

wwPDB X-ray Structure Validation Summary Report (i)

Jan 16, 2023 – 06:08 PM JST

PDB ID : 7YK9

Title : Neutron Structure of PcyA I86D Mutant Complexed with Biliverdin at Room

Temperature

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Deposited on : 2022-07-22

Resolution : 1.90 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
A 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 (1)) were used in the production of this report:

MolProbity: 4.02b-467

Mogul : 1.8.5 (274361), CSD as 541 be (2020)

Xtriage (Phenix) : 1.13

EDS : FAILED

buster-report : 1.1.7 (2018)

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)

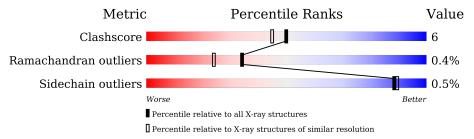
Validation Pipeline (wwPDB-VP) : 2.31.3

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 1.90 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	Similar resolution		
Wiedite	$(\# \mathrm{Entries})$	$(\# \text{Entries, resolution range}(\mathring{A}))$		
Clashscore	141614	6847 (1.90-1.90)		
Ramachandran outliers	138981	6760 (1.90-1.90)		
Sidechain outliers	138945	6760 (1.90-1.90)		

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 >=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 <=5%

Note EDS failed to run properly.

Mol	Chain	Length	Quality of chain	
1	А	248	92%	6% •



2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 5091 atoms, of which 2030 are hydrogens and 753 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.

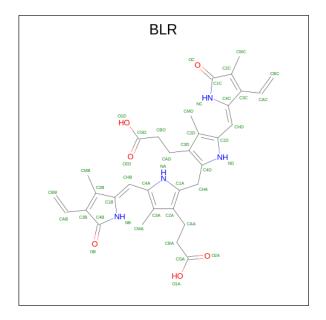
• Molecule 1 is a protein called Phycocyanobilin:ferredoxin oxidoreductase.

Mol	Chain	Residues		Atoms					ZeroOcc	AltConf	Trace	
1	Λ	243	Total	С	D	Н	N	О	S	59	210	0
1	A	240	4556	1351	449	2001	351	389	15	1 39	210	U

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	86	ASP	ILE	engineered mutation	UNP Q55891

• Molecule 2 is 3-[5-[(Z)-(4-ethenyl-3-methyl-5-oxidanylidene-pyrrol-2-ylidene)methyl]-2-[[5-[(Z)-(3-ethenyl-4-methyl-5-oxidanylidene-pyrrol-2-ylidene)methyl]-3-(3-hydroxy-3-oxopropyl) -4-methyl-1H-pyrrol-2-yl]methyl]-4-methyl-1H-pyrrol-3-yl]propanoic acid (three-letter code: BLR) (formula: $C_{33}H_{36}N_4O_6$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues		Α	ton	ns			ZeroOcc	AltConf
2	A	1	Total 76	C 33	D 4	H 29	N 4	O 6	0	0



• Molecule 3 is water.

Mo	l Chain	Residues	A	Atoms		ZeroOcc	AltConf
3	A	159	Total 459	D 300	O 159	0	1

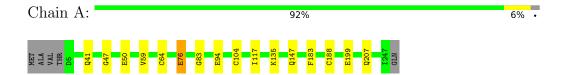


3 Residue-property plots (i)

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. 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. 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.

Note EDS failed to run properly.

• Molecule 1: Phycocyanobilin:ferredoxin oxidoreductase





4 Data and refinement statistics (i)

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

Property	Value	Source	
Space group	P 21 21 2	Depositor	
Cell constants	71.33Å 97.42Å 43.13Å	Depositor	
a, b, c, α , β , γ	90.00° 90.00° 90.00°	Depositor	
Resolution (Å)	36.91 - 1.90	Depositor	
% Data completeness	99.7 (36.91-1.90)	Depositor	
(in resolution range)	,	Depositor	
R_{merge}	(Not available)	Depositor	
R_{sym}	(Not available)	Depositor	
$< I/\sigma(I) > 1$	1.90 (at 1.89Å)	Xtriage	
Refinement program	PHENIX 1.19.2_4158	Depositor	
R, R_{free}	0.138 , 0.174	Depositor	
Wilson B-factor (Å ²)	24.7	Xtriage	
Anisotropy	0.298	Xtriage	
L-test for twinning ²	$ < L > = 0.49, < L^2> = 0.32$	Xtriage	
Estimated twinning fraction	No twinning to report.	Xtriage	
Total number of atoms	5091	wwPDB-VP	
Average B, all atoms (\mathring{A}^2)	22.0	wwPDB-VP	

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 8.10% of the height of the origin peak. No significant pseudotranslation is detected.

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.

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: BLR

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 Chair		Bo	nd lengths	Bond angles		
MIOI	Chain	RMSZ	# Z > 5	RMSZ	# Z >5	
1	A	0.79	$10/3882 \ (0.3\%)$	0.80	4/5263 (0.1%)	

The worst 5 of 10 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	\mathbf{Z}	$\operatorname{Observed}(\text{\AA})$	$Ideal(\AA)$
1	A	76[A]	GLU	CD-OE1	-5.89	1.19	1.25
1	A	76[C]	GLU	CD-OE1	-5.89	1.19	1.25
1	A	76[B]	GLU	CD-OE1	-5.89	1.19	1.25
1	A	104[A]	CYS	CB-SG	-5.12	1.73	1.81
1	A	104[B]	CYS	CB-SG	-5.12	1.73	1.81

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	\mathbf{Z}	$\mathbf{Observed}(^o)$	$\operatorname{Ideal}({}^{o})$
1	A	183[A]	PHE	CB-CG-CD2	-6.74	116.08	120.80
1	A	183[B]	PHE	CB-CG-CD2	-6.74	116.08	120.80
1	A	183[A]	PHE	CB-CG-CD1	5.78	124.84	120.80
1	A	183[B]	PHE	CB-CG-CD1	5.78	124.84	120.80

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	2555	2001	673	22	0
2	A	47	29	34	8	0
3	A	459	0	0	10	0
All	All	3061	2030	707	25	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.

The worst 5 of 25 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	$\begin{array}{c} {\rm Interatomic} \\ {\rm distance} \ ({\rm \AA}) \end{array}$	Clash overlap (Å)	
1:A:207[B]:GLN:OE1	3:A:401:HOH:O	1.80	0.99	
1:A:83[A]:GLY:O	3:A:402:HOH:O	1.92	0.87	
1:A:76[C]:GLU:OE2	3:A:403:HOH:O	2.03	0.76	
1:A:147[B]:GLN:OE1	3:A:404:HOH:O	2.17	0.61	
1:A:188[B]:CYS:SG	3:A:534:HOH:O	2.57	0.60	

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	473/248 (191%)	467 (99%)	4 (1%)	2 (0%)	34 24	

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	47[A]	GLY
1	A	47[B]	GLY



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	410/216 (190%)	408 (100%)	2 (0%)	88 89	

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	199[A]	GLU
1	A	199[B]	GLU

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)

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	В	ond leng	gths	В	ond ang	les
IVIOI	Туре		nes	Lilik	Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	BLR	A	301	-	40,46,46	4.49	15 (37%)	44,67,67	1.64	5 (11%)

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	BLR	A	301	-	-	3/24/58/58	0/4/4/4

The worst 5 of 15 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	\mathbf{Z}	$\operatorname{Observed}(\text{\AA})$	Ideal(A)
2	A	301	BLR	CHA-C4D	-22.09	1.34	1.51
2	A	301	BLR	C3D-C4D	7.93	1.51	1.39
2	A	301	BLR	C4C-NC	6.79	1.49	1.37
2	A	301	BLR	C1B-NB	5.68	1.47	1.37
2	A	301	BLR	C1C-NC	5.53	1.49	1.38

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$\mathbf{Observed}(^o)$	$\operatorname{Ideal}(^{o})$
2	A	301	BLR	CAD-C3D-C4D	-4.76	123.95	127.30
2	A	301	BLR	CAA-C2A-C1A	-4.61	124.06	127.30
2	A	301	BLR	CBA-CAA-C2A	-3.59	106.49	112.62
2	A	301	BLR	CBD-CAD-C3D	-3.52	106.61	112.62
2	A	301	BLR	CMB-C2B-C1B	-3.39	119.93	124.17

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	301	BLR	C2A-C1A-CHA-C4D
2	A	301	BLR	ND-C1D-CHD-C4C
2	A	301	BLR	C3D-C4D-CHA-C1A

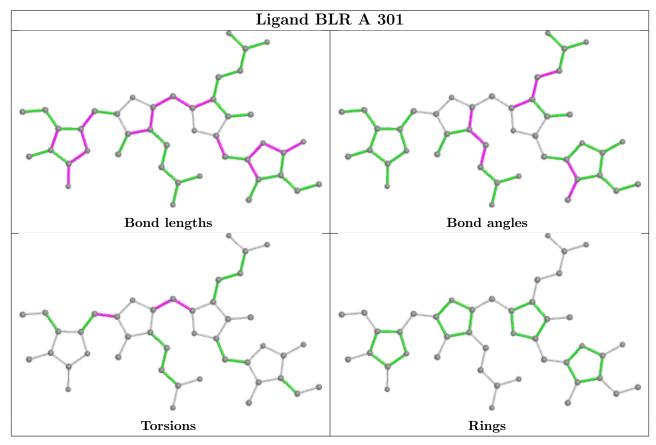
There are no ring outliers.

1 monomer is involved in 8 short contacts:



Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	301	BLR	8	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



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)

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

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

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

6.3 Carbohydrates (i)

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

6.4 Ligands (i)

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

6.5 Other polymers (i)

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

