



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 31, 2017 – 06:39 AM EDT

PDB ID : 3IUG
Title : Crystal structure of the RhoGAP domain of RICS
Authors : Nedyalkova, L.; Tempel, W.; Tong, Y.; Li, Y.; Arrowsmith, C.H.; Edwards, A.M.; Bountra, C.; Weigelt, J.; Bochkarev, A.; Park, H.; Structural Genomics Consortium (SGC)
Deposited on : unknown
Resolution : 1.77 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

<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
Xtriage (Phenix) : 1.9-1692
EDS : rb-20030345
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-20030345

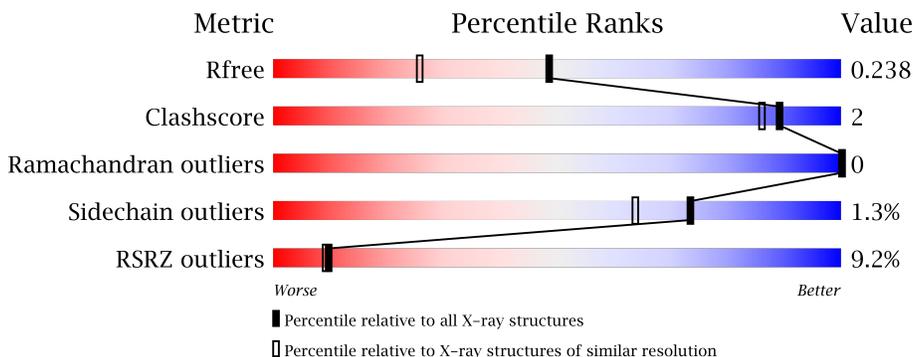
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.77 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	7172 (1.80-1.76)
Clashscore	112137	8247 (1.80-1.76)
Ramachandran outliers	110173	8154 (1.80-1.76)
Sidechain outliers	110143	8153 (1.80-1.76)
RSRZ outliers	101464	7262 (1.80-1.76)

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	229	 6% 75% 5% 20%
1	B	229	 9% 77% .. 19%

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
2	UNX	A	8	-	-	-	X
2	UNX	B	10	-	-	-	X
2	UNX	B	3	-	-	-	X
2	UNX	B	5	-	-	-	X
2	UNX	B	7	-	-	-	X

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 3315 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 Rho/Cdc42/Rac GTPase-activating protein RICS.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	184	1498	971	248	273	6	0	7	0
1	B	186	1497	969	248	274	6	0	8	0

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	349	MET	-	EXPRESSION TAG	UNP A7KAX9
A	350	HIS	-	EXPRESSION TAG	UNP A7KAX9
A	351	HIS	-	EXPRESSION TAG	UNP A7KAX9
A	352	HIS	-	EXPRESSION TAG	UNP A7KAX9
A	353	HIS	-	EXPRESSION TAG	UNP A7KAX9
A	354	HIS	-	EXPRESSION TAG	UNP A7KAX9
A	355	HIS	-	EXPRESSION TAG	UNP A7KAX9
A	356	SER	-	EXPRESSION TAG	UNP A7KAX9
A	357	SER	-	EXPRESSION TAG	UNP A7KAX9
A	358	GLY	-	EXPRESSION TAG	UNP A7KAX9
A	359	ARG	-	EXPRESSION TAG	UNP A7KAX9
A	360	GLU	-	EXPRESSION TAG	UNP A7KAX9
A	361	ASN	-	EXPRESSION TAG	UNP A7KAX9
A	362	LEU	-	EXPRESSION TAG	UNP A7KAX9
A	363	TYR	-	EXPRESSION TAG	UNP A7KAX9
A	364	PHE	-	EXPRESSION TAG	UNP A7KAX9
A	365	GLN	-	EXPRESSION TAG	UNP A7KAX9
A	366	GLY	-	EXPRESSION TAG	UNP A7KAX9
B	349	MET	-	EXPRESSION TAG	UNP A7KAX9
B	350	HIS	-	EXPRESSION TAG	UNP A7KAX9
B	351	HIS	-	EXPRESSION TAG	UNP A7KAX9
B	352	HIS	-	EXPRESSION TAG	UNP A7KAX9
B	353	HIS	-	EXPRESSION TAG	UNP A7KAX9
B	354	HIS	-	EXPRESSION TAG	UNP A7KAX9
B	355	HIS	-	EXPRESSION TAG	UNP A7KAX9

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Chain	Residue	Modelled	Actual	Comment	Reference
B	356	SER	-	EXPRESSION TAG	UNP A7KAX9
B	357	SER	-	EXPRESSION TAG	UNP A7KAX9
B	358	GLY	-	EXPRESSION TAG	UNP A7KAX9
B	359	ARG	-	EXPRESSION TAG	UNP A7KAX9
B	360	GLU	-	EXPRESSION TAG	UNP A7KAX9
B	361	ASN	-	EXPRESSION TAG	UNP A7KAX9
B	362	LEU	-	EXPRESSION TAG	UNP A7KAX9
B	363	TYR	-	EXPRESSION TAG	UNP A7KAX9
B	364	PHE	-	EXPRESSION TAG	UNP A7KAX9
B	365	GLN	-	EXPRESSION TAG	UNP A7KAX9
B	366	GLY	-	EXPRESSION TAG	UNP A7KAX9

- Molecule 2 is UNKNOWN ATOM OR ION (three-letter code: UNX) (formula: X).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	9	Total X 9 9	0	0
2	A	2	Total X 2 2	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	175	Total O 175 175	0	0
3	B	133	Total O 134 134	0	1

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	102.26Å 117.37Å 37.72Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 1.77 19.93 – 1.77	Depositor EDS
% Data completeness (in resolution range)	99.9 (20.00-1.77) 99.9 (19.93-1.77)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.23 (at 1.77Å)	Xtrriage
Refinement program	REFMAC 5.5.0102	Depositor
R, R_{free}	0.199 , 0.245 0.201 , 0.238	Depositor DCC
R_{free} test set	1027 reflections (2.33%)	DCC
Wilson B-factor (Å ²)	25.1	Xtrriage
Anisotropy	0.057	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 50.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	3315	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 14.94% 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, 0.333 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: UNX

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	0.83	0/1554	0.79	1/2114 (0.0%)
1	B	0.81	0/1555	0.80	2/2117 (0.1%)
All	All	0.82	0/3109	0.80	3/4231 (0.1%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	407	ARG	NE-CZ-NH1	6.81	123.70	120.30
1	B	531	ARG	NE-CZ-NH1	-5.98	117.31	120.30
1	A	438	ASP	CB-CG-OD2	5.57	123.31	118.30

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	A	1498	0	1486	7	0
1	B	1497	0	1473	7	0
2	A	2	0	0	0	0
2	B	9	0	0	0	0
3	A	175	0	0	3	0
3	B	134	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	3315	0	2959	13	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 (13) 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:560:LEU:O	1:A:563[A]:VAL:HG23	1.79	0.81
1:A:406:TYR:O	1:A:524[A]:VAL:HG11	2.05	0.57
1:B:568:SER:O	1:B:569:GLY:O	2.30	0.47
1:B:470:VAL:O	1:B:478:ARG:HD3	2.15	0.47
1:A:509:ASP:OD2	1:B:407:ARG:NH1	2.50	0.44
1:B:472:ALA:O	1:B:478:ARG:NH1	2.51	0.43
1:A:562:HIS:HE1	3:A:184:HOH:O	2.02	0.42
1:B:369:VAL:HG22	1:B:377:HIS:CE1	2.56	0.41
1:B:418:LEU:HD23	1:B:418:LEU:HA	1.95	0.41
1:A:560:LEU:O	1:A:563[A]:VAL:CG2	2.59	0.41
1:A:431:THR:HG22	3:A:185:HOH:O	2.21	0.40
1:B:531:ARG:HD2	3:B:154:HOH:O	2.21	0.40
1:A:416:GLN:HG2	3:A:134:HOH:O	2.21	0.40

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	187/229 (82%)	184 (98%)	3 (2%)	0	100	100
1	B	190/229 (83%)	186 (98%)	4 (2%)	0	100	100
All	All	377/458 (82%)	370 (98%)	7 (2%)	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	A	168/205 (82%)	165 (98%)	3 (2%)	64	50
1	B	166/205 (81%)	165 (99%)	1 (1%)	89	85
All	All	334/410 (82%)	330 (99%)	4 (1%)	73	67

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	427	VAL
1	A	470	VAL
1	A	532	SER
1	B	470	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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

Of 11 ligands modelled in this entry, 11 are unknown - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

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

There are no such residues in this entry.

5.8 Polymer linkage issues

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	184/229 (80%)	0.34	14 (7%) 15 14	14, 20, 37, 51	0
1	B	186/229 (81%)	0.52	20 (10%) 6 6	15, 22, 42, 55	0
All	All	370/458 (80%)	0.43	34 (9%) 10 9	14, 21, 40, 55	0

All (34) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	549	VAL	8.1
1	B	569	GLY	6.4
1	B	424	SER	5.9
1	A	435	TYR	5.8
1	B	551	ILE	5.2
1	A	431	THR	5.2
1	B	380	ASN	4.5
1	B	426	HIS	4.4
1	A	568	SER	4.4
1	A	436	VAL	3.6
1	B	425	GLU	3.5
1	B	411	VAL	3.5
1	B	532	SER	3.3
1	B	550	ARG	3.2
1	B	437	GLN	3.2
1	B	383	PHE	2.9
1	A	434	PRO	2.8
1	A	383	PHE	2.7
1	B	382	GLY	2.7
1	A	429	ASP	2.5
1	B	381	SER	2.4
1	A	433	GLU	2.3
1	A	374	LEU	2.2
1	B	420	HIS	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	568	SER	2.2
1	A	380	ASN	2.2
1	A	507[A]	LEU	2.2
1	B	463	TYR	2.1
1	A	401	ILE	2.1
1	A	381	SER	2.1
1	B	479	LEU	2.1
1	B	379	LEU	2.0
1	A	532	SER	2.0
1	B	388	VAL	2.0

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(Å ²)	Q<0.9
2	UNX	B	3	1/1	-0.09	1.80	114.81	2,2,2,2	1
2	UNX	A	8	1/1	0.32	2.01	76.39	2,2,2,2	1
2	UNX	B	5	1/1	0.54	3.17	75.21	2,2,2,2	1
2	UNX	B	10	1/1	-0.26	2.15	49.64	2,2,2,2	1
2	UNX	B	7	1/1	-0.87	1.12	16.78	2,2,2,2	1
2	UNX	A	6	1/1	-0.19	2.35	-	2,2,2,2	1
2	UNX	B	4	1/1	-0.25	1.11	-	2,2,2,2	1
2	UNX	B	2	1/1	0.45	1.71	-	2,2,2,2	1
2	UNX	B	9	1/1	-0.16	2.38	-	2,2,2,2	1
2	UNX	B	11	1/1	-0.38	1.78	-	2,2,2,2	1
2	UNX	B	1	1/1	-0.21	2.12	-	2,2,2,2	1

6.5 Other polymers [i](#)

There are no such residues in this entry.