Full wwPDB X-ray Structure Validation Report (i)

Nov 4, 2023 – 11:49 PM EDT

PDB ID	:	1F86
Title	:	TRANSTHYRETIN THR119MET PROTEIN STABILISATION
Authors	:	Sebastiao, M.P.
Deposited on	:	2000-06-29
Resolution	:	1.10 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 (i)) were used in the production of this report:

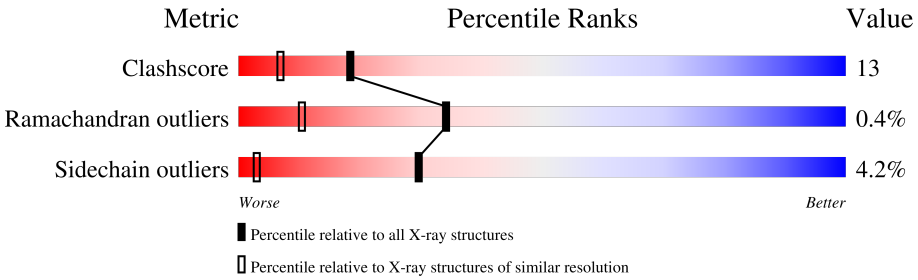
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.10 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	1671 (1.14-1.06)
Ramachandran outliers	138981	1615 (1.14-1.06)
Sidechain outliers	138945	1613 (1.14-1.06)

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%

Mol	Chain	Length	Quality of chain
1	A	115	73% 23% .
1	B	115	72% 25% .

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 2182 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.

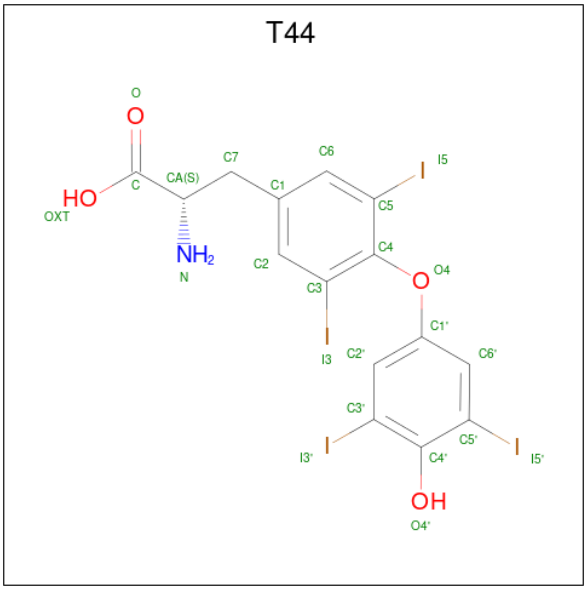
- Molecule 1 is a protein called TRANSTHYRETIN THR119MET VARIANT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	115	Total	C	N	O	S	0	23	0
			961	612	149	194	6			
1	B	115	Total	C	N	O	S	1	11	0
			932	597	147	184	4			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	119	MET	THR	engineered mutation	UNP P02766
B	119	MET	THR	engineered mutation	UNP P02766

- Molecule 2 is 3,5,3',5'-TETRAIODO-L-THYRONINE (three-letter code: T44) (formula: $C_{15}H_{11}I_4NO_4$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	I	O	0	0
			19	13	4	2		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	1	Total C I O 19 13 4 2	0	0

- Molecule 3 is water.

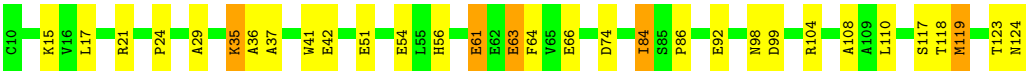
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	139	Total O 139 139	0	0
3	B	112	Total O 112 112	0	0

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.

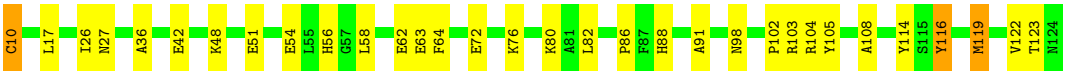
• Molecule 1: TRANSTHYRETIN THR119MET VARIANT

Chain A:



• Molecule 1: TRANSTHYRETIN THR119MET VARIANT

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α, β, γ	42.68Å 85.77Å 63.69Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	5.00 – 1.10 5.00 – 1.10	Depositor EDS
% Data completeness (in resolution range)	(Not available) (5.00-1.10) 85.1 (5.00-1.10)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.86 (at 1.10Å)	Xtriage
Refinement program	SHELXL-97	Depositor
R, R_{free}	0.147 , 0.177 0.209 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å^2)	11.2	Xtriage
Anisotropy	0.097	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	1.10 , 107.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	2182	wwPDB-VP
Average B, all atoms (Å^2)	20.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows:

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: T44

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	0.80	0/1092	1.44	13/1485 (0.9%)
1	B	0.76	0/1000	1.43	16/1362 (1.2%)
All	All	0.78	0/2092	1.44	29/2847 (1.0%)

There are no bond length outliers.

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	123	THR	C-N-CA	11.50	150.46	121.70
1	A	63[A]	GLU	OE1-CD-OE2	10.10	135.42	123.30
1	A	63[B]	GLU	OE1-CD-OE2	10.10	135.42	123.30
1	A	64	PHE	CB-CG-CD2	-8.02	115.18	120.80
1	B	64	PHE	CB-CG-CD1	7.83	126.28	120.80
1	A	119[A]	MET	CB-CA-C	7.05	124.49	110.40
1	A	119[B]	MET	CB-CA-C	7.05	124.49	110.40
1	A	119[A]	MET	CG-SD-CE	-6.83	89.28	100.20
1	A	119[B]	MET	CG-SD-CE	-6.83	89.28	100.20
1	A	119[A]	MET	CA-CB-CG	-6.56	102.16	113.30
1	A	119[B]	MET	CA-CB-CG	-6.56	102.16	113.30
1	B	116[A]	TYR	N-CA-CB	6.41	122.13	110.60
1	B	116[B]	TYR	N-CA-CB	6.41	122.13	110.60
1	B	114	TYR	CB-CG-CD1	-6.40	117.16	121.00
1	A	63[A]	GLU	CA-CB-CG	-6.33	99.48	113.40
1	A	63[B]	GLU	CA-CB-CG	-6.33	99.48	113.40
1	B	98	ASN	C-N-CA	-6.04	106.61	121.70
1	A	84	ILE	CB-CA-C	-5.65	100.30	111.60
1	B	116[A]	TYR	CZ-CE2-CD2	-5.62	114.74	119.80
1	B	116[B]	TYR	CZ-CE2-CD2	-5.62	114.74	119.80
1	B	116[A]	TYR	CG-CD1-CE1	-5.52	116.88	121.30
1	B	116[B]	TYR	CG-CD1-CE1	-5.52	116.88	121.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	64	PHE	CB-CG-CD1	5.46	124.62	120.80
1	B	105	TYR	CB-CG-CD2	5.46	124.28	121.00
1	B	114	TYR	CB-CG-CD2	5.30	124.18	121.00
1	B	116[A]	TYR	CB-CG-CD1	-5.26	117.84	121.00
1	B	116[B]	TYR	CB-CG-CD1	-5.26	117.84	121.00
1	B	10	CYS	CA-C-O	5.24	131.11	120.10
1	B	105	TYR	CB-CG-CD1	-5.09	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	961	0	933	32	0
1	B	932	0	894	19	0
2	A	19	0	4	5	0
2	B	19	0	4	5	0
3	A	139	0	0	8	0
3	B	112	0	0	6	0
All	All	2182	0	1835	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 13.

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:A:17[B]:LEU:HD11	2:A:428:T44:I3	2.05	1.26
1:B:17[A]:LEU:HD21	2:B:528:T44:I3	2.13	1.17
1:A:110[B]:LEU:HG	2:A:428:T44:I5'	2.18	1.13
1:B:17[B]:LEU:HD11	2:B:528:T44:I3	2.28	1.03
1:A:17[B]:LEU:CD1	2:A:428:T44:I3	2.83	0.96
1:B:17[B]:LEU:CD1	2:B:528:T44:I3	2.96	0.83
1:B:17[A]:LEU:CD2	2:B:528:T44:I3	2.98	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:92:GLU:HG2	3:B:594:HOH:O	1.87	0.75
1:A:36:ALA:HB2	1:A:42:GLU:HG3	1.68	0.75
1:B:102:PRO:HB2	1:B:122:VAL:HG12	1.67	0.75
1:A:61[A]:GLU:HG2	3:A:518:HOH:O	1.87	0.74
1:B:72[A]:GLU:HG2	3:B:574:HOH:O	1.88	0.74
1:A:118[B]:THR:HG23	3:B:559:HOH:O	1.89	0.72
1:B:26:ILE:HD13	1:B:51:GLU:OE2	1.89	0.72
1:B:62:GLU:OE2	1:B:63[A]:GLU:HG3	1.94	0.67
1:A:37:ALA:HB3	3:A:536:HOH:O	1.94	0.67
1:A:110[B]:LEU:CG	2:A:428:T44:I5'	3.08	0.64
1:B:76:LYS:HG2	1:B:80:LYS:HD3	1.82	0.62
1:B:27[A]:ASN:OD1	1:B:48:LYS:HE3	2.00	0.61
1:A:29:ALA:HB3	1:A:74[B]:ASP:OD1	2.04	0.58
1:B:104:ARG:HG2	3:B:535:HOH:O	2.04	0.58
1:B:88:HIS:HD2	3:B:533:HOH:O	1.85	0.57
1:A:104:ARG:HB2	1:A:123[A]:THR:HG23	1.89	0.54
1:A:63[A]:GLU:HG3	3:A:502:HOH:O	2.08	0.54
1:A:66[A]:GLU:OE1	1:A:99[A]:ASP:OD1	2.29	0.51
1:A:54:GLU:OE1	1:A:56:HIS:HE1	1.94	0.51
1:A:66[A]:GLU:HG2	1:A:98:ASN:O	2.11	0.51
1:B:91:ALA:HB1	1:B:116[B]:TYR:CZ	2.47	0.50
1:A:110[B]:LEU:HB2	1:A:117[B]:SER:OG	2.11	0.49
1:A:61[B]:GLU:HB3	3:A:467:HOH:O	2.12	0.49
1:A:36:ALA:HB2	1:A:42:GLU:CG	2.40	0.48
1:B:36:ALA:HB2	1:B:42:GLU:HG3	1.96	0.46
1:A:21:ARG:NH1	3:A:545:HOH:O	2.49	0.46
1:A:35[A]:LYS:HG2	1:A:41:TRP:CZ3	2.52	0.45
1:A:108:ALA:HB1	2:A:428:T44:H6'	1.99	0.45
1:B:119[A]:MET:HE3	1:B:119[A]:MET:HB2	1.67	0.45
1:A:15[A]:LYS:HD3	1:A:54:GLU:HG2	1.99	0.45
1:A:21:ARG:HH21	1:A:21:ARG:HG3	1.82	0.45
1:B:108:ALA:HB1	2:B:528:T44:H6'	1.99	0.43
1:A:15[A]:LYS:HD3	1:A:54:GLU:CG	2.48	0.43
1:B:58:LEU:HD12	3:B:569:HOH:O	2.17	0.43
1:A:51:GLU:HG2	3:A:493:HOH:O	2.17	0.43
1:A:35[B]:LYS:HE3	1:A:35[B]:LYS:HB2	1.69	0.43
1:B:54:GLU:OE1	1:B:56:HIS:HE1	2.02	0.41
1:A:17[B]:LEU:HD23	1:A:24:PRO:HA	2.03	0.41
1:A:63[B]:GLU:HG3	3:A:543:HOH:O	2.20	0.41
1:B:82:LEU:HA	1:B:82:LEU:HD23	1.86	0.40
1:A:84:ILE:HA	1:A:84:ILE:HD13	1.85	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:123[A]:THR:HG22	3:A:452:HOH:O	2.21	0.40
1:A:21:ARG:HG3	1:A:21:ARG:NH2	2.37	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	A	136/115 (118%)	134 (98%)	2 (2%)	0	100 100
1	B	124/115 (108%)	121 (98%)	2 (2%)	1 (1%)	19 3
All	All	260/230 (113%)	255 (98%)	4 (2%)	1 (0%)	34 10

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	86	PRO

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	120/96 (125%)	112 (93%)	8 (7%)	16 1
1	B	107/96 (112%)	103 (96%)	4 (4%)	34 4
All	All	227/192 (118%)	215 (95%)	12 (5%)	30 2

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	35[A]	LYS
1	A	35[B]	LYS
1	A	61[A]	GLU
1	A	61[B]	GLU
1	A	86	PRO
1	A	119[A]	MET
1	A	119[B]	MET
1	A	124	ASN
1	B	10	CYS
1	B	103	ARG
1	B	119[A]	MET
1	B	119[B]	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	56	HIS
1	A	90	HIS
1	A	124	ASN
1	B	56	HIS
1	B	88	HIS

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	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	T44	A	428	1	20,20,25	1.12	2 (10%)	29,29,36	2.03	8 (27%)
2	T44	B	528	-	20,20,25	1.17	1 (5%)	29,29,36	2.00	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
2	T44	A	428	1	-	0/4/4/12	0/2/2/2
2	T44	B	528	-	-	0/4/4/12	0/2/2/2

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	528	T44	C2'-C1'	-3.36	1.33	1.38
2	A	428	T44	C2'-C1'	-3.09	1.33	1.38
2	A	428	T44	C6'-C1'	2.03	1.42	1.38

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	528	T44	C1'-O4-C4	5.59	127.48	118.48
2	A	428	T44	C1'-O4-C4	-5.07	110.32	118.48
2	A	428	T44	O4-C1'-C2'	4.41	132.95	119.10
2	A	428	T44	O4-C1'-C6'	-4.31	105.58	119.10
2	B	528	T44	C2'-C3'-I3'	-3.32	112.49	118.61
2	A	428	T44	C4-C5-I5	3.07	124.66	119.42
2	B	528	T44	C7-C1-C6	-2.86	116.71	120.94
2	B	528	T44	C7-C1-C2	2.82	125.11	120.94
2	A	428	T44	O4'-C4'-C5'	2.64	127.04	120.33
2	A	428	T44	C6-C5-I5	-2.57	113.87	118.61
2	B	528	T44	C6'-C5'-I5'	2.54	123.29	118.61
2	B	528	T44	C4'-C3'-I3'	2.53	123.32	119.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	528	T44	O4-C4-C5	-2.39	116.43	120.28
2	B	528	T44	O4-C4-C3	2.21	123.85	120.28
2	B	528	T44	C4-C5-I5	2.19	123.16	119.42
2	A	428	T44	O4-C4-C5	2.13	123.72	120.28
2	B	528	T44	C6'-C1'-C2'	2.12	124.36	120.98
2	A	428	T44	C6'-C5'-I5'	2.07	122.43	118.61
2	B	528	T44	C2-C3-I3	2.05	122.39	118.61

There are no chirality outliers.

There are no torsion outliers.

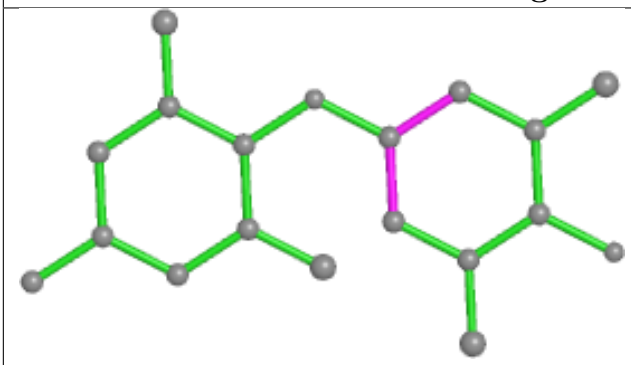
There are no ring outliers.

2 monomers are involved in 10 short contacts:

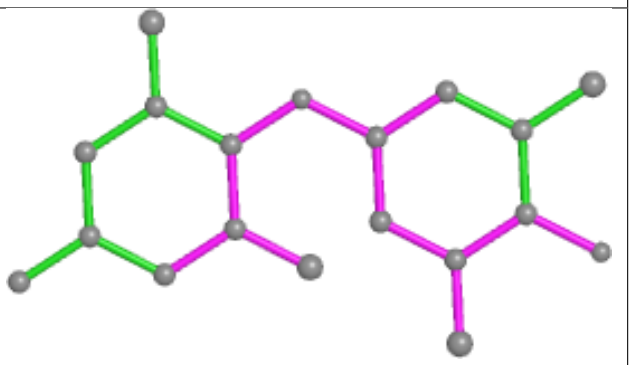
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	428	T44	5	0
2	B	528	T44	5	0

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.

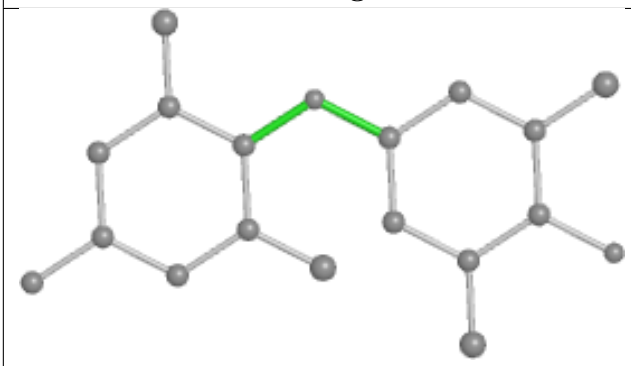
Ligand T44 A 428



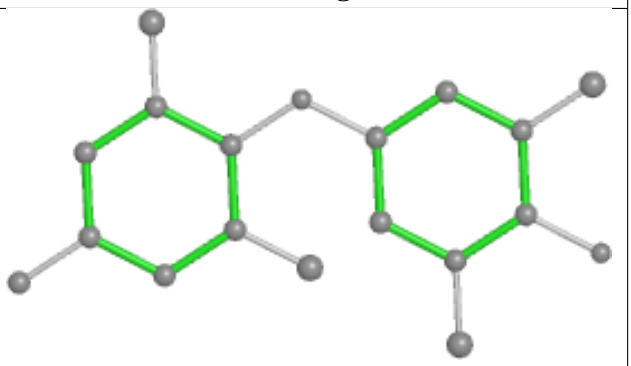
Bond lengths



Bond angles

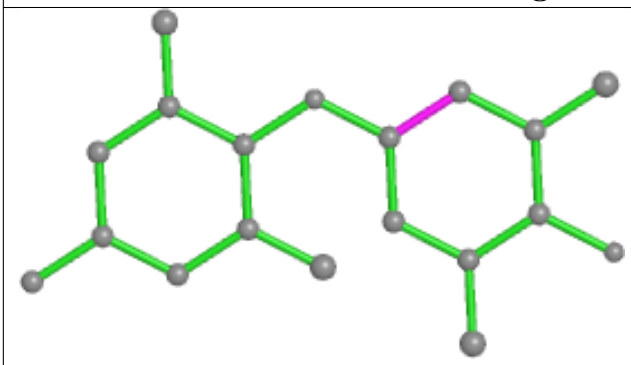


Torsions

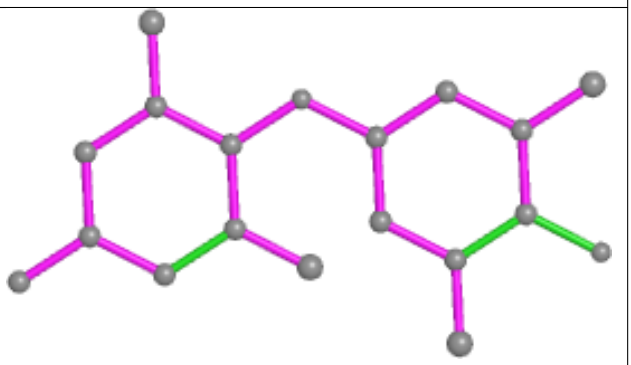


Rings

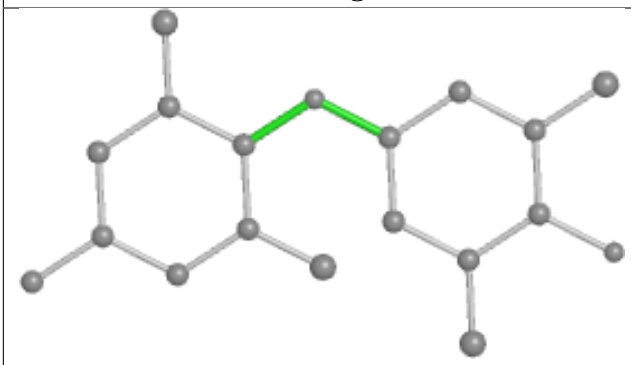
Ligand T44 B 528



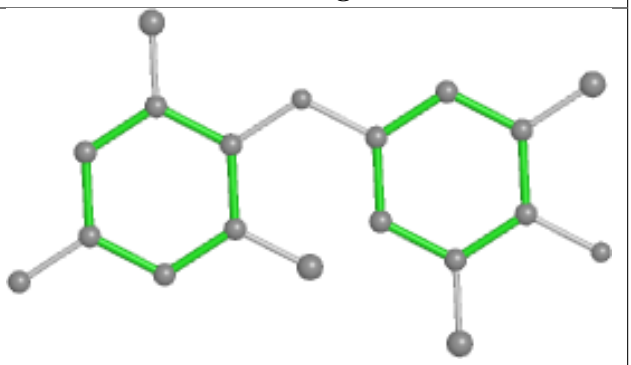
Bond lengths



Bond angles



Torsions



Rings

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

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

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

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

6.3 Carbohydrates

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

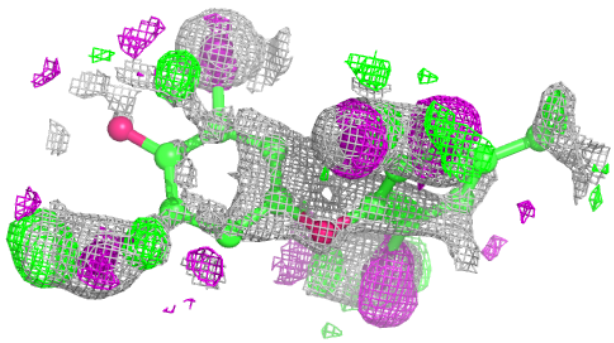
6.4 Ligands

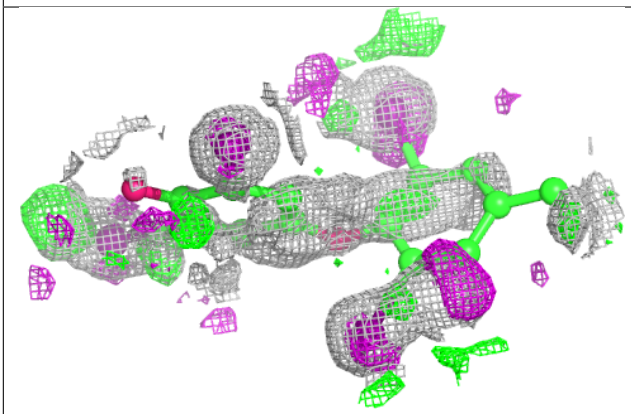
Unable to reproduce the depositors R factor - this section is therefore empty.

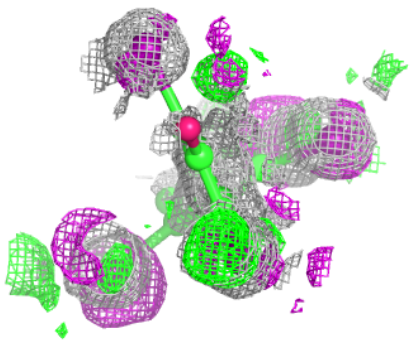
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around T44 A 428:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

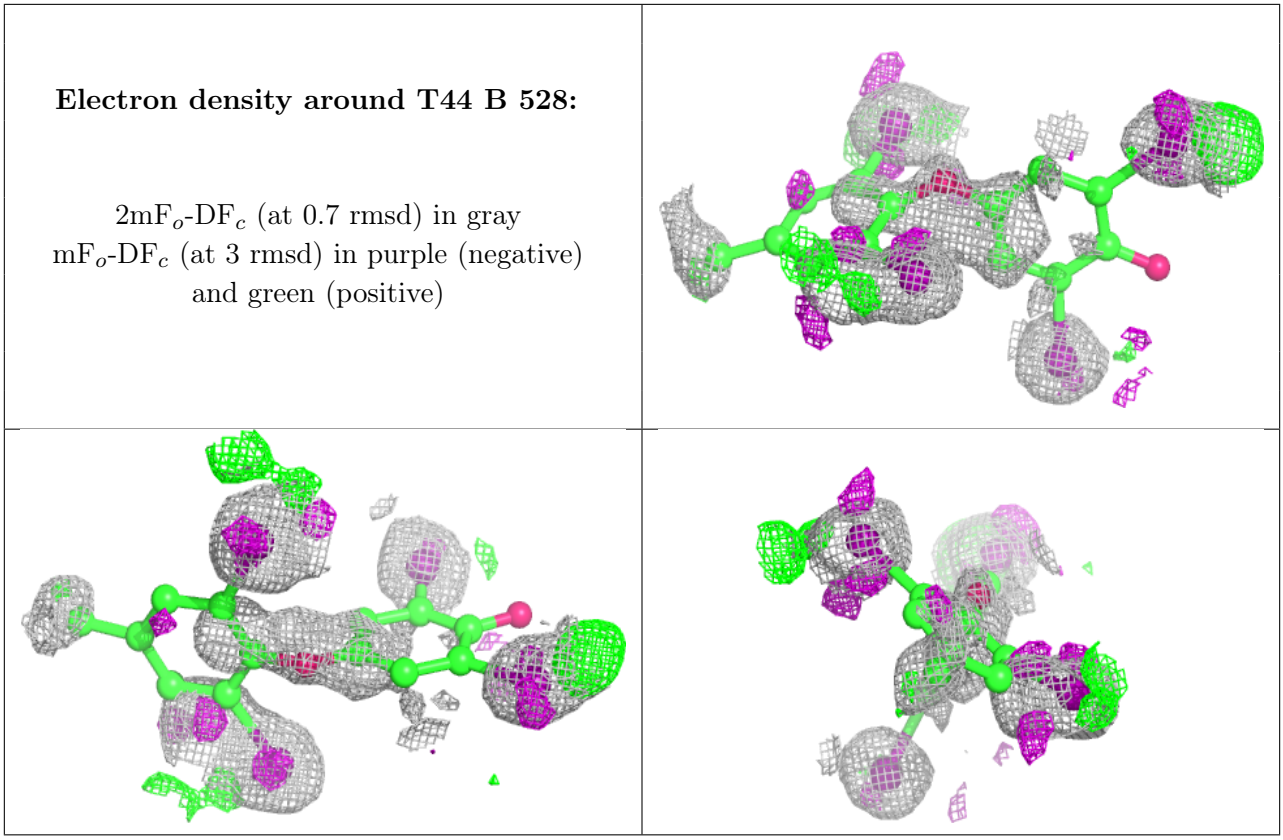






Electron density around T44 B 528:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



6.5 Other polymers (i)

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