

wwPDB X-ray Structure Validation Summary Report (i)

Oct 26, 2021 – 05:03 pm BST

:	6TXB
:	Crystal structure of Mindy1 mutant (P138A) in complex with Lys48 linked
	di-ubiquitin
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	2020-01-14
:	2.18 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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

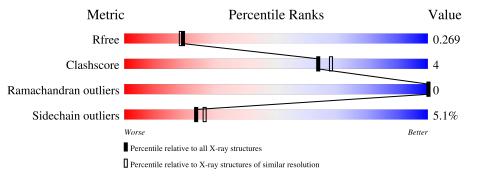
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.23.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0267
CCP4	:	7.1.010 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.23.2

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: $X\text{-}RAY \, DIFFRACTION$

The reported resolution of this entry is 2.18 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	$egin{array}{c} { m Whole \ archive} \ (\#{ m Entries}) \end{array}$	${f Similar\ resolution}\ (\#{ m Entries,\ resolution\ range}({ m \AA}))$
R_{free}	130704	6864 (2.20-2.16)
Clashscore	141614	7689 (2.20-2.16)
Ramachandran outliers	138981	7564 (2.20-2.16)
Sidechain outliers	138945	7564 (2.20-2.16)

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 <=5%

Mol	Chain	Length	Quality of chain	
1	А	289	82% 8	% • 9%
2	D	76	84%	16%
2	Н	76	91%	5% • •
2	L	76	39% 16% • 43%	



2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 3634 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 MINDY-1.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace		
1	А	263	Total 2052	C 1314	N 337	O 389	S 12	0	0	0

Chain	Residue	Modelled	Actual	Comment	Reference
A	96	GLY	-	expression tag	UNP Q8N5J2
А	97	PRO	-	expression tag	UNP Q8N5J2
А	98	LEU	-	expression tag	UNP Q8N5J2
А	99	GLY	-	expression tag	UNP Q8N5J2
А	100	SER	-	expression tag	UNP Q8N5J2
А	101	PRO	-	expression tag	UNP Q8N5J2
А	102	GLU	-	expression tag	UNP Q8N5J2
А	103	PHE	-	expression tag	UNP Q8N5J2
А	104	PRO	-	expression tag	UNP Q8N5J2
А	105	GLY	-	expression tag	UNP Q8N5J2
А	106	ARG	-	expression tag	UNP Q8N5J2
А	107	LEU	-	expression tag	UNP Q8N5J2
А	108	GLU	-	expression tag	UNP Q8N5J2
А	109	MET	-	expression tag	UNP Q8N5J2
А	137	ALA	CYS	engineered mutation	UNP Q8N5J2
А	138	ALA	PRO	engineered mutation	UNP Q8N5J2

There are 16 discrepancies between the modelled and reference sequences:

• Molecule 2 is a protein called Polyubiquitin-C.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
2	D	76	Total C N O S 594 374 104 115 1	0	0	0
2	Н	74	Total C N O S 593 374 103 115 1	0	0	0
2	L	43	Total C N O 332 205 60 67	0	0	0



• Molecule 3 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	А	3	Total Na 3 3	0	0
3	D	1	Total Na 1 1	0	0

• Molecule 4 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	А	2	Total Cl 2 2	0	0

• Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	А	48	Total O 48 48	0	0
5	D	2	Total O 2 2	0	0
5	Н	3	Total O 3 3	0	0
5	L	4	Total O 4 4	0	0



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. 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. 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: Ubiquitin carboxyl-terminal hydrolase MINDY-1

Chain A:		82%				8% • 9%)	
GLY PRO LEU GLY GLU PRO GLU FRO FRO FRO FRO FRO FRO FRO FRO FRO FRO	M109 1130 134 134 134 134 136 136	0187 L188 V200 R213	D219 P224 L231	D243 P244 Q245 F248	V262 1266	K2 <mark>69</mark> R316 N318 N318	T335 D336 Q337	P 2 2 A
12370 GLY CLYS GLY PRU GLY GLY GLY SER SER SER	PR0 GLU							
• Molecule 2: Pol	yubiquitin-C							
Chain D:		84%				16%	_	
M1 F4 19 K29 K23 K48 K48	161 161 962 863 863 863 863 863 863 863 863 875 875 876							
• Molecule 2: Pol	yubiquitin-C							
Chain H:		91%				5%•	·	
M1 31 41 41 41 41 41 87 87 87 81 81 81 81 81 81 81 81 81 81 81 81 81								
• Molecule 2: Pol	yubiquitin-C							
Chain L:	39%	16%	•		43%		-	
MET GLN GLN LLE VAL LYS LYS THR CLY CLY THR THR THR THR THR	THR LEU GLU GLU PRO 123 V26 V26 V26	K29 130 031 132 K33 K33 E34	Q41 R42 L43 144 PHE	ALA GLY K48 T55	<mark>Y59</mark> ASN ILE GLN	LYS GLU SER THR LEU H68 I.69	ARG GLY GT V	1 19



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 41 2 2	Depositor
Cell constants	74.03Å 74.03Å 202.85Å	Depositor
a, b, c, α , β , γ	90.00° 90.00° 90.00°	Depositor
Resolution (Å)	41.84 - 2.18	Depositor
Resolution (A)	41.84 - 2.18	EDS
% Data completeness	99.9(41.84-2.18)	Depositor
(in resolution range)	$100.0 \ (41.84-2.18)$	EDS
R _{merge}	0.07	Depositor
R _{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	2.24 (at 2.18\AA)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.212 , 0.246	Depositor
II, II, <i>free</i>	0.239 , 0.269	DCC
R_{free} test set	1508 reflections $(4.97%)$	wwPDB-VP
Wilson B-factor $(Å^2)$	48.6	Xtriage
Anisotropy	0.436	Xtriage
Bulk solvent $k_{sol}(e/Å^3), B_{sol}(Å^2)$	(Not available), (Not available)	EDS
L-test for twinning ²	$ L > = 0.49, < L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	3634	wwPDB-VP
Average B, all atoms $(Å^2)$	67.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 4.57% of the height of the origin peak. No significant pseudotranslation is detected.

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.



¹Intensities estimated from amplitudes.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: NA, CL

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		
	Unam	RMSZ	# Z > 5	RMSZ	# Z > 5	
1	А	0.40	0/2101	0.56	0/2864	
2	D	0.42	0/600	0.62	0/808	
2	Н	0.30	0/599	0.59	0/806	
2	L	0.43	0/332	0.65	0/444	
All	All	0.39	0/3632	0.58	0/4922	

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	А	2052	0	1983	18	0
2	D	594	0	616	5	0
2	Н	593	0	620	4	0
2	L	332	0	323	9	0
3	А	3	0	0	0	0
3	D	1	0	0	0	0
4	А	2	0	0	0	0
5	А	48	0	0	0	0
5	D	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	Н	3	0	0	0	0
5	L	4	0	0	0	0
All	All	3634	0	3542	30	0

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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 4.

The worst 5 of 30 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)
2:L:41:GLN:HB2	2:L:69:LEU:HD11	1.52	0.91
2:H:31:GLN:O	2:H:31:GLN:HG3	1.93	0.67
1:A:231:LEU:HD23	2:L:73:LEU:HD11	1.78	0.65
2:D:61:ILE:HD13	2:D:67:LEU:HD21	1.81	0.63
2:D:4:PHE:CE2	2:D:64:GLU:HA	2.36	0.60

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	Perce	ntiles
1	А	261/289~(90%)	255~(98%)	6(2%)	0	100	100
2	D	74/76~(97%)	73~(99%)	1 (1%)	0	100	100
2	Н	72/76~(95%)	72 (100%)	0	0	100	100
2	L	37/76~(49%)	36~(97%)	1 (3%)	0	100	100
All	All	444/517~(86%)	436 (98%)	8 (2%)	0	100	100

There are no Ramachandran outliers to report.



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 side chain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percen	tiles
1	А	226/251~(90%)	216~(96%)	10 (4%)	28	33
2	D	66/68~(97%)	61 (92%)	5 (8%)	13	12
2	Н	68/68~(100%)	66~(97%)	2(3%)	42	51
2	L	35/68~(52%)	32~(91%)	3~(9%)	10	9
All	All	395/455~(87%)	375~(95%)	20~(5%)	24	26

5 of 20 residues with a non-rotameric sidechain are listed below:

Mol	Chain	\mathbf{Res}	Type
2	D	63	LYS
2	L	30	ILE
2	L	73	LEU
2	L	55	THR
1	А	248	GLU

Sometimes side chains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such side chains are listed below:

Mol	Chain	Res	Type
2	L	41	GLN

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 monosaccharides in this entry.



5.6 Ligand geometry (i)

Of 6 ligands modelled in this entry, 6 are monoatomic - leaving 0 for Mogul analysis. There are no bond length outliers. There are no bond angle outliers. There are no chirality outliers. There are no torsion outliers. There are no ring outliers. No monomer is involved in short contacts.

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)

Unable to reproduce the depositors R factor - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

6.3 Carbohydrates (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

6.4 Ligands (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

6.5 Other polymers (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

