



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 31, 2020 – 06:20 AM BST

PDB ID : 5NFE
Title : Neutron structure of human transthyretin (TTR) T119M mutant at room temperature to 1.85Å resolution
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Deposited on : 2017-03-14
Resolution : 1.85 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 ⓘ symbol.

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

MolProbity : 4.02b-467
Xtrriage (Phenix) : 1.13
EDS : **FAILED**
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) : 2.13

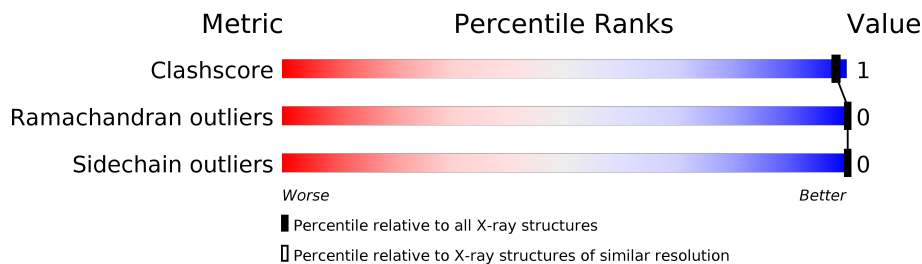
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION, NEUTRON DIFFRACTION

The reported resolution of this entry is 1.85 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))
Clashscore	141614	2625 (1.86-1.86)
Ramachandran outliers	138981	2592 (1.86-1.86)
Sidechain outliers	138945	2592 (1.86-1.86)

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 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 $\leq 5\%$.

Note EDS failed to run properly.

Mol	Chain	Length	Quality of chain
1	A	130	85% 11%
1	B	130	88% 11%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 4031 atoms, of which 356 are hydrogens and 1827 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 Transthyretin.

Mol	Chain	Residues	Atoms							ZeroOcc	AltConf	Trace
			Total	C	D	H	N	O	S			
1	A	116	1965	580	882	178	148	174	3	44	109	0
1	B	116	1966	580	883	178	148	174	3	42	109	0

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	GLY	-	expression tag	UNP P02766
A	-1	ALA	-	expression tag	UNP P02766
A	0	MET	-	expression tag	UNP P02766
A	119	MET	THR	conflict	UNP P02766
B	-2	GLY	-	expression tag	UNP P02766
B	-1	ALA	-	expression tag	UNP P02766
B	0	MET	-	expression tag	UNP P02766
B	119	MET	THR	conflict	UNP P02766

- Molecule 2 is water.


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	D	O		
2	A	26	68	42	26	0	0
2	B	12	32	20	12	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. 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.

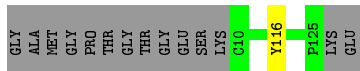
- Molecule 1: Transthyretin

Chain A:  85% 11%



- Molecule 1: Transthyretin

Chain B:  88% 11%



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	43.71Å 86.32Å 65.34Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	43.16 – 1.85	Depositor
% Data completeness (in resolution range)	96.3 (43.16-1.85)	Depositor
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	13.58 (at 1.86Å)	Xtrriage
Refinement program	PHENIX (1.10.1_2155: ???)	Depositor
R, R_{free}	0.165 , 0.194	Depositor
Wilson B-factor (Å ²)	24.4	Xtrriage
Anisotropy	0.137	Xtrriage
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
Total number of atoms	4031	wwPDB-VP
Average B, all atoms (Å ²)	34.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 37.53 % 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 4.2325e-04.*

¹ Intensities estimated from amplitudes.

² 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 [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	1.03	8/1787 (0.4%)	0.93	2/2438 (0.1%)
1	B	0.83	0/1787	0.83	2/2438 (0.1%)
All	All	0.93	8/3574 (0.2%)	0.88	4/4876 (0.1%)

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	66[A]	GLU	CB-CG	-8.40	1.36	1.52
1	A	66[B]	GLU	CB-CG	-8.40	1.36	1.52
1	A	72[A]	GLU	CB-CG	-7.19	1.38	1.52
1	A	72[B]	GLU	CB-CG	-7.19	1.38	1.52
1	A	63[A]	GLU	CB-CG	-5.94	1.40	1.52
1	A	63[B]	GLU	CB-CG	-5.94	1.40	1.52
1	A	46[A]	SER	CB-OG	5.35	1.49	1.42
1	A	46[B]	SER	CB-OG	5.35	1.49	1.42

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	116[A]	TYR	CB-CG-CD2	-5.31	117.81	121.00
1	A	116[B]	TYR	CB-CG-CD2	-5.31	117.81	121.00
1	B	116[A]	TYR	CB-CG-CD2	-5.08	117.95	121.00
1	B	116[B]	TYR	CB-CG-CD2	-5.08	117.95	121.00

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	1787	178	71	0	0
1	B	1788	178	71	0	0
2	A	68	0	0	1	0
2	B	32	0	0	0	0
All	All	3675	356	142	1	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 1.

All (1) 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)
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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	222/130 (171%)	220 (99%)	2 (1%)	0	100	100
1	B	222/130 (171%)	213 (96%)	9 (4%)	0	100	100
All	All	444/260 (171%)	433 (98%)	11 (2%)	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	Percentiles	
1	A	187/106 (176%)	187 (100%)	0	100	100
1	B	187/106 (176%)	187 (100%)	0	100	100
All	All	374/212 (176%)	374 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Some 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](#)

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

6.1 Protein, DNA and RNA chains

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

6.2 Non-standard residues in protein, DNA, RNA chains

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

6.3 Carbohydrates

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

6.4 Ligands

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

6.5 Other polymers

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