

Full wwPDB X-ray Structure Validation Report (i)

May 25, 2020 – 02:08 pm BST

PDB ID : 5QOM

Title: PanDDA analysis group deposition - Crystal Structure of DCP2 (NUDT20)

in complex with FMOPL000576a

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Deposited on : 2019-02-22

Resolution : 1.87 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 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 as541be (2020)

Xtriage (Phenix) : 1.13 EDS : 2.11

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)

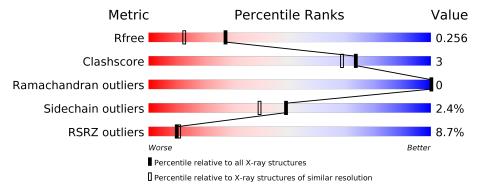
Validation Pipeline (wwPDB-VP) : 2.11

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 1.87 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	$\begin{array}{c} \text{Whole archive} \\ (\#\text{Entries}) \end{array}$	$egin{aligned} ext{Similar resolution} \ (\# ext{Entries}, ext{resolution range}(ext{Å})) \end{aligned}$
R_{free}	130704	9470 (1.90-1.86)
Clashscore	141614	10282 (1.90-1.86)
Ramachandran outliers	138981	10152 (1.90-1.86)
Sidechain outliers	138945	10152 (1.90-1.86)
RSRZ outliers	127900	9303 (1.90-1.86)

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 <=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		
			8%		
1	A	167	78%	10%	11%



2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 1317 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.

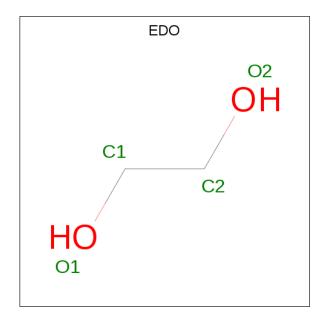
• Molecule 1 is a protein called DCP2 (NUDT20).

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace		
1	Α	149	Total	С	N	О	S	0	1	0
	11	149	1201	778	203	214	6			U

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Α	94	SER	-	expression tag	UNP Q8IU60

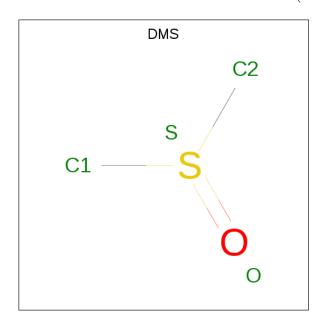
• Molecule 2 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C₂H₆O₂).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C O 4 2 2	0	0
2	A	1	Total C O 4 2 2	0	0

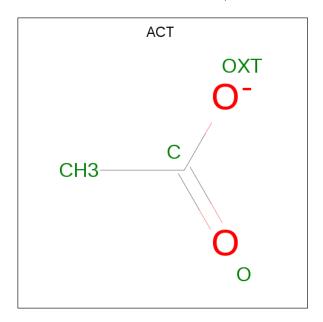


 \bullet Molecule 3 is DIMETHYL SULFOXIDE (three-letter code: DMS) (formula: $\mathrm{C_2H_6OS}).$



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf		
3	A	1	Total 4	C 2	O 1	S 1	0	0

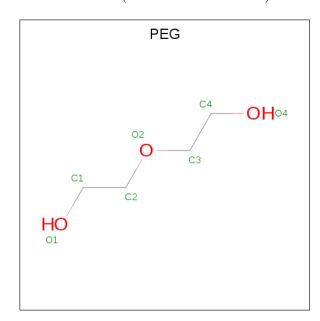
 \bullet Molecule 4 is ACETATE ION (three-letter code: ACT) (formula: $\mathrm{C_2H_3O_2}).$



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 4 2 2	0	0
4	A	1	Total C O 4 2 2	0	0

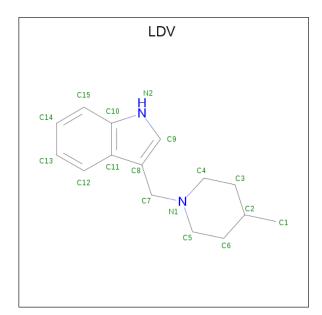


• Molecule 5 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: C₄H₁₀O₃).



Mol	Chain	Residues	Atoms		Atoms		ZeroOcc	AltConf
5	A	1	Total C 7 4	O 3	0	0		

• Molecule 6 is 3-[(4-methylpiperidin-1-yl)methyl]-1H-indole (three-letter code: LDV) (formula: $C_{15}H_{20}N_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total C N 17 15 2	0	0



• Molecule 7 is water.

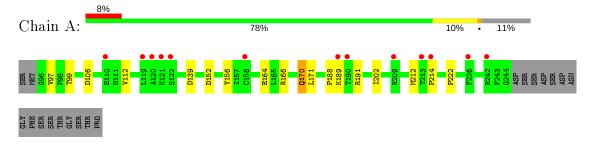
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	72	Total O 72 72	0	0



3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA 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.

• Molecule 1: DCP2 (NUDT20)





4 Data and refinement statistics (i)

Property	Value	Source	
Space group	P 21 21 21	Depositor	
Cell constants	47.92Å 61.25Å 65.57Å	Depositor	
a, b, c, α , β , γ	90.00° 90.00° 90.00°	Depositor	
Resolution (Å)	44.76 - 1.87	Depositor	
Resolution (A)	38.69 - 1.87	EDS	
% Data completeness	99.4 (44.76-1.87)	Depositor	
(in resolution range)	99.5 (38.69-1.87)	EDS	
R_{merge}	0.08	Depositor	
R_{sym}	(Not available)	Depositor	
$< I/\sigma(I) > 1$	1.54 (at 1.87Å)	Xtriage	
Refinement program	REFMAC 5.8.0189	Depositor	
D D.	0.200 , 0.252	Depositor	
R, R_{free}	0.217 , 0.256	DCC	
R_{free} test set	794 reflections (4.83%)	wwPDB-VP	
Wilson B-factor (Å ²)	35.8	Xtriage	
Anisotropy	0.170	Xtriage	
Bulk solvent $k_{sol}(e/Å^3)$, $B_{sol}(Å^2)$	0.31, 52.5	EDS	
L-test for twinning ²	$ < L >=0.49, < L^2>=0.32$	Xtriage	
Estimated twinning fraction	No twinning to report.	Xtriage	
F_o, F_c correlation	0.95	EDS	
Total number of atoms	1317	wwPDB-VP	
Average B, all atoms (Å ²)	45.0	wwPDB-VP	

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 8.11% 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: ACT, DMS, PEG, EDO, LDV

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	Boı	nd lengths	Bo	nd angles
IVIOI	Chain	RMSZ	# Z > 5	RMSZ	# Z > 5
1	A	0.95	$1/1233 \ (0.1\%)$	0.96	5/1672 (0.3%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	\mathbf{Z}	${f Observed(\AA)}$	$\operatorname{Ideal}(ext{\AA})$
1	Α	156	TYR	CB-CG	-5.62	1.43	1.51

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	\mathbf{Z}	$Observed(^o)$	$\operatorname{Ideal}({}^o)$
1	A	152	ASP	CB-CG-OD1	6.94	124.54	118.30
1	A	139	ASP	CB-CG-OD2	-5.45	113.40	118.30
1	A	139	ASP	CB-CG-OD1	5.42	123.18	118.30
1	A	166	ARG	NE-CZ-NH1	5.08	122.84	120.30
1	A	106	ASP	CB-CG-OD2	-5.03	113.78	118.30

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	1201	0	1170	7	0
2	A	8	0	12	1	0

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Continued	trom	nromanne	naae
\circ	110116	picolous	puyc

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	4	0	6	0	0
4	A	8	0	6	0	0
5	A	7	0	10	0	0
6	A	17	0	0	2	0
7	A	72	0	0	0	0
All	All	1317	0	1204	8	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 3.

All (8) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic	$\operatorname{Clash}_{\stackrel{\circ}{}}$	
7100111 1	7100H1 2	$\operatorname{distance}\left(ilde{\mathbf{A}} ight)$	overlap(A)	
1:A:99:THR:HG23	1:A:170:GLN:NE2	2.15	0.61	
1:A:188:PRO:HD2	6:A:307:LDV:C13	2.39	0.53	
1:A:97:VAL:O	1:A:170:GLN:NE2	2.48	0.46	
1:A:112:VAL:HG13	1:A:202:ILE:HD11	2.01	0.42	
1:A:164:GLU:OE2	1:A:171:LEU:HD21	2.20	0.42	
6:A:307:LDV:C9	6:A:307:LDV:C5	2.99	0.41	
1:A:222:PRO:HB2	2:A:302:EDO:H21	2.03	0.41	
1:A:212:MET:C	1:A:214:PRO:HD2	2.41	0.41	

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	Perce	$_{ m ntiles}$
1	A	148/167 (89%)	143 (97%)	5 (3%)	0	100	100

There are no Ramachandran outliers to report.



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.

Mo	ol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1		Α	124/147 (84%)	121 (98%)	3 (2%)	49 39	

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	${f Res}$	Type
1	A	170	GLN
1	A	189	LYS
1	A	191	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	170	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 (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

7 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).

Mol	Tree	Chain	Res	Link	В	ond leng	gths	Bond angles		
MIOI	Type	Chain	nes	Lilik	Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	ACT	A	304	-	1,3,3	2.30	1 (100%)	0,3,3	0.00	-
5	PEG	A	306	-	6,6,6	0.42	0	5,5,5	0.57	0
2	EDO	A	302	_	3,3,3	0.72	0	2,2,2	0.50	0
3	DMS	A	303	_	3,3,3	0.57	0	3,3,3	0.76	0
2	EDO	A	301	-	3,3,3	0.69	0	2,2,2	0.21	0
4	ACT	A	305	_	1,3,3	2.02	1 (100%)	0,3,3	0.00	_
6	LDV	A	307	-	18,19,19	0.89	1 (5%)	21,26,26	0.93	1 (4%)

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	EDO	A	301	_	-	1/1/1/1	-
2	EDO	A	302	_	-	1/1/1/1	-
6	LDV	A	307	_	-	0/3/14/14	0/3/3/3
5	PEG	A	306	_	-	1/4/4/4	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	\mathbf{Z}	${f Observed(\AA)}$	$\mathbf{Ideal}(\mathbf{\AA})$
6	A	307	LDV	C7-N1	2.39	1.52	1.47
4	A	304	ACT	СН3-С	2.30	1.51	1.48
4	A	305	ACT	СН3-С	2.02	1.51	1.48

All (1) bond angle outliers are listed below:

\mathbf{Mol}	Chain	\mathbf{Res}	Type	Atoms	\mathbf{Z}	$\mathbf{Observed}(^{o})$	$ \ \mathbf{Ideal}(^o) $
6	A	307	LDV	C14-C15-C10	-2.02	117.18	120.08

There are no chirality outliers.

All (3) torsion outliers are listed below:



Mol	Chain	Res	Type	Atoms
2	A	302	EDO	O1-C1-C2-O2
2	A	301	EDO	O1-C1-C2-O2
5	A	306	PEG	C4-C3-O2-C2

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	302	EDO	1	0
6	A	307	LDV	2	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, 95^{th} 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	$\langle { m RSRZ} \rangle$	$\#\mathrm{RSRZ}{>}2$		$OWAB(Å^2)$	Q < 0.9
1	A	149/167~(89%)	0.24	13 (8%)	10 11	26, 41, 70, 91	12 (8%)

All (13) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	158[A]	CYS	8.4
1	A	226	PHE	8.1
1	A	120	ALA	5.7
1	A	119	LEU	5.4
1	A	209	ARG	4.8
1	A	213	THR	4.6
1	A	122	SER	4.5
1	A	110	GLU	4.0
1	A	121	LYS	3.9
1	A	214	PRO	2.9
1	A	242	ARG	2.7
1	A	190	THR	2.5
1	A	189	LYS	2.5

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 carbohydrates 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, 95^{th} 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	$\mathbf{B} ext{-}\mathbf{factors}(\mathbf{\mathring{A}}^2)$	Q < 0.9
2	EDO	A	301	4/4	0.66	0.17	65,65,67,69	0
6	LDV	A	307	17/17	0.77	0.22	50,55,68,68	17
5	PEG	A	306	7/7	0.83	0.17	72,80,114,119	0
2	EDO	A	302	4/4	0.88	0.27	64,65,69,73	0
4	ACT	A	304	4/4	0.89	0.30	62,67,70,74	0
4	ACT	A	305	4/4	0.95	0.12	53,66,66,77	0
3	DMS	A	303	4/4	0.98	0.09	68,71,77,80	0

6.5 Other polymers (i)

There are no such residues in this entry.

