



Full wwPDB X-ray Structure Validation Report ⓘ

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PDB ID : 5Q4C / pdb_00005q4c
Title : PanDDA analysis group deposition – Crystal Structure of DCLRE1A after initial refinement with no ligand modelled (structure 77)
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Deposited on : 2017-05-25
Resolution : 2.73 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	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

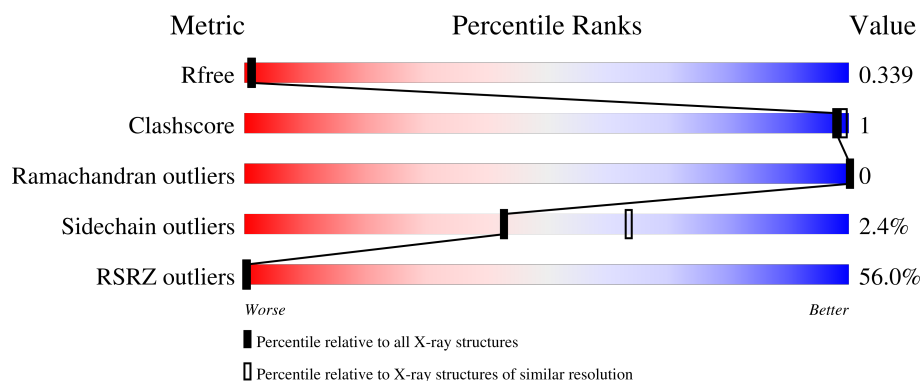
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.73 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 (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1819 (2.76-2.72)
Clashscore	190562	1866 (2.76-2.72)
Ramachandran outliers	187476	1830 (2.76-2.72)
Sidechain outliers	187428	1831 (2.76-2.72)
RSRZ outliers	180081	1819 (2.76-2.72)

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 $\leq 5\%$. 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	A	343	56% 96% ..

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 3044 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 DCLRE1A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	341	2726	1765	450	491	20	0	4	0

- Molecule 2 is MALONATE ION (CCD ID: MLI) (formula: $C_3H_2O_4$).



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

- Molecule 3 is NICKEL (II) ION (CCD ID: NI) (formula: Ni).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Ni	0	0
			1	1		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	310	Total 310	O 310	0	0

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	52.08Å 57.53Å 116.24Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	52.07 – 2.73 52.07 – 2.73	Depositor EDS
% Data completeness (in resolution range)	99.9 (52.07-2.73) 99.9 (52.07-2.73)	Depositor EDS
R_{merge}	1.15	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.34 (at 2.73Å)	Xtriage
Refinement program	REFMAC 5.8.0155	Depositor
R, R_{free}	0.271 , 0.338 0.275 , 0.339	Depositor DCC
R_{free} test set	484 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å ²)	34.7	Xtriage
Anisotropy	0.121	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 53.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.74	EDS
Total number of atoms	3044	wwPDB-VP
Average B, all atoms (Å ²)	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.00% 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.

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: 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	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.72	0/2802	0.88	1/3809 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	830	GLN	N-CA-C	5.86	116.28	108.38

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	2726	0	2676	4	0
2	A	7	0	2	0	0
3	A	1	0	0	0	0
4	A	310	0	0	3	0
All	All	3044	0	2678	4	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 1.

All (4) 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:909:GLN:NE2	4:A:1201:HOH:O	2.12	0.80
1:A:876[B]:CYS:SG	4:A:1203:HOH:O	2.56	0.59
1:A:843:SER:OG	1:A:845:GLU:OE1	2.33	0.45
1:A:851:GLN:NE2	4:A:1217:HOH:O	2.52	0.43

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	343/343 (100%)	331 (96%)	12 (4%)	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.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	299/305 (98%)	292 (98%)	7 (2%)	44	65

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	816	PHE

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Mol	Chain	Res	Type
1	A	829	ASP
1	A	830	GLN
1	A	879	TYR
1	A	928	LEU
1	A	957	LEU
1	A	1029	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	768	GLN
1	A	869	ASN
1	A	909	GLN
1	A	943	GLN
1	A	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 2 ligands modelled in this entry, 1 is monoatomic - leaving 1 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
2	MLI	A	1101	3	6,6,6	1.09	0	7,7,7	1.17	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
2	MLI	A	1101	3	-	4/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1101	MLI	C3-C1-C2-O6
2	A	1101	MLI	C3-C1-C2-O7
2	A	1101	MLI	C2-C1-C3-O9
2	A	1101	MLI	C2-C1-C3-O8

There are no ring outliers.

No monomer is involved in short contacts.

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 ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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, 95th 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	A	341/343 (99%)	2.35	191 (56%) 0 0	10, 31, 61, 117	4 (1%)

All (191) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	968	ASN	8.2
1	A	970	PHE	7.9
1	A	971	THR	7.8
1	A	962	THR	6.7
1	A	967	SER	6.5
1	A	964	TRP	6.3
1	A	966	HIS	6.1
1	A	829	ASP	5.8
1	A	879	TYR	5.4
1	A	973	ILE	5.3
1	A	972	ARG	5.3
1	A	768	GLN	5.1
1	A	703	PHE	5.0
1	A	919	LEU	5.0
1	A	965	THR	4.9
1	A	982	GLY	4.9
1	A	960	ARG	4.8
1	A	958	ALA	4.8
1	A	875	VAL	4.8
1	A	969	LYS	4.8
1	A	725	CYS	4.7
1	A	764[A]	HIS	4.6
1	A	767	GLU	4.6
1	A	981	LYS	4.5
1	A	950	GLY	4.5
1	A	745	PHE	4.5
1	A	986	ILE	4.5

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Mol	Chain	Res	Type	RSRZ
1	A	947	LYS	4.5
1	A	963	GLY	4.5
1	A	708	PRO	4.4
1	A	872	ALA	4.3
1	A	769	TYR	4.3
1	A	917	ASN	4.2
1	A	748	PRO	4.2
1	A	880	SER	4.1
1	A	949	CYS	4.1
1	A	915	GLU	4.1
1	A	700	THR	4.1
1	A	856	ARG	4.0
1	A	1023	SER	4.0
1	A	825	SER	4.0
1	A	977	ILE	4.0
1	A	847	THR	3.9
1	A	710	THR	3.9
1	A	1040	TYR	3.8
1	A	702	PRO	3.8
1	A	724	GLY	3.8
1	A	927	SER	3.8
1	A	961	PRO	3.8
1	A	744	HIS	3.7
1	A	948	LYS	3.7
1	A	891	ALA	3.6
1	A	707	ILE	3.6
1	A	784	VAL	3.6
1	A	926	SER	3.6
1	A	935	MET	3.5
1	A	959	PHE	3.5
1	A	1032	ARG	3.5
1	A	738	TYR	3.5
1	A	980	THR	3.5
1	A	763	LEU	3.4
1	A	866	VAL	3.4
1	A	846	TYR	3.4
1	A	848	PHE	3.4
1	A	937	ILE	3.4
1	A	862	ALA	3.4
1	A	902	GLN	3.3
1	A	800	ILE	3.3
1	A	804	LEU	3.3

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Mol	Chain	Res	Type	RSRZ
1	A	720	GLY	3.3
1	A	746	THR	3.2
1	A	974	ALA	3.2
1	A	1028[A]	GLU	3.2
1	A	894	LEU	3.2
1	A	852	GLN	3.2
1	A	987	TYR	3.1
1	A	806	ASN	3.0
1	A	1012	ILE	3.0
1	A	976	VAL	3.0
1	A	913	ILE	3.0
1	A	828	ALA	3.0
1	A	863	PHE	3.0
1	A	916	ILE	3.0
1	A	942	LEU	2.9
1	A	834	MET	2.9
1	A	704	TYR	2.9
1	A	754	ILE	2.9
1	A	895	GLY	2.9
1	A	991	TYR	2.9
1	A	983	ASN	2.8
1	A	743	LYS	2.8
1	A	925	CYS	2.8
1	A	723	GLU	2.8
1	A	1039	GLY	2.8
1	A	824	ARG	2.8
1	A	770	ILE	2.8
1	A	954	ASN	2.8
1	A	854	VAL	2.8
1	A	760	LYS	2.8
1	A	782	ASN	2.8
1	A	946	LEU	2.8
1	A	1024	ARG	2.8
1	A	952	LYS	2.7
1	A	953	TYR	2.7
1	A	1036	LEU	2.7
1	A	821	SER	2.7
1	A	1015	THR	2.7
1	A	945	HIS	2.7
1	A	809	VAL	2.7
1	A	721	VAL	2.7
1	A	929	VAL	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	869	ASN	2.6
1	A	914	PRO	2.6
1	A	701	CYS	2.6
1	A	881	ILE	2.6
1	A	857	PHE	2.6
1	A	990	PRO	2.6
1	A	985	SER	2.6
1	A	905	TYR	2.6
1	A	845	GLU	2.6
1	A	709	GLY	2.6
1	A	774	PRO	2.6
1	A	870	PRO	2.6
1	A	920	ILE	2.5
1	A	867	THR	2.5
1	A	864	GLU	2.5
1	A	749	VAL	2.5
1	A	912	ASN	2.5
1	A	730	LEU	2.5
1	A	788	LEU	2.5
1	A	812	HIS	2.5
1	A	711	GLY	2.5
1	A	855	ILE	2.5
1	A	797	ALA	2.5
1	A	1022	LYS	2.4
1	A	944	SER	2.4
1	A	1037	GLU	2.4
1	A	718	GLN	2.4
1	A	719	TYR	2.4
1	A	893	VAL	2.4
1	A	997	TYR	2.4
1	A	753	GLU	2.4
1	A	910	CYS	2.4
1	A	1020	THR	2.4
1	A	717	PHE	2.4
1	A	741	LEU	2.3
1	A	975	ASP	2.3
1	A	827	LEU	2.3
1	A	873	LEU	2.3
1	A	808	THR	2.3
1	A	853	GLU	2.3
1	A	957	LEU	2.3
1	A	871	HIS	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	752	SER	2.3
1	A	956	ILE	2.3
1	A	909	GLN	2.3
1	A	1019	GLY	2.3
1	A	932	LEU	2.3
1	A	939	PHE	2.3
1	A	833	HIS	2.2
1	A	830	GLN	2.2
1	A	908	LEU	2.2
1	A	780	ILE	2.2
1	A	831	LYS	2.2
1	A	1031	PHE	2.2
1	A	930	HIS	2.2
1	A	722	VAL	2.2
1	A	874	VAL	2.2
1	A	1006	TRP	2.2
1	A	943	GLN	2.2
1	A	765	VAL	2.2
1	A	766	GLN	2.2
1	A	706	LYS	2.2
1	A	761	ASN	2.1
1	A	826	LEU	2.1
1	A	726	THR	2.1
1	A	810	ILE	2.1
1	A	901	SER	2.1
1	A	882	GLY	2.1
1	A	739	ALA	2.1
1	A	911	LEU	2.1
1	A	998	LEU	2.1
1	A	1000	MET	2.0
1	A	773	LEU	2.0
1	A	888	LEU	2.0
1	A	859	ILE	2.0
1	A	984	ILE	2.0
1	A	832	VAL	2.0
1	A	868	LEU	2.0
1	A	928	LEU	2.0
1	A	1004	VAL	2.0

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

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no oligosaccharides 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, 95th 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	B-factors($\text{\AA}^2$)	Q<0.9
2	MLI	A	1101	7/7	0.88	0.12	22,23,23,26	0
3	NI	A	1102	1/1	0.98	0.04	14,14,14,14	0

6.5 Other polymers [i](#)

There are no such residues in this entry.