



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 05:22 AM UTC

PDB ID : 4JGW / pdb_00004jgw
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 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

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

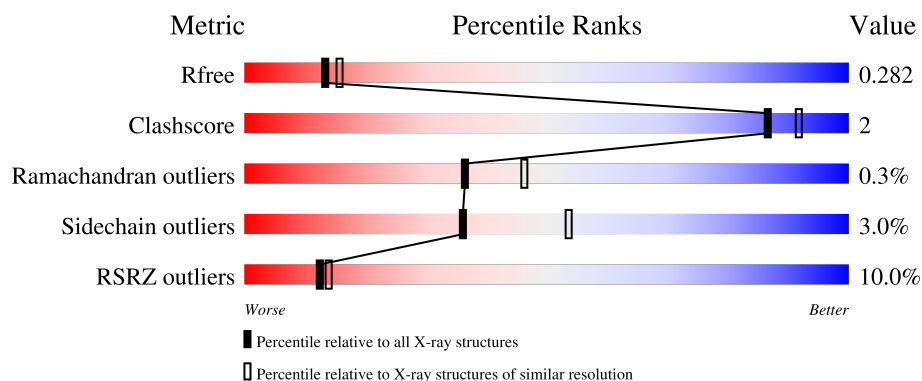
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

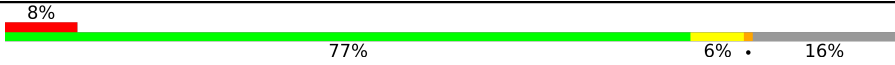
The reported resolution of this entry is 2.30 Å.

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}	180053	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. 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	473	 8% 77% 6% • 16%
1	B	473	 9% 77% 6% • 16%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 6299 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 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

- Molecule 1: Ral guanine nucleotide dissociation stimulator-like 2



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) 98.6 (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 0.249 , 0.282	Depositor DCC
R_{free} test set	2335 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	39.3	Xtriage
Anisotropy	0.276	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 26.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	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.

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](#)

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	0.42	0/3117	0.80	0/4240
1	B	0.44	0/3118	0.83	4/4237 (0.1%)
All	All	0.43	0/6235	0.81	4/8477 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	277	ARG	CA-C-N	5.91	127.23	119.84
1	B	277	ARG	C-N-CA	5.91	127.23	119.84
1	B	511	GLU	CA-C-N	5.87	123.95	119.66
1	B	511	GLU	C-N-CA	5.87	123.95	119.66

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	3059	0	3037	13	0
1	B	3058	0	3029	13	0
2	A	101	0	0	0	0
2	B	81	0	0	0	0
All	All	6299	0	6066	26	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 (26) 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:B:266:GLN:HE22	1:B:286:SER:H	1.53	0.56
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:A:308:ALA:HB3	1:A:498:LEU:HD11	1.95	0.48
1:B:181:GLN:HE21	1:B:181:GLN:H	1.61	0.48
1:A:492:LEU:HA	1:A:495:LEU:HD22	1.97	0.47
1:A:62:GLU:O	1:A:63:ASP:C	2.58	0.45
1:B:238:ASP:O	1:B:241:VAL:HG22	2.17	0.45
1:B:308:ALA:HB3	1:B:498:LEU:HD11	1.97	0.45
1:B:115:MET:HA	1:B:115:MET:HE2	1.99	0.44
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: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%)	36	46
1	B	384/473 (81%)	377 (98%)	6 (2%)	1 (0%)	36	46
All	All	768/946 (81%)	756 (98%)	10 (1%)	2 (0%)	36	46

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%)	321 (97%)	9 (3%)	39	58
1	B	326/399 (82%)	315 (97%)	11 (3%)	32	49
All	All	656/798 (82%)	636 (97%)	20 (3%)	36	53

All (20) 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	144	LEU
1	A	152	LEU
1	A	250	GLN
1	A	470	LEU
1	A	475	LYS
1	A	495	LEU
1	B	104	LEU
1	B	120	LEU
1	B	133	LEU

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Mol	Chain	Res	Type
1	B	167	LEU
1	B	181	GLN
1	B	250	GLN
1	B	428	VAL
1	B	432	LEU
1	B	470	LEU
1	B	471	LEU
1	B	478	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	73	GLN
1	A	359	GLN
1	B	181	GLN
1	B	246	HIS
1	B	266	GLN
1	B	282	HIS
1	B	359	GLN

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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%)	0.75	36 (9%) 15 16	25, 39, 59, 78	0
1	B	396/473 (83%)	0.87	43 (10%) 10 12	31, 42, 61, 93	0
All	All	792/946 (83%)	0.81	79 (9%) 12 14	25, 40, 60, 93	0

All (79) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	74	TYR	5.3
1	B	402	THR	5.1
1	B	204	SER	4.8
1	A	231	ASP	4.4
1	A	400	LEU	4.3
1	B	194	TYR	4.2
1	B	400	LEU	4.0
1	A	398	ARG	4.0
1	B	189	LEU	3.9
1	A	402	THR	3.8
1	B	53	ALA	3.7
1	B	399	GLU	3.7
1	B	217	PRO	3.7
1	B	487	ASP	3.3
1	A	283	LEU	3.3
1	A	401	LEU	3.3
1	A	375	ARG	3.3
1	B	216	ASP	3.2
1	A	360	SER	3.2
1	A	314	GLY	3.2
1	B	318	VAL	3.1
1	A	272	TRP	3.1
1	A	397	SER	3.1
1	B	401	LEU	3.1

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Mol	Chain	Res	Type	RSRZ
1	B	360	SER	3.0
1	A	318	VAL	3.0
1	B	182	LEU	3.0
1	A	388	PHE	2.9
1	A	399	GLU	2.9
1	A	63	ASP	2.9
1	A	270	GLY	2.9
1	B	190	LEU	2.8
1	B	147	TYR	2.8
1	A	483	ARG	2.8
1	B	510	VAL	2.7
1	A	208	ILE	2.7
1	A	51	GLU	2.6
1	B	388	PHE	2.6
1	B	146	SER	2.6
1	A	54	SER	2.6
1	A	507	SER	2.6
1	B	83	LEU	2.6
1	B	205	ALA	2.6
1	B	213	ALA	2.6
1	B	114	MET	2.6
1	B	210	ASN	2.5
1	A	52	GLU	2.5
1	B	279	GLY	2.5
1	B	379	ARG	2.4
1	A	311	ILE	2.4
1	A	50	GLU	2.4
1	B	513	PRO	2.3
1	A	146	SER	2.3
1	A	313	GLU	2.3
1	A	498	LEU	2.3
1	B	82	PRO	2.3
1	A	204	SER	2.3
1	B	386	GLN	2.3
1	B	490	GLN	2.3
1	B	143	ALA	2.2
1	B	282	HIS	2.2
1	A	214	ARG	2.2
1	A	512	PRO	2.2
1	B	512	PRO	2.2
1	B	383	SER	2.2
1	B	150	GLY	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	496	GLN	2.2
1	B	514	GLY	2.2
1	A	194	TYR	2.1
1	B	149	PRO	2.1
1	B	191	ARG	2.1
1	A	55	VAL	2.1
1	A	62	GLU	2.0
1	A	182	LEU	2.0
1	A	484	PRO	2.0
1	B	278	PRO	2.0
1	A	90	ARG	2.0
1	B	212	ARG	2.0
1	B	483	ARG	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.