



wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 22, 2016 – 05:42 AM EDT

PDB ID : 5HYW
Title : The crystal structure of the D3-ASK1 complex
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Deposited on : 2016-02-02
Resolution : 3.01 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

<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-20027939
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-20027939

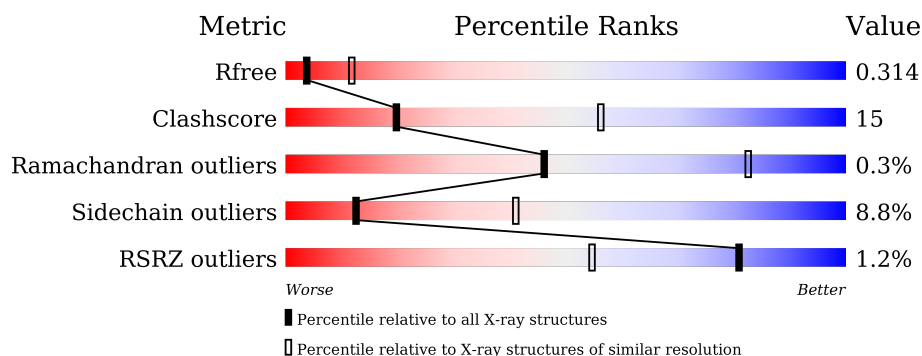
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.01 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	1773 (3.04-3.00)
Clashscore	102246	2117 (3.04-3.00)
Ramachandran outliers	100387	2050 (3.04-3.00)
Sidechain outliers	100360	2053 (3.04-3.00)
RSRZ outliers	91569	1788 (3.04-3.00)

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 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	740	<div> <div></div> <div>55% 20% • 22%</div> </div>
1	C	740	<div> <div>2%</div> <div>57% 17% • • 22%</div> </div>
2	B	169	<div> <div>2%</div> <div>34% 8% • 56%</div> </div>
2	D	169	<div> <div>2%</div> <div>34% 5% • 59%</div> </div>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 10174 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	A	580	Total	C	N	O	S	0	0	0
			4510	2885	785	813	27			
1	C	575	Total	C	N	O	S	0	0	0
			4478	2866	783	802	27			

There are 40 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	GLY	-	expression tag	UNP Q5VMP0
A	-18	ALA	-	expression tag	UNP Q5VMP0
A	-17	MET	-	expression tag	UNP Q5VMP0
A	-16	GLY	-	expression tag	UNP Q5VMP0
A	-15	SER	-	expression tag	UNP Q5VMP0
A	-14	GLY	-	expression tag	UNP Q5VMP0
A	-13	ILE	-	expression tag	UNP Q5VMP0
A	-12	GLN	-	expression tag	UNP Q5VMP0
A	-11	ARG	-	expression tag	UNP Q5VMP0
A	-10	PRO	-	expression tag	UNP Q5VMP0
A	-9	THR	-	expression tag	UNP Q5VMP0
A	-8	SER	-	expression tag	UNP Q5VMP0
A	-7	THR	-	expression tag	UNP Q5VMP0
A	-6	SER	-	expression tag	UNP Q5VMP0
A	-5	SER	-	expression tag	UNP Q5VMP0
A	-4	LEU	-	expression tag	UNP Q5VMP0
A	-3	VAL	-	expression tag	UNP Q5VMP0
A	-2	ALA	-	expression tag	UNP Q5VMP0
A	-1	ALA	-	expression tag	UNP Q5VMP0
A	0	ALA	-	expression tag	UNP Q5VMP0
C	-19	GLY	-	expression tag	UNP Q5VMP0
C	-18	ALA	-	expression tag	UNP Q5VMP0
C	-17	MET	-	expression tag	UNP Q5VMP0
C	-16	GLY	-	expression tag	UNP Q5VMP0
C	-15	SER	-	expression tag	UNP Q5VMP0

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-14	GLY	-	expression tag	UNP Q5VMP0
C	-13	ILE	-	expression tag	UNP Q5VMP0
C	-12	GLN	-	expression tag	UNP Q5VMP0
C	-11	ARG	-	expression tag	UNP Q5VMP0
C	-10	PRO	-	expression tag	UNP Q5VMP0
C	-9	THR	-	expression tag	UNP Q5VMP0
C	-8	SER	-	expression tag	UNP Q5VMP0
C	-7	THR	-	expression tag	UNP Q5VMP0
C	-6	SER	-	expression tag	UNP Q5VMP0
C	-5	SER	-	expression tag	UNP Q5VMP0
C	-4	LEU	-	expression tag	UNP Q5VMP0
C	-3	VAL	-	expression tag	UNP Q5VMP0
C	-2	ALA	-	expression tag	UNP Q5VMP0
C	-1	ALA	-	expression tag	UNP Q5VMP0
C	0	ALA	-	expression tag	UNP Q5VMP0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	74	Total	C	N	O	S	0	0	0
			609	385	98	123	3			
2	D	70	Total	C	N	O	S	0	0	0
			577	365	94	115	3			

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-8	MET	-	expression tag	UNP Q39255
B	-7	ASP	-	expression tag	UNP Q39255
B	-6	TYR	-	expression tag	UNP Q39255
B	-5	LYS	-	expression tag	UNP Q39255
B	-4	ASP	-	expression tag	UNP Q39255
B	-3	ASP	-	expression tag	UNP Q39255
B	-2	ASP	-	expression tag	UNP Q39255
B	-1	ASP	-	expression tag	UNP Q39255
B	0	LYS	-	expression tag	UNP Q39255
D	-8	MET	-	expression tag	UNP Q39255
D	-7	ASP	-	expression tag	UNP Q39255
D	-6	TYR	-	expression tag	UNP Q39255
D	-5	LYS	-	expression tag	UNP Q39255
D	-4	ASP	-	expression tag	UNP Q39255
D	-3	ASP	-	expression tag	UNP Q39255

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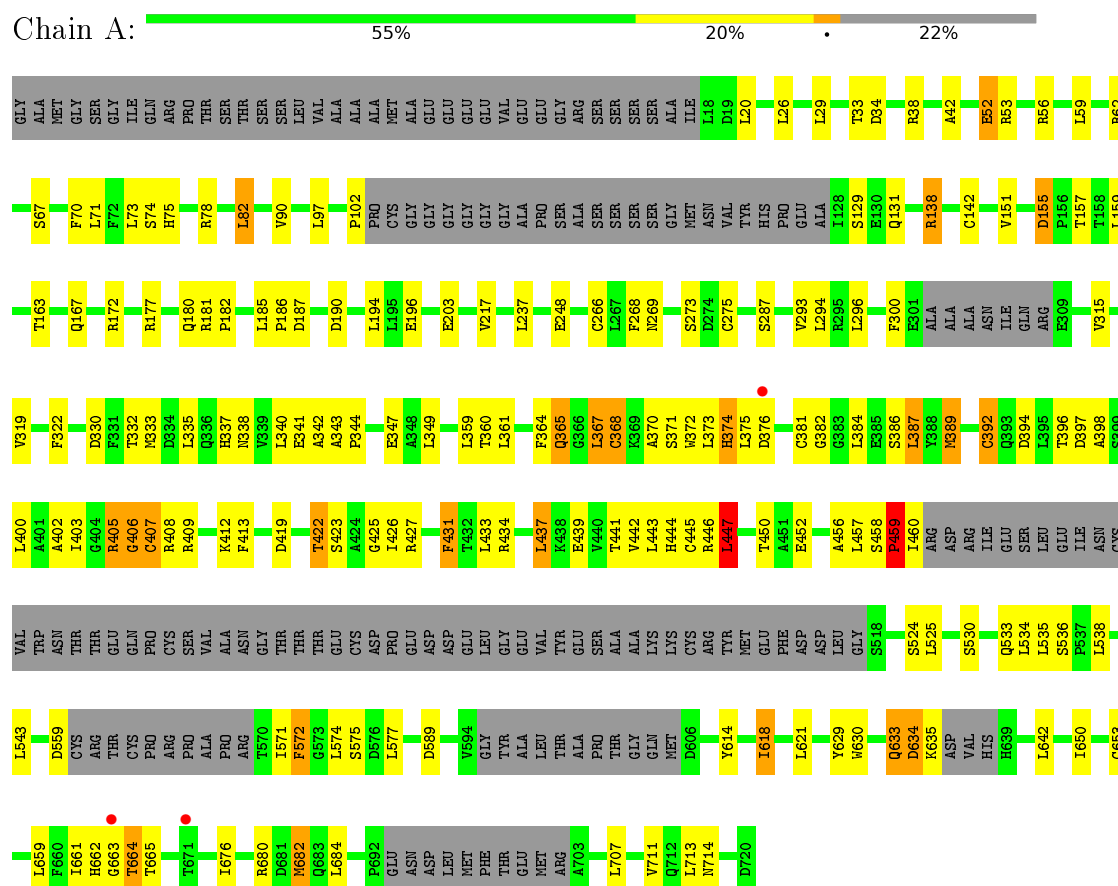
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Chain	Residue	Modelled	Actual	Comment	Reference
D	-2	ASP	-	expression tag	UNP Q39255
D	-1	ASP	-	expression tag	UNP Q39255
D	0	LYS	-	expression tag	UNP Q39255

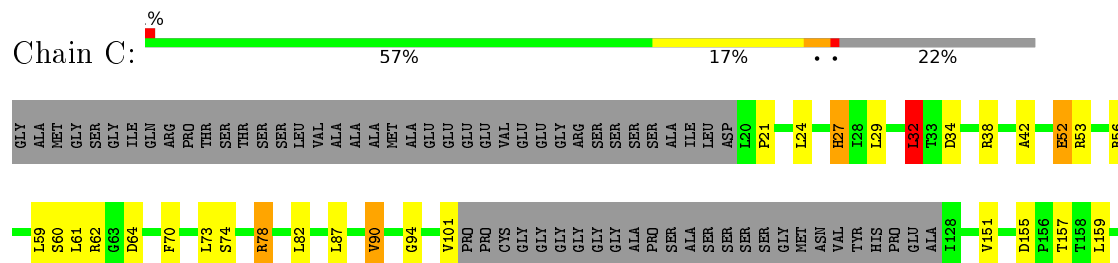
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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 ($\text{RSRZ} > 2$). 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: F-box/LRR-repeat MAX2 homolog



• Molecule 1: F-box/LRR-repeat MAX2 homolog



4 Data and refinement statistics

Property	Value	Source
Space group	P 43	Depositor
Cell constants a, b, c, α , β , γ	79.27 Å 79.27 Å 327.58 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	81.89 – 3.01 37.26 – 3.01	Depositor EDS
% Data completeness (in resolution range)	81.3 (81.89-3.01) 81.3 (37.26-3.01)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.05 (at 3.01 Å)	Xtriage
Refinement program	REFMAC 5.8.0123	Depositor
R, R_{free}	0.235 , 0.312 0.246 , 0.314	Depositor DCC
R_{free} test set	1631 reflections (5.30%)	DCC
Wilson B-factor (Å ²)	65.1	Xtriage
Anisotropy	0.021	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 24.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.478 for h,-k,-l	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	10174	wwPDB-VP
Average B, all atoms (Å ²)	62.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.14% 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	A	0.59	0/4612	0.99	27/6268 (0.4%)
1	C	0.59	1/4580 (0.0%)	1.00	31/6223 (0.5%)
2	B	0.54	0/618	0.76	1/835 (0.1%)
2	D	0.58	0/585	0.81	3/790 (0.4%)
All	All	0.59	1/10395 (0.0%)	0.97	62/14116 (0.4%)

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
1	A	0	3
1	C	0	3
All	All	0	6

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	459	PRO	N-CD	8.86	1.60	1.47

The worst 5 of 62 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	405	ARG	CB-CA-C	-11.76	86.89	110.40
1	A	386	SER	N-CA-C	10.67	139.81	111.00
1	A	572	PHE	CB-CA-C	10.61	131.62	110.40
1	C	542	GLY	N-CA-C	10.53	139.44	113.10
1	C	458	SER	C-N-CD	-9.39	99.94	120.60

There are no chirality outliers.

5 of 6 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	300	PHE	Peptide
1	A	422	THR	Peptide
1	A	447	LEU	Peptide
1	C	364	PHE	Peptide
1	C	94	GLY	Peptide

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	4510	0	4529	144	0
1	C	4478	0	4511	123	0
2	B	609	0	591	18	0
2	D	577	0	569	23	0
All	All	10174	0	10200	303	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 15.

The worst 5 of 303 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:D:91:MET:C	2:D:92:LYS:HD3	1.24	1.50
2:D:91:MET:O	2:D:92:LYS:HD3	1.28	1.26
1:A:372:TRP:O	1:A:374:HIS:CE1	1.89	1.26
1:C:375:LEU:HD23	1:C:375:LEU:O	1.34	1.25
2:B:92:LYS:O	2:B:93:ILE:HG13	1.35	1.22

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	564/740 (76%)	497 (88%)	66 (12%)	1 (0%)	52	87
1	C	559/740 (76%)	496 (89%)	62 (11%)	1 (0%)	52	87
2	B	72/169 (43%)	67 (93%)	4 (6%)	1 (1%)	14	50
2	D	68/169 (40%)	63 (93%)	4 (6%)	1 (2%)	13	48
All	All	1263/1818 (70%)	1123 (89%)	136 (11%)	4 (0%)	46	82

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	459	PRO
1	C	459	PRO
2	D	93	ILE
2	B	93	ILE

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	488/615 (79%)	438 (90%)	50 (10%)	9	32
1	C	485/615 (79%)	448 (92%)	37 (8%)	16	49
2	B	67/146 (46%)	62 (92%)	5 (8%)	17	50
2	D	64/146 (44%)	59 (92%)	5 (8%)	16	48
All	All	1104/1522 (72%)	1007 (91%)	97 (9%)	12	41

5 of 97 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	534	LEU
2	B	152	ARG
1	C	628	ASP
1	A	559	ASP

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Mol	Chain	Res	Type
1	A	682	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 6 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	374	HIS
2	D	109	ASN
1	A	533	GLN
1	A	365	GLN
1	C	75	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 [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	580/740 (78%)	0.07	3 (0%) 91 76	29, 58, 97, 128	0
1	C	575/740 (77%)	0.08	6 (1%) 84 60	30, 57, 94, 129	0
2	B	74/169 (43%)	0.17	4 (5%) 29 11	34, 74, 97, 115	0
2	D	70/169 (41%)	0.23	3 (4%) 39 16	38, 78, 99, 107	0
All	All	1299/1818 (71%)	0.09	16 (1%) 81 55	29, 59, 97, 129	0

The worst 5 of 16 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	376	ASP	4.6
2	B	142	ASP	4.1
2	D	101	LEU	3.7
2	B	97	THR	3.5
2	D	94	ASP	3.5

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.