Full wwPDB X-ray Structure Validation Report ⓘ

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PDB ID	:	3ISU
Title	:	Crystal structure of the RGC domain of IQGAP3
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Deposited on	:	2009-08-27
Resolution	:	1.88 Å(reported)

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1 Overall quality at a glance ⓘ

The reported resolution of this entry is 1.88 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	Percentile Ranks	Value
Rfree			0.245
Clashscore			5
Ramachandran outliers			0
Sidechain outliers			0
RSRZ outliers			2.0%

Worse   *Better*

▌ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution
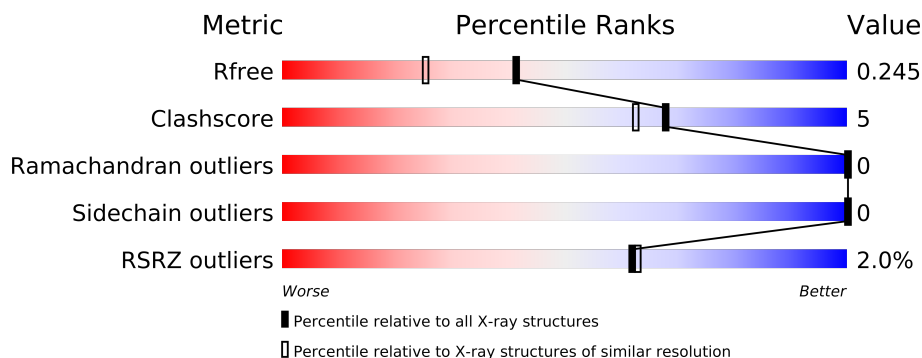
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	66092	5260 (1.90-1.86)
Clashscore	79885	6268 (1.90-1.86)
Ramachandran outliers	78287	6195 (1.90-1.86)
Sidechain outliers	78261	6196 (1.90-1.86)
RSRZ outliers	66119	5262 (1.90-1.86)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	121	

2 Entry composition ⓘ

There are 2 unique types of molecules in this entry. The entry contains 874 atoms, of which 0 are hydrogen and 0 are deuterium.

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 Ras GTPase-activating-likeprotein IQGAP3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	102	821	543	132	144	2	0	1	0

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1511	MET	-	EXPRESSION TAG	UNP Q86VI3
A	1512	HIS	-	EXPRESSION TAG	UNP Q86VI3
A	1513	HIS	-	EXPRESSION TAG	UNP Q86VI3
A	1514	HIS	-	EXPRESSION TAG	UNP Q86VI3
A	1515	HIS	-	EXPRESSION TAG	UNP Q86VI3
A	1516	HIS	-	EXPRESSION TAG	UNP Q86VI3
A	1517	HIS	-	EXPRESSION TAG	UNP Q86VI3
A	1518	SER	-	EXPRESSION TAG	UNP Q86VI3
A	1519	SER	-	EXPRESSION TAG	UNP Q86VI3
A	1520	GLY	-	EXPRESSION TAG	UNP Q86VI3
A	1521	ARG	-	EXPRESSION TAG	UNP Q86VI3
A	1522	GLU	-	EXPRESSION TAG	UNP Q86VI3
A	1523	ASN	-	EXPRESSION TAG	UNP Q86VI3
A	1524	LEU	-	EXPRESSION TAG	UNP Q86VI3
A	1525	TYR	-	EXPRESSION TAG	UNP Q86VI3
A	1526	PHE	-	EXPRESSION TAG	UNP Q86VI3
A	1527	GLN	-	EXPRESSION TAG	UNP Q86VI3
A	1528	GLY	-	EXPRESSION TAG	UNP Q86VI3

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
2	A	53	53	53	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 errors 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: Ras GTPase-activating-likeprotein IQGAP3

Chain A:
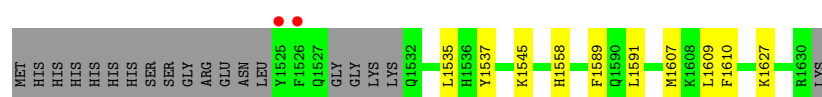
4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α, β, γ	58.12Å 58.12Å 78.29Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	40.00 – 1.88 30.90 – 1.88	Depositor EDS
% Data completeness (in resolution range)	99.9 (40.00-1.88) 99.9 (30.90-1.88)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	5.70 (at 1.88Å)	Xtriage
Refinement program	REFMAC 5.5.0102, coot, molprobity	Depositor
R, R_{free}	0.207 , 0.244 0.210 , 0.245	Depositor DCC
R_{free} test set	627 reflections (5.12%)	DCC
Wilson B-factor (Å^2)	30.3	Xtriage
Anisotropy	0.101	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 39.3	EDS
Estimated twinning fraction	0.034 for -h,-k,l	Xtriage
L-test for twinning	$< |L| > = 0.49, < L^2 > = 0.33$	Xtriage
Outliers	0 of 12877 reflections	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	874	wwPDB-VP
Average B, all atoms (Å^2)	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.88% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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	0.81	0/841	0.83	2/1136 (0.2%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1591	LEU	CA-CB-CG	5.41	127.74	115.30
1	A	1607	MET	CA-CB-CG	5.08	121.93	113.30

There are no chirality outliers.

There are no planarity outliers.

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	821	0	810	8	0
2	A	53	0	0	1	0
All	All	874	0	810	8	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 5.

All (8) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:1535:LEU:HD21	1:A:1627:LYS:HB3	1.65	0.79
1:A:1558:HIS:ND1	2:A:45:HOH:O	2.30	0.65
1:A:1535:LEU:HD21	1:A:1627:LYS:CB	2.30	0.61
1:A:1589:PHE:HZ	1:A:1609:LEU:HD22	1.81	0.45
1:A:1537:TYR:CE1	1:A:1545:LYS:HE3	2.53	0.44
1:A:1589:PHE:CZ	1:A:1609:LEU:HD22	2.52	0.44
1:A:1589:PHE:HE2	1:A:1610:PHE:CZ	2.37	0.43
1:A:1535:LEU:HD21	1:A:1627:LYS:CG	2.49	0.42

There are no symmetry-related clashes.

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	99/121 (82%)	97 (98%)	2 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	84/106 (79%)	84 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

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

5.3.3 RNA ⓘ

There are no RNA chains in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

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	102/121 (84%)	-0.09	2 (1%) 62	63	19, 29, 47, 57	0

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1525	TYR	3.0
1	A	1526	PHE	2.3

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

There are no non-standard protein/DNA/RNA residues in this entry.

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.