



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 25, 2026 – 01:18 PM EDT

PDB ID : 6BRQ / pdb_00006brq
Title : Crystal structure of rice ASK1-D3 ubiquitin ligase complex crystal form 3
Authors : Shabek, N.; Zheng, N.; Mao, H.; Hinds, T.R.; Ticchiarelli, F.; Leyser, O.
Deposited on : 2017-11-30
Resolution : 2.99 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	:	4-5-2 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

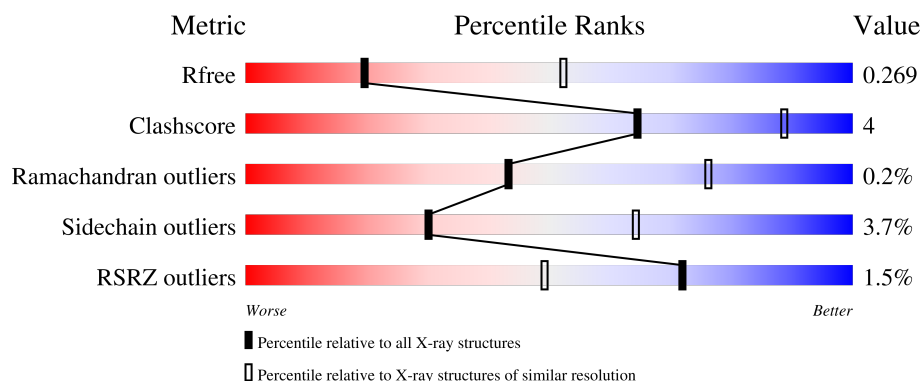
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.99 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	2672 (3.00-3.00)
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)
RSRZ outliers	180081	2671 (3.00-3.00)

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	B	688	
1	D	688	
2	A	160	
2	C	160	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 10771 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 F-box/LRR-repeat MAX2 homolog.

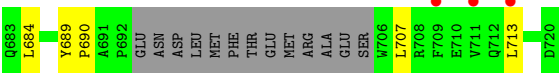
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	581	Total	C	N	O	S	0	0	0
			4500	2876	784	811	29			
1	D	592	Total	C	N	O	S	0	0	0
			4602	2944	801	828	29			

There are 14 discrepancies between the modelled and reference sequences:

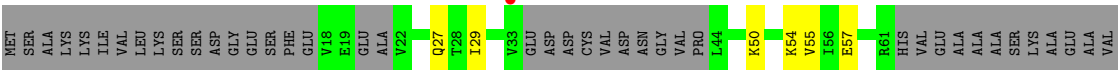
Chain	Residue	Modelled	Actual	Comment	Reference
B	509	GLU	-	linker	UNP Q5VMP0
B	510	ASN	-	linker	UNP Q5VMP0
B	511	LEU	-	linker	UNP Q5VMP0
B	512	TYR	-	linker	UNP Q5VMP0
B	513	PHE	-	linker	UNP Q5VMP0
B	514	GLN	-	linker	UNP Q5VMP0
B	515	SER	-	linker	UNP Q5VMP0
D	509	GLU	-	linker	UNP Q5VMP0
D	510	ASN	-	linker	UNP Q5VMP0
D	511	LEU	-	linker	UNP Q5VMP0
D	512	TYR	-	linker	UNP Q5VMP0
D	513	PHE	-	linker	UNP Q5VMP0
D	514	GLN	-	linker	UNP Q5VMP0
D	515	SER	-	linker	UNP Q5VMP0

- Molecule 2 is a protein called SKP1-like protein 1A.

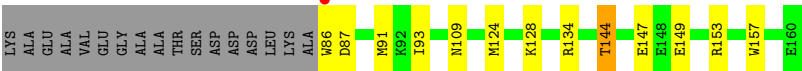
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	A	106	Total	C	N	O	S	0	0	0
			858	545	140	168	5			
2	C	99	Total	C	N	O	S	0	0	0
			811	516	133	158	4			



• Molecule 2: SKP1-like protein 1A



• Molecule 2: SKP1-like protein 1A



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	77.91Å 113.31Å 92.86Å 90.00° 99.00° 90.00°	Depositor
Resolution (Å)	91.71 – 2.99 91.71 – 2.99	Depositor EDS
% Data completeness (in resolution range)	(Not available) (91.71-2.99) 96.0 (91.71-2.99)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.13	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.82 (at 3.01Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.220 , 0.256 0.228 , 0.269	Depositor DCC
R_{free} test set	1582 reflections (4.88%)	wwPDB-VP
Wilson B-factor (Å ²)	62.1	Xtriage
Anisotropy	0.244	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 21.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	10771	wwPDB-VP
Average B, all atoms (Å ²)	65.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.64% 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

5.1 Standard geometry

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	B	0.54	0/4601	0.94	2/6253 (0.0%)
1	D	0.55	0/4705	0.93	2/6392 (0.0%)
2	A	0.56	0/867	0.99	0/1168
2	C	0.58	0/822	1.01	0/1108
All	All	0.55	0/10995	0.95	4/14921 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	155	ASP	CA-C-N	5.12	126.24	119.84
1	D	155	ASP	C-N-CA	5.12	126.24	119.84
1	B	155	ASP	CA-C-N	5.11	126.23	119.84
1	B	155	ASP	C-N-CA	5.11	126.23	119.84

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	B	4500	0	4537	32	0
1	D	4602	0	4628	38	0
2	A	858	0	859	10	0
2	C	811	0	804	9	0
All	All	10771	0	10828	85	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 (85) 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:D:224:PRO:HA	1:D:227:THR:HG22	1.61	0.82
1:B:224:PRO:HA	1:B:227:THR:HG22	1.63	0.81
1:D:187:ASP:HB2	1:D:218:ARG:HE	1.48	0.78
1:B:423:SER:O	1:B:427:ARG:HG3	1.87	0.74
1:B:309:GLU:HG3	1:B:337:HIS:HD2	1.57	0.70
1:B:254:ALA:O	1:D:78:ARG:HD3	1.93	0.67
2:A:27:GLN:HB2	2:A:109:ASN:HB3	1.83	0.61
2:C:27:GLN:HB2	2:C:109:ASN:HB3	1.83	0.61
2:C:144:THR:HG23	2:C:147:GLU:HB2	1.82	0.60
2:A:124:MET:O	2:A:128:LYS:HE2	2.02	0.60
1:D:260:ARG:NH2	1:D:290:ARG:HE	2.00	0.60
2:C:124:MET:O	2:C:128:LYS:HE2	2.02	0.60
1:D:368:CYS:HB2	1:D:378:VAL:HG12	1.85	0.58
1:B:427:ARG:HG2	1:B:456:ALA:HA	1.85	0.58
2:C:50:LYS:HE3	2:C:50:LYS:H	1.69	0.57
1:B:368:CYS:HB2	1:B:378:VAL:HG12	1.86	0.57
2:A:143:PHE:HD1	2:A:147:GLU:HG3	1.69	0.57
1:D:670:MET:HE3	1:D:682:MET:HE2	1.87	0.57
2:A:54:LYS:HA	2:A:57:GLU:HG2	1.86	0.56
1:D:670:MET:HE2	1:D:684:LEU:HB2	1.87	0.56
1:D:266:CYS:HB2	1:D:268:PHE:CE2	2.41	0.55
1:B:266:CYS:HB2	1:B:268:PHE:CE2	2.42	0.54
1:B:54:ALA:HA	1:B:80:PRO:HD2	1.92	0.52
1:D:54:ALA:HA	1:D:80:PRO:HD2	1.92	0.52
1:B:370:ALA:HB3	1:B:398:ALA:HB1	1.92	0.51
1:D:360:THR:HG23	1:D:388:TYR:HB3	1.92	0.51
1:B:360:THR:HG23	1:B:388:TYR:HB3	1.92	0.51
1:B:434:ARG:HD2	1:B:463:ARG:HH21	1.76	0.51
1:B:633:GLN:HG2	1:B:634:ASP:N	2.26	0.51
1:D:650:ILE:HB	1:D:673:PHE:HE1	1.76	0.51
1:B:329:GLU:HG2	1:B:355:ARG:HB3	1.92	0.50
1:B:159:LEU:HD13	1:B:194:LEU:HG	1.94	0.49
1:D:159:LEU:HD13	1:D:194:LEU:HG	1.95	0.49
1:D:329:GLU:HG2	1:D:355:ARG:HB3	1.93	0.48
2:A:144:THR:HG22	2:A:145:PRO:HD2	1.95	0.48
2:A:91:MET:C	2:A:93:ILE:H	2.23	0.47
1:B:364:PHE:HB3	1:B:367:LEU:HD21	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:355:ARG:NH1	1:D:357:LYS:NZ	2.62	0.47
1:B:589:ASP:HA	1:B:630:TRP:HB2	1.97	0.47
1:D:233:LEU:HB2	1:D:259:LEU:HD21	1.96	0.47
1:D:400:LEU:HD13	1:D:429:LEU:HD22	1.97	0.47
1:B:39:HIS:CD2	1:B:56:ARG:HH22	2.33	0.46
2:C:91:MET:C	2:C:93:ILE:H	2.23	0.46
1:D:21:PRO:HD2	1:D:24:LEU:HD12	1.97	0.46
1:D:39:HIS:CD2	1:D:56:ARG:HH22	2.33	0.46
1:B:21:PRO:HD2	1:B:24:LEU:HD12	1.98	0.46
1:B:400:LEU:HD13	1:B:429:LEU:HD22	1.98	0.46
1:D:589:ASP:HA	1:D:630:TRP:HB2	1.98	0.46
1:B:233:LEU:HB2	1:B:259:LEU:HD21	1.97	0.46
1:B:293:VAL:HA	1:B:330:ASP:HB3	1.98	0.45
1:D:308:ARG:HD2	1:D:308:ARG:HA	1.76	0.45
1:D:364:PHE:HB3	1:D:367:LEU:HD21	1.97	0.45
1:D:293:VAL:HA	1:D:330:ASP:HB3	1.99	0.45
1:D:70:PHE:HB2	2:C:157:TRP:CH2	2.53	0.44
1:D:689:TYR:HA	1:D:690:PRO:HA	1.72	0.44
2:A:143:PHE:CD1	2:A:147:GLU:HG3	2.51	0.44
1:D:295:ARG:HA	1:D:332:THR:HB	1.99	0.43
1:D:355:ARG:NH1	1:D:357:LYS:HZ1	2.17	0.43
1:B:461:ARG:HG3	1:B:519:TRP:CD2	2.53	0.43
1:B:295:ARG:HA	1:B:332:THR:HB	1.99	0.43
2:A:149:GLU:O	2:A:153:ARG:HB2	2.18	0.43
1:D:163:THR:N	1:D:164:PRO:HD2	2.33	0.43
1:B:473:TRP:CE2	1:B:537:PRO:HG2	2.54	0.42
1:B:163:THR:N	1:B:164:PRO:HD2	2.34	0.42
2:A:55:VAL:HG11	2:A:108:LEU:HD13	2.00	0.42
1:B:689:TYR:HA	1:B:690:PRO:HA	1.71	0.42
1:D:308:ARG:NH1	1:D:393:GLN:HG3	2.35	0.42
1:B:539:ILE:HD13	1:B:576:ASP:HB3	2.01	0.42
1:D:473:TRP:CE2	1:D:537:PRO:HG2	2.55	0.42
1:B:647:VAL:HG21	1:B:667:GLU:HG3	2.01	0.42
2:C:149:GLU:O	2:C:153:ARG:HB2	2.19	0.42
1:D:608:SER:HB2	1:D:645:PRO:HG3	2.01	0.41
1:B:70:PHE:HB2	2:A:157:TRP:CH2	2.56	0.41
1:B:676:ILE:HD12	1:B:679:LEU:HD22	2.03	0.41
1:B:388:TYR:HE1	1:B:390:LYS:HG2	1.86	0.41
1:D:412:LYS:HG2	1:D:439:GLU:HB2	2.03	0.41
1:D:651:GLN:NE2	1:D:672:PHE:HB3	2.37	0.40
1:B:417:GLY:HA2	1:B:444:HIS:O	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:44:ALA:O	2:C:134:ARG:HD2	2.21	0.40
1:D:260:ARG:NH2	1:D:290:ARG:NE	2.69	0.40
1:D:388:TYR:HE1	1:D:390:LYS:HG2	1.87	0.40
1:D:417:GLY:HA2	1:D:444:HIS:O	2.22	0.40
1:D:670:MET:CE	1:D:682:MET:HE2	2.50	0.40
2:C:86:TRP:HB3	2:C:87:ASP:H	1.72	0.40
1:D:439:GLU:HG2	1:D:466:SER:HB3	2.04	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	B	565/688 (82%)	546 (97%)	18 (3%)	1 (0%)	43	76
1	D	574/688 (83%)	554 (96%)	19 (3%)	1 (0%)	43	76
2	A	98/160 (61%)	95 (97%)	3 (3%)	0	100	100
2	C	93/160 (58%)	89 (96%)	4 (4%)	0	100	100
All	All	1330/1696 (78%)	1284 (96%)	44 (3%)	2 (0%)	43	76

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	156	PRO
1	D	156	PRO

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	B	488/575 (85%)	471 (96%)	17 (4%)	32	65
1	D	498/575 (87%)	481 (97%)	17 (3%)	32	66
2	A	96/137 (70%)	93 (97%)	3 (3%)	35	68
2	C	89/137 (65%)	83 (93%)	6 (7%)	15	46
All	All	1171/1424 (82%)	1128 (96%)	43 (4%)	30	64

All (43) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	82	LEU
1	B	126	GLU
1	B	128	ILE
1	B	180	GLN
1	B	336	GLN
1	B	380	VAL
1	B	410	LEU
1	B	455	THR
1	B	523	ARG
1	B	526	SER
1	B	569	ARG
1	B	608	SER
1	B	609	LEU
1	B	612	ARG
1	B	665	THR
1	B	667	GLU
1	B	671	THR
2	A	29	ILE
2	A	50	LYS
2	A	144	THR
1	D	82	LEU
1	D	126	GLU
1	D	128	ILE
1	D	131	GLN
1	D	308	ARG
1	D	310	GLU
1	D	410	LEU
1	D	455	THR
1	D	526	SER
1	D	544	ASP

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Mol	Chain	Res	Type
1	D	570	THR
1	D	609	LEU
1	D	642	LEU
1	D	667	GLU
1	D	668	HIS
1	D	707	LEU
1	D	713	LEU
2	C	24	LEU
2	C	25	GLU
2	C	29	ILE
2	C	50	LYS
2	C	61	ARG
2	C	144	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	337	HIS
2	A	109	ASN
1	D	180	GLN
1	D	337	HIS
1	D	393	GLN
2	C	109	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 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 ⓘ

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	B	581/688 (84%)	0.08	4 (0%) 84 66	42, 60, 89, 120	0
1	D	592/688 (86%)	0.09	11 (1%) 66 43	41, 60, 87, 132	0
2	A	106/160 (66%)	0.35	2 (1%) 66 43	48, 71, 94, 105	0
2	C	99/160 (61%)	0.31	4 (4%) 42 23	51, 83, 116, 125	0
All	All	1378/1696 (81%)	0.12	21 (1%) 72 49	41, 62, 97, 132	0

All (21) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	125	PRO	5.7
2	A	87	ASP	4.1
1	D	370	ALA	3.3
1	D	72	PHE	3.2
2	C	23	ALA	3.2
1	D	713	LEU	2.9
1	D	711	VAL	2.8
2	A	33	VAL	2.8
1	D	103	PRO	2.7
1	B	566	PRO	2.6
1	D	393	GLN	2.5
2	C	58	TYR	2.5
1	B	127	ALA	2.4
1	D	709	PHE	2.3
1	D	667	GLU	2.3
2	C	47	VAL	2.3
1	B	607	LEU	2.3
2	C	86	TRP	2.2
1	D	447	LEU	2.2
1	D	300	PHE	2.2
1	D	102	PRO	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 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.