



wwPDB X-ray Structure Validation Summary Report ⓘ

Jan 31, 2016 – 08:40 PM GMT

PDB ID : 1LB1
Title : Crystal Structure of the Dbl and Pleckstrin homology domains of Dbs in complex with RhoA
Authors : Snyder, J.T.; Worthylake, D.K.; Rossman, K.L.; Betts, L.; Pruitt, W.M.; Siderovski, D.P.; Der, C.J.; Sodek, J.
Deposited on : 2002-04-01
Resolution : 2.81 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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/validation/2016/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
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

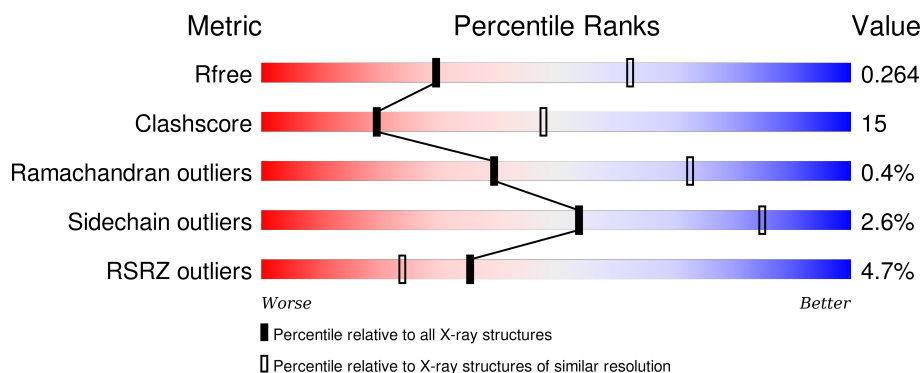
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.81 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}	91344	2676 (2.84-2.80)
Clashscore	102246	3124 (2.84-2.80)
Ramachandran outliers	100387	3072 (2.84-2.80)
Sidechain outliers	100360	3074 (2.84-2.80)
RSRZ outliers	91569	2690 (2.84-2.80)

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. 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	353	<div> <div>0%</div> <div>68% 22% 8%</div> </div>
1	C	353	<div> <div>2%</div> <div>65% 25% 8%</div> </div>
1	E	353	<div> <div>3%</div> <div>66% 24% 8%</div> </div>
1	G	353	<div> <div>11%</div> <div>67% 23% 8%</div> </div>
2	B	192	<div> <div>3%</div> <div>61% 30% 7%</div> </div>

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Mol	Chain	Length	Quality of chain
2	D	192	<div><div>%</div><div><div></div><div>62%</div><div>29%</div><div>• 7%</div></div></div>
2	F	192	<div><div>3%</div><div><div></div><div>61%</div><div>30%</div><div>• 7%</div></div></div>
2	H	192	<div><div>12%</div><div><div></div><div>59%</div><div>32%</div><div>• 7%</div></div></div>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 16236 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 Guanine nucleotide exchange factor DBS.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	324	Total	C	N	O	S	0	0	0
			2646	1682	452	491	21			
1	C	324	Total	C	N	O	S	0	0	0
			2646	1682	452	491	21			
1	E	324	Total	C	N	O	S	0	0	0
			2646	1682	452	491	21			
1	G	324	Total	C	N	O	S	0	0	0
			2646	1682	452	491	21			

There are 56 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	622	MET	-	SEE REMARK 999	UNP Q64096
A	696	ILE	ASN	SEE REMARK 999	UNP Q64096
A	697	PHE	ILE	SEE REMARK 999	UNP Q64096
A	698	LEU	PRO	SEE REMARK 999	UNP Q64096
A	699	ARG	ALA	SEE REMARK 999	UNP Q64096
A	700	GLU	GLY	SEE REMARK 999	UNP Q64096
A	701	LEU	VAL	SEE REMARK 999	UNP Q64096
A	968	GLU	-	EXPRESSION TAG	UNP Q64096
A	969	HIS	-	EXPRESSION TAG	UNP Q64096
A	970	HIS	-	EXPRESSION TAG	UNP Q64096
A	971	HIS	-	EXPRESSION TAG	UNP Q64096
A	972	HIS	-	EXPRESSION TAG	UNP Q64096
A	973	HIS	-	EXPRESSION TAG	UNP Q64096
A	974	HIS	-	EXPRESSION TAG	UNP Q64096
C	622	MET	-	SEE REMARK 999	UNP Q64096
C	696	ILE	ASN	SEE REMARK 999	UNP Q64096
C	697	PHE	ILE	SEE REMARK 999	UNP Q64096
C	698	LEU	PRO	SEE REMARK 999	UNP Q64096
C	699	ARG	ALA	SEE REMARK 999	UNP Q64096
C	700	GLU	GLY	SEE REMARK 999	UNP Q64096
C	701	LEU	VAL	SEE REMARK 999	UNP Q64096

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Chain	Residue	Modelled	Actual	Comment	Reference
C	968	GLU	-	EXPRESSION TAG	UNP Q64096
C	969	HIS	-	EXPRESSION TAG	UNP Q64096
C	970	HIS	-	EXPRESSION TAG	UNP Q64096
C	971	HIS	-	EXPRESSION TAG	UNP Q64096
C	972	HIS	-	EXPRESSION TAG	UNP Q64096
C	973	HIS	-	EXPRESSION TAG	UNP Q64096
C	974	HIS	-	EXPRESSION TAG	UNP Q64096
E	622	MET	-	SEE REMARK 999	UNP Q64096
E	696	ILE	ASN	SEE REMARK 999	UNP Q64096
E	697	PHE	ILE	SEE REMARK 999	UNP Q64096
E	698	LEU	PRO	SEE REMARK 999	UNP Q64096
E	699	ARG	ALA	SEE REMARK 999	UNP Q64096
E	700	GLU	GLY	SEE REMARK 999	UNP Q64096
E	701	LEU	VAL	SEE REMARK 999	UNP Q64096
E	968	GLU	-	EXPRESSION TAG	UNP Q64096
E	969	HIS	-	EXPRESSION TAG	UNP Q64096
E	970	HIS	-	EXPRESSION TAG	UNP Q64096
E	971	HIS	-	EXPRESSION TAG	UNP Q64096
E	972	HIS	-	EXPRESSION TAG	UNP Q64096
E	973	HIS	-	EXPRESSION TAG	UNP Q64096
E	974	HIS	-	EXPRESSION TAG	UNP Q64096
G	622	MET	-	SEE REMARK 999	UNP Q64096
G	696	ILE	ASN	SEE REMARK 999	UNP Q64096
G	697	PHE	ILE	SEE REMARK 999	UNP Q64096
G	698	LEU	PRO	SEE REMARK 999	UNP Q64096
G	699	ARG	ALA	SEE REMARK 999	UNP Q64096
G	700	GLU	GLY	SEE REMARK 999	UNP Q64096
G	701	LEU	VAL	SEE REMARK 999	UNP Q64096
G	968	GLU	-	EXPRESSION TAG	UNP Q64096
G	969	HIS	-	EXPRESSION TAG	UNP Q64096
G	970	HIS	-	EXPRESSION TAG	UNP Q64096
G	971	HIS	-	EXPRESSION TAG	UNP Q64096
G	972	HIS	-	EXPRESSION TAG	UNP Q64096
G	973	HIS	-	EXPRESSION TAG	UNP Q64096
G	974	HIS	-	EXPRESSION TAG	UNP Q64096

- Molecule 2 is a protein called Transforming protein RhoA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	178	Total	C	N	O	S	0	0	0
			1413	894	239	270	10			
2	D	178	Total	C	N	O	S	0	0	0
			1413	894	239	270	10			

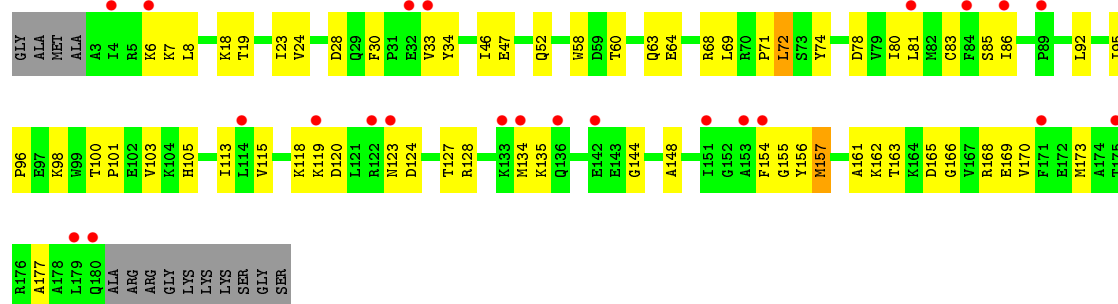
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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	F	178	Total	C	N	O	S	0	0	0
			1413	894	239	270	10			
2	H	178	Total	C	N	O	S	0	0	0
			1413	894	239	270	10			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-1	GLY	-	SEE REMARK 999	UNP P61586
B	0	ALA	-	SEE REMARK 999	UNP P61586
B	190	SER	CYS	ENGINEERED	UNP P61586
D	-1	GLY	-	SEE REMARK 999	UNP P61586
D	0	ALA	-	SEE REMARK 999	UNP P61586
D	190	SER	CYS	ENGINEERED	UNP P61586
F	-1	GLY	-	SEE REMARK 999	UNP P61586
F	0	ALA	-	SEE REMARK 999	UNP P61586
F	190	SER	CYS	ENGINEERED	UNP P61586
H	-1	GLY	-	SEE REMARK 999	UNP P61586
H	0	ALA	-	SEE REMARK 999	UNP P61586
H	190	SER	CYS	ENGINEERED	UNP P61586



4 Data and refinement statistics

Property	Value	Source
Space group	P 43	Depositor
Cell constants a, b, c, α , β , γ	158.90Å 158.90Å 151.79Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.70 – 2.81 47.70 – 2.81	Depositor EDS
% Data completeness (in resolution range)	93.7 (47.70-2.81) 93.7 (47.70-2.81)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.96 (at 2.81Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.236 , 0.266 0.236 , 0.264	Depositor DCC
R_{free} test set	4358 reflections (5.07%)	DCC
Wilson B-factor (Å ²)	68.0	Xtriage
Anisotropy	0.322	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 43.9	EDS
Estimated twinning fraction	0.029 for -h,-l,-k 0.028 for -h,l,k 0.030 for l,-k,h 0.033 for -l,-k,-h 0.238 for h,-k,-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.27$	Xtriage
Outliers	0 of 85993 reflections	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	16236	wwPDB-VP
Average B, all atoms (Å ²)	80.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.73% of the height of the origin peak. No significant pseudotranslation is detected.*

¹ Intensities estimated from amplitudes.

² Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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	0.44	0/2697	0.59	0/3624
1	C	0.45	0/2697	0.60	0/3624
1	E	0.39	0/2697	0.57	0/3624
1	G	0.37	0/2697	0.57	0/3624
2	B	0.33	0/1441	0.58	0/1949
2	D	0.39	0/1441	0.60	0/1949
2	F	0.33	0/1441	0.57	0/1949
2	H	0.30	0/1441	0.56	0/1949
All	All	0.39	0/16552	0.58	0/22292

There are no bond length outliers.

There are no bond angle outliers.

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	2646	0	2641	72	0
1	C	2646	0	2641	110	1
1	E	2646	0	2641	107	0
1	G	2646	0	2641	67	1
2	B	1413	0	1405	44	0
2	D	1413	0	1405	43	0
2	F	1413	0	1405	46	0
2	H	1413	0	1405	47	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	16236	0	16184	487	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 15.

The worst 5 of 487 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:953:ARG:HD2	1:E:949:LEU:O	1.45	1.17
2:D:123:ASN:HA	2:D:128:ARG:HH21	1.25	1.00
2:F:123:ASN:HA	2:F:128:ARG:HH21	1.24	0.99
2:H:123:ASN:HA	2:H:128:ARG:HH21	1.26	0.99
2:B:123:ASN:HA	2:B:128:ARG:HH21	1.25	0.98

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:C:953:ARG:O	1:G:627:GLU:OE2 3_554	2.13	0.07

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	320/353 (91%)	299 (93%)	19 (6%)	2 (1%)	30	63
1	C	320/353 (91%)	298 (93%)	20 (6%)	2 (1%)	30	63
1	E	320/353 (91%)	299 (93%)	19 (6%)	2 (1%)	30	63
1	G	320/353 (91%)	300 (94%)	18 (6%)	2 (1%)	30	63
2	B	176/192 (92%)	165 (94%)	11 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	D	176/192 (92%)	164 (93%)	12 (7%)	0	100	100
2	F	176/192 (92%)	165 (94%)	11 (6%)	0	100	100
2	H	176/192 (92%)	164 (93%)	12 (7%)	0	100	100
All	All	1984/2180 (91%)	1854 (93%)	122 (6%)	8 (0%)	39	73

5 of 8 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	854	ALA
1	C	854	ALA
1	E	854	ALA
1	G	854	ALA
1	A	918	ASN

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	290/316 (92%)	281 (97%)	9 (3%)	47	80
1	C	290/316 (92%)	281 (97%)	9 (3%)	47	80
1	E	290/316 (92%)	282 (97%)	8 (3%)	51	83
1	G	290/316 (92%)	282 (97%)	8 (3%)	51	83
2	B	156/164 (95%)	153 (98%)	3 (2%)	65	90
2	D	156/164 (95%)	152 (97%)	4 (3%)	54	85
2	F	156/164 (95%)	153 (98%)	3 (2%)	65	90
2	H	156/164 (95%)	153 (98%)	3 (2%)	65	90
All	All	1784/1920 (93%)	1737 (97%)	47 (3%)	54	85

5 of 47 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	D	33	VAL

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Mol	Chain	Res	Type
1	E	685	ASN
1	G	948	GLN
2	D	157	MET
1	E	707	CYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 65 such sidechains are listed below:

Mol	Chain	Res	Type
2	D	52	GLN
1	E	685	ASN
1	G	893	GLN
2	D	105	HIS
1	E	669	HIS

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 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	324/353 (91%)	0.15	2 (0%) 90 86	29, 57, 104, 166	0
1	C	324/353 (91%)	0.21	7 (2%) 65 54	26, 52, 102, 194	0
1	E	324/353 (91%)	0.41	10 (3%) 52 40	46, 74, 123, 189	0
1	G	324/353 (91%)	0.80	39 (12%) 6 3	47, 98, 154, 191	0
2	B	178/192 (92%)	0.29	6 (3%) 49 37	39, 82, 129, 159	0
2	D	178/192 (92%)	0.21	2 (1%) 82 75	33, 62, 115, 151	0
2	F	178/192 (92%)	0.39	5 (2%) 56 44	48, 87, 137, 176	0
2	H	178/192 (92%)	0.81	23 (12%) 5 2	60, 122, 160, 176	0
All	All	2008/2180 (92%)	0.40	94 (4%) 35 24	26, 73, 142, 194	0

The worst 5 of 94 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	952	CYS	11.1
1	G	908	GLY	9.8
1	C	953	ARG	7.9
1	G	907	LYS	7.6
1	E	952	CYS	7.3

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.