



Full wwPDB X-ray Structure Validation Report

Feb 27, 2014 – 11:53 AM GMT

PDB ID : 4CB0
Title : Crystal structure of CpxAHDC in complex with ATP (hexagonal form)
Authors : Mechaly, A.E.; Sassoon, N.; Betton, J.M.; Alzari, P.M.
Deposited on : 2013-10-09
Resolution : 3.30 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

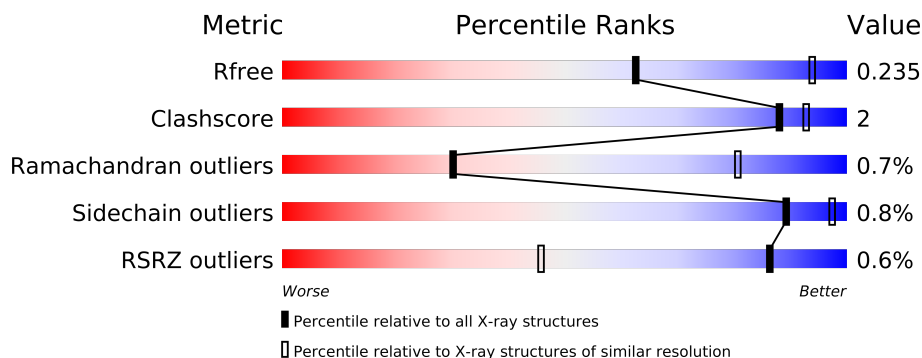
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

The reported resolution of this entry is 3.30 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}	66092	1341 (3.40-3.20)
Clashscore	79885	1696 (3.40-3.20)
Ramachandran outliers	78287	1664 (3.40-3.20)
Sidechain outliers	78261	1662 (3.40-3.20)
RSRZ outliers	66119	1342 (3.40-3.20)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	298	
1	B	298	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
3	SO4	B	1456	-	X

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 3716 atoms, of which 0 are hydrogen and 0 are deuterium.

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 SENSOR PROTEIN CPXA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	240	Total	C	N	O	Se	0	0	0
			1891	1180	339	366	6			
1	B	220	Total	C	N	O	Se	0	0	0
			1738	1088	310	335	5			

There are 56 discrepancies between the modelled and reference sequences:

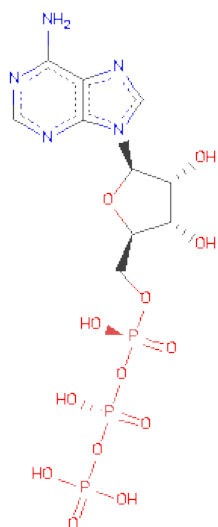
Chain	Residue	Modelled	Actual	Comment	Reference
A	160	MSE	-	EXPRESSION TAG	UNP P0AE82
A	161	GLY	-	EXPRESSION TAG	UNP P0AE82
A	162	SER	-	EXPRESSION TAG	UNP P0AE82
A	163	SER	-	EXPRESSION TAG	UNP P0AE82
A	164	HIS	-	EXPRESSION TAG	UNP P0AE82
A	165	HIS	-	EXPRESSION TAG	UNP P0AE82
A	166	HIS	-	EXPRESSION TAG	UNP P0AE82
A	167	HIS	-	EXPRESSION TAG	UNP P0AE82
A	168	HIS	-	EXPRESSION TAG	UNP P0AE82
A	169	HIS	-	EXPRESSION TAG	UNP P0AE82
A	170	SER	-	EXPRESSION TAG	UNP P0AE82
A	171	SER	-	EXPRESSION TAG	UNP P0AE82
A	172	GLY	-	EXPRESSION TAG	UNP P0AE82
A	173	LEU	-	EXPRESSION TAG	UNP P0AE82
A	174	VAL	-	EXPRESSION TAG	UNP P0AE82
A	175	PRO	-	EXPRESSION TAG	UNP P0AE82
A	176	ARG	-	EXPRESSION TAG	UNP P0AE82
A	177	GLY	-	EXPRESSION TAG	UNP P0AE82
A	178	SER	-	EXPRESSION TAG	UNP P0AE82
A	179	HIS	-	EXPRESSION TAG	UNP P0AE82
A	180	MSE	-	EXPRESSION TAG	UNP P0AE82
A	181	GLU	-	EXPRESSION TAG	UNP P0AE82
A	182	ASN	-	EXPRESSION TAG	UNP P0AE82
A	183	LEU	-	EXPRESSION TAG	UNP P0AE82
A	184	TYR	-	EXPRESSION TAG	UNP P0AE82

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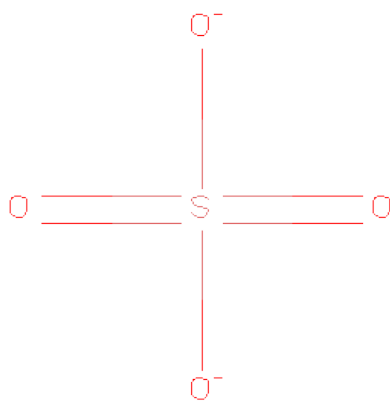
Chain	Residue	Modelled	Actual	Comment	Reference
A	185	PHE	-	EXPRESSION TAG	UNP P0AE82
A	186	GLN	-	EXPRESSION TAG	UNP P0AE82
A	187	GLY	-	EXPRESSION TAG	UNP P0AE82
B	160	MSE	-	EXPRESSION TAG	UNP P0AE82
B	161	GLY	-	EXPRESSION TAG	UNP P0AE82
B	162	SER	-	EXPRESSION TAG	UNP P0AE82
B	163	SER	-	EXPRESSION TAG	UNP P0AE82
B	164	HIS	-	EXPRESSION TAG	UNP P0AE82
B	165	HIS	-	EXPRESSION TAG	UNP P0AE82
B	166	HIS	-	EXPRESSION TAG	UNP P0AE82
B	167	HIS	-	EXPRESSION TAG	UNP P0AE82
B	168	HIS	-	EXPRESSION TAG	UNP P0AE82
B	169	HIS	-	EXPRESSION TAG	UNP P0AE82
B	170	SER	-	EXPRESSION TAG	UNP P0AE82
B	171	SER	-	EXPRESSION TAG	UNP P0AE82
B	172	GLY	-	EXPRESSION TAG	UNP P0AE82
B	173	LEU	-	EXPRESSION TAG	UNP P0AE82
B	174	VAL	-	EXPRESSION TAG	UNP P0AE82
B	175	PRO	-	EXPRESSION TAG	UNP P0AE82
B	176	ARG	-	EXPRESSION TAG	UNP P0AE82
B	177	GLY	-	EXPRESSION TAG	UNP P0AE82
B	178	SER	-	EXPRESSION TAG	UNP P0AE82
B	179	HIS	-	EXPRESSION TAG	UNP P0AE82
B	180	MSE	-	EXPRESSION TAG	UNP P0AE82
B	181	GLU	-	EXPRESSION TAG	UNP P0AE82
B	182	ASN	-	EXPRESSION TAG	UNP P0AE82
B	183	LEU	-	EXPRESSION TAG	UNP P0AE82
B	184	TYR	-	EXPRESSION TAG	UNP P0AE82
B	185	PHE	-	EXPRESSION TAG	UNP P0AE82
B	186	GLN	-	EXPRESSION TAG	UNP P0AE82
B	187	GLY	-	EXPRESSION TAG	UNP P0AE82

- Molecule 2 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
2	B	1	Total	C	N	O	P	0	0
			31	10	5	13	3		

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		

4 Data and refinement statistics

Property	Value	Source
Space group	P 61 2 2	Depositor
Cell constants a, b, c, α , β , γ	145.20Å 145.20Å 246.05Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	47.53 – 3.30 47.53 – 3.30	Depositor EDS
% Data completeness (in resolution range)	99.7 (47.53-3.30) 100.0 (47.53-3.30)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.27 (at 3.33Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.203 , 0.229 0.213 , 0.235	Depositor DCC
R_{free} test set	1217 reflections (5.13%)	DCC
Wilson B-factor (Å ²)	112.0	Xtriage
Anisotropy	0.782	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 158.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Outliers	0 of 23763 reflections	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	3716	wwPDB-VP
Average B, all atoms (Å ²)	189.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.55% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: SO4, ATP

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	0.62	0/1917	0.92	4/2585 (0.2%)
1	B	0.58	0/1762	0.86	3/2377 (0.1%)
All	All	0.60	0/3679	0.89	7/4962 (0.1%)

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	A	0	1

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	292	LEU	CA-CB-CG	7.32	132.13	115.30
1	A	418	GLY	N-CA-C	-6.49	96.88	113.10
1	A	432	ARG	NE-CZ-NH2	-5.55	117.53	120.30
1	A	223	ALA	N-CA-C	5.30	125.30	111.00
1	B	241	ARG	NE-CZ-NH2	-5.29	117.66	120.30
1	A	219	LEU	CB-CG-CD2	5.28	119.97	111.00
1	B	453	LEU	CA-CB-CG	5.08	126.99	115.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	217	GLU	Peptide

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1891	0	0	6	0
1	B	1738	0	0	4	0
2	A	31	0	0	0	0
2	B	31	0	0	1	0
3	A	20	0	0	0	0
3	B	5	0	0	0	0
All	All	3716	0	0	9	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 2.

All (9) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:283:ARG:NH2	1:B:316:GLU:OE1	2.27	0.67
1:A:330:LYS:NZ	1:A:362:LEU:O	2.38	0.56
1:A:251:ARG:NH2	1:A:289:ASN:OD1	2.41	0.53
1:B:330:LYS:NZ	1:B:362:LEU:O	2.46	0.49
1:A:248:HIS:NE2	2:B:501:ATP:O1G	2.46	0.48
1:A:280:GLU:OE1	1:B:256:ARG:NH1	2.48	0.47
1:A:396:ARG:NH2	1:A:439:ASP:OD1	2.47	0.47
1:A:218:PHE:C	1:A:220:ALA:N	2.70	0.43
1:B:324:GLU:OE2	1:B:359:ARG:NH2	2.54	0.41

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	238/298 (80%)	227 (95%)	8 (3%)	3 (1%)	18	69
1	B	214/298 (72%)	210 (98%)	4 (2%)	0	100	100
All	All	452/596 (76%)	437 (97%)	12 (3%)	3 (1%)	30	81

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	217	GLU
1	A	304	VAL
1	A	221	ALA

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	204/243 (84%)	203 (100%)	1 (0%)	94	98
1	B	188/243 (77%)	186 (99%)	2 (1%)	84	96
All	All	392/486 (81%)	389 (99%)	3 (1%)	89	97

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

Mol	Chain	Res	Type
1	A	254	LEU
1	B	291	LEU
1	B	381	THR

Some 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 chains in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

7 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	$\# Z > 2$
3	SO4	A	1456	-	4,4,4	0.15	0	6,6,6	0.11	0
3	SO4	A	1457	-	4,4,4	0.13	0	6,6,6	0.32	0
3	SO4	A	1458	-	4,4,4	0.26	0	6,6,6	0.37	0
3	SO4	A	1459	-	4,4,4	0.20	0	6,6,6	0.14	0
2	ATP	A	501	-	33,33,33	0.97	2 (6%)	52,52,52	1.83	9 (17%)
3	SO4	B	1456	-	4,4,4	0.18	0	6,6,6	0.18	0
2	ATP	B	501	-	33,33,33	1.05	2 (6%)	52,52,52	1.81	8 (15%)

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
3	SO4	A	1456	-	-	0/0/0/0	0/0/0/0
3	SO4	A	1457	-	-	0/0/0/0	0/0/0/0
3	SO4	A	1458	-	-	0/0/0/0	0/0/0/0
3	SO4	A	1459	-	-	0/0/0/0	0/0/0/0
2	ATP	A	501	-	-	0/22/38/38	0/1/3/3
3	SO4	B	1456	-	-	0/0/0/0	0/0/0/0
2	ATP	B	501	-	-	0/22/38/38	0/1/3/3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	501	ATP	C5-C4	3.26	1.47	1.40
2	A	501	ATP	C5-C4	2.91	1.47	1.40
2	B	501	ATP	C4-N9	-2.62	1.33	1.37
2	A	501	ATP	C4-N9	-2.45	1.34	1.37

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	501	ATP	N3-C2-N1	-5.86	123.81	128.71
2	B	501	ATP	N3-C2-N1	-5.82	123.84	128.71
2	B	501	ATP	N3-C4-N9	4.80	134.10	125.43
2	B	501	ATP	O4'-C1'-N9	4.79	112.89	108.44
2	A	501	ATP	N3-C4-N9	4.73	133.98	125.43
2	B	501	ATP	PA-O3A-PB	-4.67	118.00	131.68
2	A	501	ATP	O4'-C1'-N9	4.49	112.61	108.44
2	A	501	ATP	PA-O3A-PB	-4.35	118.91	131.68
2	A	501	ATP	C2'-C1'-N9	-3.20	105.05	113.27
2	B	501	ATP	C4-C5-N7	-3.05	106.91	109.52
2	B	501	ATP	C5-C4-N3	-2.99	119.20	125.70
2	A	501	ATP	C5-C4-N3	-2.98	119.21	125.70
2	A	501	ATP	C4-C5-N7	-2.89	107.05	109.52
2	A	501	ATP	C2-N3-C4	2.39	120.81	114.01
2	A	501	ATP	PB-O3B-PG	-2.29	124.96	131.68
2	B	501	ATP	C2-N3-C4	2.29	120.54	114.01
2	B	501	ATP	PB-O3B-PG	-2.17	125.33	131.68

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

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	240/298 (80%)	0.04	1 (0%)	90 57	143, 185, 244, 314	0
1	B	220/298 (73%)	0.06	1 (0%)	88 51	147, 179, 235, 277	0
All	All	460/596 (77%)	0.05	2 (0%)	86 57	143, 183, 240, 314	0

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	293	VAL	2.6
1	A	303	LEU	2.1

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

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	RSR	LLDF	B-factors(Å ²)	Q<0.9
3	SO4	B	1456	5/5	0.99	32.05	279,282,283,289	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
3	SO4	A	1456	5/5	0.25	0.12	217,222,227,227	0
2	ATP	A	501	31/31	0.25	-0.04	153,187,256,259	0
2	ATP	B	501	31/31	0.20	-0.52	151,196,223,226	0
3	SO4	A	1457	5/5	0.14	-1.26	202,202,207,210	0
3	SO4	A	1458	5/5	0.14	-1.69	222,225,234,246	0
3	SO4	A	1459	5/5	0.18	-2.51	281,281,285,286	0

6.5 Other polymers ⓘ

There are no such residues in this entry.