



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 1, 2023 – 11:56 PM EDT

PDB ID : 6MOH
Title : Dimeric DARPin C_R3 complex with EpoR
Authors : Jude, K.M.; Mohan, K.; Garcia, K.C.
Deposited on : 2018-10-04
Resolution : 3.20 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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : **FAILED**
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtrriage (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

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.20 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 5 unique types of molecules in this entry. The entry contains 5510 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 Dimeric DARPin E2C (C_R3).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	155	1139	717	200	219	3	0	0	0
1	B	155	1127	709	198	217	3	0	0	0

- Molecule 2 is a protein called Erythropoietin receptor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	C	203	1583	1011	274	291	7	0	0	0
2	D	211	1619	1033	279	300	7	0	0	0

There are 26 discrepancies between the modelled and reference sequences:

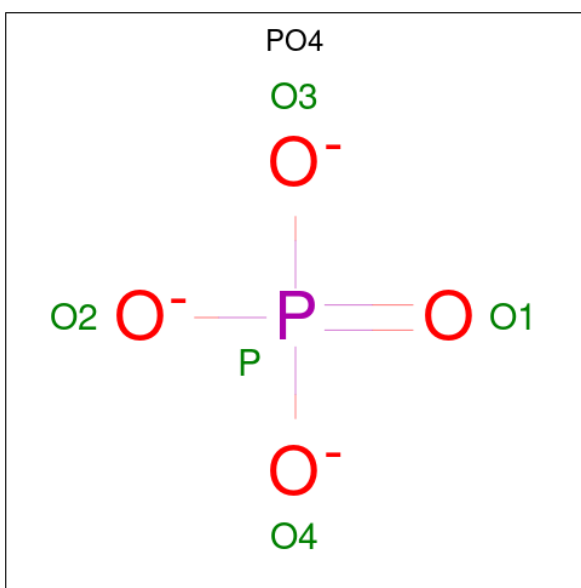
Chain	Residue	Modelled	Actual	Comment	Reference
C	3	PHE	-	expression tag	UNP P19235
C	4	ALA	-	expression tag	UNP P19235
C	5	GLY	-	expression tag	UNP P19235
C	6	SER	-	expression tag	UNP P19235
C	7	ALA	-	expression tag	UNP P19235
C	52	GLN	ASN	conflict	UNP P19235
C	164	GLN	ASN	conflict	UNP P19235
C	226	LYS	-	expression tag	UNP P19235
C	227	GLU	-	expression tag	UNP P19235
C	228	LYS	-	expression tag	UNP P19235
C	229	ALA	-	expression tag	UNP P19235
C	230	ALA	-	expression tag	UNP P19235
C	231	ALA	-	expression tag	UNP P19235
D	3	PHE	-	expression tag	UNP P19235
D	4	ALA	-	expression tag	UNP P19235
D	5	GLY	-	expression tag	UNP P19235

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Chain	Residue	Modelled	Actual	Comment	Reference
D	6	SER	-	expression tag	UNP P19235
D	7	ALA	-	expression tag	UNP P19235
D	52	GLN	ASN	conflict	UNP P19235
D	164	GLN	ASN	conflict	UNP P19235
D	226	LYS	-	expression tag	UNP P19235
D	227	GLU	-	expression tag	UNP P19235
D	228	LYS	-	expression tag	UNP P19235
D	229	ALA	-	expression tag	UNP P19235
D	230	ALA	-	expression tag	UNP P19235
D	231	ALA	-	expression tag	UNP P19235

- Molecule 3 is PHOSPHATE ION (three-letter code: PO4) (formula: O₄P).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total O P 5 4 1	0	0
3	A	1	Total O P 5 4 1	0	0
3	A	1	Total O P 5 4 1	0	0
3	B	1	Total O P 5 4 1	0	0
3	B	1	Total O P 5 4 1	0	0
3	B	1	Total O P 5 4 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	C	1	Total O P 5 4 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

- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total O 1 1	0	0
5	B	4	Total O 4 4	0	0
5	C	1	Total O 1 1	0	0

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

3 Data and refinement statistics

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

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	96.19Å 96.19Å 286.40Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	68.02 – 3.20	Depositor
% Data completeness (in resolution range)	80.0 (68.02-3.20)	Depositor
R_{merge}	0.89	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.38 (at 3.19Å)	Xtrriage
Refinement program	PHENIX (1.13_2998: ???)	Depositor
R, R_{free}	0.236 , 0.277	Depositor
Wilson B-factor (Å ²)	29.7	Xtrriage
Anisotropy	0.184	Xtrriage
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.27$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
Total number of atoms	5510	wwPDB-VP
Average B, all atoms (Å ²)	46.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.74% 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.

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 8 ligands modelled in this entry, 1 is monoatomic - leaving 7 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	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	PO4	A	203	-	4,4,4	0.91	0	6,6,6	0.43	0
3	PO4	B	201	-	4,4,4	0.91	0	6,6,6	0.44	0
3	PO4	B	203	-	4,4,4	0.91	0	6,6,6	0.44	0
3	PO4	B	202	-	4,4,4	0.92	0	6,6,6	0.42	0
3	PO4	A	201	4	4,4,4	0.91	0	6,6,6	0.44	0
3	PO4	A	202	-	4,4,4	0.91	0	6,6,6	0.43	0
3	PO4	C	301	-	4,4,4	0.92	0	6,6,6	0.44	0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

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

5.1 Protein, DNA and RNA chains

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

5.2 Non-standard residues in protein, DNA, RNA chains

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

5.3 Carbohydrates

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

5.4 Ligands

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

5.5 Other polymers

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