wwPDB X-ray Structure Validation Summary Report (i)

Feb 17, 2024 – 10:38 PM EST

PDB ID	:	4DGL
Title	:	Crystal Structure of the CK2 Tetrameric Holoenzyme
Authors	:	Lolli, G.; Battistutta, R.
Deposited on	:	2012-01-26
Resolution	:	3.00 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 (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (1)) were used in the production of this report:

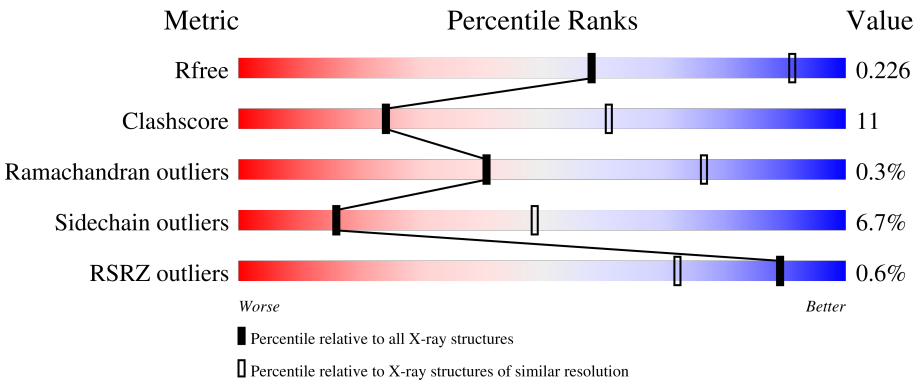
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

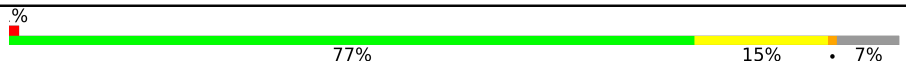
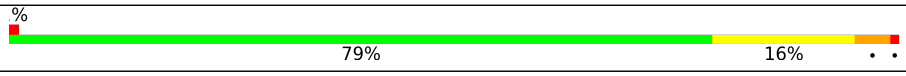
The reported resolution of this entry is 3.00 Å.

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	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (3.00-3.00)

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 of 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 <=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	215	
1	B	215	
2	C	335	
2	D	335	

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 8877 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 Casein kinase II subunit beta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	200	1633	1050	279	289	15	0	0	0
1	B	201	1643	1053	275	300	15	0	0	0

- Molecule 2 is a protein called Casein kinase II subunit alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	C	334	2815	1799	500	504	12	0	0	0
2	D	328	2772	1775	490	496	11	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	125	ARG	TYR	engineered mutation	UNP P68400
D	125	ARG	TYR	engineered mutation	UNP P68400

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Zn		
3	A	1	1	1	0	0
3	B	1	1	1	0	0

- Molecule 4 is water.

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

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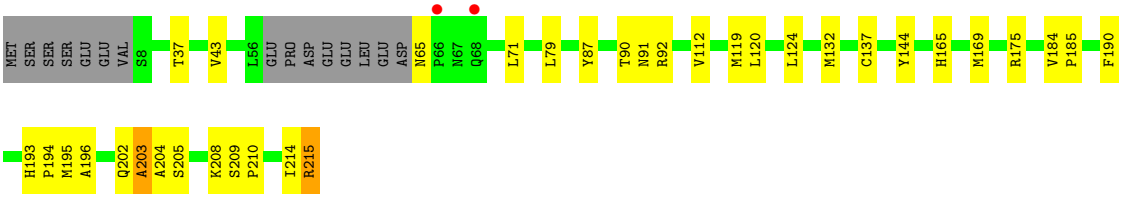
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	B	2	2	2	0	0
			Total	O		
4	C	4	4	4	0	0
			Total	O		
4	D	5	5	5	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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.

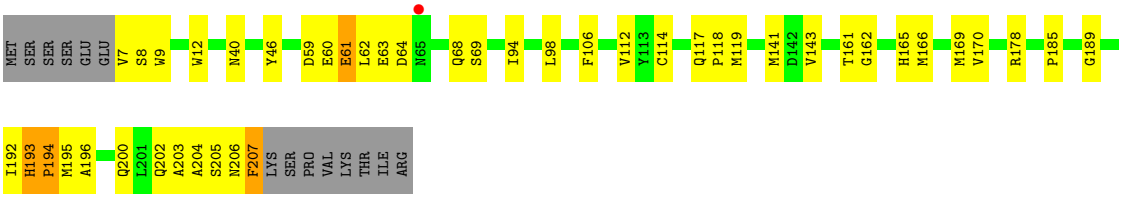
• Molecule 1: Casein kinase II subunit beta

Chain A:



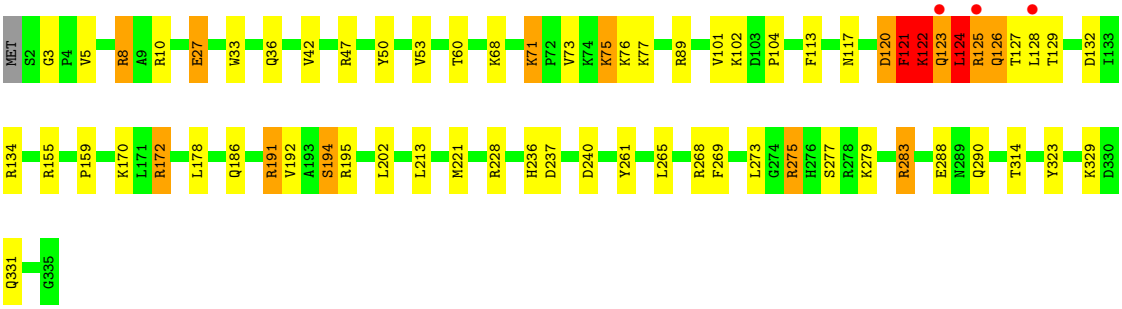
• Molecule 1: Casein kinase II subunit beta

Chain B:



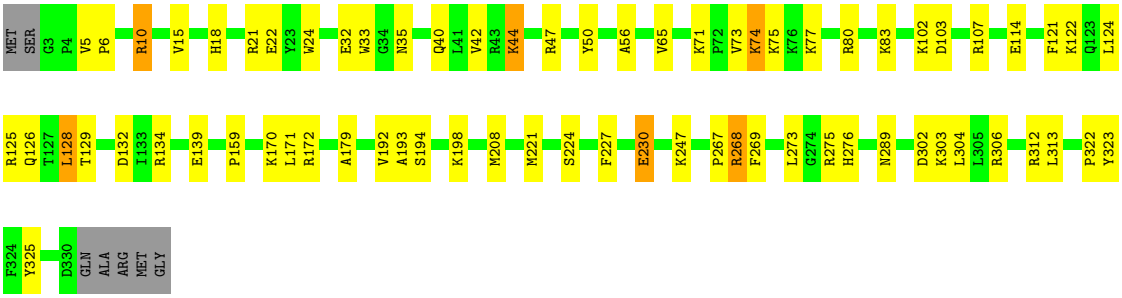
• Molecule 2: Casein kinase II subunit alpha

Chain C:



• Molecule 2: Casein kinase II subunit alpha

Chain D:


MET
SER
G3
P4
V5
P6
R10
V15
H18
R21
E22
Y23
W24
E32
W33
G34
N35
Q40
L41
V42
R43
K44
R47
Y50
A56
V65
K71
P72
V73
K74
K75
K76
K77
R80
K83
K102
D103
R107
E114
F121
K122
Q123
L124
R125
Q126
T127
L128
T129
D132
I133
R134
E139
P159
K170
L171
R172
A179
V192
A193
S194
K198
M208
M221
S224
F227
E230
K247
P267
R268
F269
L273
G274
R275
H276
N289
D302
K303
L304
L305
R306
R312
L313
P322
Y323
F324
Y325
D330
GLN
ALA
ARG
MET
GLY

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 63	Depositor
Cell constants a, b, c, α, β, γ	175.65Å 175.65Å 96.26Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	152.12 – 3.00 44.86 – 3.00	Depositor EDS
% Data completeness (in resolution range)	99.7 (152.12-3.00) 100.0 (44.86-3.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.12	Depositor
$< I/\sigma(I) >$ [1]	2.94 (at 3.01Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.195 , 0.222 0.198 , 0.226	Depositor DCC
R_{free} test set	1726 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å^2)	70.3	Xtriage
Anisotropy	0.857	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 34.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.033 for h,-h-k,-l	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	8877	wwPDB-VP
Average B, all atoms (Å^2)	92.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.29% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ 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: ZN

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	0.77	0/1682	0.73	1/2277 (0.0%)
1	B	0.83	4/1693 (0.2%)	0.85	3/2296 (0.1%)
2	C	0.79	1/2889 (0.0%)	0.85	8/3904 (0.2%)
2	D	0.78	3/2846 (0.1%)	0.79	1/3848 (0.0%)
All	All	0.79	8/9110 (0.1%)	0.81	13/12325 (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
2	C	0	1

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	24	TRP	CD2-CE2	5.92	1.48	1.41
2	D	114	GLU	CD-OE2	5.90	1.32	1.25
1	B	9	TRP	CD2-CE2	5.76	1.48	1.41
2	D	50	TYR	CE1-CZ	5.75	1.46	1.38
2	C	33	TRP	CD2-CE2	5.72	1.48	1.41

The worst 5 of 13 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	3	GLY	N-CA-C	-9.85	88.48	113.10
2	C	122	LYS	N-CA-C	-7.86	89.79	111.00
2	C	124	LEU	CB-CA-C	7.21	123.91	110.20
2	C	124	LEU	N-CA-C	-6.94	92.25	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	61	GLU	CB-CA-C	-6.94	96.51	110.40

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	C	71	LYS	Peptide

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	1633	0	1574	45	0
1	B	1643	0	1556	50	0
2	C	2815	0	2764	75	0
2	D	2772	0	2721	43	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	1	0	0	0	0
4	B	2	0	0	0	0
4	C	4	0	0	0	0
4	D	5	0	0	0	0
All	All	8877	0	8615	192	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 11.

The worst 5 of 192 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:61:GLU:O	1:B:62:LEU:HG	1.39	1.21
2:C:124:LEU:HD23	2:C:124:LEU:N	1.58	1.15
2:D:268:ARG:HH11	2:D:268:ARG:HG2	1.15	1.11
1:B:193:HIS:CG	1:B:194:PRO:HD2	1.85	1.10
2:C:8:ARG:HG2	2:C:8:ARG:HH11	1.14	1.08

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	196/215 (91%)	185 (94%)	10 (5%)	1 (0%)	29	68
1	B	199/215 (93%)	190 (96%)	8 (4%)	1 (0%)	29	68
2	C	332/335 (99%)	305 (92%)	26 (8%)	1 (0%)	41	76
2	D	326/335 (97%)	306 (94%)	20 (6%)	0	100	100
All	All	1053/1100 (96%)	986 (94%)	64 (6%)	3 (0%)	41	76

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	203	ALA
1	B	203	ALA
2	C	75	LYS

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	176/191 (92%)	168 (96%)	8 (4%)	27	64
1	B	177/191 (93%)	169 (96%)	8 (4%)	27	64
2	C	306/307 (100%)	278 (91%)	28 (9%)	9	34
2	D	302/307 (98%)	282 (93%)	20 (7%)	16	49

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	961/996 (96%)	897 (93%)	64 (7%)	16 49

5 of 64 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	D	170	LYS
2	D	208	MET
2	C	120	ASP
2	C	117	ASN
2	D	230	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 20 such sidechains are listed below:

Mol	Chain	Res	Type
2	C	331	GLN
2	D	186	GLN
2	D	290	GLN
2	D	276	HIS
1	B	193	HIS

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)

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

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 (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	200/215 (93%)	-0.29	2 (1%)	82	59	72, 102, 155, 190	0
1	B	201/215 (93%)	-0.57	1 (0%)	91	75	71, 89, 123, 174	0
2	C	334/335 (99%)	-0.55	3 (0%)	84	63	59, 83, 123, 180	0
2	D	328/335 (97%)	-0.62	0	100	100	58, 85, 116, 158	0
All	All	1063/1100 (96%)	-0.53	6 (0%)	89	72	58, 88, 133, 190	0

The worst 5 of 6 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	65	ASN	3.0
2	C	125	ARG	3.0
1	A	66	PRO	2.4
2	C	123	GLN	2.2
2	C	128	LEU	2.1

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(Å^2)	Q<0.9
3	ZN	A	301	1/1	0.99	0.15	75,75,75,75	0
3	ZN	B	301	1/1	0.99	0.12	73,73,73,73	0

6.5 Other polymers (i)

There are no such residues in this entry.