



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 5, 2026 – 12:25 PM UTC

PDB ID : 3L2O / pdb_00003l2o
Title : Structure-Based Mechanism of Dimerization-Dependent Ubiquitination by the SCFFbx4 Ubiquitin Ligase
Authors : Li, Y.; Hao, B.
Deposited on : 2009-12-15
Resolution : 2.80 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

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

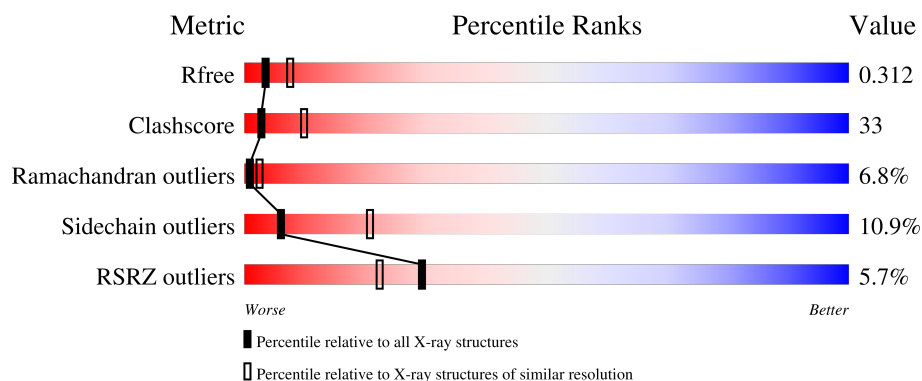
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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}	180053	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

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 of 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	149	11% 46% 38% 9% .
2	B	312	3% 49% 27% 11% . 12%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 3425 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 S-phase kinase-associated protein 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	145	Total	C	N	O	S	0	0	0
			1142	723	186	227	6			

There are 23 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1002	ALA	PRO	engineered mutation	UNP P63208
A	?	-	ASP	deletion	UNP P63208
A	?	-	ASP	deletion	UNP P63208
A	?	-	GLU	deletion	UNP P63208
A	?	-	GLY	deletion	UNP P63208
A	?	-	ASP	deletion	UNP P63208
A	?	-	ASP	deletion	UNP P63208
A	?	-	PRO	deletion	UNP P63208
A	?	-	PRO	deletion	UNP P63208
A	?	-	GLU	deletion	UNP P63208
A	?	-	ASP	deletion	UNP P63208
A	?	-	ASP	deletion	UNP P63208
A	?	-	GLU	deletion	UNP P63208
A	?	-	ASN	deletion	UNP P63208
A	?	-	LYS	deletion	UNP P63208
A	?	-	GLU	deletion	UNP P63208
A	?	-	LYS	deletion	UNP P63208
A	?	-	ARG	deletion	UNP P63208
A	1078	GLY	-	insertion	UNP P63208
A	1079	GLY	-	insertion	UNP P63208
A	1080	SER	-	insertion	UNP P63208
A	1081	GLY	-	insertion	UNP P63208

- Molecule 2 is a protein called F-box only protein 4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	274	Total	C	N	O	S	0	0	0
			2207	1423	364	406	14			

There are 21 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	?	-	THR	deletion	UNP Q9UKT5
B	?	-	ARG	deletion	UNP Q9UKT5
B	?	-	ARG	deletion	UNP Q9UKT5
B	?	-	ALA	deletion	UNP Q9UKT5
B	?	-	SER	deletion	UNP Q9UKT5
B	?	-	LYS	deletion	UNP Q9UKT5
B	?	-	SER	deletion	UNP Q9UKT5
B	?	-	SER	deletion	UNP Q9UKT5
B	?	-	ARG	deletion	UNP Q9UKT5
B	?	-	PRO	deletion	UNP Q9UKT5
B	?	-	MET	deletion	UNP Q9UKT5
B	?	-	TYR	deletion	UNP Q9UKT5
B	?	-	GLY	deletion	UNP Q9UKT5
B	?	-	ALA	deletion	UNP Q9UKT5
B	?	-	VAL	deletion	UNP Q9UKT5
B	?	-	THR	deletion	UNP Q9UKT5
B	?	-	SER	deletion	UNP Q9UKT5
B	?	-	PHE	deletion	UNP Q9UKT5
B	?	-	LEU	deletion	UNP Q9UKT5
B	?	-	HIS	deletion	UNP Q9UKT5
B	?	-	SER	deletion	UNP Q9UKT5

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	20	Total	O	0	0
			20	20		
3	B	56	Total	O	0	0
			56	56		

4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α , β , γ	92.19Å 92.19Å 148.07Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	50.00 – 2.80 50.00 – 2.80	Depositor EDS
% Data completeness (in resolution range)	99.5 (50.00-2.80) 99.5 (50.00-2.80)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.87 (at 2.80Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, R_{free}	0.249 , 0.295 0.267 , 0.312	Depositor DCC
R_{free} test set	915 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å ²)	77.0	Xtriage
Anisotropy	0.034	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 88.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.52$, $\langle L^2 \rangle = 0.36$	Xtriage
Estimated twinning fraction	0.019 for -h,-k,l	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	3425	wwPDB-VP
Average B, all atoms (Å ²)	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.45% 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 [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	1.03	1/1161 (0.1%)	1.31	13/1572 (0.8%)
2	B	1.09	4/2266 (0.2%)	1.29	17/3087 (0.6%)
All	All	1.07	5/3427 (0.1%)	1.30	30/4659 (0.6%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1082	THR	CA-CB	6.69	1.61	1.52
2	B	171	LEU	C-N	6.35	1.41	1.33
2	B	354	ASN	CA-C	5.26	1.59	1.52
2	B	147	CYS	C-N	5.18	1.39	1.34
2	B	339	MET	CA-C	-5.04	1.47	1.52

The worst 5 of 30 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1144	ASP	CB-CA-C	-10.32	89.88	110.42
1	A	1133	GLU	CB-CA-C	-9.88	90.75	110.42
2	B	106	ASP	CB-CA-C	-8.62	93.27	110.42
1	A	1144	ASP	N-CA-C	8.57	129.05	110.80
2	B	105	ARG	N-CA-C	-8.56	99.23	110.53

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	1142	0	1139	90	0
2	B	2207	0	2148	135	0
3	A	20	0	0	1	0
3	B	56	0	0	1	0
All	All	3425	0	3287	219	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 33.

The worst 5 of 219 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:1136:ARG:HA	1:A:1141:ILE:HD11	1.26	1.13
1:A:1132:PRO:O	1:A:1134:GLU:N	1.84	1.10
2:B:198:MET:CE	2:B:221:VAL:HG21	1.81	1.09
1:A:1136:ARG:CA	1:A:1141:ILE:HD11	1.85	1.06
2:B:198:MET:HE1	2:B:221:VAL:HG21	1.12	1.06

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	143/149 (96%)	111 (78%)	17 (12%)	15 (10%)	0	1
2	B	268/312 (86%)	231 (86%)	24 (9%)	13 (5%)	1	6
All	All	411/461 (89%)	342 (83%)	41 (10%)	28 (7%)	1	2

5 of 28 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1012	GLU

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Mol	Chain	Res	Type
1	A	1013	ILE
1	A	1037	ASP
1	A	1068	ASP
1	A	1080	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	129/133 (97%)	117 (91%)	12 (9%)	8	27
2	B	247/280 (88%)	218 (88%)	29 (12%)	5	18
All	All	376/413 (91%)	335 (89%)	41 (11%)	6	21

5 of 41 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	229	HIS
2	B	314	THR
2	B	235	ILE
2	B	276	ILE
2	B	327	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 16 such sidechains are listed below:

Mol	Chain	Res	Type
2	B	280	GLN
2	B	232	ASN
2	B	87	HIS
2	B	229	HIS
2	B	86	ASN

5.3.3 RNA ⓘ

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 oligosaccharides 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, 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	145/149 (97%)	0.80	16 (11%) 10 8	30, 43, 68, 72	0
2	B	274/312 (87%)	0.24	8 (2%) 53 43	33, 45, 54, 63	0
All	All	419/461 (90%)	0.44	24 (5%) 29 22	30, 45, 61, 72	0

The worst 5 of 24 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1081	GLY	6.2
1	A	1078	GLY	4.9
1	A	1082	THR	4.0
1	A	1159	TRP	3.3
1	A	1079	GLY	3.1

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 oligosaccharides 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.