



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 28, 2014 – 04:12 PM GMT

PDB ID : 4JGW
Title : The conformation of a docking site for SH3 domains is pre-selected in the Guanine Nucleotide Exchange Factor Rlf
Authors : Rehmann, H.; Popovic, M.; Jakobi, A.J.
Deposited on : 2013-03-04
Resolution : 2.30 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

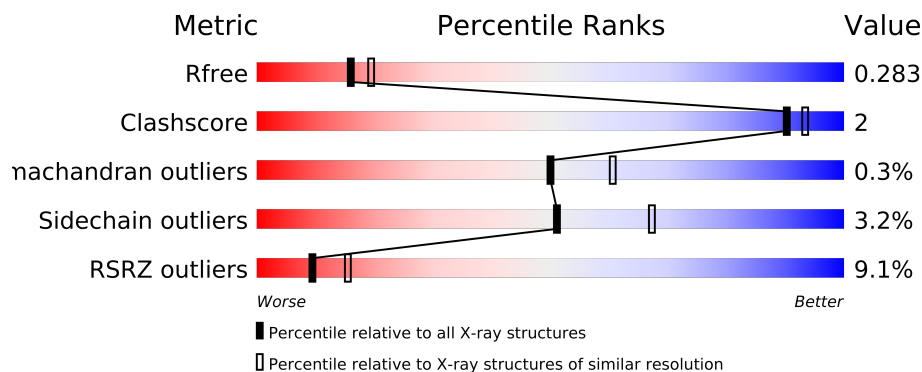
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

The reported resolution of this entry is 2.30 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}	66092	2929 (2.30-2.30)
Clashscore	79885	3679 (2.30-2.30)
Ramachandran outliers	78287	3642 (2.30-2.30)
Sidechain outliers	78261	3641 (2.30-2.30)
RSRZ outliers	66119	2930 (2.30-2.30)

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	473	
1	B	473	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 6299 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 Ral guanine nucleotide dissociation stimulator-like 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	396	Total	C	N	O	S	0	0	0
			3059	1936	535	579	9			
1	B	396	Total	C	N	O	S	0	0	0
			3058	1933	546	570	9			

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	42	GLY	-	EXPRESSION TAG	UNP Q61193
A	43	PRO	-	EXPRESSION TAG	UNP Q61193
A	44	LEU	-	EXPRESSION TAG	UNP Q61193
A	45	GLY	-	EXPRESSION TAG	UNP Q61193
A	46	SER	-	EXPRESSION TAG	UNP Q61193
A	47	PRO	-	EXPRESSION TAG	UNP Q61193
A	48	ASN	-	EXPRESSION TAG	UNP Q61193
A	49	SER	-	EXPRESSION TAG	UNP Q61193
A	147	TYR	HIS	SEE REMARK 999	UNP Q61193
A	402	THR	MET	SEE REMARK 999	UNP Q61193
B	42	GLY	-	EXPRESSION TAG	UNP Q61193
B	43	PRO	-	EXPRESSION TAG	UNP Q61193
B	44	LEU	-	EXPRESSION TAG	UNP Q61193
B	45	GLY	-	EXPRESSION TAG	UNP Q61193
B	46	SER	-	EXPRESSION TAG	UNP Q61193
B	47	PRO	-	EXPRESSION TAG	UNP Q61193
B	48	ASN	-	EXPRESSION TAG	UNP Q61193
B	49	SER	-	EXPRESSION TAG	UNP Q61193
B	147	TYR	HIS	SEE REMARK 999	UNP Q61193
B	402	THR	MET	SEE REMARK 999	UNP Q61193

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	101	Total 101	O 101	0	0
2	B	81	Total 81	O 81	0	0

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	70.93Å 75.62Å 101.33Å 90.00° 98.15° 90.00°	Depositor
Resolution (Å)	30.98 – 2.30 30.98 – 2.30	Depositor EDS
% Data completeness (in resolution range)	100.0 (30.98-2.30) 98.7 (30.98-2.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.28 (at 2.31Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.252 , 0.288 0.250 , 0.283	Depositor DCC
R_{free} test set	2335 reflections (5.27%)	DCC
Wilson B-factor (Å ²)	39.3	Xtriage
Anisotropy	0.276	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 27.4	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 46676 reflections	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	6299	wwPDB-VP
Average B, all atoms (Å ²)	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.86% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities 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	0.32	0/3117	0.48	0/4240
1	B	0.32	0/3118	0.48	0/4237
All	All	0.32	0/6235	0.48	0/8477

There are no bond length outliers.

There are no bond angle outliers.

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	3059	0	3037	13	0
1	B	3058	0	3029	12	0
2	A	101	0	0	0	0
2	B	81	0	0	0	0
All	All	6299	0	6066	25	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 2.

All (25) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:266:GLN:HE22	1:B:286:SER:H	1.53	0.56

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:472:ARG:O	1:A:475:LYS:HD3	2.08	0.54
1:B:255:ASP:HB3	1:B:429:VAL:HG11	1.91	0.52
1:A:304:SER:OG	1:A:335:TRP:NE1	2.39	0.50
1:A:352:TYR:HA	1:A:355:VAL:HG12	1.92	0.50
1:B:311:ILE:HD11	1:B:319:THR:HG23	1.93	0.50
1:B:260:LEU:HD22	1:B:478:ARG:HH11	1.75	0.49
1:A:156:THR:O	1:A:160:ILE:HG12	2.13	0.49
1:B:181:GLN:HE21	1:B:181:GLN:H	1.61	0.48
1:A:308:ALA:HB3	1:A:498:LEU:HD11	1.95	0.48
1:A:492:LEU:HA	1:A:495:LEU:HD22	1.97	0.47
1:B:308:ALA:HB3	1:B:498:LEU:HD11	1.97	0.45
1:B:238:ASP:O	1:B:241:VAL:HG22	2.17	0.45
1:B:510:VAL:HG12	1:B:511:GLU:HG3	1.99	0.43
1:B:182:LEU:HD13	1:B:211:LEU:HD23	2.01	0.43
1:A:187:SER:O	1:A:191:ARG:HB2	2.18	0.43
1:B:181:GLN:H	1:B:181:GLN:NE2	2.16	0.42
1:B:85:PRO:HA	1:B:86:PRO:HD3	1.88	0.42
1:A:255:ASP:HB3	1:A:429:VAL:HG11	2.02	0.41
1:A:301:VAL:HG22	1:A:335:TRP:CE3	2.55	0.41
1:B:274:HIS:HB3	1:B:277:ARG:HD2	2.02	0.41
1:A:236:PRO:HB2	1:A:304:SER:HA	2.03	0.41
1:A:325:PRO:HB2	1:A:326:PRO:HD3	2.02	0.41
1:A:62:GLU:O	1:A:63:ASP:C	2.58	0.41
1:A:475:LYS:HA	1:A:478:ARG:HH11	1.86	0.41

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	384/473 (81%)	379 (99%)	4 (1%)	1 (0%)	50	60
1	B	384/473 (81%)	377 (98%)	6 (2%)	1 (0%)	50	60
All	All	768/946 (81%)	756 (98%)	10 (1%)	2 (0%)	50	60

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	63	ASP
1	B	278	PRO

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	330/399 (83%)	320 (97%)	10 (3%)	53	70
1	B	326/399 (82%)	315 (97%)	11 (3%)	49	64
All	All	656/798 (82%)	635 (97%)	21 (3%)	51	67

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	104	LEU
1	A	114	MET
1	A	120	LEU
1	A	134	PHE
1	A	152	LEU
1	A	250	GLN
1	A	367	ARG
1	A	470	LEU
1	A	475	LYS
1	A	495	LEU
1	B	104	LEU
1	B	120	LEU
1	B	133	LEU
1	B	134	PHE
1	B	167	LEU
1	B	181	GLN
1	B	250	GLN
1	B	432	LEU
1	B	471	LEU
1	B	478	ARG
1	B	483	ARG

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	359	GLN
1	B	181	GLN
1	B	246	HIS
1	B	266	GLN
1	B	493	GLN

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	396/473 (83%)	0.68	32 (8%) 12 18	25, 39, 59, 78	0
1	B	396/473 (83%)	0.68	40 (10%) 7 12	31, 42, 61, 93	0
All	All	792/946 (83%)	0.68	72 (9%) 9 15	25, 40, 60, 93	0

All (72) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	74	TYR	6.8
1	A	400	LEU	6.4
1	A	231	ASP	5.6
1	B	400	LEU	5.0
1	A	51	GLU	4.4
1	A	63	ASP	4.1
1	A	311	ILE	4.0
1	A	283	LEU	3.9
1	B	194	TYR	3.6
1	A	483	ARG	3.6
1	B	149	PRO	3.5
1	B	147	TYR	3.5
1	B	146	SER	3.4
1	B	53	ALA	3.4
1	B	367	ARG	3.4
1	A	50	GLU	3.4
1	A	232	SER	3.3
1	B	190	LEU	3.3
1	B	243	LEU	3.2
1	B	379	ARG	3.1
1	B	513	PRO	3.1
1	A	233	PRO	3.1
1	B	193	GLY	3.0
1	B	514	GLY	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	119	ALA	3.0
1	B	504	HIS	3.0
1	B	364	HIS	3.0
1	A	272	TRP	3.0
1	A	118	PRO	2.9
1	B	365	ARG	2.9
1	B	114	MET	2.9
1	B	217	PRO	2.8
1	A	399	GLU	2.8
1	A	162	VAL	2.8
1	A	121	LEU	2.8
1	B	402	THR	2.8
1	B	143	ALA	2.8
1	B	493	GLN	2.7
1	B	496	GLN	2.7
1	B	512	PRO	2.7
1	A	117	THR	2.7
1	A	122	ALA	2.6
1	A	270	GLY	2.6
1	B	216	ASP	2.6
1	B	386	GLN	2.6
1	B	478	ARG	2.5
1	A	397	SER	2.5
1	B	311	ILE	2.5
1	B	399	GLU	2.5
1	A	386	GLN	2.4
1	B	151	GLU	2.4
1	B	401	LEU	2.4
1	B	205	ALA	2.4
1	A	361	SER	2.4
1	A	271	LEU	2.3
1	B	490	GLN	2.3
1	A	375	ARG	2.3
1	A	464	PHE	2.3
1	B	282	HIS	2.3
1	B	122	ALA	2.3
1	A	398	ARG	2.2
1	B	481	ASP	2.2
1	A	108	ARG	2.2
1	B	87	ARG	2.1
1	A	318	VAL	2.1
1	A	52	GLU	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	451	GLU	2.1
1	A	243	LEU	2.0
1	B	189	LEU	2.0
1	A	54	SER	2.0
1	B	434	THR	2.0
1	B	192	THR	2.0

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.