

Full wwPDB X-ray Structure Validation Report (i)

Nov 14, 2023 – 03:26 AM JST

PDB ID	:	8W48
Title	:	Neutron and X-ray joint structure of WT-TTR in complex with piceatannol
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Deposited on		
Resolution	:	1.19 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 (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:

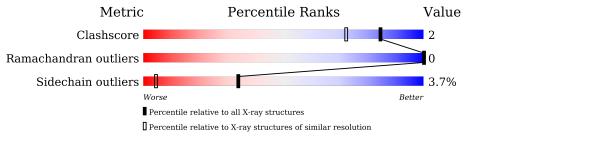
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	FAILED
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson 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-RAY DIFFRACTION, NEUTRON DIFFRACTION

The reported resolution of this entry is 1.19 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	$\begin{array}{c} \textbf{Whole archive} \\ (\#\textbf{Entries}) \end{array}$	${f Similar\ resolution}\ (\#{ m Entries,\ resolution\ range}({ m \AA}))$
Clashscore	141614	1286 (1.22-1.18)
Ramachandran outliers	138981	1240 (1.22-1.18)
Sidechain outliers	138945	1239 (1.22-1.18)

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%

Note EDS failed to run properly.

Mol	Chain	Length	Quality of chain					
1	А	159	70%	·	27%			
1	В	159	69%	•	28%			



2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 4093 atoms, of which 1722 are hydrogens and 462 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.

Mol	Chain	Residues		Atoms					ZeroOcc	AltConf	Trace	
1	Λ	116	Total	С	D	Η	Ν	Ο	S	32	109	0
			1947	573	183	868	147	174	2			
1	р	114	Total	С	D	Η	Ν	0	S	46	108	0
	D	114	1894	561	175	844	141	171	2			0

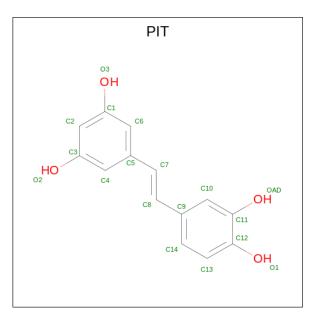
• Molecule 1 is a protein called Transthyretin.

Chain	Residue	Modelled	Actual	Comment	Reference
А	-31	MET	-	expression tag	UNP P02766
А	-30	ARG	-	expression tag	UNP P02766
А	-29	GLY	-	expression tag	UNP P02766
А	-28	SER	-	expression tag	UNP P02766
А	-27	HIS	-	expression tag	UNP P02766
A	-26	HIS	-	expression tag	UNP P02766
А	-25	HIS	-	expression tag	UNP P02766
A	-24	HIS	-	expression tag	UNP P02766
А	-23	HIS	-	expression tag	UNP P02766
А	-22	HIS	-	expression tag	UNP P02766
A	-21	GLY	-	expression tag	UNP P02766
А	-20	SER	-	expression tag	UNP P02766
В	-31	MET	-	expression tag	UNP P02766
В	-30	ARG	-	expression tag	UNP P02766
В	-29	GLY	-	expression tag	UNP P02766
В	-28	SER	-	expression tag	UNP P02766
В	-27	HIS	-	expression tag	UNP P02766
В	-26	HIS	-	expression tag	UNP P02766
В	-25	HIS	-	expression tag	UNP P02766
В	-24	HIS	-	expression tag	UNP P02766
В	-23	HIS	-	expression tag	UNP P02766
В	-22	HIS	-	expression tag	UNP P02766
В	-21	GLY	-	expression tag	UNP P02766
В	-20	SER	_	expression tag	UNP P02766

There are 24 discrepancies between the modelled and reference sequences:



• Molecule 2 is PICEATANNOL (three-letter code: PIT) (formula: $C_{14}H_{12}O_4$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
9	Λ	1	Total	С	D	Н	Ο	0	0
		1	30	14	7	5	4	0	0
0	р	1	Total	С	D	Η	Ο	0	0
	D	1	30	14	7	5	4	0	0

• Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	А	57	Total D O 109 52 57	2	0
3	В	45	Total D O 83 38 45	2	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. 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. 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.

Note EDS failed to run properly.

• Molecule 1: Transthyretin

Chain A:	70%	•	27%					
MET ARG GLY GLY HIS HIS HIS HIS HIS	CALS CALS CALS CALS CALS CALS CALS CALS	GLY GLU SER LYS C10 K35	E92 S100 P125 LYS GLU					
• Molecule 1: Transthyretin								
Chain B:	69%	·	28%					
MET ARG GLY GLY HIS HIS HIS HIS HIS	ALLS ALLA ALLA ALLA ALLA ALLA ALLA ALLA	GLY GLU SER LYS C10 E66	E92 P102 ASN ASN LYS GLU					



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants	43.67Å 85.01Å 65.35Å	Depositor
a, b, c, α , β , γ	90.00° 90.00° 90.00°	Depositor
Resolution (Å)	42.51 - 1.19	Depositor
% Data completeness	99.8 (42.51-1.19)	Depositor
(in resolution range)	· · · · · · · · · · · · · · · · · · ·	-
R_{merge}	(Not available)	Depositor
R _{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	$1.92 (at 1.19 \text{\AA})$	Xtriage
Refinement program	unknown	Depositor
R, R_{free}	0.179 , 0.202	Depositor
Wilson B-factor $(Å^2)$	17.8	Xtriage
Anisotropy	0.135	Xtriage
L-test for twinning ²	$ < L >=0.48, < L^2>=0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	4093	wwPDB-VP
Average B, all atoms $(Å^2)$	31.0	wwPDB-VP

EDS failed to run properly - this section is therefore incomplete.

Xtriage's analysis on translational NCS is as follows: The analyses of the Patterson function reveals a significant off-origin peak that is 29.65 % 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 1.4946e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.

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.



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: DOD, PIT

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	А	0.58	0/1785	0.72	0/2438	
1	В	0.47	0/1748	0.65	0/2386	
All	All	0.53	0/3533	0.68	0/4824	

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	А	1079	868	49	0	0
1	В	1050	844	42	1	0
2	А	25	5	9	0	0
2	В	25	5	11	0	0
3	А	109	0	0	0	0
3	В	83	0	0	2	0
All	All	2371	1722	111	3	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 2.

All (3) close contacts within the same asymmetric unit are listed below, sorted by their clash



magnitude.

Atom 1	Atom-2	Interatomic	Clash	
Atom-1		distance (\AA)	overlap (Å)	

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	ntiles
1	А	222/159~(140%)	220~(99%)	2(1%)	0	100	100
1	В	218/159~(137%)	206~(94%)	12~(6%)	0	100	100
All	All	440/318~(138%)	426 (97%)	14(3%)	0	100	100

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	Percen	tiles
1	А	187/131~(143%)	179~(96%)	8 (4%)	29	3
1	В	182/131~(139%)	176~(97%)	6 (3%)	38	5
All	All	369/262~(141%)	355~(96%)	14 (4%)	34	4

All (14) residues with a non-rotameric sidechain are listed below:



Mol	Chain	Res	Type
1	А	10[A]	CYS
1	А	10[B]	CYS
1	А	35[A]	LYS
1	А	35[B]	LYS
1	А	92[A]	GLU
1	А	92[B]	GLU
1	А	100[A]	SER
1	А	100[B]	SER
1	В	10[A]	CYS
1	В	10[B]	CYS
1	В	66[A]	GLU
1	В	66[B]	GLU
1	В	92[A]	GLU
1	В	92[B]	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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)

2 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	Turne	Chain	Dec	Link	Bo	ond leng	\mathbf{ths}	B	ond ang	les
IVIOI	Type	Chain	Res	LIIIK	Counts	RMSZ	# Z >2	Counts	RMSZ	# Z >2
2	PIT	А	201	-	19,19,19	1.25	3 (15%)	26,26,26	1.03	1 (3%)
2	PIT	В	201	-	19,19,19	1.33	3 (15%)	26,26,26	0.82	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.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	PIT	А	201	-	-	0/5/5/5	0/2/2/2
2	PIT	В	201	-	-	0/5/5/5	0/2/2/2

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$\operatorname{Observed}(\operatorname{\AA})$	Ideal(Å)
2	В	201	PIT	C8-C7	4.27	1.52	1.31
2	А	201	PIT	C8-C7	3.87	1.50	1.31
2	А	201	PIT	C9-C8	-2.74	1.39	1.47
2	В	201	PIT	C5-C7	-2.51	1.40	1.47
2	В	201	PIT	C9-C8	-2.38	1.40	1.47
2	А	201	PIT	C5-C7	-2.35	1.40	1.47

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
2	А	201	PIT	C9-C10-C11	-2.79	118.76	120.76

There are no chirality outliers.

There are no torsion outliers.

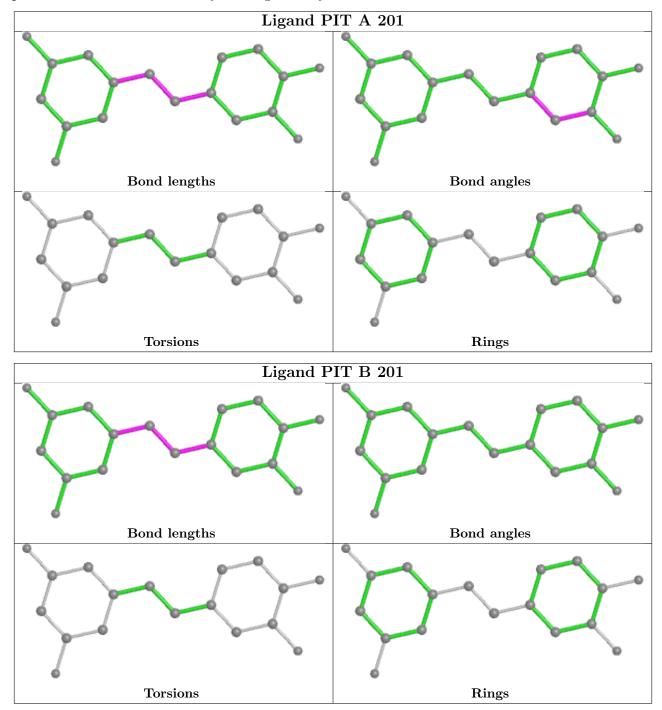
There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and



any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



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)

EDS failed to run properly - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains (i)

EDS failed to run properly - this section is therefore empty.

6.3 Carbohydrates (i)

EDS failed to run properly - this section is therefore empty.

6.4 Ligands (i)

EDS failed to run properly - this section is therefore empty.

6.5 Other polymers (i)

EDS failed to run properly - this section is therefore empty.

