



# Full wwPDB X-ray Structure Validation Report ⓘ

May 26, 2020 – 10:06 am BST

PDB ID : 3T19  
Title : Crystal structure of HIV-1 reverse transcriptase (wild type) in complex with inhibitor M05  
Authors : Yan, Y.; Reid, J.  
Deposited on : 2011-07-21  
Resolution : 2.60 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

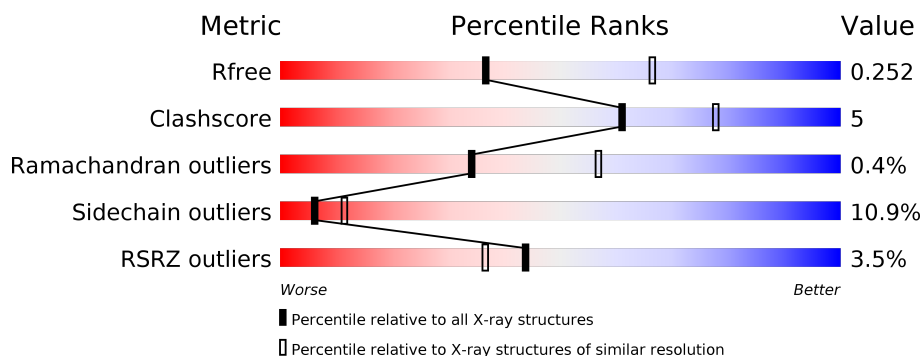
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.60 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	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)

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	563	<div> <div>3%</div> <div> <div></div> <div>77%</div> <div>20%</div> <div>••</div> </div> </div>
1	B	563	<div> <div>3%</div> <div> <div></div> <div>57%</div> <div>13%</div> <div>•</div> <div>29%</div> </div> </div>

## 2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 8043 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.

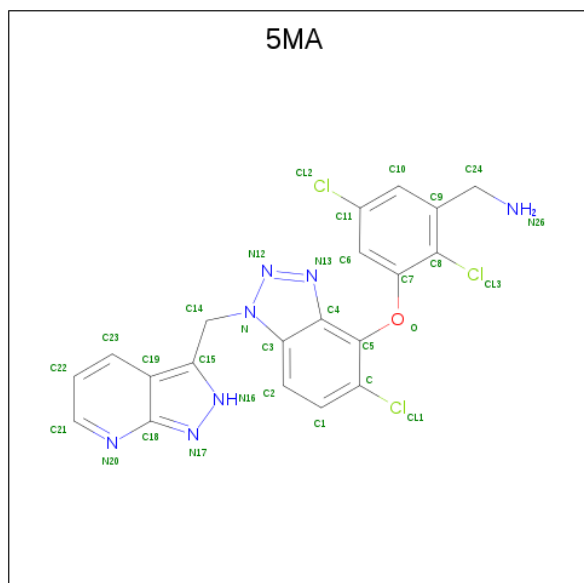
- Molecule 1 is a protein called Reverse Transcriptase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	554	Total	C	N	O	S	0	0	0
			4504	2913	751	832	8			
1	B	400	Total	C	N	O	S	0	0	0
			3312	2157	548	601	6			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	MET	-	EXPRESSION TAG	UNP P04585
A	-1	ASN	-	EXPRESSION TAG	UNP P04585
A	0	SER	-	EXPRESSION TAG	UNP P04585
B	-2	MET	-	EXPRESSION TAG	UNP P04585
B	-1	ASN	-	EXPRESSION TAG	UNP P04585
B	0	SER	-	EXPRESSION TAG	UNP P04585

- Molecule 2 is 1-(2,5-dichloro-3-{[5-chloro-1-(2H-pyrazolo[3,4-b]pyridin-3-ylmethyl)-1H-benzotriazol-4-yl]oxy}phenyl)methanamine (three-letter code: 5MA) (formula: C<sub>20</sub>H<sub>14</sub>Cl<sub>3</sub>N<sub>7</sub>O).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	Cl	N	O	0	0
			31	20	3	7	1		

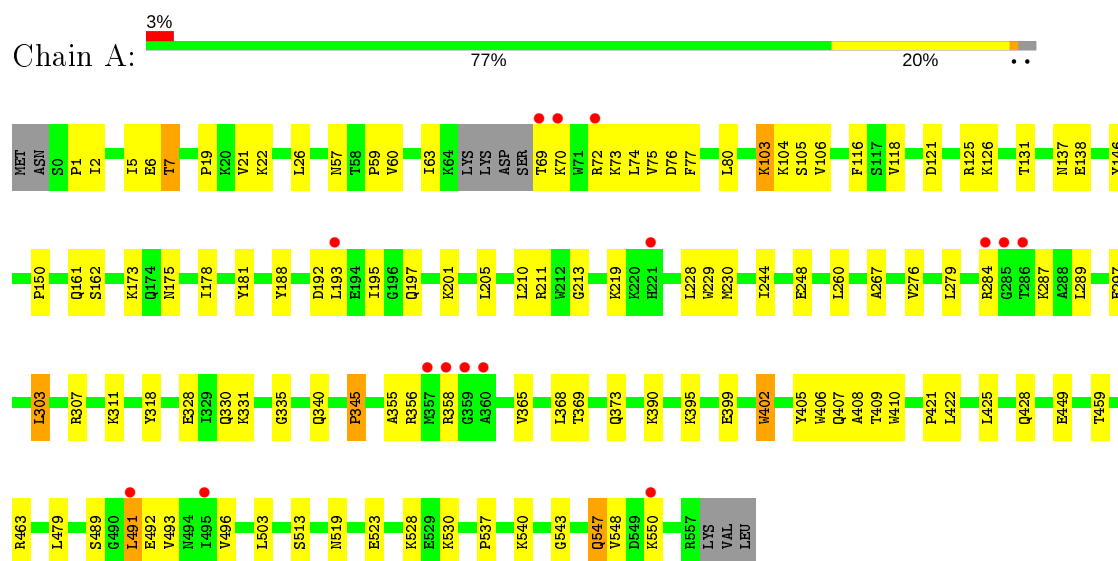
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	121	Total	O	0	0
			121	121		
3	B	75	Total	O	0	0
			75	75		

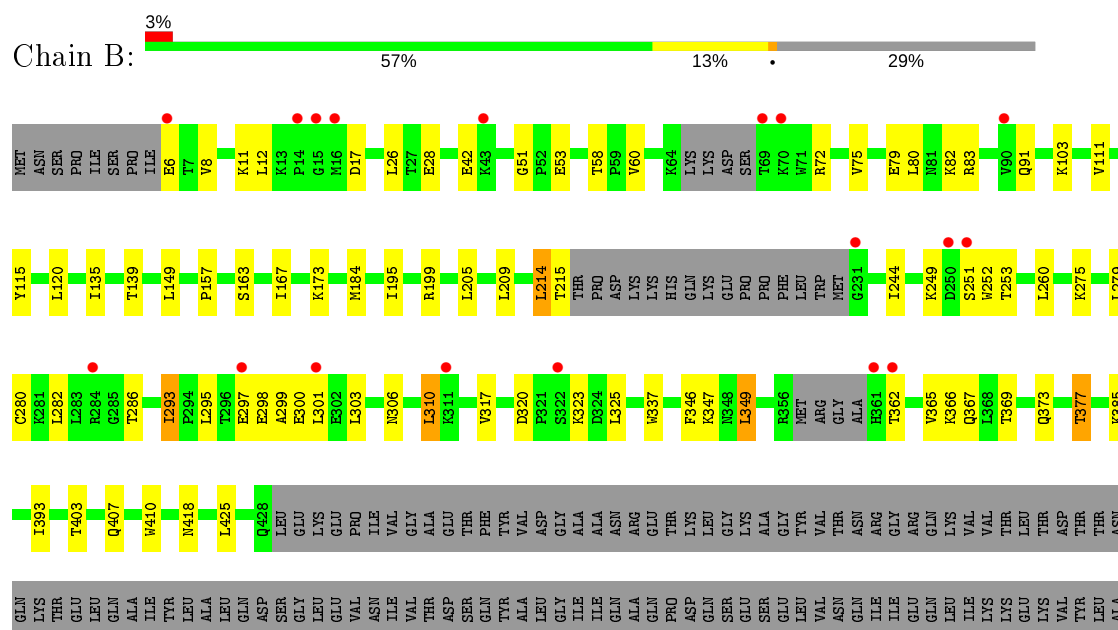
### 3 Residue-property plots

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



#### • Molecule 1: Reverse Transcriptase



TRP VAL  
PRO ALA  
HIS LYS  
GLY ILE  
GLY GLY  
ASN GLU  
GLN VAL  
ASP LYS  
LEU VAL  
SER ALA  
GLY ILE  
ARG LYS  
VAL VAL  
LEU

## 4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	118.06Å 153.66Å 154.88Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	26.21 – 2.60 25.96 – 2.60	Depositor EDS
% Data completeness (in resolution range)	95.9 (26.21-2.60) 96.1 (25.96-2.60)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	0.06	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.33 (at 2.60Å)	Xtriage
Refinement program	BUSTER 2.9.7	Depositor
R, $R_{free}$	0.199 , 0.248 0.199 , 0.252	Depositor DCC
$R_{free}$ test set	2098 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	50.9	Xtriage
Anisotropy	0.232	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 58.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	8043	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	54.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.83% 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: 5MA

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	0.51	0/4620	0.76	1/6279 (0.0%)
1	B	0.50	0/3405	0.75	0/4627
All	All	0.51	0/8025	0.76	1/10906 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	345	PRO	C-N-CA	6.22	137.26	121.70

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	4504	0	4547	39	0
1	B	3312	0	3333	34	0
2	A	31	0	14	4	0
3	A	121	0	0	0	0
3	B	75	0	0	1	0
All	All	8043	0	7894	71	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 5.

All (71) 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:B:214:LEU:HD23	1:B:214:LEU:H	1.51	0.75
1:A:103:LYS:H	2:A:561:5MA:HN16	1.36	0.74
1:B:282:LEU:HB3	1:B:293:ILE:HD11	1.70	0.72
1:A:406:TRP:CH2	1:B:418:ASN:HA	2.30	0.66
1:A:330:GLN:HE22	1:A:340:GLN:HE22	1.41	0.66
1:B:337:TRP:HE1	1:B:367:GLN:HE21	1.45	0.65
1:A:193:LEU:HB3	1:A:197:GLN:HG3	1.82	0.62
1:B:373:GLN:O	1:B:377:THR:HG23	2.00	0.61
1:A:537:PRO:HB2	1:A:540:LYS:HG3	1.86	0.58
1:A:405:TYR:CE2	1:A:407:GLN:HB3	2.39	0.58
1:A:492:GLU:HG2	1:A:530:LYS:HB2	1.85	0.58
1:A:365:VAL:O	1:A:369:THR:HG23	2.05	0.57
1:B:362:THR:CG2	1:B:367:GLN:HG3	2.35	0.57
1:A:7:THR:HG21	1:A:121:ASP:HA	1.87	0.57
1:A:318:TYR:CZ	2:A:561:5MA:H14A	2.41	0.56
1:B:215:THR:HA	3:B:619:HOH:O	2.04	0.56
1:A:328:GLU:HG2	1:A:390:LYS:HB2	1.87	0.56
1:B:297:GLU:HA	1:B:300:GLU:HB2	1.88	0.54
1:B:362:THR:HG23	1:B:366:LYS:HE3	1.88	0.54
1:B:115:TYR:HB3	1:B:149:LEU:HB2	1.88	0.54
1:B:373:GLN:NE2	1:B:407:GLN:H	2.05	0.54
1:B:244:ILE:HB	1:B:310:LEU:HG	1.91	0.53
1:A:330:GLN:NE2	1:A:340:GLN:HE22	2.07	0.53
1:A:73:LYS:NZ	1:A:146:TYR:OH	2.42	0.52
1:B:275:LYS:H	1:B:306:ASN:HD21	1.56	0.52
1:B:317:VAL:HG12	1:B:349:LEU:HD13	1.91	0.51
1:A:399:GLU:HA	1:A:402:TRP:CE3	2.45	0.51
1:B:373:GLN:HE22	1:B:407:GLN:H	1.58	0.51
1:A:181:TYR:HB2	1:A:188:TYR:HB2	1.93	0.51
1:A:19:PRO:HG3	1:A:80:LEU:HB2	1.93	0.50
1:A:60:VAL:HG12	1:A:75:VAL:HG22	1.93	0.50
1:A:330:GLN:HE22	1:A:340:GLN:NE2	2.09	0.50
1:A:59:PRO:HG2	1:A:76:ASP:HB3	1.93	0.49
1:A:175:ASN:HD21	1:A:201:LYS:NZ	2.11	0.49
1:B:346:PHE:N	1:B:346:PHE:CD2	2.81	0.48
1:A:103:LYS:HD2	2:A:561:5MA:H1	1.95	0.48
1:B:295:LEU:HB3	1:B:300:GLU:OE1	2.13	0.48
1:B:362:THR:HG22	1:B:367:GLN:HG3	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:77:PHE:CE2	1:A:150:PRO:HB2	2.48	0.48
1:B:377:THR:HG22	1:B:410:TRP:HZ2	1.77	0.48
1:A:7:THR:CG2	1:A:121:ASP:HA	2.44	0.47
1:A:303:LEU:O	1:A:307:ARG:HG3	2.15	0.47
1:B:279:LEU:HD13	1:B:299:ALA:HB1	1.97	0.47
1:B:365:VAL:O	1:B:369:THR:HG23	2.16	0.46
1:A:63:ILE:HG12	1:A:74:LEU:HD11	1.98	0.46
1:A:547:GLN:HA	1:A:550:LYS:HE2	1.98	0.46
1:B:60:VAL:HG23	1:B:75:VAL:HG22	1.98	0.46
1:A:104:LYS:HB2	1:A:192:ASP:HA	1.97	0.46
1:A:57:ASN:ND2	1:A:131:THR:OG1	2.49	0.45
1:A:408:ALA:O	1:B:393:ILE:HG13	2.17	0.45
1:B:28:GLU:HA	1:B:135:ILE:HD11	1.98	0.44
1:A:175:ASN:HB3	1:A:178:ILE:HD12	1.99	0.44
1:A:125:ARG:HG2	1:A:146:TYR:O	2.17	0.44
1:B:320:ASP:OD2	1:B:323:LYS:HG3	2.18	0.44
1:A:2:ILE:HD12	1:A:116:PHE:O	2.17	0.44
1:A:318:TYR:CE1	2:A:561:5MA:H14A	2.53	0.44
1:B:377:THR:HG22	1:B:410:TRP:CZ2	2.53	0.43
1:A:229:TRP:CE2	1:A:230:MET:HG3	2.52	0.43
1:B:157:PRO:HG3	1:B:184:MET:HA	2.00	0.43
1:A:331:LYS:HB3	1:A:421:PRO:HG2	2.00	0.43
1:A:335:GLY:O	1:A:355:ALA:HA	2.19	0.43
1:B:79:GLU:HG3	1:B:83:ARG:HE	1.84	0.42
1:A:244:ILE:HD13	1:A:267:ALA:HB2	2.00	0.42
1:B:362:THR:HG21	1:B:367:GLN:HG3	2.02	0.42
1:A:513:SER:H	1:A:519:ASN:HD21	1.67	0.41
1:A:1:PRO:HB2	1:A:213:GLY:HA2	2.02	0.41
1:B:195:ILE:O	1:B:199:ARG:HG3	2.20	0.41
1:B:51:GLY:HA3	1:B:53:GLU:OE1	2.20	0.41
1:B:163:SER:O	1:B:167:ILE:HG13	2.20	0.41
1:B:249:LYS:HB2	1:B:252:TRP:CE2	2.56	0.41
1:B:325:LEU:HD12	1:B:385:LYS:HG3	2.02	0.41

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	550/563 (98%)	519 (94%)	27 (5%)	4 (1%)	22	43
1	B	392/563 (70%)	379 (97%)	13 (3%)	0	100	100
All	All	942/1126 (84%)	898 (95%)	40 (4%)	4 (0%)	34	57

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	491	LEU
1	A	543	GLY
1	A	195	ILE
1	A	345	PRO

### 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	492/503 (98%)	434 (88%)	58 (12%)	5	9
1	B	364/503 (72%)	329 (90%)	35 (10%)	8	16
All	All	856/1006 (85%)	763 (89%)	93 (11%)	6	11

All (93) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	ILE
1	A	6	GLU

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Mol	Chain	Res	Type
1	A	7	THR
1	A	21	VAL
1	A	22	LYS
1	A	26	LEU
1	A	69	THR
1	A	70	LYS
1	A	72	ARG
1	A	103	LYS
1	A	105	SER
1	A	106	VAL
1	A	118	VAL
1	A	126	LYS
1	A	137	ASN
1	A	138	GLU
1	A	161	GLN
1	A	162	SER
1	A	173	LYS
1	A	205	LEU
1	A	210	LEU
1	A	211	ARG
1	A	219	LYS
1	A	228	LEU
1	A	248	GLU
1	A	260	LEU
1	A	276	VAL
1	A	279	LEU
1	A	284	ARG
1	A	287	LYS
1	A	289	LEU
1	A	297	GLU
1	A	303	LEU
1	A	311	LYS
1	A	356	ARG
1	A	358	ARG
1	A	368	LEU
1	A	373	GLN
1	A	395	LYS
1	A	402	TRP
1	A	409	THR
1	A	410	TRP
1	A	422	LEU
1	A	425	LEU

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Mol	Chain	Res	Type
1	A	428	GLN
1	A	449	GLU
1	A	459	THR
1	A	463	ARG
1	A	479	LEU
1	A	489	SER
1	A	491	LEU
1	A	493	VAL
1	A	496	VAL
1	A	503	LEU
1	A	523	GLU
1	A	528	LYS
1	A	547	GLN
1	A	548	VAL
1	B	6	GLU
1	B	8	VAL
1	B	11	LYS
1	B	12	LEU
1	B	17	ASP
1	B	26	LEU
1	B	42	GLU
1	B	58	THR
1	B	72	ARG
1	B	80	LEU
1	B	82	LYS
1	B	91	GLN
1	B	103	LYS
1	B	111	VAL
1	B	120	LEU
1	B	139	THR
1	B	173	LYS
1	B	205	LEU
1	B	209	LEU
1	B	214	LEU
1	B	251	SER
1	B	253	THR
1	B	260	LEU
1	B	280	CYS
1	B	286	THR
1	B	293	ILE
1	B	298	GLU
1	B	301	LEU

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Mol	Chain	Res	Type
1	B	303	LEU
1	B	310	LEU
1	B	347	LYS
1	B	349	LEU
1	B	377	THR
1	B	403	THR
1	B	425	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	57	ASN
1	A	147	ASN
1	A	175	ASN
1	A	198	HIS
1	A	258	GLN
1	A	330	GLN
1	A	334	GLN
1	A	407	GLN
1	A	519	ASN
1	B	96	HIS
1	B	147	ASN
1	B	161	GLN
1	B	175	ASN
1	B	182	GLN
1	B	208	HIS
1	B	255	ASN
1	B	258	GLN
1	B	306	ASN
1	B	336	GLN
1	B	367	GLN
1	B	373	GLN
1	B	428	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 ⓘ

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	5MA	A	561	-	33,35,35	1.70	8 (24%)	29,51,51	1.34	3 (10%)

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	5MA	A	561	-	-	1/9/10/10	0/5/5/5

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	561	5MA	C21-N20	4.63	1.41	1.32
2	A	561	5MA	C14-C15	3.26	1.55	1.51
2	A	561	5MA	C10-C11	3.16	1.43	1.38
2	A	561	5MA	C22-C23	2.98	1.43	1.36
2	A	561	5MA	C2-C1	2.45	1.41	1.36
2	A	561	5MA	C23-C19	2.25	1.46	1.42
2	A	561	5MA	C6-C11	2.07	1.41	1.38
2	A	561	5MA	N12-N	2.01	1.38	1.34

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	561	5MA	O-C5-C	-4.05	115.81	120.51
2	A	561	5MA	C6-C11-CL2	-3.12	115.25	119.15
2	A	561	5MA	C10-C11-CL2	2.08	121.75	119.15

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	561	5MA	C8-C7-O-C5

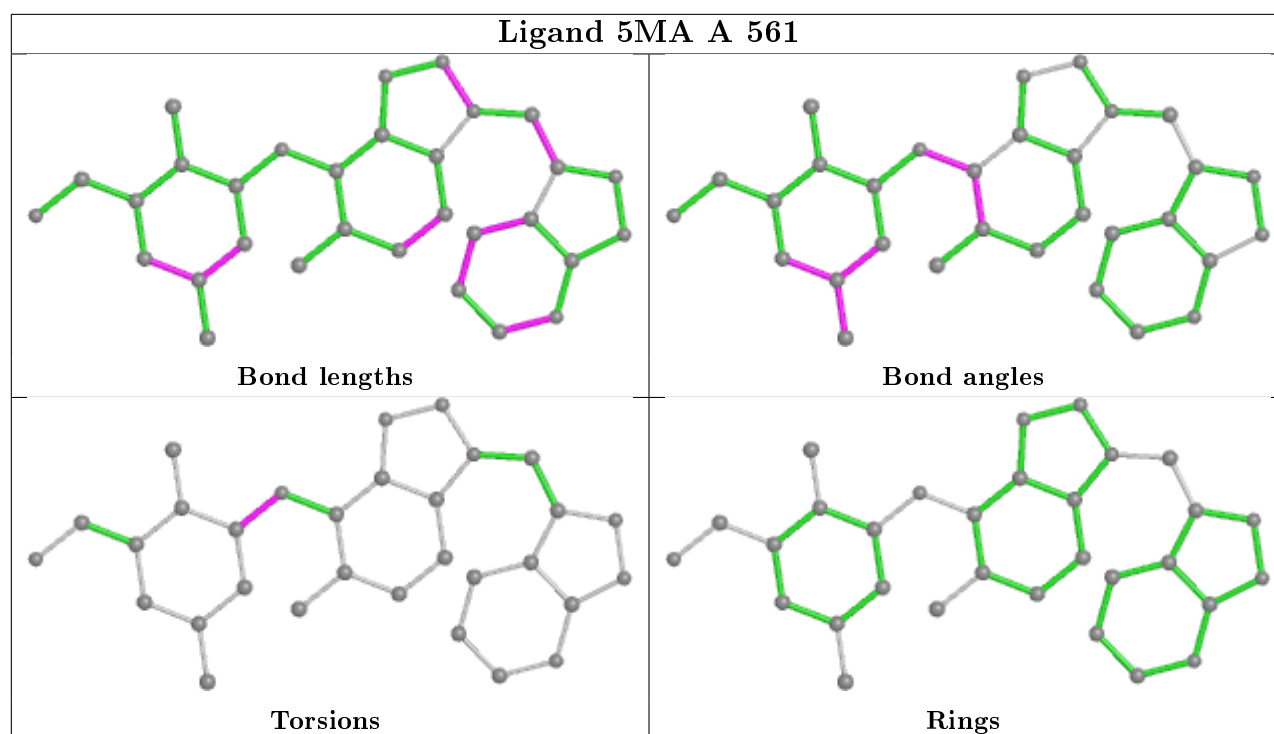
There are no ring outliers.

1 monomer is involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	561	5MA	4	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

### 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	554/563 (98%)	-0.15	15 (2%) 54 48	30, 51, 77, 98	0
1	B	400/563 (71%)	-0.10	18 (4%) 33 26	30, 52, 83, 104	0
All	All	954/1126 (84%)	-0.13	33 (3%) 44 36	30, 51, 80, 104	0

All (33) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	15	GLY	5.3
1	B	361	HIS	5.2
1	B	14	PRO	4.9
1	B	362	THR	4.7
1	B	231	GLY	4.5
1	B	250	ASP	4.0
1	A	284	ARG	3.9
1	A	69	THR	3.6
1	A	358	ARG	3.6
1	A	286	THR	3.4
1	A	359	GLY	3.4
1	B	69	THR	3.3
1	A	491	LEU	3.1
1	B	251	SER	3.0
1	A	70	LYS	2.8
1	B	90	VAL	2.7
1	B	284	ARG	2.6
1	A	360	ALA	2.6
1	A	221	HIS	2.6
1	B	301	LEU	2.5
1	B	43	LYS	2.5
1	A	285	GLY	2.4
1	B	311	LYS	2.4
1	A	193	LEU	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	550	LYS	2.4
1	B	297	GLU	2.4
1	B	70	LYS	2.4
1	A	72	ARG	2.4
1	A	495	ILE	2.3
1	B	322	SER	2.2
1	B	16	MET	2.2
1	B	6	GLU	2.1
1	A	357	MET	2.1

## 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](#)

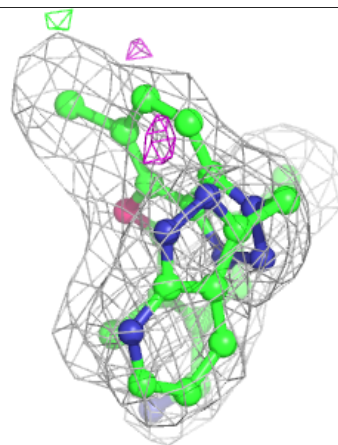
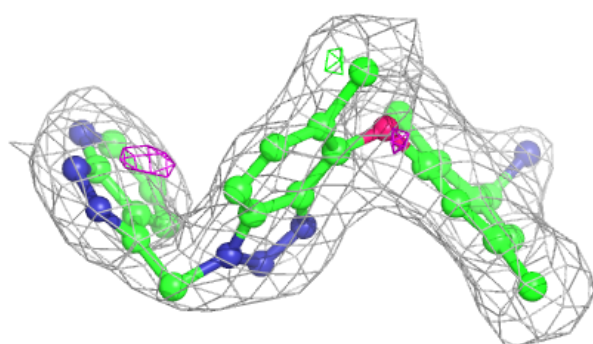
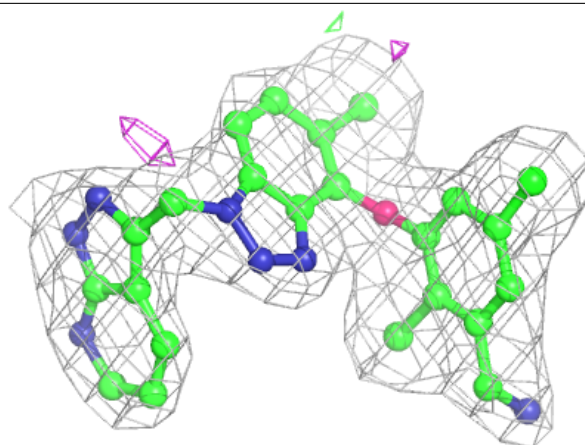
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	5MA	A	561	31/31	0.98	0.14	35,43,49,50	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.

**Electron density around 5MA A 561:**

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



## 6.5 Other polymers ⓘ

There are no such residues in this entry.