



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 07:16 PM GMT

PDB ID : 1EUV
Title : X-RAY STRUCTURE OF THE C-TERMINAL ULP1 PROTEASE DOMAIN
IN COMPLEX WITH SMT3, THE YEAST ORTHOLOG OF SUMO.
Authors : Mossessova, E.; Lima, C.D.
Deposited on : 2000-04-17
Resolution : 1.60 Å(reported)

This is a Full wwPDB X-ray Structure Validation 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 : 1.7 (RC4), CSD as536be (2015)
Xtrriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

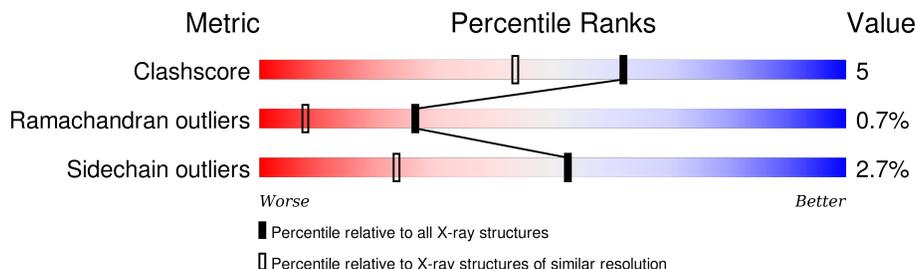
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.60 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))
Clashscore	102246	2732 (1.60-1.60)
Ramachandran outliers	100387	2654 (1.60-1.60)
Sidechain outliers	100360	2653 (1.60-1.60)

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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	221	 81% 14% ••
2	B	86	 84% 7% • 8%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 2849 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 ULP1 PROTEASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	221	1801	1145	308	338	10	7	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	401	GLY	LYS	CLONING ARTIFACTS	UNP Q02724
A	402	SER	LYS	CLONING ARTIFACTS	UNP Q02724

- Molecule 2 is a protein called UBITQUTIN-LIKE PROTEIN SMT3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	79	616	383	112	118	3	0	0	0

- Molecule 3 is water.

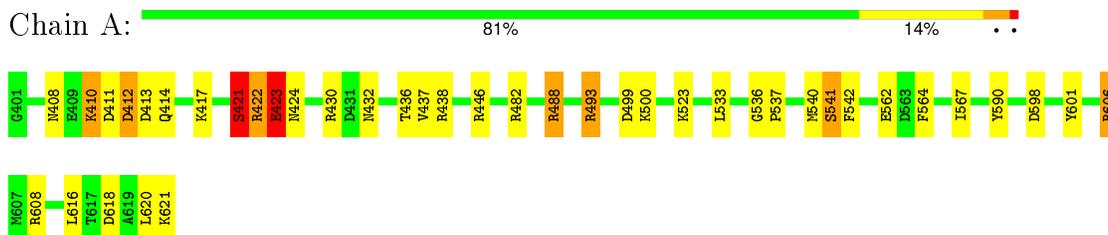
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	330	Total 330	O 330	0	0
3	B	102	Total 102	O 102	0	0

3 Residue-property plots [i](#)

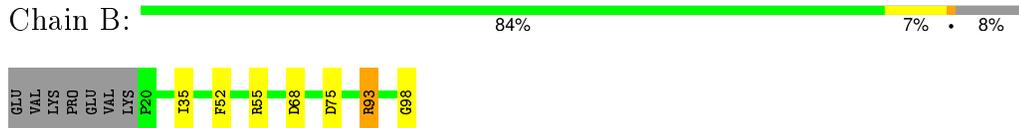
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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 ($RSRZ > 2$). 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.

Note EDS was not executed.

- Molecule 1: ULP1 PROTEASE



- Molecule 2: UBITQUTIN-LIKE PROTEIN SMT3



4 Data and refinement statistics

Xtrriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	125.77Å 53.17Å 54.26Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	25.00 – 1.60	Depositor
% Data completeness (in resolution range)	96.6 (25.00-1.60)	Depositor
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	REFMAC	Depositor
R, R_{free}	0.190 , 0.251	Depositor
Estimated twinning fraction	No twinning to report.	Xtrriage
Total number of atoms	2849	wwPDB-VP
Average B, all atoms (Å ²)	31.0	wwPDB-VP

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	0.79	1/1838 (0.1%)	1.59	23/2482 (0.9%)
2	B	0.59	1/624 (0.2%)	1.23	1/834 (0.1%)
All	All	0.74	2/2462 (0.1%)	1.51	24/3316 (0.7%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	422	ARG	CA-CB	-15.45	1.20	1.53
2	B	98	GLY	C-O	7.73	1.36	1.23

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	446	ARG	NE-CZ-NH2	-22.71	108.94	120.30
1	A	446	ARG	NE-CZ-NH1	21.29	130.94	120.30
1	A	422	ARG	CB-CA-C	10.65	131.69	110.40
1	A	412	ASP	CB-CG-OD1	10.47	127.72	118.30
1	A	601	TYR	CB-CG-CD1	-9.86	115.08	121.00
1	A	423	GLU	CB-CG-CD	9.57	140.04	114.20
1	A	446	ARG	CD-NE-CZ	-8.84	111.22	123.60
1	A	601	TYR	CB-CG-CD2	8.05	125.83	121.00
1	A	421	SER	N-CA-CB	7.86	122.29	110.50
1	A	606	ARG	NE-CZ-NH1	7.28	123.94	120.30
1	A	499	ASP	CB-CG-OD1	7.27	124.84	118.30
1	A	598	ASP	CB-CG-OD1	7.14	124.73	118.30
1	A	422	ARG	CA-CB-CG	7.04	128.88	113.40
1	A	608	ARG	NE-CZ-NH2	-6.63	116.98	120.30
1	A	482	ARG	CD-NE-CZ	6.60	132.84	123.60
2	B	93	ARG	CD-NE-CZ	6.33	132.46	123.60
1	A	590	TYR	CB-CG-CD1	5.74	124.45	121.00
1	A	564	PHE	CB-CG-CD1	5.70	124.79	120.80
1	A	500	LYS	CA-CB-CG	-5.62	101.04	113.40
1	A	541	SER	CA-CB-OG	5.52	126.11	111.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	430	ARG	CD-NE-CZ	-5.40	116.04	123.60
1	A	618	ASP	CB-CG-OD1	5.15	122.93	118.30
1	A	590	TYR	CB-CG-CD2	-5.11	117.93	121.00
1	A	437	VAL	CA-CB-CG2	-5.02	103.37	110.90

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	1801	0	1787	24	0
2	B	616	0	599	3	0
3	A	330	0	0	12	6
3	B	102	0	0	1	0
All	All	2849	0	2386	26	6

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 5.

All (26) 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:421:SER:HB3	3:A:743:HOH:O	1.73	0.88
1:A:424:ASN:ND2	1:A:438:ARG:H	1.83	0.77
1:A:424:ASN:HD21	1:A:438:ARG:H	1.40	0.68
1:A:413:ASP:O	1:A:417:LYS:HG3	1.96	0.66
1:A:567:ILE:HD12	3:A:673:HOH:O	1.99	0.62
1:A:621:LYS:HD3	3:A:763:HOH:O	1.99	0.62
2:B:93:ARG:HG2	3:B:138:HOH:O	2.01	0.60
1:A:422:ARG:O	1:A:423:GLU:HB2	2.09	0.53
1:A:410:LYS:HG2	1:A:411:ASP:N	2.24	0.52
1:A:621:LYS:HG2	3:A:765:HOH:O	2.10	0.51
1:A:488:ARG:HD2	3:A:855:HOH:O	2.11	0.50
1:A:562:GLU:HG2	3:A:799:HOH:O	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:414:GLN:HG2	1:A:616:LEU:HD13	1.94	0.50
1:A:493:ARG:HG2	2:B:68:ASP:HB3	1.94	0.49
1:A:606:ARG:HD2	3:A:725:HOH:O	2.12	0.49
1:A:412:ASP:CG	3:A:935:HOH:O	2.51	0.49
1:A:408:ASN:HD21	1:A:410:LYS:NZ	2.12	0.48
1:A:562:GLU:HG2	3:A:715:HOH:O	2.19	0.43
1:A:536:GLY:O	1:A:537:PRO:C	2.57	0.42
1:A:542:PHE:HB3	3:A:917:HOH:O	2.20	0.41
2:B:35:ILE:HD12	2:B:52:PHE:CD1	2.56	0.41
1:A:523:LYS:HE2	3:A:848:HOH:O	2.21	0.40
1:A:424:ASN:HD21	1:A:436:THR:HB	1.87	0.40
1:A:620:LEU:O	1:A:621:LYS:C	2.59	0.40
1:A:533:LEU:HD12	1:A:533:LEU:HA	1.97	0.40
1:A:541:SER:HB3	3:A:705:HOH:O	2.20	0.40

All (6) 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)
3:A:625:HOH:O	3:A:892:HOH:O 3_548	1.28	0.92
3:A:625:HOH:O	3:A:895:HOH:O 3_548	1.62	0.58
3:A:672:HOH:O	3:A:908:HOH:O 3_558	1.68	0.52
3:A:662:HOH:O	3:A:931:HOH:O 3_558	2.07	0.13
3:A:642:HOH:O	3:A:931:HOH:O 3_558	2.18	0.02
3:A:645:HOH:O	3:A:908:HOH:O 3_558	2.18	0.02

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	219/221 (99%)	213 (97%)	5 (2%)	1 (0%)	34 12

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	77/86 (90%)	74 (96%)	2 (3%)	1 (1%)	15	2
All	All	296/307 (96%)	287 (97%)	7 (2%)	2 (1%)	26	8

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	423	GLU
2	B	75	ASP

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	199/199 (100%)	193 (97%)	6 (3%)	48	19
2	B	64/77 (83%)	63 (98%)	1 (2%)	70	47
All	All	263/276 (95%)	256 (97%)	7 (3%)	52	23

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	410	LYS
1	A	421	SER
1	A	432	ASN
1	A	488	ARG
1	A	493	ARG
1	A	540	MET
2	B	55	ARG

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

Mol	Chain	Res	Type
1	A	424	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 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

6.1 Protein, DNA and RNA chains

EDS was not executed - this section will therefore be empty.

6.2 Non-standard residues in protein, DNA, RNA chains

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates

EDS was not executed - this section will therefore be empty.

6.4 Ligands

EDS was not executed - this section will therefore be empty.

6.5 Other polymers

EDS was not executed - this section will therefore be empty.