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wwPDB X-ray Structure Validation Summary Report (i)

Aug 29, 2023 – 07:42 AM EDT

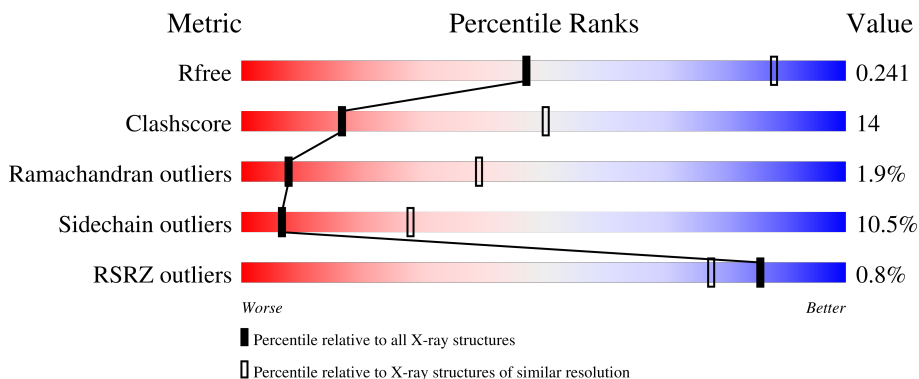|		
PDB ID	:	3ODW
Title	:	Crystal Structure of the Linker-DH/PH domains of p115-RhoGEF
Authors	:	Chen, Z.; Guo, L.; Sprang, S.R.; Sternweis, P.C.
Deposited on	:	2010-08-11
Resolution	:	3.20 Å(reported)

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 3.20 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		0.241
Clashscore		14
Ramachandran outliers		1.9%
Sidechain outliers		10.5%
RSRZ outliers		0.8%

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}	130704	1133 (3.20-3.20)
Clashscore	141614	1253 (3.20-3.20)
Ramachandran outliers	138981	1234 (3.20-3.20)
Sidechain outliers	138945	1233 (3.20-3.20)
RSRZ outliers	127900	1095 (3.20-3.20)

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 <=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	536	45% 14% • 38%
1	B	536	.% 36% 21% • 39%

2 Entry composition ⓘ

There is only 1 type of molecule in this entry. The entry contains 5416 atoms, of which 0 are hydrogens and 0 are deuteriums.
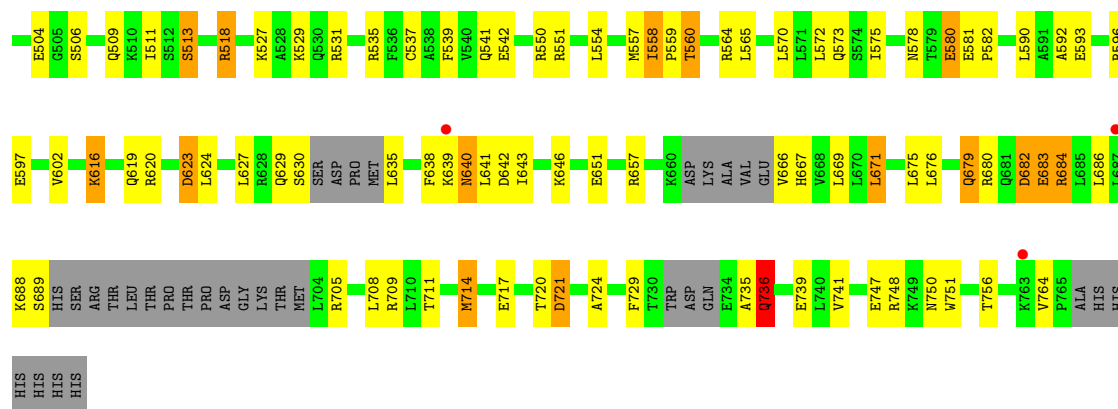
In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Rho guanine nucleotide exchange factor 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	331	Total	C	N	O	S	0	0	0
			2729	1730	490	493	16			
1	B	326	Total	C	N	O	S	0	0	0
			2687	1704	483	486	14			

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	237	GLN	-	expression tag	UNP Q92888
A	238	THR	-	expression tag	UNP Q92888
A	239	SER	-	expression tag	UNP Q92888
A	767	HIS	-	expression tag	UNP Q92888
A	768	HIS	-	expression tag	UNP Q92888
A	769	HIS	-	expression tag	UNP Q92888
A	770	HIS	-	expression tag	UNP Q92888
A	771	HIS	-	expression tag	UNP Q92888
A	772	HIS	-	expression tag	UNP Q92888
B	237	GLN	-	expression tag	UNP Q92888
B	238	THR	-	expression tag	UNP Q92888
B	239	SER	-	expression tag	UNP Q92888
B	767	HIS	-	expression tag	UNP Q92888
B	768	HIS	-	expression tag	UNP Q92888
B	769	HIS	-	expression tag	UNP Q92888
B	770	HIS	-	expression tag	UNP Q92888
B	771	HIS	-	expression tag	UNP Q92888
B	772	HIS	-	expression tag	UNP Q92888

3 Residue-property plots ⓘ

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes 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: Rho guanine nucleotide exchange factor 1

Chain A:

• Molecule 1: Rho guanine nucleotide exchange factor 1

Chain B:

E504 G505 S506 Q509 K510 I511 S512 S513 R518 K527 A528 K529 Q530 R531 R535 F536 C537 A538 F539 V540 Q541 E542 R550 R551 L554 M557 I558 P559 T560 R564 L565 L570 L571 L572 Q573 S574 I575 N578 T579 E580 E581 P582 L590 A591 A592 E593 R596

E597 V602 K616 Q619 R620 D623 L624 L627 R628 Q629 S630 SER ASP PRO MET L635 F638 K639 N640 L641 D642 I643 K646 E651 R657 K660 ASP LYS ALA VAL GLU V666 H667 V668 L669 L670 L671 L675 L676 Q679 R680 Q681 D682 E683 R684 L685 L686 L687

K688 S689 HIS SER ARG THR LEU THR PRO THR PRO ASP GLY LYS THR MET L704 R705 L708 R709 L710 T711 M714 E717 T720 D721 A724 F729 T730 TRP ASP GLN E734 A735 Q736 E739 L740 V741 E747 R748 K749 N750 W751 T756 K763 V764 P765 ALA HIS HIS

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4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 32	Depositor
Cell constants a, b, c, α, β, γ	111.64Å 111.64Å 97.88Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	43.67 – 3.20 43.67 – 3.20	Depositor EDS
% Data completeness (in resolution range)	99.5 (43.67-3.20) 99.5 (43.67-3.20)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.54 (at 3.19Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, R_{free}	0.231 , 0.289 0.229 , 0.241	Depositor DCC
R_{free} test set	1147 reflections (5.11%)	wwPDB-VP
Wilson B-factor (Å^2)	72.1	Xtriage
Anisotropy	0.072	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 41.0	EDS
L-test for twinning[2]	$< |L| > = 0.50, < L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.008 for -h,-k,l 0.448 for h,-h-k,-l 0.012 for -k,-h,-l	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	5416	wwPDB-VP
Average B, all atoms (Å^2)	96.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.91% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.
[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

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	0.73	4/2770 (0.1%)	0.84	4/3721 (0.1%)
1	B	0.94	4/2727 (0.1%)	1.05	7/3664 (0.2%)
All	All	0.84	8/5497 (0.1%)	0.95	11/7385 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	684	ARG	CZ-NH1	16.19	1.54	1.33
1	A	684	ARG	CD-NE	13.16	1.68	1.46
1	B	623	ASP	CB-CG	11.23	1.75	1.51
1	A	684	ARG	CZ-NH1	-8.02	1.22	1.33
1	B	684	ARG	CZ-NH2	6.82	1.42	1.33

The worst 5 of 11 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	684	ARG	NE-CZ-NH1	-31.79	104.41	120.30
1	B	684	ARG	NH1-CZ-NH2	12.23	132.85	119.40
1	A	684	ARG	NE-CZ-NH2	12.22	126.41	120.30
1	A	623	ASP	CB-CG-OD2	-11.42	108.02	118.30
1	A	623	ASP	CB-CG-OD1	10.73	127.96	118.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

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Mol	Chain	Res	Type	Group
1	B	684	ARG	Sidechain

5.2 Too-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 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	2729	0	2802	66	0
1	B	2687	0	2762	94	1
All	All	5416	0	5564	156	1

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 14.

The worst 5 of 156 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:623:ASP:CB	1:B:623:ASP:CG	1.75	1.55
1:A:684:ARG:NE	1:A:684:ARG:CD	1.68	1.54
1:B:717:GLU:HG3	1:B:748:ARG:HH12	1.05	1.19
1:A:634:MET:HE2	1:A:635:LEU:HD12	1.31	1.12
1:B:717:GLU:HG3	1:B:748:ARG:NH1	1.67	1.09

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:504:GLU:OE1	1:B:535:ARG:NH1[2_654]	2.18	0.02

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	319/536 (60%)	285 (89%)	27 (8%)	7 (2%)	6	35
1	B	314/536 (59%)	265 (84%)	44 (14%)	5 (2%)	9	43
All	All	633/1072 (59%)	550 (87%)	71 (11%)	12 (2%)	8	39

5 of 12 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	635	LEU
1	A	721	ASP
1	B	490	GLU
1	B	721	ASP
1	A	565	LEU

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	306/476 (64%)	276 (90%)	30 (10%)	8	31
1	B	301/476 (63%)	267 (89%)	34 (11%)	6	25
All	All	607/952 (64%)	543 (90%)	64 (10%)	7	28

5 of 64 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	689	SER
1	B	711	THR
1	A	679	GLN
1	A	677	LEU
1	B	714	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 8 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	667	HIS
1	B	604	GLN
1	B	509	GLN
1	B	414	GLN
1	B	573	GLN

5.3.3 RNA ⓘ

There are no RNA molecules 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 monosaccharides 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(Å²)	Q<0.9
1	A	331/536 (61%)	-0.02	1 (0%)	94	92	53, 85, 140, 199	0
1	B	326/536 (60%)	0.02	4 (1%)	79	67	62, 98, 145, 202	0
All	All	657/1072 (61%)	-0.00	5 (0%)	86	78	53, 95, 143, 202	0

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	763	LYS	2.8
1	B	639	LYS	2.5
1	B	687	LEU	2.3
1	A	628	ARG	2.3
1	B	499	ARG	2.1

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 monosaccharides 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.

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