



Full wwPDB X-ray Structure Validation Report ⓘ

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PDB ID : 5Q8E / pdb_00005q8e
Title : PanDDA analysis group deposition – Crystal Structure of DCLRE1A after initial refinement with no ligand modelled (structure 223)
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Deposited on : 2017-05-25
Resolution : 1.63 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

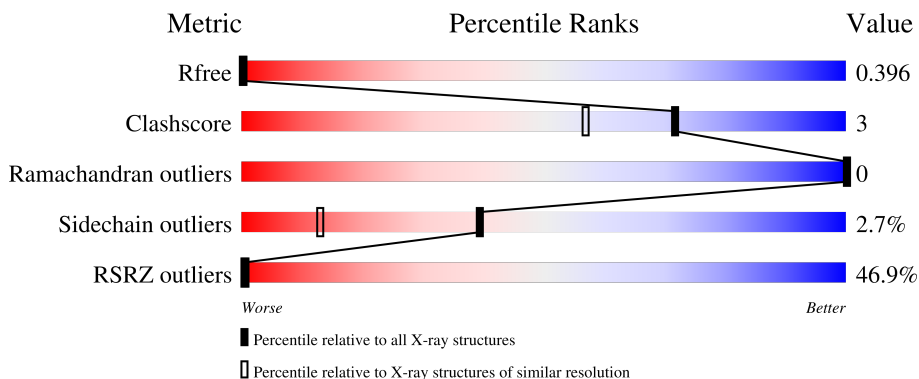
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.63 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	1141 (1.64-1.64)
Clashscore	190562	1171 (1.64-1.64)
Ramachandran outliers	187476	1151 (1.64-1.64)
Sidechain outliers	187428	1150 (1.64-1.64)
RSRZ outliers	180081	1141 (1.64-1.64)

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	47% 91% 8% ..

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	51.80Å 57.89Å 114.51Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	28.63 – 1.63 28.63 – 1.63	Depositor EDS
% Data completeness (in resolution range)	99.9 (28.63-1.63) 99.9 (28.63-1.63)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.46 (at 1.63Å)	Xtriage
Refinement program	REFMAC 5.8.0155	Depositor
R, R_{free}	0.312 , 0.374 0.332 , 0.396	Depositor DCC
R_{free} test set	2117 reflections (4.83%)	wwPDB-VP
Wilson B-factor (Å ²)	23.4	Xtriage
Anisotropy	0.482	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 38.8	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	0.91	EDS
Total number of atoms	3044	wwPDB-VP
Average B, all atoms (Å ²)	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.17% 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: MLI, NI

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	0.88	0/2802	0.99	2/3809 (0.1%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	830	GLN	N-CA-C	6.10	117.50	108.60
1	A	913	ILE	N-CA-C	-5.25	104.12	108.63

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	18	0
2	A	7	0	2	0	0
3	A	1	0	0	0	0
4	A	310	0	0	11	1
All	All	3044	0	2678	18	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 3.

All (18) 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:1202:HOH:O	2.11	0.84
1:A:867:THR:O	4:A:1201:HOH:O	2.08	0.70
1:A:1032:ARG:NE	4:A:1216:HOH:O	2.44	0.50
1:A:743:LYS:HG3	1:A:744:HIS:CE1	2.46	0.50
1:A:875:VAL:HG23	1:A:956:ILE:HG23	1.95	0.48
1:A:1032:ARG:CZ	4:A:1216:HOH:O	2.62	0.48
1:A:871:HIS:CE1	4:A:1338:HOH:O	2.66	0.47
1:A:851:GLN:NE2	4:A:1223:HOH:O	2.47	0.47
1:A:760:LYS:O	1:A:764[A]:HIS:HA	2.15	0.46
1:A:983:ASN:ND2	4:A:1219:HOH:O	2.45	0.45
1:A:1029:LYS:NZ	4:A:1207:HOH:O	2.37	0.44
1:A:973:ILE:N	4:A:1227:HOH:O	2.50	0.44
1:A:924:MET:N	4:A:1218:HOH:O	2.45	0.44
1:A:973:ILE:HG22	4:A:1227:HOH:O	2.17	0.44
1:A:717:PHE:CE1	1:A:728:TYR:HB3	2.54	0.43
1:A:859:ILE:HD11	1:A:889:ALA:HB1	2.00	0.42
1:A:874:VAL:HG11	1:A:890:ILE:HG21	2.03	0.41
1:A:856:ARG:HA	1:A:856:ARG:HE	1.86	0.40

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)
4:A:1376:HOH:O	4:A:1420:HOH:O[3_545]	2.17	0.03

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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%)	327 (95%)	16 (5%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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%)	291 (97%)	8 (3%)	39	13

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	816	PHE
1	A	829	ASP
1	A	830	GLN
1	A	879	TYR
1	A	893	VAL
1	A	928	LEU
1	A	975	ASP
1	A	1029	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	744	HIS
1	A	766	GLN
1	A	768	GLN
1	A	851	GLN
1	A	909	GLN
1	A	943	GLN
1	A	966	HIS
1	A	979	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

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	1.29	0	7,7,7	1.02	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-O8
2	A	1101	MLI	C2-C1-C3-O9

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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%)	2.59	160 (46%) 0 1	15, 39, 105, 153	4 (1%)

All (160) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	984	ILE	11.6
1	A	745	PHE	10.9
1	A	987	TYR	9.5
1	A	977	ILE	9.2
1	A	973	ILE	9.1
1	A	937	ILE	8.8
1	A	939	PHE	8.7
1	A	956	ILE	8.7
1	A	765	VAL	8.6
1	A	970	PHE	8.5
1	A	986	ILE	8.3
1	A	982	GLY	8.2
1	A	942	LEU	8.0
1	A	976	VAL	7.9
1	A	980	THR	7.8
1	A	866	VAL	7.5
1	A	974	ALA	7.3
1	A	747	PHE	7.3
1	A	781	VAL	7.2
1	A	770	ILE	7.0
1	A	865	ALA	6.9
1	A	711	GLY	6.9
1	A	769	TYR	6.9
1	A	966	HIS	6.8
1	A	971	THR	6.7
1	A	985	SER	6.7
1	A	946	LEU	6.5

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Mol	Chain	Res	Type	RSRZ
1	A	722	VAL	6.5
1	A	750	TYR	6.4
1	A	744	HIS	6.4
1	A	862	ALA	6.4
1	A	954	ASN	6.3
1	A	978	PRO	6.3
1	A	951	GLY	6.3
1	A	868	LEU	6.1
1	A	941	GLY	6.0
1	A	741	LEU	6.0
1	A	967	SER	5.9
1	A	928	LEU	5.9
1	A	988	GLY	5.9
1	A	780	ILE	5.7
1	A	961	PRO	5.6
1	A	968	ASN	5.6
1	A	964	TRP	5.6
1	A	957	LEU	5.6
1	A	959	PHE	5.4
1	A	981	LYS	5.4
1	A	759	LEU	5.3
1	A	768	GLN	5.1
1	A	746	THR	5.1
1	A	983	ASN	5.0
1	A	953	TYR	5.0
1	A	742	SER	4.9
1	A	979	GLN	4.9
1	A	763	LEU	4.9
1	A	972	ARG	4.9
1	A	739	ALA	4.9
1	A	873	LEU	4.9
1	A	748	PRO	4.8
1	A	721	VAL	4.8
1	A	784	VAL	4.8
1	A	950	GLY	4.6
1	A	779	CYS	4.6
1	A	963	GLY	4.4
1	A	932	LEU	4.4
1	A	989	ILE	4.4
1	A	879	TYR	4.4
1	A	764[A]	HIS	4.4
1	A	861	THR	4.4

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Mol	Chain	Res	Type	RSRZ
1	A	955	GLN	4.3
1	A	867	THR	4.3
1	A	740	GLY	4.2
1	A	772	PRO	4.2
1	A	938	ASN	4.2
1	A	828	ALA	4.1
1	A	940	LYS	4.1
1	A	724	GLY	4.0
1	A	857	PHE	4.0
1	A	743	LYS	4.0
1	A	863	PHE	4.0
1	A	709	GLY	4.0
1	A	773	LEU	4.0
1	A	935	MET	4.0
1	A	960	ARG	3.9
1	A	943	GLN	3.9
1	A	717	PHE	3.9
1	A	847	THR	3.8
1	A	771	HIS	3.8
1	A	782	ASN	3.8
1	A	749	VAL	3.7
1	A	875	VAL	3.7
1	A	766	GLN	3.7
1	A	726	THR	3.7
1	A	965	THR	3.7
1	A	874	VAL	3.7
1	A	871	HIS	3.7
1	A	894	LEU	3.6
1	A	962	THR	3.6
1	A	969	LYS	3.5
1	A	860	ASN	3.5
1	A	856	ARG	3.4
1	A	945	HIS	3.4
1	A	936	GLN	3.4
1	A	975	ASP	3.4
1	A	712	PHE	3.3
1	A	767	GLU	3.3
1	A	958	ALA	3.3
1	A	848	PHE	3.3
1	A	775	LEU	3.2
1	A	826	LEU	3.2
1	A	927	SER	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	893	VAL	3.2
1	A	719	TYR	3.1
1	A	870	PRO	3.1
1	A	700	THR	3.1
1	A	804	LEU	3.1
1	A	876[A]	CYS	3.0
1	A	934	MET	2.9
1	A	727	ALA	2.9
1	A	827	LEU	2.9
1	A	725	CYS	2.9
1	A	944	SER	2.9
1	A	738	TYR	2.9
1	A	878	THR	2.8
1	A	716	ALA	2.8
1	A	952	LYS	2.8
1	A	710	THR	2.8
1	A	864	GLU	2.8
1	A	949	CYS	2.8
1	A	736	ASP	2.8
1	A	720	GLY	2.8
1	A	729	PHE	2.7
1	A	895	GLY	2.7
1	A	925	CYS	2.7
1	A	869	ASN	2.7
1	A	704	TYR	2.7
1	A	948	LYS	2.7
1	A	805	PRO	2.6
1	A	854	VAL	2.6
1	A	774	PRO	2.6
1	A	947	LYS	2.6
1	A	777	THR	2.6
1	A	703	PHE	2.6
1	A	926	SER	2.5
1	A	707	ILE	2.5
1	A	858	ALA	2.5
1	A	723	GLU	2.5
1	A	832	VAL	2.5
1	A	852	GLN	2.4
1	A	783	GLY	2.4
1	A	872	ALA	2.4
1	A	829	ASP	2.3
1	A	990	PRO	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	1018	VAL	2.2
1	A	824	ARG	2.1
1	A	859	ILE	2.1
1	A	778	GLU	2.1
1	A	908	LEU	2.1
1	A	931	LEU	2.1
1	A	849	PRO	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 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	0.90	0.09	28,36,40,43	0
3	NI	A	1102	1/1	0.98	0.06	24,24,24,24	0

6.5 Other polymers [i](#)

There are no such residues in this entry.