



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 01:45 PM UTC

PDB ID : 5Q74 / pdb_00005q74
Title : PanDDA analysis group deposition – Crystal Structure of DCLRE1A after initial refinement with no ligand modelled (structure 177)
Authors : Newman, J.A.; Aitkenhead, H.; Lee, S.Y.; Kupinska, K.; Burgess-Brown, N.; Tallon, R.; Krojer, T.; von Delft, F.; Arrowsmith, C.H.; Edwards, A.; Bountra, C.; Gileadi, O.
Deposited on : 2017-05-25
Resolution : 1.21 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

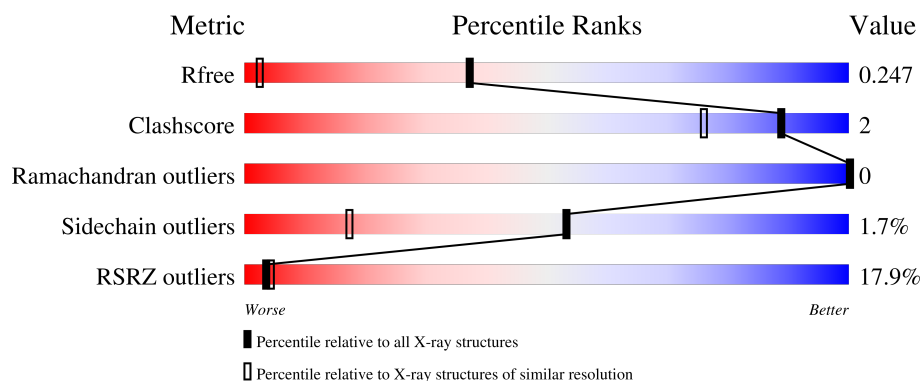
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.21 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	2002 (1.24-1.20)
Clashscore	190562	2061 (1.24-1.20)
Ramachandran outliers	187476	2009 (1.24-1.20)
Sidechain outliers	187428	2008 (1.24-1.20)
RSRZ outliers	180081	2000 (1.24-1.20)

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	18% 85% 13% ..

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	52.12Å 57.09Å 115.29Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	52.11 – 1.21 52.11 – 1.21	Depositor EDS
% Data completeness (in resolution range)	97.5 (52.11-1.21) 97.5 (52.11-1.21)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.47 (at 1.21Å)	Xtriage
Refinement program	REFMAC 5.8.0155	Depositor
R, R_{free}	0.217 , 0.237 0.225 , 0.247	Depositor DCC
R_{free} test set	5180 reflections (4.90%)	wwPDB-VP
Wilson B-factor (Å ²)	14.5	Xtriage
Anisotropy	0.078	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 29.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	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)	23.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.41% 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	1.72	31/2802 (1.1%)	1.37	16/3809 (0.4%)

All (31) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	989	ILE	CA-C	7.26	1.60	1.52
1	A	961	PRO	N-CA	-6.96	1.38	1.47
1	A	879	TYR	N-CA	6.69	1.52	1.46
1	A	707	ILE	CA-C	6.58	1.58	1.53
1	A	891	ALA	C-O	6.50	1.31	1.24
1	A	961	PRO	CA-C	6.35	1.59	1.52
1	A	840	THR	C-O	6.00	1.31	1.24
1	A	835	LEU	N-CA	5.89	1.53	1.46
1	A	961	PRO	C-O	5.72	1.29	1.23
1	A	956	ILE	N-CA	5.72	1.52	1.46
1	A	1006	TRP	C-O	5.71	1.30	1.24
1	A	798	VAL	N-CA	5.64	1.52	1.46
1	A	892	ASP	C-O	5.62	1.30	1.24
1	A	888	LEU	C-O	5.61	1.30	1.24
1	A	1012	ILE	N-CA	5.53	1.52	1.46
1	A	860	ASN	N-CA	5.49	1.53	1.46
1	A	1035	LYS	CA-CB	-5.46	1.44	1.53
1	A	830	GLN	C-O	-5.39	1.17	1.23
1	A	864	GLU	C-O	5.39	1.30	1.24
1	A	852	GLN	N-CA	5.30	1.52	1.46
1	A	793	HIS	N-CA	5.29	1.49	1.46
1	A	759	LEU	C-O	5.23	1.30	1.24
1	A	1020	THR	C-O	5.22	1.30	1.23
1	A	1023	SER	N-CA	5.12	1.52	1.46
1	A	862	ALA	C-O	5.12	1.30	1.24
1	A	793	HIS	C-O	5.12	1.27	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	739	ALA	N-CA	5.11	1.52	1.46
1	A	945	HIS	CA-C	5.10	1.59	1.52
1	A	955	GLN	CA-C	5.02	1.58	1.52
1	A	992	SER	N-CA	5.01	1.52	1.46
1	A	921	THR	N-CA	5.00	1.52	1.46

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	829	ASP	N-CA-C	7.90	122.49	113.01
1	A	961	PRO	CB-CA-C	6.36	118.55	111.11
1	A	869	ASN	CA-C-N	6.25	125.93	119.56
1	A	869	ASN	C-N-CA	6.25	125.93	119.56
1	A	898	VAL	CA-C-N	6.00	127.39	121.57
1	A	898	VAL	C-N-CA	6.00	127.39	121.57
1	A	713	THR	O-C-N	5.89	131.00	123.11
1	A	766	GLN	CA-C-N	5.74	128.24	120.38
1	A	766	GLN	C-N-CA	5.74	128.24	120.38
1	A	966	HIS	N-CA-C	5.65	118.98	111.75
1	A	961	PRO	N-CA-C	-5.60	101.42	110.55
1	A	747	PHE	CA-C-N	5.32	125.48	119.90
1	A	747	PHE	C-N-CA	5.32	125.48	119.90
1	A	741	LEU	CA-C-O	-5.26	115.98	121.55
1	A	735	SER	CA-C-O	-5.09	115.15	120.55
1	A	900	MET	CA-C-O	-5.03	116.05	121.38

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	10	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	10	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 2.

All (10) 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:1018:VAL:HG22	4:A:1275:HOH:O	1.86	0.76
1:A:909:GLN:NE2	4:A:1202:HOH:O	2.18	0.75
1:A:830:GLN:HB2	4:A:1321:HOH:O	2.02	0.59
1:A:1028[A]:GLU:OE2	4:A:1201:HOH:O	2.17	0.58
1:A:743:LYS:HB3	1:A:764[B]:HIS:O	2.10	0.51
1:A:743:LYS:CB	1:A:764[B]:HIS:O	2.62	0.47
1:A:701:CYS:N	4:A:1213:HOH:O	2.50	0.43
1:A:937:ILE:HG21	1:A:960:ARG:CG	2.50	0.42
1:A:829:ASP:OD1	1:A:829:ASP:N	2.52	0.42
1:A:705:LYS:NZ	4:A:1204:HOH:O	2.42	0.40

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:1374:HOH:O	4:A:1450:HOH:O[1_455]	2.06	0.14
1:A:829:ASP:OD2	1:A:966:HIS:N[3_545]	2.08	0.12
4:A:1215:HOH:O	4:A:1464:HOH:O[1_455]	2.15	0.05

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%)	334 (97%)	9 (3%)	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%)	294 (98%)	5 (2%)	53	17

All (5) 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	960	ARG
1	A	1029	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	768	GLN
1	A	851	GLN
1	A	860	ASN
1	A	869	ASN
1	A	917	ASN
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 [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	1.65	2 (33%)	7,7,7	1.15	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	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1101	MLI	O7-C2	-2.46	1.22	1.30
2	A	1101	MLI	C1-C3	2.14	1.54	1.51

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-O9
2	A	1101	MLI	C3-C1-C2-O6
2	A	1101	MLI	C2-C1-C3-O8
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, 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%)	0.98	61 (17%) 3 4	7, 20, 38, 88	4 (1%)

All (61) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	970	PHE	6.6
1	A	964	TRP	5.2
1	A	703	PHE	5.1
1	A	879	TYR	4.8
1	A	968	ASN	4.3
1	A	700	THR	4.3
1	A	971	THR	4.3
1	A	721	VAL	4.2
1	A	965	THR	3.9
1	A	966	HIS	3.8
1	A	969	LYS	3.8
1	A	925	CYS	3.7
1	A	724	GLY	3.6
1	A	709	GLY	3.6
1	A	745	PHE	3.5
1	A	769	TYR	3.3
1	A	740	GLY	3.3
1	A	746	THR	3.3
1	A	720	GLY	3.3
1	A	747	PHE	3.1
1	A	963	GLY	3.1
1	A	830	GLN	3.1
1	A	829	ASP	3.1
1	A	832	VAL	3.0
1	A	744	HIS	2.9
1	A	710	THR	2.8
1	A	928	LEU	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	967	SER	2.8
1	A	950	GLY	2.8
1	A	708	PRO	2.7
1	A	704	TYR	2.7
1	A	701	CYS	2.6
1	A	726	THR	2.6
1	A	742	SER	2.6
1	A	741	LEU	2.6
1	A	764[A]	HIS	2.6
1	A	973	ILE	2.6
1	A	826	LEU	2.6
1	A	979	GLN	2.6
1	A	972	ARG	2.5
1	A	974	ALA	2.5
1	A	765	VAL	2.4
1	A	702	PRO	2.4
1	A	707	ILE	2.4
1	A	977	ILE	2.4
1	A	957	LEU	2.4
1	A	828	ALA	2.4
1	A	725	CYS	2.3
1	A	962	THR	2.3
1	A	975	ASP	2.3
1	A	738	TYR	2.3
1	A	936	GLN	2.3
1	A	743	LYS	2.3
1	A	722	VAL	2.2
1	A	960	ARG	2.2
1	A	763	LEU	2.1
1	A	711	GLY	2.1
1	A	1032	ARG	2.1
1	A	924	MET	2.1
1	A	719	TYR	2.0
1	A	1018	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	0.95	0.08	16,20,26,32	0
3	NI	A	1102	1/1	0.99	0.05	14,14,14,14	0

6.5 Other polymers [i](#)

There are no such residues in this entry.