



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 17, 2017 – 04:19 PM EST

PDB ID : 5H2W
Title : Crystal structure of the karyopherin Kap60p bound to the SUMO protease Ulp1p (150-340)
Authors : Hirano, H.; Matsuura, Y.
Deposited on : 2016-10-18
Resolution : 2.50 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	:	unknown
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20028442
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-20028442

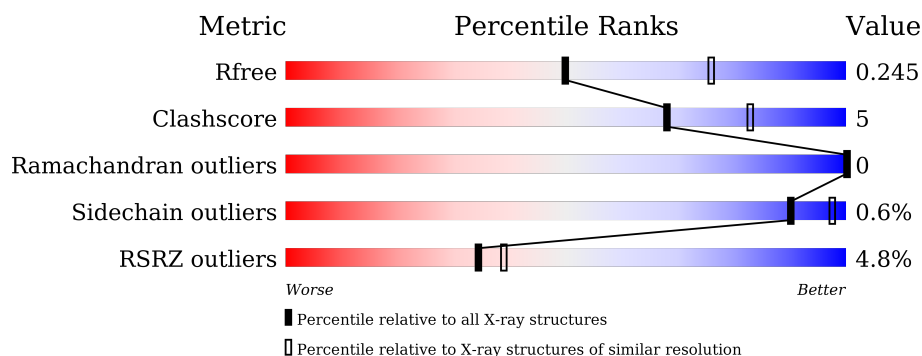
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	3553 (2.50-2.50)
Clashscore	102246	4242 (2.50-2.50)
Ramachandran outliers	100387	4156 (2.50-2.50)
Sidechain outliers	100360	4158 (2.50-2.50)
RSRZ outliers	91569	3562 (2.50-2.50)

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	423	<div> <div>4%</div> <div>86%</div> <div>12%</div> <div>.</div> </div>
1	C	423	<div> <div>4%</div> <div>88%</div> <div>10%</div> <div>.</div> </div>
2	B	191	<div> <div>%</div> <div>7%</div> <div>91%</div> <div>..</div> </div>
2	D	191	<div> <div>2%</div> <div>7%</div> <div>90%</div> <div>.</div> </div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 6752 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 Importin subunit alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	416	Total	C	N	O	S	0	0	0
			3171	2015	534	606	16			
1	C	414	Total	C	N	O	S	0	0	0
			3171	2011	529	615	16			

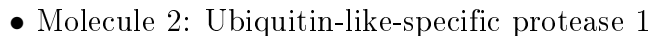
- Molecule 2 is a protein called Ubiquitin-like-specific protease 1.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	B	17	Total	C	N	O	0	0	0
			155	99	36	20			
2	D	19	Total	C	N	O	0	0	0
			170	107	38	25			

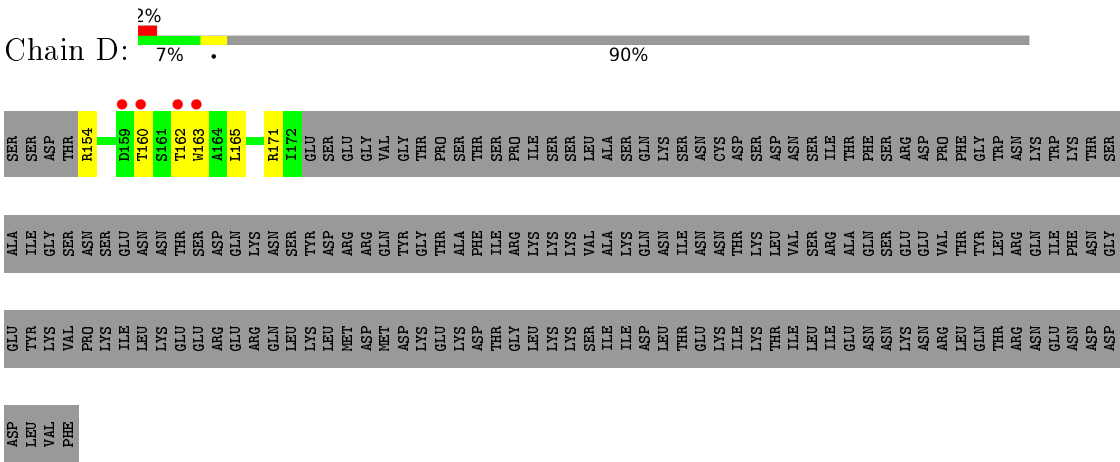
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	30	Total	O	0	0
			30	30		
3	B	4	Total	O	0	0
			4	4		
3	C	48	Total	O	0	0
			48	48		
3	D	3	Total	O	0	0
			3	3		

- Molecule 1: Importin subunit alpha



● Molecule 2: Ubiquitin-like-specific protease 1



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	52.61Å 63.54Å 80.91Å 106.09° 107.72° 90.50°	Depositor
Resolution (Å)	27.03 – 2.50 27.03 – 2.50	Depositor EDS
% Data completeness (in resolution range)	90.5 (27.03-2.50) 81.3 (27.03-2.50)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.14 (at 2.50Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.9_1692)	Depositor
R, R_{free}	0.213 , 0.247 0.214 , 0.245	Depositor DCC
R_{free} test set	1540 reflections (5.16%)	DCC
Wilson B-factor (Å ²)	29.8	Xtriage
Anisotropy	0.633	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 33.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.028 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	6752	wwPDB-VP
Average B, all atoms (Å ²)	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.71% 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	0.22	0/3222	0.43	0/4392
1	C	0.22	0/3221	0.41	0/4389
2	B	0.37	0/158	0.45	0/207
2	D	0.32	0/174	0.58	0/231
All	All	0.23	0/6775	0.43	0/9219

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	D	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	D	160	THR	Peptide

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	3171	0	3198	33	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	3171	0	3191	27	0
2	B	155	0	167	7	0
2	D	170	0	179	5	0
3	A	30	0	0	0	0
3	B	4	0	0	0	0
3	C	48	0	0	1	0
3	D	3	0	0	0	0
All	All	6752	0	6735	63	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 5.

All (63) 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:244:ARG:NH2	2:B:165:LEU:O	2.09	0.84
1:C:244:ARG:NH2	2:D:165:LEU:O	2.11	0.80
1:A:247:LYS:HB2	2:B:162:THR:HG21	1.65	0.78
1:A:95:GLN:HG3	1:A:103:GLU:HG2	1.64	0.77
1:A:192:GLN:HE21	2:B:171:ARG:HH11	1.32	0.76
1:C:95:GLN:NE2	1:C:103:GLU:OE1	2.25	0.69
1:C:463:LYS:HZ3	1:C:471:ASN:N	1.93	0.67
1:C:310:HIS:HD2	1:C:312:SER:H	1.42	0.66
1:A:310:HIS:HD2	1:A:312:SER:H	1.43	0.66
1:A:310:HIS:CD2	1:A:312:SER:H	2.20	0.60
1:A:460:GLU:O	1:A:463:LYS:HB2	2.02	0.58
1:C:310:HIS:CD2	1:C:312:SER:H	2.20	0.58
1:C:414:GLY:HA3	1:C:421:ILE:HG12	1.86	0.57
1:A:299:ARG:HH11	1:A:299:ARG:HG3	1.70	0.56
1:A:95:GLN:HG2	1:A:107:ALA:HB2	1.86	0.56
1:A:106:SER:OG	1:A:110:LYS:NZ	2.39	0.55
1:A:209:ASP:O	1:A:213:GLN:HG2	2.07	0.55
1:C:392:LEU:HD22	1:C:407:ILE:HD12	1.89	0.54
1:A:365:ILE:HG21	1:A:388:LEU:HD11	1.92	0.52
1:A:464:GLU:OE1	1:A:464:GLU:N	2.40	0.51
1:A:192:GLN:HE21	2:B:171:ARG:NH1	2.05	0.50
1:A:392:LEU:HD22	1:A:407:ILE:HD12	1.93	0.50
2:B:163:TRP:CE3	2:B:163:TRP:HA	2.46	0.50
1:A:354:LYS:HE2	1:A:357:ILE:HG13	1.93	0.50
1:A:481:GLY:O	1:A:485:LYS:HG2	2.12	0.49
1:C:279:TRP:CD2	1:C:318:PRO:HB3	2.46	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:282:SER:HB2	1:C:321:ARG:HG3	1.95	0.48
1:C:247:LYS:HA	1:C:248:PRO:HA	1.66	0.48
1:C:471:ASN:HB3	1:C:474:ALA:HB3	1.96	0.47
1:C:138:PHE:HB3	1:C:147:LEU:HG	1.97	0.46
1:C:493:GLU:H	1:C:493:GLU:CD	2.18	0.46
1:A:98:SER:O	1:A:134:ARG:NH2	2.48	0.46
1:C:365:ILE:HG21	1:C:388:LEU:HD11	1.98	0.46
1:C:493:GLU:OE1	1:C:493:GLU:N	2.46	0.46
1:A:187:VAL:HB	1:A:228:LYS:HD2	1.98	0.46
1:A:137:GLU:O	1:A:140:ARG:HG3	2.16	0.45
1:A:478:GLU:OE1	1:A:479:LYS:HD2	2.17	0.45
1:A:122:PRO:HB2	1:A:125:VAL:HG22	1.98	0.44
2:B:163:TRP:HE3	2:B:163:TRP:HA	1.82	0.44
1:A:246:LYS:HB2	2:B:162:THR:HG23	2.00	0.44
1:A:228:LYS:HD3	1:A:231:LEU:HB2	1.99	0.44
1:C:298:VAL:HG23	1:C:300:ILE:HG13	2.00	0.44
1:C:359:LYS:HD3	1:C:398:LYS:HG3	2.00	0.44
1:A:122:PRO:HB2	1:A:125:VAL:CG2	2.48	0.44
1:A:279:TRP:CD2	1:A:318:PRO:HB3	2.53	0.44
1:C:226:SER:OG	1:C:228:LYS:HB2	2.18	0.43
1:A:463:LYS:HE3	1:A:471:ASN:N	2.33	0.43
1:C:192:GLN:HE21	2:D:171:ARG:NH1	2.16	0.43
2:D:162:THR:O	2:D:163:TRP:CD1	2.72	0.43
1:C:358:LYS:NZ	3:C:611:HOH:O	2.52	0.42
1:A:496:LYS:O	1:A:500:LYS:HB2	2.20	0.42
1:A:417:ARG:HA	1:A:418:PRO:HD2	1.88	0.42
1:A:138:PHE:HB3	1:A:147:LEU:HG	2.01	0.42
1:A:450:ASP:OD1	1:A:500:LYS:HE2	2.20	0.42
1:A:298:VAL:HG23	1:A:300:ILE:HG13	2.01	0.41
1:C:434:CYS:SG	1:C:482:GLY:HA3	2.61	0.41
1:C:397:TYR:CE2	1:C:401:LYS:HD2	2.56	0.41
1:C:431:LYS:HB3	1:C:432:PRO:HD3	2.03	0.41
1:C:452:LEU:HD13	1:C:486:ILE:HD11	2.03	0.41
1:C:192:GLN:NE2	2:D:171:ARG:HD3	2.37	0.40
1:A:127:ILE:HD13	1:A:168:VAL:HG21	2.02	0.40
1:C:354:LYS:HA	1:C:354:LYS:HD2	1.82	0.40
1:C:247:LYS:CB	2:D:162:THR:HG21	2.51	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	412/423 (97%)	403 (98%)	9 (2%)	0	100	100
1	C	410/423 (97%)	404 (98%)	6 (2%)	0	100	100
2	B	13/191 (7%)	13 (100%)	0	0	100	100
2	D	17/191 (9%)	15 (88%)	2 (12%)	0	100	100
All	All	852/1228 (69%)	835 (98%)	17 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	344/364 (94%)	343 (100%)	1 (0%)	94	99
1	C	347/364 (95%)	346 (100%)	1 (0%)	94	99
2	B	16/178 (9%)	15 (94%)	1 (6%)	22	40
2	D	18/178 (10%)	17 (94%)	1 (6%)	26	47
All	All	725/1084 (67%)	721 (99%)	4 (1%)	90	97

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	491	GLN
2	B	163	TRP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	290	GLU
2	D	154	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	192	GLN
1	A	310	HIS
1	A	494	ASN
1	C	95	GLN
1	C	142	ASN
1	C	192	GLN
1	C	213	GLN
1	C	310	HIS

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 ⓘ

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	416/423 (98%)	0.36	19 (4%) 36 41	27, 39, 60, 74	0
1	C	414/423 (97%)	0.32	17 (4%) 41 46	25, 36, 60, 80	0
2	B	17/191 (8%)	0.40	2 (11%) 6 6	31, 39, 77, 84	0
2	D	19/191 (9%)	0.81	4 (21%) 1 1	32, 46, 83, 84	0
All	All	866/1228 (70%)	0.35	42 (4%) 34 39	25, 37, 62, 84	0

All (42) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	118	GLU	3.8
2	D	160	THR	3.6
1	A	365	ILE	3.5
1	A	332	LEU	3.3
1	A	227	ASN	3.3
1	A	464	GLU	3.2
1	A	348	LEU	3.2
1	C	493	GLU	3.1
2	B	162	THR	3.1
1	A	502	TYR	3.1
1	C	142	ASN	3.0
2	D	162	THR	3.0
1	C	365	ILE	2.9
1	C	90	PRO	2.9
1	C	415	LEU	2.8
1	C	246	LYS	2.8
1	A	415	LEU	2.8
1	A	353	PRO	2.8
1	A	441	ASP	2.7
1	A	119	HIS	2.7
1	C	494	ASN	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	495	ASP	2.6
1	C	498	TYR	2.6
1	C	227	ASN	2.5
1	A	89	LEU	2.5
2	B	163	TRP	2.5
1	C	89	LEU	2.5
1	A	498	TYR	2.5
1	A	140	ARG	2.4
1	C	416	GLN	2.4
1	A	383	ASN	2.4
2	D	159	ASP	2.4
1	A	493	GLU	2.3
2	D	163	TRP	2.3
1	A	460	GLU	2.3
1	C	141	GLU	2.3
1	C	463	LYS	2.2
1	A	351	SER	2.2
1	C	193	ALA	2.1
1	A	381	ASP	2.1
1	C	403	ALA	2.1
1	A	407	ILE	2.1

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.