



# Full wwPDB X-ray Structure Validation Report ⓘ

May 16, 2020 – 06:38 pm BST

PDB ID : 1XZX  
Title : Thyroxine-Thyroid Hormone Receptor Interactions  
Authors : Sandler, B.; Webb, P.; Apriletti, J.W.; Huber, B.R.; Togashi, M.; Cunha Lima, S.T.; Juric, S.; Nilsson, S.; Wagner, R.; Fletterick, R.J.; Baxter, J.D.  
Deposited on : 2004-11-12  
Resolution : 2.50 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](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.

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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 : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.11

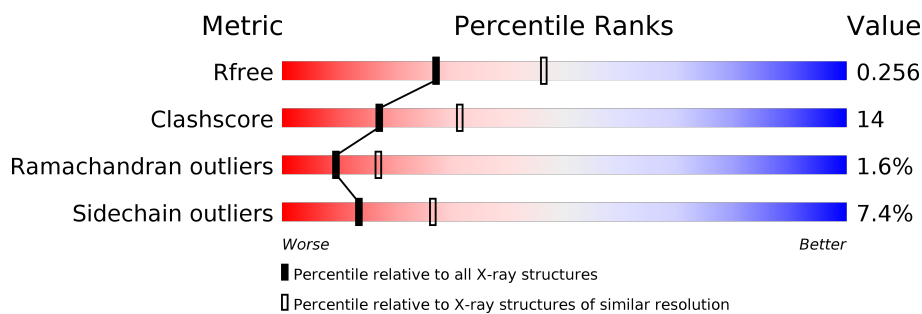
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.50 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))
$R_{free}$	130704	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)

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  $\geq 3$ , 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  $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	X	281	

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 2011 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 Thyroid hormone receptor beta-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	X	249	1916	1231	323	346	16	0	0	0

There are 21 discrepancies between the modelled and reference sequences:

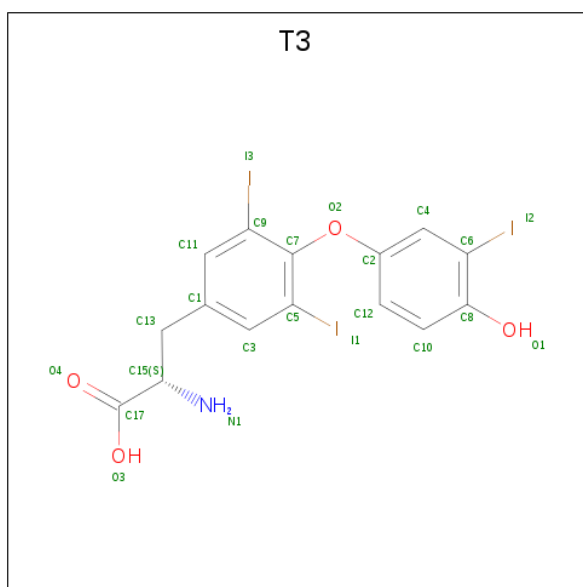
Chain	Residue	Modelled	Actual	Comment	Reference
X	181	MET	-	EXPRESSION TAG	UNP P10828
X	182	GLY	-	EXPRESSION TAG	UNP P10828
X	183	SER	-	EXPRESSION TAG	UNP P10828
X	184	SER	-	EXPRESSION TAG	UNP P10828
X	185	HIS	-	EXPRESSION TAG	UNP P10828
X	186	HIS	-	EXPRESSION TAG	UNP P10828
X	187	HIS	-	EXPRESSION TAG	UNP P10828
X	188	HIS	-	EXPRESSION TAG	UNP P10828
X	189	HIS	-	EXPRESSION TAG	UNP P10828
X	190	HIS	-	EXPRESSION TAG	UNP P10828
X	191	SER	-	EXPRESSION TAG	UNP P10828
X	192	SER	-	EXPRESSION TAG	UNP P10828
X	193	GLY	-	EXPRESSION TAG	UNP P10828
X	194	LEU	-	EXPRESSION TAG	UNP P10828
X	195	VAL	-	EXPRESSION TAG	UNP P10828
X	196	PRO	-	EXPRESSION TAG	UNP P10828
X	197	ARG	-	EXPRESSION TAG	UNP P10828
X	198	GLY	-	EXPRESSION TAG	UNP P10828
X	199	SER	-	EXPRESSION TAG	UNP P10828
X	200	HIS	-	EXPRESSION TAG	UNP P10828
X	201	MET	-	EXPRESSION TAG	UNP P10828

- Molecule 2 is CACODYLATE ION (three-letter code: CAC) (formula:  $C_2H_6AsO_2$ ).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	X	1	Total 1	As 1	0	0
2	X	1	Total 1	As 1	0	0
2	X	1	Total 1	As 1	0	0
2	X	1	Total 1	As 1	0	0
2	X	1	Total 1	As 1	0	0
2	X	1	Total 1	As 1	0	0

- Molecule 3 is 3,5,3'-TRIIODOTHYRONINE (three-letter code: T3) (formula:  $C_{15}H_{12}I_3NO_4$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	X	1	Total	C	I	N	O	0	0
			23	15	3	1	4		

- Molecule 4 is water.

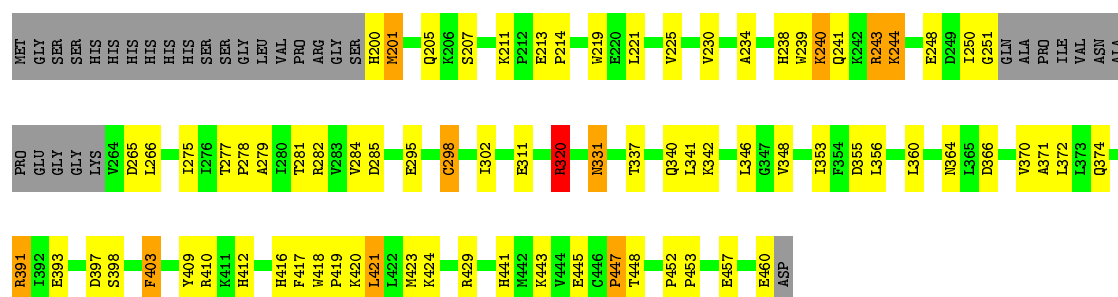
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	X	66	Total	O	0	0
			66	66		

### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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.

- Molecule 1: Thyroid hormone receptor beta-1

Chain X: 



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	68.76 Å 68.76 Å 130.94 Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	19.84 – 2.50 19.85 – 2.30	Depositor EDS
% Data completeness (in resolution range)	100.0 (19.84-2.50) 99.8 (19.85-2.30)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.09	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.84 (at 2.30 Å)	Xtriage
Refinement program	REFMAC	Depositor
R, $R_{free}$	0.185 , 0.244 0.198 , 0.256	Depositor DCC
$R_{free}$ test set	1648 reflections (9.99%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	43.8	Xtriage
Anisotropy	0.209	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 40.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.028 for -h,-k,l	Xtriage
$F_o, F_c$ correlation	0.89	EDS
Total number of atoms	2011	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	49.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.13% 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 [i](#)

### 5.1 Standard geometry [i](#)

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

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	X	1.41	6/1959 (0.3%)	1.24	14/2659 (0.5%)

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	X	0	2

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	X	409	TYR	CD1-CE1	6.79	1.49	1.39
1	X	248	GLU	CG-CD	6.44	1.61	1.51
1	X	342	LYS	CE-NZ	6.25	1.64	1.49
1	X	311	GLU	CD-OE2	6.15	1.32	1.25
1	X	284	VAL	CB-CG2	5.50	1.64	1.52
1	X	348	VAL	CB-CG2	-5.09	1.42	1.52

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	320	ARG	NE-CZ-NH2	-8.31	116.14	120.30
1	X	285	ASP	CB-CG-OD2	7.97	125.47	118.30
1	X	282	ARG	NE-CZ-NH2	-7.69	116.46	120.30
1	X	366	ASP	CB-CG-OD1	7.31	124.88	118.30
1	X	320	ARG	NE-CZ-NH1	5.94	123.27	120.30
1	X	355	ASP	CB-CG-OD2	5.92	123.63	118.30
1	X	265	ASP	CB-CG-OD2	5.87	123.58	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	429	ARG	NE-CZ-NH1	5.81	123.20	120.30
1	X	410	ARG	NE-CZ-NH1	5.42	123.01	120.30
1	X	282	ARG	NE-CZ-NH1	5.42	123.01	120.30
1	X	397	ASP	CB-CG-OD2	5.34	123.10	118.30
1	X	251	GLY	CA-C-O	-5.26	111.12	120.60
1	X	366	ASP	OD1-CG-OD2	-5.22	113.38	123.30
1	X	391	ARG	NE-CZ-NH2	-5.04	117.78	120.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	X	250	ILE	Peptide
1	X	447	PRO	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	X	1916	0	1866	51	0
2	X	6	0	0	1	0
3	X	23	0	10	3	0
4	X	66	0	0	20	0
All	All	2011	0	1876	51	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 14.

All (51) 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:X:201:MET:O	4:X:15:HOH:O	1.83	0.96
1:X:298:CYS:HB2	2:X:503:CAC:AS	2.35	0.85
1:X:279:ALA:HB2	1:X:331:ASN:OD1	1.84	0.76
1:X:460:GLU:CB	4:X:46:HOH:O	2.33	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:460:GLU:HA	4:X:46:HOH:O	1.87	0.73
1:X:416:HIS:O	1:X:420:LYS:HG3	1.89	0.72
1:X:460:GLU:CA	4:X:46:HOH:O	2.40	0.67
1:X:353:ILE:HD13	3:X:500:T3:I3	2.64	0.67
1:X:201:MET:CB	4:X:24:HOH:O	2.42	0.66
1:X:443:LYS:NZ	1:X:448:THR:HG23	2.14	0.62
1:X:277:THR:O	1:X:281:THR:HG23	2.01	0.61
1:X:239:TRP:CD2	1:X:320:ARG:HD2	2.37	0.60
1:X:418:TRP:HB3	1:X:419:PRO:HD3	1.84	0.60
1:X:337:THR:OG1	1:X:340:GLN:HG3	2.03	0.59
1:X:412:HIS:CD2	1:X:417:PHE:CE2	2.92	0.58
1:X:205:GLN:HB2	4:X:15:HOH:O	2.04	0.57
1:X:393:GLU:CB	4:X:65:HOH:O	2.56	0.54
1:X:443:LYS:HE2	4:X:25:HOH:O	2.06	0.54
1:X:417:PHE:CE2	1:X:421:LEU:HD22	2.42	0.54
1:X:341:LEU:HD11	1:X:346:LEU:HD12	1.90	0.53
1:X:205:GLN:CB	4:X:15:HOH:O	2.57	0.52
1:X:364:ASN:OD1	4:X:29:HOH:O	2.19	0.52
1:X:277:THR:OG1	4:X:51:HOH:O	2.19	0.51
1:X:205:GLN:CG	4:X:15:HOH:O	2.60	0.50
1:X:420:LYS:HA	1:X:423:MET:CE	2.42	0.50
1:X:214:PRO:HB2	1:X:219:TRP:NE1	2.26	0.49
1:X:275:ILE:HG13	3:X:500:T3:I1	2.83	0.49
1:X:205:GLN:HG3	4:X:15:HOH:O	2.12	0.49
1:X:225:VAL:HG12	1:X:371:ALA:HB1	1.95	0.49
1:X:353:ILE:CD1	3:X:500:T3:I3	3.30	0.48
1:X:200:HIS:O	1:X:201:MET:CB	2.61	0.47
1:X:453:PRO:O	1:X:457:GLU:HG3	2.15	0.47
1:X:372:LEU:O	4:X:63:HOH:O	2.20	0.46
1:X:230:VAL:O	4:X:56:HOH:O	2.21	0.46
1:X:452:PRO:HA	1:X:453:PRO:HD3	1.85	0.46
1:X:372:LEU:HD13	1:X:403:PHE:HA	1.98	0.45
1:X:364:ASN:HB3	4:X:55:HOH:O	2.17	0.45
1:X:238:HIS:CD2	4:X:66:HOH:O	2.70	0.45
1:X:372:LEU:HB3	4:X:63:HOH:O	2.16	0.45
1:X:200:HIS:CB	4:X:50:HOH:O	2.65	0.44
1:X:221:LEU:O	1:X:225:VAL:HG23	2.18	0.44
1:X:277:THR:N	1:X:278:PRO:HD2	2.33	0.44
1:X:213:GLU:HB3	1:X:214:PRO:CD	2.48	0.43
1:X:211:LYS:HD2	1:X:211:LYS:HA	1.86	0.43
1:X:370:VAL:O	1:X:374:GLN:HG3	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:360:LEU:HD23	1:X:360:LEU:HA	1.78	0.42
1:X:441:HIS:HB3	4:X:27:HOH:O	2.20	0.42
1:X:244:LYS:O	1:X:244:LYS:HG3	2.19	0.41
1:X:240:LYS:HD2	1:X:243:ARG:NH2	2.35	0.41
1:X:420:LYS:HA	1:X:423:MET:HE3	2.00	0.41
1:X:356:LEU:HD11	1:X:424:LYS:HD2	2.03	0.40

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	X	245/281 (87%)	232 (95%)	9 (4%)	4 (2%)	9	17

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	X	445	GLU
1	X	447	PRO
1	X	201	MET
1	X	234	ALA

### 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	X	203/246 (82%)	188 (93%)	15 (7%)	13	27

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	X	207	SER
1	X	240	LYS
1	X	241	GLN
1	X	243	ARG
1	X	244	LYS
1	X	266	LEU
1	X	295	GLU
1	X	298	CYS
1	X	302	ILE
1	X	320	ARG
1	X	331	ASN
1	X	391	ARG
1	X	398	SER
1	X	403	PHE
1	X	421	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	X	235	GLN
1	X	241	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry

Of 7 ligands modelled in this entry, 6 are modelled with single atom - leaving 1 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	T3	X	500	-	21,24,24	1.73	5 (23%)	29,34,34	1.95	11 (37%)

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	T3	X	500	-	-	1/8/12/12	0/2/2/2

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	X	500	T3	O2-C7	-4.25	1.30	1.39
3	X	500	T3	C10-C8	-2.74	1.34	1.39
3	X	500	T3	O1-C8	-2.42	1.31	1.36
3	X	500	T3	C5-I1	2.32	2.15	2.10
3	X	500	T3	C8-C6	2.10	1.43	1.39

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	X	500	T3	C8-C6-I2	-5.24	114.60	119.81
3	X	500	T3	C10-C8-C6	-3.55	115.90	119.27
3	X	500	T3	C11-C9-C7	-3.12	115.26	121.59
3	X	500	T3	C11-C9-I3	2.61	123.43	118.61
3	X	500	T3	C3-C5-I1	2.52	123.27	118.61
3	X	500	T3	C4-C6-I2	2.23	122.72	118.61
3	X	500	T3	C11-C1-C3	2.16	121.95	118.98
3	X	500	T3	O1-C8-C10	2.11	125.08	119.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	X	500	T3	C3-C5-C7	-2.10	117.33	121.59
3	X	500	T3	C10-C12-C2	2.08	122.27	119.73
3	X	500	T3	C13-C15-C17	-2.05	107.37	110.69

There are no chirality outliers.

All (1) torsion outliers are listed below:

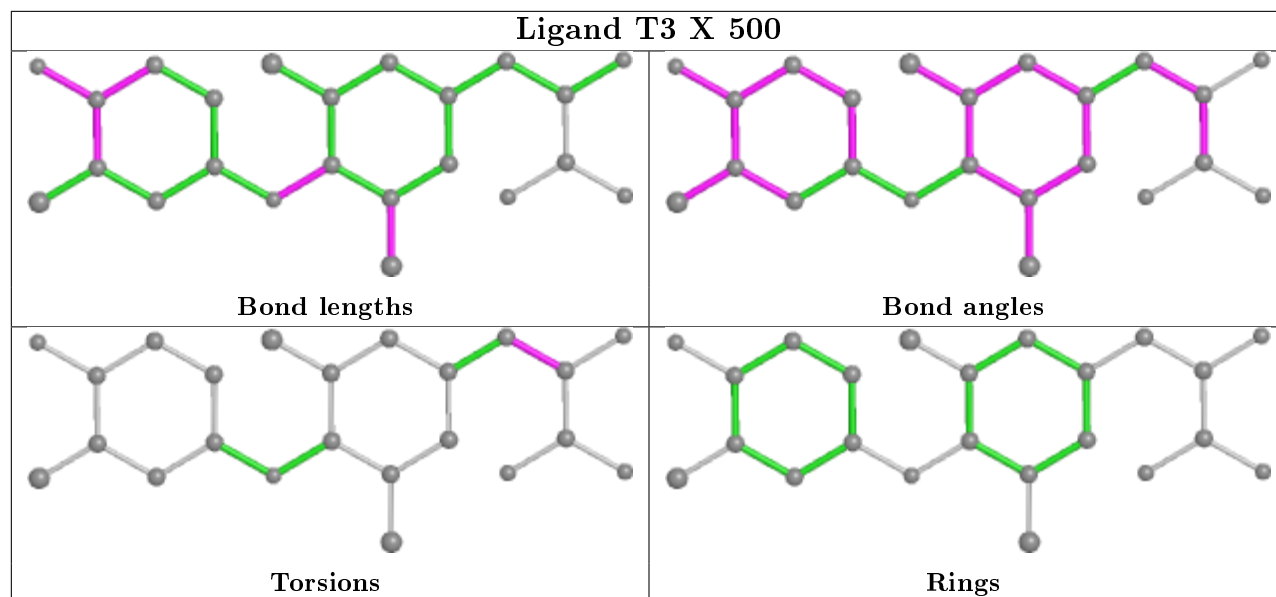
Mol	Chain	Res	Type	Atoms
3	X	500	T3	C1-C13-C15-N1

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	X	500	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 than 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](#)

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

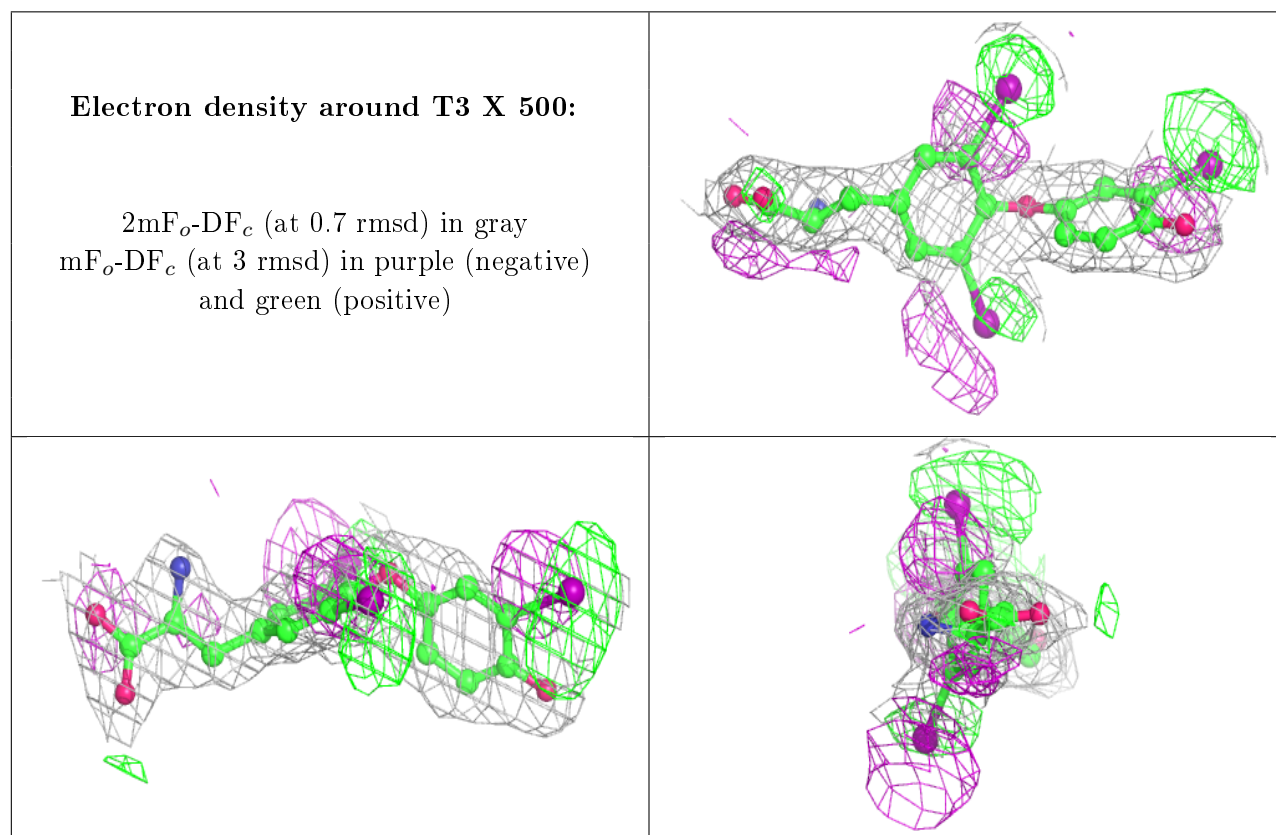
### 6.3 Carbohydrates [i](#)

Unable to reproduce the depositors R factor - this section is therefore empty.

### 6.4 Ligands [i](#)

Unable to reproduce the depositors R factor - this section is therefore empty.

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.





## 6.5 Other polymers

Unable to reproduce the depositors R factor - this section is therefore empty.