



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 9, 2026 – 04:04 PM UTC

PDB ID : 5TTR / pdb_00005ttr
Title : LEU 55 PRO TRANSTHYRETIN CRYSTAL STRUCTURE
Authors : Sebastiao, M.P.; Saraiva, M.J.; Damas, A.M.
Deposited on : 1998-04-30
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 ⓘ 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 ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

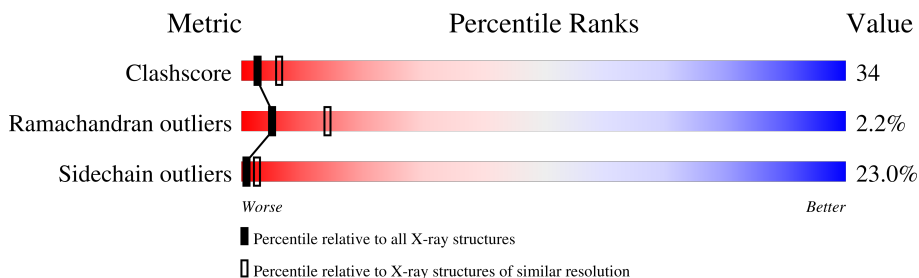
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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 (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	127	14% 40% 32% 5% 9%
1	B	127	19% 32% 31% 9% 9%
1	C	127	13% 50% 23% 6% 9%
1	D	127	16% 38% 30% 8% 9%
1	E	127	20% 33% 27% 11% 9%
1	F	127	20% 35% 27% 9% 9%
1	G	127	21% 30% 31% 9% 9%
1	H	127	17% 43% 24% 8% 9%

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 7147 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 TRANSTHYRETIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	116	Total	C	N	O	S	4	0	0
			895	572	147	174	2			
1	B	116	Total	C	N	O	S	18	0	0
			890	569	145	174	2			
1	C	116	Total	C	N	O	S	7	0	0
			895	572	147	174	2			
1	D	116	Total	C	N	O	S	0	0	0
			891	570	147	172	2			
1	E	116	Total	C	N	O	S	11	0	0
			895	572	147	174	2			
1	F	116	Total	C	N	O	S	0	0	0
			895	572	147	174	2			
1	G	116	Total	C	N	O	S	7	0	0
			891	570	147	172	2			
1	H	116	Total	C	N	O	S	4	0	0
			895	572	147	174	2			

There are 8 discrepancies between the modelled and reference sequences:

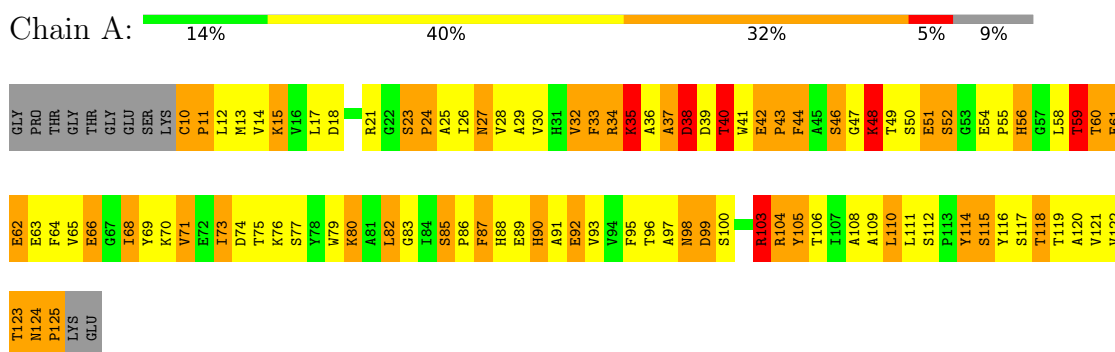
Chain	Residue	Modelled	Actual	Comment	Reference
A	55	PRO	LEU	engineered mutation	UNP P02766
B	55	PRO	LEU	engineered mutation	UNP P02766
C	55	PRO	LEU	engineered mutation	UNP P02766
D	55	PRO	LEU	engineered mutation	UNP P02766
E	55	PRO	LEU	engineered mutation	UNP P02766
F	55	PRO	LEU	engineered mutation	UNP P02766
G	55	PRO	LEU	engineered mutation	UNP P02766
H	55	PRO	LEU	engineered mutation	UNP P02766

3 Residue-property plots [i](#)

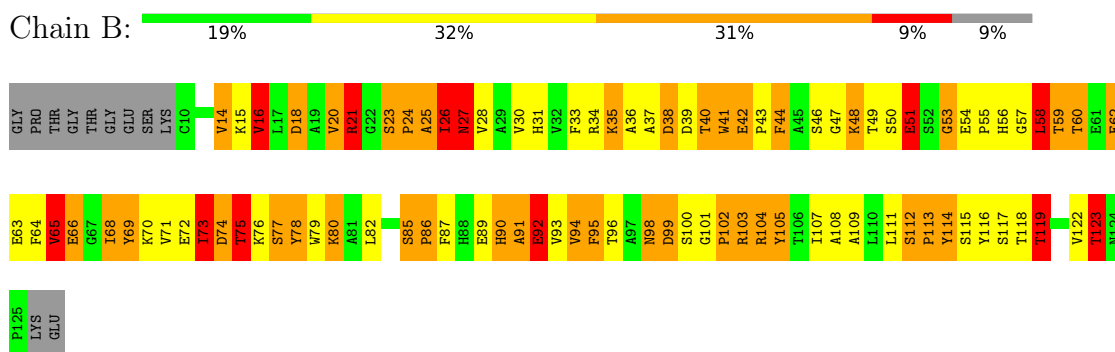
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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 was not executed.

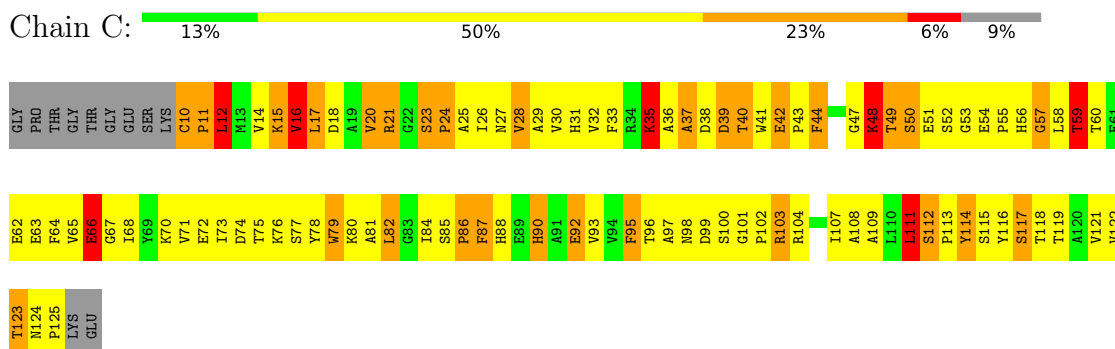
• Molecule 1: TRANSTHYRETIN



• Molecule 1: TRANSTHYRETIN

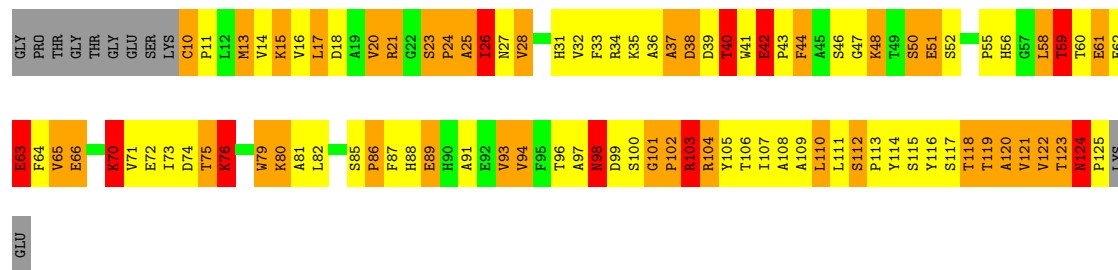


• Molecule 1: TRANSTHYRETIN

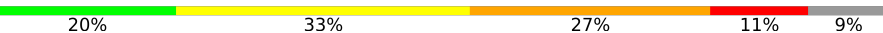


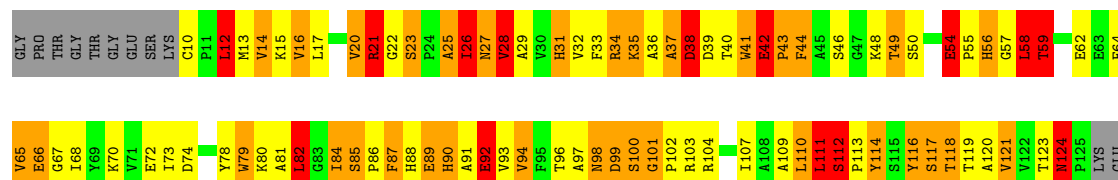
- Molecule 1: TRANSTHYRETIN

Chain D: 

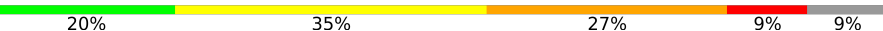


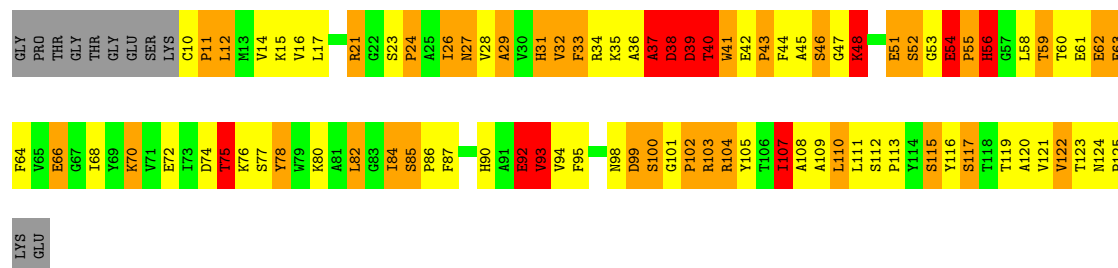
- Molecule 1: TRANSTHYRETIN

Chain E: 



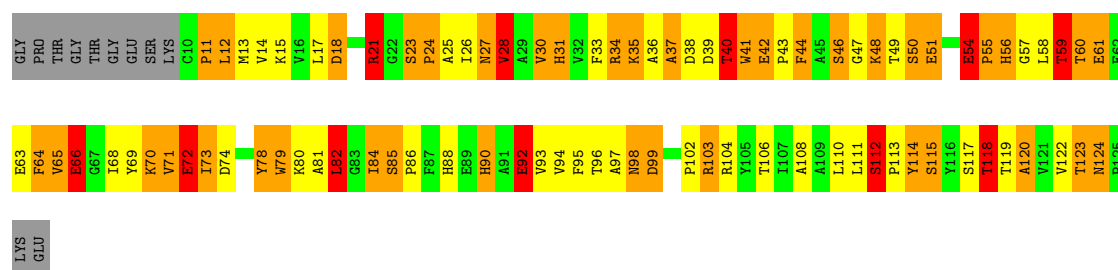
- Molecule 1: TRANSTHYRETIN

Chain F: 

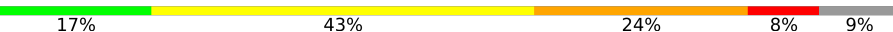


- Molecule 1: TRANSTHYRETIN

Chain G: 



- Molecule 1: TRANSTHYRETIN

Chain H: 

GLY	PRO	THR	GLY	THR	GLY	GLU	SER	LYS	C10	P11		V14	K15	V16	L17	D18	A19	V20	R21	G22	S23	P24	A25	I26	N27	V28	A29	V30	H31	V32	F33	R34	K35	A36	A37	D38	D39	T40	W41	E42	P43	F44	A45	S46	G47	K48	T49	S50	E51	S52	G53	E54	P55	H56	G57	L58	T59	T60	E61
E62	E63	F64	V65	E66	G67	I68	Y69	K70	V71	E72	I73	D74	T75	K76	S77	Y78	W79		S85	P86	F87	H88	E89	H90	A91	E92	V93	V94	F95	T96	A97	N98	D99		P102	R103	R104	Y105		A108	A109	L110	L111	S112	P113	Y114	S115	Y116	S117	T118	T119		V122	T123	N124	P125	LYS	GLU	

4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	149.99Å 78.74Å 98.95Å 90.00° 100.50° 90.00°	Depositor
Resolution (Å)	8.00 – 2.70	Depositor
% Data completeness (in resolution range)	98.0 (8.00-2.70)	Depositor
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	PROLSQ	Depositor
R, R_{free}	0.199 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	7147	wwPDB-VP
Average B, all atoms (Å ²)	31.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

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	1.47	4/920 (0.4%)	3.36	134/1257 (10.7%)
1	B	1.44	4/914 (0.4%)	3.25	151/1249 (12.1%)
1	C	1.71	3/920 (0.3%)	3.40	164/1257 (13.0%)
1	D	1.35	2/916 (0.2%)	3.23	153/1252 (12.2%)
1	E	1.39	3/920 (0.3%)	3.24	137/1257 (10.9%)
1	F	1.31	1/920 (0.1%)	3.21	139/1257 (11.1%)
1	G	1.36	3/916 (0.3%)	4.01	152/1252 (12.1%)
1	H	1.39	3/920 (0.3%)	3.35	142/1257 (11.3%)
All	All	1.43	23/7346 (0.3%)	3.39	1172/10038 (11.7%)

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	C	1	0
1	E	0	1
1	G	0	1
All	All	1	2

The worst 5 of 23 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	125	PRO	CA-C	26.54	2.08	1.52
1	B	123	THR	C-N	17.06	1.68	1.33
1	G	124	ASN	C-N	12.91	1.55	1.34
1	G	39	ASP	C-O	8.43	1.34	1.24
1	F	39	ASP	C-O	7.97	1.34	1.24

The worst 5 of 1172 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	124	ASN	O-C-N	-75.39	25.90	121.64
1	A	21	ARG	CD-NE-CZ	39.60	179.85	124.40
1	H	27	ASN	CA-CB-CG	29.78	142.38	112.60
1	G	35	LYS	CG-CD-CE	28.84	177.63	111.30
1	C	54	GLU	CA-CB-CG	18.93	151.96	114.10

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	C	125	PRO	CA

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	E	124	ASN	Peptide
1	G	124	ASN	Mainchain

5.2 Too-close contacts

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	895	0	865	69	0
1	B	890	0	860	75	0
1	C	895	0	864	52	0
1	D	891	0	861	74	0
1	E	895	0	865	59	0
1	F	895	0	865	52	0
1	G	891	0	860	60	0
1	H	895	0	865	56	0
All	All	7147	0	6905	470	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 34.

The worst 5 of 470 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:D:26:ILE:CD1	1:D:51:GLU:HA	1.24	1.62
1:C:21:ARG:NH2	1:C:82:LEU:HD11	1.29	1.48
1:C:21:ARG:NH2	1:C:82:LEU:CD1	1.82	1.42
1:F:44:PHE:CZ	1:F:59:THR:HG21	1.63	1.33
1:C:44:PHE:CZ	1:C:59:THR:HG21	1.63	1.32

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	114/127 (90%)	107 (94%)	4 (4%)	3 (3%)	4	11
1	B	114/127 (90%)	105 (92%)	5 (4%)	4 (4%)	3	6
1	C	114/127 (90%)	109 (96%)	2 (2%)	3 (3%)	4	11
1	D	114/127 (90%)	108 (95%)	4 (4%)	2 (2%)	6	18
1	E	114/127 (90%)	103 (90%)	8 (7%)	3 (3%)	4	11
1	F	114/127 (90%)	105 (92%)	7 (6%)	2 (2%)	6	18
1	G	114/127 (90%)	106 (93%)	7 (6%)	1 (1%)	14	35
1	H	114/127 (90%)	109 (96%)	3 (3%)	2 (2%)	6	18
All	All	912/1016 (90%)	852 (93%)	40 (4%)	20 (2%)	5	14

5 of 20 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	G	37	ALA
1	H	37	ALA
1	D	39	ASP
1	E	56	HIS
1	F	37	ALA

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	97/105 (92%)	76 (78%)	21 (22%)	1	3
1	B	96/105 (91%)	74 (77%)	22 (23%)	1	2
1	C	97/105 (92%)	77 (79%)	20 (21%)	1	3
1	D	96/105 (91%)	70 (73%)	26 (27%)	0	1
1	E	97/105 (92%)	72 (74%)	25 (26%)	0	2
1	F	97/105 (92%)	73 (75%)	24 (25%)	1	2
1	G	96/105 (91%)	71 (74%)	25 (26%)	0	2
1	H	97/105 (92%)	82 (84%)	15 (16%)	2	7
All	All	773/840 (92%)	595 (77%)	178 (23%)	1	2

5 of 178 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	F	26	ILE
1	G	34	ARG
1	F	43	PRO
1	F	86	PRO
1	G	58	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 13 such sidechains are listed below:

Mol	Chain	Res	Type
1	E	124	ASN
1	F	27	ASN
1	H	88	HIS
1	G	27	ASN
1	G	90	HIS

5.3.3 RNA ⓘ

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 [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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	B	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	123:THR	C	124:ASN	N	1.68

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates [i](#)

EDS was not executed - this section is therefore empty.

6.4 Ligands [i](#)

EDS was not executed - this section is therefore empty.

6.5 Other polymers [i](#)

EDS was not executed - this section is therefore empty.