Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 04:34 PM UTC

PDB ID	:	5Q2Q / pdb_00005q2q
Title	:	PanDDA analysis group deposition – Crystal Structure of DCLRE1A after initial refinement with no ligand modelled (structure 18)
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Deposited on	:	2017-05-25
Resolution	:	1.44 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:

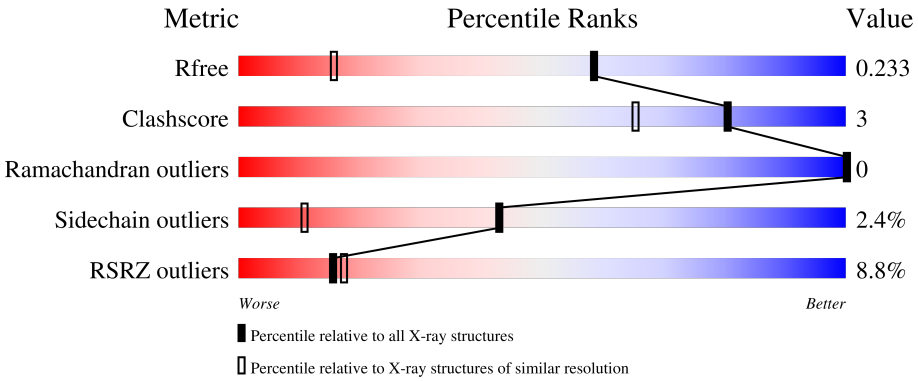
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 1.44 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	3234 (1.46-1.42)
Clashscore	190562	3289 (1.46-1.42)
Ramachandran outliers	187476	3248 (1.46-1.42)
Sidechain outliers	187428	3248 (1.46-1.42)
RSRZ outliers	180081	3234 (1.46-1.42)

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 <=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	9% 82% 15%

2 Entry composition (i)

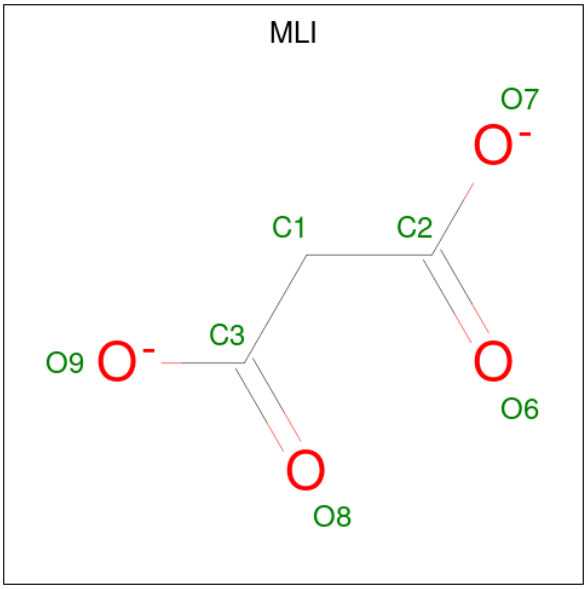
There are 4 unique types of molecules in this entry. The entry contains 3044 atoms, of which 0 are hydrogens and 0 are deuteriums.

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
			Total	Ni		
3	A	1	1	1	0	0

- Molecule 4 is water.

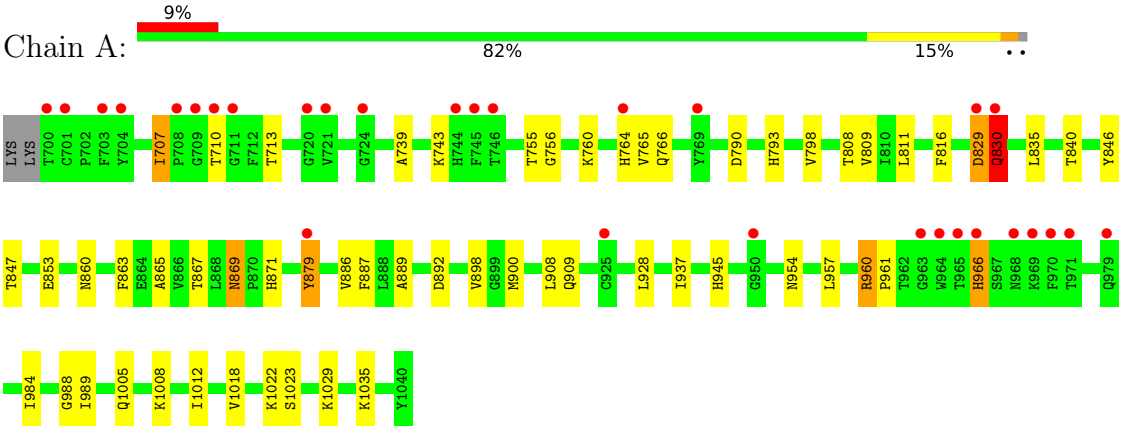
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	A	310	310	310	0	0

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: DCLRE1A

Chain A:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	52.20Å 57.20Å 115.24Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	28.60 – 1.44 28.60 – 1.44	Depositor EDS
% Data completeness (in resolution range)	99.7 (28.60-1.44) 99.7 (28.60-1.44)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.04 (at 1.44Å)	Xtriage
Refinement program	REFMAC 5.8.0155	Depositor
R, R_{free}	0.194 , 0.222 0.203 , 0.233	Depositor DCC
R_{free} test set	3050 reflections (4.82%)	wwPDB-VP
Wilson B-factor (Å^2)	18.2	Xtriage
Anisotropy	0.018	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 30.3	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	0.96	EDS
Total number of atoms	3044	wwPDB-VP
Average B, all atoms (Å^2)	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.23% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical 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.

5 Model quality

5.1 Standard geometry

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	1.73	34/2802 (1.2%)	1.42	13/3809 (0.3%)

All (34) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	989	ILE	CA-C	7.78	1.61	1.52
1	A	1005	GLN	N-CA	7.67	1.55	1.46
1	A	793	HIS	N-CA	7.41	1.50	1.46
1	A	835	LEU	N-CA	6.89	1.54	1.46
1	A	860	ASN	N-CA	6.81	1.54	1.46
1	A	840	THR	C-O	6.80	1.31	1.24
1	A	879	TYR	N-CA	6.74	1.52	1.46
1	A	830	GLN	C-O	-6.68	1.16	1.23
1	A	961	PRO	N-CA	-6.64	1.39	1.47
1	A	1023	SER	N-CA	6.60	1.54	1.46
1	A	707	ILE	CA-C	6.56	1.58	1.53
1	A	809	VAL	CA-C	6.42	1.60	1.52
1	A	1012	ILE	C-O	6.02	1.30	1.24
1	A	790	ASP	CG-OD2	-6.01	1.14	1.25
1	A	853	GLU	N-CA	5.95	1.53	1.46
1	A	798	VAL	N-CA	5.92	1.52	1.46
1	A	1008	LYS	CA-CB	5.73	1.56	1.52
1	A	886	VAL	C-O	5.51	1.30	1.24
1	A	811	LEU	CA-CB	-5.36	1.46	1.53
1	A	755	THR	C-O	5.36	1.30	1.24
1	A	863	PHE	C-O	5.34	1.30	1.24
1	A	1023	SER	C-O	5.32	1.30	1.24
1	A	739	ALA	N-CA	5.19	1.52	1.46
1	A	892	ASP	C-O	5.18	1.30	1.24
1	A	1035	LYS	CA-CB	-5.18	1.45	1.53
1	A	847	THR	CA-C	5.17	1.58	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	988	GLY	C-N	5.17	1.39	1.33
1	A	808	THR	N-CA	5.17	1.52	1.46
1	A	867	THR	N-CA	5.16	1.52	1.46
1	A	865	ALA	C-O	5.11	1.30	1.24
1	A	984	ILE	N-CA	5.05	1.52	1.46
1	A	954	ASN	N-CA	5.04	1.52	1.46
1	A	846	TYR	C-O	5.04	1.30	1.23
1	A	889	ALA	C-O	5.03	1.30	1.24

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	829	ASP	N-CA-C	8.02	122.64	113.01
1	A	713	THR	O-C-N	6.49	131.80	123.11
1	A	756	GLY	CA-C-O	-6.27	114.30	120.75
1	A	898	VAL	CA-C-N	5.86	127.25	121.57
1	A	898	VAL	C-N-CA	5.86	127.25	121.57
1	A	869	ASN	CA-C-N	5.67	125.37	119.82
1	A	869	ASN	C-N-CA	5.67	125.37	119.82
1	A	887	PHE	N-CA-C	-5.53	105.26	112.23
1	A	961	PRO	CB-CA-C	5.38	117.97	111.46
1	A	766	GLN	CA-C-N	5.33	127.73	120.54
1	A	766	GLN	C-N-CA	5.33	127.73	120.54
1	A	945	HIS	N-CA-C	5.08	116.82	111.28
1	A	966	HIS	N-CA-C	5.05	118.22	111.75

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	14	1
2	A	7	0	2	0	0
3	A	1	0	0	0	0
4	A	310	0	0	6	2

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	3044	0	2678	14	3

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 (14) 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:830:GLN:HB2	4:A:1292:HOH:O	1.84	0.77
1:A:909:GLN:NE2	4:A:1201:HOH:O	2.18	0.76
1:A:1018:VAL:HG22	4:A:1332:HOH:O	1.85	0.75
1:A:1022:LYS:HE3	4:A:1221:HOH:O	1.98	0.63
1:A:1022:LYS:CE	4:A:1221:HOH:O	2.55	0.53
1:A:743:LYS:CB	1:A:764[B]:HIS:O	2.60	0.50
1:A:743:LYS:HB3	1:A:764[B]:HIS:HB2	1.95	0.48
1:A:764[A]:HIS:HE1	4:A:1345:HOH:O	1.96	0.47
1:A:937:ILE:HG21	1:A:960:ARG:CG	2.46	0.46
1:A:764[A]:HIS:O	1:A:765:VAL:C	2.59	0.46
1:A:707:ILE:O	1:A:710:THR:OG1	2.31	0.44
1:A:869:ASN:ND2	1:A:871:HIS:H	2.16	0.43
1:A:900:MET:SD	1:A:908:LEU:HD12	2.59	0.42
1:A:760:LYS:O	1:A:764[A]:HIS:HA	2.19	0.42

All (3) 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:1404:HOH:O	4:A:1435:HOH:O[1_655]	2.00	0.20
4:A:1423:HOH:O	4:A:1449:HOH:O[1_455]	2.02	0.18
1:A:829:ASP:OD2	1:A:966:HIS:N[3_545]	2.12	0.08

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%)	337 (98%)	6 (2%)	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 12

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

Mol	Chain	Res	Type
1	A	816	PHE
1	A	830	GLN
1	A	879	TYR
1	A	928	LEU
1	A	957	LEU
1	A	960	ARG
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	768	GLN
1	A	851	GLN
1	A	869	ASN
1	A	943	GLN
1	A	966	HIS
1	A	968	ASN
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	1.21	0	7,7,7	1.09	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	C2-C1-C3-O8
2	A	1101	MLI	C3-C1-C2-O6
2	A	1101	MLI	C2-C1-C3-O9
2	A	1101	MLI	C3-C1-C2-O7

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, 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	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	341/343 (99%)	0.51	30 (8%)	15	17	8, 22, 43, 100	4 (1%)

All (30) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	970	PHE	5.4
1	A	703	PHE	4.4
1	A	968	ASN	4.3
1	A	966	HIS	3.8
1	A	700	THR	3.7
1	A	964	TRP	3.4
1	A	879	TYR	3.4
1	A	721	VAL	3.3
1	A	746	THR	2.9
1	A	965	THR	2.9
1	A	709	GLY	2.9
1	A	724	GLY	2.8
1	A	830	GLN	2.8
1	A	971	THR	2.8
1	A	745	PHE	2.7
1	A	969	LYS	2.7
1	A	829	ASP	2.6
1	A	764[A]	HIS	2.5
1	A	950	GLY	2.5
1	A	925	CYS	2.4
1	A	720	GLY	2.4
1	A	769	TYR	2.4
1	A	701	CYS	2.4
1	A	744	HIS	2.3
1	A	710	THR	2.3
1	A	704	TYR	2.3
1	A	979	GLN	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	963	GLY	2.1
1	A	708	PRO	2.1
1	A	711	GLY	2.0

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, 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	B-factors(Å^2)	Q<0.9
2	MLI	A	1101	7/7	0.96	0.07	15,18,25,27	0
3	NI	A	1102	1/1	0.99	0.04	13,13,13,13	0

6.5 Other polymers (i)

There are no such residues in this entry.