WORLDWIDE wwPDB PROTEIN DATA BANK

wwPDB X-ray Structure Validation Summary Report (i)

Nov 5, 2023 – 05:59 AM EST

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PDB ID	:	2H79
Title	:	Crystal Structure of human TR alpha bound T3 in orthorhombic space group
Authors	:	Nascimento, A.S.; Dias, S.M.G.; Nunes, F.M.; Aparicio, R.; Bleicher, L.; Ambrosio, A.L.B.; Figueira, A.C.M.; Santos, M.A.M.; Neto, M.O.; Fischer, H.; Togashi, H.F.M.; Craievich, A.F.; Garrat, R.C.; Baxter, J.D.; Webb, P.; Polikarpov, I.
Deposited on	:	2006-06-01
Resolution	:	1.87 Å(reported)

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 1.87 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.
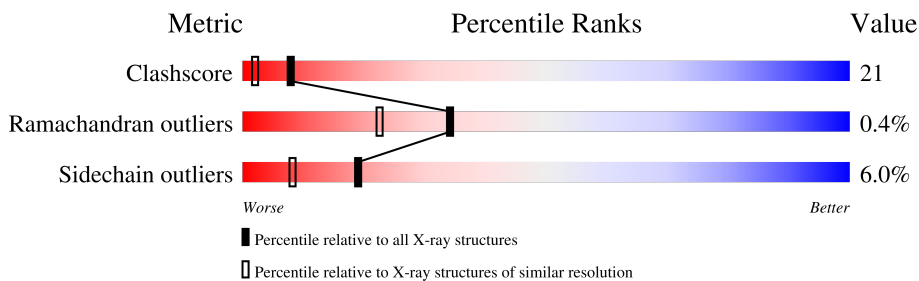
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	10282 (1.90-1.86)
Ramachandran outliers	138981	10152 (1.90-1.86)
Sidechain outliers	138945	10152 (1.90-1.86)

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 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 was not executed.

Mol	Chain	Length	Quality of chain
1	A	269	62% 28% 6% ··

2   Entry composition ⓘ

There are 3 unique types of molecules in this entry. The entry contains 2687 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 THRA protein.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	As	C	N	O	S			
1	A	267	2237	6	1412	373	425	21	20	31	0

There are 11 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	142	ALA	-	cloning artifact	UNP Q6FH41
A	143	ARG	-	cloning artifact	UNP Q6FH41
A	144	GLY	-	cloning artifact	UNP Q6FH41
A	145	SER	-	cloning artifact	UNP Q6FH41
A	146	HIS	-	cloning artifact	UNP Q6FH41
A	147	MET	-	cloning artifact	UNP Q6FH41
A	244	CAS	CYS	modified residue	UNP Q6FH41
A	334	CAS	CYS	modified residue	UNP Q6FH41
A	380	CAS	CYS	modified residue	UNP Q6FH41
A	388	CAS	MET	engineered mutation	UNP Q6FH41
A	392	CAS	CYS	modified residue	UNP Q6FH41

- Molecule 2 is 3,5,3'TRIIODOTHYRONINE (three-letter code: T3) (formula: $C_{15}H_{12}I_3NO_4$).
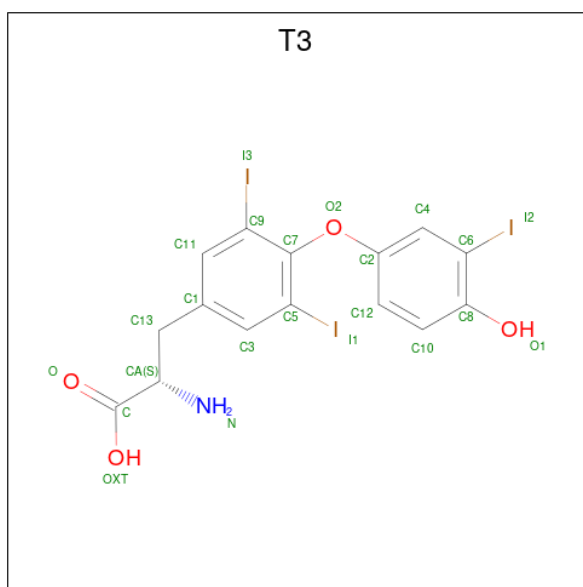
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total 23	C 15	I 3	N 1	O 4	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	427	Total 427	O 427	3	0

3 Residue-property plots ⓘ

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: THRA protein

Chain A:
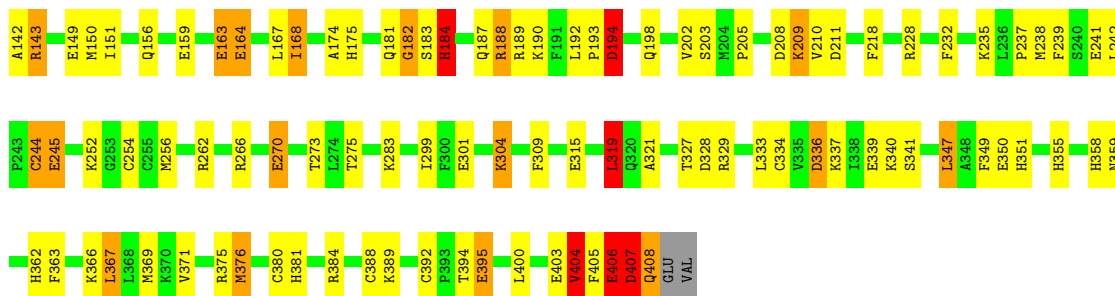
4 Data and refinement statistics ⓘ

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

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	59.98Å 80.80Å 102.21Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	63.25 – 1.87	Depositor
% Data completeness (in resolution range)	98.2 (63.25-1.87)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.149 , 0.187	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	2687	wwPDB-VP
Average B, all atoms (Å^2)	29.0	wwPDB-VP

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: T3, CAS

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	1.81	38/2369 (1.6%)	1.63	42/3187 (1.3%)

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	3

The worst 5 of 38 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	184	HIS	CG-CD2	-16.72	1.07	1.35
1	A	408	GLN	N-CA	13.90	1.74	1.46
1	A	142	ALA	C-N	-12.89	1.04	1.34
1	A	190	LYS	CG-CD	-11.95	1.11	1.52
1	A	245	GLU	CD-OE2	11.28	1.38	1.25

The worst 5 of 42 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	408	GLN	CB-CG-CD	22.57	170.28	111.60
1	A	142	ALA	O-C-N	16.53	149.15	122.70
1	A	142	ALA	CA-C-N	-15.49	83.12	117.20
1	A	304	LYS	CD-CE-NZ	12.28	139.94	111.70
1	A	190	LYS	CB-CG-CD	12.03	142.88	111.60

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	184	HIS	Sidechain
1	A	406[A]	GLU	Peptide
1	A	407[B]	ASP	Peptide

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	2237	0	2162	95	1
2	A	23	0	6	3	0
3	A	427	0	0	57	4
All	All	2687	0	2168	96	4

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 21.

The worst 5 of 96 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:304:LYS:CE	1:A:304:LYS:NZ	1.75	1.48
1:A:256:MET:CE	1:A:256:MET:SD	2.02	1.47
1:A:376[B]:MET:HE3	3:A:634:HOH:O	1.08	1.25
1:A:355:HIS:CE1	3:A:799:HOH:O	1.86	1.22
1:A:333[B]:LEU:HD11	3:A:580:HOH:O	1.03	1.19

All (4) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:765:HOH:O	3:A:782:HOH:O[3_655]	1.75	0.45
1:A:244[A]:CAS:CE1	3:A:799:HOH:O[4_555]	1.94	0.26
3:A:712:HOH:O	3:A:830:HOH:O[4_455]	2.12	0.08
3:A:518:HOH:O	3:A:789:HOH:O[4_455]	2.17	0.03

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	290/269 (108%)	283 (98%)	6 (2%)	1 (0%)	41	30

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	182	GLY

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	262/234 (112%)	246 (94%)	16 (6%)	18	8

5 of 16 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	404[B]	VAL
1	A	404[A]	VAL
1	A	319	LEU
1	A	395[B]	GLU
1	A	270	GLU

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	175	HIS
1	A	351	HIS
1	A	358	HIS
1	A	381	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

6 non-standard protein/DNA/RNA residues 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	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#|Z| > 2$	Counts	RMSZ	$\#|Z| > 2$
1	CAS	A	388	1	5,8,9	1.28	1 (20%)	1,9,11	4.50	1 (100%)
1	CAS	A	244[A]	-	5,8,9	2.14	2 (40%)	1,9,11	0.20	0
1	CAS	A	334	1	5,8,9	7.31	2 (40%)	1,9,11	2.35	1 (100%)
1	CAS	A	380	1	5,8,9	1.52	1 (20%)	1,9,11	1.00	0
1	CAS	A	392	1	5,8,9	2.36	1 (20%)	1,9,11	2.08	1 (100%)
1	CAS	A	244[B]	-	5,8,9	1.92	1 (20%)	1,9,11	0.11	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
1	CAS	A	388	1	-	0/0/7/9	-
1	CAS	A	244[A]	-	-	0/0/7/9	-
1	CAS	A	334	1	-	0/0/7/9	-
1	CAS	A	380	1	-	0/0/7/9	-
1	CAS	A	392	1	-	0/0/7/9	-
1	CAS	A	244[B]	-	-	0/0/7/9	-

The worst 5 of 8 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	334	CAS	AS-CE1	-15.95	1.54	1.96
1	A	392	CAS	AS-CE1	-4.57	1.84	1.96
1	A	244[A]	CAS	CB-CA	3.91	1.62	1.53
1	A	244[B]	CAS	CB-CA	3.91	1.62	1.53
1	A	334	CAS	AS-CE2	3.46	2.05	1.96

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	388	CAS	CA-CB-SG	-4.50	95.50	114.43
1	A	334	CAS	CA-CB-SG	-2.35	104.56	114.43
1	A	392	CAS	CA-CB-SG	-2.08	105.67	114.43

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	244[A]	CAS	0	1
1	A	244[B]	CAS	1	0

5.5   Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6   Ligand geometry ⓘ

1 ligand is 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	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
2	T3	A	1	-	23,24,24	1.65	4 (17%)	33,34,34	1.43	6 (18%)

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	T3	A	1	-	-	3/12/12/12	0/2/2/2

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1	T3	C8-C6	4.18	1.48	1.39
2	A	1	T3	C9-I3	3.74	2.18	2.10
2	A	1	T3	C12-C10	2.14	1.42	1.38
2	A	1	T3	C4-C6	2.03	1.43	1.39

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1	T3	C12-C2-C4	3.87	125.86	120.53
2	A	1	T3	C2-O2-C7	3.58	124.24	118.48
2	A	1	T3	O1-C8-C6	-2.98	115.58	119.19
2	A	1	T3	C13-C1-C3	-2.74	115.73	120.44
2	A	1	T3	C11-C1-C3	2.24	122.06	118.98

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1	T3	C3-C1-C13-CA
2	A	1	T3	OXT-C-CA-C13
2	A	1	T3	C11-C1-C13-CA

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1	T3	3	0

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.
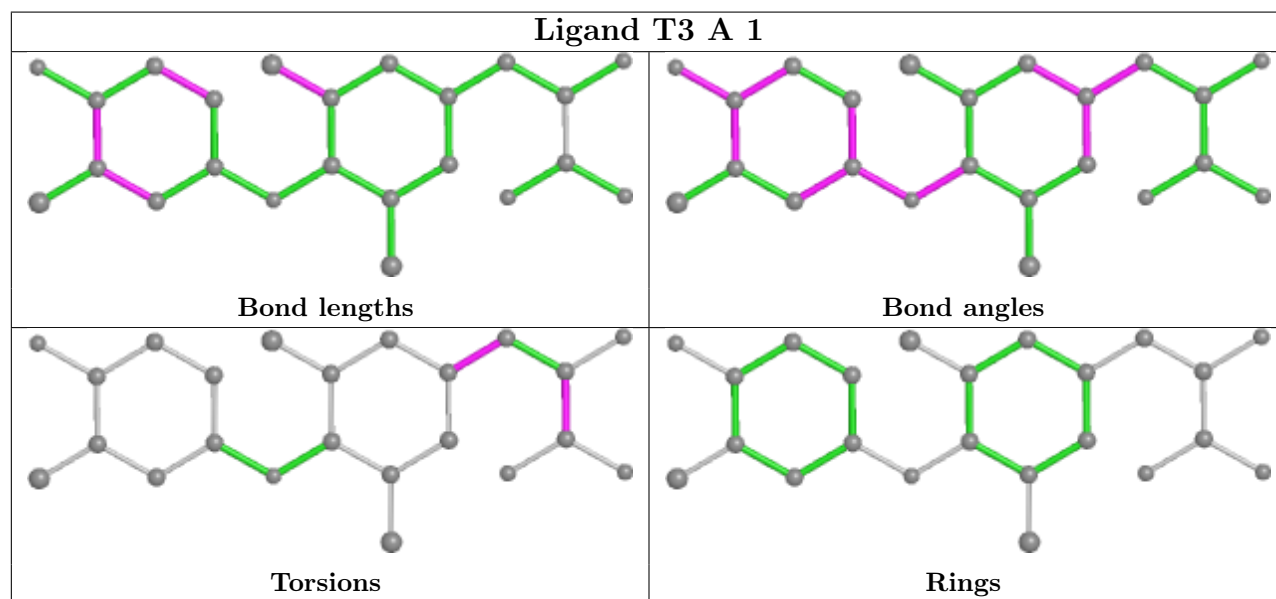
5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	142:ALA	C	143:ARG	N	1.04

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates ⓘ

EDS was not executed - this section is therefore empty.

6.4 Ligands ⓘ

EDS was not executed - this section is therefore empty.

6.5 Other polymers ⓘ

EDS was not executed - this section is therefore empty.