



wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 29, 2016 – 02:57 PM EDT

PDB ID : 5B83
Title : Crystal structure of Optineurin UBAN in complex with linear ubiquitin
Authors : Ishii, R.; Nureki, O.
Deposited on : 2016-06-12
Resolution : 2.69 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

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity	:	4.02b-467
Mogul	:	unknown
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20027939
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20027939

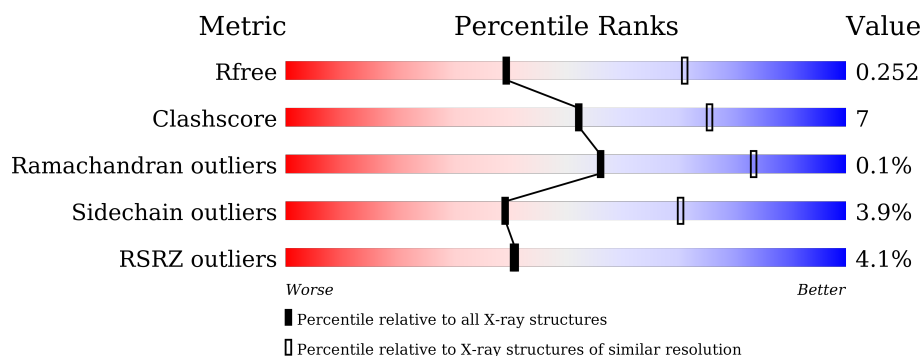
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.69 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}	91344	2103 (2.70-2.70)
Clashscore	102246	2422 (2.70-2.70)
Ramachandran outliers	100387	2382 (2.70-2.70)
Sidechain outliers	100360	2382 (2.70-2.70)
RSRZ outliers	91569	2107 (2.70-2.70)

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 ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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	304	<div> <div>7%</div> <div> <div></div> <div>78%</div> <div>20%</div> <div>..</div> </div> </div>
1	D	304	<div> <div>2%</div> <div> <div></div> <div>84%</div> <div>14%</div> <div>..</div> </div> </div>
2	B	102	<div> <div>2%</div> <div> <div></div> <div>48%</div> <div>8%</div> <div>42%</div> </div> </div>
2	C	102	<div> <div>4%</div> <div> <div></div> <div>47%</div> <div>10%</div> <div>40%</div> </div> </div>
2	E	102	<div> <div></div> <div> <div></div> <div>37%</div> <div>12%</div> <div>51%</div> </div> </div>
2	F	102	<div> <div>2%</div> <div> <div></div> <div>43%</div> <div>13%</div> <div>42%</div> </div> </div>

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 6702 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 tetra ubiquitin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	302	Total	C	N	O	S	0	0	0
			2396	1508	418	466	4			
1	D	300	Total	C	N	O	S	0	0	0
			2377	1496	413	464	4			

- Molecule 2 is a protein called Optineurin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	59	Total	C	N	O	S	0	0	0
			483	299	83	96	5			
2	C	61	Total	C	N	O	S	0	0	0
			496	305	85	102	4			
2	E	50	Total	C	N	O	S	0	0	0
			412	256	71	82	3			
2	F	59	Total	C	N	O	S	0	0	0
			479	296	83	96	4			

There are 28 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	409	GLY	-	expression tag	UNP Q96CV9
B	410	PRO	-	expression tag	UNP Q96CV9
B	411	LEU	-	expression tag	UNP Q96CV9
B	412	GLY	-	expression tag	UNP Q96CV9
B	413	SER	-	expression tag	UNP Q96CV9
B	414	HIS	-	expression tag	UNP Q96CV9
B	415	MET	-	expression tag	UNP Q96CV9
C	409	GLY	-	expression tag	UNP Q96CV9
C	410	PRO	-	expression tag	UNP Q96CV9
C	411	LEU	-	expression tag	UNP Q96CV9
C	412	GLY	-	expression tag	UNP Q96CV9
C	413	SER	-	expression tag	UNP Q96CV9

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Chain	Residue	Modelled	Actual	Comment	Reference
C	414	HIS	-	expression tag	UNP Q96CV9
C	415	MET	-	expression tag	UNP Q96CV9
E	409	GLY	-	expression tag	UNP Q96CV9
E	410	PRO	-	expression tag	UNP Q96CV9
E	411	LEU	-	expression tag	UNP Q96CV9
E	412	GLY	-	expression tag	UNP Q96CV9
E	413	SER	-	expression tag	UNP Q96CV9
E	414	HIS	-	expression tag	UNP Q96CV9
E	415	MET	-	expression tag	UNP Q96CV9
F	409	GLY	-	expression tag	UNP Q96CV9
F	410	PRO	-	expression tag	UNP Q96CV9
F	411	LEU	-	expression tag	UNP Q96CV9
F	412	GLY	-	expression tag	UNP Q96CV9
F	413	SER	-	expression tag	UNP Q96CV9
F	414	HIS	-	expression tag	UNP Q96CV9
F	415	MET	-	expression tag	UNP Q96CV9

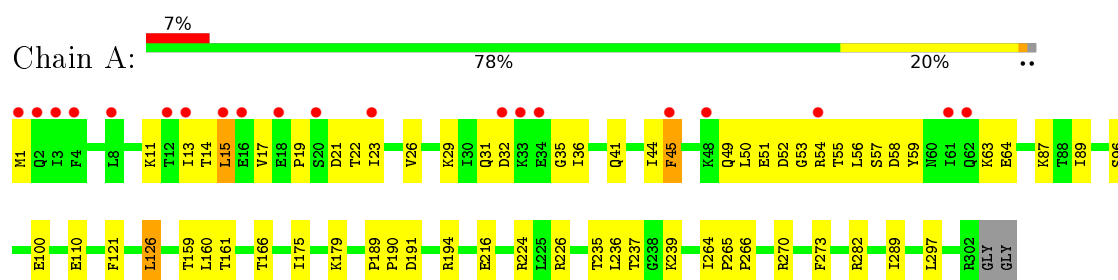
- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	23	Total O 23 23	0	0
3	B	3	Total O 3 3	0	0
3	C	3	Total O 3 3	0	0
3	D	25	Total O 25 25	0	0
3	E	5	Total O 5 5	0	0

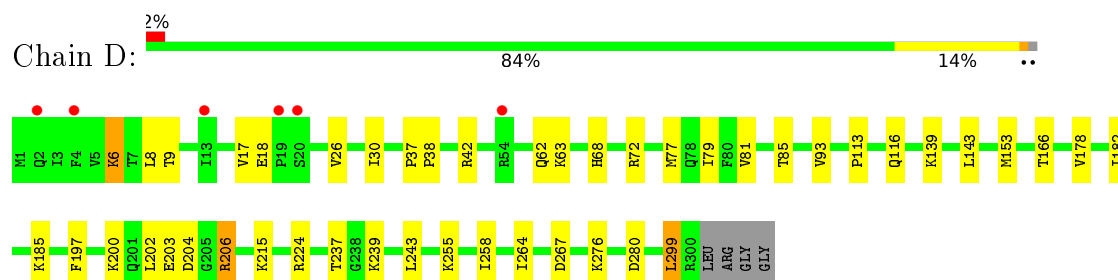
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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 ($\text{RSRZ} > 2$). 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.

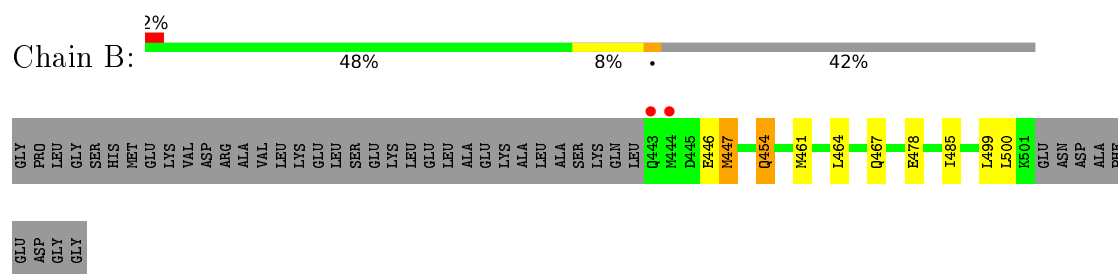
• Molecule 1: tetra ubiquitin



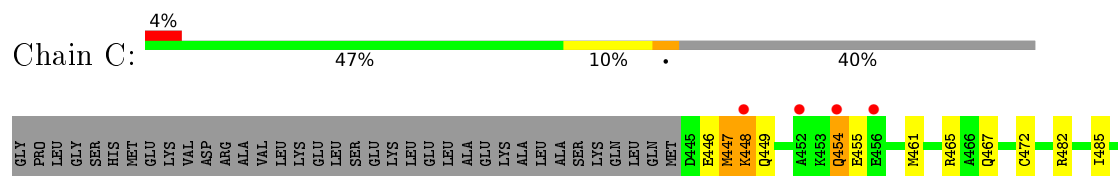
• Molecule 1: tetra ubiquitin



• Molecule 2: Optineurin

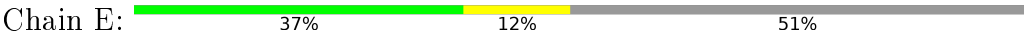


• Molecule 2: Optineurin



D504	ASP
ASP	PHE
PHE	GLU
GLU	ASP
ASP	GLY
GLY	GLY

• Molecule 2: Optineurin



GLY	PRO	LEU	GLY	SER	HIS	MET	GLU	LYS	VAL	ASP	ARG	ALA	VAL	LEU	LYS	GLU	LEU	SER	GLU	LYS	LEU	GLU	LEU	ALA	GLU	LYS	ALA	LEU	ALA	SER	LYS	GLN	LEU	GLN	MET	ASP	GLU	MET	LYS	GLN	THR	ILE	ALA	R483	Q454	L464	M468	S473	D474	F475	R479	R482	E483	K484
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I485	E488	K489	L492	E502	ASN	ASP	ALA	ALA	PHE	GLU	ASP	GLY
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• Molecule 2: Optineurin



GLY	PRO	LEU	GLY	SER	HIS	MET	GLU	LYS	VAL	ASP	ARG	ALA	VAL	LEU	LYS	GLU	LEU	SER	GLU	LYS	LEU	GLU	LEU	ALA	GLU	LYS	ALA	LEU	ALA	SER	LYS	GLN	LEU	GLN	MET	ASP	GLU	R447	K448	Q449	T450	I451	Q454	L458	E459	T462	R465	M468	E469	D474	E478
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I485	K501	E502	R503	D504	A505	PHE	GLU	GLU	ASP	GLY	GLY
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4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	71.33Å 82.04Å 244.85Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.06 – 2.69 49.06 – 2.69	Depositor EDS
% Data completeness (in resolution range)	99.4 (49.06-2.69) 95.1 (49.06-2.69)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.67 (at 2.69Å)	Xtriage
Refinement program	PHENIX (1.10.1 _2155: ???)	Depositor
R, R_{free}	0.201 , 0.254 0.199 , 0.252	Depositor DCC
R_{free} test set	1942 reflections (5.02%)	DCC
Wilson B-factor (Å ²)	45.1	Xtriage
Anisotropy	0.265	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 43.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	6702	wwPDB-VP
Average B, all atoms (Å ²)	62.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.18% 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	0.46	0/2423	0.68	1/3263 (0.0%)
1	D	0.46	0/2404	0.65	0/3238
2	B	0.53	0/486	0.67	0/648
2	C	0.51	0/499	0.66	1/667 (0.1%)
2	E	0.58	0/415	0.58	0/554
2	F	0.56	0/482	0.67	0/644
All	All	0.48	0/6709	0.66	2/9014 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	482	ARG	NE-CZ-NH1	6.12	123.36	120.30
1	A	191	ASP	CB-CG-OD1	6.02	123.72	118.30

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	2396	0	2504	38	1
1	D	2377	0	2480	26	1
2	B	483	0	485	11	0
2	C	496	0	489	10	0
2	E	412	0	411	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	F	479	0	479	12	0
3	A	23	0	0	2	0
3	B	3	0	0	0	0
3	C	3	0	0	0	0
3	D	25	0	0	0	0
3	E	5	0	0	0	0
All	All	6702	0	6848	90	1

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 7.

The worst 5 of 90 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:E:479:ARG:NH2	2:F:478:GLU:OE2	2.12	0.82
1:A:1:MET:N	1:A:17:VAL:O	2.13	0.81
1:A:237:THR:HG21	1:A:239:LYS:HZ2	1.46	0.80
1:A:36:ILE:O	1:A:41:GLN:NE2	2.21	0.73
1:D:224:ARG:NH2	2:F:474:ASP:OD1	2.24	0.70

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:282:ARG:NH2	1:D:204:ASP:OD2[3_655]	2.06	0.14

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	300/304 (99%)	284 (95%)	15 (5%)	1 (0%)	46 75

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	298/304 (98%)	286 (96%)	12 (4%)	0	100	100
2	B	57/102 (56%)	56 (98%)	1 (2%)	0	100	100
2	C	59/102 (58%)	56 (95%)	3 (5%)	0	100	100
2	E	48/102 (47%)	48 (100%)	0	0	100	100
2	F	57/102 (56%)	52 (91%)	5 (9%)	0	100	100
All	All	819/1016 (81%)	782 (96%)	36 (4%)	1 (0%)	56	83

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	52	ASP

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	272/272 (100%)	263 (97%)	9 (3%)	45	76
1	D	270/272 (99%)	266 (98%)	4 (2%)	72	91
2	B	52/86 (60%)	49 (94%)	3 (6%)	25	52
2	C	53/86 (62%)	46 (87%)	7 (13%)	5	12
2	E	44/86 (51%)	41 (93%)	3 (7%)	20	43
2	F	51/86 (59%)	48 (94%)	3 (6%)	24	51
All	All	742/888 (84%)	713 (96%)	29 (4%)	39	70

5 of 29 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	C	448	LYS
2	C	467	GLN
2	F	468	MET
2	C	454	GLN
2	C	472	CYS

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

Mol	Chain	Res	Type
2	F	454	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 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, 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	302/304 (99%)	0.06	20 (6%) 22 20	26, 48, 145, 187	0
1	D	300/304 (98%)	-0.09	6 (2%) 68 69	28, 49, 121, 143	0
2	B	59/102 (57%)	-0.10	2 (3%) 49 49	25, 47, 119, 140	0
2	C	61/102 (59%)	0.20	4 (6%) 22 20	27, 50, 133, 166	0
2	E	50/102 (49%)	-0.15	0 100 100	29, 58, 127, 147	0
2	F	59/102 (57%)	0.06	2 (3%) 49 49	34, 52, 129, 153	0
All	All	831/1016 (81%)	-0.01	34 (4%) 41 41	25, 50, 138, 187	0

The worst 5 of 34 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	61	ILE	5.2
1	A	15	LEU	5.0
1	A	4	PHE	4.8
1	A	1	MET	3.7
1	A	20	SER	3.7

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.