



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 27, 2023 – 07:55 AM EDT

PDB ID : 3IPY  
Title : X-Ray structure of Human Deoxycytidine Kinase in complex with an inhibitor  
Authors : Tari, L.W.; Swanson, R.V.; Hunter, M.; Hoffman, I.; Stouch, T.R.; Carson, K.G.  
Deposited on : 2009-08-18  
Resolution : 2.54 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.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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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 : 2.35  
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) : 2.35

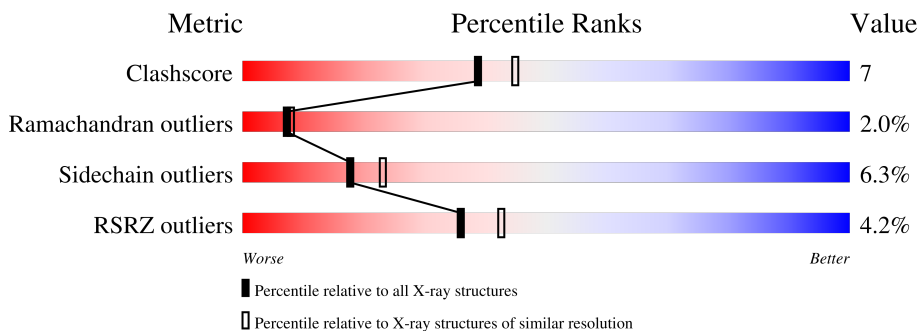
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.54 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	1332 (2.56-2.52)
Ramachandran outliers	138981	1315 (2.56-2.52)
Sidechain outliers	138945	1315 (2.56-2.52)
RSRZ outliers	127900	1272 (2.56-2.52)

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  $\geq 3$ , 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	241	
1	B	241	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	MLT	B	262	X	-	-	-

## 2 Entry composition [i](#)

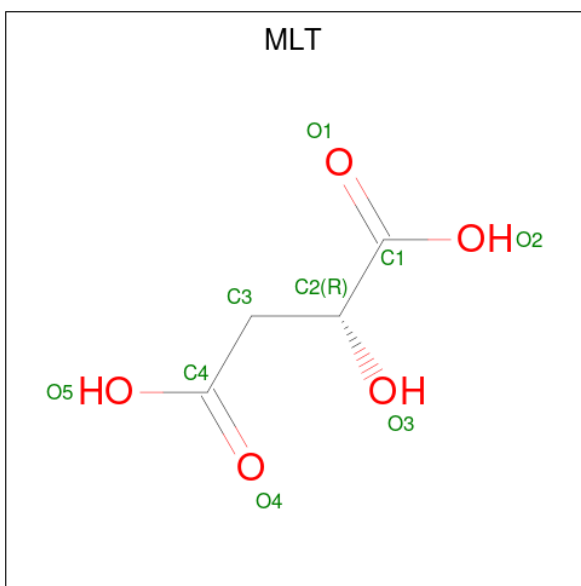
There are 4 unique types of molecules in this entry. The entry contains 3987 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Deoxycytidine kinase.

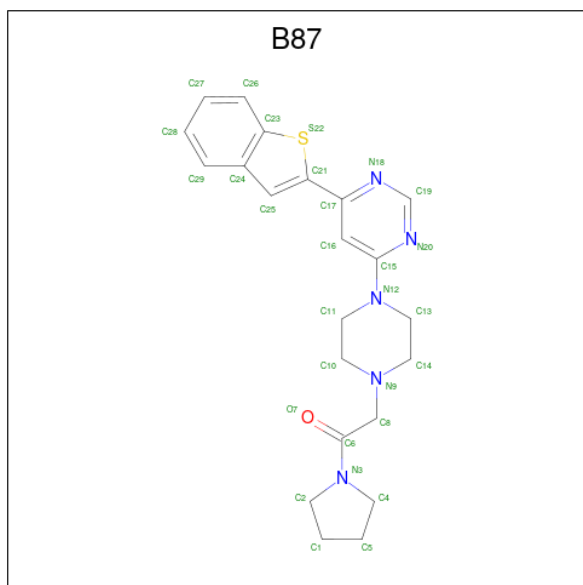
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	225	Total 1872	C 1200	N 311	O 352	S 9	20	0	0
1	B	225	Total 1871	C 1200	N 311	O 351	S 9	26	0	0

- Molecule 2 is D-MALATE (three-letter code: MLT) (formula:  $C_4H_6O_5$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
2	A	1	Total 9	C 4	O 5	0	0
2	B	1	Total 9	C 4	O 5	0	0

- Molecule 3 is 4-(1-benzothiophen-2-yl)-6-[4-(2-oxo-2-pyrrolidin-1-ylethyl)piperazin-1-yl]pyrimidine (three-letter code: B87) (formula:  $C_{22}H_{25}N_5OS$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	S		
3	A	1	Total	C	N	O	S	0	0
			29	22	5	1	1		
3	A	1	Total	C	N	O	S	0	0
			29	22	5	1	1		
3	B	1	Total	C	N	O	S	0	0
			29	22	5	1	1		
3	B	1	Total	C	N	O	S	0	0
			29	22	5	1	1		

- Molecule 4 is water.

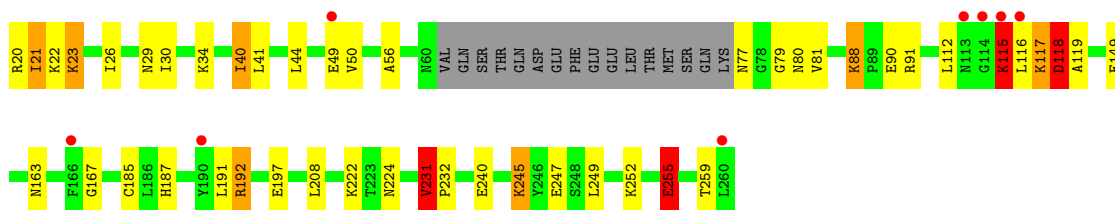
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	53	Total	O	0	0
			53	53		
4	B	57	Total	O	0	0
			57	57		

### 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 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.

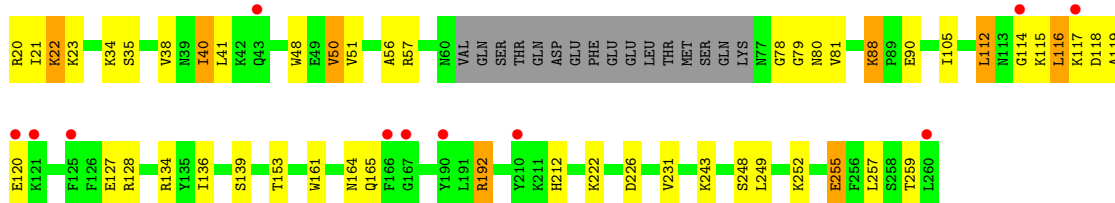
- Molecule 1: Deoxycytidine kinase

Chain A: 



- Molecule 1: Deoxycytidine kinase

Chain B: 



## 4 Data and refinement statistics i

Property	Value	Source
Space group	I 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	74.56Å 74.43Å 239.10Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	119.52 – 2.54 48.20 – 2.54	Depositor EDS
% Data completeness (in resolution range)	94.5 (119.52-2.54) 89.9 (48.20-2.54)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.34 (at 2.54Å)	Xtrriage
Refinement program	REFMAC 5.2.0005	Depositor
R, $R_{free}$	0.214 , 0.273 0.218 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	39.3	Xtrriage
Anisotropy	0.423	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.39 , 29.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	0.468 for -k,-h,-l	Xtrriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	3987	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	43.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.70% 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: B87, MLT

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	1.04	9/1916 (0.5%)	0.82	10/2589 (0.4%)
1	B	1.41	14/1915 (0.7%)	1.20	17/2589 (0.7%)
All	All	1.24	23/3831 (0.6%)	1.03	27/5178 (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	A	0	1
1	B	1	0
All	All	1	1

All (23) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	57	ARG	CZ-NH2	-40.17	0.80	1.33
1	A	240	GLU	CG-CD	-27.67	1.10	1.51
1	B	252	LYS	CE-NZ	-18.92	1.01	1.49
1	B	56	ALA	CA-CB	-15.48	1.20	1.52
1	B	164	ASN	CB-CG	-14.77	1.17	1.51
1	A	255	GLU	CB-CG	-14.50	1.24	1.52
1	B	21	ILE	CB-CG2	-13.50	1.10	1.52
1	A	21	ILE	CB-CG2	-12.64	1.13	1.52
1	B	88	LYS	CE-NZ	12.63	1.80	1.49
1	A	56	ALA	CA-CB	-11.67	1.27	1.52
1	B	51	VAL	CB-CG2	-10.14	1.31	1.52
1	A	40	ILE	CB-CG1	-9.91	1.26	1.54
1	B	243	LYS	CE-NZ	-9.74	1.24	1.49
1	A	22	LYS	CG-CD	-8.96	1.22	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	22	LYS	CG-CD	-8.92	1.22	1.52
1	B	50	VAL	CB-CG1	-8.71	1.34	1.52
1	B	231	VAL	CB-CG2	8.52	1.70	1.52
1	A	255	GLU	CD-OE1	7.95	1.34	1.25
1	A	255	GLU	CG-CD	-7.04	1.41	1.51
1	B	153	THR	CB-CG2	-6.80	1.29	1.52
1	B	112	LEU	CG-CD2	6.60	1.76	1.51
1	A	50	VAL	CB-CG1	-6.19	1.39	1.52
1	B	248	SER	CB-OG	-5.49	1.35	1.42

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	57	ARG	NE-CZ-NH2	32.19	136.40	120.30
1	B	57	ARG	NH1-CZ-NH2	-14.89	103.02	119.40
1	B	40	ILE	CG1-CB-CG2	14.39	143.05	111.40
1	B	112	LEU	CD1-CG-CD2	-13.55	69.84	110.50
1	B	22	LYS	CB-CG-CD	13.37	146.35	111.60
1	A	231	VAL	CG1-CB-CG2	-12.62	90.71	110.90
1	B	41	LEU	CB-CG-CD1	-11.34	91.72	111.00
1	A	56	ALA	N-CA-CB	10.35	124.58	110.10
1	A	40	ILE	CG1-CB-CG2	10.30	134.06	111.40
1	A	41	LEU	CB-CG-CD1	-9.81	94.32	111.00
1	B	112	LEU	CB-CG-CD2	-9.79	94.36	111.00
1	B	164	ASN	CA-CB-CG	9.33	133.93	113.40
1	B	51	VAL	CA-CB-CG2	9.21	124.71	110.90
1	B	164	ASN	CB-CG-OD1	-8.26	105.07	121.60
1	B	50	VAL	CA-CB-CG1	-8.01	98.89	110.90
1	B	252	LYS	CD-CE-NZ	-7.95	93.41	111.70
1	B	153	THR	CA-CB-CG2	7.76	123.27	112.40
1	A	21	ILE	CA-CB-CG2	7.75	126.41	110.90
1	B	21	ILE	CG1-CB-CG2	7.74	128.42	111.40
1	A	252	LYS	CD-CE-NZ	-6.73	96.21	111.70
1	B	22	LYS	CG-CD-CE	-6.55	92.26	111.90
1	A	22	LYS	CB-CG-CD	6.49	128.47	111.60
1	A	255	GLU	CA-CB-CG	6.28	127.21	113.40
1	B	164	ASN	OD1-CG-ND2	5.58	134.74	121.90
1	A	255	GLU	CG-CD-OE2	-5.37	107.57	118.30
1	B	105	ILE	CB-CG1-CD1	5.36	128.91	113.90
1	A	240	GLU	CG-CD-OE2	5.33	128.95	118.30

All (1) chirality outliers are listed below:



Mol	Chain	Res	Type	Atom
1	B	40	ILE	CB

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	255	GLU	Sidechain

## 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	1872	0	1820	28	0
1	B	1871	0	1820	24	0
2	A	9	0	4	1	0
2	B	9	0	4	1	0
3	A	58	0	50	3	0
3	B	58	0	50	2	0
4	A	53	0	0	3	0
4	B	57	0	0	3	0
All	All	3987	0	3748	56	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 7.

All (56) 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:192:ARG:HG2	1:B:192:ARG:HH21	1.32	0.92
1:A:90:GLU:HG2	3:A:264:B87:H2A	1.51	0.88
1:A:192:ARG:HH21	1:A:192:ARG:HG2	1.40	0.84
1:B:192:ARG:HH21	1:B:192:ARG:CG	2.01	0.72
1:A:192:ARG:HH21	1:A:192:ARG:CG	2.07	0.68
1:B:34:LYS:HE2	1:B:128:ARG:NH2	2.11	0.66
1:A:149:GLU:HG2	4:A:289:HOH:O	1.95	0.66
2:B:262:MLT:O4	4:B:332:HOH:O	2.15	0.63
1:B:192:ARG:HG2	1:B:192:ARG:NH2	2.08	0.62
1:A:77:ASN:N	1:A:80:ASN:HB2	2.14	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:88:LYS:HE2	1:A:91:ARG:HB2	1.82	0.61
1:B:116:LEU:C	1:B:118:ASP:H	2.04	0.59
1:A:34:LYS:NZ	2:A:261:MLT:O2	2.35	0.59
1:A:163:ASN:O	1:A:167:GLY:HA3	2.05	0.56
1:A:23:LYS:HD2	1:A:112:LEU:HD21	1.88	0.56
1:A:192:ARG:HG2	1:A:192:ARG:NH2	2.16	0.56
1:B:48:TRP:CZ2	1:B:257:LEU:HD12	2.41	0.55
1:B:78:GLY:C	1:B:80:ASN:H	2.11	0.54
1:A:115:LYS:HA	1:A:117:LYS:HG3	1.91	0.52
1:A:117:LYS:O	1:A:119:ALA:N	2.43	0.51
1:B:161:TRP:O	1:B:165:GLN:HG2	2.11	0.51
1:A:187:HIS:O	1:A:191:LEU:HG	2.10	0.50
1:A:30:ILE:HD12	1:A:208:LEU:HD12	1.93	0.49
1:A:245:LYS:HA	4:A:292:HOH:O	2.12	0.49
1:B:116:LEU:O	1:B:118:ASP:N	2.46	0.49
1:A:49:GLU:HG2	1:A:116:LEU:HD13	1.96	0.47
1:A:115:LYS:C	1:A:117:LYS:H	2.18	0.47
1:B:118:ASP:HA	1:B:119:ALA:HA	1.79	0.46
1:B:116:LEU:O	1:B:116:LEU:HG	2.15	0.46
1:A:90:GLU:HG2	3:A:264:B87:C2	2.35	0.45
1:A:118:ASP:CG	1:A:119:ALA:N	2.70	0.45
1:B:136:ILE:HG21	1:B:212:HIS:CE1	2.52	0.45
1:A:21:ILE:HD12	1:A:112:LEU:HD23	1.99	0.45
1:B:78:GLY:O	1:B:80:ASN:N	2.49	0.45
3:B:265:B87:H16	3:B:265:B87:H11A	1.75	0.44
1:A:247:GLU:HG2	4:A:292:HOH:O	2.17	0.44
1:A:192:ARG:NH2	1:A:197:GLU:OE1	2.47	0.43
1:B:34:LYS:HE2	1:B:128:ARG:CZ	2.48	0.43
1:B:116:LEU:C	1:B:118:ASP:N	2.72	0.43
1:B:192:ARG:NH2	4:B:320:HOH:O	2.52	0.42
1:B:134:ARG:O	1:B:139:SER:HB2	2.19	0.42
1:A:23:LYS:HB2	1:A:23:LYS:HE3	1.82	0.42
1:B:114:GLY:HA2	1:B:115:LYS:HG2	2.01	0.42
1:B:78:GLY:C	1:B:80:ASN:N	2.72	0.42
3:B:266:B87:H16	3:B:266:B87:H13	1.83	0.42
1:A:26:ILE:HG22	1:A:34:LYS:HG2	2.02	0.41
1:A:255:GLU:O	1:A:259:THR:HG23	2.20	0.41
1:A:245:LYS:HB3	1:A:245:LYS:HE2	1.76	0.41
1:B:38:VAL:HG13	1:B:50:VAL:HG21	2.03	0.41
1:B:90:GLU:H	1:B:90:GLU:CD	2.24	0.41
1:B:114:GLY:HA2	1:B:115:LYS:CG	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:231:VAL:HA	1:A:232:PRO:HD3	1.95	0.41
1:A:29:ASN:HB3	1:A:185:CYS:SG	2.62	0.40
1:B:35:SER:HB2	4:B:331:HOH:O	2.21	0.40
3:A:263:B87:H11A	3:A:263:B87:H16	1.85	0.40
1:B:255:GLU:O	1:B:259:THR:HG23	2.22	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	221/241 (92%)	205 (93%)	11 (5%)	5 (2%)	6	6
1	B	221/241 (92%)	211 (96%)	6 (3%)	4 (2%)	8	10
All	All	442/482 (92%)	416 (94%)	17 (4%)	9 (2%)	7	8

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	118	ASP
1	B	116	LEU
1	B	117	LYS
1	A	79	GLY
1	B	79	GLY
1	A	44	LEU
1	B	120	GLU
1	A	117	LYS
1	A	115	LYS

### 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	205/223 (92%)	192 (94%)	13 (6%)	18	23
1	B	205/223 (92%)	192 (94%)	13 (6%)	18	23
All	All	410/446 (92%)	384 (94%)	26 (6%)	18	23

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	20	ARG
1	A	23	LYS
1	A	40	ILE
1	A	81	VAL
1	A	88	LYS
1	A	115	LYS
1	A	118	ASP
1	A	192	ARG
1	A	222	LYS
1	A	224	ASN
1	A	231	VAL
1	A	245	LYS
1	A	249	LEU
1	B	20	ARG
1	B	22	LYS
1	B	23	LYS
1	B	40	ILE
1	B	81	VAL
1	B	88	LYS
1	B	112	LEU
1	B	127	GLU
1	B	192	ARG
1	B	222	LYS
1	B	226	ASP
1	B	249	LEU
1	B	255	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	39	ASN
1	A	97	GLN
1	B	39	ASN
1	B	80	ASN
1	B	97	GLN
1	B	163	ASN

### 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](#)

6 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
3	B87	B	265	-	31,33,33	1.67	2 (6%)	35,46,46	2.61	12 (34%)
3	B87	A	264	-	31,33,33	1.75	1 (3%)	35,46,46	2.62	12 (34%)
3	B87	B	266	-	31,33,33	1.83	1 (3%)	35,46,46	2.80	12 (34%)
2	MLT	A	261	-	8,8,8	1.04	0	10,10,10	1.76	2 (20%)
2	MLT	B	262	-	8,8,8	1.16	0	10,10,10	1.86	4 (40%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	B87	A	263	-	31,33,33	1.77	1 (3%)	35,46,46	2.59	12 (34%)

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	B87	B	265	-	-	1/12/33/33	0/5/5/5
3	B87	A	264	-	-	4/12/33/33	0/5/5/5
3	B87	B	266	-	-	7/12/33/33	0/5/5/5
2	MLT	A	261	-	-	4/8/8/8	-
2	MLT	B	262	-	1/1/3/3	5/8/8/8	-
3	B87	A	263	-	-	1/12/33/33	0/5/5/5

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	266	B87	C23-S22	-8.71	1.67	1.74
3	A	263	B87	C23-S22	-8.57	1.67	1.74
3	A	264	B87	C23-S22	-8.36	1.67	1.74
3	B	265	B87	C23-S22	-7.70	1.68	1.74
3	B	265	B87	C28-C29	2.00	1.41	1.36

All (54) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	266	B87	C14-N9-C10	7.73	126.23	108.83
3	B	266	B87	C19-N20-C15	7.72	121.69	114.94
3	A	264	B87	C19-N20-C15	6.81	120.89	114.94
3	A	263	B87	C19-N20-C15	6.58	120.69	114.94
3	B	265	B87	C14-N9-C10	6.24	122.88	108.83
3	B	265	B87	C19-N20-C15	6.12	120.28	114.94
3	A	263	B87	C14-N9-C10	5.98	122.29	108.83
3	A	264	B87	C14-N9-C10	5.94	122.21	108.83
3	B	266	B87	N18-C19-N20	-5.75	119.69	128.68
3	A	263	B87	C8-N9-C10	5.29	119.30	111.09
3	A	264	B87	C8-N9-C14	5.16	119.10	111.09
3	B	265	B87	C8-N9-C10	5.12	119.04	111.09
3	B	265	B87	N18-C19-N20	-5.08	120.74	128.68
3	A	264	B87	N18-C19-N20	-4.95	120.95	128.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	264	B87	C8-N9-C10	4.89	118.69	111.09
3	A	263	B87	N18-C19-N20	-4.87	121.06	128.68
3	A	263	B87	C8-N9-C14	4.71	118.40	111.09
3	B	265	B87	C13-N12-C11	4.69	121.86	111.52
3	B	266	B87	C19-N18-C17	4.63	121.78	115.40
3	B	266	B87	C8-N9-C10	4.52	118.11	111.09
3	B	265	B87	C8-N9-C14	4.50	118.08	111.09
3	B	266	B87	C10-C11-N12	-4.47	102.01	110.70
3	A	263	B87	C13-N12-C11	4.43	121.29	111.52
3	A	264	B87	C19-N18-C17	4.26	121.27	115.40
3	A	264	B87	C13-N12-C11	4.22	120.84	111.52
3	A	263	B87	C19-N18-C17	4.20	121.18	115.40
3	B	265	B87	C19-N18-C17	4.00	120.91	115.40
2	A	261	MLT	O2-C1-C2	3.56	120.55	112.72
3	A	264	B87	C16-C17-N18	-3.32	118.80	121.54
2	B	262	MLT	O2-C1-O1	-3.14	116.97	124.09
3	A	263	B87	C16-C17-N18	-3.13	118.96	121.54
3	B	265	B87	C10-C11-N12	-3.11	104.65	110.70
2	A	261	MLT	O2-C1-O1	-2.99	117.31	124.09
3	B	266	B87	C8-N9-C14	2.91	115.61	111.09
3	B	266	B87	C14-C13-N12	-2.85	105.17	110.70
3	B	266	B87	C16-C17-N18	-2.76	119.26	121.54
3	B	265	B87	N20-C15-N12	2.76	120.92	116.79
3	B	266	B87	N20-C15-N12	2.68	120.80	116.79
3	A	263	B87	C4-N3-C2	2.52	114.80	111.34
3	B	265	B87	C16-C17-N18	-2.47	119.50	121.54
3	B	265	B87	C16-C15-N12	-2.46	119.38	122.30
2	B	262	MLT	O2-C1-C2	2.44	118.09	112.72
3	A	264	B87	C16-C15-N20	-2.35	118.65	122.73
3	B	266	B87	C13-N12-C11	2.34	116.68	111.52
3	A	263	B87	C10-C11-N12	-2.29	106.25	110.70
3	B	265	B87	C4-N3-C2	2.24	114.42	111.34
3	B	266	B87	C16-C15-N20	-2.22	118.88	122.73
2	B	262	MLT	C3-C2-C1	2.18	115.49	110.33
3	A	263	B87	N20-C15-N12	2.14	119.99	116.79
3	A	264	B87	C10-C11-N12	-2.14	106.55	110.70
3	A	263	B87	C16-C15-N20	-2.13	119.05	122.73
3	A	264	B87	C4-N3-C2	2.11	114.24	111.34
3	A	264	B87	N20-C15-N12	2.11	119.95	116.79
2	B	262	MLT	C2-C3-C4	-2.00	107.18	112.13

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	B	262	MLT	C2

All (22) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	264	B87	O7-C6-N3-C2
3	A	264	B87	C8-C6-N3-C2
3	A	264	B87	O7-C6-N3-C4
3	A	264	B87	C8-C6-N3-C4
3	B	266	B87	O7-C6-N3-C2
3	B	266	B87	C8-C6-N3-C2
3	B	266	B87	O7-C6-N3-C4
3	B	266	B87	C8-C6-N3-C4
2	B	262	MLT	O1-C1-C2-O3
2	B	262	MLT	O2-C1-C2-O3
3	A	263	B87	C6-C8-N9-C14
3	B	266	B87	C6-C8-N9-C14
3	B	266	B87	O7-C6-C8-N9
3	B	266	B87	N3-C6-C8-N9
3	B	265	B87	C6-C8-N9-C14
2	A	261	MLT	O3-C2-C3-C4
2	B	262	MLT	O3-C2-C3-C4
2	A	261	MLT	C1-C2-C3-C4
2	A	261	MLT	O1-C1-C2-O3
2	A	261	MLT	O2-C1-C2-O3
2	B	262	MLT	O1-C1-C2-C3
2	B	262	MLT	O2-C1-C2-C3

There are no ring outliers.

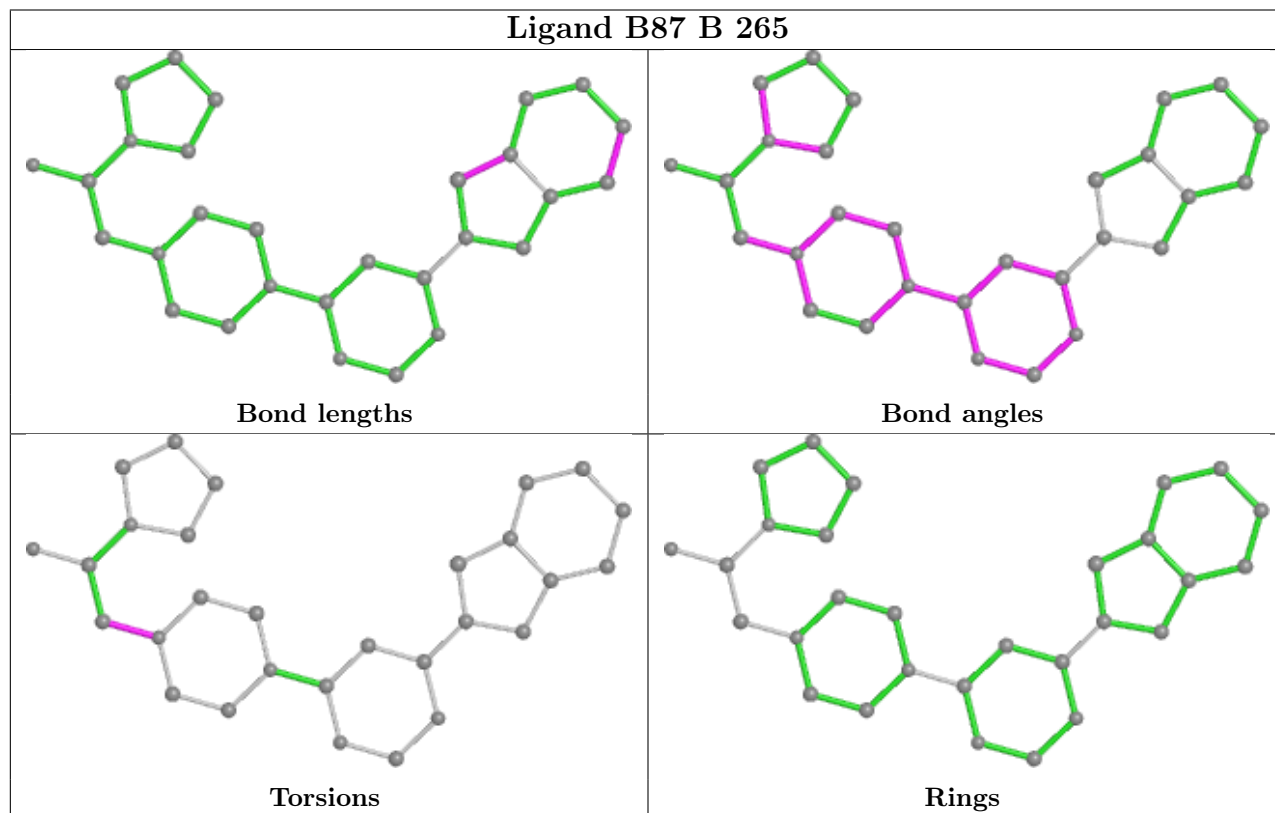
6 monomers are involved in 7 short contacts:

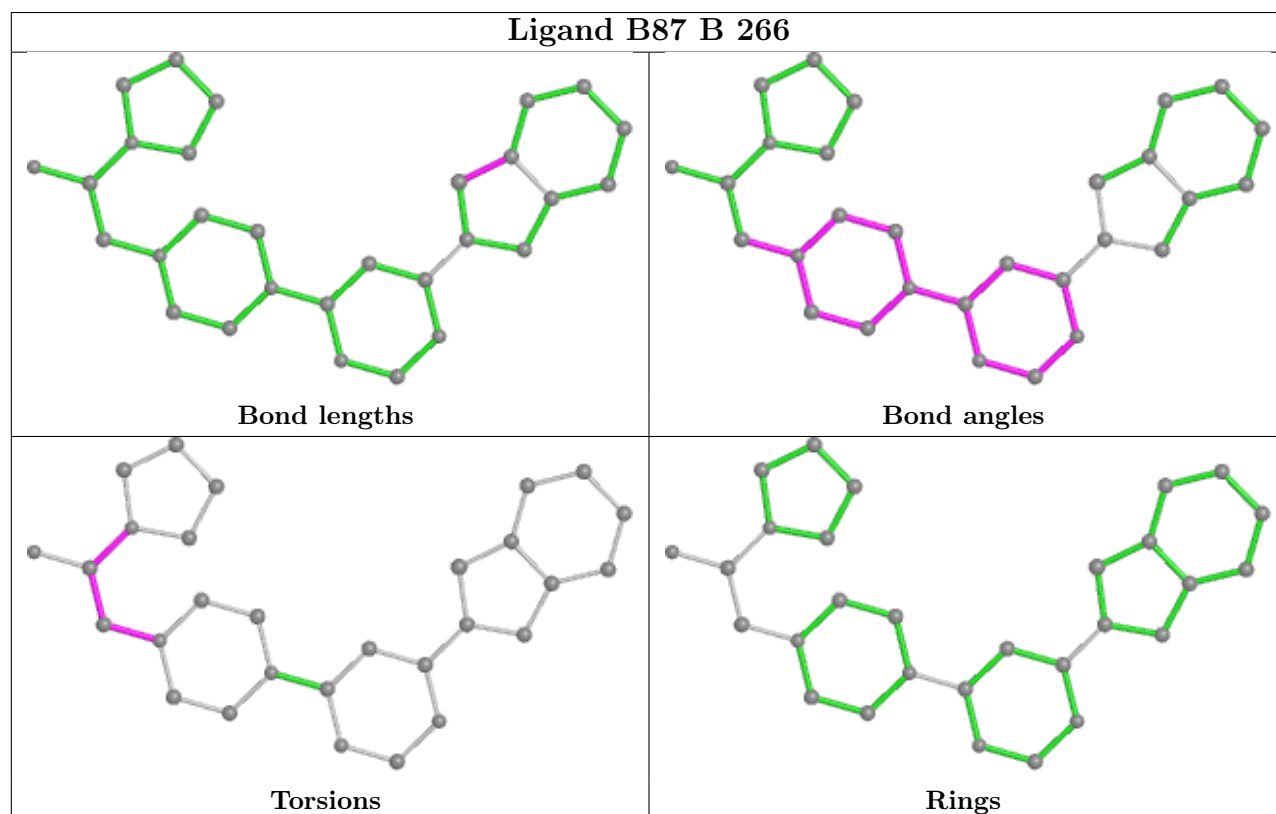
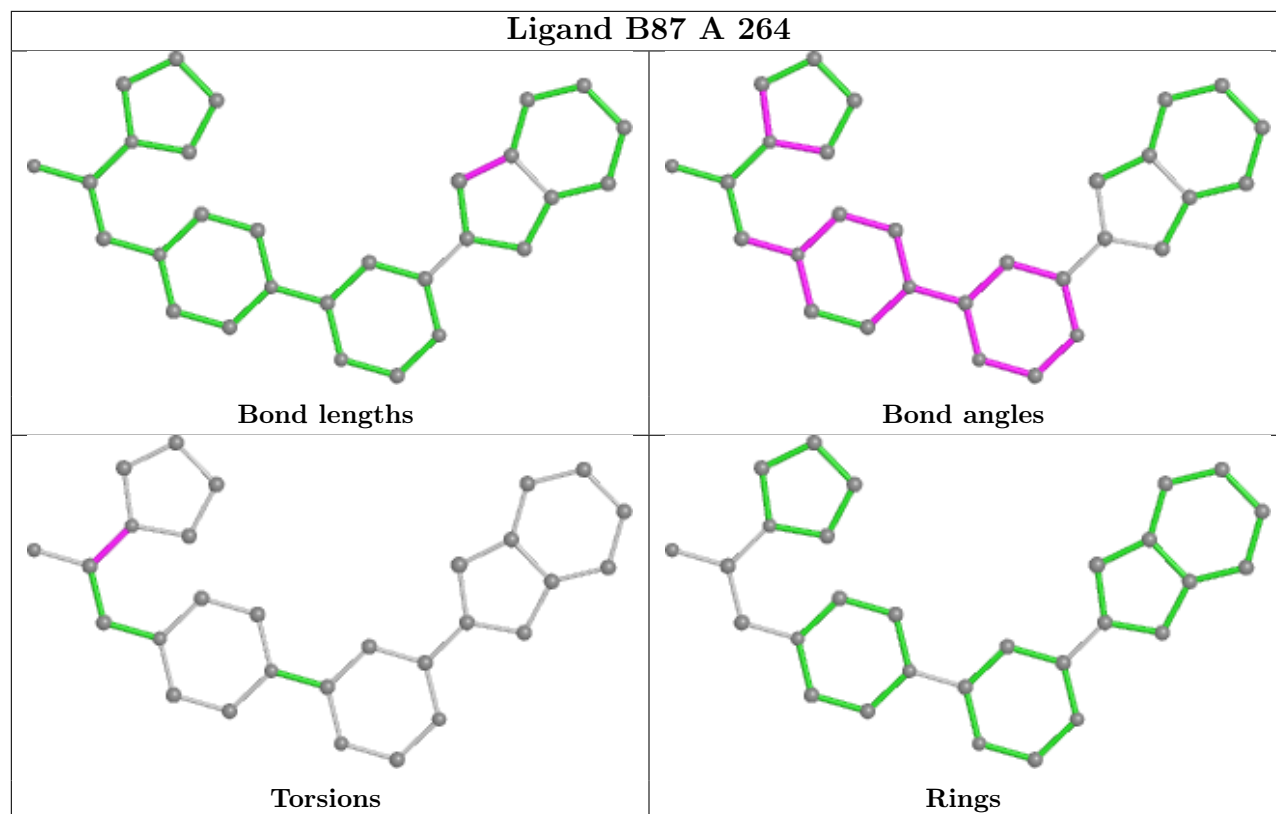
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	265	B87	1	0
3	A	264	B87	2	0
3	B	266	B87	1	0
2	A	261	MLT	1	0
2	B	262	MLT	1	0
3	A	263	B87	1	0

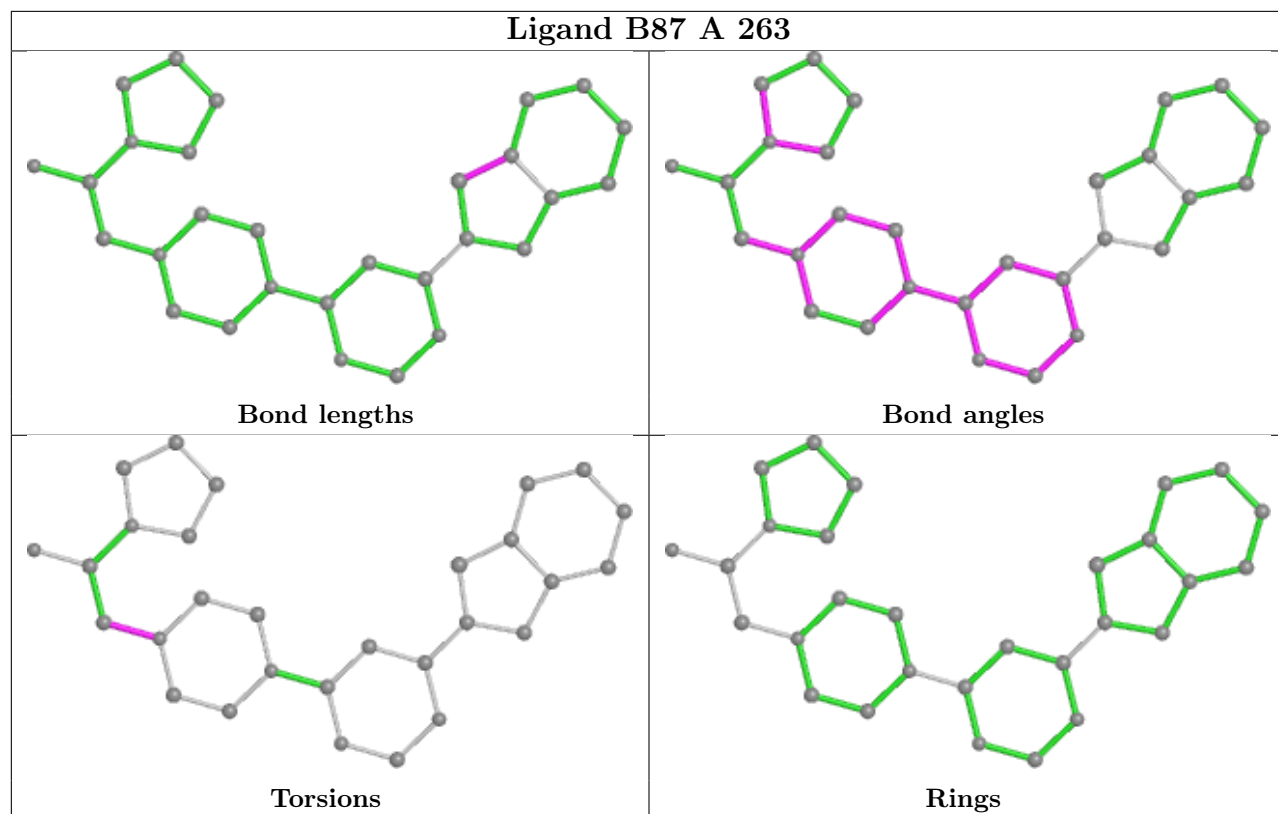
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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](#)

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	225/241 (93%)	0.55	8 (3%) 42 49	28, 42, 64, 77	12 (5%)
1	B	225/241 (93%)	0.59	11 (4%) 29 35	28, 43, 64, 77	18 (8%)
All	All	450/482 (93%)	0.57	19 (4%) 36 42	28, 43, 64, 77	30 (6%)

All (19) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	115	LYS	5.3
1	B	120	GLU	3.7
1	A	166	PHE	3.2
1	B	166	PHE	2.9
1	A	49	GLU	2.8
1	A	113	ASN	2.7
1	B	114	GLY	2.7
1	A	114	GLY	2.6
1	B	121	LYS	2.4
1	A	116	LEU	2.3
1	B	260	LEU	2.3
1	B	167	GLY	2.2
1	A	260	LEU	2.2
1	B	210	TYR	2.1
1	B	43	GLN	2.1
1	B	117	LYS	2.1
1	A	190	TYR	2.0
1	B	190	TYR	2.0
1	B	125	PHE	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](#)

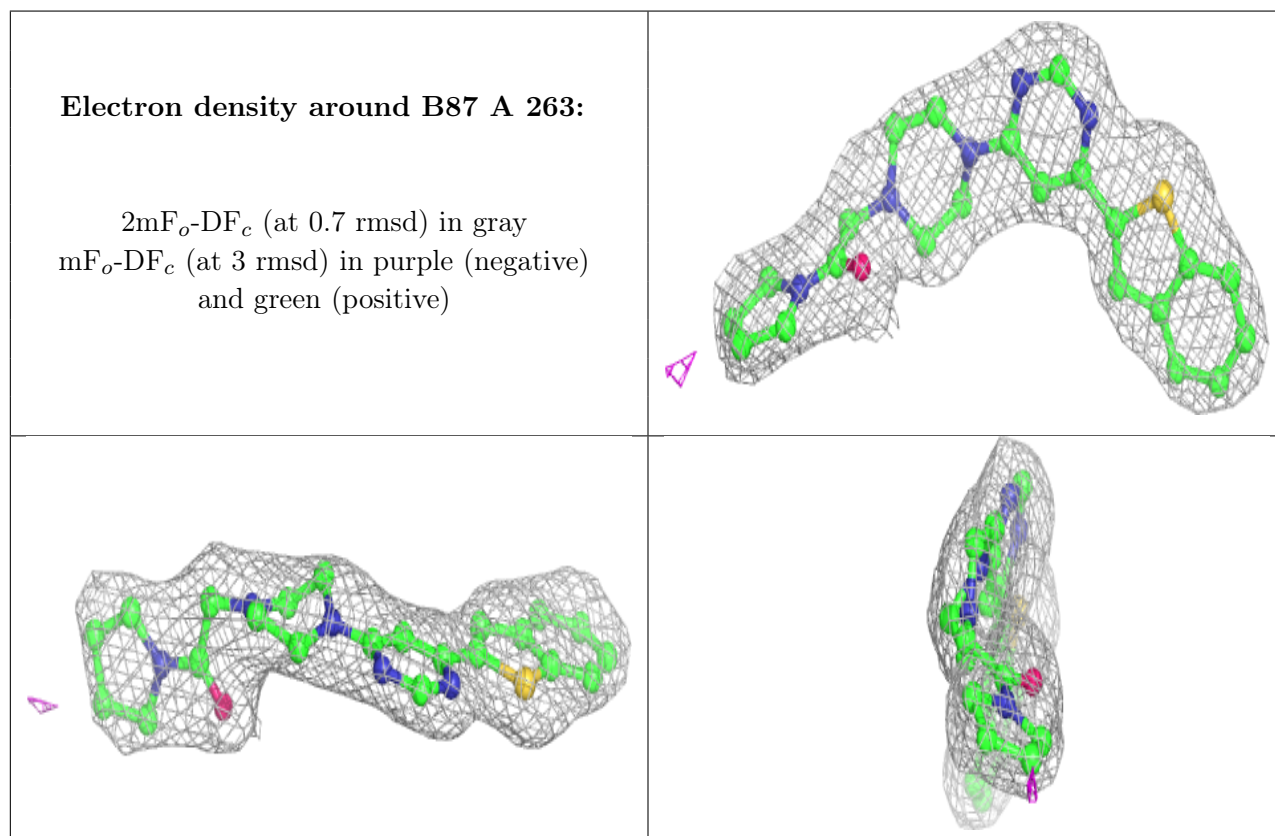
There are no monosaccharides in this entry.

### 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.

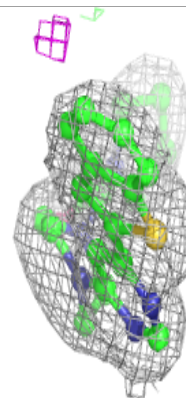
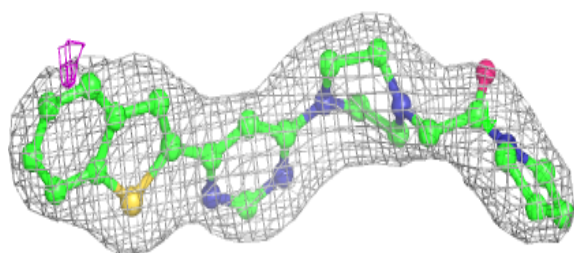
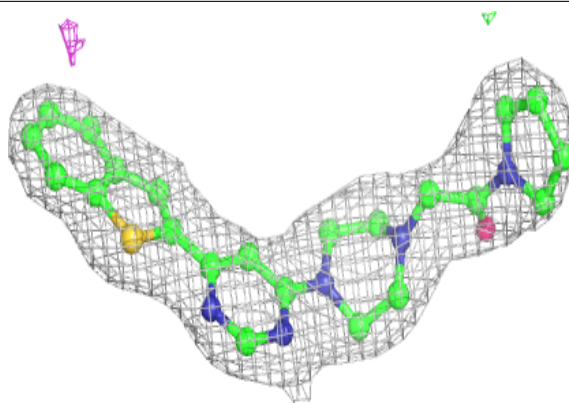
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
2	MLT	A	261	9/9	0.89	0.20	47,49,49,49	0
2	MLT	B	262	9/9	0.90	0.22	45,49,51,51	0
3	B87	A	263	29/29	0.96	0.17	30,32,34,34	0
3	B87	A	264	29/29	0.96	0.19	34,37,51,52	0
3	B87	B	266	29/29	0.96	0.20	32,35,53,53	0
3	B87	B	265	29/29	0.97	0.16	33,34,34,36	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.

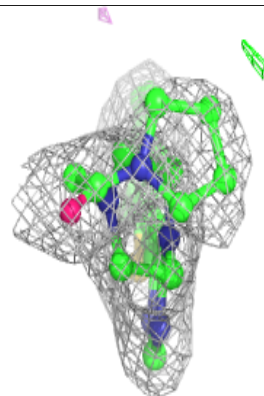
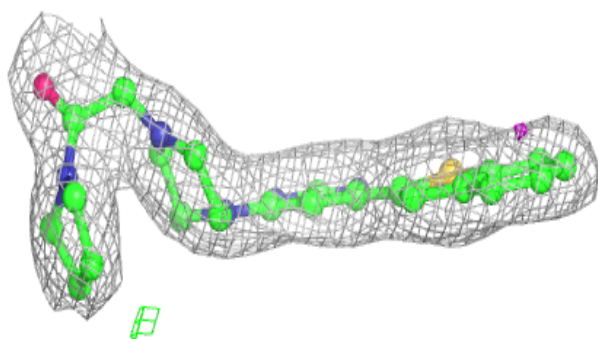
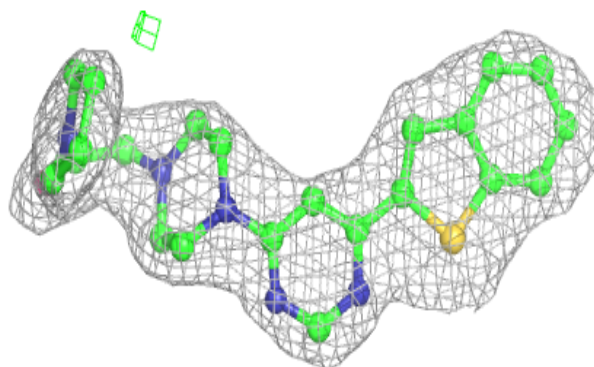


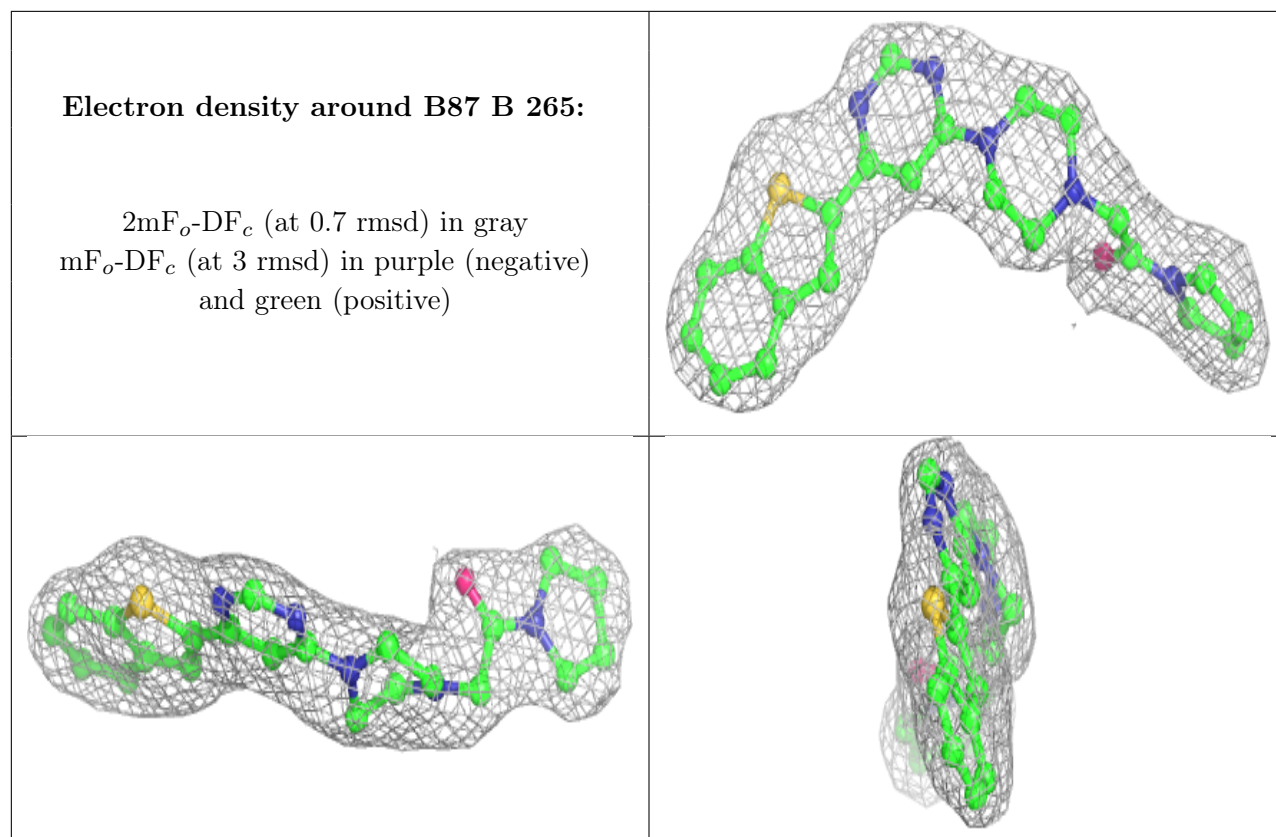
**Electron density around B87 A 264:**

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

**Electron density around B87 B 266:**

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





## 6.5 Other polymers [i](#)

There are no such residues in this entry.