



wwPDB X-ray Structure Validation Summary Report ⓘ

Jan 10, 2018 – 05:20 PM EST

PDB ID : 6BCA
Title : A Complex between PH Domain of LbcRhoGEF (AKAP-Lbc) and Activated RhoA Bound to a GTP Analog
Authors : Sternweis, P.C.; Chen, Z.
Deposited on : 2017-10-20
Resolution : 2.00 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 : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20030736
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
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) : rb-20030736

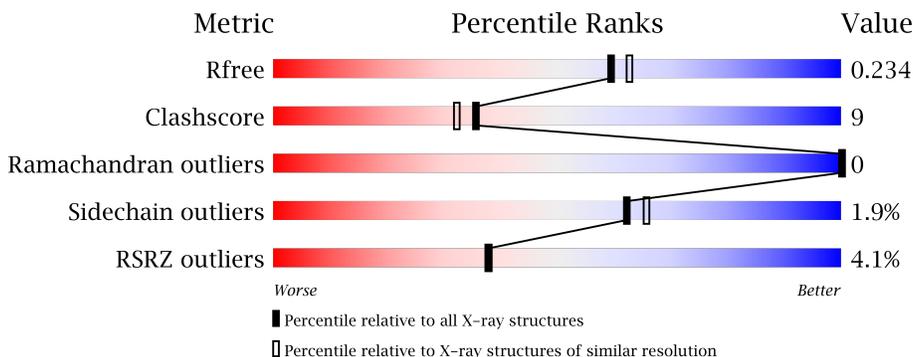
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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	6609 (2.00-2.00)
Clashscore	112137	7775 (2.00-2.00)
Ramachandran outliers	110173	7679 (2.00-2.00)
Sidechain outliers	110143	7678 (2.00-2.00)
RSRZ outliers	101464	6696 (2.00-2.00)

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	C	185	 5% (red), 81% (green), 15% (yellow), 8% (grey)
1	F	185	 3% (red), 78% (green), 19% (yellow), 8% (grey)
2	A	151	 3% (red), 74% (green), 17% (yellow), 8% (grey)
2	B	151	 3% (red), 72% (green), 17% (yellow), 8% (grey)

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 10841 atoms, of which 5197 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 Transforming protein RhoA.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
1	F	179	2829	897	1410	240	272	10	0	0	0
1	C	179	2829	897	1410	240	272	10	0	0	0

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	-3	GLY	-	expression tag	UNP P61586
F	-2	ILE	-	expression tag	UNP P61586
F	-1	LEU	-	expression tag	UNP P61586
F	0	ASP	-	expression tag	UNP P61586
C	-3	GLY	-	expression tag	UNP P61586
C	-2	ILE	-	expression tag	UNP P61586
C	-1	LEU	-	expression tag	UNP P61586
C	0	ASP	-	expression tag	UNP P61586

- Molecule 2 is a protein called A-kinase anchor protein 13.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
2	A	139	2293	713	1171	194	210	5	0	0	0
2	B	139	2311	719	1180	198	209	5	0	0	0

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	2189	GLY	-	expression tag	UNP Q12802
A	2190	ILE	-	expression tag	UNP Q12802
A	2191	LEU	-	expression tag	UNP Q12802
A	2192	ASP	-	expression tag	UNP Q12802

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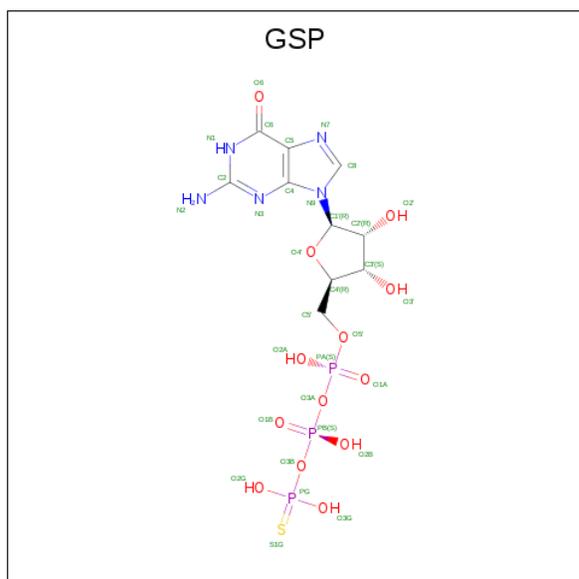
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Chain	Residue	Modelled	Actual	Comment	Reference
A	2334	HIS	-	expression tag	UNP Q12802
A	2335	HIS	-	expression tag	UNP Q12802
A	2336	HIS	-	expression tag	UNP Q12802
A	2337	HIS	-	expression tag	UNP Q12802
A	2338	HIS	-	expression tag	UNP Q12802
A	2339	HIS	-	expression tag	UNP Q12802
B	2189	GLY	-	expression tag	UNP Q12802
B	2190	ILE	-	expression tag	UNP Q12802
B	2191	LEU	-	expression tag	UNP Q12802
B	2192	ASP	-	expression tag	UNP Q12802
B	2334	HIS	-	expression tag	UNP Q12802
B	2335	HIS	-	expression tag	UNP Q12802
B	2336	HIS	-	expression tag	UNP Q12802
B	2337	HIS	-	expression tag	UNP Q12802
B	2338	HIS	-	expression tag	UNP Q12802
B	2339	HIS	-	expression tag	UNP Q12802

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	C	1	Total Mg 1 1	0	0
3	F	1	Total Mg 1 1	0	0

- Molecule 4 is 5'-GUANOSINE-DIPHOSPHATE-MONOTHIOPHOSPHATE (three-letter code: GSP) (formula: C₁₀H₁₆N₅O₁₃P₃S).



Mol	Chain	Residues	Atoms							ZeroOcc	AltConf
			Total	C	H	N	O	P	S		
4	F	1	45	10	13	5	13	3	1	0	0
4	C	1	45	10	13	5	13	3	1	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	F	156	Total 156	O 156	0	0
5	A	87	Total 87	O 87	0	0
5	B	89	Total 89	O 89	0	0
5	C	155	Total 155	O 155	0	0



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	51.35Å 60.52Å 63.62Å 91.83° 92.97° 90.01°	Depositor
Resolution (Å)	34.21 – 2.00 39.15 – 2.00	Depositor EDS
% Data completeness (in resolution range)	97.1 (34.21-2.00) 96.4 (39.15-2.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.10	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.23 (at 2.00Å)	Xtrriage
Refinement program	PHENIX 1.8_1069	Depositor
R, R_{free}	0.196 , 0.234 0.197 , 0.234	Depositor DCC
R_{free} test set	2500 reflections (4.95%)	DCC
Wilson B-factor (Å ²)	22.8	Xtrriage
Anisotropy	0.144	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.41 , 43.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	0.165 for -h,k,-l	Xtrriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	10841	wwPDB-VP
Average B, all atoms (Å ²)	24.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.11% of the height of the origin peak. No significant pseudotranslation is detected.*

¹ Intensities estimated from amplitudes.

² Theoretical 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: GSP, MG

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	C	0.68	0/1447	0.77	2/1956 (0.1%)
1	F	0.74	2/1447 (0.1%)	0.83	4/1956 (0.2%)
2	A	0.57	0/1133	0.70	1/1511 (0.1%)
2	B	0.60	0/1144	0.72	1/1526 (0.1%)
All	All	0.66	2/5171 (0.0%)	0.76	8/6949 (0.1%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	107	CYS	CB-SG	-6.32	1.71	1.82
1	F	34	TYR	CD2-CE2	-5.48	1.31	1.39

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	122	ARG	NE-CZ-NH2	-11.39	114.61	120.30
1	F	122	ARG	NE-CZ-NH1	10.08	125.34	120.30
1	C	70	ARG	NE-CZ-NH2	-7.23	116.68	120.30
1	C	70	ARG	NE-CZ-NH1	6.41	123.50	120.30
1	F	70	ARG	NE-CZ-NH1	5.42	123.01	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	C	1419	1410	1408	21	0
1	F	1419	1410	1408	25	0
2	A	1122	1171	1179	19	0
2	B	1131	1180	1183	36	0
3	C	1	0	0	0	0
3	F	1	0	0	0	0
4	C	32	13	12	0	0
4	F	32	13	12	0	0
5	A	87	0	0	2	0
5	B	89	0	0	8	0
5	C	155	0	0	1	0
5	F	156	0	0	3	0
All	All	5644	5197	5202	95	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 9.

The worst 5 of 95 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)
2:B:2312:GLU:OE2	2:B:2314:HIS:HE1	1.67	0.77
2:A:2204:ILE:O	2:A:2208:THR:HG23	1.85	0.77
2:B:2259:LEU:HD13	2:B:2259:LEU:C	2.05	0.77
1:F:167:VAL:O	1:F:170:VAL:HG12	1.85	0.75
2:A:2217:LYS:HD2	2:A:2307:ASP:O	1.86	0.74

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	C	177/185 (96%)	171 (97%)	6 (3%)	0	100	100
1	F	177/185 (96%)	171 (97%)	6 (3%)	0	100	100
2	A	135/151 (89%)	131 (97%)	4 (3%)	0	100	100
2	B	135/151 (89%)	131 (97%)	4 (3%)	0	100	100
All	All	624/672 (93%)	604 (97%)	20 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	C	156/160 (98%)	155 (99%)	1 (1%)	89	92
1	F	156/160 (98%)	154 (99%)	2 (1%)	73	78
2	A	126/137 (92%)	124 (98%)	2 (2%)	68	72
2	B	127/137 (93%)	121 (95%)	6 (5%)	30	26
All	All	565/594 (95%)	554 (98%)	11 (2%)	62	66

5 of 11 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	2208	THR
2	B	2238	VAL
2	B	2275	ASP
2	A	2329	GLN
2	B	2273	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
2	A	2314	HIS
2	B	2314	HIS

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](#)

Of 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 for Mogul analysis.

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
4	GSP	C	202	3	26,34,34	1.57	4 (15%)	24,54,54	2.23	6 (25%)
4	GSP	F	202	3	26,34,34	1.27	2 (7%)	24,54,54	1.77	4 (16%)

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
4	GSP	C	202	3	-	0/17/38/38	0/3/3/3
4	GSP	F	202	3	-	0/17/38/38	0/3/3/3

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	202	GSP	PG-S1G	-3.75	1.83	1.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	F	202	GSP	PG-S1G	-3.73	1.83	1.90
4	C	202	GSP	PA-O1A	-2.36	1.42	1.50
4	C	202	GSP	C2-N1	2.49	1.39	1.35
4	F	202	GSP	C6-N1	3.09	1.38	1.33

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	202	GSP	N3-C2-N1	-5.28	119.75	127.46
4	F	202	GSP	N3-C2-N1	-4.64	120.68	127.46
4	C	202	GSP	C5-C6-N1	-4.09	117.66	123.48
4	C	202	GSP	C4-C5-N7	-3.70	105.83	109.41
4	F	202	GSP	C5-C6-N1	-3.45	118.58	123.48

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	C	179/185 (96%)	0.47	10 (5%) 25 25	10, 15, 38, 47	0
1	F	179/185 (96%)	0.46	6 (3%) 46 46	10, 15, 35, 51	0
2	A	139/151 (92%)	0.24	5 (3%) 43 44	12, 21, 42, 51	0
2	B	139/151 (92%)	0.37	5 (3%) 43 44	12, 23, 46, 55	0
All	All	636/672 (94%)	0.39	26 (4%) 38 38	10, 18, 40, 55	0

The worst 5 of 26 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	2195	TYR	5.7
1	F	181	ALA	4.8
2	B	2267	GLN	4.0
1	C	181	ALA	3.6
2	B	2266	ASP	3.0

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
4	GSP	C	202	32/32	0.97	0.14	0.08	10,12,15,18	0
4	GSP	F	202	32/32	0.97	0.14	-0.09	9,11,14,16	0
3	MG	C	201	1/1	0.99	0.15	-0.18	10,10,10,10	0
3	MG	F	201	1/1	0.97	0.11	-1.51	10,10,10,10	0

6.5 Other polymers [i](#)

There are no such residues in this entry.