W O R L D W I D E

wwPDB

PROTEIN DATA BANK

wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 13, 2017 – 03:26 am GMT

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PDB ID	:	2GNG
Title	:	Protein kinase A fivefold mutant model of Rho-kinase
Authors	:	Bonn, S.; Herrero, S.; Breitenlechner, C.B.; Engh, R.A.; Gassel, M.; Bossemeyer, D.
Deposited on	:	2006-04-10
Resolution	:	1.87 Å(reported)

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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 1.87 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.
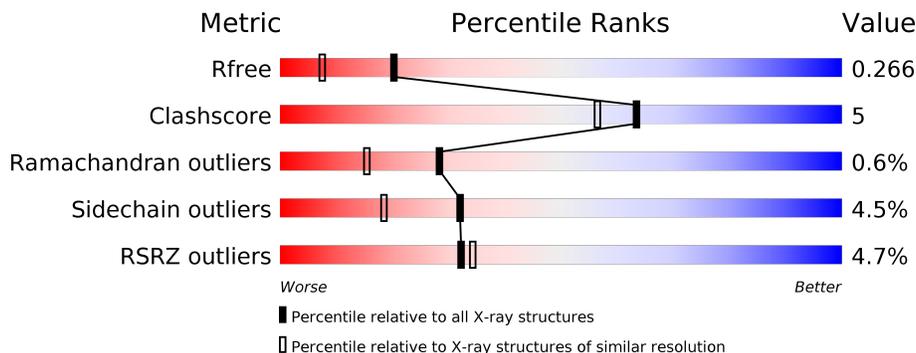
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	100719	7505 (1.90-1.86)
Clashscore	112137	8369 (1.90-1.86)
Ramachandran outliers	110173	8279 (1.90-1.86)
Sidechain outliers	110143	8280 (1.90-1.86)
RSRZ outliers	101464	7571 (1.90-1.86)

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 <=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	350	
2	I	20	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
1	SEP	A	10	-	-	X	-

2 Entry composition ⓘ

There are 3 unique types of molecules in this entry. The entry contains 3214 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 cAMP-dependent protein kinase, alpha-catalytic subunit.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	341	Total 2821	C 1823	N 472	O 513	P 3	S 10	0	0	0

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	10	SEP	SER	MODIFIED RESIDUE	UNP P00517
A	49	ILE	LEU	ENGINEERED	UNP P00517
A	123	MET	VAL	ENGINEERED	UNP P00517
A	127	ASP	GLU	ENGINEERED	UNP P00517
A	181	LYS	GLN	ENGINEERED	UNP P00517
A	183	ALA	THR	ENGINEERED	UNP P00517
A	197	TPO	THR	MODIFIED RESIDUE	UNP P00517
A	338	SEP	SER	MODIFIED RESIDUE	UNP P00517

- Molecule 2 is a protein called cAMP-dependent protein kinase inhibitor alpha.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	I	20	Total 157	C 94	N 32	O 31	0	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	213	Total 213	O 213	0	0
3	I	23	Total 23	O 23	0	0

3 Residue-property plots ⓘ

These plots are drawn for all protein, RNA and DNA 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: cAMP-dependent protein kinase, alpha-catalytic subunit
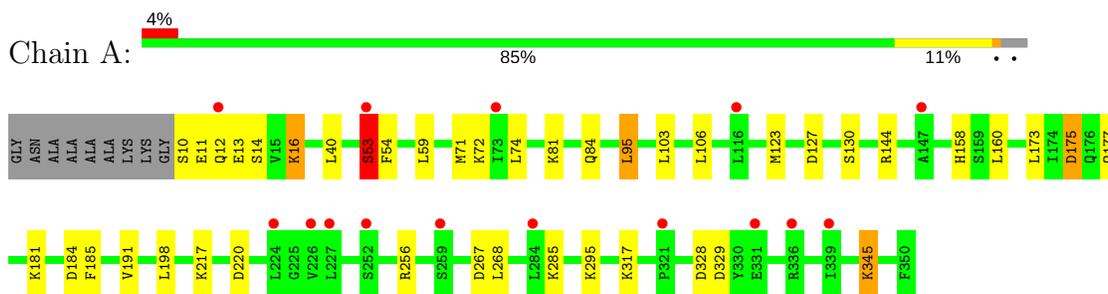
• Molecule 2: cAMP-dependent protein kinase inhibitor alpha
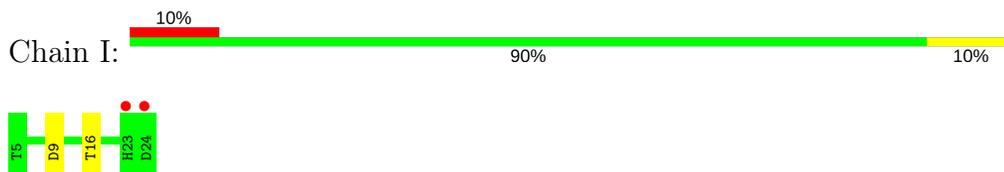
4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	71.91Å 76.40Å 80.72Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	21.98 – 1.87 21.96 – 1.76	Depositor EDS
% Data completeness (in resolution range)	79.1 (21.98-1.87) 78.0 (21.96-1.76)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.05 (at 1.76Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.195 , 0.258 0.206 , 0.266	Depositor DCC
R_{free} test set	1524 reflections (5.43%)	DCC
Wilson B-factor (Å^2)	30.9	Xtriage
Anisotropy	0.489	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 43.6	EDS
L-test for twinning[2]	$< |L| > = 0.49, < L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	3214	wwPDB-VP
Average B, all atoms (Å^2)	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.55% of the height of the origin peak. No significant pseudotranslation is detected.*

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[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 ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: TPO, SEP

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	0.79	1/2861 (0.0%)	0.86	8/3851 (0.2%)
2	I	0.70	0/159	1.08	1/212 (0.5%)
All	All	0.78	1/3020 (0.0%)	0.88	9/4063 (0.2%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	71	MET	SD-CE	-6.38	1.42	1.77

The worst 5 of 9 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	127	ASP	CB-CG-OD2	9.01	126.41	118.30
1	A	144	ARG	NE-CZ-NH2	-7.37	116.61	120.30
1	A	144	ARG	NE-CZ-NH1	6.95	123.77	120.30
1	A	191	VAL	CB-CA-C	-6.59	98.88	111.40
1	A	328	ASP	CB-CG-OD2	6.57	124.21	118.30

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	2821	0	2793	29	2
2	I	157	0	146	0	1
3	A	213	0	0	8	5
3	I	23	0	0	0	2
All	All	3214	0	2939	29	5

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 29 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:10:SEP:HA	1:A:13:GLU:HB2	1.38	1.06
1:A:54:PHE:CE2	1:A:84:GLN:HG3	2.06	0.90
1:A:10:SEP:N	1:A:13:GLU:HG3	1.89	0.86
1:A:123:MET:HE1	1:A:175:ASP:HB3	1.59	0.85
1:A:11:GLU:HG2	1:A:12:GLN:NE2	1.94	0.81

All (5) 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)
2:I:16:THR:CB	3:A:527:HOH:O[2_655]	1.70	0.50
3:A:391:HOH:O	3:I:599:HOH:O[2_654]	1.72	0.48
1:A:53:SER:OG	3:A:595:HOH:O[4_555]	1.95	0.25
1:A:13:GLU:CB	3:A:610:HOH:O[3_644]	2.06	0.14
3:A:486:HOH:O	3:I:579:HOH:O[2_654]	2.16	0.04

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	337/350 (96%)	323 (96%)	12 (4%)	2 (1%)	28	15
2	I	18/20 (90%)	17 (94%)	1 (6%)	0	100	100
All	All	355/370 (96%)	340 (96%)	13 (4%)	2 (1%)	28	15

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	53	SER
1	A	184	ASP

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	298/301 (99%)	284 (95%)	14 (5%)	30	17
2	I	15/15 (100%)	15 (100%)	0	100	100
All	All	313/316 (99%)	299 (96%)	14 (4%)	32	18

5 of 14 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	160	LEU
1	A	198	LEU
1	A	295	LYS
1	A	95	LEU
1	A	285	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	12	GLN
1	A	42	GLN
1	A	77	GLN
1	A	113	ASN

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Mol	Chain	Res	Type
1	A	158	HIS

5.3.3   RNA ⓘ

There are no RNA molecules in this entry.

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

3 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	SEP	A	10	1	9,9,10	1.62	2 (22%)	9,12,14	1.62	1 (11%)
1	TPO	A	197	1	9,10,11	0.77	0	10,14,16	1.09	1 (10%)
1	SEP	A	338	1	9,9,10	1.52	2 (22%)	9,12,14	1.91	2 (22%)

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	SEP	A	10	1	-	0/5/8/10	0/0/0/0
1	TPO	A	197	1	-	0/8/11/13	0/0/0/0
1	SEP	A	338	1	-	0/5/8/10	0/0/0/0

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	10	SEP	CA-C	2.10	1.53	1.50
1	A	338	SEP	P-O1P	2.64	1.59	1.50
1	A	338	SEP	CA-C	2.91	1.54	1.50
1	A	10	SEP	P-O1P	3.30	1.62	1.50

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	338	SEP	OG-P-O1P	2.13	112.45	106.47
1	A	197	TPO	OG1-P-O1P	2.13	117.62	109.26
1	A	10	SEP	OG-CB-CA	3.81	111.92	108.17
1	A	338	SEP	OG-CB-CA	4.71	112.81	108.17

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	10	SEP	5	0

5.5 Carbohydrates (i)

There are no carbohydrates 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	338/350 (96%)	0.24	15 (4%)	35	37	25, 36, 51, 60	6 (1%)
2	I	20/20 (100%)	0.10	2 (10%)	8	8	28, 31, 58, 62	0
All	All	358/370 (96%)	0.23	17 (4%)	32	34	25, 35, 51, 62	6 (1%)

The worst 5 of 17 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	12	GLN	5.7
2	I	24	ASP	3.4
1	A	339	ILE	3.2
1	A	331	GLU	3.0
2	I	23	HIS	2.7

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

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(Å^2)	Q<0.9
1	SEP	A	10	10/11	0.70	0.53	-	55,56,60,60	10
1	SEP	A	338	10/11	0.95	0.15	-	47,48,49,50	0
1	TPO	A	197	11/12	0.98	0.07	-	25,28,30,31	0

6.3   Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

There are no ligands in this entry.

6.5 Other polymers ⓘ

There are no such residues in this entry.