



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 09:02 AM UTC

PDB ID : 6SG4 / pdb_00006sg4
Title : Structure of CDK2/cyclin A M246Q, S247EN
Authors : Salamina, M.; Basle, A.; Massa, B.; Noble, M.E.M.; Endicott, J.A.
Deposited on : 2019-08-02
Resolution : 2.43 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 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	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

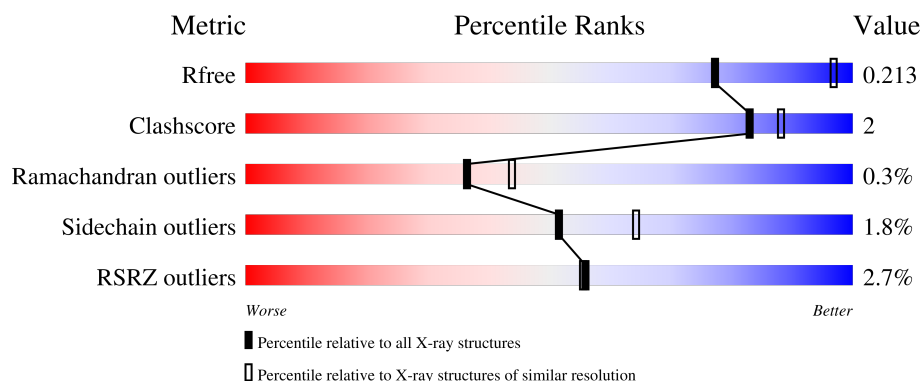
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.43 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}	180053	2340 (2.46-2.42)
Clashscore	190562	2400 (2.46-2.42)
Ramachandran outliers	187476	2379 (2.46-2.42)
Sidechain outliers	187428	2379 (2.46-2.42)
RSRZ outliers	180081	2340 (2.46-2.42)

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	302	
1	C	302	
2	B	269	
2	D	269	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 8485 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 Cyclin-dependent kinase 2.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	262	Total	C	N	O	P	S	0	1	0
			2112	1378	354	371	1	8			
1	C	261	Total	C	N	O	P	S	0	0	0
			2103	1372	358	365	1	7			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-3	GLY	-	expression tag	UNP P24941
A	-2	PRO	-	expression tag	UNP P24941
A	-1	GLY	-	expression tag	UNP P24941
A	0	SER	-	expression tag	UNP P24941
C	-3	GLY	-	expression tag	UNP P24941
C	-2	PRO	-	expression tag	UNP P24941
C	-1	GLY	-	expression tag	UNP P24941
C	0	SER	-	expression tag	UNP P24941

- Molecule 2 is a protein called Cyclin-A2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	258	Total	C	N	O	S	0	0	0
			2087	1350	341	386	10			
2	D	258	Total	C	N	O	S	0	0	0
			2086	1349	341	386	10			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	173	MET	-	initiating methionine	UNP P20248
B	246	GLN	MET	conflict	UNP P20248
B	247	GLU	-	insertion	UNP P20248
B	248	ASN	SER	conflict	UNP P20248

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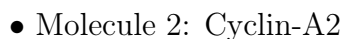
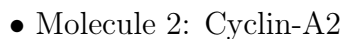
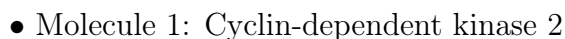
Chain	Residue	Modelled	Actual	Comment	Reference
B	434	LEU	-	expression tag	UNP P20248
B	435	GLU	-	expression tag	UNP P20248
B	436	HIS	-	expression tag	UNP P20248
B	437	HIS	-	expression tag	UNP P20248
B	438	HIS	-	expression tag	UNP P20248
B	439	HIS	-	expression tag	UNP P20248
B	440	HIS	-	expression tag	UNP P20248
B	441	HIS	-	expression tag	UNP P20248
D	173	MET	-	initiating methionine	UNP P20248
D	246	GLN	MET	conflict	UNP P20248
D	247	GLU	-	insertion	UNP P20248
D	248	ASN	SER	conflict	UNP P20248
D	434	LEU	-	expression tag	UNP P20248
D	435	GLU	-	expression tag	UNP P20248
D	436	HIS	-	expression tag	UNP P20248
D	437	HIS	-	expression tag	UNP P20248
D	438	HIS	-	expression tag	UNP P20248
D	439	HIS	-	expression tag	UNP P20248
D	440	HIS	-	expression tag	UNP P20248
D	441	HIS	-	expression tag	UNP P20248

- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	38	Total O 38 38	0	0
3	B	33	Total O 33 33	0	0
3	C	16	Total O 16 16	0	0
3	D	10	Total O 10 10	0	0

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- Molecule 1: Cyclin-dependent kinase 2



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	40.31Å 137.85Å 109.77Å 90.00° 99.81° 90.00°	Depositor
Resolution (Å)	85.10 – 2.43 85.10 – 2.43	Depositor EDS
% Data completeness (in resolution range)	99.4 (85.10-2.43) 99.5 (85.10-2.43)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.73 (at 2.42Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.201 , 0.251 (Not available) , 0.213	Depositor DCC
R_{free} test set	2130 reflections (4.32%)	wwPDB-VP
Wilson B-factor (Å ²)	37.5	Xtriage
Anisotropy	0.207	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 32.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.027 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	8485	wwPDB-VP
Average B, all atoms (Å ²)	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 27.89 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 2.0304e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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: TPO

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	1.04	1/2160 (0.0%)	1.39	3/2934 (0.1%)
1	C	1.05	1/2149 (0.0%)	1.43	0/2919
2	B	1.04	0/2137	1.48	2/2903 (0.1%)
2	D	1.02	0/2134	1.51	0/2895
All	All	1.04	2/8580 (0.0%)	1.45	5/11651 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	209	ILE	C-O	5.97	1.31	1.24
1	C	209	ILE	C-O	5.96	1.32	1.24

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	83	LEU	CA-C-N	5.54	129.13	120.82
1	A	83	LEU	C-N-CA	5.54	129.13	120.82
2	B	401	LYS	CA-C-N	5.17	126.55	120.09
2	B	401	LYS	C-N-CA	5.17	126.55	120.09
1	A	172	GLU	CB-CA-C	-5.00	102.18	110.68

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	2112	0	2152	10	0
1	C	2103	0	2144	18	0
2	B	2087	0	2102	13	0
2	D	2086	0	2099	6	0
3	A	38	0	0	0	0
3	B	33	0	0	0	0
3	C	16	0	0	0	0
3	D	10	0	0	0	0
All	All	8485	0	8497	40	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 2.

All (40) 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:278:LYS:NZ	2:B:181:ASP:OD2	2.16	0.78
1:A:177:CYS:SG	1:A:233:MET:SD	2.86	0.74
2:D:363:LEU:O	2:D:367:THR:HG23	1.92	0.69
1:A:252:VAL:HG11	1:A:255:LEU:HD12	1.76	0.68
2:B:190:GLU:O	2:B:194:LYS:HE3	1.96	0.65
1:C:177:CYS:SG	1:C:233:MET:SD	2.97	0.63
1:C:156:VAL:HG22	1:C:159:TYR:CE2	2.38	0.58
1:A:154:VAL:O	2:B:317:THR:CG2	2.55	0.55
1:C:64:VAL:HG21	1:C:144:ALA:HB2	1.88	0.54
1:C:162:GLU:OE2	1:C:208:GLU:OE1	2.27	0.53
2:B:206:ILE:HG22	2:B:210:MET:HE1	1.91	0.53
2:D:389:LYS:HB3	2:D:390:PRO:HD3	1.92	0.52
1:A:78:LEU:HD12	1:A:78:LEU:N	2.26	0.51
1:A:155:PRO:HD2	2:B:317:THR:HG23	1.92	0.50
1:A:154:VAL:O	2:B:317:THR:HG22	2.12	0.50
2:B:190:GLU:O	2:B:194:LYS:CE	2.59	0.50
2:B:203:GLN:HG2	2:B:206:ILE:HD11	1.94	0.49
1:C:154:VAL:O	2:D:317:THR:HG22	2.13	0.48
1:C:155:PRO:HD2	2:D:317:THR:HG23	1.96	0.47
1:C:35:ILE:HG22	1:C:77:TYR:CD1	2.50	0.46
2:D:210:MET:HE1	2:D:251:ARG:HB2	1.96	0.46
1:C:36:ARG:HD2	1:C:76:LEU:HD23	1.96	0.46
1:C:227:TRP:O	1:C:230:VAL:HG22	2.16	0.45
2:B:206:ILE:HG22	2:B:210:MET:CE	2.46	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:346:ASP:HA	2:B:347:PRO:HA	1.77	0.44
2:B:218:LEU:HB3	2:B:262:MET:CE	2.48	0.44
1:C:122:ARG:HA	1:C:152:PHE:CE1	2.53	0.43
1:C:156:VAL:CG2	1:C:159:TYR:CE2	3.02	0.43
1:C:158:THR:HA	1:C:178:LYS:O	2.19	0.42
2:B:218:LEU:HD13	2:B:262:MET:HE2	2.00	0.42
1:A:189:LEU:HD12	1:A:189:LEU:HA	1.81	0.42
1:C:51:GLU:O	1:C:55:LEU:HB2	2.20	0.42
1:C:116:ALA:O	1:C:120:SER:HB2	2.21	0.41
1:C:35:ILE:HG22	1:C:77:TYR:CE1	2.56	0.41
1:C:167:TRP:CD1	1:C:204:PRO:HA	2.56	0.41
1:A:154:VAL:O	2:B:317:THR:HG23	2.21	0.41
1:C:239:SER:O	1:C:240:PHE:C	2.63	0.41
2:D:182:ILE:O	2:D:186:LEU:HG	2.21	0.40
1:A:252:VAL:HG11	1:A:255:LEU:CD1	2.48	0.40
1:C:88:LYS:HB2	1:C:130:PRO:HB2	2.03	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	258/302 (85%)	249 (96%)	8 (3%)	1 (0%)	30	36
1	C	256/302 (85%)	238 (93%)	16 (6%)	2 (1%)	16	18
2	B	256/269 (95%)	254 (99%)	2 (1%)	0	100	100
2	D	255/269 (95%)	250 (98%)	5 (2%)	0	100	100
All	All	1025/1142 (90%)	991 (97%)	31 (3%)	3 (0%)	36	44

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	84	HIS
1	A	164	VAL
1	C	230	VAL

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	232/264 (88%)	231 (100%)	1 (0%)	84	89
1	C	230/264 (87%)	222 (96%)	8 (4%)	32	44
2	B	232/243 (96%)	228 (98%)	4 (2%)	53	66
2	D	231/243 (95%)	227 (98%)	4 (2%)	53	66
All	All	925/1014 (91%)	908 (98%)	17 (2%)	51	64

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	239	SER
2	B	194	LYS
2	B	282	ILE
2	B	317	THR
2	B	369	THR
1	C	33	LYS
1	C	44	VAL
1	C	120	SER
1	C	122	ARG
1	C	135	ILE
1	C	156	VAL
1	C	230	VAL
1	C	265	GLN
2	D	317	THR
2	D	332	SER
2	D	386	GLU
2	D	415	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10)

such sidechains are listed below:

Mol	Chain	Res	Type
1	A	85	GLN
1	A	268	HIS
2	B	297	HIS
2	B	420	HIS
2	B	432	ASN
1	C	62	ASN
2	D	314	GLN
2	D	327	ASN
2	D	420	HIS
2	D	432	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

2 non-standard protein/DNA/RNA residues 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	$\# Z > 2$
1	TPO	A	160	1	8,10,11	0.64	0	10,14,16	0.88	0
1	TPO	C	160	1	8,10,11	0.68	0	10,14,16	0.82	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
1	TPO	A	160	1	-	0/9/11/13	-
1	TPO	C	160	1	-	1/9/11/13	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	C	160	TPO	C-CA-CB-CG2

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

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	261/302 (86%)	-0.23	1 (0%) 88 90	15, 36, 65, 81	2 (0%)
1	C	260/302 (86%)	0.29	15 (5%) 29 25	29, 52, 87, 110	0
2	B	258/269 (95%)	-0.27	2 (0%) 82 83	22, 38, 55, 69	0
2	D	258/269 (95%)	0.28	10 (3%) 43 40	34, 53, 89, 98	0
All	All	1037/1142 (90%)	0.02	28 (2%) 56 55	15, 44, 80, 110	2 (0%)

All (28) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	43	GLY	4.2
2	B	193	CYS	3.9
1	C	161	HIS	3.3
1	C	295	HIS	3.3
1	C	35	ILE	3.2
1	C	225	VAL	3.1
2	B	175	VAL	3.1
1	C	29	VAL	3.0
1	C	239	SER	3.0
1	C	36	ARG	2.9
2	D	193	CYS	2.8
1	C	32	LEU	2.7
2	D	250	LEU	2.6
1	C	293	VAL	2.5
2	D	324	GLN	2.4
2	D	175	VAL	2.4
2	D	176	PRO	2.4
1	C	242	LYS	2.4
1	C	238	PRO	2.2
2	D	178	TYR	2.2
2	D	282	ILE	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	213	PHE	2.2
2	D	325	PRO	2.1
1	C	163	VAL	2.1
2	D	249	VAL	2.1
1	A	35	ILE	2.1
1	C	96	LEU	2.0
2	D	281	TYR	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [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
1	TPO	C	160	11/12	0.91	0.10	60,65,67,70	0
1	TPO	A	160	11/12	0.98	0.05	35,37,39,40	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.