



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 04:28 PM UTC

PDB ID : 3IPY / pdb_00003ipy
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

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>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

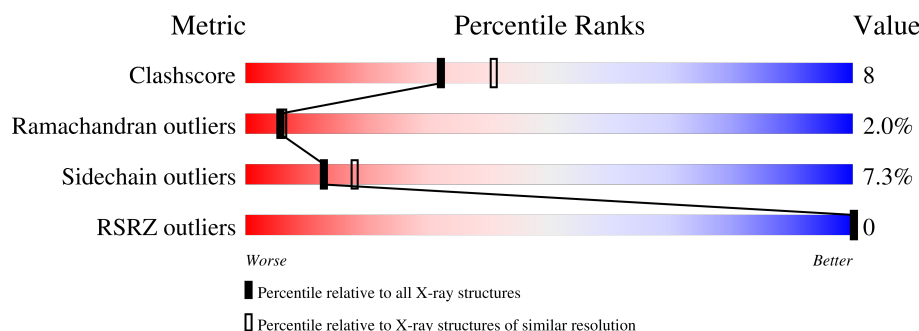
1 Overall quality at a glance

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	190562	1120 (2.54-2.54)
Ramachandran outliers	187476	1106 (2.54-2.54)
Sidechain outliers	187428	1106 (2.54-2.54)
RSRZ outliers	180081	1091 (2.54-2.54)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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](#)

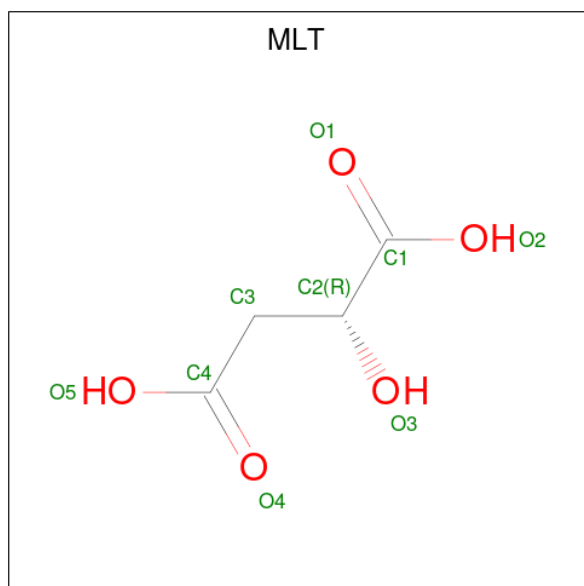
There are 4 unique types of molecules in this entry. The entry contains 3987 atoms, of which 0 are hydrogens and 0 are deuteriums.

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.

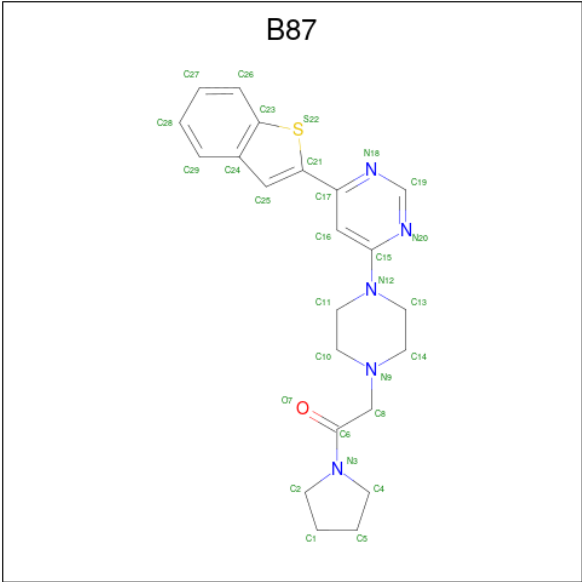
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	225	Total	C	N	O	S	20	0	0
			1872	1200	311	352	9			
1	B	225	Total	C	N	O	S	26	0	0
			1871	1200	311	351	9			

- Molecule 2 is D-MALATE (CCD ID: MLT) (formula: C₄H₆O₅).



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

- Molecule 3 is 4-(1-benzothiophen-2-yl)-6-[4-(2-oxo-2-pyrrolidin-1-ylethyl)piperazin-1-yl]pyrimidine (CCD ID: B87) (formula: C₂₂H₂₅N₅OS).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
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		

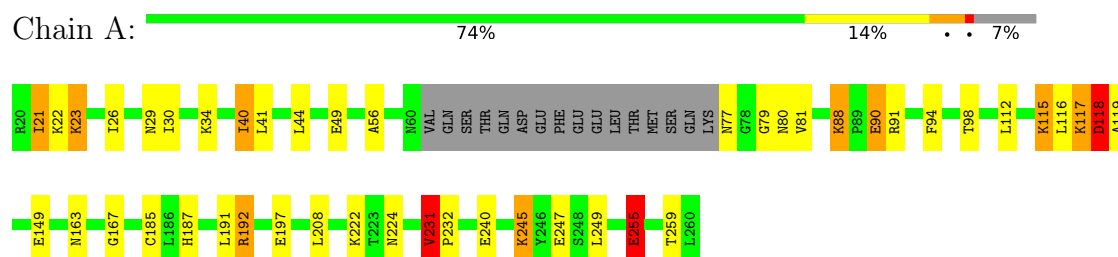
- Molecule 4 is water.

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

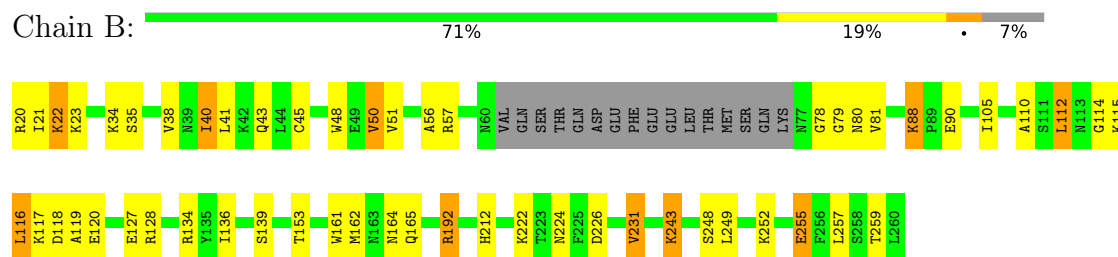
3 Residue-property plots

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



• Molecule 1: Deoxycytidine kinase



4 Data and refinement statistics

Property	Value	Source
Space group	I 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	74.56Å 74.43Å 239.10Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	119.52 – 2.54 119.52 – 2.54	Depositor EDS
% Data completeness (in resolution range)	94.5 (119.52-2.54) 89.9 (119.52-2.54)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.34 (at 2.54Å)	Xtriage
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 ²)	39.3	Xtriage
Anisotropy	0.423	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 31.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.468 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	3987	wwPDB-VP
Average B, all atoms (Å ²)	43.0	wwPDB-VP

Xtriage'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.*

¹Intensities estimated from amplitudes.

²Theoretical 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

5.1 Standard geometry

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	0.95	6/1916 (0.3%)	0.98	7/2589 (0.3%)
1	B	1.44	17/1915 (0.9%)	1.30	19/2589 (0.7%)
All	All	1.22	23/3831 (0.6%)	1.15	26/5178 (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	-40.48	0.80	1.33
1	B	56	ALA	CA-CB	-21.55	1.20	1.53
1	A	240	GLU	CG-CD	-16.64	1.10	1.52
1	A	56	ALA	CA-CB	-16.39	1.27	1.53
1	B	252	LYS	CE-NZ	-15.87	1.01	1.49
1	B	164	ASN	CB-CG	-13.99	1.17	1.52
1	A	40	ILE	CB-CG1	-13.57	1.26	1.53
1	B	21	ILE	CB-CG2	-12.59	1.10	1.52
1	A	21	ILE	CB-CG2	-11.78	1.13	1.52
1	B	88	LYS	CE-NZ	10.43	1.80	1.49
1	A	22	LYS	CG-CD	-10.15	1.22	1.52
1	B	22	LYS	CG-CD	-10.11	1.22	1.52
1	A	255	GLU	CB-CG	-9.28	1.24	1.52
1	B	243	LYS	CE-NZ	-8.22	1.24	1.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	105	ILE	CG1-CD1	-8.12	1.20	1.51
1	B	112	LEU	CG-CD2	7.19	1.76	1.52
1	B	162	MET	SD-CE	-6.99	1.62	1.79
1	B	153	THR	CB-CG2	-6.86	1.29	1.52
1	B	40	ILE	CB-CG1	-6.55	1.40	1.53
1	B	51	VAL	CB-CG2	-6.36	1.31	1.52
1	B	231	VAL	CB-CG2	5.51	1.70	1.52
1	B	50	VAL	CB-CG1	-5.45	1.34	1.52
1	B	110	ALA	CA-CB	5.17	1.61	1.53

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	164	ASN	CA-CB-CG	21.33	133.93	112.60
1	B	57	ARG	NE-CZ-NH2	19.11	136.40	119.20
1	B	112	LEU	CD1-CG-CD2	-18.62	69.84	110.80
1	B	22	LYS	CB-CG-CD	15.24	146.35	111.30
1	B	57	ARG	NH1-CZ-NH2	-12.52	103.02	119.30
1	B	164	ASN	OD1-CG-ND2	12.14	134.74	122.60
1	B	40	ILE	CG1-CB-CG2	10.78	143.05	110.70
1	A	56	ALA	N-CA-CB	10.05	124.58	110.01
1	A	21	ILE	CA-CB-CG2	9.36	126.41	110.50
1	A	231	VAL	CG1-CB-CG2	-9.13	90.71	110.80
1	B	51	VAL	CA-CB-CG2	8.42	124.71	110.40
1	B	22	LYS	CG-CD-CE	-8.28	92.26	111.30
1	B	164	ASN	CB-CG-OD1	-7.86	105.07	120.80
1	A	40	ILE	CG1-CB-CG2	7.79	134.06	110.70
1	B	153	THR	CA-CB-CG2	7.51	123.27	110.50
1	A	22	LYS	CB-CG-CD	7.46	128.47	111.30
1	B	105	ILE	CB-CG1-CD1	7.19	128.91	113.80
1	B	50	VAL	CA-CB-CG1	-6.77	98.89	110.40
1	A	255	GLU	CA-CB-CG	6.56	127.21	114.10
1	B	248	SER	CA-CB-OG	6.46	124.01	111.10
1	B	41	LEU	CB-CG-CD1	-6.33	91.72	110.70
1	B	21	ILE	CG1-CB-CG2	5.91	128.42	110.70
1	B	252	LYS	CD-CE-NZ	-5.78	93.41	111.90
1	A	41	LEU	CB-CG-CD1	-5.46	94.32	110.70
1	B	112	LEU	CB-CG-CD2	-5.45	94.36	110.70
1	B	45	CYS	N-CA-C	5.20	116.98	109.07

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	31	0
1	B	1871	0	1820	25	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	60	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 8.

All (60) 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
1:B:116:LEU:C	1:B:118:ASP:H	2.04	0.64
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:77:ASN:N	1:A:80:ASN:HB2	2.14	0.62
1:A:88:LYS:HE2	1:A:91:ARG:HB2	1.82	0.61
1:A:34:LYS:NZ	2:A:261:MLT:O2	2.35	0.59
1:B:78:GLY:C	1:B:80:ASN:H	2.11	0.58
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:A:115:LYS:HA	1:A:117:LYS:HG3	1.91	0.52
1:A:115:LYS:C	1:A:117:LYS:H	2.18	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:118:ASP:CG	1:A:119:ALA:N	2.70	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:B:116:LEU:C	1:B:118:ASP:N	2.72	0.48
1:B:78:GLY:C	1:B:80:ASN:N	2.72	0.47
1:A:49:GLU:HG2	1:A:116:LEU:HD13	1.96	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:B:90:GLU:H	1:B:90:GLU:CD	2.24	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:H	1:A:247:GLU:CD	2.25	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:114:GLY:HA3	1:B:115:LYS:C	2.43	0.43
1:B:34:LYS:HE2	1:B:128:ARG:CZ	2.48	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
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:115:LYS:C	1:A:117:LYS:N	2.79	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:245:LYS:HB3	1:A:245:LYS:HE2	1.76	0.41
1:A:94:PHE:CD2	1:A:94:PHE:C	2.99	0.41
1:B:38:VAL:HG13	1:B:50:VAL:HG21	2.03	0.41
1:B:114:GLY:HA2	1:B:115:LYS:CG	2.51	0.41
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%)	5	4
1	B	221/241 (92%)	211 (96%)	6 (3%)	4 (2%)	6	7
All	All	442/482 (92%)	416 (94%)	17 (4%)	9 (2%)	6	6

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 ⓘ

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%)	16	23
1	B	205/223 (92%)	188 (92%)	17 (8%)	10	14
All	All	410/446 (92%)	380 (93%)	30 (7%)	13	18

All (30) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	23	LYS
1	A	40	ILE
1	A	81	VAL
1	A	88	LYS
1	A	90	GLU
1	A	98	THR
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	43	GLN
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	224	ASN
1	B	226	ASP
1	B	231	VAL

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Mol	Chain	Res	Type
1	B	243	LYS
1	B	249	LEU
1	B	255	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	39	ASN
1	A	195	ASN
1	A	224	ASN
1	B	39	ASN
1	B	43	GLN
1	B	140	ASN
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 oligosaccharides 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	A	263	-	33,33,33	1.20	3 (9%)	45,46,46	2.87	17 (37%)
3	B87	A	264	-	33,33,33	1.05	3 (9%)	45,46,46	2.84	16 (35%)
2	MLT	B	262	-	8,8,8	1.20	0	10,10,10	1.84	3 (30%)
3	B87	B	266	-	33,33,33	1.20	3 (9%)	45,46,46	3.10	16 (35%)
2	MLT	A	261	-	8,8,8	1.07	0	10,10,10	1.79	3 (30%)
3	B87	B	265	-	33,33,33	1.13	3 (9%)	45,46,46	2.83	16 (35%)

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	A	263	-	-	1/16/33/33	0/5/5/5
3	B87	A	264	-	-	4/16/33/33	0/5/5/5
2	MLT	B	262	-	1/1/3/3	5/8/8/8	-
3	B87	B	266	-	-	7/16/33/33	0/5/5/5
2	MLT	A	261	-	-	4/8/8/8	-
3	B87	B	265	-	-	1/16/33/33	0/5/5/5

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	265	B87	C24-C23	3.76	1.48	1.41
3	B	266	B87	C23-S22	-3.54	1.67	1.74
3	A	263	B87	C23-S22	-3.49	1.67	1.74
3	A	263	B87	C17-C21	3.49	1.51	1.46
3	B	266	B87	C24-C23	3.42	1.47	1.41
3	A	264	B87	C23-S22	-3.41	1.67	1.74
3	A	264	B87	C24-C23	3.37	1.47	1.41
3	A	263	B87	C24-C23	3.32	1.47	1.41
3	B	265	B87	C23-S22	-3.15	1.68	1.74
3	B	266	B87	C17-C21	2.27	1.49	1.46
3	B	265	B87	C17-C21	2.25	1.49	1.46
3	A	264	B87	C17-C21	2.03	1.49	1.46

All (71) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	266	B87	C19-N18-C17	10.59	121.78	115.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	264	B87	C19-N18-C17	9.69	121.27	115.81
3	A	263	B87	C19-N18-C17	9.53	121.18	115.81
3	B	265	B87	C19-N18-C17	9.05	120.91	115.81
3	B	266	B87	C14-N9-C10	8.07	126.23	108.84
3	B	266	B87	C19-N20-C15	8.03	121.69	114.95
3	A	264	B87	C19-N20-C15	7.07	120.89	114.95
3	A	263	B87	C19-N20-C15	6.84	120.69	114.95
3	B	265	B87	C14-N9-C10	6.52	122.88	108.84
3	B	265	B87	C19-N20-C15	6.36	120.28	114.95
3	A	263	B87	C14-N9-C10	6.24	122.29	108.84
3	A	264	B87	C14-N9-C10	6.21	122.21	108.84
3	B	266	B87	N20-C19-N18	-5.87	119.69	128.58
3	A	263	B87	C8-N9-C10	5.25	119.30	111.14
3	B	265	B87	N20-C19-N18	-5.18	120.74	128.58
3	A	264	B87	C8-N9-C14	5.12	119.10	111.14
3	B	265	B87	C8-N9-C10	5.08	119.04	111.14
3	A	264	B87	N20-C19-N18	-5.04	120.95	128.58
3	A	263	B87	N20-C19-N18	-4.97	121.06	128.58
3	A	264	B87	C8-N9-C10	4.85	118.69	111.14
3	A	263	B87	C8-N9-C14	4.66	118.40	111.14
3	B	265	B87	C13-N12-C11	4.58	121.86	111.57
3	B	266	B87	C8-N9-C10	4.48	118.11	111.14
3	B	265	B87	C8-N9-C14	4.46	118.08	111.14
3	A	263	B87	C13-N12-C11	4.32	121.29	111.57
3	B	266	B87	C10-C11-N12	-4.17	102.01	110.78
3	A	264	B87	C13-N12-C11	4.12	120.84	111.57
3	B	266	B87	C17-C21-S22	-4.02	112.64	119.58
3	B	265	B87	C17-C21-S22	-3.85	112.94	119.58
3	A	264	B87	C16-C17-N18	-3.73	118.80	123.27
2	A	261	MLT	O2-C1-C2	3.69	120.55	112.74
3	A	263	B87	C16-C17-N18	-3.59	118.96	123.27
3	A	263	B87	C17-C21-S22	-3.44	113.65	119.58
3	A	263	B87	C23-S22-C21	3.40	95.50	91.12
3	B	266	B87	C16-C17-N18	-3.34	119.26	123.27
3	A	264	B87	C17-C21-S22	-3.17	114.11	119.58
3	B	265	B87	C16-C17-N18	-3.14	119.50	123.27
2	B	262	MLT	O2-C1-O1	-3.13	116.97	124.08
3	B	266	B87	C17-C21-C25	3.07	134.59	129.05
3	A	263	B87	C17-C21-C25	3.00	134.47	129.05
2	A	261	MLT	O2-C1-O1	-2.98	117.31	124.08
3	B	266	B87	C23-S22-C21	2.96	94.94	91.12
3	B	265	B87	C21-C17-N18	2.96	120.30	116.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	265	B87	C10-C11-N12	-2.92	104.65	110.78
3	B	265	B87	N20-C15-N12	2.91	120.92	116.76
3	B	266	B87	C8-N9-C14	2.87	115.61	111.14
3	B	266	B87	C21-C17-N18	2.85	120.16	116.44
3	B	266	B87	N20-C15-N12	2.83	120.80	116.76
3	B	265	B87	C17-C21-C25	2.75	134.01	129.05
3	A	264	B87	C21-C17-N18	2.74	120.01	116.44
3	B	265	B87	C23-S22-C21	2.67	94.56	91.12
3	A	263	B87	C21-C17-N18	2.67	119.92	116.44
3	B	266	B87	C14-C13-N12	-2.67	105.17	110.78
3	A	263	B87	C4-N3-C2	2.59	114.80	111.37
3	A	264	B87	C23-S22-C21	2.55	94.40	91.12
2	B	262	MLT	O2-C1-C2	2.53	118.09	112.74
3	A	264	B87	C16-C15-N20	-2.50	118.65	122.82
3	B	265	B87	C16-C15-N12	-2.47	119.38	122.35
3	B	266	B87	C16-C15-N20	-2.37	118.88	122.82
3	B	265	B87	C4-N3-C2	2.30	114.42	111.37
3	B	266	B87	C13-N12-C11	2.27	116.68	111.57
3	A	263	B87	C16-C15-N20	-2.27	119.05	122.82
3	A	263	B87	N20-C15-N12	2.26	119.99	116.76
3	A	264	B87	N20-C15-N12	2.23	119.95	116.76
3	A	264	B87	C17-C21-C25	2.21	133.04	129.05
3	A	264	B87	C4-N3-C2	2.17	114.24	111.37
3	A	263	B87	C10-C11-N12	-2.15	106.25	110.78
3	A	263	B87	C26-C23-C24	2.05	123.71	121.16
2	A	261	MLT	O5-C4-C3	2.03	120.32	114.00
2	B	262	MLT	C3-C2-C1	2.02	115.49	110.53
3	A	264	B87	C10-C11-N12	-2.01	106.55	110.78

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

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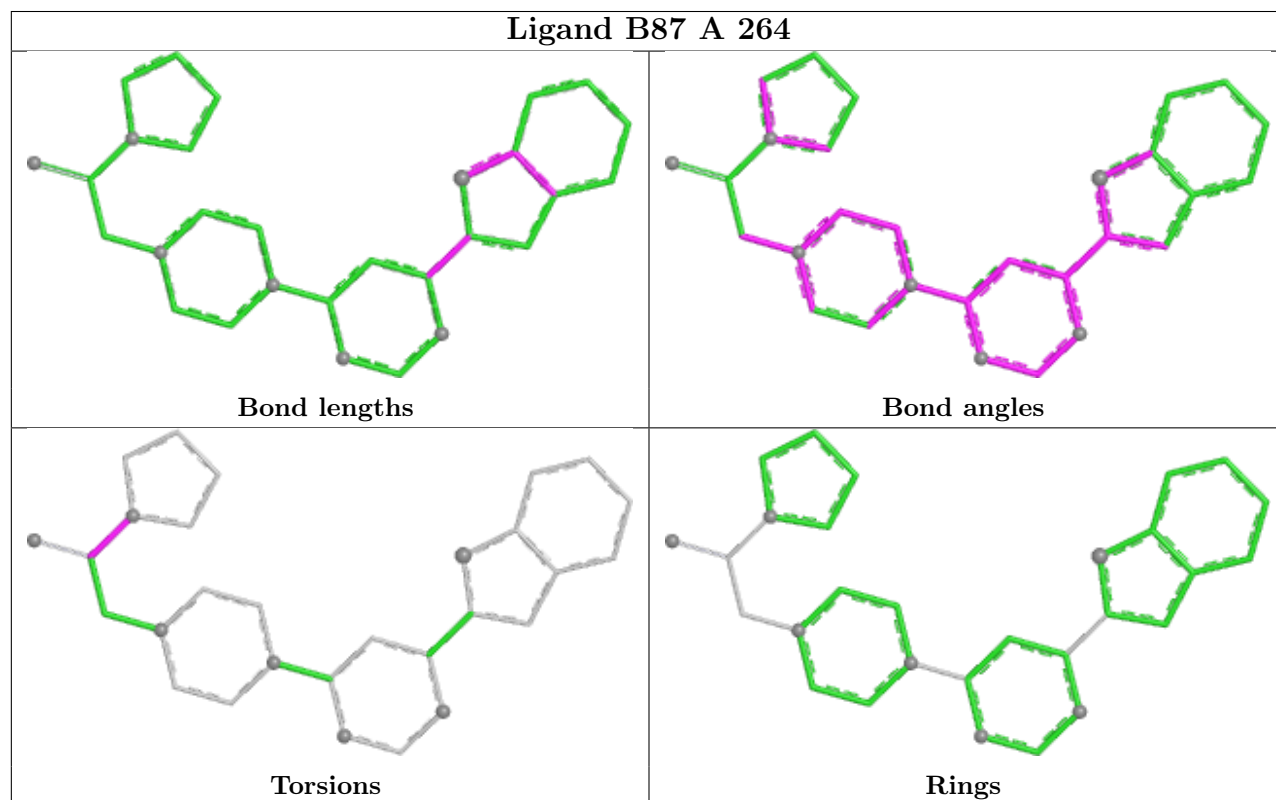
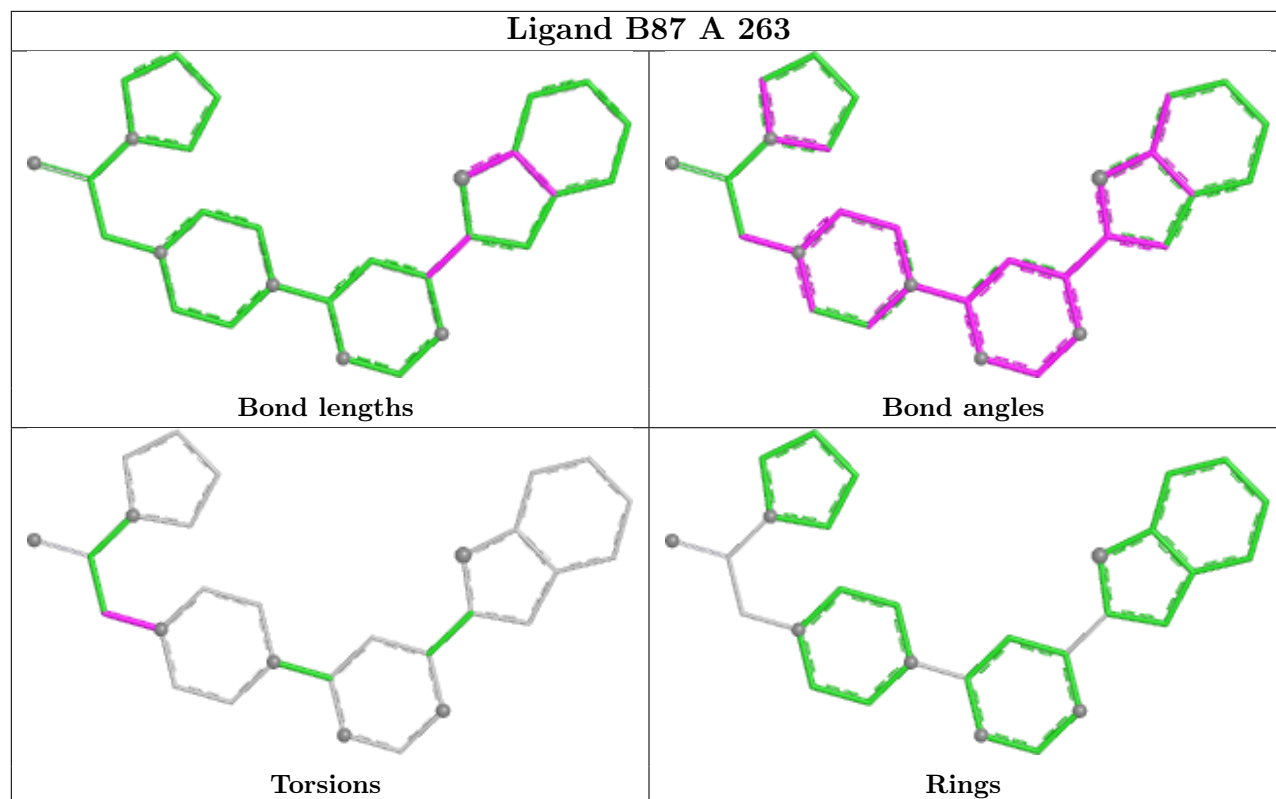
Mol	Chain	Res	Type	Atoms
3	B	266	B87	C8-C6-N3-C2
3	B	266	B87	O7-C6-N3-C4
3	B	266	B87	C8-C6-N3-C4
2	B	262	MLT	O1-C1-C2-O3
2	B	262	MLT	O2-C1-C2-O3
3	B	266	B87	O7-C6-C8-N9
3	B	266	B87	N3-C6-C8-N9
3	A	263	B87	C6-C8-N9-C14
3	B	266	B87	C6-C8-N9-C14
3	B	265	B87	C6-C8-N9-C14
2	A	261	MLT	O3-C2-C3-C4
2	B	262	MLT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

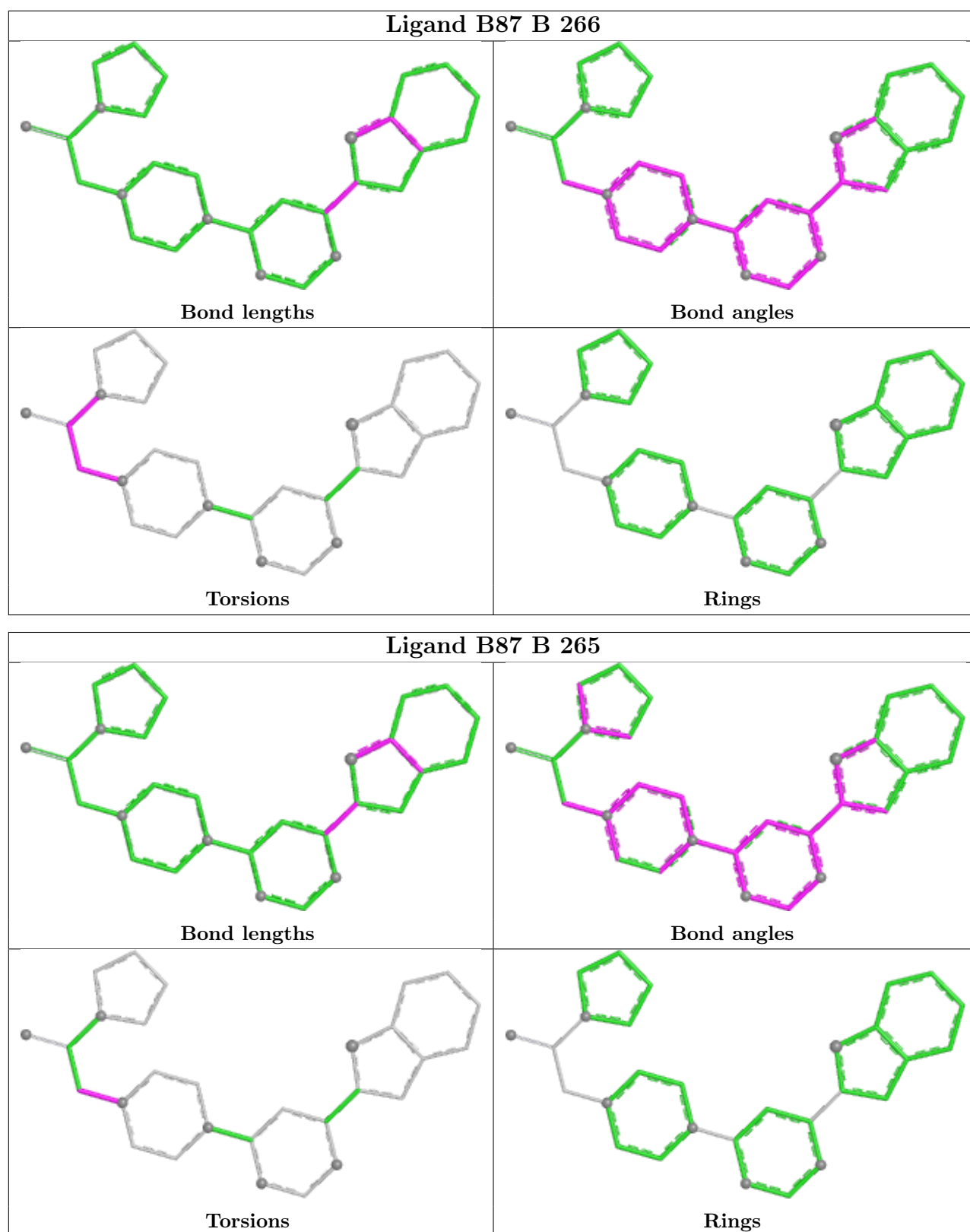
There are no ring outliers.

6 monomers are involved in 7 short contacts:

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

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, 95th 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 ²)	Q<0.9
1	A	225/241 (93%)	-1.19	0 100 100	24, 42, 64, 77	12 (5%)
1	B	225/241 (93%)	-1.17	0 100 100	28, 42, 64, 77	18 (8%)
All	All	450/482 (93%)	-1.18	0 100 100	24, 42, 64, 77	30 (6%)

There are no RSRZ outliers to report.

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 oligosaccharides in this entry.

6.4 Ligands [i](#)

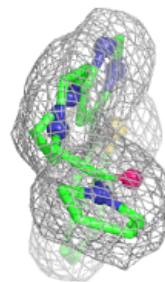
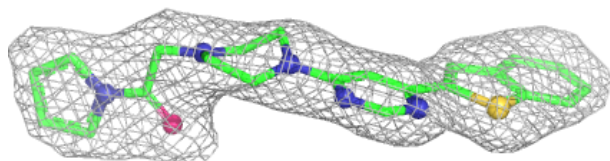
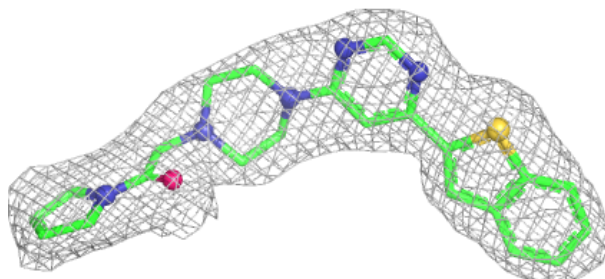
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	MLT	A	261	9/9	0.98	0.06	47,49,49,49	0
2	MLT	B	262	9/9	0.99	0.06	45,49,51,51	0
3	B87	A	263	29/29	0.99	0.03	30,32,34,34	0
3	B87	A	264	29/29	0.99	0.05	34,37,51,52	0
3	B87	B	265	29/29	0.99	0.04	33,34,34,36	0
3	B87	B	266	29/29	0.99	0.05	32,35,53,53	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.

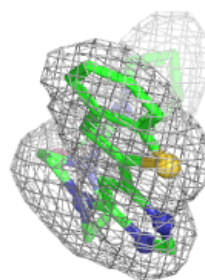
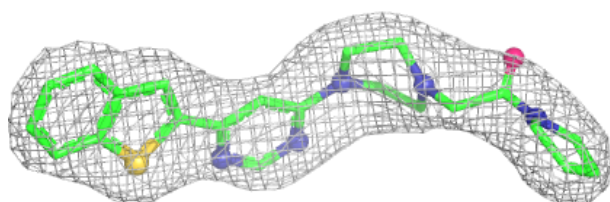
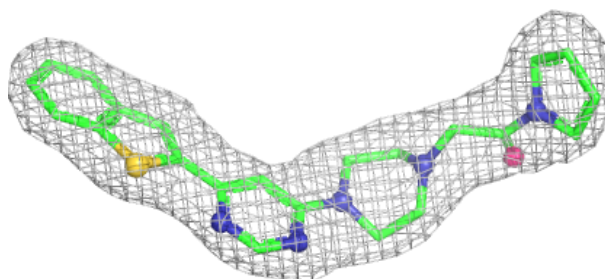
Electron density around B87 A 263:

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

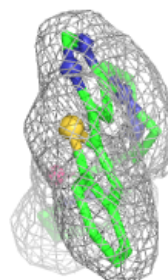
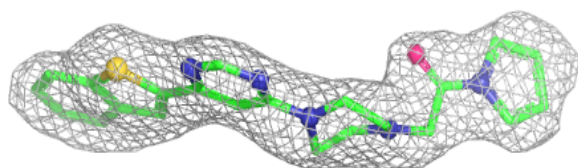
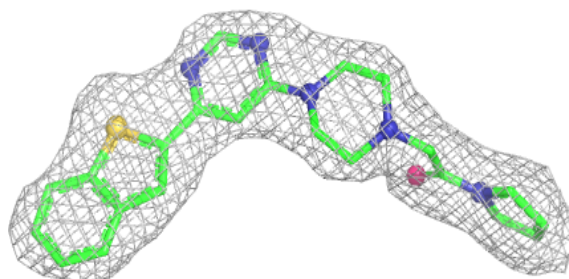


Electron density around B87 A 264:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

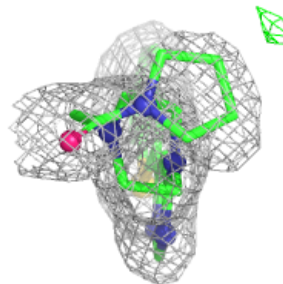
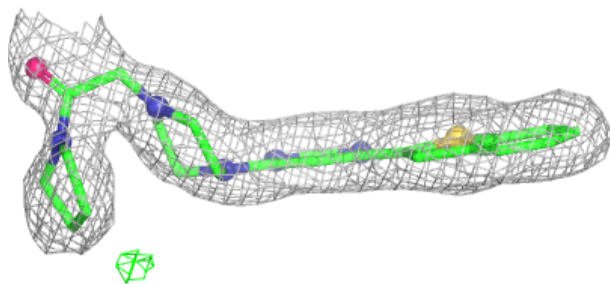
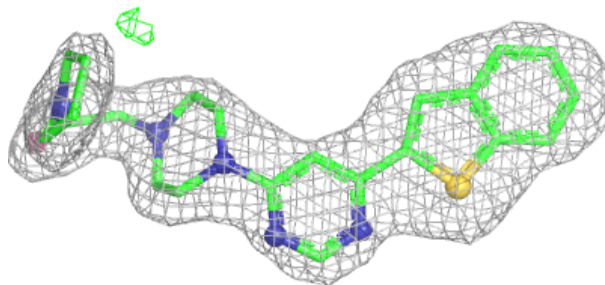
**Electron density around B87 B 265:**

$2mF_o-DF_c$ (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.