

# Full wwPDB X-ray Structure Validation Report (i)

#### Aug 21, 2020 – 02:03 PM BST

PDB ID	:	5Q1K
Title	:	PanDDA analysis group deposition – Crystal Structure of DCLRE1A in com-
		plex with FMOPL000074a
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		Tallon, R.; Krojer, T.; von Delft, F.; Arrowsmith, C.H.; Edwards, A.; Bountra,
		C.; Gileadi, O.
Deposited on	:	2017-05-15
$\operatorname{Resolution}$	:	1.42  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:

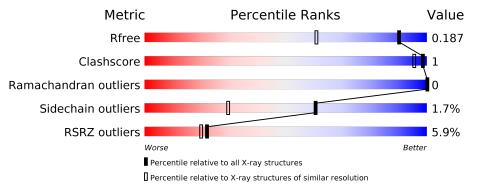
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
$\mathbf{X}$ triage (Phenix)	:	1.13
$\mathrm{EDS}$	:	2.13.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
$\operatorname{CCP4}$	:	$7.0.044 (\mathrm{Gargrove})$
Ideal geometry (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 (i)

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

The reported resolution of this entry is 1.42 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	$egin{array}{c} { m Whole \ archive} \ (\#{ m Entries}) \end{array}$	${f Similar\ resolution}\ (\#{ m Entries},{ m resolution\ range}({ m \AA}))$
$R_{free}$	130704	2579(1.44-1.40)
Clashscore	141614	2696 (1.44-1.40)
Ramachandran outliers	138981	2632(1.44-1.40)
Sidechain outliers	138945	2631(1.44-1.40)
RSRZ outliers	127900	2528 (1.44-1.40)

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
1	Λ	242	6%
1	A	545	97% ••



#### 5Q1K

## 2 Entry composition (i)

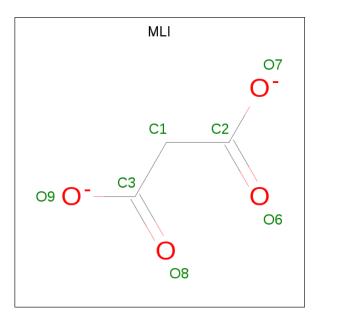
There are 5 unique types of molecules in this entry. The entry contains 3143 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 DNA cross-link repair 1A protein.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace		
1	А	341	Total 2806	C 1815	N 462	O 508	S 21	0	14	0

• Molecule 2 is MALONATE ION (three-letter code: MLI) (formula:  $C_3H_2O_4$ ).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	А	1	Total C 7 3	0 4	0	0

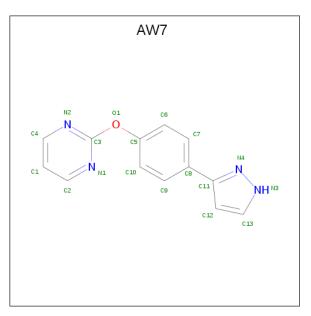
• Molecule 3 is NICKEL (II) ION (three-letter code: NI) (formula: Ni).

[	Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
	3	А	1	Total Ni 1 1	0	0

• Molecule 4 is 2-[4-(1 {H}-pyrazol-3-yl)phenoxy]pyrimidine (three-letter code: AW7)



(formula:  $C_{13}H_{10}N_4O$ ).



[	Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
	4	А	1	Total 18	C 13	N 4	0 1	0	1

• Molecule 5 is water.

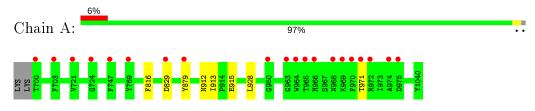
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	А	311	Total O 311 311	0	3



## 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 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: DNA cross-link repair 1A protein





## 4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants	52.05Å $57.22$ Å $115.26$ Å	Depositor
a, b, c, $\alpha$ , $\beta$ , $\gamma$	$90.00^{\circ}$ $90.00^{\circ}$ $90.00^{\circ}$	Depositor
Resolution (Å)	52.05 - 1.42	Depositor
Resolution (A)	51.25 - 1.42	EDS
% Data completeness	99.1 (52.05-1.42)	Depositor
(in resolution range)	99.1 (51.25-1.42)	EDS
R <sub>merge</sub>	0.07	Depositor
R <sub>sym</sub>	(Not available)	Depositor
$< I/\sigma(I) > 1$	$1.47 (at 1.42 \text{\AA})$	Xtriage
Refinement program	REFMAC 5.8.0155	Depositor
D D.	0.153 , $0.187$	Depositor
$R, R_{free}$	0.154 , $0.187$	DCC
$R_{free}$ test set	3150 reflections $(4.83%)$	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	18.1	Xtriage
Anisotropy	0.148	Xtriage
Bulk solvent $k_{sol}(e/Å^3), B_{sol}(Å^2)$	0.32 , $44.8$	EDS
L-test for twinning <sup>2</sup>	$ \langle L  \rangle = 0.49, \langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	3143	wwPDB-VP
Average B, all atoms $(Å^2)$	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 5.57% of the height of the origin peak. No significant pseudotranslation is detected.

<sup>&</sup>lt;sup>2</sup>Theoretical 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.



<sup>&</sup>lt;sup>1</sup>Intensities 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: AW7, NI, MLI  $\,$ 

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		
	Chain	RMSZ	# Z  > 5	RMSZ	# Z  > 5	
1	А	0.56	0/2883	0.65	0/3920	

There are no bond length outliers.

There are no bond angle outliers.

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	А	2806	0	2758	3	0
2	А	7	0	2	0	0
3	А	1	0	0	0	0
4	А	18	0	0	1	0
5	А	311	0	0	2	1
All	All	3143	0	2760	3	1

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 1.

All (3) 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:A:915[D]:GLU:OE2	4:A:1103[D]:AW7:C10	2.37	0.72
1:A:912[D]:ASN:HA	5:A:1201:HOH:O	2.18	0.43
1:A:913[D]:ILE:HG22	5:A:1281:HOH:O	2.19	0.42

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:1207:HOH:O	5:A:1396:HOH:O[3_555]	2.03	0.17

### 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	Percentil	es
1	А	353/343~(103%)	344~(98%)	9~(2%)	0	100 100	0

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.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	А	310/305~(102%)	305~(98%)	5(2%)	62 32	

All (5) residues with a non-rotameric sidechain are listed below:



Mol	Chain	Res	Type
1	А	816	PHE
1	А	829	ASP
1	А	879	TYR
1	А	928	LEU
1	А	971	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	А	851	GLN
1	А	869	ASN
1	А	943	GLN
1	А	979	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 monosaccharides in this entry.

## 5.6 Ligand geometry (i)

Of 3 ligands modelled in this entry, 1 is monoatomic - leaving 2 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	$\mathbf{Res}$	Link	Bo	ond leng	$\mathbf{ths}$	В	ond ang	les
	Type	Cham	nes		Counts	RMSZ	# Z >2	Counts	RMSZ	# Z  > 2
2	MLI	А	1101	3	$0,\!6,\!6$	0.00	-	$0,\!7,\!7$	0.00	-



Mol	Type	Chain	Res	Link	Bo	ond leng	ths	В	ond ang	les
IVI0I	туре	Unam	nes	LINK	Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z >2
4	AW7	А	1103[D]	-	20,20,20	0.46	0	24,26,26	0.98	2 (8%)

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	$\mathbf{Res}$	Link	Chirals	Torsions	Rings
2	MLI	А	1101	3	-	0/0/4/4	-
4	AW7	А	1103[D]	-	-	2/8/8/8	0/3/3/3

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
4	А	1103[D]	AW7	C3-O1-C5	2.36	124.85	118.78
4	А	1103[D]	AW7	O1-C3-N1	2.04	122.21	115.82

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	$\operatorname{Res}$	Type	Atoms
4	А	1103[D]	AW7	C10-C5-O1-C3
4	А	1103[D]	AW7	C6-C5-O1-C3

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	А	1103[D]	AW7	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, 95<sup>th</sup> 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	А	341/343~(99%)	0.11	20 (5%) 22 20	11, 24, 45, 111	0

All (20) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	А	970	PHE	7.8
1	А	971	THR	7.2
1	А	969	LYS	6.2
1	А	966	HIS	5.4
1	А	964	TRP	5.2
1	А	950	GLY	4.9
1	А	968	ASN	4.8
1	А	965	THR	4.5
1	А	963	GLY	4.4
1	А	703	PHE	4.1
1	А	721	VAL	3.6
1	А	974	ALA	3.5
1	А	700	THR	3.4
1	А	879	TYR	3.2
1	А	972	ARG	2.9
1	А	975	ASP	2.6
1	А	829	ASP	2.5
1	А	724	GLY	2.3
1	А	769	TYR	2.2
1	А	747	PHE	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,  $95^{th}$  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	$\mathbf{RSR}$	$\mathbf{B} ext{-factors}(\mathrm{\AA}^2)$	Q<0.9
4	AW7	А	1103[D]	18/18	0.77	0.26	24,29,40,41	18
2	MLI	А	1101	7/7	0.98	0.08	16, 18, 21, 27	0
3	NI	А	1102	1/1	1.00	0.04	14,14,14,14	0

## 6.5 Other polymers (i)

There are no such residues in this entry.

