



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 22, 2025 – 01:20 AM EDT

PDB ID : 6V3N / pdb_00006v3n
Title : Crystal structure of CDYL2 in complex with H3K27me3
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Structural Genomics Consortium; Structural Genomics Consortium (SGC)
Deposited on : 2019-11-26
Resolution : 2.70 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	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0rc1
EDS	:	FAILED
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.42

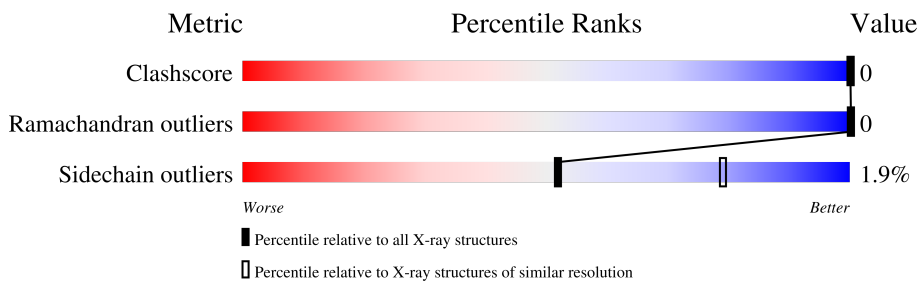
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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))
Clashscore	180529	3684 (2.70-2.70)
Ramachandran outliers	177936	3633 (2.70-2.70)
Sidechain outliers	177891	3633 (2.70-2.70)

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 $\leq 5\%$.

Note EDS failed to run properly.

Mol	Chain	Length	Quality of chain
1	A	64	92% 6%
1	B	64	95% . .
2	C	17	88% 12%
2	D	17	82% 18%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 1207 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 Y-like protein 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	60	Total	C	N	O	S	0	1	0
			500	318	85	95	2			
1	B	62	Total	C	N	O	S	0	0	1
			501	317	85	97	2			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	GLY	-	expression tag	UNP Q8N8U2
B	1	GLY	-	expression tag	UNP Q8N8U2

- Molecule 2 is a protein called ACE-GLN-LEU-ALA-THR-LYS-ALA-ALA-ARG-M3L-SER-ALA-PRO-ALA-THR-TYR-NH2.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	C	15	Total	C	N	O	0	0	1
			99	63	19	17			
2	D	14	Total	C	N	O	0	0	1
			95	60	18	17			

- Molecule 3 is UNKNOWN ATOM OR ION (CCD ID: UNX) (formula: X).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	10	Total	X	0	0
			10	10		
3	B	2	Total	X	0	0
			2	2		

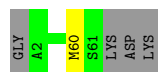
3 Residue-property plots [i](#)

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. 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. 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.

Note EDS failed to run properly.

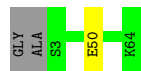
- Molecule 1: Chromodomain Y-like protein 2

Chain A:  92% 6%




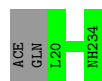
- Molecule 1: Chromodomain Y-like protein 2

Chain B:  95% 2%




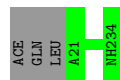
- Molecule 2: ACE-GLN-LEU-ALA-THR-LYS-ALA-ALA-ARG-M3L-SER-ALA-PRO-ALA-TH R-TYR-NH2

Chain C:  88% 12%



- Molecule 2: ACE-GLN-LEU-ALA-THR-LYS-ALA-ALA-ARG-M3L-SER-ALA-PRO-ALA-TH R-TYR-NH2

Chain D:  82% 18%



4 Data and refinement statistics

EDS failed to run properly - this section is therefore incomplete.

Property	Value	Source
Space group	P 43 2 2	Depositor
Cell constants a, b, c, α , β , γ	60.79Å 60.79Å 178.60Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	44.65 – 2.70	Depositor
% Data completeness (in resolution range)	99.9 (44.65-2.70)	Depositor
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.55 (at 2.69Å)	Xtriage
Refinement program	BUSTER 2.10.3	Depositor
R, R_{free}	0.240 , 0.258	Depositor
Wilson B-factor (Å ²)	70.3	Xtriage
Anisotropy	0.451	Xtriage
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
Total number of atoms	1207	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 6.31% 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: NH2, M3L, UNX

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	0.49	0/517	0.71	0/700
1	B	0.44	0/516	0.70	0/701
2	C	0.56	0/87	0.68	0/118
2	D	0.43	0/83	0.72	0/113
All	All	0.47	0/1203	0.70	0/1632

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	500	0	435	0	0
1	B	501	0	414	0	0
2	C	99	0	95	0	0
2	D	95	0	96	0	0
3	A	10	0	0	0	0
3	B	2	0	0	0	0
All	All	1207	0	1040	0	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 0.

There are no clashes within the asymmetric unit.

There are no symmetry-related clashes.

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	58/64 (91%)	58 (100%)	0	0	100	100
1	B	60/64 (94%)	58 (97%)	2 (3%)	0	100	100
2	C	12/17 (71%)	12 (100%)	0	0	100	100
2	D	11/17 (65%)	11 (100%)	0	0	100	100
All	All	141/162 (87%)	139 (99%)	2 (1%)	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	48/57 (84%)	47 (98%)	1 (2%)	48	76
1	B	46/57 (81%)	45 (98%)	1 (2%)	47	76
2	C	5/9 (56%)	5 (100%)	0	100	100
2	D	6/9 (67%)	6 (100%)	0	100	100
All	All	105/132 (80%)	103 (98%)	2 (2%)	52	79

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	60	MET
1	B	50	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

2 non-standard protein/DNA/RNA residues are modelled in this entry.

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	M3L	C	27	2	10,11,12	0.68	0	9,14,16	0.41	0
2	M3L	D	27	2	10,11,12	0.60	0	9,14,16	0.49	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	M3L	C	27	2	-	1/9/10/12	-
2	M3L	D	27	2	-	2/9/10/12	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	27	M3L	CE-CD-CG-CB
2	D	27	M3L	CE-CD-CG-CB
2	D	27	M3L	N-CA-CB-CG

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 12 ligands modelled in this entry, 12 are unknown - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

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

EDS failed to run properly - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains

EDS failed to run properly - this section is therefore empty.

6.3 Carbohydrates

EDS failed to run properly - this section is therefore empty.

6.4 Ligands

EDS failed to run properly - this section is therefore empty.

6.5 Other polymers

EDS failed to run properly - this section is therefore empty.