



Full wwPDB X-ray Structure Validation Report ⓘ

May 21, 2020 – 10:08 pm BST

PDB ID : 5WOP
Title : High Resolution Structure of Mutant CA09-PB2cap
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Deposited on : 2017-08-02
Resolution : 1.52 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (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

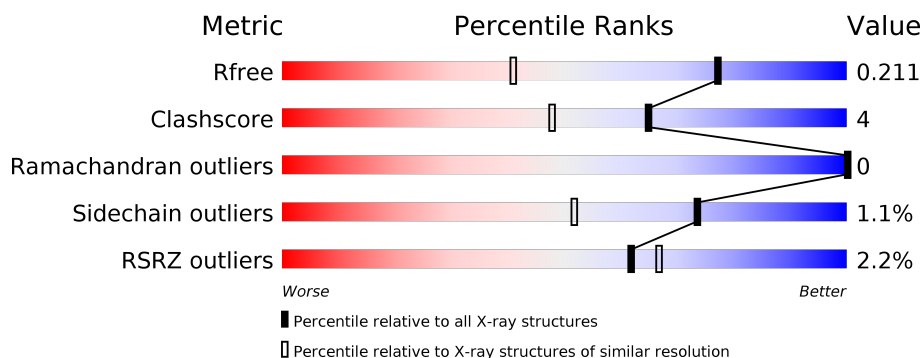
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.52 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	4009 (1.54-1.50)
Clashscore	141614	4249 (1.54-1.50)
Ramachandran outliers	138981	4148 (1.54-1.50)
Sidechain outliers	138945	4146 (1.54-1.50)
RSRZ outliers	127900	3943 (1.54-1.50)

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	159	<div> <div>3%</div> <div> <div></div> <div>87%</div> <div>11%</div> </div> </div>
1	B	159	<div> <div>2%</div> <div> <div></div> <div>90%</div> <div>10%</div> </div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	GOL	B	501	-	X	-	-

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 5442 atoms, of which 2593 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 Polymerase PB2.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	159	Total	C	H	N	O	S	55	0	0
			2527	783	1282	223	229	10			
1	B	159	Total	C	H	N	O	S	55	0	0
			2523	783	1279	222	229	10			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	421	GLY	-	linker	UNP F4MEU3
A	422	SER	-	linker	UNP F4MEU3
A	423	GLY	-	linker	UNP F4MEU3
B	421	GLY	-	linker	UNP F4MEU3
B	422	SER	-	linker	UNP F4MEU3
B	423	GLY	-	linker	UNP F4MEU3

- Molecule 2 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C H O 14 3 8 3	2	0
2	A	1	Total C H O 14 3 8 3	2	0
2	A	1	Total C H O 14 3 8 3	2	0
2	B	1	Total C H O 14 3 8 3	2	0

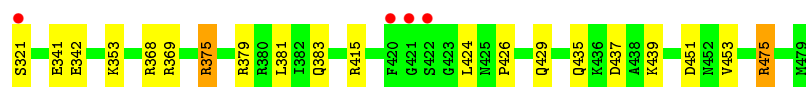
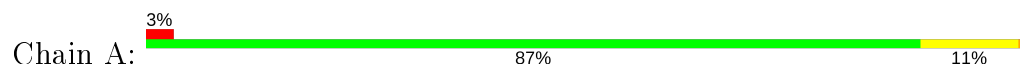
- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	177	Total O 177 177	0	0
3	B	159	Total O 159 159	0	0

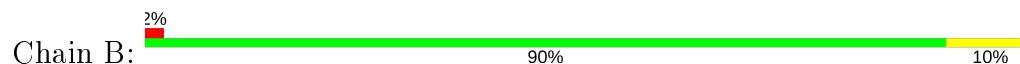
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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 and electron density. 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. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). 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.

• Molecule 1: Polymerase PB2



• Molecule 1: Polymerase PB2



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	36.86Å 72.43Å 61.32Å 90.00° 103.18° 90.00°	Depositor
Resolution (Å)	39.00 – 1.52 36.21 – 1.52	Depositor EDS
% Data completeness (in resolution range)	99.2 (39.00-1.52) 99.2 (36.21-1.52)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.11 (at 1.52Å)	Xtriage
Refinement program	REFMAC 5.8.0158	Depositor
R, R_{free}	0.148 , 0.210 0.151 , 0.211	Depositor DCC
R_{free} test set	2438 reflections (5.09%)	wwPDB-VP
Wilson B-factor (Å ²)	13.4	Xtriage
Anisotropy	0.039	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 50.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.98	EDS
Total number of atoms	5442	wwPDB-VP
Average B, all atoms (Å ²)	21.0	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 55.28 % 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 3.2342e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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: GOL

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	1.27	1/1262 (0.1%)	1.16	8/1689 (0.5%)
1	B	1.27	2/1261 (0.2%)	1.20	5/1687 (0.3%)
All	All	1.27	3/2523 (0.1%)	1.18	13/3376 (0.4%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	342	GLU	CD-OE1	9.59	1.36	1.25
1	B	405	SER	CB-OG	-6.63	1.33	1.42
1	B	380	ARG	CD-NE	5.26	1.55	1.46

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	451	ASP	CB-CG-OD2	-6.76	112.21	118.30
1	B	389	ARG	NE-CZ-NH1	-6.61	116.99	120.30
1	B	380	ARG	NE-CZ-NH2	6.59	123.59	120.30
1	B	390	ASP	CB-CG-OD1	6.14	123.82	118.30
1	A	375	ARG	NE-CZ-NH2	5.95	123.27	120.30
1	A	368	ARG	CG-CD-NE	5.75	123.87	111.80
1	B	469	MET	CG-SD-CE	5.74	109.39	100.20
1	A	475	ARG	NE-CZ-NH2	-5.53	117.53	120.30
1	A	437	ASP	CB-CG-OD1	5.25	123.03	118.30
1	A	379	ARG	NE-CZ-NH2	-5.24	117.68	120.30
1	A	475	ARG	NE-CZ-NH1	5.23	122.91	120.30
1	A	381	LEU	CB-CG-CD2	5.21	119.86	111.00
1	B	451	ASP	CB-CG-OD2	-5.08	113.73	118.30

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	1245	1282	1276	15	1
1	B	1244	1279	1275	7	0
2	A	18	24	24	7	0
2	B	6	8	8	2	1
3	A	177	0	0	3	1
3	B	159	0	0	1	0
All	All	2849	2593	2583	21	2

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 4.

All (21) 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:475:ARG:HE	2:A:503:GOL:H2	1.54	0.72
1:A:426:PRO:HA	1:A:429:GLN:HE21	1.55	0.72
1:A:375:ARG:HE	1:A:383:GLN:HE21	1.39	0.69
1:B:426:PRO:HA	1:B:429:GLN:HE21	1.64	0.62
1:A:375:ARG:HE	1:A:383:GLN:NE2	2.01	0.59
1:A:475:ARG:NE	2:A:503:GOL:H2	2.18	0.58
1:B:369:ARG:NE	2:B:501:GOL:O2	2.38	0.56
1:B:339:LYS:HG2	1:B:357:HIS:CE1	2.41	0.56
1:A:415:ARG:HH21	2:A:502:GOL:C1	2.19	0.55
1:B:373:ILE:CG2	3:B:732:HOH:O	2.56	0.54
1:A:435:GLN:NE2	3:A:604:HOH:O	2.44	0.49
1:B:392:GLN:HB3	2:B:501:GOL:H31	1.95	0.49
1:A:453:VAL:HB	2:A:503:GOL:H32	1.95	0.48
1:A:415:ARG:HH21	2:A:502:GOL:H12	1.81	0.45
1:A:321:SER:HB2	3:A:630:HOH:O	2.16	0.44
1:B:339:LYS:HD2	1:B:355:ARG:NH2	2.33	0.43
1:A:353:LYS:O	1:A:426:PRO:HG2	2.20	0.42
1:A:415:ARG:HE	2:A:502:GOL:H32	1.83	0.42
1:A:369:ARG:NH2	1:B:375:ARG:HH22	2.17	0.41
1:A:424:LEU:HD12	2:A:501:GOL:O2	2.21	0.41
1:A:321:SER:CB	3:A:630:HOH:O	2.69	0.40

All (2) 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)
1:A:375:ARG:HH22	2:B:501:GOL:HO2[1_556]	1.31	0.29
3:A:697:HOH:O	3:A:773:HOH:O[1_655]	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	157/159 (99%)	153 (98%)	4 (2%)	0	100	100
1	B	157/159 (99%)	155 (99%)	2 (1%)	0	100	100
All	All	314/318 (99%)	308 (98%)	6 (2%)	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	137/137 (100%)	135 (98%)	2 (2%)	65	38
1	B	136/137 (99%)	135 (99%)	1 (1%)	84	69
All	All	273/274 (100%)	270 (99%)	3 (1%)	73	52

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	341	GLU
1	A	439	LYS
1	B	420	PHE

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

Mol	Chain	Res	Type
1	A	383	GLN
1	A	429	GLN
1	A	435	GLN
1	B	357	HIS
1	B	419	ASN
1	B	429	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](#)

4 ligands 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	GOL	A	503	-	5,5,5	0.49	0	5,5,5	1.74	2 (40%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	GOL	A	501	-	5,5,5	0.36	0	5,5,5	0.68	0
2	GOL	B	501	-	5,5,5	2.86	3 (60%)	5,5,5	1.53	1 (20%)
2	GOL	A	502	-	5,5,5	0.62	0	5,5,5	1.23	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	GOL	A	503	-	-	0/4/4/4	-
2	GOL	A	501	-	-	2/4/4/4	-
2	GOL	B	501	-	-	2/4/4/4	-
2	GOL	A	502	-	-	2/4/4/4	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	501	GOL	O3-C3	4.78	1.62	1.42
2	B	501	GOL	O2-C2	3.16	1.52	1.43
2	B	501	GOL	C1-C2	2.38	1.61	1.51

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	501	GOL	O2-C2-C3	-2.60	97.68	109.12
2	A	503	GOL	C3-C2-C1	-2.55	101.80	111.70
2	A	503	GOL	O3-C3-C2	2.28	121.14	110.20

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	501	GOL	C1-C2-C3-O3
2	A	501	GOL	C1-C2-C3-O3
2	A	501	GOL	O2-C2-C3-O3
2	A	502	GOL	O2-C2-C3-O3
2	B	501	GOL	O2-C2-C3-O3
2	A	502	GOL	C1-C2-C3-O3

There are no ring outliers.

4 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	503	GOL	3	0
2	A	501	GOL	1	0
2	B	501	GOL	2	1
2	A	502	GOL	3	0

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	159/159 (100%)	-0.54	4 (2%) 57 62	9, 15, 42, 85	0
1	B	159/159 (100%)	-0.55	3 (1%) 66 71	10, 16, 41, 84	0
All	All	318/318 (100%)	-0.55	7 (2%) 62 67	9, 16, 42, 85	0

All (7) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	420	PHE	7.8
1	B	420	PHE	6.5
1	A	422	SER	3.7
1	B	421	GLY	3.5
1	A	421	GLY	3.4
1	A	321	SER	3.0
1	B	422	SER	3.0

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 carbohydrates 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(\AA^2)	Q<0.9
2	GOL	A	503	6/6	0.74	0.35	60,75,92,93	2
2	GOL	B	501	6/6	0.74	0.28	54,128,140,142	2
2	GOL	A	501	6/6	0.79	0.20	50,85,88,89	2
2	GOL	A	502	6/6	0.80	0.28	39,53,65,66	2

6.5 Other polymers [i](#)

There are no such residues in this entry.