



wwPDB X-ray Structure Validation Summary Report ⓘ

Jan 31, 2016 – 10:40 PM GMT

PDB ID : 1UNL
Title : STRUCTURAL MECHANISM FOR THE INHIBITION OF CD5-P25 FROM
THE ROSCOVITINE, ALOISINE AND INDIRUBIN.
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Deposited on : 2003-09-10
Resolution : 2.20 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
<http://wwpdb.org/validation/2016/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 : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

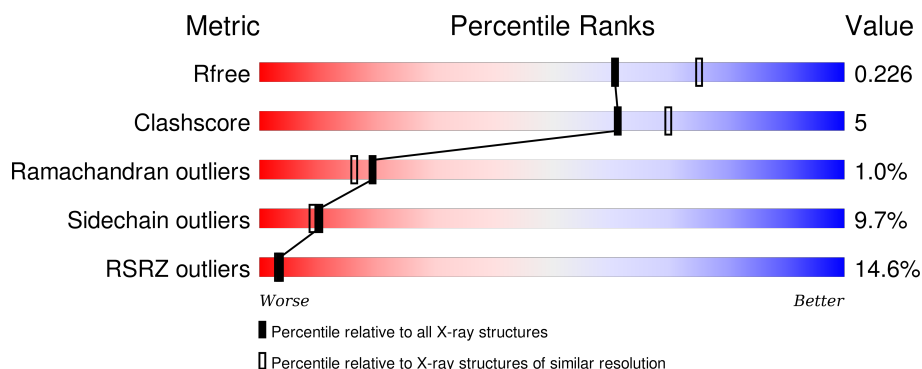
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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}	91344	3774 (2.20-2.20)
Clashscore	102246	4477 (2.20-2.20)
Ramachandran outliers	100387	4404 (2.20-2.20)
Sidechain outliers	100360	4405 (2.20-2.20)
RSRZ outliers	91569	3781 (2.20-2.20)

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. 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	292	<div> <div>8%</div> <div>77%</div> <div>18%</div> <div>• •</div> </div>
1	B	292	<div> <div>17%</div> <div>78%</div> <div>17%</div> <div>• •</div> </div>
2	D	208	<div> <div>63%</div> <div>8%</div> <div>28%</div> <div>•</div> </div>
2	E	208	<div> <div>26%</div> <div>55%</div> <div>14%</div> <div>28%</div> <div>•</div> </div>

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 7424 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 5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	292	Total	C	N	O	S	0	0	0
			2346	1505	403	426	12			
1	B	292	Total	C	N	O	S	0	0	0
			2346	1505	403	426	12			

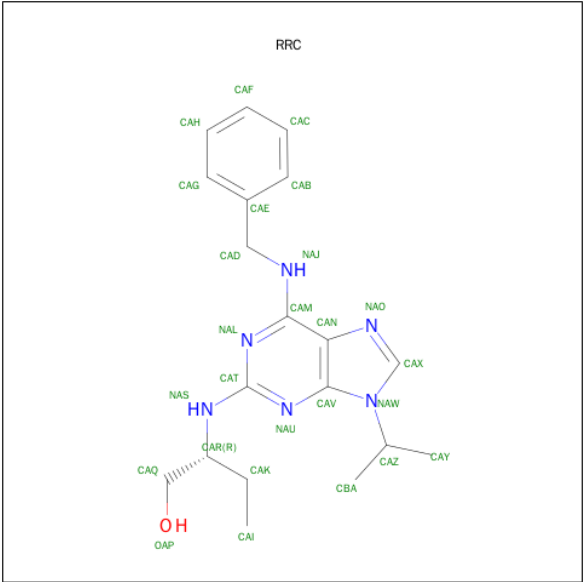
There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	144	ASN	ASP	ENGINEERED MUTATION	UNP Q00535
B	144	ASN	ASP	ENGINEERED MUTATION	UNP Q00535

- Molecule 2 is a protein called CYCLIN-DEPENDENT KINASE 5 ACTIVATOR 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	150	Total	C	N	O	S	0	0	1
			1202	771	199	221	11			
2	E	150	Total	C	N	O	S	0	0	1
			1202	771	199	221	11			

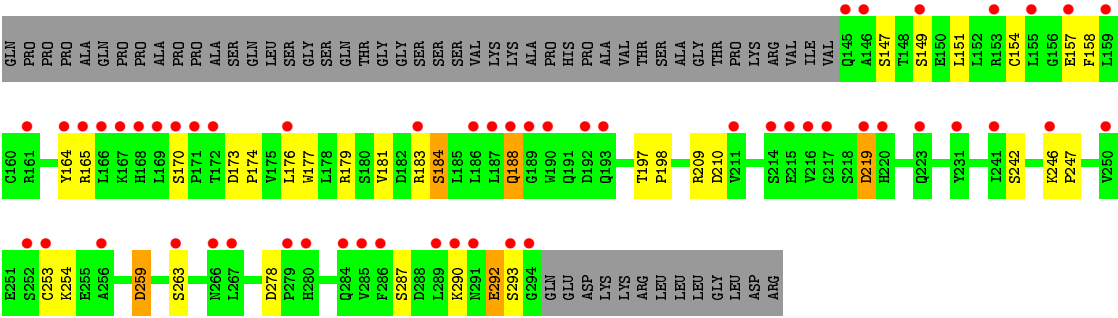
- Molecule 3 is R-ROSCOVITINE (three-letter code: RRC) (formula: C₁₉H₂₆N₆O).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			26	19	6	1		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	142	Total	O	0	0
			142	142		
4	B	80	Total	O	0	0
			80	80		
4	D	58	Total	O	0	0
			58	58		
4	E	22	Total	O	0	0
			22	22		



4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α , β , γ	117.99Å 117.99Å 156.17Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	19.76 – 2.20 19.66 – 2.20	Depositor EDS
% Data completeness (in resolution range)	94.4 (19.76-2.20) 94.4 (19.66-2.20)	Depositor EDS
R_{merge}	0.01	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.29 (at 2.21Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.216 , 0.219 0.218 , 0.226	Depositor DCC
R_{free} test set	3057 reflections (5.31%)	DCC
Wilson B-factor (Å ²)	36.4	Xtriage
Anisotropy	0.198	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.41 , 65.8	EDS
Estimated twinning fraction	0.022 for -h,-k,l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Outliers	1 of 60593 reflections (0.002%)	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	7424	wwPDB-VP
Average B, all atoms (Å ²)	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.52% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: RRC

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	0.84	5/2402 (0.2%)	0.97	16/3251 (0.5%)
1	B	0.68	1/2402 (0.0%)	0.92	16/3251 (0.5%)
2	D	0.79	0/1230	0.86	8/1669 (0.5%)
2	E	0.44	0/1230	0.67	4/1669 (0.2%)
All	All	0.72	6/7264 (0.1%)	0.89	44/9840 (0.4%)

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
1	A	0	2

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	73	ASP	C-N	-6.98	1.18	1.34
1	B	43	GLY	N-CA	6.62	1.55	1.46
1	A	53	CYS	CB-SG	-6.08	1.72	1.82
1	A	180	SER	CB-OG	5.44	1.49	1.42
1	A	74	LYS	N-CA	-5.30	1.35	1.46

The worst 5 of 44 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	198	ALA	N-CA-CB	11.59	126.33	110.10
1	A	72	SER	C-N-CA	-9.02	99.15	121.70
1	B	198	ALA	N-CA-CB	8.85	122.48	110.10
2	D	209	ARG	NE-CZ-NH1	8.21	124.41	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	235	ASP	CB-CG-OD2	8.12	125.61	118.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	41	ASP	Peptide
1	A	72	SER	Peptide

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	2346	0	2364	34	0
1	B	2346	0	2365	31	0
2	D	1202	0	1187	8	0
2	E	1202	0	1187	10	0
3	A	26	0	26	1	0
4	A	142	0	0	2	0
4	B	80	0	0	2	0
4	D	58	0	0	1	0
4	E	22	0	0	1	0
All	All	7424	0	7129	78	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 5.

The worst 5 of 78 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:73:ASP:OD1	1:A:74:LYS:N	1.85	1.08
1:A:73:ASP:OD1	1:A:75:LYS:N	1.89	1.04
1:A:72:SER:O	1:A:73:ASP:HB3	1.62	0.96
1:B:40:ASP:N	1:B:40:ASP:OD1	1.81	0.96
1:B:40:ASP:CG	1:B:41:ASP:N	2.30	0.85

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	290/292 (99%)	273 (94%)	15 (5%)	2 (1%)	26	25
1	B	290/292 (99%)	265 (91%)	19 (7%)	6 (2%)	9	5
2	D	148/208 (71%)	146 (99%)	2 (1%)	0	100	100
2	E	148/208 (71%)	142 (96%)	5 (3%)	1 (1%)	26	25
All	All	876/1000 (88%)	826 (94%)	41 (5%)	9 (1%)	19	16

5 of 9 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	40	ASP
1	B	11	GLY
1	B	163	VAL
1	A	73	ASP
1	A	163	VAL

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	260/260 (100%)	239 (92%)	21 (8%)	15	14
1	B	260/260 (100%)	230 (88%)	30 (12%)	7	6
2	D	138/186 (74%)	133 (96%)	5 (4%)	42	52

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	E	138/186 (74%)	117 (85%)	21 (15%)	3	2
All	All	796/892 (89%)	719 (90%)	77 (10%)	10	9

5 of 77 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	73	ASP
1	B	219	LEU
2	E	254	LYS
1	B	74	LYS
1	B	136	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 13 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	226	GLN
1	A	270	ASN
1	B	206	ASN
1	A	135	ASN
1	B	137	ASN

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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

1 ligand is 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	RRC	A	1293	-	24,28,28	0.89	2 (8%)	29,38,38	3.41	10 (34%)

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	RRC	A	1293	-	-	0/17/17/17	0/3/3/3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1293	RRC	CAN-CAV	-2.29	1.35	1.40
3	A	1293	RRC	CAX-NAO	2.13	1.38	1.34

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1293	RRC	CAZ-NAW-CAV	-9.11	116.33	127.15
3	A	1293	RRC	NAU-CAT-NAL	-5.28	118.12	126.22
3	A	1293	RRC	CAQ-CAR-NAS	-3.53	103.14	109.33
3	A	1293	RRC	CAK-CAR-CAQ	-2.64	107.39	111.62
3	A	1293	RRC	CAT-NAL-CAM	2.75	122.55	116.92

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1293	RRC	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 [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	292/292 (100%)	0.36	23 (7%) 15 15	18, 23, 33, 53	0
1	B	292/292 (100%)	0.96	51 (17%) 2 2	18, 24, 32, 53	0
2	D	150/208 (72%)	-0.01	1 (0%) 89 88	19, 23, 29, 32	0
2	E	150/208 (72%)	1.76	54 (36%) 0 0	20, 24, 25, 26	0
All	All	884/1000 (88%)	0.73	129 (14%) 3 3	18, 24, 31, 53	0

The worst 5 of 129 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	290	CYS	10.9
1	A	292	PRO	10.7
1	A	291	PRO	10.5
1	A	290	CYS	9.6
1	B	43	GLY	9.2

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 carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(\AA^2)	Q<0.9
3	RRC	A	1293	26/26	0.88	0.16	-0.23	19,23,24,25	0

6.5 Other polymers [i](#)

There are no such residues in this entry.