



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 22, 2020 – 11:10 AM BST

PDB ID : 2CKO
Title : Crystal structure of Human Choline Kinase alpha 2
Authors : Malito, E.; Lavie, A.
Deposited on : 2006-04-20
Resolution : 2.15 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 : 2.13.1
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) : 2.13.1

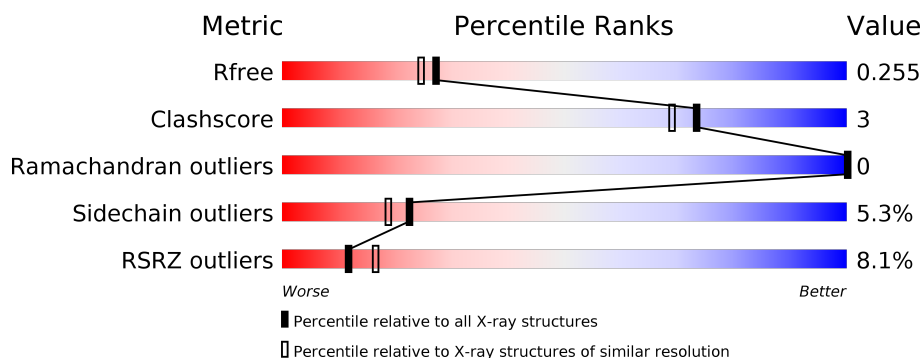
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.15 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	1479 (2.16-2.16)
Clashscore	141614	1585 (2.16-2.16)
Ramachandran outliers	138981	1560 (2.16-2.16)
Sidechain outliers	138945	1559 (2.16-2.16)
RSRZ outliers	127900	1456 (2.16-2.16)

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	390	<div> <div>9%</div> <div> <div></div> <div>79%</div> <div>8%</div> <div>12%</div> </div> </div>
1	B	390	<div> <div>6%</div> <div> <div></div> <div>79%</div> <div>9%</div> <div>11%</div> </div> </div>

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 6119 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.

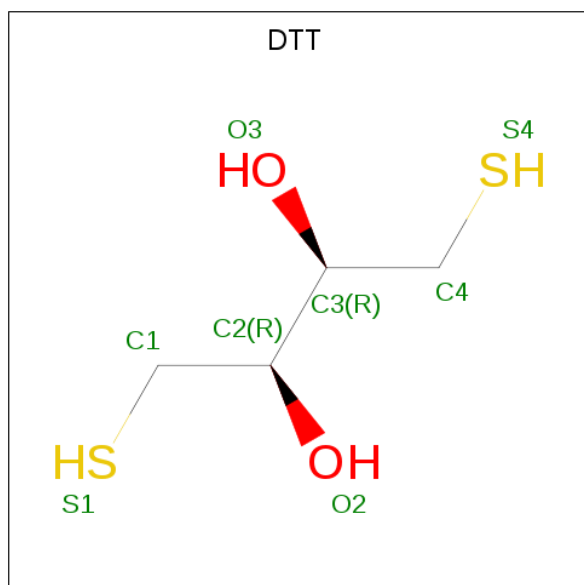
- Molecule 1 is a protein called CHOLINE KINASE ALPHA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	344	Total	C	N	O	S	0	0	0
			2830	1836	476	502	16			
1	B	346	Total	C	N	O	S	0	0	0
			2856	1852	480	508	16			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	220	SER	GLY	conflict	UNP P35790
A	422	LEU	GLN	conflict	UNP P35790
B	220	SER	GLY	conflict	UNP P35790
B	422	LEU	GLN	conflict	UNP P35790

- Molecule 2 is 2,3-DIHYDROXY-1,4-DITHIOBUTANE (three-letter code: DTT) (formula: C₄H₁₀O₂S₂).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total 8	C 4	O 2	S 2	0	0
2	B	1	Total 8	C 4	O 2	S 2	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	214	Total 214	O 214	0	0
3	B	203	Total 203	O 203	0	0

- Molecule 1: CHOLINE KINASE ALPHA



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	56.18Å 122.82Å 132.17Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.15 29.59 – 2.15	Depositor EDS
% Data completeness (in resolution range)	100.0 (30.00-2.15) 100.0 (29.59-2.15)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.72 (at 2.16Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.199 , 0.256 0.199 , 0.255	Depositor DCC
R_{free} test set	5080 reflections (10.05%)	wwPDB-VP
Wilson B-factor (Å ²)	33.4	Xtriage
Anisotropy	0.034	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 50.6	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	0.94	EDS
Total number of atoms	6119	wwPDB-VP
Average B, all atoms (Å ²)	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.37% 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

5.1 Standard geometry

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

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	0.68	0/2903	0.67	0/3907
1	B	0.67	0/2930	0.67	0/3945
All	All	0.67	0/5833	0.67	0/7852

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

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	2830	0	2789	14	0
1	B	2856	0	2820	22	0
2	A	8	0	10	0	0
2	B	8	0	10	1	0
3	A	214	0	0	2	0
3	B	203	0	0	4	0
All	All	6119	0	5629	37	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 3.

All (37) 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:104:ARG:HG2	1:A:104:ARG:HH11	1.42	0.82
1:B:339:ARG:CZ	1:B:405:MET:HE2	2.10	0.82
1:B:123:MET:HE2	1:B:123:MET:H	1.48	0.78
1:B:331:PHE:HE2	3:B:2023:HOH:O	1.70	0.74
1:A:392:ASN:OD1	3:A:2183:HOH:O	2.12	0.68
1:B:305:ASN:HD21	1:B:337:ASN:HD22	1.47	0.62
1:B:331:PHE:CE2	3:B:2023:HOH:O	2.47	0.61
1:A:195:LYS:H	1:A:207:GLN:HE21	1.49	0.60
1:B:389:ASP:OD1	3:B:2169:HOH:O	2.17	0.59
1:B:308:GLN:HE21	1:B:310:GLY:H	1.50	0.57
1:B:305:ASN:ND2	1:B:337:ASN:HD22	2.05	0.54
1:A:308:GLN:HE21	1:A:310:GLY:H	1.56	0.54
1:A:265:PHE:CD1	1:A:270:ARG:HD3	2.43	0.54
1:B:210:PRO:HB2	1:B:316:GLU:HG2	1.91	0.53
1:B:453:ARG:NH1	3:B:2200:HOH:O	2.28	0.52
1:B:383:LEU:HD21	1:B:405:MET:CE	2.39	0.51
1:A:387:GLN:NE2	3:A:2179:HOH:O	2.32	0.50
1:B:339:ARG:NH2	1:B:405:MET:HE2	2.26	0.50
1:A:116:ILE:HD11	1:A:126:GLN:HB2	1.93	0.50
1:B:396:GLU:O	1:B:400:ILE:HG12	2.13	0.49
1:A:126:GLN:HE21	1:A:142:LYS:NZ	2.11	0.49
1:B:131:ASP:N	1:B:131:ASP:OD1	2.44	0.48
1:A:104:ARG:HG2	1:A:104:ARG:NH1	2.18	0.48
1:A:204:ARG:HD2	1:A:206:GLU:OE1	2.14	0.48
1:A:313:LEU:O	1:A:326:LEU:HA	2.13	0.47
1:B:187:LEU:HD13	1:B:331:PHE:CD2	2.50	0.47
1:A:263:ILE:HD11	1:A:425:ILE:HG22	1.97	0.46
1:B:345:ASN:ND2	1:B:420:TRP:HE1	2.13	0.46
1:B:187:LEU:HD13	1:B:331:PHE:CE2	2.52	0.45
1:B:357:GLU:H	1:B:357:GLU:CD	2.19	0.45
2:B:1458:DTT:H12	2:B:1458:DTT:H41	1.57	0.44
1:A:89:ARG:HG3	1:A:108:GLU:OE2	2.20	0.42
1:B:448:TYR:CE2	1:B:452:LYS:HD2	2.55	0.41
1:A:387:GLN:HG3	1:A:390:PHE:HB2	2.01	0.41
1:B:256:TYR:O	1:B:260:VAL:HG23	2.20	0.41
1:B:383:LEU:HD21	1:B:405:MET:HE1	2.01	0.41
1:B:123:MET:HE2	1:B:123:MET:N	2.27	0.40

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	338/390 (87%)	323 (96%)	15 (4%)	0	100	100
1	B	342/390 (88%)	329 (96%)	13 (4%)	0	100	100
All	All	680/780 (87%)	652 (96%)	28 (4%)	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	A	301/349 (86%)	285 (95%)	16 (5%)	22	19
1	B	305/349 (87%)	289 (95%)	16 (5%)	23	19
All	All	606/698 (87%)	574 (95%)	32 (5%)	22	19

All (32) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	104	ARG
1	A	110	GLU
1	A	124	LEU
1	A	128	SER
1	A	145	LEU
1	A	179	LEU
1	A	192	LEU
1	A	257	LEU

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Mol	Chain	Res	Type
1	A	268	GLU
1	A	308	GLN
1	A	328	LEU
1	A	342	ASP
1	A	367	ARG
1	A	373	LYS
1	A	429	LYS
1	A	451	GLN
1	B	93	LEU
1	B	123	MET
1	B	131	ASP
1	B	177	MET
1	B	192	LEU
1	B	199	ILE
1	B	202	GLN
1	B	259	GLU
1	B	264	LYS
1	B	272	LYS
1	B	318	ARG
1	B	391	GLU
1	B	395	THR
1	B	399	SER
1	B	406	LEU
1	B	451	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	112	HIS
1	A	126	GLN
1	A	207	GLN
1	A	308	GLN
1	A	377	HIS
1	A	392	ASN
1	A	451	GLN
1	B	305	ASN
1	B	308	GLN
1	B	345	ASN
1	B	392	ASN
1	B	410	ASN
1	B	451	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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

2 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	DTT	A	1458	-	7,7,7	0.59	0	4,8,8	1.90	1 (25%)
2	DTT	B	1458	-	7,7,7	0.54	0	4,8,8	0.48	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	DTT	A	1458	-	-	4/8/8/8	-
2	DTT	B	1458	-	-	6/8/8/8	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
2	A	1458	DTT	C3-C4-S4	-3.40	104.59	114.47

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1458	DTT	C1-C2-C3-O3
2	A	1458	DTT	C1-C2-C3-C4
2	A	1458	DTT	O2-C2-C3-O3
2	A	1458	DTT	O2-C2-C3-C4
2	B	1458	DTT	S1-C1-C2-O2
2	B	1458	DTT	S1-C1-C2-C3
2	B	1458	DTT	C1-C2-C3-O3
2	B	1458	DTT	C1-C2-C3-C4
2	B	1458	DTT	O2-C2-C3-O3
2	B	1458	DTT	O2-C2-C3-C4

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	1458	DTT	1	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

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	344/390 (88%)	0.31	34 (9%) 7 11	17, 31, 68, 75	0
1	B	346/390 (88%)	0.22	22 (6%) 19 26	19, 33, 56, 65	0
All	All	690/780 (88%)	0.26	56 (8%) 12 16	17, 32, 63, 75	0

All (56) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	132	THR	6.0
1	B	320	ASN	5.5
1	A	150	ALA	5.0
1	A	149	GLY	4.9
1	A	148	TYR	4.8
1	B	120	LEU	4.7
1	B	388	ASN	4.1
1	A	151	ILE	4.1
1	B	317	GLY	4.0
1	B	119	GLY	4.0
1	A	121	SER	3.9
1	A	118	GLY	3.9
1	B	321	SER	3.8
1	A	109	ASP	3.7
1	A	115	VAL	3.7
1	A	131	ASP	3.5
1	A	116	ILE	3.2
1	B	333	TYR	3.2
1	B	115	VAL	3.0
1	A	433	ILE	2.9
1	B	389	ASP	2.9
1	A	136	LEU	2.8
1	A	112	HIS	2.8
1	A	135	THR	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	322	GLU	2.7
1	A	432	SER	2.7
1	B	319	GLU	2.7
1	B	228	ILE	2.7
1	B	176	ALA	2.7
1	A	147	LEU	2.7
1	A	123	MET	2.6
1	B	392	ASN	2.6
1	A	235	PHE	2.6
1	A	130	PRO	2.5
1	A	129	LEU	2.5
1	A	113	ILE	2.5
1	B	307	CYS	2.4
1	A	357	GLU	2.4
1	B	329	ILE	2.4
1	A	137	GLY	2.4
1	A	89	ARG	2.4
1	B	343	ILE	2.4
1	B	318	ARG	2.3
1	A	127	CYS	2.3
1	B	235	PHE	2.3
1	A	395	THR	2.3
1	B	357	GLU	2.2
1	A	105	GLY	2.2
1	A	331	PHE	2.2
1	A	134	ALA	2.2
1	A	144	LEU	2.1
1	B	177	MET	2.1
1	A	389	ASP	2.1
1	B	262	ARG	2.1
1	A	124	LEU	2.0
1	A	307	CYS	2.0

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 monosaccharides 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	DTT	A	1458	8/8	0.85	0.31	68,69,70,73	0
2	DTT	B	1458	8/8	0.87	0.14	66,66,67,68	0

6.5 Other polymers [i](#)

There are no such residues in this entry.