



wwPDB X-ray Structure Validation Summary Report ⓘ

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PDB ID : 4I6J / pdb_00004i6j
Title : A ubiquitin ligase-substrate complex
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Deposited on : 2012-11-29
Resolution : 2.70 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

<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	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

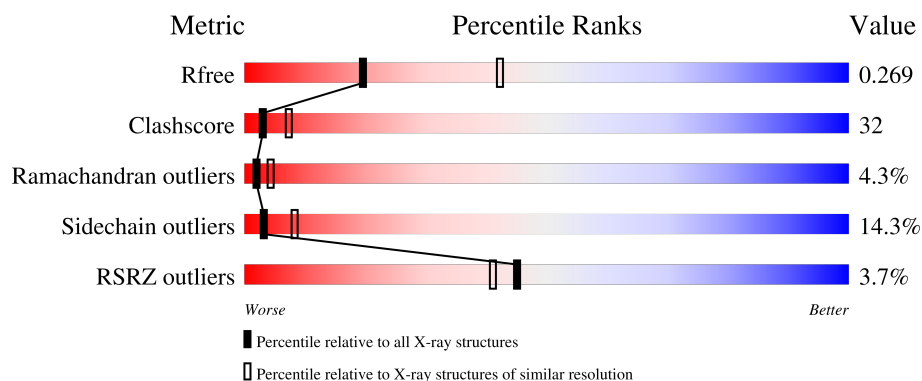
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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}	180053	3538 (2.70-2.70)
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (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 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 $\leq 5\%$. 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	544	2% 51% 33% 8% 8%
2	B	428	% 50% 33% 8% 8%
3	C	163	15% 15% 45% 17% 20%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 8435 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 Cryptochrome-2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	503	Total	C	N	O	S	0	0	0
			4079	2616	723	718	22			

- Molecule 2 is a protein called F-box/LRR-repeat protein 3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	394	Total	C	N	O	S	0	0	0
			3156	2022	538	574	22			

- Molecule 3 is a protein called S-phase kinase-associated protein 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	130	Total	C	N	O	S	0	0	0
			1044	667	168	204	5			

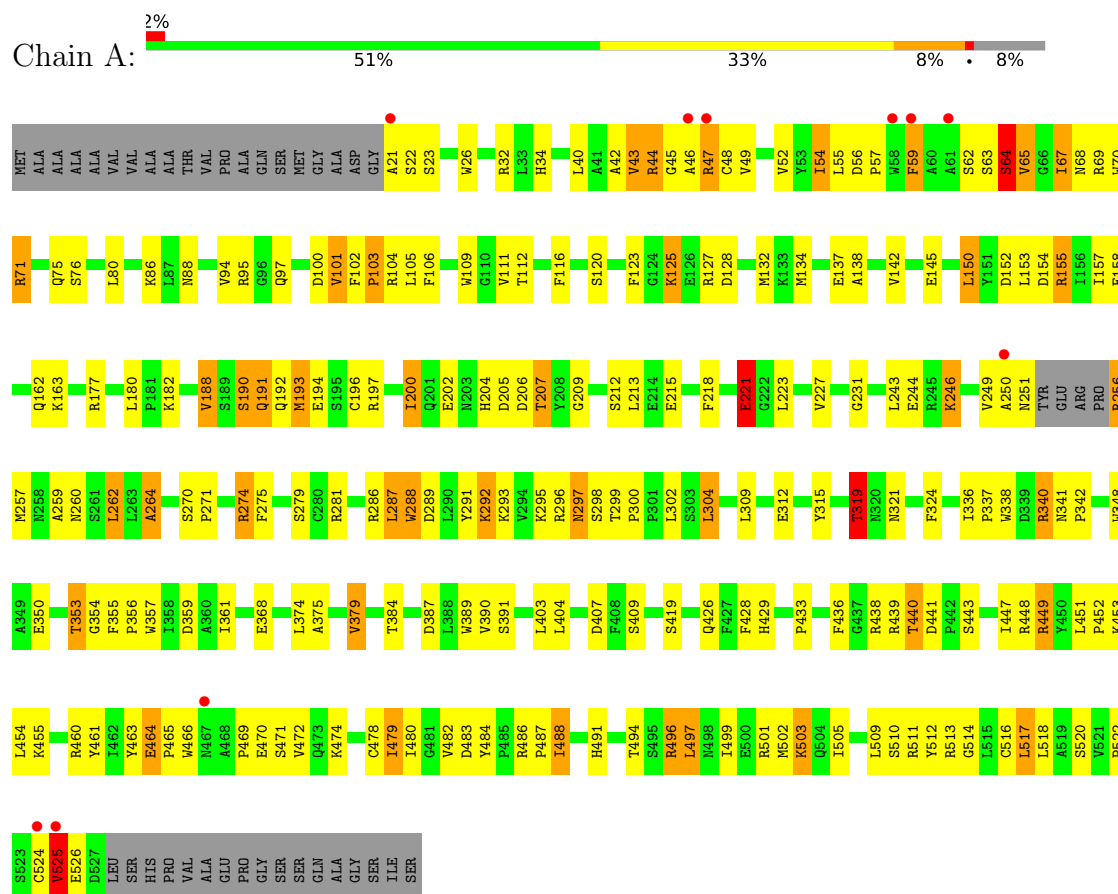
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	93	Total	O	0	0
			93	93		
4	B	58	Total	O	0	0
			58	58		
4	C	5	Total	O	0	0
			5	5		

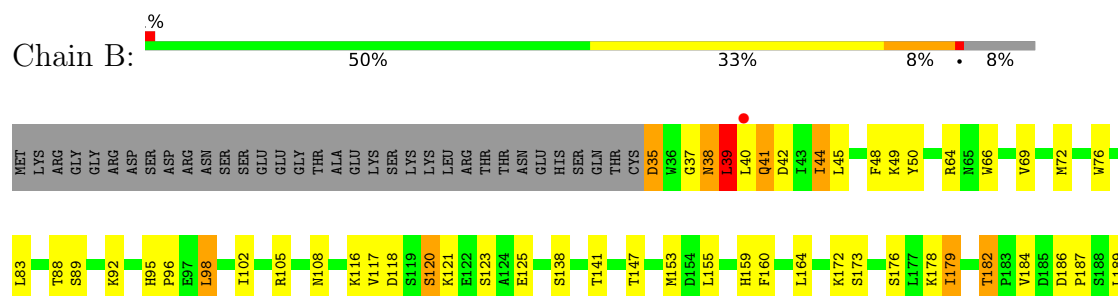
3 Residue-property plots

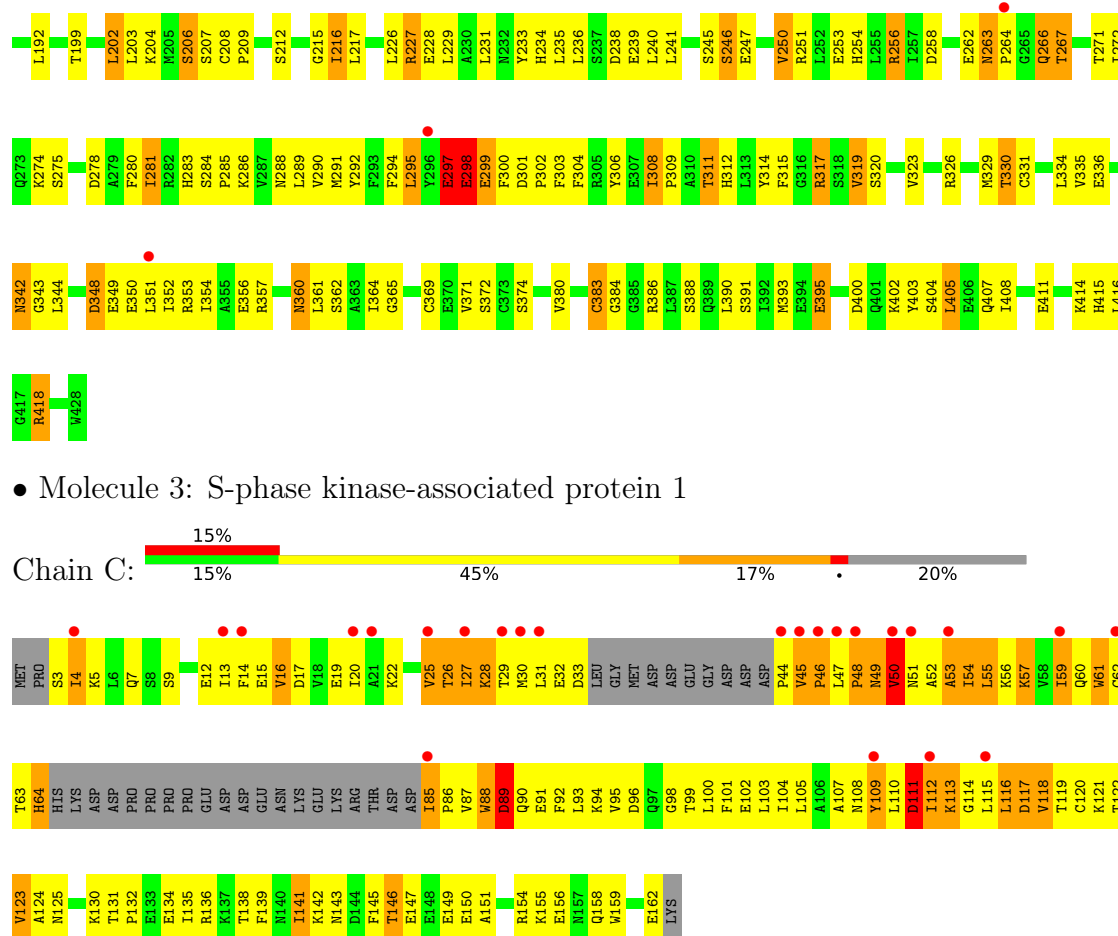
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Cryptochrome-2



• Molecule 2: F-box/LRR-repeat protein 3





• Molecule 3: S-phase kinase-associated protein 1

4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α , β , γ	125.39Å 125.39Å 145.71Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	47.52 – 2.70 47.52 – 2.70	Depositor EDS
% Data completeness (in resolution range)	99.8 (47.52-2.70) 95.6 (47.52-2.70)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.03 (at 2.48Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.1_743)	Depositor
R, R_{free}	0.203 , 0.265 0.206 , 0.269	Depositor DCC
R_{free} test set	2304 reflections (3.59%)	wwPDB-VP
Wilson B-factor (Å ²)	42.6	Xtriage
Anisotropy	0.284	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 44.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.021 for -h,-k,l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	8435	wwPDB-VP
Average B, all atoms (Å ²)	49.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.98% 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	0.58	2/4195 (0.0%)	0.95	13/5691 (0.2%)
2	B	0.57	0/3233	0.95	7/4384 (0.2%)
3	C	0.47	0/1059	0.95	4/1430 (0.3%)
All	All	0.56	2/8487 (0.0%)	0.95	24/11505 (0.2%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	341	ASN	C-N	5.70	1.41	1.34
1	A	342	PRO	N-CD	5.30	1.55	1.47

The worst 5 of 24 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	13	ILE	N-CA-C	10.37	120.30	111.90
2	B	208	CYS	CA-C-N	7.82	127.89	119.28
2	B	208	CYS	C-N-CA	7.82	127.89	119.28
2	B	303	PHE	N-CA-C	7.54	122.59	111.96
2	B	299	GLU	N-CA-C	-7.05	104.56	113.02

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	4079	0	4012	210	0
2	B	3156	0	3153	180	0
3	C	1044	0	1054	155	0
4	A	93	0	0	9	0
4	B	58	0	0	31	0
4	C	5	0	0	0	0
All	All	8435	0	8219	524	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 32.

The worst 5 of 524 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:B:311:THR:HG23	2:B:312:HIS:CD2	1.77	1.20
3:C:112:ILE:HG22	3:C:115:LEU:N	1.57	1.20
3:C:112:ILE:CG2	3:C:115:LEU:H	1.52	1.19
3:C:112:ILE:HG21	3:C:115:LEU:CB	1.74	1.17
2:B:216:ILE:HD11	2:B:235:LEU:HB3	1.11	1.06

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	499/544 (92%)	441 (88%)	44 (9%)	14 (3%)	4	9
2	B	392/428 (92%)	347 (88%)	35 (9%)	10 (3%)	4	11
3	C	124/163 (76%)	80 (64%)	24 (19%)	20 (16%)	0	0
All	All	1015/1135 (89%)	868 (86%)	103 (10%)	44 (4%)	2	4

5 of 44 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	221	GLU
1	A	259	ALA
1	A	297	ASN
1	A	525	VAL
1	A	526	GLU

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	432/460 (94%)	376 (87%)	56 (13%)	4	10
2	B	360/390 (92%)	305 (85%)	55 (15%)	3	7
3	C	119/150 (79%)	100 (84%)	19 (16%)	2	6
All	All	911/1000 (91%)	781 (86%)	130 (14%)	3	8

5 of 130 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	C	50	VAL
3	C	59	ILE
1	A	497	LEU
1	A	496	ARG
3	C	64	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 8 such sidechains are listed below:

Mol	Chain	Res	Type
3	C	64	HIS
3	C	7	GLN
2	B	266	GLN
2	B	195	ASN
2	B	312	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 oligosaccharides 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	503/544 (92%)	-0.17	10 (1%) 65 62	20, 38, 83, 119	0
2	B	394/428 (92%)	-0.28	4 (1%) 79 78	23, 42, 68, 95	0
3	C	130/163 (79%)	1.03	24 (18%) 3 3	44, 87, 139, 160	0
All	All	1027/1135 (90%)	-0.06	38 (3%) 45 41	20, 43, 101, 160	0

The worst 5 of 38 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	C	20	ILE	4.1
3	C	31	LEU	3.6
1	A	250	ALA	3.5
1	A	46	ALA	3.5
1	A	61	ALA	3.4

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 oligosaccharides 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.