



# wwPDB X-ray Structure Validation Summary Report ⓘ

Oct 12, 2024 – 08:25 pm BST

PDB ID : 5FWU  
Title : Wnt modulator Kremen crystal form II at 2.8Å  
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Deposited on : 2016-02-21  
Resolution : 2.80 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](mailto: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>.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

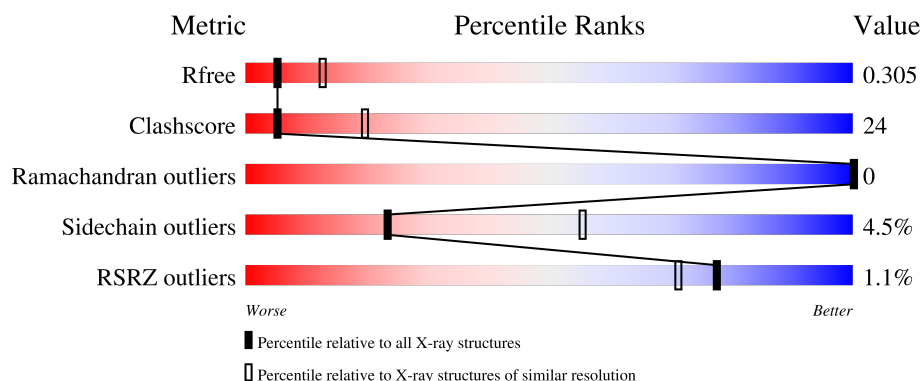
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.80 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))
$R_{free}$	164625	3657 (2.80-2.80)
Clashscore	180529	4123 (2.80-2.80)
Ramachandran outliers	177936	4071 (2.80-2.80)
Sidechain outliers	177891	4073 (2.80-2.80)
RSRZ outliers	164620	3659 (2.80-2.80)

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  $\geq 3$ , 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	406	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	NAG	A	1326	X	-	-	-

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 2132 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 KREMEN PROTEIN 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	271	Total	C	N	O	S	0	0	0
			2102	1344	348	390	20			

There are 61 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-10	MET	-	initiating methionine	UNP Q96MU8
A	-9	GLY	-	expression tag	UNP Q96MU8
A	-8	ILE	-	expression tag	UNP Q96MU8
A	-7	LEU	-	expression tag	UNP Q96MU8
A	-6	PRO	-	expression tag	UNP Q96MU8
A	-5	SER	-	expression tag	UNP Q96MU8
A	-4	PRO	-	expression tag	UNP Q96MU8
A	-3	GLY	-	expression tag	UNP Q96MU8
A	-2	MET	-	expression tag	UNP Q96MU8
A	-1	PRO	-	expression tag	UNP Q96MU8
A	0	ALA	-	expression tag	UNP Q96MU8
A	1	LEU	-	expression tag	UNP Q96MU8
A	2	LEU	-	expression tag	UNP Q96MU8
A	3	SER	-	expression tag	UNP Q96MU8
A	4	LEU	-	expression tag	UNP Q96MU8
A	5	VAL	-	expression tag	UNP Q96MU8
A	6	SER	-	expression tag	UNP Q96MU8
A	7	LEU	-	expression tag	UNP Q96MU8
A	8	LEU	-	expression tag	UNP Q96MU8
A	9	SER	-	expression tag	UNP Q96MU8
A	10	VAL	-	expression tag	UNP Q96MU8
A	11	LEU	-	expression tag	UNP Q96MU8
A	12	LEU	-	expression tag	UNP Q96MU8
A	13	MET	-	expression tag	UNP Q96MU8
A	14	GLY	-	expression tag	UNP Q96MU8
A	15	CYS	-	expression tag	UNP Q96MU8
A	16	VAL	-	expression tag	UNP Q96MU8

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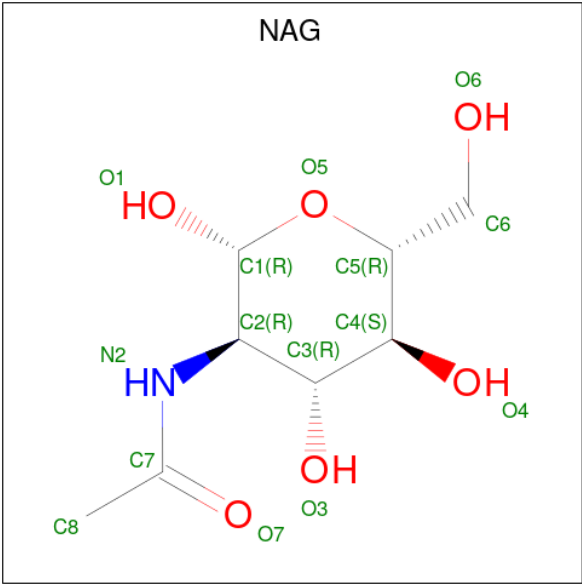
Chain	Residue	Modelled	Actual	Comment	Reference
A	17	ALA	-	expression tag	UNP Q96MU8
A	18	GLU	-	expression tag	UNP Q96MU8
A	19	THR	-	expression tag	UNP Q96MU8
A	20	GLY	-	expression tag	UNP Q96MU8
A	21	ALA	-	expression tag	UNP Q96MU8
A	22	PRO	-	expression tag	UNP Q96MU8
A	23	SER	-	expression tag	UNP Q96MU8
A	24	PRO	-	expression tag	UNP Q96MU8
A	25	GLY	-	expression tag	UNP Q96MU8
A	26	LEU	-	expression tag	UNP Q96MU8
A	27	GLY	-	expression tag	UNP Q96MU8
A	28	PRO	-	expression tag	UNP Q96MU8
A	325	GLY	-	insertion	UNP Q96MU8
A	326	SER	-	insertion	UNP Q96MU8
A	327	GLU	-	insertion	UNP Q96MU8
A	328	ASN	-	insertion	UNP Q96MU8
A	329	LEU	-	insertion	UNP Q96MU8
A	330	TYR	-	insertion	UNP Q96MU8
A	331	PHE	-	insertion	UNP Q96MU8
A	332	GLN	-	insertion	UNP Q96MU8
A	333	GLY	-	insertion	UNP Q96MU8
A	334	GLY	-	insertion	UNP Q96MU8
A	335	SER	-	insertion	UNP Q96MU8
A	385	THR	-	expression tag	UNP Q96MU8
A	386	HIS	-	expression tag	UNP Q96MU8
A	387	HIS	-	expression tag	UNP Q96MU8
A	388	HIS	-	expression tag	UNP Q96MU8
A	389	HIS	-	expression tag	UNP Q96MU8
A	390	HIS	-	expression tag	UNP Q96MU8
A	391	HIS	-	expression tag	UNP Q96MU8
A	392	HIS	-	expression tag	UNP Q96MU8
A	393	HIS	-	expression tag	UNP Q96MU8
A	394	HIS	-	expression tag	UNP Q96MU8
A	395	HIS	-	expression tag	UNP Q96MU8

- Molecule 2 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	2	Total Cl 2 2	0	0

- Molecule 3 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula:

C<sub>8</sub>H<sub>15</sub>NO<sub>6</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	A	1	Total	C	N	O	0	0
			14	8	1	5		



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 43	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	65.78Å 65.78Å 75.01Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	65.78 – 2.80 65.78 – 2.80	Depositor EDS
% Data completeness (in resolution range)	99.8 (65.78-2.80) 99.8 (65.78-2.80)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.44 (at 2.81Å)	Xtriage
Refinement program	REFMAC 5.8.0103	Depositor
R, $R_{free}$	0.216 , 0.307 0.218 , 0.305	Depositor DCC
$R_{free}$ test set	366 reflections (4.61%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	82.4	Xtriage
Anisotropy	0.189	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 74.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.051 for h,-k,-l	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	2132	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	91.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.53% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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

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

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	0.95	0/2170	0.98	7/2950 (0.2%)

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	1

There are no bond length outliers.

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
1	A	262	ARG	NE-CZ-NH2	-8.94	115.83	120.30
1	A	85	ARG	NE-CZ-NH1	8.57	124.59	120.30
1	A	262	ARG	NE-CZ-NH1	7.26	123.93	120.30
1	A	85	ARG	NE-CZ-NH2	-5.77	117.42	120.30
1	A	162	GLU	OE1-CD-OE2	-5.38	116.84	123.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	289	PRO	Peptide



## 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	2102	0	1909	97	0
2	A	2	0	0	0	0
3	A	28	0	26	0	0
All	All	2132	0	1935	97	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 24.

The worst 5 of 97 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:A:185:GLU:OE1	1:A:203:ARG:NE	1.82	1.10
1:A:59:ASN:O	1:A:62:PHE:CE2	2.04	1.10
1:A:188:SER:HB2	1:A:199:GLY:O	1.76	0.86
1:A:61:THR:OG1	1:A:66:TYR:O	1.97	0.83
1:A:239:VAL:HG13	1:A:303:PHE:O	1.79	0.82

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	261/406 (64%)	253 (97%)	8 (3%)	0	<b>100</b> <b>100</b>

There are no Ramachandran outliers to report.

### 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	223/339 (66%)	213 (96%)	10 (4%)	23 55

5 of 10 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	223	SER
1	A	233	THR
1	A	263	ASP
1	A	138	THR
1	A	161	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	81	HIS
1	A	145	GLN
1	A	251	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

Of 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 for Mogul analysis.

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	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	NAG	A	1325	1	14,14,15	0.47	0	17,19,21	1.23	1 (5%)
3	NAG	A	1326	1	14,14,15	0.81	1 (7%)	17,19,21	2.31	5 (29%)

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.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	A	1325	1	-	0/6/23/26	0/1/1/1
3	NAG	A	1326	1	1/1/5/7	1/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1326	NAG	C1-C2	2.16	1.55	1.52

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1326	NAG	C1-C2-N2	5.94	120.64	110.49
3	A	1326	NAG	O5-C1-C2	-4.63	103.98	111.29
3	A	1325	NAG	C1-O5-C5	3.51	116.95	112.19
3	A	1326	NAG	C1-O5-C5	2.78	115.95	112.19
3	A	1326	NAG	C2-N2-C7	2.47	126.42	122.90

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	A	1326	NAG	C1

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1326	NAG	C3-C2-N2-C7

There are no ring outliers.

No monomer is involved in short contacts.

## 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	271/406 (66%)	-0.00	3 (1%) 77 71	52, 84, 137, 152	0

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	69	LEU	3.3
1	A	30	PRO	2.7
1	A	150	PHE	2.2

### 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<sup>th</sup> 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	B-factors(Å <sup>2</sup> )	Q<0.9
3	NAG	A	1326	14/15	0.79	0.13	101,116,122,126	0
2	CL	A	1324	1/1	0.84	0.18	96,96,96,96	0
3	NAG	A	1325	14/15	0.87	0.10	86,99,108,120	0
2	CL	A	1323	1/1	0.89	0.17	107,107,107,107	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.