



wwPDB X-ray Structure Validation Summary Report ⓘ

Dec 15, 2016 – 11:11 AM EST

PDB ID : 2CO0
Title : WDR5 and unmodified Histone H3 complex at 2.25 angstrom
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Deposited on : 2006-05-25
Resolution : 2.25 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-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

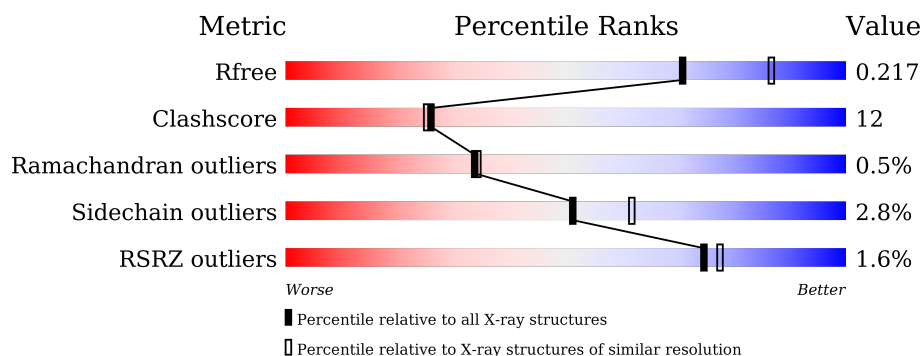
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.25 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	1640 (2.28-2.24)
Clashscore	102246	1095 (2.26-2.26)
Ramachandran outliers	100387	1063 (2.26-2.26)
Sidechain outliers	100360	1063 (2.26-2.26)
RSRZ outliers	91569	1647 (2.28-2.24)

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	315	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, orange 1%, yellow 21%, green 74%, grey 4%);"></div> <div style="display: flex; justify-content: space-between; width: 90%; margin: 0 auto;"> % 74% 21% .. </div> </div>
2	B	15	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 13%, orange 13%, yellow 7%, green 33%, grey 60%);"></div> <div style="display: flex; justify-content: space-between; width: 90%; margin: 0 auto;"> 13% 33% 7% 60% </div> </div>
2	D	15	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, yellow 7%, green 33%, grey 60%);"></div> <div style="display: flex; justify-content: space-between; width: 90%; margin: 0 auto;"> 33% 7% 60% </div> </div>
3	C	315	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, orange 1%, yellow 26%, green 69%, grey 4%);"></div> <div style="display: flex; justify-content: space-between; width: 90%; margin: 0 auto;"> % 69% 26% .. </div> </div>

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 5092 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 WD-REPEAT PROTEIN 5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	304	Total	C	N	O	S	0	0	0
			2356	1500	391	452	13			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	38	MET	LYS	CONFLICT	UNP P61964
A	162	MET	LYS	CONFLICT	UNP P61964
A	237	ASP	THR	CONFLICT	UNP P61964
A	282	MET	LEU	CONFLICT	UNP P61964

- Molecule 2 is a protein called HISTONE H3 DIMETHYL-LYSINE 4.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	B	6	Total	C	N	O	0	0	1
			42	24	11	7			
2	D	6	Total	C	N	O	0	0	1
			42	24	11	7			

- Molecule 3 is a protein called WD-REPEAT PROTEIN 5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	304	Total	C	N	O	S	0	0	0
			2355	1500	391	451	13			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	38	MET	LYS	CONFLICT	UNP P61964
C	162	MET	LYS	CONFLICT	UNP P61964
C	282	MET	LEU	CONFLICT	UNP P61964

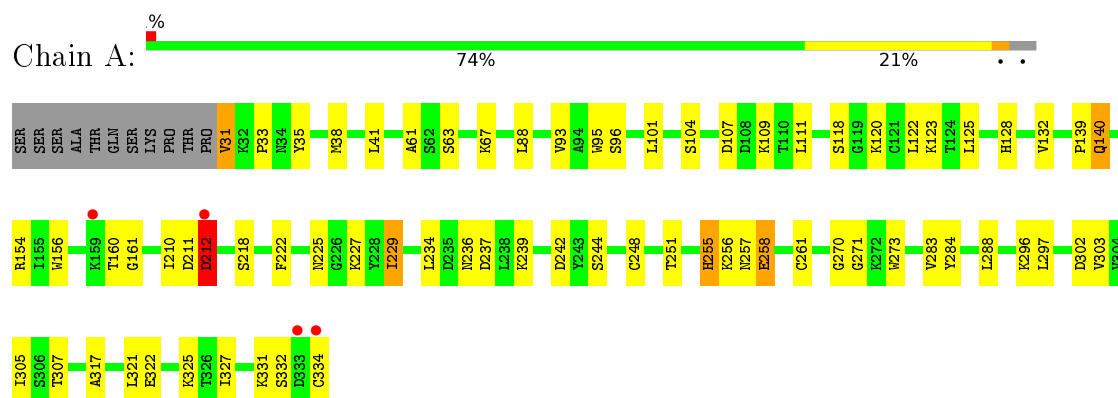
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	140	Total 140	O 140	0	0
4	B	9	Total 9	O 9	0	0
4	C	142	Total 142	O 142	0	0
4	D	6	Total 6	O 6	0	0

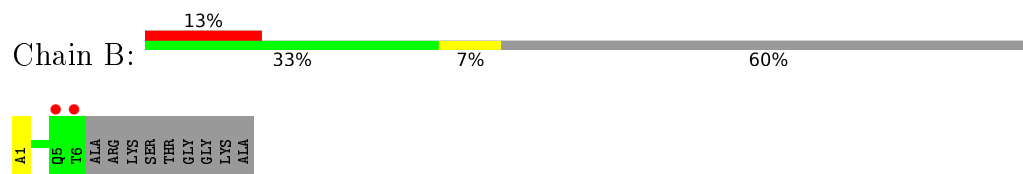
3 Residue-property plots [i](#)

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 ($RSRZ > 2$). 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.

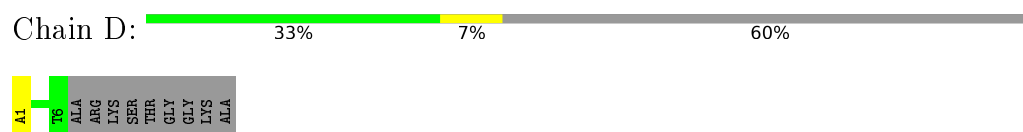
- Molecule 1: WD-REPEAT PROTEIN 5



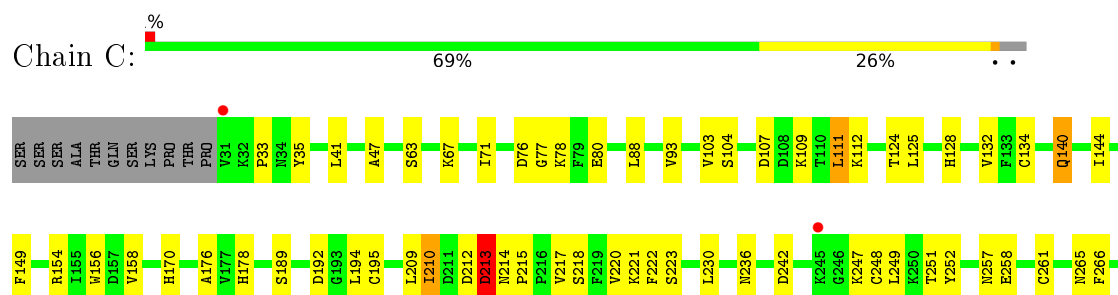
- Molecule 2: HISTONE H3 DIMETHYL-LYSINE 4

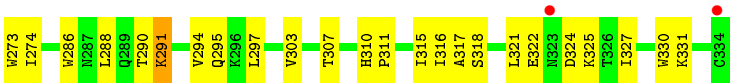


- Molecule 2: HISTONE H3 DIMETHYL-LYSINE 4



- Molecule 3: WD-REPEAT PROTEIN 5





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	64.92Å 47.03Å 101.77Å 90.00° 107.01° 90.00°	Depositor
Resolution (Å)	20.00 – 2.25 19.73 – 2.24	Depositor EDS
% Data completeness (in resolution range)	95.4 (20.00-2.25) 94.9 (19.73-2.24)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.35 (at 2.23Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.190 , 0.226 0.185 , 0.217	Depositor DCC
R_{free} test set	1309 reflections (5.10%)	DCC
Wilson B-factor (Å ²)	21.3	Xtriage
Anisotropy	0.306	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 52.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.033 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	5092	wwPDB-VP
Average B, all atoms (Å ²)	23.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 22.84 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 5.2555e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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	0.34	0/2412	0.70	1/3270 (0.0%)
2	B	0.77	0/41	0.66	0/53
2	D	0.73	0/41	0.63	0/53
3	C	0.34	0/2411	0.69	1/3269 (0.0%)
All	All	0.35	0/4905	0.70	2/6645 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	242	ASP	N-CA-C	-5.37	96.51	111.00
3	C	242	ASP	N-CA-C	-5.30	96.69	111.00

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	2356	0	2326	58	0
2	B	42	0	48	2	0
2	D	42	0	48	1	0
3	C	2355	0	2329	63	0
4	A	140	0	0	4	0
4	B	9	0	0	0	0
4	C	142	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	D	6	0	0	0	0
All	All	5092	0	4751	118	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 12.

The worst 5 of 118 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)
3:C:236:ASN:HD22	3:C:257:ASN:H	1.13	0.97
3:C:140:GLN:HE21	3:C:140:GLN:H	1.00	0.94
1:A:236:ASN:HD22	1:A:257:ASN:H	1.15	0.92
1:A:107:ASP:OD2	2:B:1:ALA:HB2	1.76	0.86
1:A:140:GLN:H	1:A:140:GLN:HE21	1.19	0.86

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	302/315 (96%)	281 (93%)	19 (6%)	2 (1%)	26	26
2	B	4/15 (27%)	4 (100%)	0	0	100	100
2	D	4/15 (27%)	4 (100%)	0	0	100	100
3	C	302/315 (96%)	284 (94%)	17 (6%)	1 (0%)	46	52
All	All	612/660 (93%)	573 (94%)	36 (6%)	3 (0%)	34	34

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	212	ASP

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Mol	Chain	Res	Type
1	A	234	LEU
3	C	213	ASP

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	266/276 (96%)	259 (97%)	7 (3%)	54	65
2	B	4/10 (40%)	4 (100%)	0	100	100
2	D	4/10 (40%)	4 (100%)	0	100	100
3	C	266/276 (96%)	258 (97%)	8 (3%)	48	59
All	All	540/572 (94%)	525 (97%)	15 (3%)	51	62

5 of 15 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	258	GLU
3	C	111	LEU
3	C	213	ASP
1	A	255	HIS
3	C	210	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 10 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	265	ASN
3	C	100	ASN
3	C	178	HIS
1	A	255	HIS
3	C	140	GLN

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	304/315 (96%)	-0.07	4 (1%) 79 82	10, 20, 36, 51	0
2	B	6/15 (40%)	0.58	2 (33%) 0 0	17, 19, 42, 42	0
2	D	6/15 (40%)	0.09	0 100 100	18, 23, 36, 39	0
3	C	304/315 (96%)	-0.09	4 (1%) 79 82	13, 22, 35, 48	0
All	All	620/660 (93%)	-0.07	10 (1%) 74 77	10, 21, 36, 51	0

The worst 5 of 10 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	334	CYS	4.4
3	C	334	CYS	3.9
1	A	212	ASP	3.6
3	C	31	VAL	3.0
2	B	6	THR	3.0

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 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.