



Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 07:39 AM GMT

PDB ID : 2D0N
Title : Crystal structure of the C-terminal SH3 domain of the adaptor protein GADS
in complex with SLP-76 motif peptide reveals a unique SH3-SH3 interaction
Authors : Dimasi, N.
Deposited on : 2005-08-04
Resolution : 1.57 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>

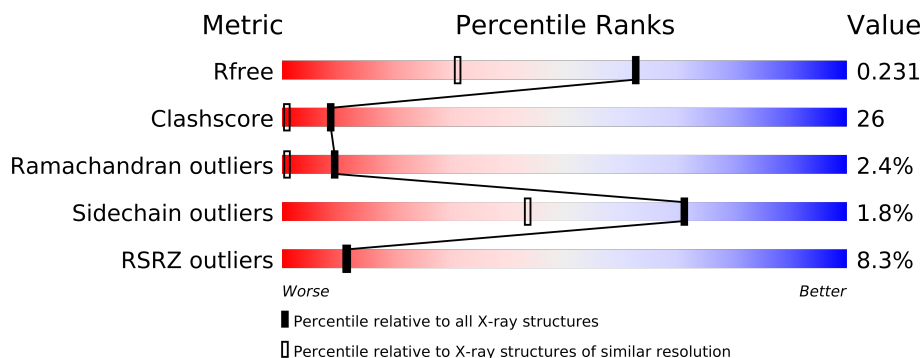
The following versions of software and data (see [references](#)) were used in the production of this report:

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 1.57 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	2778 (1.60-1.56)
Clashscore	79885	3207 (1.60-1.56)
Ramachandran outliers	78287	3107 (1.60-1.56)
Sidechain outliers	78261	3104 (1.60-1.56)
RSRZ outliers	66119	2778 (1.60-1.56)

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	59	
1	C	59	
2	B	9	
2	D	9	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 1258 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 GRB2-related adaptor protein 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	59	Total	C	N	O	S	0	0	0
			469	301	77	89	2			
1	C	56	Total	C	N	O	S	0	0	0
			450	291	74	84	1			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	264	GLY	-	CLONING ARTIFACT	UNP O89100
A	265	SER	-	CLONING ARTIFACT	UNP O89100
A	266	PRO	-	CLONING ARTIFACT	UNP O89100
C	264	GLY	-	CLONING ARTIFACT	UNP O89100
C	265	SER	-	CLONING ARTIFACT	UNP O89100
C	266	PRO	-	CLONING ARTIFACT	UNP O89100

- Molecule 2 is a protein called SLP-76 binding peptide.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	B	9	Total	C	N	O	0	0	0
			70	42	13	15			
2	D	9	Total	C	N	O	0	0	0
			70	42	13	15			

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	90	Total	O	0	0
			90	90		
3	B	18	Total	O	0	0
			18	18		
3	C	80	Total	O	0	0
			80	80		

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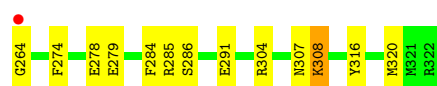
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	D	11	Total	O	0	0
			11	11		

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: GRB2-related adaptor protein 2

Chain A: 



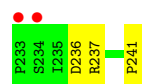
- Molecule 1: GRB2-related adaptor protein 2

Chain C: 



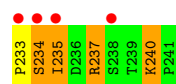
- Molecule 2: SLP-76 binding peptide

Chain B: 



- Molecule 2: SLP-76 binding peptide

Chain D: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 42 21 2	Depositor
Cell constants a, b, c, α , β , γ	58.62Å 58.62Å 74.10Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	7.90 – 1.57 7.94 – 1.57	Depositor EDS
% Data completeness (in resolution range)	(Not available) (7.90-1.57) 89.3 (7.94-1.57)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	0.18	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.32 (at 1.57Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.221 , 0.284 0.226 , 0.231	Depositor DCC
R_{free} test set	856 reflections (5.47%)	DCC
Wilson B-factor (Å ²)	18.4	Xtriage
Anisotropy	0.027	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.56 , 66.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 18493 reflections	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	1258	wwPDB-VP
Average B, all atoms (Å ²)	20.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.61% 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	1.49	4/484 (0.8%)	1.24	3/658 (0.5%)
1	C	1.49	6/465 (1.3%)	1.58	7/634 (1.1%)
2	B	1.21	0/71	1.07	0/93
2	D	0.77	0/71	1.21	1/93 (1.1%)
All	All	1.44	10/1091 (0.9%)	1.38	11/1478 (0.7%)

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	C	0	1

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	318	ALA	CA-CB	6.32	1.65	1.52
1	C	288	GLU	CG-CD	6.18	1.61	1.51
1	C	284	PHE	CE2-CZ	5.80	1.48	1.37
1	A	284	PHE	CE2-CZ	5.56	1.48	1.37
1	A	286	SER	CB-OG	-5.50	1.35	1.42
1	C	307	ASN	CB-CG	5.38	1.63	1.51
1	C	288	GLU	CD-OE2	-5.18	1.20	1.25
1	C	291	GLU	CD-OE1	5.14	1.31	1.25
1	A	274	PHE	CD1-CE1	5.09	1.49	1.39
1	A	291	GLU	CG-CD	5.08	1.59	1.51

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	318	ALA	C-N-CD	-13.66	90.54	120.60
1	C	269	ARG	NE-CZ-NH2	-12.92	113.84	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	318	ALA	C-N-CA	8.76	158.79	122.00
1	C	269	ARG	NE-CZ-NH1	7.46	124.03	120.30
1	C	320	MET	CB-CA-C	-6.75	96.90	110.40
1	A	320	MET	CG-SD-CE	6.21	110.14	100.20
1	C	304	ARG	NE-CZ-NH1	-5.51	117.55	120.30
1	A	304	ARG	NE-CZ-NH2	-5.46	117.57	120.30
2	D	237	ARG	NE-CZ-NH2	-5.26	117.67	120.30
1	A	285	ARG	NE-CZ-NH2	-5.18	117.71	120.30
1	C	318	ALA	CB-CA-C	-5.01	102.58	110.10

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	320	MET	Peptide

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	469	0	432	12	2
1	C	450	0	416	30	2
2	B	70	0	72	4	0
2	D	70	0	72	9	0
3	A	90	0	0	12	0
3	B	18	0	0	3	0
3	C	80	0	0	8	0
3	D	11	0	0	4	1
All	All	1258	0	992	53	3

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 26.

All (53) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:318:ALA:HA	3:C:191:HOH:O	1.44	1.18
1:C:267:TRP:H	1:C:321:MET:HA	1.32	0.89
1:A:316:TYR:HB3	3:A:199:HOH:O	1.73	0.88
1:A:279:GLU:HG3	3:A:171:HOH:O	1.73	0.86
1:C:275:GLU:CG	3:C:76:HOH:O	2.25	0.83
2:D:233:PRO:HA	3:D:79:HOH:O	1.76	0.83
2:D:233:PRO:O	2:D:234:SER:HB3	1.81	0.78
1:C:291:GLU:HG2	3:C:195:HOH:O	1.85	0.76
1:C:320:MET:HB2	1:C:321:MET:O	1.87	0.74
1:C:275:GLU:HG2	3:C:76:HOH:O	1.83	0.74
1:C:275:GLU:CD	3:C:76:HOH:O	2.27	0.72
1:A:316:TYR:CD2	3:A:199:HOH:O	2.43	0.71
3:A:171:HOH:O	1:C:308:LYS:HE3	1.90	0.70
1:C:304:ARG:HD2	3:C:190:HOH:O	1.92	0.69
1:C:269:ARG:H	1:C:318:ALA:HB2	1.59	0.67
2:D:233:PRO:O	2:D:234:SER:CB	2.43	0.67
1:C:267:TRP:N	1:C:321:MET:HA	2.09	0.66
2:D:234:SER:N	3:D:79:HOH:O	2.28	0.66
1:C:318:ALA:CB	1:C:319:PRO:CA	2.75	0.65
1:C:267:TRP:H	1:C:321:MET:CA	2.06	0.64
1:C:318:ALA:HB1	1:C:319:PRO:C	2.20	0.62
1:C:277:LEU:C	1:C:278:GLU:HG3	2.20	0.62
1:A:307:ASN:CG	3:A:194:HOH:O	2.39	0.61
1:A:264:GLY:N	3:A:50:HOH:O	2.34	0.61
1:C:318:ALA:HB1	1:C:319:PRO:CA	2.32	0.59
2:D:234:SER:O	2:D:235:ILE:O	2.22	0.57
1:C:269:ARG:H	1:C:318:ALA:CB	2.18	0.57
2:B:236:ASP:HA	3:B:192:HOH:O	2.07	0.55
1:C:320:MET:CB	1:C:321:MET:O	2.56	0.53
2:D:233:PRO:CA	3:D:79:HOH:O	2.46	0.52
2:D:234:SER:O	2:D:235:ILE:C	2.49	0.50
1:C:268:ALA:HA	1:C:318:ALA:HB3	1.94	0.50
1:C:277:LEU:HD21	3:C:156:HOH:O	2.11	0.50
1:C:318:ALA:HB3	1:C:319:PRO:HA	1.94	0.50
2:B:236:ASP:CA	3:B:192:HOH:O	2.60	0.49
1:A:316:TYR:CB	3:A:199:HOH:O	2.45	0.48
2:D:237:ARG:O	2:D:240:LYS:HG3	2.12	0.48
1:C:268:ALA:HA	1:C:319:PRO:HA	1.96	0.47
1:C:307:ASN:ND2	3:C:193:HOH:O	2.38	0.47
1:A:308:LYS:HD2	3:A:184:HOH:O	2.15	0.46
2:B:241:PRO:HB2	1:C:293:LEU:HD22	1.98	0.46
2:D:233:PRO:C	3:D:79:HOH:O	2.55	0.45
1:C:266:PRO:HD2	1:C:292:VAL:O	2.15	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:237:ARG:N	3:B:192:HOH:O	2.48	0.45
1:C:277:LEU:C	1:C:278:GLU:CG	2.84	0.45
1:A:279:GLU:CG	3:A:171:HOH:O	2.48	0.45
1:C:318:ALA:HB3	1:C:319:PRO:CA	2.46	0.44
1:A:278:GLU:HG3	3:A:18:HOH:O	2.18	0.43
1:C:268:ALA:CA	1:C:318:ALA:HB3	2.50	0.41
1:A:307:ASN:O	1:C:279:GLU:HB2	2.19	0.41
1:C:293:LEU:HD23	1:C:293:LEU:HA	1.85	0.41
1:A:316:TYR:HD2	3:A:199:HOH:O	1.93	0.41
1:A:307:ASN:ND2	3:A:194:HOH:O	2.54	0.40

All (3) 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	Distance(Å)	Clash(Å)
3:D:79:HOH:O	3:D:79:HOH:O[2_445]	1.89	0.31
1:A:278:GLU:OE1	1:C:307:ASN:ND2[2_545]	2.01	0.19
1:A:264:GLY:O	1:C:320:MET:CE[5_454]	2.09	0.11

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	57/59 (97%)	56 (98%)	1 (2%)	0	100	100
1	C	54/59 (92%)	52 (96%)	1 (2%)	1 (2%)	12	1
2	B	7/9 (78%)	7 (100%)	0	0	100	100
2	D	7/9 (78%)	5 (71%)	0	2 (29%)	0	0
All	All	125/136 (92%)	120 (96%)	2 (2%)	3 (2%)	9	1

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	318	ALA
2	D	235	ILE

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Mol	Chain	Res	Type
2	D	234	SER

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	48/49 (98%)	47 (98%)	1 (2%)	66	36
1	C	46/49 (94%)	46 (100%)	0	100	100
2	B	9/9 (100%)	9 (100%)	0	100	100
2	D	9/9 (100%)	8 (89%)	1 (11%)	9	1
All	All	112/116 (97%)	110 (98%)	2 (2%)	71	43

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	308	LYS
2	D	240	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	306	HIS
1	C	306	HIS

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	59/59 (100%)	-0.14	1 (1%) 67 69	9, 13, 24, 34	0
1	C	56/59 (94%)	0.49	4 (7%) 16 15	11, 18, 29, 37	0
2	B	9/9 (100%)	1.31	2 (22%) 1 1	14, 18, 44, 47	0
2	D	9/9 (100%)	2.69	4 (44%) 1 1	24, 28, 49, 52	0
All	All	133/136 (97%)	0.41	11 (8%) 11 11	9, 16, 34, 52	0

All (11) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	321	MET	12.0
2	D	234	SER	10.8
2	B	234	SER	7.0
2	D	233	PRO	6.0
1	A	264	GLY	5.4
2	B	233	PRO	4.3
1	C	318	ALA	3.2
2	D	235	ILE	2.9
1	C	307	ASN	2.3
2	D	238	SER	2.3
1	C	285	ARG	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.