



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 1, 2026 – 08:42 PM UTC

PDB ID : 8D4Y / pdb_00008d4y
Title : C-terminal SANT-SLIDE domain of human Chromodomain-helicase-DNA-binding protein 4 (CHD4)
Authors : Moghaddas Sani, H.; Deshpande, C.N.; Panjikar, S.; Patel, K.; Mackay, J.P.
Deposited on : 2022-06-03
Resolution : 2.90 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
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

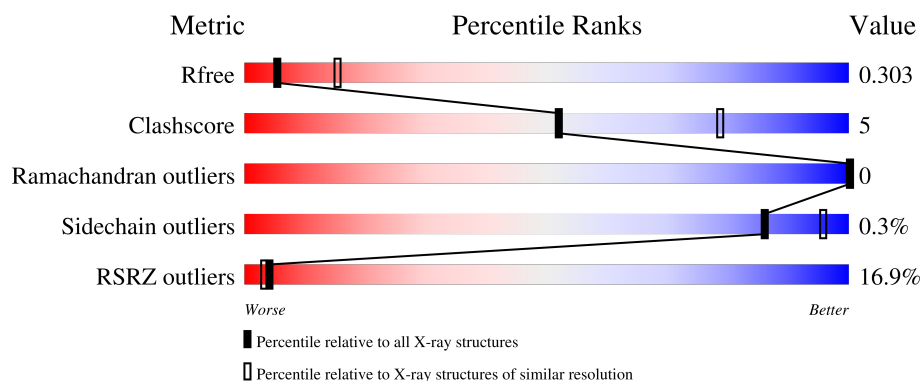
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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	2481 (2.90-2.90)
Clashscore	190562	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)
RSRZ outliers	180081	2481 (2.90-2.90)

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	431	11% 42% 7% 51%
1	B	431	6% 45% 5% 50%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 3557 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.

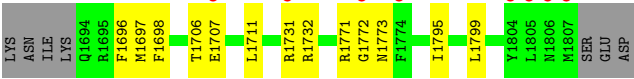
- Molecule 1 is a protein called Chromodomain-helicase-DNA-binding protein 4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	210	Total	C	N	O	S	0	0	0
			1740	1116	322	293	9			
1	B	217	Total	C	N	O	S	0	0	0
			1811	1161	339	302	9			

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total	O	0	0
			2	2		
2	B	4	Total	O	0	0
			4	4		

PRO
MET
GLU
THR
GLU
PRO
LYS
GLY
ALA
ALA
ASP
VAL
GLU
LYS
VAL
GLU
GLU
LYS
SER
ALA
ILE
ASP
LEU
THR
PRO
ILE
VAL
VAL
GLU
ASP
LYS
GLU
GLU
LYS
LYS
GLU
GLU
GLU
LYS
LYS
GLU
VAL
MET
LEU
GLN
ASN
GLY
GLY
THR
PRO
LYS
ASP
LEU
ASN
ASP
GLU
LYS
GLN
LYS



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	65.43Å 66.67Å 99.37Å 90.00° 100.77° 90.00°	Depositor
Resolution (Å)	19.90 – 2.90 19.90 – 2.90	Depositor EDS
% Data completeness (in resolution range)	98.0 (19.90-2.90) 97.8 (19.90-2.90)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.16 (at 2.88Å)	Xtriage
Refinement program	PHENIX 1.19.2_4158	Depositor
R, R_{free}	0.263 , 0.301 0.262 , 0.303	Depositor DCC
R_{free} test set	902 reflections (4.77%)	wwPDB-VP
Wilson B-factor (Å ²)	81.6	Xtriage
Anisotropy	0.102	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 51.3	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	0.90	EDS
Total number of atoms	3557	wwPDB-VP
Average B, all atoms (Å ²)	90.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.35% 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](#)

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	0.60	0/1780	0.97	0/2391
1	B	0.48	0/1852	0.77	0/2488
All	All	0.54	0/3632	0.87	0/4879

There are no bond length outliers.

There are no bond angle outliers.

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	1740	0	1729	20	0
1	B	1811	0	1819	16	0
2	A	2	0	0	0	0
2	B	4	0	0	0	0
All	All	3557	0	3548	36	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 5.

All (36) 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:1505:LYS:HD3	1:A:1509:PHE:HE1	1.59	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1445:VAL:O	1:B:1449:ARG:N	2.32	0.60
1:B:1698:PHE:O	1:B:1731:ARG:NH1	2.40	0.55
1:B:1445:VAL:O	1:B:1448:LEU:N	2.41	0.52
1:A:1505:LYS:HD3	1:A:1509:PHE:CE1	2.44	0.51
1:B:1707:GLU:O	1:B:1711:LEU:HG	2.11	0.51
1:B:1795:ILE:O	1:B:1799:LEU:HG	2.12	0.49
1:B:1706:THR:HG23	1:B:1795:ILE:HD12	1.95	0.47
1:A:1403:LEU:HA	1:A:1414:LEU:HD23	1.96	0.47
1:B:1696:PHE:CZ	1:B:1732:ARG:HA	2.51	0.46
1:B:1435:PRO:O	1:B:1438:ALA:N	2.39	0.45
1:A:1403:LEU:HD12	1:A:1414:LEU:HG	1.97	0.45
1:A:1417:ASN:HB3	1:A:1420:GLN:OE1	2.16	0.45
1:B:1698:PHE:HD2	1:B:1731:ARG:CG	2.30	0.45
1:A:1403:LEU:O	1:A:1413:VAL:HA	2.17	0.44
1:A:1438:ALA:O	1:A:1439:PHE:C	2.60	0.44
1:B:1436:GLN:O	1:B:1437:ASP:C	2.59	0.44
1:B:1772:GLY:O	1:B:1773:ASN:C	2.59	0.44
1:A:1763:GLU:N	1:A:1764:PRO:HD2	2.32	0.44
1:A:1488:SER:HA	1:A:1491:HIS:CG	2.54	0.43
1:A:1464:MET:O	1:A:1465:ARG:C	2.62	0.43
1:A:1517:SER:HA	1:A:1736:TRP:CE2	2.54	0.42
1:A:1518:MET:HE2	1:A:1518:MET:HB2	1.76	0.42
1:A:1412:GLU:HA	1:A:1416:PHE:O	2.19	0.42
1:A:1774:PHE:HA	1:A:1777:ILE:HD12	2.02	0.42
1:B:1467:LEU:O	1:B:1468:CYS:C	2.63	0.42
1:B:1698:PHE:HD2	1:B:1731:ARG:HG3	1.84	0.42
1:B:1771:ARG:O	1:B:1771:ARG:HG2	2.20	0.41
1:A:1488:SER:HA	1:A:1491:HIS:HB2	2.00	0.41
1:A:1417:ASN:ND2	1:A:1419:ARG:H	2.18	0.41
1:B:1706:THR:HG23	1:B:1795:ILE:CD1	2.50	0.41
1:B:1512:VAL:HG11	1:B:1697:MET:HB2	2.03	0.41
1:A:1423:ALA:O	1:A:1424:PHE:C	2.64	0.41
1:A:1716:GLU:O	1:A:1720:THR:HG23	2.21	0.41
1:A:1462:LEU:C	1:A:1462:LEU:HD13	2.46	0.40
1:A:1773:ASN:N	1:A:1773:ASN:OD1	2.52	0.40

There are no symmetry-related clashes.

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	202/431 (47%)	193 (96%)	9 (4%)	0	100	100
1	B	209/431 (48%)	202 (97%)	7 (3%)	0	100	100
All	All	411/862 (48%)	395 (96%)	16 (4%)	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	178/374 (48%)	177 (99%)	1 (1%)	78	93
1	B	186/374 (50%)	186 (100%)	0	100	100
All	All	364/748 (49%)	363 (100%)	1 (0%)	86	96

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1436	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1417	ASN
1	A	1730	HIS

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Mol	Chain	Res	Type
1	A	1806	ASN
1	B	1410	ASN
1	B	1442	GLN
1	B	1743	ASN

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](#)

There are no ligands in this entry.

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	210/431 (48%)	1.16	46 (21%)	2 2	30, 85, 145, 176	0
1	B	217/431 (50%)	0.88	26 (11%)	9 7	30, 78, 144, 191	0
All	All	427/862 (49%)	1.02	72 (16%)	4 3	30, 82, 145, 191	0

All (72) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1510	GLU	5.2
1	A	1439	PHE	5.1
1	B	1522	ALA	5.0
1	B	1806	ASN	4.8
1	B	1805	LEU	4.5
1	B	1487	LEU	4.3
1	A	1400	LEU	4.1
1	A	1511	HIS	4.1
1	A	1411	ILE	3.9
1	B	1441	THR	3.9
1	B	1772	GLY	3.8
1	B	1774	PHE	3.8
1	A	1433	MET	3.5
1	A	1414	LEU	3.5
1	B	1443	TRP	3.4
1	B	1731	ARG	3.4
1	A	1512	VAL	3.4
1	A	1488	SER	3.4
1	B	1807	MET	3.3
1	B	1400	LEU	3.3
1	A	1446	ARG	3.3
1	B	1438	ALA	3.3
1	B	1455	GLU	3.3
1	A	1417	ASN	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	1445	VAL	3.2
1	A	1464	MET	3.2
1	B	1444	LEU	3.1
1	A	1403	LEU	3.1
1	A	1448	LEU	3.1
1	A	1805	LEU	3.0
1	A	1463	PHE	3.0
1	A	1413	VAL	2.8
1	B	1406	ARG	2.8
1	A	1416	PHE	2.8
1	B	1437	ASP	2.6
1	B	1445	VAL	2.6
1	A	1808	SER	2.6
1	A	1468	CYS	2.6
1	A	1462	LEU	2.6
1	A	1515	ARG	2.6
1	A	1435	PRO	2.6
1	B	1414	LEU	2.6
1	A	1405	ALA	2.6
1	A	1466	HIS	2.5
1	B	1450	GLY	2.5
1	A	1514	GLY	2.5
1	A	1702	ASP	2.4
1	B	1410	ASN	2.4
1	A	1725	THR	2.4
1	B	1707	GLU	2.4
1	B	1436	GLN	2.4
1	A	1806	ASN	2.3
1	A	1736	TRP	2.3
1	A	1419	ARG	2.3
1	B	1468	CYS	2.3
1	A	1456	PHE	2.2
1	A	1492	VAL	2.2
1	A	1804	TYR	2.2
1	A	1504	LYS	2.2
1	A	1704	GLY	2.2
1	B	1804	TYR	2.1
1	A	1420	GLN	2.1
1	B	1447	ASP	2.1
1	A	1520	GLU	2.1
1	B	1405	ALA	2.1
1	A	1412	GLU	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	1418	ALA	2.1
1	A	1507	GLN	2.0
1	A	1401	PRO	2.0
1	A	1406	ARG	2.0
1	A	1703	GLY	2.0
1	A	1460	VAL	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](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.