Full wwPDB X-ray Structure Validation Report (i)

Dec 3, 2023 – 12:40 pm GMT

PDB ID	:	1OKW
Title	:	Cyclin A binding groove inhibitor Ac-Arg-Arg-Leu-Asn-(m-Cl-Phe)-NH2
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Deposited on	:	2003-07-31
Resolution	:	2.50 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 (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 (i)) were used in the production of this report:

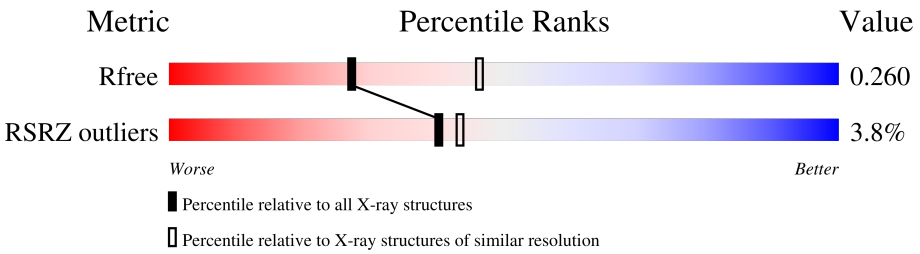
MolProbity	:	FAILED
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson 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 2.50 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	4661 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

MolProbity failed to run properly - the sequence quality summary graphics cannot be shown.

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 9569 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 CELL DIVISION PROTEIN KINASE 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	296	2378	1547	403	420	8	0	0	0
1	C	296	2378	1547	403	420	8	0	0	0

- Molecule 2 is a protein called CYCLIN A2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	258	2083	1350	339	383	11	0	0	0
2	D	258	2083	1350	339	383	11	0	0	0

- Molecule 3 is a protein called ACE-ARG-ARG-LEU-ASN-FCL-NH2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	Cl	N	O			
3	E	7	54	33	1	13	7	0	0	1
3	F	7	54	33	1	13	7	0	0	1

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	A	137	137	137	0	0
4	B	115	115	115	0	0
4	C	146	146	146	0	0
4	D	131	131	131	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	E	6	6	6	0	0
			Total	O		
4	F	4	4	4	0	0

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3 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	74.54Å 114.05Å 156.18Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	15.00 – 2.50 19.70 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.1 (15.00-2.50) 99.1 (19.70-2.50)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.56 (at 2.50Å)	Xtriage
Refinement program	REFMAC 5.0	Depositor
R, R_{free}	0.173 , 0.253 0.183 , 0.260	Depositor DCC
R_{free} test set	1437 reflections (3.10%)	wwPDB-VP
Wilson B-factor (Å^2)	29.8	Xtriage
Anisotropy	1.166	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 48.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	9569	wwPDB-VP
Average B, all atoms (Å^2)	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.45% 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.

4 Model quality (i)

4.1 Standard geometry (i)

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4.2 Too-close contacts (i)

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4.3 Torsion angles (i)

4.3.1 Protein backbone (i)

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4.3.2 Protein sidechains (i)

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4.3.3 RNA (i)

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4.4 Non-standard residues in protein, DNA, RNA chains (i)

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	$\#\|Z\| > 2$
3	FCL	E	506	3	11,12,13	0.77	1 (9%)	12,15,17	1.51	2 (16%)
3	FCL	F	506	3	11,12,13	0.79	0	12,15,17	2.45	4 (33%)

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	FCL	E	506	3	-	4/5/6/8	0/1/1/1
3	FCL	F	506	3	-	3/5/6/8	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	506	FCL	CE1-CL1	2.22	1.79	1.74

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	F	506	FCL	CG-CB-CA	-4.61	104.76	114.10
3	F	506	FCL	CB-CG-CD2	-4.33	112.32	120.91
3	E	506	FCL	CG-CB-CA	-3.97	106.06	114.10
3	F	506	FCL	CB-CG-CD1	3.79	126.94	120.44
3	F	506	FCL	CE1-CD1-CG	-2.44	116.88	119.71
3	E	506	FCL	CB-CG-CD2	-2.17	116.59	120.91

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	E	506	FCL	C-CA-CB-CG
3	F	506	FCL	C-CA-CB-CG
3	F	506	FCL	N-CA-CB-CG
3	E	506	FCL	N-CA-CB-CG
3	E	506	FCL	CA-CB-CG-CD2
3	F	506	FCL	CA-CB-CG-CD2
3	E	506	FCL	CA-CB-CG-CD1

There are no ring outliers.

No monomer is involved in short contacts.

4.5 Carbohydrates (i)

There are no monosaccharides in this entry.

4.6 Ligand geometry (i)

There are no ligands in this entry.

4.7 Other polymers (i)

There are no such residues in this entry.

4.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

5 Fit of model and data (i)

5.1 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	296/298 (99%)	-0.02	9 (3%) 50 53	25, 44, 88, 108	1 (0%)
1	C	296/298 (99%)	-0.02	14 (4%) 31 33	23, 42, 86, 122	0
2	B	258/260 (99%)	-0.11	12 (4%) 31 33	25, 42, 71, 116	0
2	D	258/260 (99%)	-0.05	6 (2%) 60 63	19, 43, 73, 111	0
3	E	4/7 (57%)	-0.03	0 100 100	30, 39, 52, 70	4 (100%)
3	F	4/7 (57%)	0.20	1 (25%) 0 0	41, 57, 58, 75	0
All	All	1116/1130 (98%)	-0.05	42 (3%) 40 43	19, 43, 83, 122	5 (0%)

All (42) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	39	THR	6.3
1	C	40	GLU	5.8
2	B	175	VAL	4.8
1	A	95	ALA	4.7
1	C	14	THR	4.3
1	A	296	LEU	4.1
1	C	163	VAL	4.1
2	B	325	ALA	3.9
1	A	96	LEU	3.7
2	B	176	PRO	3.6
2	D	323	GLN	3.5
1	A	159	TYR	3.3
2	B	324	PRO	3.0
2	D	325	ALA	3.0
2	D	432	LEU	2.8
1	C	98	GLY	2.7
1	C	95	ALA	2.7
1	C	165	THR	2.7
2	B	378	ARG	2.6

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Mol	Chain	Res	Type	RSRZ
1	C	13	GLY	2.6
2	B	179	HIS	2.5
1	C	38	ASP	2.5
1	A	163	VAL	2.4
1	C	36	ARG	2.4
2	B	178	TYR	2.4
1	A	177	CYS	2.3
3	F	505	ASN	2.3
1	C	295	HIS	2.3
1	C	96	LEU	2.3
1	A	160	THR	2.3
1	A	36	ARG	2.2
1	C	164	VAL	2.2
1	C	296	LEU	2.2
2	B	423	LEU	2.2
2	B	201	LYS	2.2
2	B	323	GLN	2.1
2	D	359	ALA	2.1
2	D	358	ALA	2.1
2	D	179	HIS	2.1
2	B	432	LEU	2.1
2	B	345	ASP	2.0
1	A	243	TRP	2.0

5.2 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
3	FCL	F	506	12/13	0.79	0.22	52,60,71,75	0
3	FCL	E	506	12/13	0.88	0.18	55,62,68,71	12

5.3 Carbohydrates (i)

There are no monosaccharides in this entry.

5.4 Ligands (i)

There are no ligands in this entry.

5.5 Other polymers (i)

There are no such residues in this entry.