



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 9, 2018 – 06:12 pm GMT

PDB ID : 3E6C
Title : CprK OCPA DNA Complex
Authors : Levy, C.
Deposited on : 2008-08-15
Resolution : 1.80 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
Mogul : 1.7.3 (157068), CSD as539be (2018)
Xtriage (Phenix) : 1.13
EDS : trunk30967
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)
Refmac : 5.8.0158
CCP4 : 7.0 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk30967

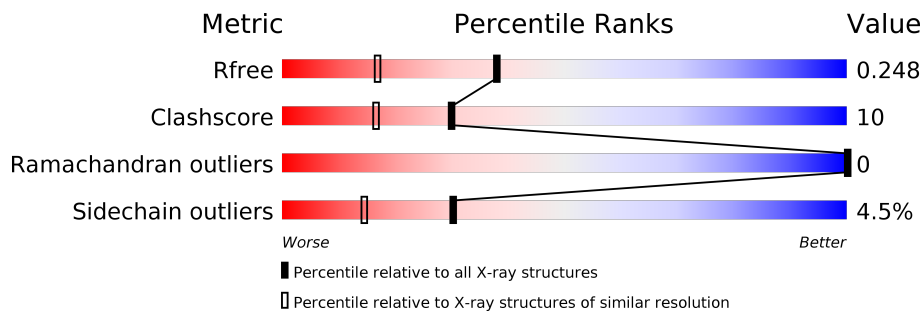
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.80 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}	111664	5253 (1.80-1.80)
Clashscore	122126	6077 (1.80-1.80)
Ramachandran outliers	120053	6011 (1.80-1.80)
Sidechain outliers	120020	6010 (1.80-1.80)

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. 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 $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	C	250	
2	B	13	
3	A	13	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 2506 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 Cyclic nucleotide-binding protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	C	225	Total	C	N	O	S	0	1	0
			1809	1164	296	339	10			

There are 19 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	200	SER	CYS	ENGINEERED	UNP Q18R04
C	233	SER	-	EXPRESSION TAG	UNP Q18R04
C	234	ASP	-	EXPRESSION TAG	UNP Q18R04
C	235	PRO	-	EXPRESSION TAG	UNP Q18R04
C	236	ASN	-	EXPRESSION TAG	UNP Q18R04
C	237	SER	-	EXPRESSION TAG	UNP Q18R04
C	238	SER	-	EXPRESSION TAG	UNP Q18R04
C	239	SER	-	EXPRESSION TAG	UNP Q18R04
C	240	VAL	-	EXPRESSION TAG	UNP Q18R04
C	241	ASP	-	EXPRESSION TAG	UNP Q18R04
C	242	LYS	-	EXPRESSION TAG	UNP Q18R04
C	243	LEU	-	EXPRESSION TAG	UNP Q18R04
C	244	ALA	-	EXPRESSION TAG	UNP Q18R04
C	245	ALA	-	EXPRESSION TAG	UNP Q18R04
C	246	ALA	-	EXPRESSION TAG	UNP Q18R04
C	247	LEU	-	EXPRESSION TAG	UNP Q18R04
C	248	ASP	-	EXPRESSION TAG	UNP Q18R04
C	249	HIS	-	EXPRESSION TAG	UNP Q18R04
C	250	HIS	-	EXPRESSION TAG	UNP Q18R04

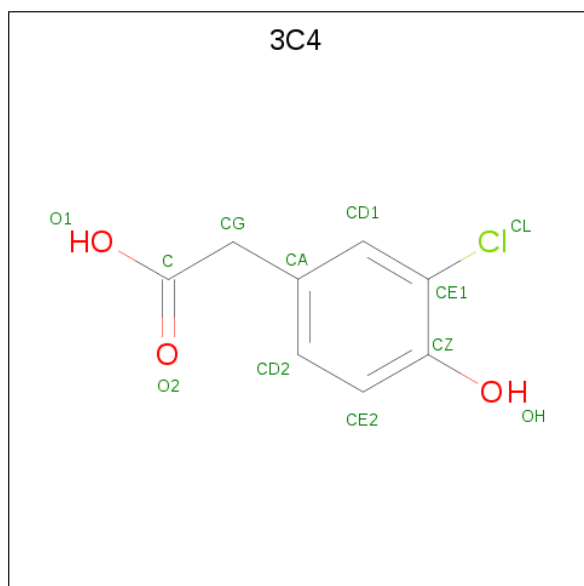
- Molecule 2 is a DNA chain called DNA (5'-D(P*DGP*DCP*DAP*DTP*DTP*DAP*DAP*DCP*DAP*DTP*DGP*DCP*DC)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	13	Total	C	N	O	P	0	0	0
			264	126	48	77	13			

- Molecule 3 is a DNA chain called DNA (5'-D(P*DGP*DGP*DCP*DAP*DTP*DGP*DTP*DTP*DAP*DAP*DTP*DGP*DC)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	A	13	Total	C	N	O	P	0	0	0
			269	128	49	79	13			

- Molecule 4 is (3-CHLORO-4-HYDROXYPHENYL)ACETIC ACID (three-letter code: 3C4) (formula: C₈H₇ClO₃).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	C	1	Total	C	Cl	O	0	0
			12	8	1	3		

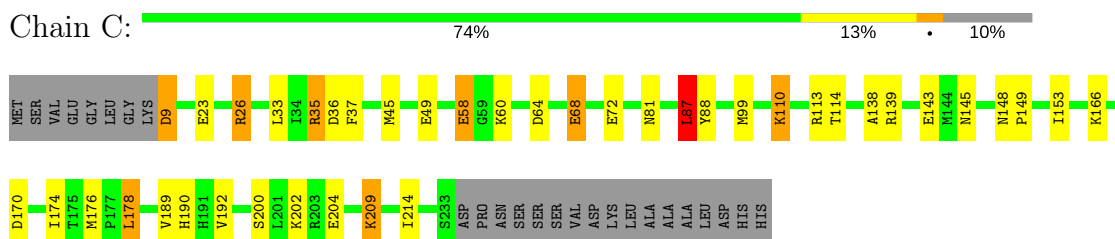
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	C	136	Total	O	0	0
			136	136		
5	B	6	Total	O	0	0
			6	6		
5	A	10	Total	O	0	0
			10	10		

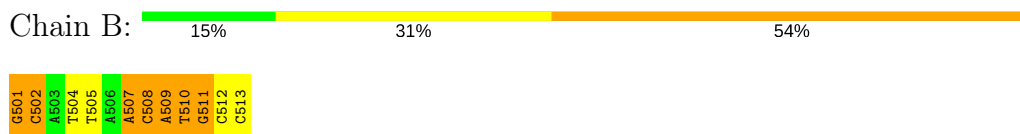
3 Residue-property plots [i](#)

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. 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.

- Molecule 1: Cyclic nucleotide-binding protein



- Molecule 2: DNA (5'-D(P*DGP*DCP*DAP*DTP*DTP*DAP*DAP*DCP*DAP*DTP*DGP*DCP*DC)-3')



- Molecule 3: DNA (5'-D(P*DGP*DGP*DCP*DAP*DTP*DGP*DTP*DTP*DAP*DAP*DTP*DGP*DC)-3')



4 Data and refinement statistics

Property	Value	Source
Space group	P 62 2 2	Depositor
Cell constants a, b, c, α , β , γ	100.60Å 100.60Å 149.66Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	27.48 – 1.80 25.72 – 1.80	Depositor EDS
% Data completeness (in resolution range)	99.4 (27.48-1.80) 99.4 (25.72-1.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.55 (at 1.80Å)	Xtriage
Refinement program	REFMAC 5.2	Depositor
R, R_{free}	0.217 , 0.250 0.221 , 0.248	Depositor DCC
R_{free} test set	2108 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	27.9	Xtriage
Anisotropy	0.145	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 57.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	2506	wwPDB-VP
Average B, all atoms (Å ²)	58.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.54% 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: 3C4

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	C	1.20	8/1849 (0.4%)	1.13	8/2495 (0.3%)
2	B	1.44	2/295 (0.7%)	2.40	19/452 (4.2%)
3	A	1.28	0/301	2.41	24/463 (5.2%)
All	All	1.24	10/2445 (0.4%)	1.58	51/3410 (1.5%)

The worst 5 of 10 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	36	ASP	C-O	8.76	1.40	1.23
1	C	68	GLU	CG-CD	8.11	1.64	1.51
1	C	68	GLU	CB-CG	7.65	1.66	1.52
1	C	36	ASP	CG-OD2	7.42	1.42	1.25
2	B	502	DC	C3'-O3'	-7.17	1.34	1.44

The worst 5 of 51 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	26	ARG	NE-CZ-NH1	14.64	127.62	120.30
2	B	513	DC	O4'-C4'-C3'	-13.20	98.08	106.00
1	C	26	ARG	NE-CZ-NH2	-12.36	114.12	120.30
2	B	508	DC	O4'-C1'-N1	11.99	116.39	108.00
3	A	540	DT	O4'-C1'-N1	-11.61	99.88	108.00

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	C	1809	0	1816	41	0
2	B	264	0	147	4	1
3	A	269	0	148	1	1
4	C	12	0	6	0	0
5	A	10	0	0	0	0
5	B	6	0	0	0	0
5	C	136	0	0	9	1
All	All	2506	0	2117	45	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 10.

The worst 5 of 45 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:C:190:HIS:CD2	1:C:192:VAL:HG13	1.84	1.11
1:C:190:HIS:HD2	1:C:192:VAL:HG13	1.39	0.87
1:C:214:ILE:HD11	5:C:1152:HOH:O	1.75	0.86
1:C:214:ILE:CD1	5:C:1152:HOH:O	2.26	0.83
1:C:26:ARG:HE	1:C:81:ASN:HD21	1.29	0.80

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)
2:B:501:DG:P	3:A:546:DC:O3'[11_555]	1.69	0.51
5:C:1123:HOH:O	5:C:1150:HOH:O[11_555]	1.88	0.32

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	C	224/250 (90%)	213 (95%)	11 (5%)	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	C	199/220 (90%)	190 (96%)	9 (4%)	30	14

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

Mol	Chain	Res	Type
1	C	110	LYS
1	C	209	LYS
1	C	170	ASP
1	C	58	GLU
1	C	143	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	81	ASN
1	C	180	GLN
1	C	190	HIS

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Mol	Chain	Res	Type
1	C	228	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](#)

1 ligand is 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
4	3C4	C	604	-	9,12,12	4.84	4 (44%)	13,16,16	2.92	8 (61%)

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
4	3C4	C	604	-	-	0/2/4/4	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	604	3C4	CE2-CD2	-7.83	1.25	1.38
4	C	604	3C4	CD1-CE1	-5.46	1.29	1.38
4	C	604	3C4	CE2-CZ	5.41	1.49	1.39
4	C	604	3C4	CZ-CE1	9.02	1.48	1.39

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	604	3C4	CE2-CZ-CE1	-7.84	110.87	118.55
4	C	604	3C4	CZ-CE1-CL	-2.17	115.20	119.50
4	C	604	3C4	C-CG-CA	2.14	117.75	112.43
4	C	604	3C4	CD1-CE1-CZ	2.14	122.20	120.95
4	C	604	3C4	OH-CZ-CE2	2.40	125.86	119.34

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 ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

6.3 Carbohydrates ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.

6.4 Ligands ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.

6.5 Other polymers ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.