Full wwPDB X-ray Structure Validation Report ⓘ

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PDB ID	:	6H4J
Title	:	Usp25 catalytic domain
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Deposited on	:	2018-07-21
Resolution	:	3.07 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 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:

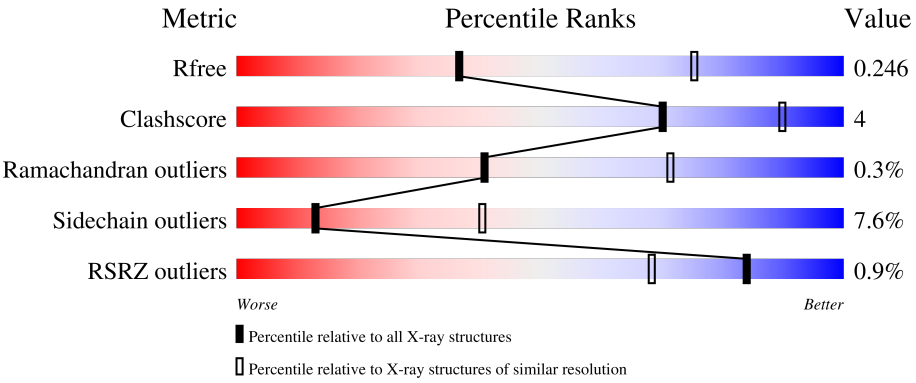
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.07 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	1447 (3.10-3.06)
Clashscore	141614	1546 (3.10-3.06)
Ramachandran outliers	138981	1487 (3.10-3.06)
Sidechain outliers	138945	1486 (3.10-3.06)
RSRZ outliers	127900	1416 (3.10-3.06)

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% 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	552	% 75% 13% 12%
1	B	552	% 71% 12% • 16%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 7588 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
1	A	488	Total	C	N	O	S	0	0	0
			3931	2504	681	730	16			
1	B	464	Total	C	N	O	S	0	1	0
			3625	2317	617	677	14			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	155	GLY	-	expression tag	UNP Q9UHP3
A	156	PRO	-	expression tag	UNP Q9UHP3
B	155	GLY	-	expression tag	UNP Q9UHP3
B	156	PRO	-	expression tag	UNP Q9UHP3

- Molecule 2 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total	Cl	0	0
			2	2		
2	B	1	Total	Cl	0	0
			1	1		

- Molecule 3 is water.

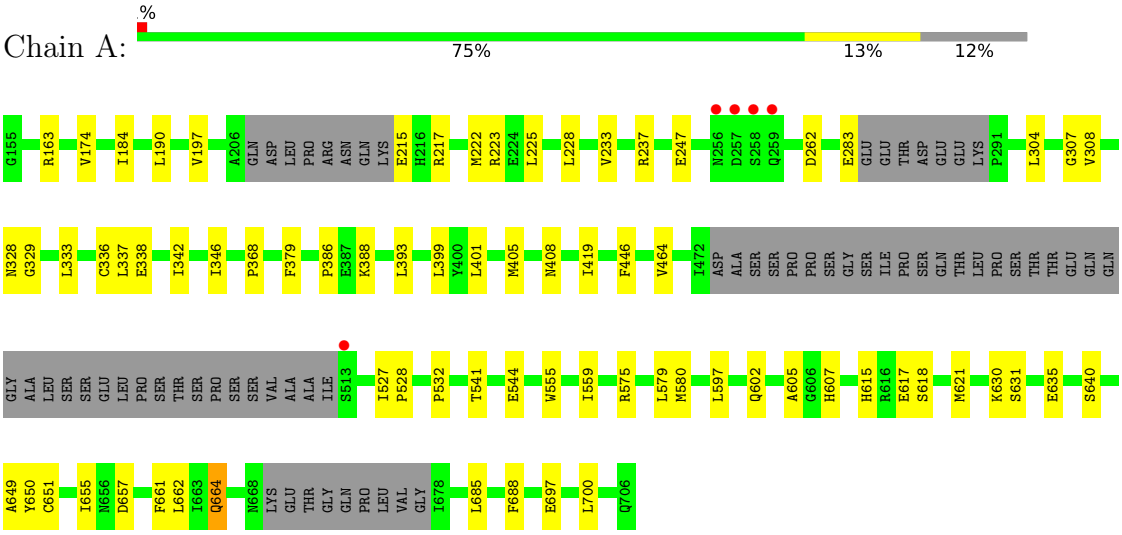
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	11	Total	O	0	0
			11	11		
3	B	18	Total	O	0	0
			18	18		

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 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.

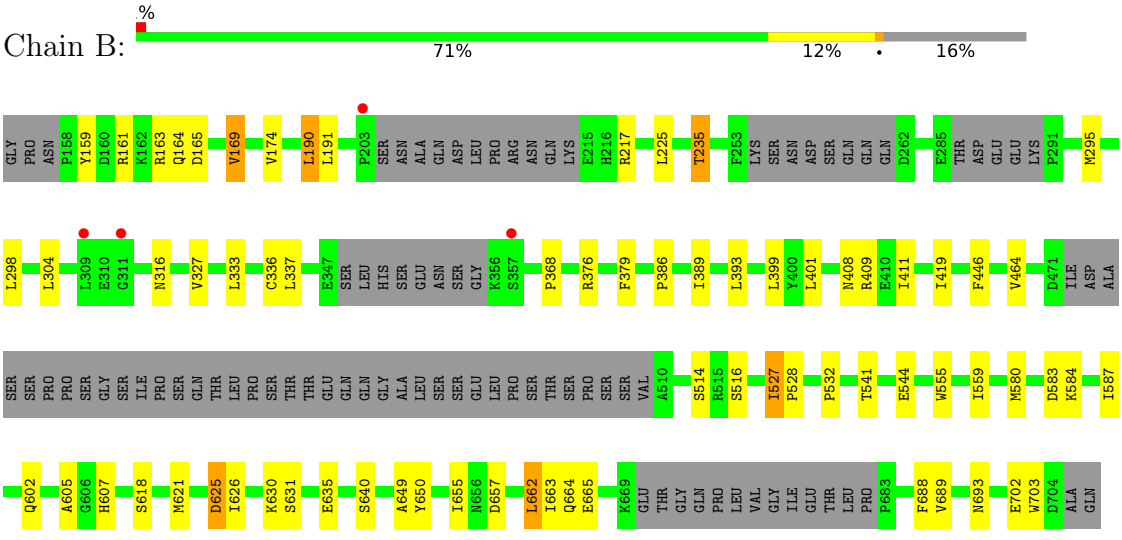
• Molecule 1: Ubiquitin carboxyl-terminal hydrolase 25

Chain A:



• Molecule 1: Ubiquitin carboxyl-terminal hydrolase 25

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	81.94Å 202.63Å 169.59Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.54 – 3.07 48.54 – 3.07	Depositor EDS
% Data completeness (in resolution range)	100.0 (48.54-3.07) 100.0 (48.54-3.07)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.47 (at 3.07Å)	Xtriage
Refinement program	BUSTER 2.10.2	Depositor
R, R_{free}	0.181 , 0.230 0.200 , 0.246	Depositor DCC
R_{free} test set	1365 reflections (5.09%)	wwPDB-VP
Wilson B-factor (Å^2)	86.6	Xtriage
Anisotropy	0.248	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 76.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	7588	wwPDB-VP
Average B, all atoms (Å^2)	104.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.06% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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

Bond lengths and bond angles in the following residue types are not validated in this section: 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	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	A	0.51	0/4031	0.67	0/5466
1	B	0.49	0/3718	0.65	0/5059
All	All	0.50	0/7749	0.66	0/10525

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

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	3931	0	3699	29	0
1	B	3625	0	3302	23	0
2	A	2	0	0	0	0
2	B	1	0	0	0	0
3	A	11	0	0	0	0
3	B	18	0	0	0	0
All	All	7588	0	7001	52	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 4.

All (52) 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:328:ASN:CG	1:A:329:GLY:H	1.72	0.91
1:A:661:PHE:HA	1:A:664:GLN:HG2	1.66	0.78
1:A:328:ASN:CG	1:A:329:GLY:N	2.45	0.69
1:A:215:GLU:HG3	1:A:217:ARG:H	1.58	0.67
1:A:602:GLN:HB2	1:A:605:ALA:HB3	1.76	0.66
1:A:405:MET:HB2	1:A:408:ASN:HD22	1.62	0.65
1:A:419:ILE:HD11	1:A:580:MET:HG2	1.80	0.64
1:B:327:VAL:HG21	1:B:376:ARG:HG2	1.80	0.64
1:A:338:GLU:O	1:A:342:ILE:HG13	2.00	0.62
1:A:697:GLU:HA	1:A:700:LEU:HD12	1.83	0.60
1:B:169:VAL:HG22	1:B:235:THR:HG23	1.83	0.60
1:A:174:VAL:HG12	1:A:174:VAL:O	2.02	0.59
1:B:191:LEU:HD13	1:B:663:ILE:HG23	1.86	0.58
1:B:408:ASN:HA	1:B:411:ILE:HD13	1.87	0.56
1:B:327:VAL:CG2	1:B:376:ARG:HG2	2.35	0.56
1:B:555:TRP:O	1:B:559:ILE:HG12	2.06	0.55
1:B:419:ILE:HD11	1:B:580:MET:HG2	1.88	0.54
1:A:555:TRP:O	1:A:559:ILE:HG12	2.08	0.53
1:A:368:PRO:HB2	1:A:662:LEU:HD11	1.90	0.53
1:A:615:HIS:CE1	1:A:655:ILE:HD11	2.43	0.52
1:B:411:ILE:HD12	1:B:411:ILE:H	1.74	0.52
1:A:661:PHE:HA	1:A:664:GLN:CG	2.39	0.51
1:B:174:VAL:HG12	1:B:174:VAL:O	2.11	0.51
1:B:602:GLN:HB2	1:B:605:ALA:HB3	1.93	0.50
1:A:307:GLY:HA2	1:A:346:ILE:HD11	1.92	0.50
1:B:333:LEU:HD23	1:B:399:LEU:HD13	1.92	0.50
1:B:640:SER:HB3	1:B:649:ALA:HB2	1.93	0.50
1:A:197:VAL:HG13	1:A:222:MET:CE	2.41	0.50
1:A:640:SER:HB3	1:A:649:ALA:HB2	1.93	0.50
1:B:625:ASP:O	1:B:626:ILE:HB	2.13	0.48
1:A:328:ASN:ND2	1:A:329:GLY:H	2.11	0.48
1:B:190:LEU:HD11	1:B:655:ILE:HD11	1.95	0.48
1:B:464:VAL:HG22	1:B:532:PRO:HB2	1.95	0.48
1:B:587:ILE:HG22	1:B:587:ILE:O	2.13	0.48
1:A:333:LEU:HD23	1:A:399:LEU:HD13	1.94	0.48
1:B:295:MET:HA	1:B:298:LEU:HD12	1.95	0.47
1:A:197:VAL:HG13	1:A:222:MET:HE1	1.96	0.47
1:A:464:VAL:HG22	1:A:532:PRO:HB2	1.98	0.46
1:A:184:ILE:HD12	1:A:225:LEU:HD11	1.98	0.45
1:B:164:GLN:HG2	1:B:165:ASP:H	1.82	0.45
1:A:541:THR:HB	1:A:544:GLU:H	1.83	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:368:PRO:HB2	1:B:662:LEU:HD21	2.00	0.44
1:B:541:THR:HB	1:B:544:GLU:H	1.82	0.43
1:A:163:ARG:HB2	1:A:237:ARG:O	2.19	0.43
1:A:575:ARG:NE	1:A:579:LEU:HD11	2.35	0.42
1:A:597:LEU:HB2	1:A:651:CYS:HB3	2.02	0.42
1:B:379:PHE:HA	1:B:386:PRO:HA	2.02	0.41
1:A:379:PHE:HA	1:A:386:PRO:HA	2.03	0.41
1:B:621:MET:SD	1:B:630:LYS:HA	2.61	0.41
1:A:527:ILE:HA	1:A:528:PRO:HD3	1.93	0.41
1:B:527:ILE:HA	1:B:528:PRO:HD3	1.89	0.40
1:A:621:MET:SD	1:A:630:LYS:HA	2.62	0.40

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	478/552 (87%)	450 (94%)	28 (6%)	0	100	100
1	B	451/552 (82%)	420 (93%)	28 (6%)	3 (1%)	22	54
All	All	929/1104 (84%)	870 (94%)	56 (6%)	3 (0%)	41	71

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	625	ASP
1	B	235	THR
1	B	689	VAL

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	412/501 (82%)	387 (94%)	25 (6%)	18 48
1	B	361/501 (72%)	327 (91%)	34 (9%)	8 30
All	All	773/1002 (77%)	714 (92%)	59 (8%)	13 40

All (59) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	190	LEU
1	A	223	ARG
1	A	228	LEU
1	A	233	VAL
1	A	247	GLU
1	A	262	ASP
1	A	283	GLU
1	A	304	LEU
1	A	308	VAL
1	A	336	CYS
1	A	337	LEU
1	A	388	LYS
1	A	393	LEU
1	A	401	LEU
1	A	446	PHE
1	A	607	HIS
1	A	617	GLU
1	A	618	SER
1	A	631	SER
1	A	635	GLU
1	A	650	TYR
1	A	657	ASP
1	A	664	GLN
1	A	685	LEU
1	A	688	PHE
1	B	159	TYR
1	B	161	ARG

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Mol	Chain	Res	Type
1	B	163	ARG
1	B	169	VAL
1	B	190	LEU
1	B	217	ARG
1	B	225	LEU
1	B	304	LEU
1	B	316	ASN
1	B	336	CYS
1	B	337	LEU
1	B	389	ILE
1	B	393	LEU
1	B	401	LEU
1	B	409	ARG
1	B	446	PHE
1	B	514	SER
1	B	516	SER
1	B	527	ILE
1	B	583	ASP
1	B	584	LYS
1	B	607	HIS
1	B	618	SER
1	B	631	SER
1	B	635	GLU
1	B	650	TYR
1	B	657	ASP
1	B	662	LEU
1	B	664	GLN
1	B	665	GLU
1	B	688	PHE
1	B	693	ASN
1	B	702	GLU
1	B	703	TRP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	173	ASN
1	A	185	GLN
1	A	322	GLN
1	A	359	GLN
1	A	408	ASN
1	B	279	GLN

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Mol	Chain	Res	Type
1	B	594	HIS

5.3.3 RNA

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

Of 3 ligands modelled in this entry, 3 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

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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, 95^{th} 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	488/552 (88%)	-0.36	5 (1%)	82	66	50, 92, 149, 182	0
1	B	464/552 (84%)	-0.30	4 (0%)	84	68	54, 109, 172, 202	0
All	All	952/1104 (86%)	-0.33	9 (0%)	84	68	50, 99, 166, 202	0

All (9) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	257	ASP	3.8
1	A	513	SER	3.6
1	A	258	SER	2.7
1	B	309	LEU	2.6
1	B	311	GLY	2.6
1	B	357	SER	2.5
1	A	256	ASN	2.5
1	B	203	PRO	2.1
1	A	259	GLN	2.0

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

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates

There are no monosaccharides in this entry.

6.4 Ligands

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,

median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	CL	B	801	1/1	0.81	0.12	125,125,125,125	0
2	CL	A	801	1/1	0.83	0.18	111,111,111,111	0
2	CL	A	802	1/1	0.91	0.35	104,104,104,104	0

6.5 Other polymers (i)

There are no such residues in this entry.