



Full wwPDB X-ray Structure Validation Report ⓘ

May 13, 2020 – 12:56 am BST

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

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

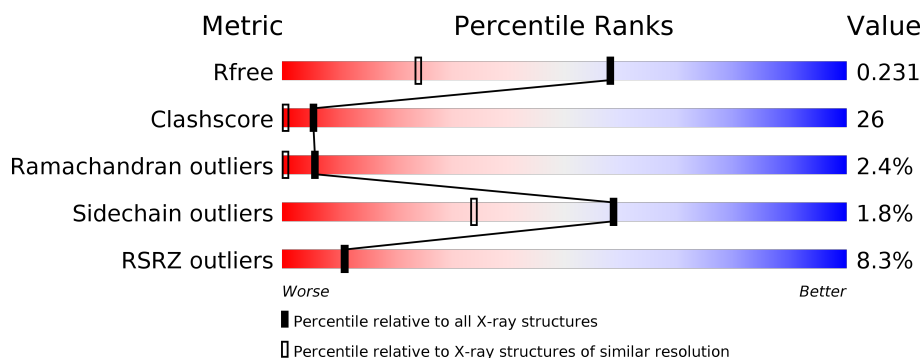
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	130704	5534 (1.60-1.56)
Clashscore	141614	5861 (1.60-1.56)
Ramachandran outliers	138981	5708 (1.60-1.56)
Sidechain outliers	138945	5703 (1.60-1.56)
RSRZ outliers	127900	5431 (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 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	59	<div> <div>2%</div> <div> <div></div> <div>78%</div> <div>20%</div> <div>•</div> </div> </div>
1	C	59	<div> <div>7%</div> <div> <div></div> <div>61%</div> <div>24%</div> <div>7%</div> <div>•</div> <div>5%</div> </div> </div>
2	B	9	<div> <div>22%</div> <div> <div></div> <div>67%</div> <div>33%</div> </div> </div>
2	D	9	<div> <div>44%</div> <div> <div></div> <div>44%</div> <div>11%</div> <div>44%</div> </div> </div>

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 1258 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 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 [i](#)

These plots are drawn for all protein, RNA and DNA 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.

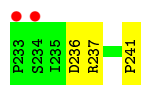
- Molecule 1: GRB2-related adaptor protein 2



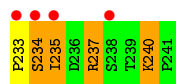
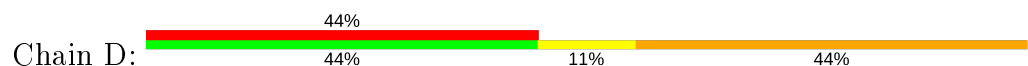
- Molecule 1: GRB2-related adaptor protein 2



- Molecule 2: SLP-76 binding peptide



- Molecule 2: SLP-76 binding peptide



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 0.225 , 0.231	Depositor DCC
R_{free} test set	856 reflections (4.63%)	wwPDB-VP
Wilson B-factor (Å ²)	18.4	Xtriage
Anisotropy	0.027	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.46 , 66.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	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.

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

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 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	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

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 26.

All (53) 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: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
1:C:266:PRO:HD2	1:C:292:VAL:O	2.15	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:233:PRO:C	3:D:79:HOH:O	2.55	0.45
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:A:307:ASN:O	1:C:279:GLU:HB2	2.19	0.41
1:C:268:ALA:CA	1:C:318:ALA:HB3	2.50	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	Interatomic distance (Å)	Clash overlap (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 [i](#)

5.3.1 Protein backbone [i](#)

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%)	8	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%)	6	0

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	318	ALA
2	D	235	ILE
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%)	53	27
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%)	6	0
All	All	112/116 (97%)	110 (98%)	2 (2%)	59	34

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 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 [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

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%)	0.03	1 (1%) 70 71	9, 13, 24, 34	0
1	C	56/59 (94%)	0.64	4 (7%) 16 16	11, 18, 29, 37	0
2	B	9/9 (100%)	1.51	2 (22%) 0 0	14, 18, 44, 47	0
2	D	9/9 (100%)	3.11	4 (44%) 0 0	24, 28, 49, 52	0
All	All	133/136 (97%)	0.59	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	11.7
2	D	234	SER	11.2
2	B	234	SER	7.8
2	D	233	PRO	6.9
1	A	264	GLY	5.8
2	B	233	PRO	4.6
2	D	235	ILE	4.3
1	C	318	ALA	3.9
2	D	238	SER	2.8
1	C	307	ASN	2.6
1	C	285	ARG	2.5

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 [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.