



wwPDB X-ray Structure Validation Summary Report ⓘ

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PDB ID : 6P5L / pdb_00006p5l
Title : Crystal Structure of Ubl123 with an EZH2 peptide
Authors : Saridakis, V.
Deposited on : 2019-05-30
Resolution : 3.30 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

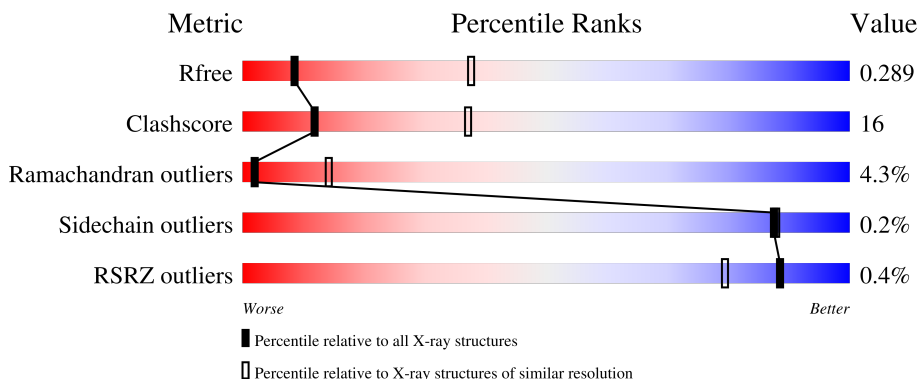
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.30 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	1169 (3.32-3.28)
Clashscore	190562	1209 (3.32-3.28)
Ramachandran outliers	187476	1188 (3.32-3.28)
Sidechain outliers	187428	1187 (3.32-3.28)
RSRZ outliers	180081	1169 (3.32-3.28)

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	356	62% 30% • •
1	B	356	63% 29% • •
2	D	8	38% 38% 25%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 5622 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 Ubiquitin carboxyl-terminal hydrolase 7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	341	Total	C	N	O	S	0	0	0
			2784	1760	474	532	18			
1	B	340	Total	C	N	O	S	0	0	0
			2780	1757	477	530	16			

- Molecule 2 is a protein called PRO-ARG-LYS-LYS-LYS-ARG-LYS-HIS.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	D	6	Total	C	N	O	0	0	0
			58	36	16	6			

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.

Chain A:

62% 30%

Residue	State
P852	Green
L853	Green
R854	Green
F868	Green
K869	Green
P870	Green
R871	Green
P873	Green
K873	Green
K874	Green
K875	Green
L876	Green
Y877	Green
Y878	Green
Q879	Green
Q880	Green
L881	Green
K882	Green
R883	Green
LYS	Green
ILE	Green
THR	Green
ASP	Green
PHE	Green
GLU	Green
ASN	Green
D839	Green
A842	Green
D843	Yellow
G844	Yellow
N845	Yellow
K846	Yellow
T847	Yellow
M848	Yellow
I849	Yellow
E850	Yellow
L851	Yellow
S852	Yellow
E855	Yellow
E856	Yellow
P857	Yellow
V858	Yellow
T859	Yellow
E863	Yellow
T864	Yellow
V865	Yellow
E868	Yellow
L869	Yellow
A870	Yellow
A871	Yellow
S872	Yellow
G873	Yellow
A874	Yellow
T875	Yellow
L876	Yellow
F879	Yellow
H883	Yellow
M891	Yellow
Y892	Yellow
N700	Yellow
H704	Yellow
I705	Yellow
Y706	Yellow
I709	Yellow
R714	Yellow
R723	Yellow
K739	Yellow
L742	Yellow
Y749	Yellow
D750	Yellow
V751	Yellow
S752	Yellow
L753	Yellow
D754	Yellow
D758	Yellow
E759	Yellow
L760	Yellow
M761	Yellow
V767	Yellow
E774	Yellow
E779	Yellow
L780	Yellow
K784	Yellow
E785	Yellow
Y786	Yellow
F787	Yellow
D795	Yellow
V796	Yellow
I797	Yellow
D800	Yellow
K801	Yellow
T802	Yellow
I803	Yellow
D806	Yellow
T812	Yellow
L813	Yellow
S814	Yellow
N815	Yellow
R816	Yellow
M817	Yellow
N818	Yellow
Y819	Yellow
K824	Yellow
Q828	Yellow
R829	Yellow
L830	Yellow
N831	Yellow
T832	Yellow
D833	Yellow
P834	Yellow
M835	Yellow
Q838	Yellow
Q843	Yellow
G844	Yellow
Y845	Yellow
R846	Yellow
D847	Yellow

[illegible]

Chain D: 38% 38% 25%

PRO
R490
R491
K492
K493
R494
K495
HIS

4 Data and refinement statistics

Property	Value	Source
Space group	P 42 21 2	Depositor
Cell constants a, b, c, α , β , γ	165.45Å 165.45Å 110.90Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.61 – 3.30 29.61 – 3.30	Depositor EDS
% Data completeness (in resolution range)	99.5 (29.61-3.30) 99.3 (29.61-3.30)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.13 (at 3.31Å)	Xtriage
Refinement program	PHENIX 1.13_2998	Depositor
R, R_{free}	0.231 , 0.289 0.240 , 0.289	Depositor DCC
R_{free} test set	2000 reflections (8.40%)	wwPDB-VP
Wilson B-factor (Å ²)	117.6	Xtriage
Anisotropy	0.133	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 69.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	5622	wwPDB-VP
Average B, all atoms (Å ²)	122.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.64% 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	0.41	0/2843	1.24	21/3840 (0.5%)
1	B	0.35	1/2838 (0.0%)	0.86	2/3832 (0.1%)
2	D	0.34	0/57	0.76	0/69
All	All	0.38	1/5738 (0.0%)	1.06	23/7741 (0.3%)

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	A	0	1
1	B	0	1
All	All	0	2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	597	LEU	CG-CD2	-5.64	1.33	1.52

The worst 5 of 23 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	645	ASN	CB-CG-OD1	28.98	178.76	120.80
1	A	645	ASN	CB-CG-ND2	-26.54	76.59	116.40
1	A	880	GLN	CG-CD-NE2	-22.18	83.14	116.40
1	A	645	ASN	OD1-CG-ND2	-19.98	102.62	122.60
1	A	880	GLN	CA-CB-CG	-10.43	93.23	114.10

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	880	GLN	Sidechain
1	B	607	GLN	Peptide

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	2784	0	2727	94	0
1	B	2780	0	2725	91	0
2	D	58	0	77	4	0
All	All	5622	0	5529	176	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 16.

The worst 5 of 176 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:B:719:VAL:HG12	1:B:723:ARG:HD2	1.50	0.91
1:B:569:ILE:HG21	1:B:613:MET:HE1	1.56	0.85
1:B:578:HIS:NE2	1:B:580:GLY:O	2.10	0.85
1:A:869:LYS:HB3	1:A:870:PRO:HD2	1.63	0.80
1:A:704:HIS:O	1:A:723:ARG:NH2	2.16	0.79

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	339/356 (95%)	293 (86%)	35 (10%)	11 (3%)	3	19
1	B	336/356 (94%)	272 (81%)	46 (14%)	18 (5%)	1	10
2	D	4/8 (50%)	2 (50%)	2 (50%)	0	100	100
All	All	679/720 (94%)	567 (84%)	83 (12%)	29 (4%)	2	14

5 of 29 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	617	GLN
1	A	645	ASN
1	A	672	SER
1	A	750	ASP
1	A	870	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	A	310/327 (95%)	310 (100%)	0	100	100
1	B	309/327 (94%)	308 (100%)	1 (0%)	86	86
2	D	6/8 (75%)	6 (100%)	0	100	100
All	All	625/662 (94%)	624 (100%)	1 (0%)	87	88

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	597	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 7 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	843	GLN
1	B	566	GLN

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Mol	Chain	Res	Type
1	B	728	GLN
1	B	617	GLN
1	A	645	ASN

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 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	341/356 (95%)	-0.29	2 (0%) 85 73	70, 106, 166, 199	0
1	B	340/356 (95%)	-0.21	1 (0%) 90 82	83, 129, 180, 211	0
2	D	6/8 (75%)	0.28	0 100 100	124, 127, 147, 156	0
All	All	687/720 (95%)	-0.24	3 (0%) 88 79	70, 116, 176, 211	0

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	847	ASP	3.9
1	B	540	LEU	3.3
1	A	816	ARG	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 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.