



Full wwPDB X-ray Structure Validation Report ⓘ

May 26, 2020 – 08:13 pm BST

PDB ID : 5O71
Title : Crystal structure of human USP25
Authors : Reverter, D.; Liu, B.
Deposited on : 2017-06-07
Resolution : 3.28 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

<https://www.wwpdb.org/validation/2017/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
Xtriage (Phenix) : 1.13
EDS : 2.11
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

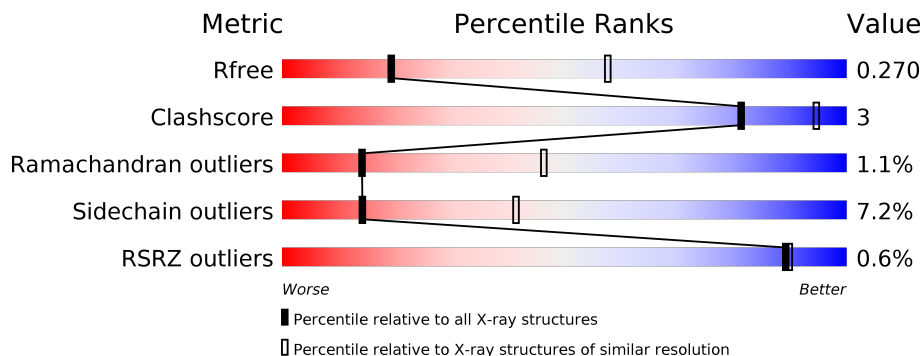
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.28 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}	130704	1177 (3.32-3.24)
Clashscore	141614	1044 (3.30-3.26)
Ramachandran outliers	138981	1026 (3.30-3.26)
Sidechain outliers	138945	1025 (3.30-3.26)
RSRZ outliers	127900	1141 (3.32-3.24)

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 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	716	

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 3963 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 25.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	474	3963	2533	685	729	16	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLY	-	expression tag	UNP Q9UHP3
A	0	SER	-	expression tag	UNP Q9UHP3

4 Data and refinement statistics

Property	Value	Source
Space group	I 4 2 2	Depositor
Cell constants a, b, c, α , β , γ	140.81Å 140.81Å 190.16Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	95.08 – 3.28 95.08 – 3.28	Depositor EDS
% Data completeness (in resolution range)	99.3 (95.08-3.28) 99.4 (95.08-3.28)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.89 (at 3.26Å)	Xtrriage
Refinement program	REFMAC 5.8.0158	Depositor
R, R_{free}	0.202 , 0.275 0.205 , 0.270	Depositor DCC
R_{free} test set	722 reflections (4.85%)	wwPDB-VP
Wilson B-factor (Å ²)	129.6	Xtrriage
Anisotropy	0.361	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 108.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtrriage
Estimated twinning fraction	0.020 for $-1/2^*h+1/2^*k-1/2^*l, 1/2^*h-1/2^*k-1/2^*l, -h-k$ 0.038 for $-1/2^*h-1/2^*k+1/2^*l, -1/2^*h-1/2^*k-1/2^*l, h-k$	Xtrriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	3963	wwPDB-VP
Average B, all atoms (Å ²)	150.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.39% of the height of the origin peak. No significant pseudotranslation is detected.*

¹ Intensities estimated from amplitudes.

² Theoretical 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	0.56	0/4060	0.79	2/5477 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	403	ARG	NE-CZ-NH1	6.62	123.61	120.30
1	A	403	ARG	CG-CD-NE	5.17	122.65	111.80

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	3963	0	3873	20	0
All	All	3963	0	3873	20	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 3.

All (20) 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:534:HIS:HB3	1:A:535:PRO:CD	2.14	0.76

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:534:HIS:HB3	1:A:535:PRO:HD3	1.81	0.60
1:A:310:GLU:O	1:A:312:LYS:N	2.38	0.56
1:A:366:LEU:HG	1:A:405:MET:HE1	1.89	0.54
1:A:379:PHE:CZ	1:A:384:GLY:O	2.65	0.50
1:A:198:LEU:O	1:A:226:ARG:NH2	2.45	0.50
1:A:637:VAL:HG13	1:A:641:PHE:CD2	2.47	0.49
1:A:467:SER:N	1:A:468:PRO:CD	2.78	0.46
1:A:218:ASN:HD21	1:A:277:ALA:HB2	1.80	0.46
1:A:662:LEU:HA	1:A:662:LEU:HD23	1.79	0.45
1:A:167:ALA:HB1	1:A:168:PRO:HD2	2.00	0.44
1:A:401:LEU:HD12	1:A:591:TYR:CD1	2.52	0.44
1:A:665:GLU:HG2	1:A:666:GLU:N	2.34	0.43
1:A:188:PHE:CE1	1:A:194:ARG:HD2	2.54	0.42
1:A:385:ARG:HB3	1:A:386:PRO:HD2	2.01	0.42
1:A:173:ASN:HD21	1:A:180:PHE:HB3	1.84	0.42
1:A:436:TYR:HD2	1:A:559:ILE:HG23	1.85	0.41
1:A:636:LEU:HD23	1:A:636:LEU:C	2.40	0.41
1:A:584:LYS:HA	1:A:587:ILE:HG22	2.02	0.41
1:A:400:TYR:CE1	1:A:590:PRO:HB3	2.55	0.41

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	462/716 (64%)	401 (87%)	56 (12%)	5 (1%)	14 46

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	534	HIS
1	A	311	GLY

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	468	PRO
1	A	667	PHE
1	A	585	SER

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	432/640 (68%)	401 (93%)	31 (7%)	14 41

All (31) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	165	ASP
1	A	169	VAL
1	A	174	VAL
1	A	178	CYS
1	A	226	ARG
1	A	266	PHE
1	A	283	GLU
1	A	360	GLU
1	A	373	GLU
1	A	389	ILE
1	A	402	ASP
1	A	403	ARG
1	A	405	MET
1	A	406	HIS
1	A	435	ARG
1	A	451	VAL
1	A	461	SER
1	A	464	VAL
1	A	521	PRO
1	A	538	ARG
1	A	541	THR
1	A	562	ASP
1	A	592	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	598	VAL
1	A	613	PHE
1	A	631	SER
1	A	648	SER
1	A	662	LEU
1	A	667	PHE
1	A	668	ASN
1	A	684	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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	474/716 (66%)	-0.04	3 (0%) 89 90	91, 144, 212, 254	0

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	603	ALA	2.4
1	A	255	SER	2.2
1	A	604	ASN	2.0

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.