

Full wwPDB X-ray Structure Validation Report (i)

Oct 2, 2023 – 03:33 PM EDT

PDB ID : 6NRR

Title : Crystal structure of Dpr11 IG1 bound to DIP-gamma IG+IG2

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Deposited on : 2019-01-24

Resolution : 2.50 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 (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 2.50 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 2462 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 Defective proboscis extension response 11, isoform B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	95	Total	С	N	O	S	0	0	0
_			759	481	139	137	2			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference	
A	112	SER	-	expression tag	UNP Q8MRE6	
A	113	ARG	-	expression tag	UNP Q8MRE6	
A	220	HIS	-	expression tag	UNP Q8MRE6	
A	221	HIS	-	expression tag	UNP Q8MRE6	
A	222	HIS	-	expression tag	UNP Q8MRE6	
A	223	HIS	-	expression tag	UNP Q8MRE6	
A	224	HIS	-	expression tag	UNP Q8MRE6	
A	225	HIS	-	expression tag	UNP Q8MRE6	

• Molecule 2 is a protein called Dpr-interacting protein gamma.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	В	199	Total 1553	C 963	N 289	O 288	S 13	0	1	0

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
В	33	SER	-	expression tag	UNP Q9VAR6
В	34	ARG	-	expression tag	UNP Q9VAR6
В	239	HIS	-	expression tag	UNP Q9VAR6
В	240	HIS	-	expression tag	UNP Q9VAR6
В	241	HIS	-	expression tag	UNP Q9VAR6
В	242	HIS	-	expression tag	UNP Q9VAR6
В	243	HIS	-	expression tag	UNP Q9VAR6
В	244	HIS	-	expression tag	UNP Q9VAR6

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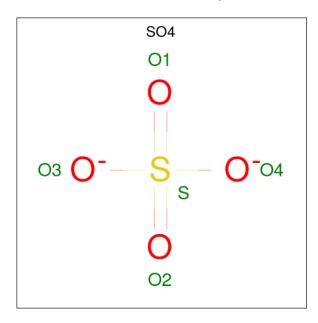
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Chain	Residue	Modelled	Actual	Comment	Reference
В	245	HIS	-	expression tag	UNP Q9VAR6

• Molecule 3 is an oligosaccharide called beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	С	4	Total 49	C 28	N 2	O 19	0	0	0

• Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total O S 5 4 1	0	0
4	A	1	Total O S 5 4 1	0	0
4	A	1	Total O S 5 4 1	0	0
4	В	1	Total O S 5 4 1	0	0

• Molecule 5 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).





Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C O 6 3 3	0	0
5	В	1	Total C O 6 3 3	0	0

• Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	22	Total O 22 22	0	0
6	В	47	Total O 47 47	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 43 21 2	Depositor
Cell constants	85.36Å 85.36Å 103.58Å	Depositor
a, b, c, α , β , γ	90.00° 90.00° 90.00°	Depositor
Resolution (Å)	44.28 - 2.50	Depositor
% Data completeness	99.7 (44.28-2.50)	Depositor
(in resolution range)	, , ,	
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	1.28 (at 2.51Å)	Xtriage
Refinement program	PHENIX dev_3374	Depositor
R, R_{free}	0.207 , 0.261	Depositor
Wilson B-factor (\mathring{A}^2)	48.3	Xtriage
Anisotropy	0.416	Xtriage
L-test for twinning ²	$ < L > = 0.48, < L^2> = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	2462	wwPDB-VP
Average B, all atoms $(Å^2)$	56.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 3.92% 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.

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)

4 monosaccharides are 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	Tuno	Chain	Res	Link	Во	ond leng	ths	Bond angles		
MIOI	Type	Chain	nes	Lilik	Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	NAG	С	1	3,2	14,14,15	0.26	0	17,19,21	0.45	0
3	NAG	С	2	3	14,14,15	0.28	0	17,19,21	0.39	0
3	BMA	С	3	3	11,11,12	0.89	0	15,15,17	0.88	0
3	FUC	С	4	3	10,10,11	0.93	0	14,14,16	1.07	2 (14%)

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
3	NAG	С	1	3,2	-	0/6/23/26	0/1/1/1
3	NAG	С	2	3	-	2/6/23/26	0/1/1/1
3	BMA	С	3	3	-	0/2/19/22	0/1/1/1
3	FUC	С	4	3	-	-	0/1/1/1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^o)$	$\operatorname{Ideal}({}^{o})$
3	С	4	FUC	O5-C5-C4	2.39	113.81	109.52
3	С	4	FUC	C1-O5-C5	2.28	117.95	112.78

There are no chirality outliers.

All (2) torsion outliers are listed below:

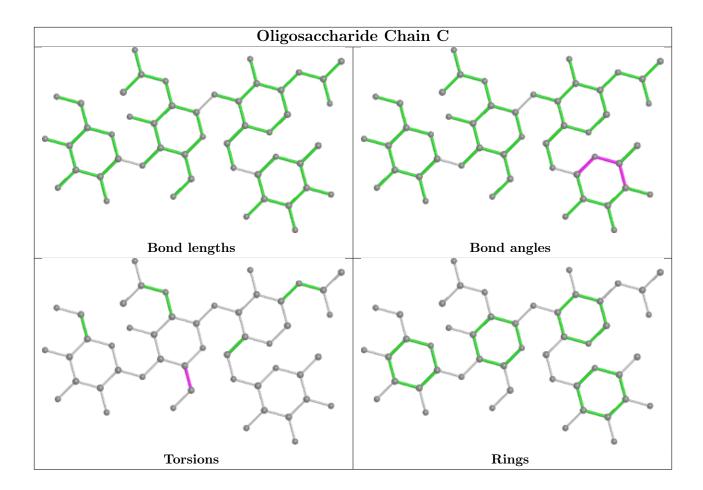
Mol	Chain	Res	Type	Atoms
3	С	2	NAG	C4-C5-C6-O6
3	С	2	NAG	O5-C5-C6-O6

There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.





4.6 Ligand geometry (i)

6 ligands are 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).

Mal	Mol Type		Dog	Res Link	Bond lengths			Bond angles						
MIOI	Type	Chain	nes	nes	nes	nes	Res	LIIIK	Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	SO4	В	905	-	4,4,4	0.14	0	6,6,6	0.15	0				
5	GOL	A	304	_	5,5,5	0.86	0	5,5,5	1.17	1 (20%)				
4	SO4	A	303	-	4,4,4	0.15	0	6,6,6	0.12	0				
4	SO4	A	301	-	4,4,4	0.14	0	6,6,6	0.13	0				
5	GOL	В	906	-	5,5,5	0.89	0	5,5,5	1.05	0				
4	SO4	A	302	_	4,4,4	0.15	0	6,6,6	0.09	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	GOL	В	906	-	-	3/4/4/4	-
5	GOL	A	304	-	-	1/4/4/4	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	\mathbf{Z}	$Observed(^o)$	$\operatorname{Ideal}({}^{o})$
5	A	304	GOL	C3-C2-C1	-2.10	103.56	111.70

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	В	906	GOL	C1-C2-C3-O3
5	В	906	GOL	O2-C2-C3-O3
5	A	304	GOL	O1-C1-C2-C3
5	В	906	GOL	O1-C1-C2-C3

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	301	SO4	0	1

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.

