



wwPDB X-ray Structure Validation Summary Report ⓘ

May 18, 2020 – 05:00 am BST

PDB ID : 6XWV
Title : Crystal structure of drosophila melanogaster CENP-C bound to CAL1
Authors : Jeyaprakash, A.A.; Medina-Pritchard, B.; Lazou, V.; Zou, J.; Byron, O.; Abad, M.A.; Rappsilber, J.; Heun, P.
Deposited on : 2020-01-24
Resolution : 2.27 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Xtrriage (Phenix) : 1.13
EDS : 2.11
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

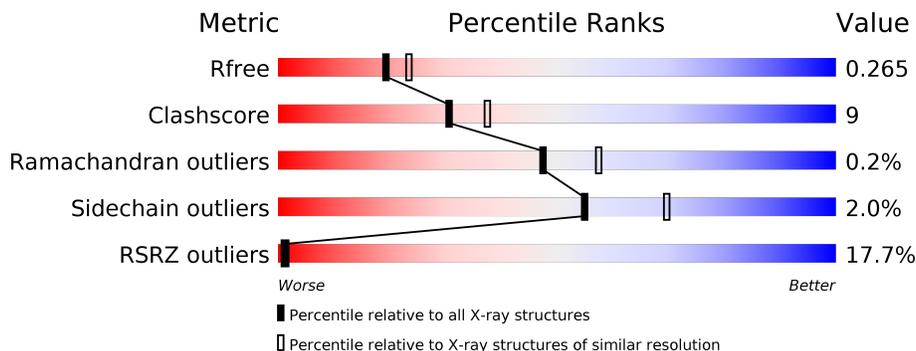
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

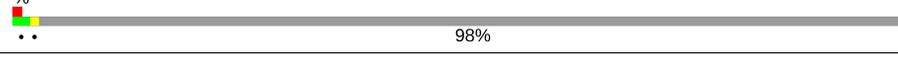
The reported resolution of this entry is 2.27 Å.

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}	130704	6980 (2.30-2.26)
Clashscore	141614	7711 (2.30-2.26)
Ramachandran outliers	138981	7597 (2.30-2.26)
Sidechain outliers	138945	7598 (2.30-2.26)
RSRZ outliers	127900	6849 (2.30-2.26)

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 on 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	1411	
1	B	1411	
1	C	1411	
1	D	1411	
2	E	979	

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 4229 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 Calmodulin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	133	1041	659	178	197	7	0	0	0
1	B	125	985	625	165	188	7	0	0	0
1	C	131	1025	650	175	193	7	0	0	0
1	D	123	969	617	160	185	7	0	0	0

- Molecule 2 is a protein called Ryanodine Receptor 2.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
2	E	24	191	126	35	30	0	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	6	Total 6 O 6	0	0
3	E	1	Total 1 O 1	0	0
3	B	3	Total 3 O 3	0	0
3	C	3	Total 3 O 3	0	0
3	D	5	Total 5 O 5	0	0

GLY	
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GLY	
LYS	

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	86.27Å 86.44Å 88.46Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.08 – 2.27 29.10 – 2.27	Depositor EDS
% Data completeness (in resolution range)	98.4 (29.08-2.27) 92.1 (29.10-2.27)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.57 (at 2.26Å)	Xtriage
Refinement program	PHENIX 1.17.1_3660	Depositor
R, R_{free}	0.237 , 0.266 0.237 , 0.265	Depositor DCC
R_{free} test set	1961 reflections (6.33%)	wwPDB-VP
Wilson B-factor (Å ²)	40.5	Xtriage
Anisotropy	1.016	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 49.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.000 for -h,l,k 0.000 for -l,-k,-h 0.000 for k,h,-l 0.000 for k,l,h 0.000 for l,h,k	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	4229	wwPDB-VP
Average B, all atoms (Å ²)	71.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 42.84 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.9248e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹ Intensities estimated from amplitudes.

² Theoretical 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	0.36	0/1058	0.71	4/1425 (0.3%)
1	B	0.48	1/1000 (0.1%)	0.82	6/1345 (0.4%)
1	C	0.36	0/1042	0.56	1/1403 (0.1%)
1	D	0.36	0/984	0.67	1/1325 (0.1%)
2	E	0.24	0/195	0.42	0/262
All	All	0.39	1/4279 (0.0%)	0.69	12/5760 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	1390	ARG	CZ-NH1	5.92	1.40	1.33

The worst 5 of 12 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	1390	ARG	NE-CZ-NH2	-11.31	114.64	120.30
1	A	1381	ARG	CG-CD-NE	9.18	131.08	111.80
1	A	1339	LYS	CA-CB-CG	8.01	131.02	113.40
1	B	1278	GLU	CB-CA-C	6.60	123.60	110.40
1	B	1315	TYR	CA-CB-CG	6.33	125.42	113.40

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	1390	ARG	Sidechain

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	1041	0	1021	18	0
1	B	985	0	962	24	0
1	C	1025	0	1009	12	0
1	D	969	0	943	22	0
2	E	191	0	192	5	0
3	A	6	0	0	0	0
3	B	3	0	0	0	0
3	C	3	0	0	0	0
3	D	5	0	0	0	0
3	E	1	0	0	0	0
All	All	4229	0	4127	77	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 9.

The worst 5 of 77 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:B:1352:HIS:HE1	1:B:1411:SER:N	1.74	0.86
1:B:1352:HIS:HE1	1:B:1411:SER:H	1.27	0.80
1:D:1352:HIS:CD2	1:D:1353:PRO:HD2	2.22	0.75
1:D:1352:HIS:ND1	1:D:1410:ARG:HB3	2.04	0.73
1:B:1352:HIS:CE1	1:B:1411:SER:N	2.57	0.73

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	129/1411 (9%)	124 (96%)	4 (3%)	1 (1%)	19	22
1	B	121/1411 (9%)	119 (98%)	2 (2%)	0	100	100
1	C	127/1411 (9%)	121 (95%)	6 (5%)	0	100	100
1	D	119/1411 (8%)	117 (98%)	2 (2%)	0	100	100
2	E	22/979 (2%)	22 (100%)	0	0	100	100
All	All	518/6623 (8%)	503 (97%)	14 (3%)	1 (0%)	47	57

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1372	GLU

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	110/1275 (9%)	107 (97%)	3 (3%)	44	59
1	B	105/1275 (8%)	102 (97%)	3 (3%)	42	56
1	C	109/1275 (8%)	106 (97%)	3 (3%)	43	57
1	D	103/1275 (8%)	103 (100%)	0	100	100
2	E	17/861 (2%)	17 (100%)	0	100	100
All	All	444/5961 (7%)	435 (98%)	9 (2%)	55	70

5 of 9 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	1315	TYR
1	C	1389	ASP
1	C	1282	LYS
1	A	1389	ASP
1	B	1343	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	1352	HIS
1	C	1316	GLN
1	D	1397	GLN

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 carbohydrates 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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	133/1411 (9%)	1.00	24 (18%) 1 1	39, 62, 111, 152	0
1	B	125/1411 (8%)	0.99	21 (16%) 1 2	41, 67, 114, 141	0
1	C	131/1411 (9%)	1.03	21 (16%) 1 2	41, 64, 126, 147	0
1	D	123/1411 (8%)	1.07	22 (17%) 1 1	43, 74, 123, 154	0
2	E	24/979 (2%)	1.10	7 (29%) 0 0	48, 61, 83, 114	0
All	All	536/6623 (8%)	1.03	95 (17%) 1 1	39, 67, 118, 154	0

The worst 5 of 95 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	1293	ALA	8.8
1	B	1315	TYR	8.6
1	D	1352	HIS	8.0
1	C	1292	ASP	7.9
1	A	1373	GLU	6.4

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 carbohydrates in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.