



wwPDB X-ray Structure Validation Summary Report ⓘ

Sep 11, 2023 – 06:05 AM EDT

PDB ID : 4MD7
Title : Crystal Structure of full-length symmetric CK2 holoenzyme
Authors : Lolli, G.; Ranchio, A.; Battistutta, R.
Deposited on : 2013-08-22
Resolution : 3.10 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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4.02b-467
Xtriage (Phenix) : 1.13
EDS : 2.35.1
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) : 2.35.1

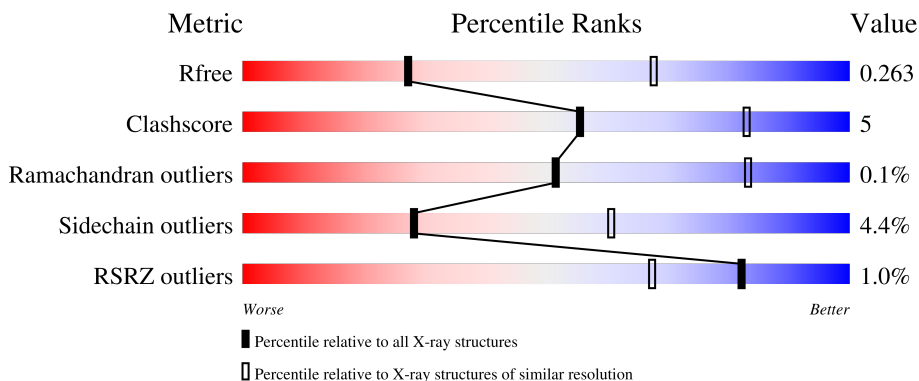
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.10 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.



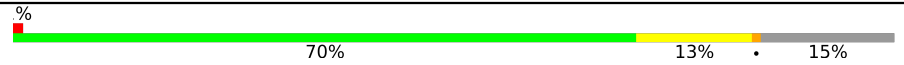


Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1094 (3.10-3.10)
Clashscore	141614	1184 (3.10-3.10)
Ramachandran outliers	138981	1141 (3.10-3.10)
Sidechain outliers	138945	1141 (3.10-3.10)
RSRZ outliers	127900	1067 (3.10-3.10)

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 $\leq 5\%$. 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	215	 81% 10% • 7%
1	B	215	 77% 13% • 9%
1	C	215	 79% 12% • 8%
1	D	215	 76% 13% • 9%
2	E	391	 72% 12% • 15%

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Mol	Chain	Length	Quality of chain
2	F	391	 <p>% 70% 13% 15%</p>
2	G	391	 <p>% 72% 12% 15%</p>
2	H	391	 <p>3% 75% 9% 16%</p>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 17621 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	199	Total 1622	C 1040	N 273	O 294	S 15	0	0	0
1	B	195	Total 1592	C 1024	N 268	O 285	S 15	0	0	0
1	C	197	Total 1605	C 1031	N 271	O 288	S 15	0	0	0
1	D	195	Total 1592	C 1024	N 268	O 285	S 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	E	332	Total 2804	C 1795	N 495	O 503	S 11	0	0	0
2	F	332	Total 2804	C 1795	N 495	O 503	S 11	0	0	0
2	G	332	Total 2804	C 1795	N 495	O 503	S 11	0	0	0
2	H	330	Total 2794	C 1790	N 493	O 500	S 11	0	0	0

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	344	GLU	THR	engineered mutation	UNP P68400
E	360	GLU	THR	engineered mutation	UNP P68400
E	362	GLU	SER	engineered mutation	UNP P68400
E	370	GLU	SER	engineered mutation	UNP P68400
F	344	GLU	THR	engineered mutation	UNP P68400
F	360	GLU	THR	engineered mutation	UNP P68400
F	362	GLU	SER	engineered mutation	UNP P68400
F	370	GLU	SER	engineered mutation	UNP P68400

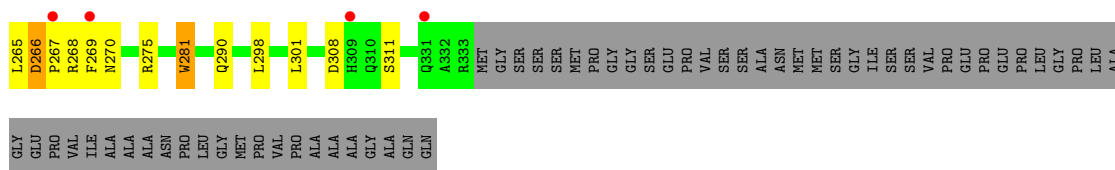
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Chain	Residue	Modelled	Actual	Comment	Reference
G	344	GLU	THR	engineered mutation	UNP P68400
G	360	GLU	THR	engineered mutation	UNP P68400
G	362	GLU	SER	engineered mutation	UNP P68400
G	370	GLU	SER	engineered mutation	UNP P68400
H	344	GLU	THR	engineered mutation	UNP P68400
H	360	GLU	THR	engineered mutation	UNP P68400
H	362	GLU	SER	engineered mutation	UNP P68400
H	370	GLU	SER	engineered mutation	UNP P68400

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

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



GLY
GLU
PRO
VAL
ILE
ALA
ALA
ALA
ASN
PRO
LEU
GLY
MET
PRO
VAL
PRO
ALA
ALA
ALA
GLY
ALA
GLN

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	142.32Å 57.96Å 186.19Å 90.00° 102.42° 90.00°	Depositor
Resolution (Å)	181.83 – 3.10 48.87 – 3.10	Depositor EDS
% Data completeness (in resolution range)	95.9 (181.83-3.10) 96.1 (48.87-3.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.16	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.52 (at 3.12Å)	Xtrriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.233 , 0.263 0.234 , 0.263	Depositor DCC
R_{free} test set	2681 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å ²)	50.5	Xtrriage
Anisotropy	0.499	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 38.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.41$, $\langle L^2 \rangle = 0.24$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.87	EDS
Total number of atoms	17621	wwPDB-VP
Average B, all atoms (Å ²)	56.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.21% 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:
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	0.56	0/1671	0.69	3/2265 (0.1%)
1	B	0.54	0/1641	0.73	4/2223 (0.2%)
1	C	0.50	1/1654 (0.1%)	0.65	3/2242 (0.1%)
1	D	0.49	1/1641 (0.1%)	0.68	4/2223 (0.2%)
2	E	0.56	3/2879 (0.1%)	0.62	0/3893
2	F	0.55	1/2879 (0.0%)	0.60	0/3893
2	G	0.52	2/2879 (0.1%)	0.61	2/3893 (0.1%)
2	H	0.51	2/2869 (0.1%)	0.57	1/3879 (0.0%)
All	All	0.53	10/18113 (0.1%)	0.63	17/24511 (0.1%)

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	216	TRP	CD2-CE2	5.55	1.48	1.41
1	C	12	TRP	CD2-CE2	5.30	1.47	1.41
2	G	33	TRP	CD2-CE2	5.27	1.47	1.41
1	D	9	TRP	CD2-CE2	5.21	1.47	1.41
2	H	281	TRP	CD2-CE2	5.16	1.47	1.41

The worst 5 of 17 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	47	ARG	NE-CZ-NH1	11.96	126.28	120.30
1	B	47	ARG	NE-CZ-NH2	-11.82	114.39	120.30
1	D	47	ARG	NE-CZ-NH2	-11.18	114.71	120.30
1	D	47	ARG	NE-CZ-NH1	11.00	125.80	120.30
1	A	47	ARG	NE-CZ-NH1	-10.54	115.03	120.30

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	1622	0	1534	21	0
1	B	1592	0	1517	26	0
1	C	1605	0	1524	27	0
1	D	1592	0	1517	25	1
2	E	2804	0	2748	26	0
2	F	2804	0	2748	34	0
2	G	2804	0	2748	27	1
2	H	2794	0	2741	16	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
All	All	17621	0	17077	177	1

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 5.

The worst 5 of 177 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:186:ARG:HG2	1:C:186:ARG:HH11	1.36	0.90
1:A:186:ARG:HH11	1:A:186:ARG:HG2	1.37	0.89
1:B:186:ARG:HH11	1:B:186:ARG:HG2	1.38	0.85
1:D:186:ARG:HG2	1:D:186:ARG:HH11	1.39	0.85
2:E:90:GLY:O	2:H:18:HIS:CG	2.32	0.83

All (1) 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:D:70:ASP:OD1	2:G:195:ARG:NH1[2_546]	2.12	0.08

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	195/215 (91%)	190 (97%)	5 (3%)	0	100	100
1	B	191/215 (89%)	186 (97%)	5 (3%)	0	100	100
1	C	193/215 (90%)	187 (97%)	6 (3%)	0	100	100
1	D	191/215 (89%)	185 (97%)	6 (3%)	0	100	100
2	E	330/391 (84%)	310 (94%)	19 (6%)	1 (0%)	41	73
2	F	330/391 (84%)	313 (95%)	17 (5%)	0	100	100
2	G	330/391 (84%)	308 (93%)	21 (6%)	1 (0%)	41	73
2	H	328/391 (84%)	312 (95%)	15 (5%)	1 (0%)	41	73
All	All	2088/2424 (86%)	1991 (95%)	94 (4%)	3 (0%)	51	83

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	G	268	ARG
2	H	269	PHE
2	E	125	TYR

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	174/191 (91%)	169 (97%)	5 (3%)	42	72
1	B	171/191 (90%)	167 (98%)	4 (2%)	50	77

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	172/191 (90%)	167 (97%)	5 (3%)	42	72
1	D	171/191 (90%)	162 (95%)	9 (5%)	22	54
2	E	305/347 (88%)	291 (95%)	14 (5%)	27	59
2	F	305/347 (88%)	289 (95%)	16 (5%)	23	55
2	G	305/347 (88%)	289 (95%)	16 (5%)	23	55
2	H	304/347 (88%)	290 (95%)	14 (5%)	27	59
All	All	1907/2152 (89%)	1824 (96%)	83 (4%)	28	61

5 of 83 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	G	47	ARG
2	H	32	GLU
2	G	119	THR
2	G	268	ARG
2	H	121	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 29 such sidechains are listed below:

Mol	Chain	Res	Type
2	F	118	ASN
2	H	234	HIS
2	F	331	GLN
2	G	310	GLN
2	F	310	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](#)

Of 4 ligands modelled in this entry, 4 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	199/215 (92%)	-0.52	0 100 100	14, 31, 61, 88	0
1	B	195/215 (90%)	-0.32	1 (0%) 91 81	21, 41, 71, 97	0
1	C	197/215 (91%)	-0.11	3 (1%) 73 54	39, 65, 109, 155	0
1	D	195/215 (90%)	-0.17	2 (1%) 82 67	36, 61, 90, 116	0
2	E	332/391 (84%)	-0.49	0 100 100	21, 36, 61, 95	0
2	F	332/391 (84%)	-0.29	2 (0%) 89 78	25, 45, 81, 100	0
2	G	332/391 (84%)	-0.14	2 (0%) 89 78	30, 61, 98, 123	0
2	H	330/391 (84%)	0.28	11 (3%) 46 24	51, 86, 116, 131	0
All	All	2112/2424 (87%)	-0.20	21 (0%) 82 67	14, 52, 103, 155	0

The worst 5 of 21 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	H	267	PRO	4.4
1	C	70	ASP	3.9
2	H	125	TYR	3.5
2	H	128	LEU	3.4
2	F	121	PHE	3.1

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	0.11	14,14,14,14	0
3	ZN	B	301	1/1	0.99	0.12	17,17,17,17	0
3	ZN	D	301	1/1	0.99	0.10	36,36,36,36	0
3	ZN	C	301	1/1	1.00	0.12	32,32,32,32	0

6.5 Other polymers [i](#)

There are no such residues in this entry.