

wwPDB X-ray Structure Validation Summary Report (i)

Dec 12, 2023 – 09:48 pm GMT

PDB ID : 2XL3

Title : WDR5 IN COMPLEX WITH AN RBBP5 PEPTIDE AND HISTONE H3

PEPTIDE

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Deposited on : 2010-07-19

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 (i) 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 (1)) were used in the production of this report:

Mol Probity : 4.02b-467

Mogul : 1.8.4, CSD as541be (2020)

Xtriage (Phenix) : 1.13 EDS : 2.36

Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)

 $Refmac \quad : \quad 5.8.0158$

CCP4 : 7.0.044 (Gargrove)

Ideal geometry (proteins) : Engh & Huber (2001) Ideal geometry (DNA, RNA) : Parkinson et al. (1996)

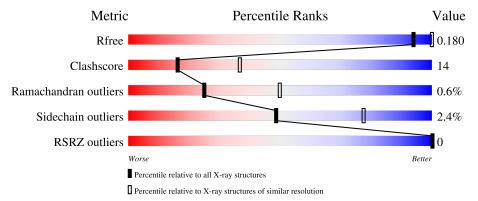
Validation Pipeline (wwPDB-VP) : 2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: $X\text{-}RAY\ DIFFRACTION$

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 $(\# \mathrm{Entries})$	$\begin{array}{c} {\rm Similar\ resolution} \\ (\#{\rm Entries,\ resolution\ range(\mathring{A})}) \end{array}$
R_{free}	130704	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (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 <=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	334		65%		25%	• 9%	
1	В	334		66%		24%	• 9%	
2	С	14	4	3%	29%	29	%	
2	Е	14	21%	36%	7%	36%		
3	D	9	11%	44%		44%		



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Mol	Chain	Length		Quality of	f chain
3	F	9	33%	11%	56%



2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 5031 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-CONTAINING PROTEIN 5.

\mathbf{Mol}	Chain	Residues	\mathbf{Atoms}				ZeroOcc	AltConf	Trace		
1	Δ	303	Total	С	N	О	S	0	1	0	
1	Λ	303	2346	1497	389	450	10				
1	B	304	Total	С	N	О	S	0	0	0	
1	ם	304	2345	1494	390	451	10			U	

• Molecule 2 is a protein called RETINOBLASTOMA-BINDING PROTEIN 5.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	С	10	Total 77	C 44			0	0	0
2	Е	9	Total 69	C 40		O 20	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chair	n Residue	Modelled	Actual	Comment	Reference
С	1	TYR	-	expression tag	UNP Q8BX09
E	1	TYR	-	expression tag	UNP Q8BX09

• Molecule 3 is a protein called HISTONE H3.1.

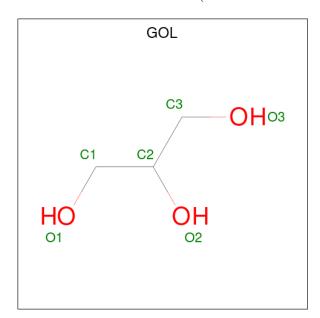
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	D	5	Total 41			O 7	0	0	0
3	F	4	Total 28	C 16	N 7	O 5	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	9	TYR	-	expression tag	UNP P68433
F	9	TYR	-	expression tag	UNP P68433



• Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 6 3 3	0	0
4	A	1	Total C O 6 3 3	0	0
4	В	1	Total C O 6 3 3	0	0

• Molecule 5 is water.

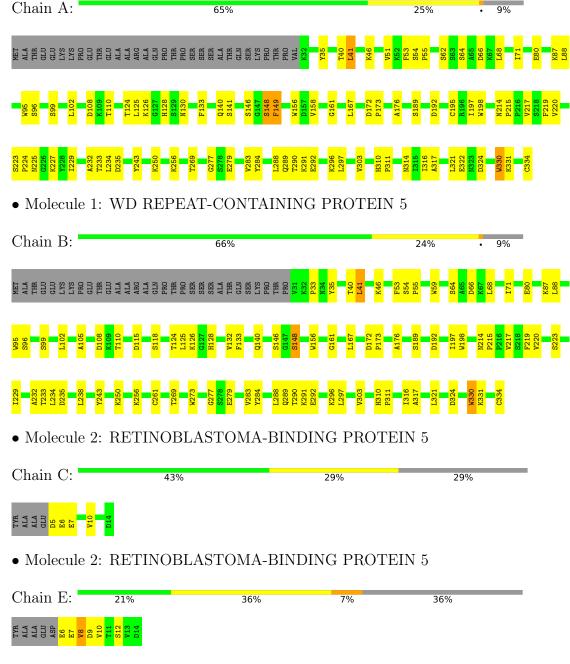
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	54	Total O 54 54	0	0
5	В	51	Total O 51 51	0	0
5	D	2	Total O 2 2	0	0



3 Residue-property plots (i)

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: WD REPEAT-CONTAINING PROTEIN 5





• Molecule 3: HISTONE H3.1

Chain D: 11% 44% 44%

A1 R2 R2 K4 Q5 Q5 THR ALA ARG

• Molecule 3: HISTONE H3.1

Chain F: 33% 11% 56%

A1
T3
K4
GLN
THR
ALA
ARG



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants	47.10Å 81.32Å 86.35Å	Donogitor
a, b, c, α , β , γ	90.00° 91.13° 90.00°	Depositor
Resolution (Å)	41.69 - 2.70	Depositor
Resolution (A)	41.69 - 2.70	EDS
% Data completeness	92.4 (41.69-2.70)	Depositor
(in resolution range)	98.7 (41.69-2.70)	EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	2.48 (at 2.69Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
D.D.	0.176 , 0.235	Depositor
R, R_{free}	0.183 , 0.180	DCC
R_{free} test set	861 reflections (4.84%)	wwPDB-VP
Wilson B-factor (Å ²)	36.2	Xtriage
Anisotropy	1.263	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$, $B_{sol}(Å^2)$	0.31 , 19.2	EDS
L-test for twinning ²	$< L > = 0.49, < L^2> = 0.32$	Xtriage
Estimated twinning fraction	0.267 for h,-k,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	5031	wwPDB-VP
Average B, all atoms (Å ²)	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 7.40% of the height of the origin peak. No significant pseudotranslation is detected.

²Theoretical values of <|L|>, $<L^2>$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.



¹Intensities estimated from amplitudes.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: GOL

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		
IVIOI		RMSZ	# Z > 5	RMSZ	# Z > 5	
1	A	0.40	0/2406	0.54	0/3266	
1	В	0.40	0/2401	0.55	0/3260	
2	С	0.32	0/76	0.52	0/102	
2	Е	0.65	0/68	0.72	0/91	
3	D	0.50	0/40	0.60	0/51	
3	F	0.48	0/27	0.73	0/35	
All	All	0.41	0/5018	0.55	0/6805	

There are no bond length outliers.

There are no bond angle outliers.

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	2346	0	2306	63	0
1	В	2345	0	2306	66	0
2	С	77	0	62	9	0
2	Е	69	0	58	8	0
3	D	41	0	48	3	0
3	F	28	0	29	5	0
4	A	12	0	16	0	0



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	.,	10	1

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	В	6	0	8	2	0
5	A	54	0	0	2	0
5	В	51	0	0	1	0
5	D	2	0	0	1	0
All	All	5031	0	4833	140	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 14.

The worst 5 of 140 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	$\begin{array}{c} {\rm Interatomic} \\ {\rm distance} \ ({\rm \AA}) \end{array}$	$\begin{array}{c} \text{Clash} \\ \text{overlap } (\text{\AA}) \end{array}$
2:E:6:GLU:HG2	2:E:6:GLU:O	1.59	0.99
1:A:224:PRO:HD2	2:C:10:VAL:HG13	1.49	0.93
2:C:10:VAL:HG13	2:C:10:VAL:O	1.79	0.81
2:C:10:VAL:O	2:C:10:VAL:CG1	2.30	0.80
1:A:233:THR:HG23	1:A:235:ASP:OD2	1.86	0.76

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	Perce	entiles
1	A	302/334 (90%)	273 (90%)	27 (9%)	2 (1%)	22	46
1	В	302/334 (90%)	275 (91%)	25 (8%)	2 (1%)	22	46
2	C	8/14 (57%)	5 (62%)	3 (38%)	0	100	100
2	\mathbf{E}	7/14 (50%)	5 (71%)	2 (29%)	0	100	100
3	D	3/9 (33%)	3 (100%)	0	0	100	100
3	F	2/9 (22%)	2 (100%)	0	0	100	100



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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	624/714 (87%)	563 (90%)	57 (9%)	4 (1%)	25 50

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	234	LEU
1	В	234	LEU
1	В	277	GLY
1	A	277	GLY

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	A	263/291 (90%)	256 (97%)	7 (3%)	44 74		
1	В	263/291 (90%)	257 (98%)	6 (2%)	50 78		
2	С	10/12 (83%)	10 (100%)	0	100 100	0	
2	E	9/12 (75%)	8 (89%)	1 (11%)	6 14		
3	D	4/7~(57%)	4 (100%)	0	100 100	0	
3	F	2/7~(29%)	2 (100%)	0	100 100	0	
All	All	551/620 (89%)	537 (98%)	14 (2%)	49 76		

5 of 14 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	В	41	LEU
1	В	140	GLN
2	Е	8	VAL
1	В	330	TRP
1	В	334	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:



Mol	Chain	Res	Type
1	A	128	HIS
1	A	265	ASN
1	В	128	HIS
1	В	265	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

3 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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| > 2 is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol Type	Chain	Chain	Chain	Chain	Chain	Chain	Chain	Chain	Chain	Chain	Chain	Res	Link	В	Bond lengths			Bond angles		
	туре		ites	LIIIK	Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2										
4	GOL	A	1336	-	5,5,5	0.43	0	5,5,5	0.21	0										
4	GOL	В	1335	-	5,5,5	0.33	0	5,5,5	0.24	0										
4	GOL	A	1335	-	5,5,5	0.41	0	5,5,5	0.20	0										

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.



\mathbf{Mol}	Type	Chain	Res	Link	Chirals	Torsions	Rings	
4	GOL	A	1336	-	-	2/4/4/4	-	
4	GOL	В	1335	-	-	2/4/4/4	-	
4	GOL	A	1335	-	-	2/4/4/4	-	

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 6 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	1335	GOL	C1-C2-C3-O3
4	A	1336	GOL	C1-C2-C3-O3
4	В	1335	GOL	C1-C2-C3-O3
4	В	1335	GOL	O2-C2-C3-O3
4	A	1335	GOL	O2-C2-C3-O3

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	В	1335	GOL	2	0

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.



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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, 95^{th} 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>	# RSRZ > 2		ZZ>2	$OWAB(Å^2)$	Q < 0.9
1	A	303/334 (90%)	-0.87	0	100	100	22, 34, 51, 68	0
1	В	304/334 (91%)	-0.86	0	100	100	22, 34, 53, 68	0
2	С	10/14 (71%)	0.00	0	100	100	40, 54, 89, 90	0
2	Е	9/14 (64%)	-0.49	0	100	100	46, 50, 76, 89	0
3	D	5/9~(55%)	-0.08	0	100	100	46, 50, 73, 78	0
3	F	4/9 (44%)	-0.26	0	100	100	49, 54, 61, 66	0
All	All	635/714 (88%)	-0.84	0	100	100	22, 34, 56, 90	0

There are no RSRZ outliers to report.

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 monosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	$ m B ext{-}factors(\AA^2)$	Q<0.9
4	GOL	A	1335	6/6	0.90	0.20	48,51,56,72	0



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Mol	Type	Chain	Res	Atoms	RSCC	RSR	${f B-factors}({f \AA}^2)$	Q < 0.9
4	GOL	В	1335	6/6	0.91	0.15	50,56,66,68	0
4	GOL	A	1336	6/6	0.92	0.12	42,54,54,69	0

6.5 Other polymers (i)

There are no such residues in this entry.

