



# Full wwPDB X-ray Structure Validation Report ⓘ

May 13, 2020 – 06:35 am BST

PDB ID : 6ECL  
Title : Crystal Structure of a 1,2,4-Triazole Allosteric RNase H Inhibitor in Complex with HIV Reverse Transcriptase  
Authors : Kirby, K.A.; Sarafianos, S.G.  
Deposited on : 2018-08-08  
Resolution : 2.38 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

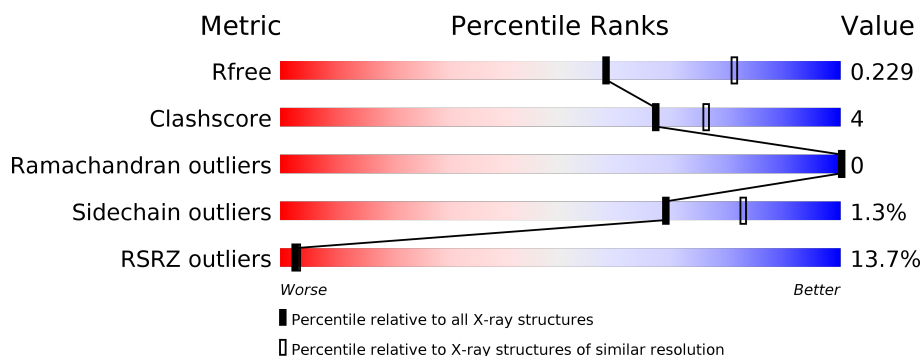
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.38 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	5509 (2.40-2.36)
Clashscore	141614	6082 (2.40-2.36)
Ramachandran outliers	138981	5973 (2.40-2.36)
Sidechain outliers	138945	5975 (2.40-2.36)
RSRZ outliers	127900	5397 (2.40-2.36)

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  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	557	<div> <div>15%</div> <div> <div></div> <div>90%</div> <div>10%</div> <div></div> </div> </div>
2	B	429	<div> <div>12%</div> <div> <div></div> <div>83%</div> <div>10%</div> <div>7%</div> <div></div> </div> </div>

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 8075 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 Reverse transcriptase/ribonuclease H.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	556	Total	C	N	O	S	0	0	0
			4524	2929	752	835	8			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	MET	-	initiating methionine	UNP P03366
A	0	VAL	-	expression tag	UNP P03366
A	280	SER	CYS	engineered mutation	UNP P03366

- Molecule 2 is a protein called Reverse transcriptase/ribonuclease H.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	401	Total	C	N	O	S	0	1	0
			3336	2175	550	605	6			

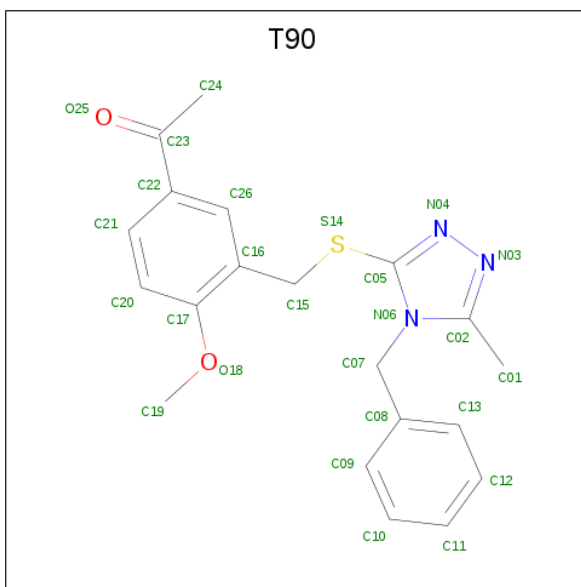
There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	0	GLY	-	expression tag	UNP P03366
B	280	SER	CYS	engineered mutation	UNP P03366

- Molecule 3 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	2	Total	Mn	0	0
			2	2		

- Molecule 4 is 1-[4-methoxy-3-[[5-methyl-4-(phenylmethyl)-1,2,4-triazol-3-yl]sulfanylmethyl]phenyl]ethanone (three-letter code: T90) (formula: C<sub>20</sub>H<sub>21</sub>N<sub>3</sub>O<sub>2</sub>S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	S	0	0
			26	20	3	2	1		

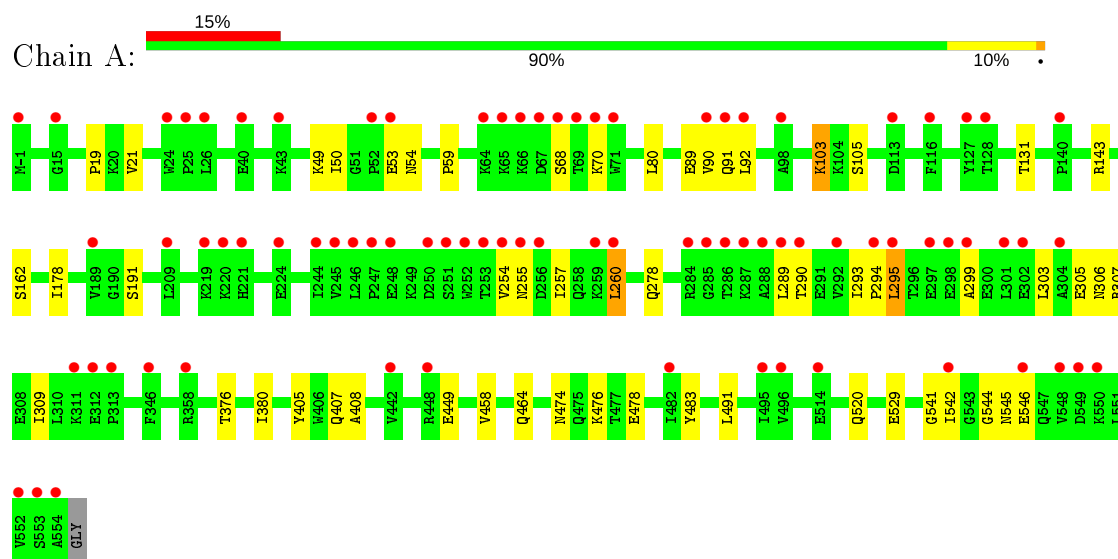
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	107	Total	O	0	0
			107	107		
5	B	80	Total	O	0	0
			80	80		

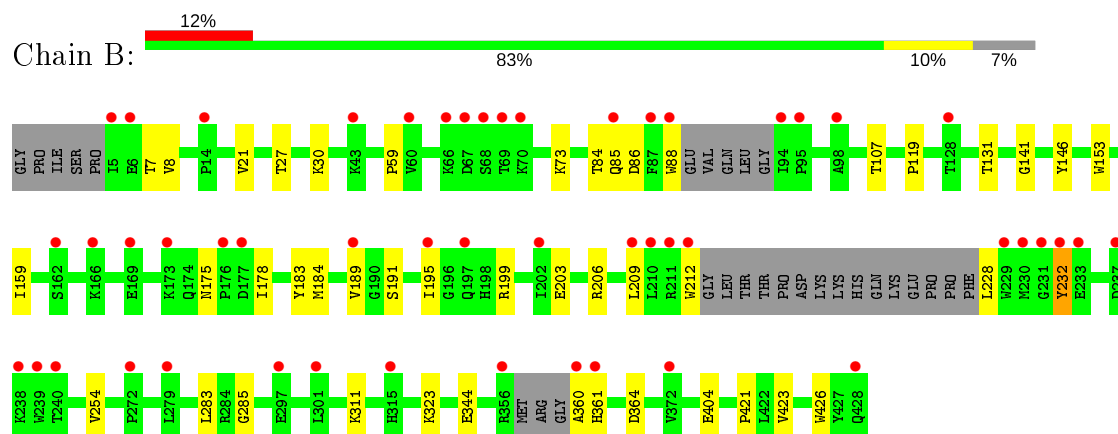
### 3 Residue-property plots [i](#)

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 and electron density. 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. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). 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: Reverse transcriptase/ribonuclease H



- Molecule 2: Reverse transcriptase/ribonuclease H



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	163.11Å 73.41Å 108.58Å 90.00° 100.43° 90.00°	Depositor
Resolution (Å)	19.77 – 2.38 19.77 – 2.38	Depositor EDS
% Data completeness (in resolution range)	97.3 (19.77-2.38) 97.4 (19.77-2.38)	Depositor EDS
$R_{merge}$	0.04	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.66 (at 2.38Å)	Xtriage
Refinement program	PHENIX 1.10.1	Depositor
R, $R_{free}$	0.185 , 0.229 0.185 , 0.229	Depositor DCC
$R_{free}$ test set	2468 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	47.2	Xtriage
Anisotropy	0.131	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 54.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	8075	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	69.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.85% 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: MN, T90

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	0.28	0/4642	0.46	0/6307
2	B	0.28	0/3431	0.45	0/4659
All	All	0.28	0/8073	0.46	0/10966

There are no bond length outliers.

There are no bond angle outliers.

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	4524	0	4588	35	0
2	B	3336	0	3360	30	0
3	A	2	0	0	0	0
4	A	26	0	0	0	0
5	A	107	0	0	0	0
5	B	80	0	0	2	0
All	All	8075	0	7948	62	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 4.

All (62) 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)
2:B:84:THR:HG21	2:B:153:TRP:HE1	1.48	0.79
1:A:255:ASN:HB2	1:A:289:LEU:HB2	1.79	0.64
1:A:303:LEU:HA	1:A:306:ASN:HB2	1.80	0.63
2:B:195:ILE:HD11	2:B:199:ARG:HH21	1.64	0.62
2:B:360:ALA:N	5:B:506:HOH:O	2.33	0.60
1:A:305:GLU:O	1:A:309:ILE:N	2.34	0.58
2:B:178:ILE:HD12	2:B:191:SER:HB3	1.83	0.58
1:A:289:LEU:HD12	1:A:290:THR:HG23	1.85	0.57
2:B:7:THR:HG22	2:B:119:PRO:HB2	1.85	0.57
1:A:257:ILE:HD12	1:A:260:LEU:HD21	1.86	0.57
2:B:30:LYS:NZ	2:B:404:GLU:OE1	2.37	0.55
1:A:293:ILE:HD12	1:A:294:PRO:HD2	1.88	0.55
2:B:203:GLU:OE1	2:B:206:ARG:NH1	2.40	0.55
1:A:458:VAL:HG23	1:A:464:GLN:HG2	1.88	0.55
2:B:195:ILE:O	2:B:199:ARG:HG2	2.08	0.54
1:A:21:VAL:HB	1:A:59:PRO:HD3	1.89	0.54
2:B:107:THR:HA	2:B:232:TYR:O	2.07	0.53
1:A:295:LEU:HG	1:A:299:ALA:HB3	1.90	0.53
2:B:73:LYS:NZ	2:B:146:TYR:OH	2.42	0.52
2:B:178:ILE:HD11	2:B:189:VAL:HG12	1.92	0.51
1:A:295:LEU:HG	1:A:299:ALA:CB	2.42	0.50
1:A:376:THR:O	1:A:380:ILE:HG12	2.11	0.50
1:A:474:ASN:O	1:A:478:GLU:HG3	2.12	0.50
1:A:405:TYR:CE2	1:A:407:GLN:HB2	2.47	0.50
1:A:408:ALA:HB1	2:B:364:ASP:HB3	1.94	0.50
1:A:491:LEU:HB3	1:A:529:GLU:HG3	1.93	0.49
2:B:209:LEU:HD22	2:B:228:LEU:HD22	1.95	0.49
2:B:175:ASN:O	2:B:178:ILE:HG22	2.12	0.49
1:A:254:VAL:HB	1:A:289:LEU:HA	1.93	0.49
1:A:19:PRO:HG3	1:A:80:LEU:HB2	1.94	0.48
1:A:449:GLU:OE1	1:A:449:GLU:N	2.46	0.47
2:B:183:TYR:CE2	2:B:184:MET:HG2	2.49	0.47
2:B:421:PRO:HB2	2:B:423:VAL:HG12	1.95	0.47
1:A:178:ILE:HD13	1:A:191:SER:HB3	1.97	0.46
2:B:311:LYS:HA	2:B:311:LYS:HD3	1.75	0.46
1:A:49:LYS:HB3	1:A:49:LYS:HE3	1.78	0.46
1:A:68:SER:HB3	1:A:70:LYS:HE2	1.97	0.46
1:A:50:ILE:HG13	1:A:143:ARG:HB3	1.97	0.46
1:A:131:THR:HG22	1:A:143:ARG:HD2	1.97	0.46
2:B:361:HIS:O	5:B:501:HOH:O	2.21	0.45
1:A:54:ASN:HB3	1:A:143:ARG:HH21	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:254:VAL:HG13	2:B:283:LEU:HD22	1.98	0.45
1:A:303:LEU:HD21	1:A:307:ARG:HE	1.82	0.45
1:A:544:GLY:N	2:B:285:GLY:O	2.50	0.44
2:B:423:VAL:HA	2:B:426:TRP:CD1	2.53	0.44
1:A:53:GLU:H	1:A:53:GLU:CD	2.22	0.43
2:B:84:THR:HG21	2:B:153:TRP:NE1	2.26	0.43
2:B:209:LEU:HD13	2:B:228:LEU:HD13	2.01	0.43
1:A:131:THR:HG23	1:A:143:ARG:HH11	1.83	0.43
2:B:21:VAL:HB	2:B:59:PRO:HD3	2.00	0.43
1:A:542:ILE:HG22	1:A:545:ASN:HB3	2.00	0.42
2:B:8:VAL:HG11	2:B:159:ILE:HG12	2.02	0.42
1:A:103:LYS:HE2	1:A:103:LYS:HB2	1.54	0.42
1:A:91:GLN:HG3	1:A:91:GLN:O	2.20	0.41
2:B:323:LYS:NZ	2:B:344:GLU:OE2	2.30	0.41
1:A:541:GLY:HA2	1:A:546:GLU:HB3	2.02	0.41
1:A:483:TYR:CE1	1:A:520:GLN:HB3	2.56	0.41
2:B:131:THR:CG2	2:B:141:GLY:HA3	2.50	0.41
2:B:86:ASP:HB3	2:B:88:TRP:NE1	2.36	0.41
1:A:380:ILE:HD12	2:B:27:THR:HG22	2.03	0.40
1:A:278:GLN:HB3	1:A:299:ALA:HB2	2.04	0.40
2:B:212:TRP:CD1	2:B:212:TRP:N	2.89	0.40

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	554/557 (100%)	538 (97%)	16 (3%)	0	100	100
2	B	394/429 (92%)	384 (98%)	10 (2%)	0	100	100
All	All	948/986 (96%)	922 (97%)	26 (3%)	0	100	100

There are no Ramachandran outliers to report.

### 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	497/497 (100%)	488 (98%)	9 (2%)	59	75
2	B	367/390 (94%)	365 (100%)	2 (0%)	88	95
All	All	864/887 (97%)	853 (99%)	11 (1%)	69	82

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	89	GLU
1	A	90	VAL
1	A	92	LEU
1	A	103	LYS
1	A	105	SER
1	A	162	SER
1	A	260	LEU
1	A	295	LEU
1	A	476	LYS
2	B	85	GLN
2	B	232	TYR

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

Mol	Chain	Res	Type
1	A	332	GLN
1	A	447	ASN

### 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 carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 3 ligands modelled in this entry, 2 are monoatomic - 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	$\# Z  > 2$
4	T90	A	602	-	25,28,28	1.16	3 (12%)	29,38,38	1.54	4 (13%)

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
4	T90	A	602	-	-	0/14/15/15	0/3/3/3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	602	T90	C05-N06	-2.50	1.34	1.36
4	A	602	T90	C05-S14	2.27	1.81	1.75
4	A	602	T90	C15-C16	2.10	1.53	1.51

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	602	T90	C15-S14-C05	6.27	107.67	101.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	602	T90	O18-C17-C16	2.71	119.74	115.97
4	A	602	T90	O18-C17-C20	-2.63	119.87	124.37
4	A	602	T90	C19-O18-C17	-2.29	114.06	117.53

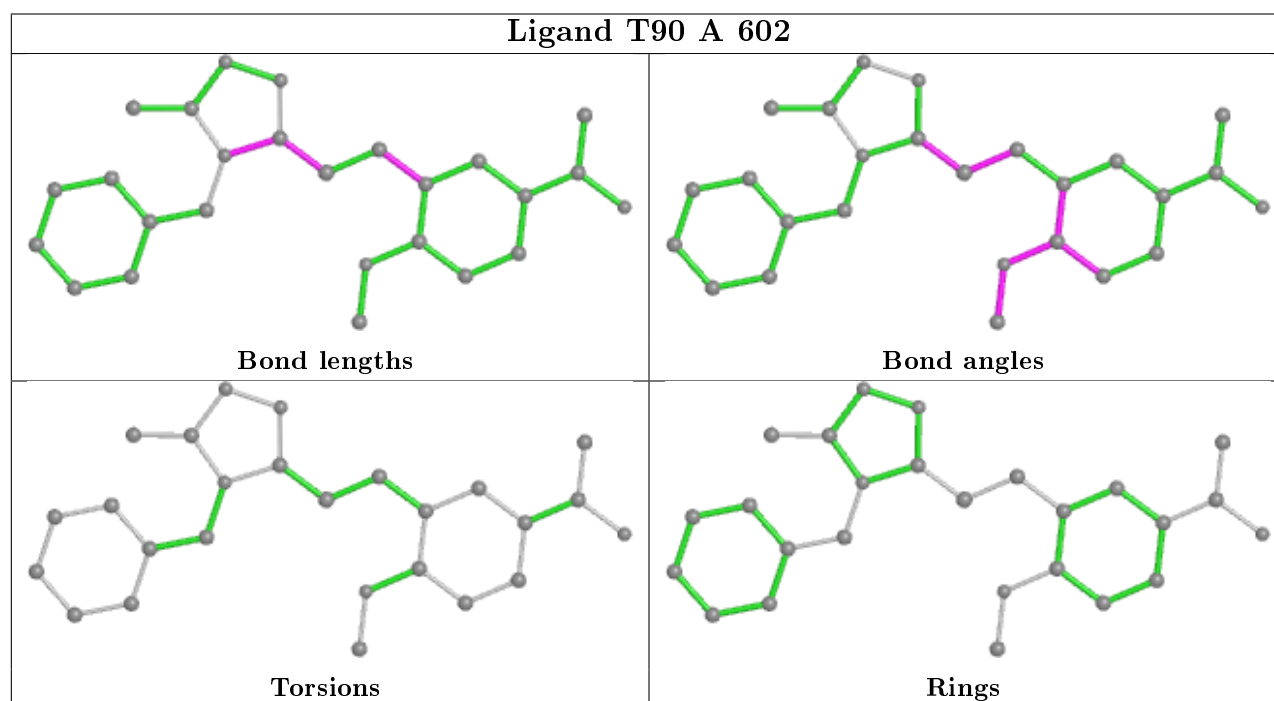
There are no chirality outliers.

There are no torsion outliers.

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 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

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å <sup>2</sup> )	Q<0.9
1	A	556/557 (99%)	0.85	81 (14%)	2 2	29, 66, 129, 171	0
2	B	401/429 (93%)	0.65	50 (12%)	3 4	32, 60, 115, 146	0
All	All	957/986 (97%)	0.76	131 (13%)	3 3	29, 64, 125, 171	0

All (131) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	67	ASP	10.7
1	A	292	VAL	8.9
1	A	297	GLU	7.8
2	B	231	GLY	7.7
2	B	229	TRP	7.7
2	B	232	TYR	7.4
2	B	239	TRP	7.4
2	B	88	TRP	7.0
1	A	289	LEU	6.9
1	A	298	GLU	6.9
1	A	301	LEU	6.8
1	A	24	TRP	6.8
2	B	210	LEU	6.7
1	A	295	LEU	6.4
1	A	311	LYS	6.3
2	B	95	PRO	6.3
1	A	69	THR	6.2
1	A	65	LYS	6.1
1	A	286	THR	5.9
1	A	70	LYS	5.7
2	B	230	MET	5.7
1	A	294	PRO	5.6
1	A	66	LYS	5.6
2	B	67	ASP	5.5

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Mol	Chain	Res	Type	RSRZ
1	A	288	ALA	5.4
1	A	304	ALA	5.4
1	A	290	THR	5.3
1	A	554	ALA	5.2
1	A	68	SER	5.2
2	B	85	GLN	5.1
1	A	546	GLU	4.9
1	A	116	PHE	4.7
1	A	245	VAL	4.6
2	B	238	LYS	4.6
2	B	94	ILE	4.6
1	A	92	LEU	4.5
2	B	189	VAL	4.5
1	A	246	LEU	4.5
2	B	360	ALA	4.4
1	A	220	LYS	4.4
1	A	52	PRO	4.2
1	A	287	LYS	4.2
2	B	237	ASP	4.2
1	A	285	GLY	4.2
1	A	284	ARG	4.1
2	B	5	ILE	4.1
2	B	428	GLN	4.0
2	B	87	PHE	3.9
1	A	43	LYS	3.7
2	B	301	LEU	3.6
1	A	482	ILE	3.6
1	A	244	ILE	3.5
1	A	358	ARG	3.5
1	A	254	VAL	3.5
1	A	495	ILE	3.4
2	B	69	THR	3.4
2	B	240	THR	3.3
1	A	90	VAL	3.3
1	A	221	HIS	3.3
1	A	252	TRP	3.2
2	B	195	ILE	3.1
1	A	-1	MET	3.1
2	B	356	ARG	3.1
1	A	251	SER	3.1
2	B	209	LEU	3.0
2	B	211	ARG	3.0

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Mol	Chain	Res	Type	RSRZ
2	B	361	HIS	2.9
1	A	552	VAL	2.9
1	A	256	ASP	2.9
1	A	259	LYS	2.9
2	B	68	SER	2.8
1	A	15	GLY	2.8
2	B	169	GLU	2.8
1	A	542	ILE	2.8
1	A	302	GLU	2.8
2	B	177	ASP	2.7
1	A	496	VAL	2.7
1	A	113	ASP	2.7
2	B	173	LYS	2.7
1	A	255	ASN	2.7
2	B	70	LYS	2.6
1	A	219	LYS	2.6
2	B	315	HIS	2.6
1	A	128	THR	2.6
2	B	212	TRP	2.6
1	A	140	PRO	2.6
1	A	250	ASP	2.6
2	B	6	GLU	2.6
1	A	514	GLU	2.5
1	A	442	VAL	2.5
2	B	372	VAL	2.5
2	B	166	LYS	2.5
1	A	299	ALA	2.5
2	B	14	PRO	2.5
2	B	197	GLN	2.5
2	B	162	SER	2.4
1	A	209	LEU	2.4
1	A	189	VAL	2.4
2	B	60	VAL	2.4
1	A	127	TYR	2.3
1	A	25	PRO	2.3
1	A	553	SER	2.3
1	A	224	GLU	2.3
1	A	253	THR	2.3
1	A	248	GLU	2.3
1	A	549	ASP	2.2
2	B	202	ILE	2.2
1	A	550	LYS	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	313	PRO	2.2
2	B	176	PRO	2.2
2	B	297	GLU	2.2
1	A	247	PRO	2.2
2	B	233	GLU	2.2
1	A	260	LEU	2.2
2	B	98	ALA	2.2
2	B	272	PRO	2.2
1	A	98	ALA	2.1
2	B	279	LEU	2.1
1	A	312	GLU	2.1
1	A	64	LYS	2.1
1	A	448	ARG	2.1
1	A	26	LEU	2.1
1	A	71	TRP	2.1
1	A	91	GLN	2.1
1	A	346	PHE	2.1
1	A	40	GLU	2.1
2	B	43	LYS	2.0
2	B	66	LYS	2.0
1	A	53	GLU	2.0
2	B	128	THR	2.0
1	A	548	VAL	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

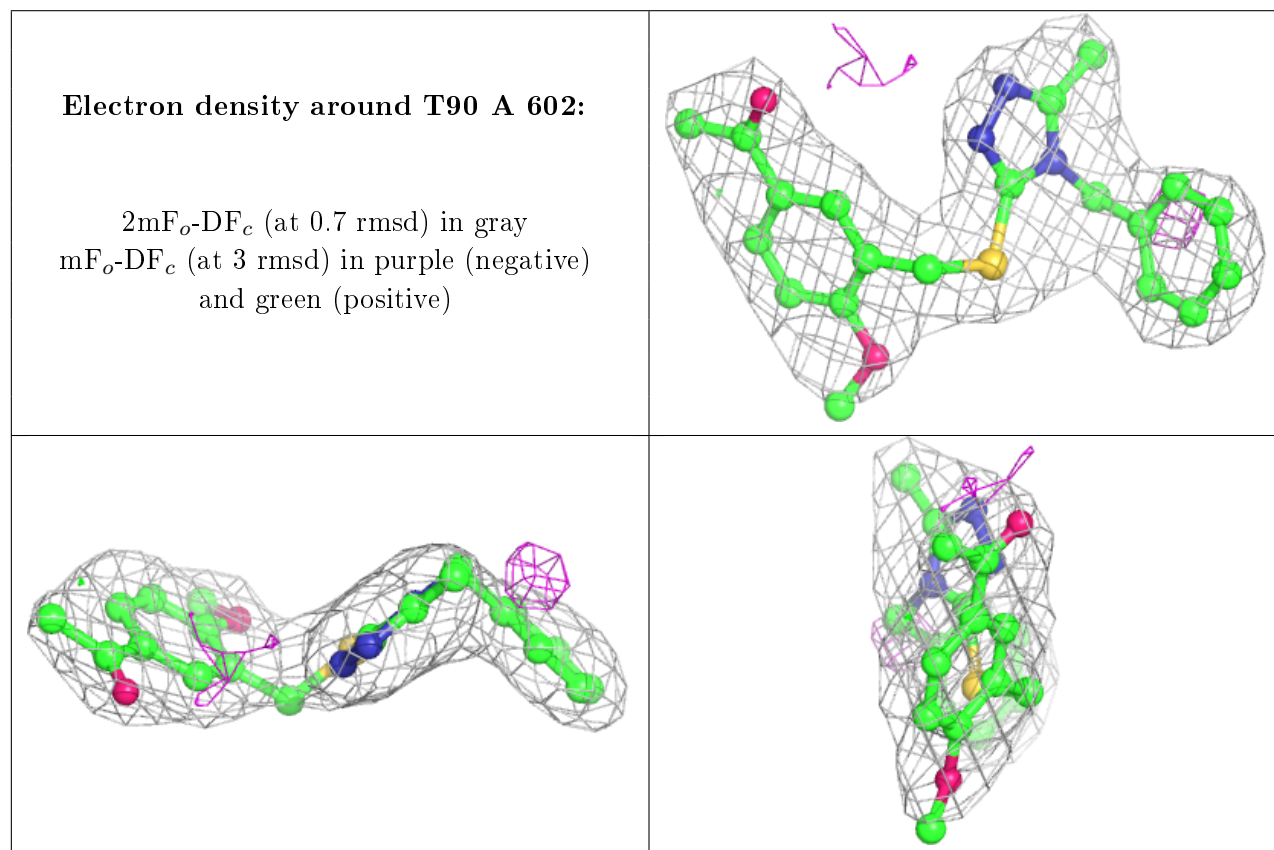
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	MN	A	601	1/1	0.26	0.18	118,118,118,118	0
3	MN	A	603	1/1	0.48	0.15	188,188,188,188	0
4	T90	A	602	26/26	0.94	0.18	49,64,74,77	0

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 [i](#)

There are no such residues in this entry.