:HD2	1.92	0.50
1:A:489:ASP:HB3	1:A:492:ILE:HG12	1.92	0.50
1:A:537:LEU:HD21	1:A:546:GLU:HG3	1.93	0.50
1:B:583:ARG:HG3	1:B:683:ARG:HG2	1.94	0.50
1:A:671:ALA:HA	1:A:764:PRO:HA	1.93	0.49
1:A:798:THR:HG23	1:A:799:PRO:HD3	1.94	0.49
1:B:798:THR:HG23	1:B:799:PRO:HD3	1.93	0.49
1:B:685:GLU:O	1:B:689:MET:HG2	2.12	0.49
1:B:526:VAL:HG12	1:B:526:VAL:O	2.14	0.48
1:B:499:PHE:HA	1:B:518:LEU:HD22	1.96	0.48
1:A:599:ALA:O	1:A:606:TRP:HZ2	1.96	0.48
1:A:532:GLU:HA	1:A:588:LYS:O	2.13	0.47
1:B:540:LEU:HD23	1:B:573:PHE:HD2	1.78	0.47
1:B:623:PHE:CE2	1:B:625:ALA:HB3	2.49	0.47
1:B:534:ILE:HB	1:B:587:LEU:HD23	1.96	0.46
1:B:742:PRO:HB2	1:B:750:ALA:HB1	1.98	0.45
1:A:534:ILE:HB	1:A:587:LEU:HD13	1.98	0.45
1:B:526:VAL:HB	1:B:529:ARG:HH22	1.82	0.45
1:A:584:THR:HA	1:A:679:VAL:O	2.17	0.44
1:A:493:ARG:HB3	1:A:494:PRO:HD2	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:623:PHE:CE2	1:A:625:ALA:HB3	2.53	0.43
1:B:676:THR:OG1	1:B:735:LEU:HB2	2.18	0.43
1:A:697:LYS:O	1:A:701:LYS:HG3	2.19	0.43
1:A:622:VAL:O	1:A:650:ASN:ND2	2.50	0.43
1:B:671:ALA:HA	1:B:764:PRO:HA	2.01	0.43
2:A:901:NAG:O3	2:A:901:NAG:O7	2.28	0.43
1:B:777:PRO:O	1:B:781:GLN:HG3	2.19	0.42
1:A:490:PRO:HA	1:B:610:LEU:HD22	2.01	0.42
1:B:470:GLY:HA3	1:B:497:LEU:HB2	2.02	0.41
1:B:606:TRP:HD1	1:B:775:LEU:HD21	1.85	0.41
1:B:525:TYR:HB2	1:B:593:ARG:O	2.21	0.41
1:B:777:PRO:HB2	1:B:779:GLU:OE1	2.22	0.40

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	287/356 (81%)	277 (96%)	10 (4%)	0	100	100
1	B	281/356 (79%)	265 (94%)	15 (5%)	1 (0%)	34	68
All	All	568/712 (80%)	542 (95%)	25 (4%)	1 (0%)	47	79

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	527	ALA

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	246/296 (83%)	243 (99%)	3 (1%)	71	87
1	B	242/296 (82%)	239 (99%)	3 (1%)	71	87
All	All	488/592 (82%)	482 (99%)	6 (1%)	71	87

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	528	CYS
1	A	607	ASN
1	A	798	THR
1	B	526	VAL
1	B	528	CYS
1	B	798	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	770	GLN
1	B	524	GLN
1	B	554	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

There are no monosaccharides in this entry.

5.6 Ligand geometry

1 ligand is 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	NAG	A	901	1	14,14,15	0.51	0	17,19,21	0.45	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	NAG	A	901	1	-	4/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	901	NAG	C1-C2-N2-C7
2	A	901	NAG	O5-C5-C6-O6
2	A	901	NAG	C4-C5-C6-O6
2	A	901	NAG	C3-C2-N2-C7

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	901	NAG	1	0

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 [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, 95th 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 ²)	Q<0.9
1	A	295/356 (82%)	0.21	8 (2%) 54 31	63, 94, 160, 199	0
1	B	291/356 (81%)	0.23	4 (1%) 75 58	62, 99, 156, 180	0
All	All	586/712 (82%)	0.22	12 (2%) 65 45	62, 97, 159, 199	0

All (12) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	681	ALA	5.5
1	A	581	ASP	3.3
1	B	750	ALA	3.1
1	B	527	ALA	2.9
1	B	554	GLN	2.4
1	A	694	ILE	2.4
1	B	694	ILE	2.2
1	A	600	GLN	2.2
1	A	580	LYS	2.2
1	A	585	TYR	2.2
1	A	582	THR	2.1
1	A	691	ASN	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](#)

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. The B-factors column lists the minimum, median, 95th 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	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	NAG	A	901	14/15	0.85	0.17	134,146,153,153	0

6.5 Other polymers [i](#)

There are no such residues in this entry.