



# wwPDB X-ray Structure Validation Summary Report ⓘ

May 16, 2020 – 06:01 am BST

PDB ID : 3S8V  
Title : Crystal structure of LRP6-Dkk1 complex  
Authors : Cheng, Z.; Xu, W.  
Deposited on : 2011-05-31  
Resolution : 3.10 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](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	:	2.11
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

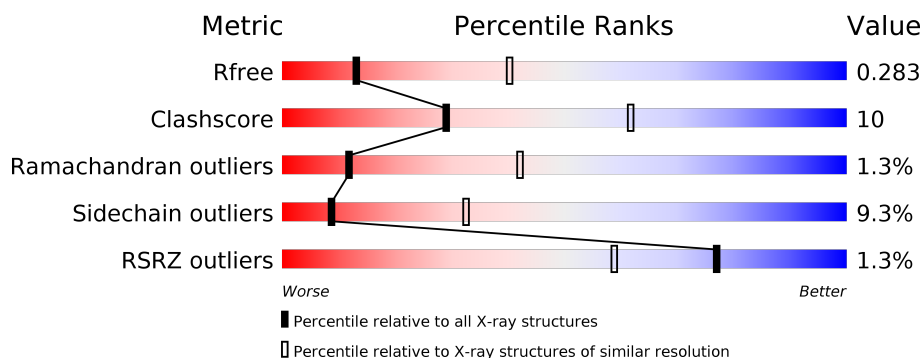
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 3.10 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	1094 (3.10-3.10)
Clashscore	141614	1184 (3.10-3.10)
Ramachandran outliers	138981	1141 (3.10-3.10)
Sidechain outliers	138945	1141 (3.10-3.10)
RSRZ outliers	127900	1067 (3.10-3.10)

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	A	623	<div> <div>70%</div> <div>22%</div> <div>• •</div> </div>
1	B	623	<div> <div>2%</div> <div>70%</div> <div>25%</div> <div>• •</div> </div>
2	X	88	<div> <div>%</div> <div>63%</div> <div>18%</div> <div>•</div> <div>17%</div> </div>

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 10177 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 Low-density lipoprotein receptor-related protein 6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	600	Total	C	N	O	S	0	0	0
			4790	3011	846	908	25			
1	B	604	Total	C	N	O	S	0	0	0
			4818	3025	854	914	25			

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	621	HIS	-	EXPRESSION TAG	UNP O75581
A	622	HIS	-	EXPRESSION TAG	UNP O75581
A	623	HIS	-	EXPRESSION TAG	UNP O75581
A	624	HIS	-	EXPRESSION TAG	UNP O75581
A	625	HIS	-	EXPRESSION TAG	UNP O75581
A	626	HIS	-	EXPRESSION TAG	UNP O75581
A	627	HIS	-	EXPRESSION TAG	UNP O75581
A	628	HIS	-	EXPRESSION TAG	UNP O75581
A	1062	ILE	VAL	CONFLICT	UNP O75581
B	621	HIS	-	EXPRESSION TAG	UNP O75581
B	622	HIS	-	EXPRESSION TAG	UNP O75581
B	623	HIS	-	EXPRESSION TAG	UNP O75581
B	624	HIS	-	EXPRESSION TAG	UNP O75581
B	625	HIS	-	EXPRESSION TAG	UNP O75581
B	626	HIS	-	EXPRESSION TAG	UNP O75581
B	627	HIS	-	EXPRESSION TAG	UNP O75581
B	628	HIS	-	EXPRESSION TAG	UNP O75581
B	1062	ILE	VAL	CONFLICT	UNP O75581

- Molecule 2 is a protein called Dickkopf-related protein 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	X	73	Total	C	N	O	S	0	0	0
			569	345	116	98	10			

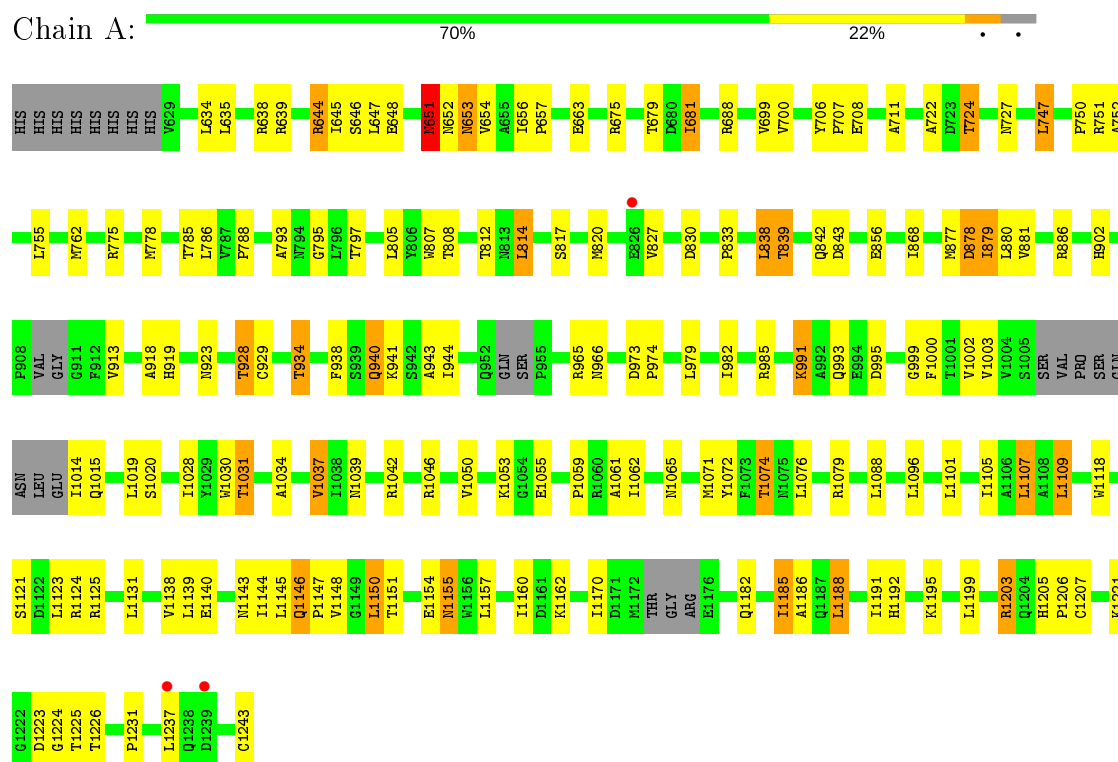
There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
X	179	GLY	-	EXPRESSION TAG	UNP O94907
X	180	PRO	-	EXPRESSION TAG	UNP O94907
X	181	GLY	-	EXPRESSION TAG	UNP O94907
X	182	SER	-	EXPRESSION TAG	UNP O94907

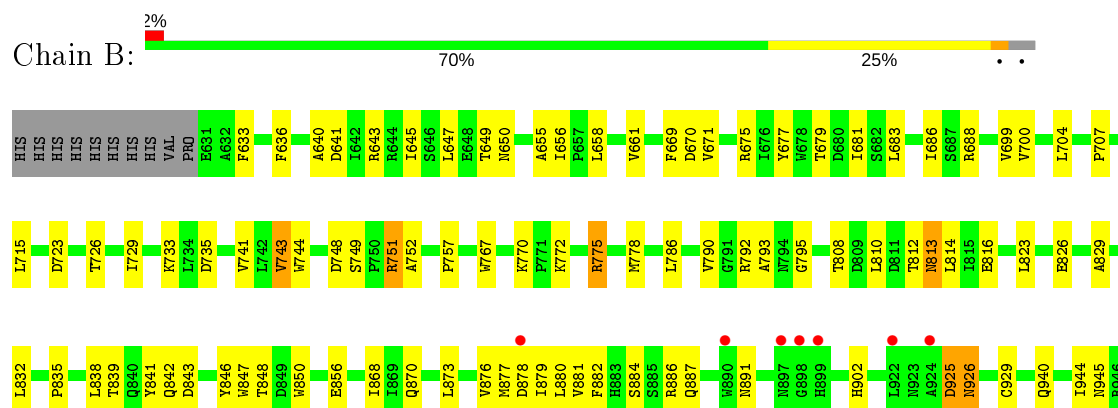
### 3 Residue-property plots

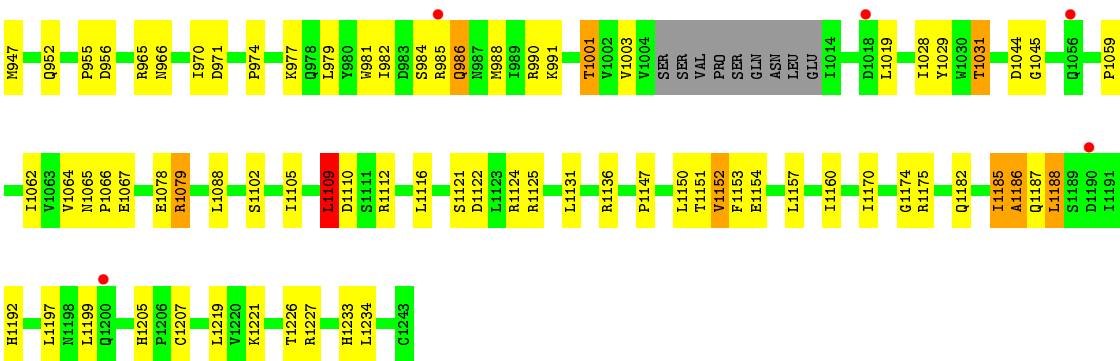
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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: Low-density lipoprotein receptor-related protein 6



- Molecule 1: Low-density lipoprotein receptor-related protein 6





● Molecule 2: Dickkopf-related protein 1



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	94.38Å 105.05Å 161.23Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 3.10 29.63 – 3.05	Depositor EDS
% Data completeness (in resolution range)	98.2 (30.00-3.10) 97.4 (29.63-3.05)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.65 (at 3.06Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, $R_{free}$	0.240 , 0.292 0.236 , 0.283	Depositor DCC
$R_{free}$ test set	1538 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	71.7	Xtriage
Anisotropy	0.612	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.26 , 49.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	10177	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	87.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.78% 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 [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	0.36	0/4889	0.57	0/6630
1	B	0.36	0/4919	0.55	1/6674 (0.0%)
2	X	0.37	0/577	0.55	0/766
All	All	0.36	0/10385	0.56	1/14070 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	1109	LEU	CA-CB-CG	5.38	127.66	115.30

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	4790	0	4676	94	0
1	B	4818	0	4705	88	0
2	X	569	0	558	14	0
All	All	10177	0	9939	194	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 10.

The worst 5 of 194 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:A:1031:THR:HG23	1:A:1062:ILE:HD11	1.19	1.12
1:B:1031:THR:HG23	1:B:1062:ILE:HD11	1.36	1.03
1:A:679:THR:HG21	1:A:707:PRO:O	1.63	0.99
1:A:1019:LEU:HD12	1:A:1028:ILE:HD11	1.44	0.97
1:B:1031:THR:HG23	1:B:1062:ILE:CD1	1.94	0.97

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	A	590/623 (95%)	529 (90%)	50 (8%)	11 (2%)	8	33
1	B	600/623 (96%)	540 (90%)	55 (9%)	5 (1%)	19	54
2	X	69/88 (78%)	65 (94%)	4 (6%)	0	100	100
All	All	1259/1334 (94%)	1134 (90%)	109 (9%)	16 (1%)	12	42

5 of 16 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	1174	GLY
1	A	878	ASP
1	A	879	ILE
1	B	926	ASN
1	B	986	GLN

### 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	A	525/546 (96%)	473 (90%)	52 (10%)	8	29
1	B	527/546 (96%)	479 (91%)	48 (9%)	9	33
2	X	64/75 (85%)	60 (94%)	4 (6%)	18	48
All	All	1116/1167 (96%)	1012 (91%)	104 (9%)	9	32

5 of 104 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1188	LEU
1	B	748	ASP
1	B	1188	LEU
1	A	1203	ARG
1	B	641	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 25 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1155	ASN
1	A	1211	ASN
2	X	223	HIS
1	A	1205	HIS
1	A	1216	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 ⓘ

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 [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	A	600/623 (96%)	-0.23	3 (0%) 91 81	45, 80, 113, 143	0
1	B	604/623 (96%)	-0.09	12 (1%) 65 44	45, 90, 113, 141	0
2	X	73/88 (82%)	-0.00	1 (1%) 75 56	65, 86, 107, 122	0
All	All	1277/1334 (95%)	-0.15	16 (1%) 77 59	45, 86, 113, 143	0

The worst 5 of 16 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	899	HIS	4.5
1	B	898	GLY	4.3
2	X	241	GLU	4.0
1	B	897	ASN	2.9
1	B	1056	GLN	2.8

### 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 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.