Full wwPDB X-ray Structure Validation Report (i)

Aug 31, 2020 – 08:12 AM BST

PDB ID	:	6FFT
Title	:	Neutron structure of human transthyretin (TTR) S52P mutant in complex with tafamidis at room temperature to 2A resolution (quasi-Laue)
Authors	:	Yee, A.W.; Moulin, M.; Blakeley, M.P.; Haertlein, M.; Mitchell, E.P.; Forsyth, V.T.
Deposited on	:	2018-01-09
Resolution	:	2.00 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 following versions of software and data (see references (1)) were used in the production of this report:

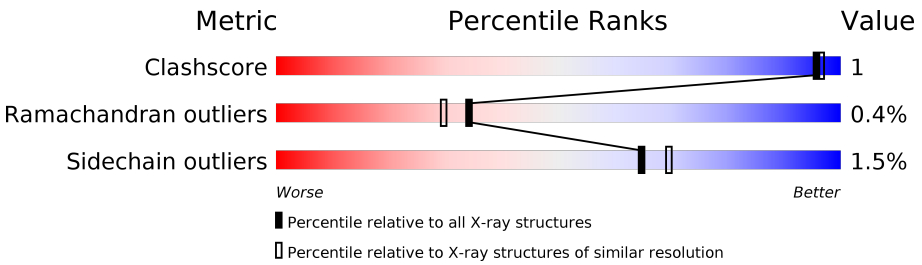
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	FAILED
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.13

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.00 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	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)

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 <=5%

Note EDS failed to run properly.

Mol	Chain	Length	Quality of chain
1	A	130	81% 8% 11%
1	B	130	82% 7% 11%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 4024 atoms, of which 368 are hydrogens and 1796 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.

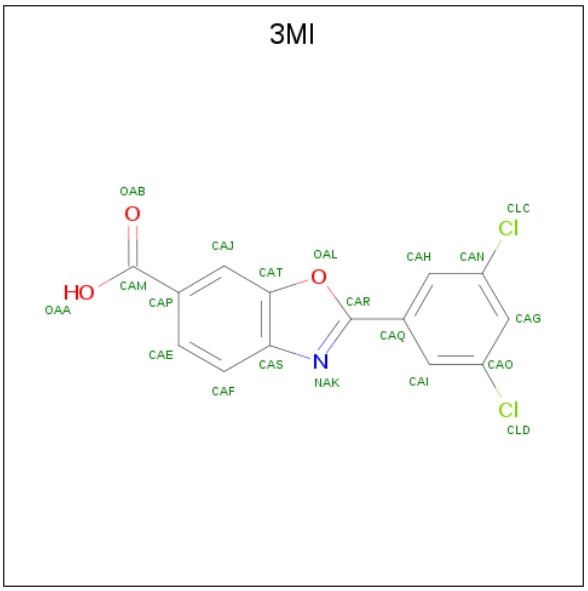
- Molecule 1 is a protein called Transthyretin.

Mol	Chain	Residues	Atoms							ZeroOcc	AltConf	Trace
			Total	C	D	H	N	O	S			
1	A	116	1947	575	872	178	147	173	2	46	108	0
1	B	116	1948	575	873	178	147	173	2	45	108	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	52	PRO	SER	engineered mutation	UNP P02766
B	-2	GLY	-	expression tag	UNP P02766
B	-1	ALA	-	expression tag	UNP P02766
B	0	MET	-	expression tag	UNP P02766
B	52	PRO	SER	engineered mutation	UNP P02766

- Molecule 2 is 2-(3,5-dichlorophenyl)-1,3-benzoxazole-6-carboxylic acid (three-letter code: 3MI) (formula: $C_{14}H_7Cl_2NO_3$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
			Total	C	Cl	H	N	O		
2	A	1	26	14	2	6	1	3	0	0
			Total	C	Cl	H	N	O		
2	B	1	26	14	2	6	1	3	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	D	O		
3	A	16	47	31	16	0	0
			Total	D	O		
3	B	10	30	20	10	0	0

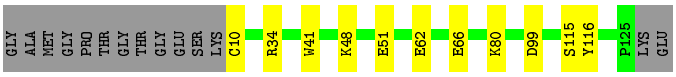
3 Residue-property plots (i)

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.

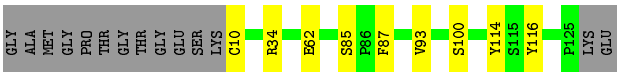
- Molecule 1: Transthyretin

Chain A:



- Molecule 1: Transthyretin

Chain B:



4 Data and refinement statistics (i)

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	43.90Å 85.70Å 65.54Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	42.85 – 2.00	Depositor
% Data completeness (in resolution range)	99.2 (42.85-2.00)	Depositor
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	23.24 (at 2.00Å)	Xtriage
Refinement program	PHENIX (1.10.1_2155: ???)	Depositor
R, R_{free}	0.157 , 0.195	Depositor
Wilson B-factor (Å^2)	23.3	Xtriage
Anisotropy	0.186	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	4024	wwPDB-VP
Average B, all atoms (Å^2)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 50.40 % 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 6.5073e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[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: 3MI

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	1.26	14/1781 (0.8%)	1.05	8/2435 (0.3%)
1	B	1.18	10/1781 (0.6%)	0.99	4/2435 (0.2%)
All	All	1.22	24/3562 (0.7%)	1.02	12/4870 (0.2%)

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	66[A]	GLU	CB-CG	-9.17	1.34	1.52
1	A	66[B]	GLU	CB-CG	-9.17	1.34	1.52
1	A	116[A]	TYR	CE2-CZ	-7.43	1.28	1.38
1	A	116[B]	TYR	CE2-CZ	-7.43	1.28	1.38
1	B	116[A]	TYR	CE2-CZ	-6.70	1.29	1.38
1	B	116[B]	TYR	CE2-CZ	-6.70	1.29	1.38
1	A	62[A]	GLU	CG-CD	6.24	1.61	1.51
1	A	62[B]	GLU	CG-CD	6.24	1.61	1.51
1	B	93[A]	VAL	CB-CG1	-5.63	1.41	1.52
1	B	93[B]	VAL	CB-CG1	-5.63	1.41	1.52
1	B	87[A]	PHE	CB-CG	-5.43	1.42	1.51
1	B	87[B]	PHE	CB-CG	-5.43	1.42	1.51
1	B	114[A]	TYR	CD1-CE1	-5.29	1.31	1.39
1	B	114[B]	TYR	CD1-CE1	-5.29	1.31	1.39
1	A	115[A]	SER	CB-OG	-5.23	1.35	1.42
1	A	115[B]	SER	CB-OG	-5.23	1.35	1.42
1	A	51[A]	GLU	CG-CD	5.18	1.59	1.51
1	A	51[B]	GLU	CG-CD	5.18	1.59	1.51
1	A	41[A]	TRP	C-N	-5.07	1.22	1.34
1	A	41[B]	TRP	C-N	-5.07	1.22	1.34
1	B	62[A]	GLU	CG-CD	5.03	1.59	1.51
1	B	62[B]	GLU	CG-CD	5.03	1.59	1.51
1	A	48[A]	LYS	CE-NZ	5.01	1.61	1.49
1	A	48[B]	LYS	CE-NZ	5.01	1.61	1.49

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	34[A]	ARG	NE-CZ-NH2	-7.82	116.39	120.30
1	B	34[B]	ARG	NE-CZ-NH2	-7.82	116.39	120.30
1	A	99[A]	ASP	CB-CG-OD2	-7.16	111.86	118.30
1	A	99[B]	ASP	CB-CG-OD2	-7.16	111.86	118.30
1	B	34[A]	ARG	CG-CD-NE	-6.21	98.76	111.80
1	B	34[B]	ARG	CG-CD-NE	-6.21	98.76	111.80
1	A	34[A]	ARG	CG-CD-NE	-5.44	100.37	111.80
1	A	34[B]	ARG	CG-CD-NE	-5.44	100.37	111.80
1	A	34[A]	ARG	NE-CZ-NH2	-5.25	117.67	120.30
1	A	34[B]	ARG	NE-CZ-NH2	-5.25	117.67	120.30
1	A	80[A]	LYS	CD-CE-NZ	-5.11	99.95	111.70
1	A	80[B]	LYS	CD-CE-NZ	-5.11	99.95	111.70

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	1769	178	56	0	0
1	B	1770	178	56	0	0
2	A	20	6	6	0	0
2	B	20	6	6	0	0
3	A	47	0	0	0	0
3	B	30	0	0	0	0
All	All	3656	368	124	0	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.

There are no clashes within the asymmetric unit.

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	221/130 (170%)	217 (98%)	4 (2%)	0	100	100
1	B	221/130 (170%)	209 (95%)	10 (4%)	2 (1%)	17	11
All	All	442/260 (170%)	426 (96%)	14 (3%)	2 (0%)	34	23

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	100[A]	SER
1	B	100[B]	SER

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	186/106 (176%)	184 (99%)	2 (1%)	73	78
1	B	186/106 (176%)	182 (98%)	4 (2%)	52	55
All	All	372/212 (176%)	366 (98%)	6 (2%)	65	67

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10[A]	CYS
1	A	10[B]	CYS
1	B	10[A]	CYS
1	B	10[B]	CYS

Continued on next page...

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Mol	Chain	Res	Type
1	B	85[A]	SER
1	B	85[B]	SER

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)

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	3MI	B	201	-	17,22,22	2.52	7 (41%)	24,32,32	1.95	5 (20%)
2	3MI	A	201	-	17,22,22	2.36	4 (23%)	24,32,32	2.45	7 (29%)

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	3MI	B	201	-	-	2/2/8/8	0/3/3/3
2	3MI	A	201	-	-	2/2/8/8	0/3/3/3

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	201	3MI	CAP-CAM	-6.70	1.41	1.47
2	B	201	3MI	CAP-CAM	-6.16	1.41	1.47
2	A	201	3MI	CAF-CAS	-4.28	1.34	1.41
2	B	201	3MI	CAO-CLD	-4.24	1.65	1.74
2	B	201	3MI	CAF-CAS	-3.89	1.35	1.41
2	B	201	3MI	CAN-CLC	3.19	1.81	1.74
2	A	201	3MI	CAO-CLD	-2.68	1.68	1.74
2	B	201	3MI	CAF-CAE	2.57	1.42	1.36
2	B	201	3MI	CAT-CAS	-2.47	1.34	1.42
2	A	201	3MI	CAN-CLC	2.36	1.79	1.74
2	B	201	3MI	CAH-CAN	2.29	1.42	1.38

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	201	3MI	CAI-CAQ-CAR	-5.11	112.58	120.06
2	A	201	3MI	CAH-CAN-CLC	4.98	125.38	119.15
2	B	201	3MI	CAH-CAQ-CAR	4.86	127.17	120.06
2	A	201	3MI	CAJ-CAP-CAM	4.68	126.52	120.36
2	A	201	3MI	CAG-CAN-CLC	-4.50	113.53	119.15
2	B	201	3MI	CAI-CAQ-CAR	-4.47	113.51	120.06
2	A	201	3MI	CAE-CAP-CAM	-4.06	114.92	120.37
2	B	201	3MI	CAH-CAN-CLC	3.61	123.66	119.15
2	B	201	3MI	CAR-NAK-CAS	3.48	110.68	103.78
2	A	201	3MI	CAH-CAQ-CAR	3.22	124.77	120.06
2	B	201	3MI	CAG-CAN-CLC	-2.89	115.54	119.15
2	A	201	3MI	CAI-CAQ-CAH	2.65	122.23	118.31

There are no chirality outliers.

All (4) torsion outliers are listed below:

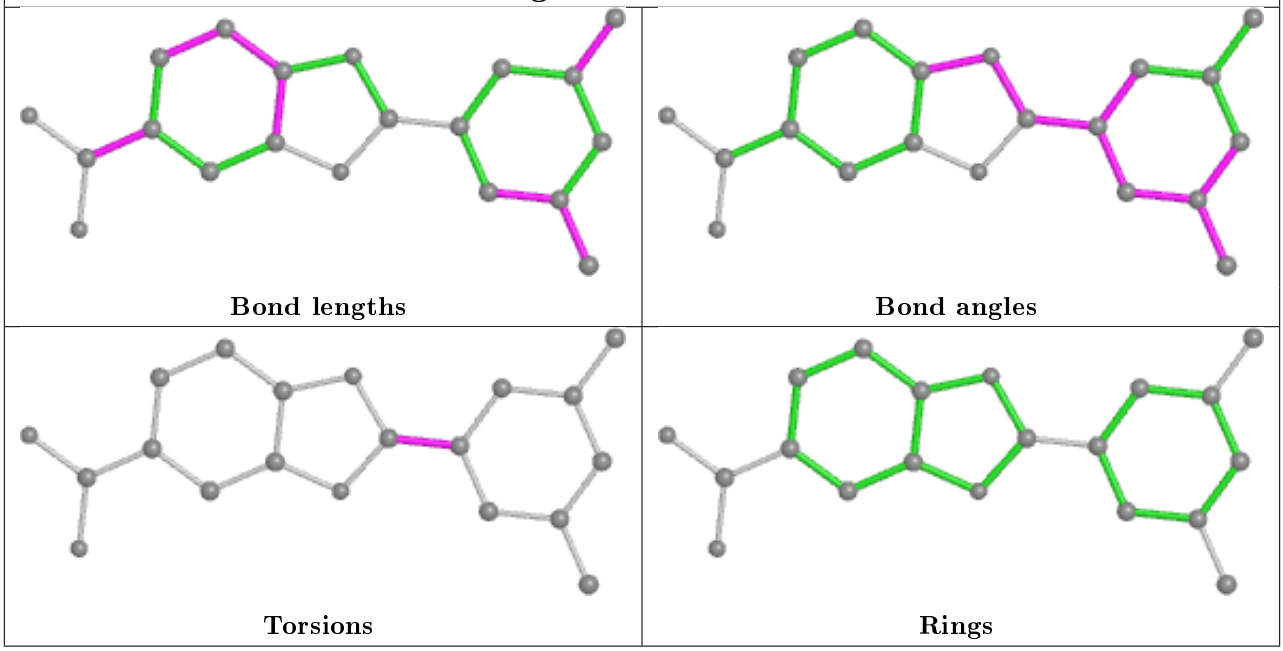
Mol	Chain	Res	Type	Atoms
2	B	201	3MI	CAH-CAQ-CAR-NAK
2	B	201	3MI	CAI-CAQ-CAR-NAK
2	A	201	3MI	CAH-CAQ-CAR-NAK
2	A	201	3MI	CAI-CAQ-CAR-NAK

There are no ring outliers.

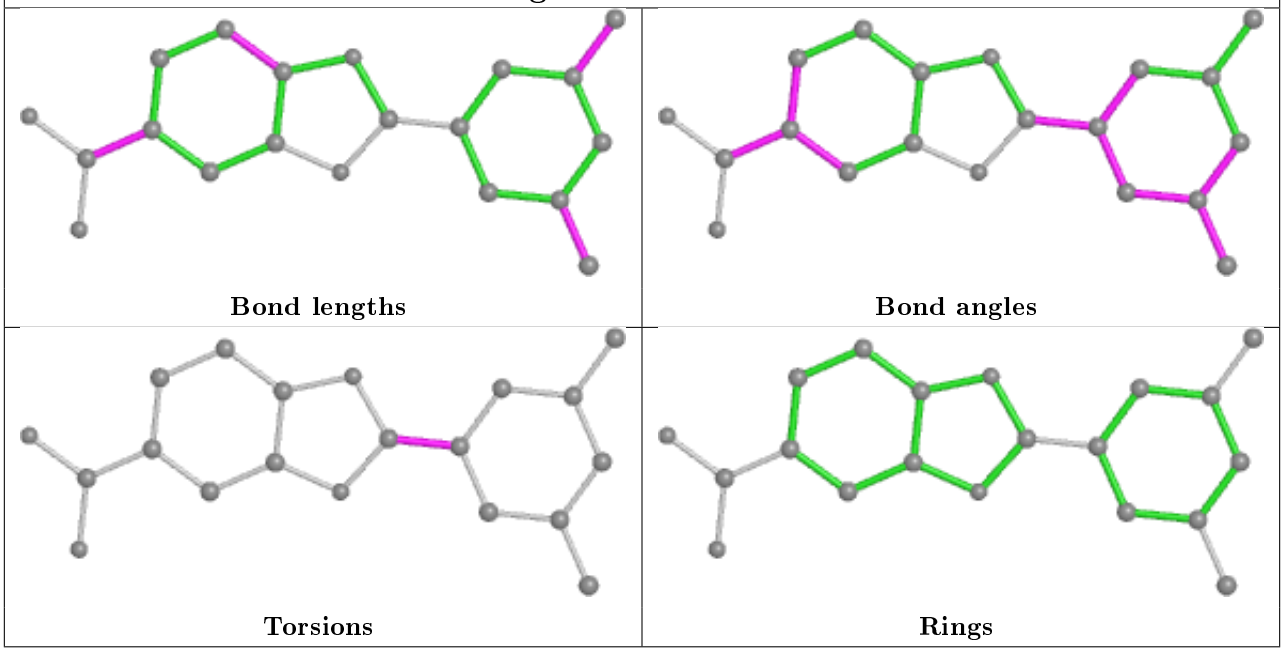
No monomer is involved in short contacts.

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 3MI B 201



Ligand 3MI A 201



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)

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

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

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

6.3 Carbohydrates (i)

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

6.4 Ligands (i)

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

6.5 Other polymers (i)

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