



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 29, 2020 – 12:32 PM BST

PDB ID : 6KPD  
Title : The crystal structure of the BALDIBIS/IDD9 bound to the homodimeric SCL3  
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Deposited on : 2019-08-15  
Resolution : 3.20 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](mailto: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.

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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 : 2.13  
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) : 2.13

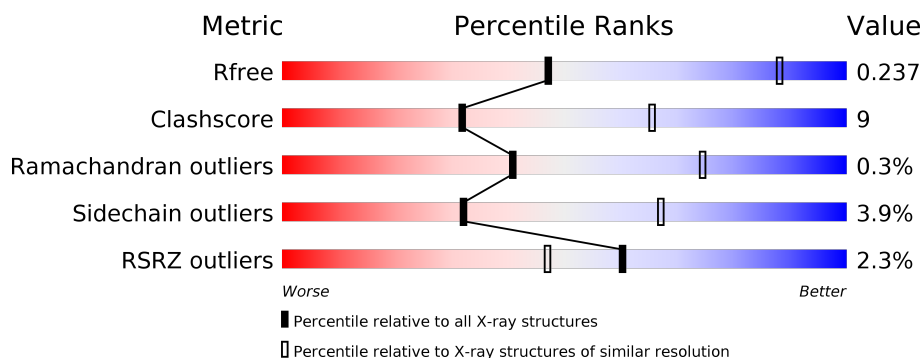
# 1 Overall quality at a glance

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	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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	C	452	<div> <div>2%</div> <div> <div></div> <div>65%</div> <div>17%</div> <div>•</div> <div>17%</div> </div> </div>
2	B	38	<div> <div>21%</div> <div>11%</div> <div>5%</div> <div>63%</div> </div>

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 3012 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 Scarecrow-like protein 3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	C	376	2920	1850	518	535	17	0	0	0

There are 34 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	-1	GLY	-	expression tag	UNP Q9LPR8
C	0	PRO	-	expression tag	UNP Q9LPR8
C	?	-	ARG	deletion	UNP Q9LPR8
C	?	-	LYS	deletion	UNP Q9LPR8
C	?	-	ASN	deletion	UNP Q9LPR8
C	?	-	CYS	deletion	UNP Q9LPR8
C	?	-	ALA	deletion	UNP Q9LPR8
C	?	-	LEU	deletion	UNP Q9LPR8
C	?	-	ARG	deletion	UNP Q9LPR8
C	?	-	PHE	deletion	UNP Q9LPR8
C	?	-	GLN	deletion	UNP Q9LPR8
C	?	-	ASN	deletion	UNP Q9LPR8
C	?	-	ASN	deletion	UNP Q9LPR8
C	?	-	PRO	deletion	UNP Q9LPR8
C	?	-	SER	deletion	UNP Q9LPR8
C	?	-	GLY	deletion	UNP Q9LPR8
C	?	-	VAL	deletion	UNP Q9LPR8
C	?	-	ASP	deletion	UNP Q9LPR8
C	?	-	LEU	deletion	UNP Q9LPR8
C	?	-	GLN	deletion	UNP Q9LPR8
C	?	-	ARG	deletion	UNP Q9LPR8
C	?	-	VAL	deletion	UNP Q9LPR8
C	?	-	LEU	deletion	UNP Q9LPR8
C	?	-	MET	deletion	UNP Q9LPR8
C	?	-	MET	deletion	UNP Q9LPR8
C	?	-	SER	deletion	UNP Q9LPR8
C	?	-	HIS	deletion	UNP Q9LPR8

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Chain	Residue	Modelled	Actual	Comment	Reference
C	?	-	GLY	deletion	UNP Q9LPR8
C	?	-	SER	deletion	UNP Q9LPR8
C	?	-	ALA	deletion	UNP Q9LPR8
C	?	-	ALA	deletion	UNP Q9LPR8
C	?	-	GLU	deletion	UNP Q9LPR8
C	?	-	ALA	deletion	UNP Q9LPR8
C	?	-	ARG	deletion	UNP Q9LPR8

- Molecule 2 is a protein called Peptide from Zinc finger protein BALDIBIS.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	14	Total	C	N	O	S	0	0	0
			92	57	16	17	2			

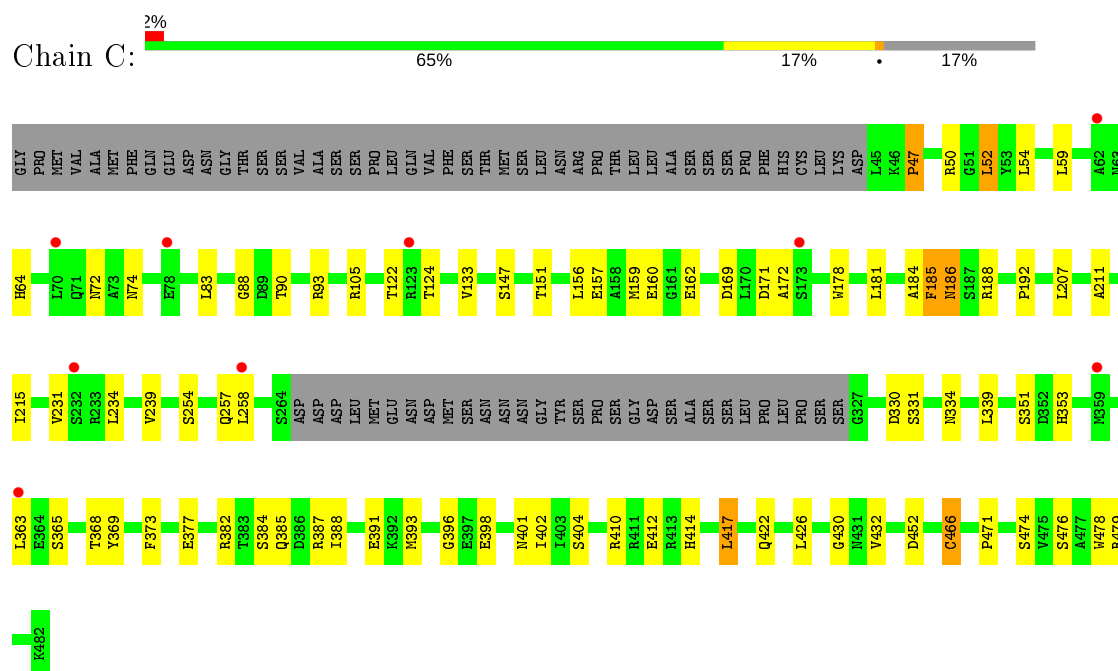
There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	346	GLY	-	expression tag	UNP Q944L3
B	347	PRO	-	expression tag	UNP Q944L3

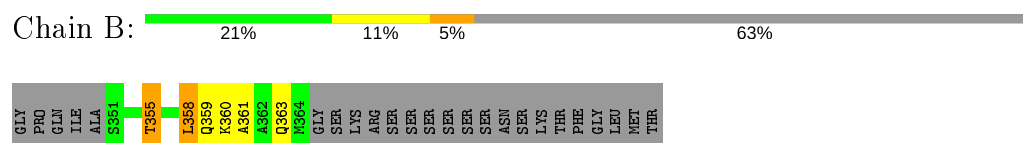
### 3 Residue-property plots [i](#)

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: Scarecrow-like protein 3



- Molecule 2: Peptide from Zinc finger protein BALDIBIS



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	103.38 Å   103.38 Å   68.69 Å 90.00°   90.00°   120.00°	Depositor
Resolution (Å)	44.77 – 3.20 44.77 – 3.20	Depositor EDS
% Data completeness (in resolution range)	99.2 (44.77-3.20) 99.2 (44.77-3.20)	Depositor EDS
$R_{merge}$	0.12	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.58 (at 3.19 Å)	Xtriage
Refinement program	PHENIX	Depositor
R, $R_{free}$	0.204 , 0.237 0.204 , 0.237	Depositor DCC
$R_{free}$ test set	394 reflections (5.49%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	79.2	Xtriage
Anisotropy	0.348	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 30.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.058 for -h,-k,l	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	3012	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	71.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.16% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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	C	0.27	0/2979	0.47	0/4043
2	B	0.30	0/91	0.52	0/122
All	All	0.27	0/3070	0.47	0/4165

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

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	C	2920	0	2845	49	0
2	B	92	0	88	6	0
All	All	3012	0	2933	53	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 9.

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:52:LEU:HD12	2:B:361:ALA:HB2	1.20	1.17
1:C:476:SER:HG	1:C:478:TRP:HE1	0.98	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:360:LYS:O	2:B:363:GLN:HG2	1.75	0.85
1:C:417:LEU:HD12	1:C:417:LEU:O	1.77	0.84
1:C:52:LEU:CD1	2:B:361:ALA:HB2	2.06	0.82
1:C:88:GLY:O	1:C:93:ARG:NH1	2.27	0.68
1:C:417:LEU:HD22	1:C:474:SER:HB2	1.78	0.66
1:C:385:GLN:NE2	1:C:385:GLN:H	1.98	0.61
1:C:186:ASN:HA	1:C:192:PRO:HG3	1.85	0.58
1:C:157:GLU:O	1:C:160:GLU:HG2	2.03	0.58
1:C:412:GLU:OE2	1:C:414:HIS:NE2	2.28	0.57
1:C:398:GLU:O	1:C:402:ILE:HG13	2.05	0.56
1:C:211:ALA:O	1:C:215:ILE:HG22	2.05	0.56
1:C:387:ARG:O	1:C:391:GLU:HG3	2.06	0.56
2:B:355:THR:O	2:B:359:GLN:HG3	2.06	0.55
1:C:156:LEU:HD11	1:C:184:ALA:HB1	1.89	0.54
1:C:47:PRO:O	1:C:50:ARG:HG2	2.08	0.54
1:C:234:LEU:HD22	1:C:257:GLN:HG3	1.90	0.53
1:C:417:LEU:HD12	1:C:417:LEU:C	2.29	0.53
1:C:239:VAL:HG12	1:C:339:LEU:HD11	1.91	0.53
1:C:147:SER:O	1:C:151:THR:HG23	2.08	0.52
1:C:93:ARG:HH21	1:C:388:ILE:HD11	1.76	0.51
2:B:355:THR:HA	2:B:358:LEU:HD21	1.93	0.51
1:C:353:HIS:CD2	1:C:365:SER:HA	2.46	0.50
1:C:369:TYR:OH	1:C:398:GLU:OE1	2.20	0.50
1:C:466:CYS:HB3	1:C:471:PRO:HA	1.92	0.50
1:C:432:VAL:HG23	1:C:479:ARG:HB2	1.93	0.50
1:C:64:HIS:CE1	1:C:72:ASN:HB3	2.47	0.49
1:C:54:LEU:HD21	1:C:83:LEU:HB3	1.94	0.49
1:C:351:SER:OG	1:C:368:THR:OG1	2.31	0.48
1:C:391:GLU:O	1:C:396:GLY:N	2.39	0.48
1:C:207:LEU:HD12	1:C:231:VAL:HG22	1.94	0.48
1:C:105:ARG:HB2	1:C:404:SER:HA	1.96	0.47
1:C:430:GLY:O	1:C:479:ARG:N	2.36	0.47
2:B:358:LEU:HD23	2:B:358:LEU:H	1.80	0.47
1:C:185:PHE:O	1:C:188:ARG:HG2	2.14	0.47
1:C:401:ASN:HD21	1:C:410:ARG:HA	1.80	0.47
1:C:384:SER:O	1:C:388:ILE:HG12	2.16	0.46
1:C:178:TRP:CE3	1:C:181:LEU:HD12	2.51	0.45
1:C:330:ASP:O	1:C:334:ASN:ND2	2.45	0.45
1:C:122:THR:O	1:C:124:THR:N	2.50	0.45
1:C:169:ASP:HB3	1:C:172:ALA:HB2	1.99	0.44
1:C:159:MET:HA	1:C:162:GLU:HG3	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:258:LEU:HD23	1:C:258:LEU:HA	1.85	0.44
1:C:422:GLN:O	1:C:426:LEU:HD23	2.19	0.43
1:C:47:PRO:O	1:C:50:ARG:N	2.43	0.43
1:C:377:GLU:OE2	1:C:382:ARG:NH2	2.52	0.42
1:C:133:VAL:HG21	1:C:393:MET:HG2	2.00	0.42
1:C:90:THR:HG23	1:C:373:PHE:HB3	2.01	0.42
1:C:59:LEU:HD11	1:C:363:LEU:HG	2.02	0.41
1:C:178:TRP:HE3	1:C:181:LEU:HD12	1.84	0.41
1:C:377:GLU:HA	1:C:387:ARG:NH2	2.36	0.41
1:C:401:ASN:ND2	1:C:410:ARG:HA	2.37	0.40

There are no symmetry-related clashes.

## 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	C	372/452 (82%)	360 (97%)	11 (3%)	1 (0%)	41	74
2	B	12/38 (32%)	11 (92%)	1 (8%)	0	100	100
All	All	384/490 (78%)	371 (97%)	12 (3%)	1 (0%)	41	74

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	47	PRO

### 5.3.2 Protein sidechains [i](#)

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	C	303/394 (77%)	293 (97%)	10 (3%)	38	71
2	B	7/30 (23%)	5 (71%)	2 (29%)	0	1
All	All	310/424 (73%)	298 (96%)	12 (4%)	32	67

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	52	LEU
1	C	74	ASN
1	C	171	ASP
1	C	185	PHE
1	C	186	ASN
1	C	254	SER
1	C	331	SER
1	C	417	LEU
1	C	452	ASP
1	C	466	CYS
2	B	355	THR
2	B	358	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	74	ASN
1	C	121	GLN
1	C	385	GLN
2	B	363	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 [i](#)

There are no monosaccharides 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 [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	C	376/452 (83%)	0.05	9 (2%) 59 44	44, 69, 93, 121	0
2	B	14/38 (36%)	-0.10	0 100 100	95, 105, 109, 114	0
All	All	390/490 (79%)	0.05	9 (2%) 60 47	44, 69, 99, 121	0

All (9) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	70	LEU	3.7
1	C	123	ARG	2.8
1	C	258	LEU	2.7
1	C	78	GLU	2.5
1	C	359	MET	2.5
1	C	173	SER	2.5
1	C	363	LEU	2.4
1	C	62	ALA	2.4
1	C	232	SER	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 monosaccharides 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.