



Full wwPDB X-ray Structure Validation Report ⓘ

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PDB ID : 5Q7J / pdb_00005q7j
Title : PanDDA analysis group deposition – Crystal Structure of DCLRE1A after initial refinement with no ligand modelled (structure 192)
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 : 1.54 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

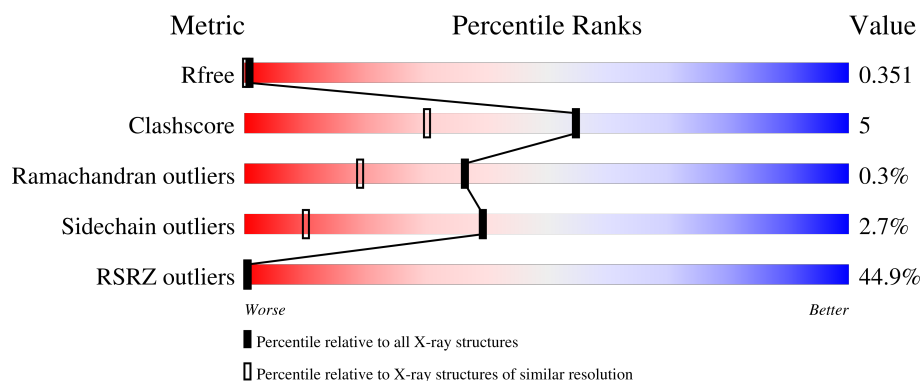
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.54 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	1003 (1.54-1.54)
Clashscore	190562	1025 (1.54-1.54)
Ramachandran outliers	187476	1007 (1.54-1.54)
Sidechain outliers	187428	1007 (1.54-1.54)
RSRZ outliers	180081	1002 (1.54-1.54)

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	45% 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	51.79Å 57.87Å 114.55Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	51.78 – 1.54 51.78 – 1.54	Depositor EDS
% Data completeness (in resolution range)	97.5 (51.78-1.54) 97.5 (51.78-1.54)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.75 (at 1.54Å)	Xtriage
Refinement program	REFMAC 5.8.0155	Depositor
R, R_{free}	0.290 , 0.339 0.300 , 0.351	Depositor DCC
R_{free} test set	2508 reflections (4.85%)	wwPDB-VP
Wilson B-factor (Å ²)	20.2	Xtriage
Anisotropy	0.351	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 32.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	3044	wwPDB-VP
Average B, all atoms (Å ²)	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.48% 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	1.04	4/2802 (0.1%)	1.09	4/3809 (0.1%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	833	HIS	C-O	5.57	1.30	1.24
1	A	1008	LYS	C-O	5.52	1.26	1.23
1	A	1012	ILE	N-CA	5.13	1.52	1.46
1	A	732	HIS	C-O	5.09	1.29	1.23

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	860	ASN	N-CA-C	7.13	118.74	110.97
1	A	830	GLN	N-CA-C	6.00	117.97	108.79
1	A	911	LEU	N-CA-C	5.76	119.93	113.02
1	A	848	PHE	CB-CA-C	5.70	117.74	110.22

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	26	0
2	A	7	0	2	0	0
3	A	1	0	0	0	0
4	A	310	0	0	14	1
All	All	3044	0	2678	26	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 5.

All (26) 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:1203:HOH:O	2.16	0.75
1:A:955:GLN:OE1	4:A:1201:HOH:O	2.15	0.65
1:A:871:HIS:CE1	4:A:1300:HOH:O	2.51	0.63
1:A:815:ASP:OD1	4:A:1202:HOH:O	2.16	0.62
1:A:980:THR:HG23	4:A:1236:HOH:O	2.11	0.51
1:A:860:ASN:O	1:A:861:THR:C	2.55	0.50
1:A:743:LYS:HG3	1:A:744:HIS:CE1	2.47	0.50
1:A:717:PHE:CE1	1:A:728:TYR:HB3	2.47	0.49
1:A:742:SER:O	1:A:765:VAL:HG22	2.12	0.49
1:A:784:VAL:HG21	4:A:1481:HOH:O	2.13	0.48
1:A:875:VAL:O	1:A:958:ALA:HA	2.16	0.46
1:A:1032:ARG:NE	4:A:1219:HOH:O	2.49	0.45
1:A:973:ILE:N	4:A:1216:HOH:O	2.49	0.45
1:A:859:ILE:HD11	1:A:889:ALA:HB1	1.99	0.45
1:A:702:PRO:HG2	1:A:705:LYS:HG3	2.00	0.43
1:A:973:ILE:HG22	4:A:1216:HOH:O	2.17	0.43
1:A:973:ILE:HD13	1:A:990:PRO:HD2	1.99	0.43
1:A:972:ARG:HB3	4:A:1216:HOH:O	2.19	0.43
1:A:1032:ARG:CZ	4:A:1219:HOH:O	2.68	0.41
1:A:864:GLU:HB2	4:A:1367:HOH:O	2.19	0.41
1:A:983:ASN:ND2	4:A:1213:HOH:O	2.45	0.41
1:A:978:PRO:HD3	4:A:1440:HOH:O	2.20	0.41
1:A:760:LYS:O	1:A:764[A]:HIS:HA	2.21	0.41
1:A:834:MET:HE2	1:A:1013:ILE:HD11	2.03	0.41
1:A:856:ARG:HE	1:A:856:ARG:HA	1.85	0.41
1:A:718:GLN:HB3	1:A:739:ALA:O	2.22	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:1391:HOH:O	4:A:1402:HOH:O[3_545]	2.15	0.05

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%)	324 (94%)	18 (5%)	1 (0%)	36 19

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	978	PRO

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%)	291 (97%)	8 (3%)	39 10

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

Mol	Chain	Res	Type
1	A	700	THR
1	A	816	PHE
1	A	830	GLN
1	A	879	TYR
1	A	893	VAL

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Mol	Chain	Res	Type
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 (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	851	GLN
1	A	943	GLN
1	A	955	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	1.33	0	7,7,7	1.44	1 (14%)

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.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1101	MLI	O7-C2-C1	2.64	122.69	114.51

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	C2-C1-C3-O9
2	A	1101	MLI	C3-C1-C2-O7
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%)	2.41	153 (44%) 0 0	13, 32, 95, 155	4 (1%)

All (153) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	745	PHE	11.3
1	A	984	ILE	10.9
1	A	939	PHE	10.7
1	A	973	ILE	10.5
1	A	942	LEU	9.6
1	A	765	VAL	9.6
1	A	970	PHE	9.5
1	A	977	ILE	9.3
1	A	986	ILE	9.1
1	A	769	TYR	8.3
1	A	747	PHE	8.3
1	A	937	ILE	8.2
1	A	987	TYR	8.2
1	A	971	THR	8.0
1	A	982	GLY	7.8
1	A	974	ALA	7.7
1	A	780	ILE	7.6
1	A	980	THR	7.6
1	A	976	VAL	7.6
1	A	941	GLY	7.5
1	A	744	HIS	7.3
1	A	946	LEU	7.2
1	A	770	ILE	6.9
1	A	968	ASN	6.9
1	A	746	THR	6.8
1	A	966	HIS	6.7
1	A	978	PRO	6.7

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Mol	Chain	Res	Type	RSRZ
1	A	750	TYR	6.5
1	A	967	SER	6.5
1	A	781	VAL	6.4
1	A	711	GLY	6.3
1	A	741	LEU	6.1
1	A	964	TRP	6.0
1	A	742	SER	6.0
1	A	928	LEU	6.0
1	A	972	ARG	5.9
1	A	722	VAL	5.7
1	A	956	ILE	5.5
1	A	985	SER	5.5
1	A	938	ASN	5.4
1	A	951	GLY	5.3
1	A	768	GLN	5.2
1	A	940	LYS	5.1
1	A	879	TYR	5.1
1	A	981	LYS	5.1
1	A	764[A]	HIS	5.1
1	A	743	LYS	5.1
1	A	943	GLN	5.0
1	A	988	GLY	5.0
1	A	983	ASN	5.0
1	A	861	THR	4.9
1	A	979	GLN	4.7
1	A	721	VAL	4.7
1	A	866	VAL	4.6
1	A	828	ALA	4.6
1	A	862	ALA	4.6
1	A	857	PHE	4.5
1	A	826	LEU	4.4
1	A	748	PRO	4.4
1	A	856	ARG	4.4
1	A	936	GLN	4.2
1	A	965	THR	4.2
1	A	771	HIS	4.2
1	A	784	VAL	4.2
1	A	763	LEU	4.2
1	A	740	GLY	4.2
1	A	766	GLN	4.2
1	A	950	GLY	4.1
1	A	957	LEU	4.1

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Mol	Chain	Res	Type	RSRZ
1	A	953	TYR	4.0
1	A	868	LEU	4.0
1	A	963	GLY	4.0
1	A	779	CYS	4.0
1	A	749	VAL	4.0
1	A	700	THR	3.9
1	A	932	LEU	3.9
1	A	935	MET	3.9
1	A	989	ILE	3.9
1	A	782	ASN	3.8
1	A	894	LEU	3.8
1	A	954	ASN	3.8
1	A	717	PHE	3.8
1	A	724	GLY	3.8
1	A	767	GLU	3.8
1	A	944	SER	3.8
1	A	863	PHE	3.7
1	A	860	ASN	3.7
1	A	709	GLY	3.7
1	A	723	GLU	3.7
1	A	961	PRO	3.7
1	A	945	HIS	3.7
1	A	975	ASP	3.6
1	A	893	VAL	3.5
1	A	759	LEU	3.5
1	A	712	PHE	3.4
1	A	969	LYS	3.4
1	A	848	PHE	3.4
1	A	871	HIS	3.2
1	A	865	ALA	3.2
1	A	726	THR	3.1
1	A	703	PHE	3.1
1	A	955	GLN	3.1
1	A	872	ALA	3.0
1	A	869	ASN	3.0
1	A	739	ALA	3.0
1	A	829	ASP	3.0
1	A	927	SER	2.9
1	A	783	GLY	2.9
1	A	960	ARG	2.9
1	A	804	LEU	2.9
1	A	949	CYS	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	962	THR	2.9
1	A	827	LEU	2.9
1	A	864	GLU	2.9
1	A	933	PRO	2.8
1	A	947	LYS	2.8
1	A	952	LYS	2.8
1	A	710	THR	2.8
1	A	719	TYR	2.8
1	A	875	VAL	2.8
1	A	925	CYS	2.8
1	A	867	THR	2.8
1	A	934	MET	2.7
1	A	948	LYS	2.7
1	A	926	SER	2.7
1	A	852	GLN	2.6
1	A	725	CYS	2.6
1	A	959	PHE	2.5
1	A	773	LEU	2.5
1	A	775	LEU	2.4
1	A	1039	GLY	2.4
1	A	870	PRO	2.4
1	A	720	GLY	2.4
1	A	895	GLY	2.4
1	A	824	ARG	2.3
1	A	735	SER	2.3
1	A	874	VAL	2.3
1	A	738	TYR	2.3
1	A	772	PRO	2.2
1	A	831	LYS	2.2
1	A	873	LEU	2.2
1	A	805	PRO	2.2
1	A	912	ASN	2.2
1	A	832	VAL	2.2
1	A	716	ALA	2.1
1	A	830	GLN	2.1
1	A	704	TYR	2.1
1	A	736	ASP	2.1
1	A	1040	TYR	2.1
1	A	1010	GLN	2.1
1	A	878	THR	2.0
1	A	718	GLN	2.0
1	A	958	ALA	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, 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	0.10	27,34,35,36	0
3	NI	A	1102	1/1	0.99	0.05	21,21,21,21	0

6.5 Other polymers [i](#)

There are no such residues in this entry.