



Full wwPDB X-ray Structure Validation Report ⓘ

May 21, 2020 – 11:39 pm BST

PDB ID : 4V0I
Title : Water Network Determines Selectivity for a Series of Pyrimidone Indoline Amide PI3KBeta Inhibitors over PI3K-Delta
Authors : Robinson, D.; Bertrand, T.; Carry, J.C.; Halley, F.; Karlsson, A.; Mathieu, M.; Minoux, H.; Perrin, M.A.; Robert, B.; Schio, L.; Sherman, W.
Deposited on : 2014-09-16
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 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

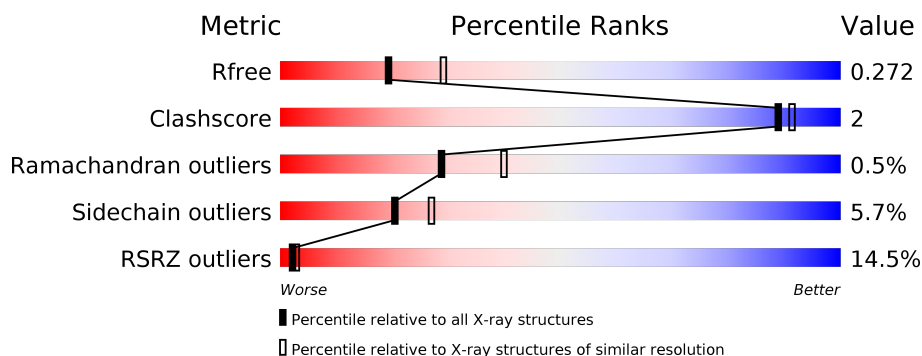
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.54 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))
R_{free}	130704	1284 (2.56-2.52)
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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	940	<div> <div>13%</div> <div>73%</div> <div>7%</div> <div>19%</div> </div>
1	B	940	<div> <div>11%</div> <div>76%</div> <div>8%</div> <div>16%</div> </div>

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 12654 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.

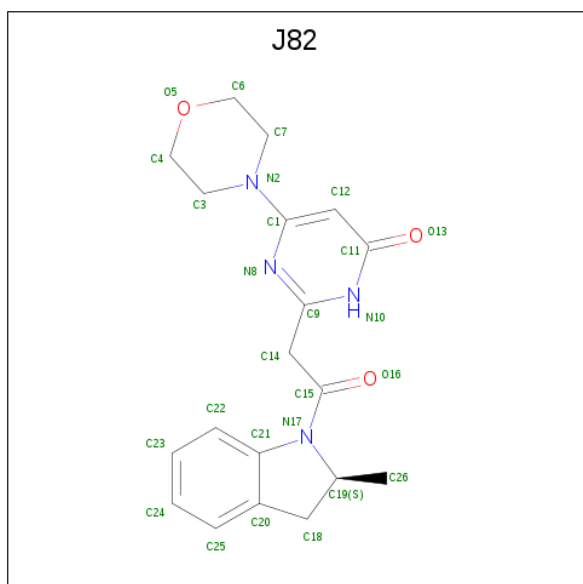
- Molecule 1 is a protein called PHOSPHATIDYLINOSITOL-4,5-BISPHOSPHATE 3-KINASE CATALYTIC SUBUNIT DELTA ISOFORM.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	759	Total	C	N	O	S	0	0	0
			6102	3913	1031	1107	51			
1	B	792	Total	C	N	O	S	0	0	0
			6360	4073	1076	1158	53			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	105	GLY	-	expression tag	UNP O35904
B	105	GLY	-	expression tag	UNP O35904

- Molecule 2 is 2-[2-(2-METHYL-2,3-DIHYDRO-INDOL-1-YL)-2-OXO-ETHYL]-6-MORPHOLIN-4-YL-3H-PYRIMIDIN-4-ONE (three-letter code: J82) (formula: C₁₉H₂₂N₄O₃).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			26	19	4	3		
2	B	1	Total	C	N	O	0	0
			26	19	4	3		

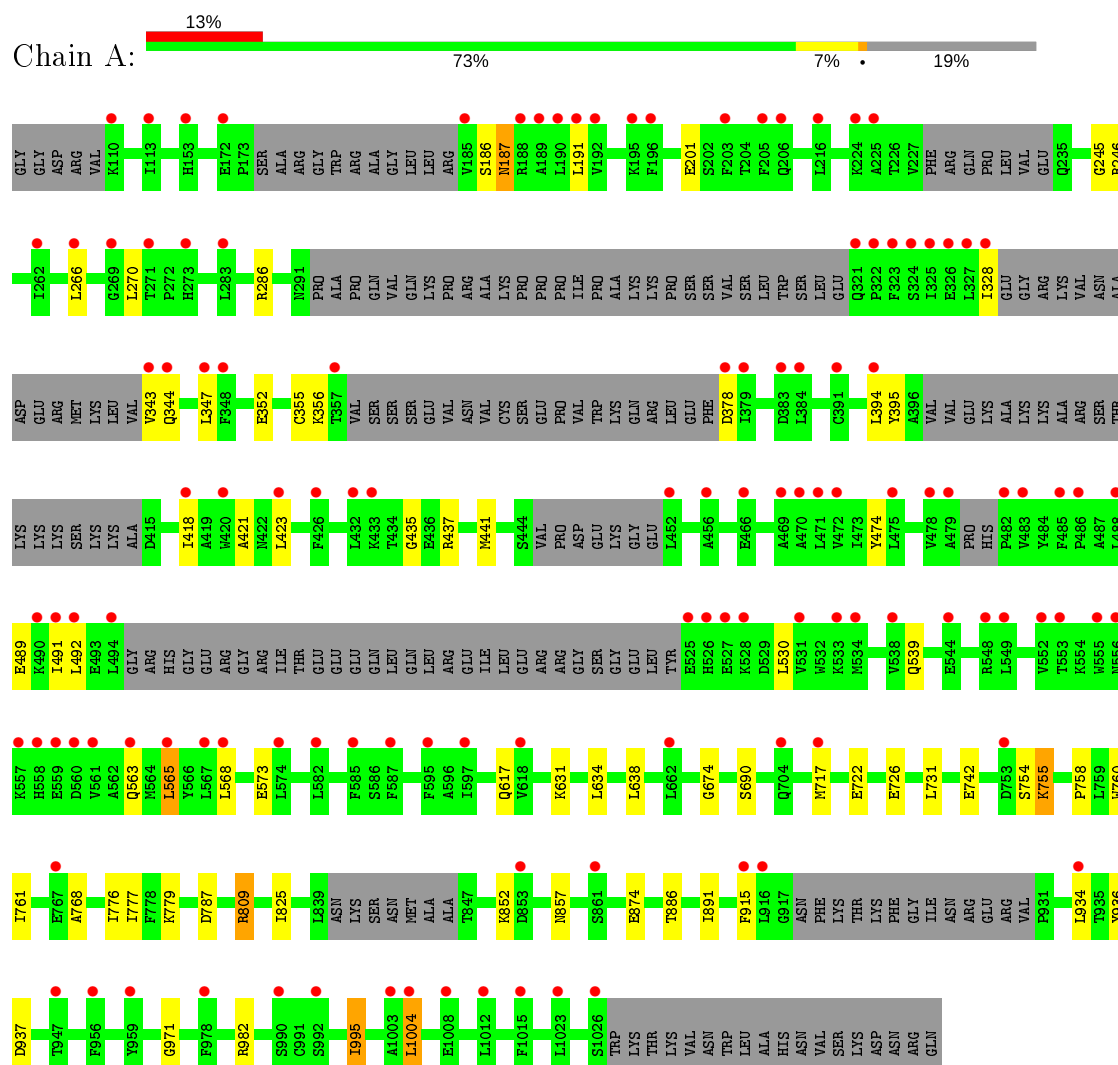
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	78	Total	O	0	0
			78	78		
3	B	62	Total	O	0	0
			62	62		

3 Residue-property plots

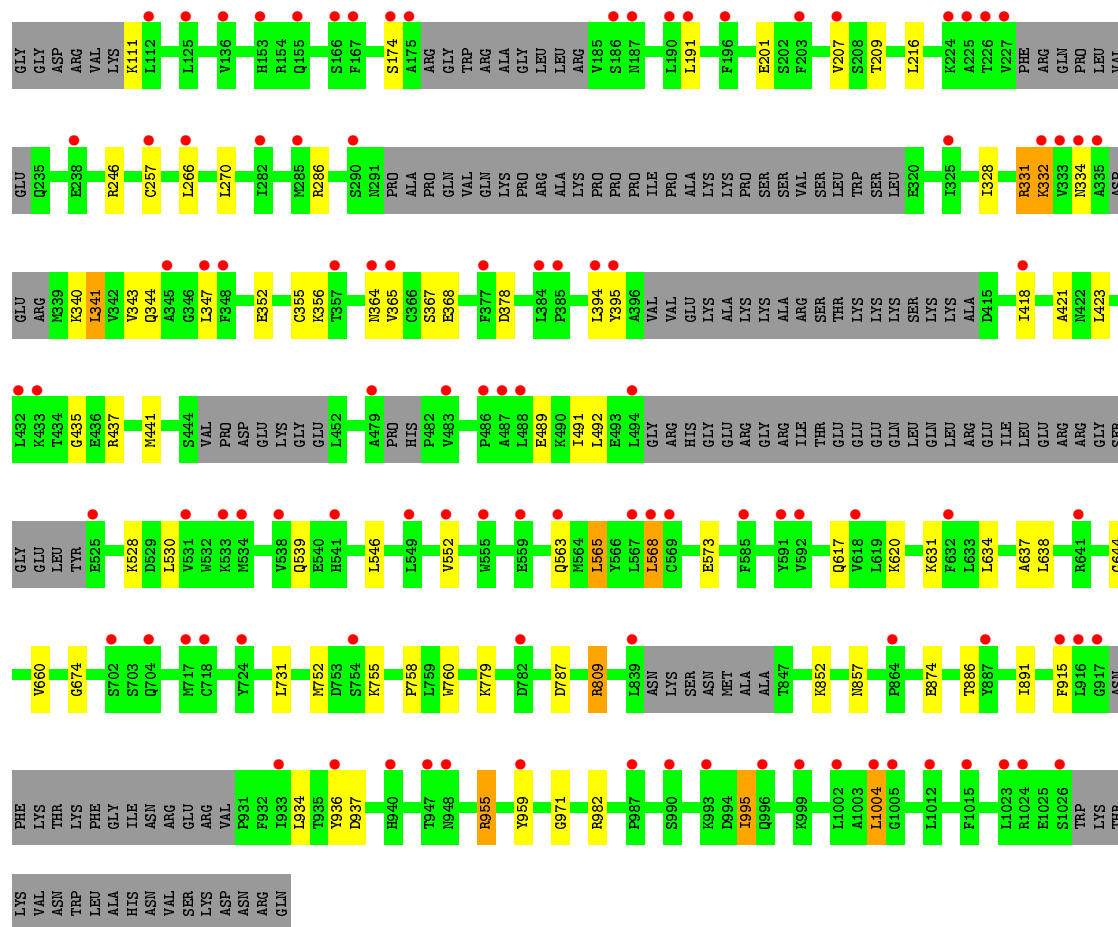
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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: PHOSPHATIDYLINOSITOL-4,5-BISPHOSPHATE 3-KINASE CATALYTIC SUBUNIT DELTA ISOFORM



• Molecule 1: PHOSPHATIDYLINOSITOL-4,5-BISPHOSPHATE 3-KINASE CATALYTIC SUBUNIT DELTA ISOFORM





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	62.00Å 216.43Å 76.97Å 90.00° 113.29° 90.00°	Depositor
Resolution (Å)	44.70 – 2.54 108.22 – 2.54	Depositor EDS
% Data completeness (in resolution range)	98.8 (44.70-2.54) 97.1 (108.22-2.54)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.99 (at 2.55Å)	Xtriage
Refinement program	BUSTER 2.9.7	Depositor
R, R_{free}	0.234 , (Not available) 0.248 , 0.272	Depositor DCC
R_{free} test set	3070 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å ²)	46.7	Xtriage
Anisotropy	0.147	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 35.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.42$, $\langle L^2 \rangle = 0.25$	Xtriage
Estimated twinning fraction	0.168 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	12654	wwPDB-VP
Average B, all atoms (Å ²)	56.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.34% 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: J82

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	0.38	0/6233	0.57	0/8406
1	B	0.38	0/6496	0.57	0/8763
All	All	0.38	0/12729	0.57	0/17169

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

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	6102	0	6074	20	0
1	B	6360	0	6331	26	0
2	A	26	0	22	2	0
2	B	26	0	22	1	0
3	A	78	0	0	0	0
3	B	62	0	0	0	0
All	All	12654	0	12449	47	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 2.

All (47) 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:332:LYS:HD2	1:B:341:LEU:HD11	1.72	0.70
1:A:355:CYS:HB2	1:A:378:ASP:HB3	1.73	0.70
1:A:186:SER:HA	1:A:187:ASN:CB	2.34	0.57
1:B:758:PRO:HB3	1:B:779:LYS:HG2	1.86	0.56
1:A:186:SER:HA	1:A:187:ASN:HB3	1.88	0.54
1:B:809:ARG:HD3	1:B:874:GLU:OE1	2.08	0.53
1:B:331:ARG:HA	1:B:367:SER:O	2.08	0.53
1:A:809:ARG:HD3	1:A:874:GLU:OE1	2.09	0.53
1:B:344:GLN:HB2	1:B:395:TYR:HE2	1.76	0.50
1:B:886:THR:HA	1:B:891:ILE:HD12	1.94	0.50
1:A:982:ARG:HD2	1:A:995:ILE:HD11	1.94	0.49
1:B:982:ARG:HD2	1:B:995:ILE:HD11	1.93	0.49
1:A:886:THR:HA	1:A:891:ILE:HD12	1.94	0.49
1:B:955:ARG:HD3	1:B:959:TYR:HE2	1.77	0.49
1:A:344:GLN:HB2	1:A:395:TYR:HE2	1.76	0.49
1:A:758:PRO:HB3	1:A:779:LYS:HG2	1.93	0.49
1:B:355:CYS:HB2	1:B:378:ASP:HB3	1.95	0.47
1:A:760:TRP:HB2	2:A:1500:J82:C24	2.45	0.47
1:B:491:ILE:HG21	1:B:565:LEU:HD22	1.98	0.46
1:A:491:ILE:HG21	1:A:565:LEU:HD22	1.98	0.46
1:A:245:GLY:HA3	1:A:768:ALA:HB2	1.98	0.45
1:B:637:ALA:HB1	1:B:644:GLY:HA2	1.97	0.45
1:B:207:VAL:HG11	1:B:216:LEU:HG	1.97	0.45
1:A:971:GLY:HA3	1:A:1004:LEU:HD21	1.98	0.44
1:A:489:GLU:HA	1:A:492:LEU:HD12	1.99	0.44
1:B:638:LEU:HD21	1:B:674:GLY:HA3	1.99	0.44
2:A:1500:J82:H263	2:A:1500:J82:H142	2.00	0.44
1:A:421:ALA:HB2	1:A:441:MET:HG2	1.99	0.44
1:B:489:GLU:HA	1:B:492:LEU:HD12	1.99	0.44
1:B:971:GLY:HA3	1:B:1004:LEU:HD21	1.99	0.44
1:B:752:MET:HB3	1:B:758:PRO:HD2	1.99	0.43
1:B:421:ALA:HB2	1:B:441:MET:HG2	2.00	0.43
1:A:638:LEU:HD21	1:A:674:GLY:HA3	2.00	0.42
1:B:760:TRP:HB2	2:B:1500:J82:C24	2.49	0.42
1:B:341:LEU:HD12	1:B:365:VAL:HA	2.02	0.42
1:A:394:LEU:HD23	1:A:418:ILE:HB	2.01	0.42
1:B:620:LYS:HG2	1:B:660:VAL:HG11	2.01	0.42
1:B:394:LEU:HD23	1:B:418:ILE:HB	2.01	0.42
1:A:777:ILE:HB	1:A:825:ILE:HB	2.01	0.42
1:B:209:THR:HG23	1:B:257:CYS:HB3	2.02	0.42
1:A:328:ILE:HD11	1:A:474:TYR:HB2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:955:ARG:HD3	1:B:959:TYR:CE2	2.54	0.41
1:A:343:VAL:HG22	1:A:394:LEU:HD12	2.03	0.41
1:B:528:LYS:HG2	1:B:552:VAL:HG12	2.02	0.41
1:B:343:VAL:HG22	1:B:394:LEU:HD12	2.03	0.40
1:B:546:LEU:HD11	1:B:568:LEU:HD12	2.03	0.40
1:A:761:ILE:HB	1:A:776:ILE:HG13	2.03	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	735/940 (78%)	714 (97%)	17 (2%)	4 (0%)	29	40
1	B	770/940 (82%)	745 (97%)	22 (3%)	3 (0%)	34	46
All	All	1505/1880 (80%)	1459 (97%)	39 (3%)	7 (0%)	29	40

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	755	LYS
1	A	742	GLU
1	B	755	LYS
1	A	187	ASN
1	B	328	ILE
1	A	435	GLY
1	B	435	GLY

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	669/827 (81%)	632 (94%)	37 (6%)	21	29
1	B	699/827 (84%)	658 (94%)	41 (6%)	19	25
All	All	1368/1654 (83%)	1290 (94%)	78 (6%)	20	27

All (78) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	191	LEU
1	A	201	GLU
1	A	246	ARG
1	A	266	LEU
1	A	270	LEU
1	A	286	ARG
1	A	347	LEU
1	A	352	GLU
1	A	356	LYS
1	A	423	LEU
1	A	437	ARG
1	A	530	LEU
1	A	539	GLN
1	A	563	GLN
1	A	565	LEU
1	A	568	LEU
1	A	573	GLU
1	A	617	GLN
1	A	631	LYS
1	A	634	LEU
1	A	690	SER
1	A	717	MET
1	A	722	GLU
1	A	726	GLU
1	A	731	LEU
1	A	754	SER
1	A	755	LYS

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Mol	Chain	Res	Type
1	A	787	ASP
1	A	809	ARG
1	A	852	LYS
1	A	857	ASN
1	A	915	PHE
1	A	934	LEU
1	A	936	TYR
1	A	937	ASP
1	A	995	ILE
1	A	1004	LEU
1	B	111	LYS
1	B	174	SER
1	B	191	LEU
1	B	201	GLU
1	B	246	ARG
1	B	266	LEU
1	B	270	LEU
1	B	286	ARG
1	B	331	ARG
1	B	332	LYS
1	B	334	ASN
1	B	340	LYS
1	B	341	LEU
1	B	347	LEU
1	B	352	GLU
1	B	356	LYS
1	B	364	ASN
1	B	368	GLU
1	B	423	LEU
1	B	437	ARG
1	B	530	LEU
1	B	539	GLN
1	B	563	GLN
1	B	565	LEU
1	B	568	LEU
1	B	573	GLU
1	B	617	GLN
1	B	631	LYS
1	B	634	LEU
1	B	731	LEU
1	B	787	ASP
1	B	809	ARG

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Mol	Chain	Res	Type
1	B	852	LYS
1	B	857	ASN
1	B	915	PHE
1	B	934	LEU
1	B	936	TYR
1	B	937	ASP
1	B	955	ARG
1	B	995	ILE
1	B	1004	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

2 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	J82	A	1500	-	28,29,29	1.49	7 (25%)	34,41,41	2.20	9 (26%)
2	J82	B	1500	-	28,29,29	1.48	7 (25%)	34,41,41	2.23	9 (26%)

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	J82	A	1500	-	-	4/10/32/32	0/4/4/4
2	J82	B	1500	-	-	4/10/32/32	0/4/4/4

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1500	J82	C9-N8	-3.22	1.29	1.33
2	B	1500	J82	C12-C1	-3.21	1.34	1.39
2	A	1500	J82	C12-C1	-3.21	1.34	1.39
2	A	1500	J82	C9-N8	-3.18	1.29	1.33
2	B	1500	J82	C19-N17	-3.04	1.45	1.48
2	A	1500	J82	C19-N17	-2.70	1.46	1.48
2	A	1500	J82	C11-N10	2.52	1.37	1.33
2	B	1500	J82	C1-N8	2.31	1.37	1.34
2	A	1500	J82	C9-N10	2.31	1.37	1.33
2	A	1500	J82	C1-N8	2.31	1.37	1.34
2	A	1500	J82	C21-C20	-2.30	1.37	1.39
2	B	1500	J82	C11-N10	2.27	1.37	1.33
2	B	1500	J82	C21-C20	-2.20	1.37	1.39
2	B	1500	J82	C9-N10	2.18	1.36	1.33

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1500	J82	C12-C11-N10	-8.28	114.41	124.08
2	A	1500	J82	C12-C11-N10	-8.10	114.63	124.08
2	B	1500	J82	O16-C15-N17	3.94	126.48	121.58
2	A	1500	J82	C26-C19-C18	-3.74	106.51	114.71
2	A	1500	J82	O16-C15-N17	3.58	126.03	121.58
2	B	1500	J82	C12-C1-N2	-3.45	118.20	122.29
2	A	1500	J82	C12-C1-N2	-3.19	118.51	122.29
2	A	1500	J82	C19-N17-C15	3.18	126.03	119.27
2	B	1500	J82	C26-C19-C18	-3.14	107.81	114.71
2	B	1500	J82	C11-C12-C1	2.91	119.77	116.19
2	B	1500	J82	C19-N17-C15	2.91	125.44	119.27
2	A	1500	J82	C11-C12-C1	2.87	119.71	116.19
2	B	1500	J82	N8-C1-N2	2.80	119.69	116.55
2	A	1500	J82	N8-C1-N2	2.68	119.56	116.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1500	J82	C14-C9-N8	2.33	121.23	117.20
2	B	1500	J82	C18-C20-C21	2.08	111.97	109.74
2	A	1500	J82	C14-C9-N8	2.03	120.71	117.20
2	A	1500	J82	C18-C20-C21	2.02	111.91	109.74

There are no chirality outliers.

All (8) torsion outliers are listed below:

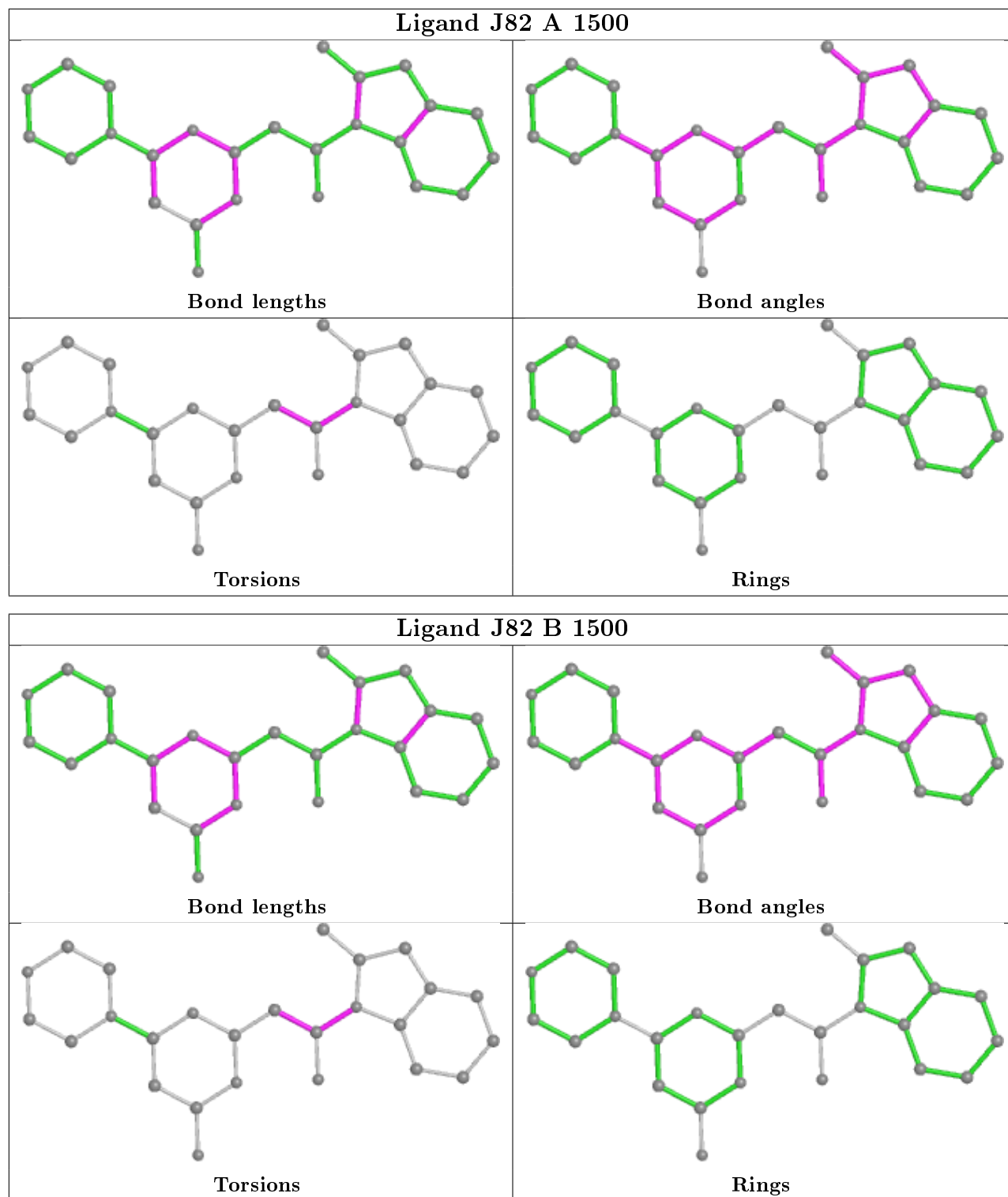
Mol	Chain	Res	Type	Atoms
2	B	1500	J82	O16-C15-N17-C19
2	A	1500	J82	C14-C15-N17-C19
2	B	1500	J82	C14-C15-N17-C19
2	A	1500	J82	O16-C15-N17-C19
2	B	1500	J82	C9-C14-C15-O16
2	B	1500	J82	C9-C14-C15-N17
2	A	1500	J82	C9-C14-C15-O16
2	A	1500	J82	C9-C14-C15-N17

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1500	J82	2	0
2	B	1500	J82	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 ⓘ

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, 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	759/940 (80%)	1.01	122 (16%)  	23, 55, 93, 120	0
1	B	792/940 (84%)	0.92	103 (13%)  	22, 54, 87, 131	0
All	All	1551/1880 (82%)	0.97	225 (14%)  	22, 54, 91, 131	0

All (225) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	323	PHE	7.0
1	A	559	GLU	6.8
1	A	534	MET	6.1
1	A	347	LEU	6.0
1	A	915	PHE	5.9
1	A	472	VAL	5.6
1	A	266	LEU	5.5
1	A	203	PHE	5.4
1	A	433	LYS	5.3
1	B	591	TYR	5.2
1	B	125	LEU	5.1
1	B	384	LEU	5.1
1	B	559	GLU	5.0
1	B	549	LEU	4.7
1	A	595	PHE	4.7
1	B	334	ASN	4.6
1	A	1003	ALA	4.6
1	A	1008	GLU	4.6
1	A	990	SER	4.5
1	A	205	PHE	4.5
1	A	206	GLN	4.4
1	B	987	PRO	4.2
1	A	357	THR	4.2
1	A	321	GLN	4.2

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Mol	Chain	Res	Type	RSRZ
1	A	110	LYS	4.2
1	B	538	VAL	4.1
1	B	993	LYS	4.1
1	A	343	VAL	4.1
1	B	936	TYR	4.1
1	A	384	LEU	4.0
1	B	1026	SER	4.0
1	A	525	GLU	4.0
1	A	549	LEU	3.9
1	B	224	LYS	3.9
1	A	557	LYS	3.8
1	A	992	SER	3.8
1	A	533	LYS	3.8
1	B	332	LYS	3.8
1	B	917	GLY	3.7
1	B	488	LEU	3.7
1	B	567	LEU	3.7
1	A	853	ASP	3.7
1	A	426	PHE	3.7
1	A	494	LEU	3.7
1	B	433	LYS	3.6
1	B	153	HIS	3.6
1	B	915	PHE	3.6
1	B	1002	LEU	3.6
1	B	947	THR	3.6
1	B	531	VAL	3.6
1	B	494	LEU	3.5
1	A	565	LEU	3.5
1	B	191	LEU	3.5
1	A	418	ILE	3.5
1	B	541	HIS	3.5
1	B	207	VAL	3.5
1	A	394	LEU	3.4
1	A	271	THR	3.4
1	B	203	PHE	3.4
1	B	916	LEU	3.4
1	B	534	MET	3.4
1	A	378	ASP	3.4
1	B	227	VAL	3.3
1	B	364	ASN	3.3
1	A	662	LEU	3.3
1	A	327	LEU	3.3

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Mol	Chain	Res	Type	RSRZ
1	A	262	ILE	3.3
1	A	328	ILE	3.3
1	A	1015	PHE	3.3
1	B	418	ILE	3.3
1	A	538	VAL	3.3
1	A	191	LEU	3.2
1	A	224	LYS	3.2
1	A	482	PRO	3.2
1	A	528	LYS	3.1
1	A	558	HIS	3.1
1	A	483	VAL	3.1
1	A	531	VAL	3.1
1	A	959	TYR	3.1
1	A	348	PHE	3.1
1	A	767	GLU	3.1
1	B	325	ILE	3.1
1	B	563	GLN	3.1
1	B	948	ASN	3.1
1	A	560	ASP	3.0
1	A	717	MET	3.0
1	B	717	MET	3.0
1	B	1004	LEU	3.0
1	B	486	PRO	3.0
1	B	377	PHE	3.0
1	B	1015	PHE	3.0
1	B	702	SER	3.0
1	A	283	LEU	3.0
1	A	582	LEU	3.0
1	B	568	LEU	3.0
1	B	864	PRO	3.0
1	A	1023	LEU	2.9
1	B	282	ILE	2.9
1	A	192	VAL	2.9
1	B	112	LEU	2.9
1	B	290	SER	2.9
1	B	136	VAL	2.8
1	B	345	ALA	2.8
1	B	479	ALA	2.8
1	B	887	TYR	2.8
1	A	466	GLU	2.8
1	B	175	ALA	2.8
1	B	1012	LEU	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	185	VAL	2.8
1	A	196	PHE	2.8
1	B	266	LEU	2.8
1	A	618	VAL	2.8
1	A	556	ASN	2.8
1	B	525	GLU	2.8
1	B	933	ILE	2.8
1	A	1004	LEU	2.8
1	B	186	SER	2.8
1	A	423	LEU	2.7
1	A	322	PRO	2.7
1	A	172	GLU	2.7
1	A	1012	LEU	2.7
1	A	488	LEU	2.7
1	A	478	VAL	2.7
1	B	483	VAL	2.7
1	A	344	GLN	2.7
1	A	526	HIS	2.6
1	A	1026	SER	2.6
1	A	324	SER	2.6
1	B	155	GLN	2.6
1	A	383	ASP	2.6
1	B	174	SER	2.6
1	A	490	LYS	2.6
1	B	347	LEU	2.6
1	A	391	CYS	2.6
1	A	552	VAL	2.6
1	B	552	VAL	2.5
1	B	704	GLN	2.5
1	A	956	PHE	2.5
1	A	947	THR	2.5
1	A	753	ASP	2.5
1	A	486	PRO	2.5
1	A	113	ILE	2.5
1	A	491	ILE	2.5
1	B	959	TYR	2.5
1	A	195	LYS	2.5
1	A	216	LEU	2.5
1	B	585	PHE	2.5
1	B	1024	ARG	2.5
1	A	470	ALA	2.5
1	B	225	ALA	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	555	TRP	2.5
1	B	1005	GLY	2.5
1	A	585	PHE	2.5
1	B	190	LEU	2.5
1	B	285	MET	2.4
1	B	641	ARG	2.4
1	B	940	HIS	2.4
1	B	238	GLU	2.4
1	A	326	GLU	2.4
1	A	379	ILE	2.4
1	B	569	CYS	2.4
1	A	567	LEU	2.4
1	B	385	PRO	2.4
1	B	187	ASN	2.4
1	A	153	HIS	2.4
1	B	226	THR	2.4
1	A	861	SER	2.4
1	A	225	ALA	2.3
1	A	456	ALA	2.3
1	B	999	LYS	2.3
1	B	990	SER	2.3
1	A	190	LEU	2.3
1	A	568	LEU	2.3
1	A	188	ARG	2.3
1	A	325	ILE	2.3
1	B	196	PHE	2.3
1	B	357	THR	2.3
1	B	632	PHE	2.3
1	B	335	ALA	2.3
1	A	273	HIS	2.3
1	A	587	PHE	2.3
1	B	333	VAL	2.2
1	A	471	LEU	2.2
1	A	269	GLY	2.2
1	B	365	VAL	2.2
1	A	574	LEU	2.2
1	A	916	LEU	2.2
1	B	394	LEU	2.2
1	B	1023	LEU	2.2
1	B	395	TYR	2.2
1	B	257	CYS	2.2
1	B	487	ALA	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	492	LEU	2.2
1	A	561	VAL	2.2
1	A	544	GLU	2.2
1	A	555	TRP	2.2
1	B	839	LEU	2.2
1	B	533	LYS	2.1
1	A	189	ALA	2.1
1	A	978	PHE	2.1
1	B	167	PHE	2.1
1	A	934	LEU	2.1
1	B	718	CYS	2.1
1	B	724	TYR	2.1
1	B	782	ASP	2.1
1	A	479	ALA	2.1
1	B	618	VAL	2.1
1	A	485	PHE	2.1
1	A	432	LEU	2.1
1	B	754	SER	2.1
1	A	527	GLU	2.1
1	A	704	GLN	2.1
1	A	469	ALA	2.1
1	A	553	THR	2.1
1	B	592	VAL	2.1
1	A	597	ILE	2.1
1	B	432	LEU	2.1
1	B	996	GLN	2.1
1	A	548	ARG	2.1
1	A	452	LEU	2.1
1	B	166	SER	2.1
1	B	348	PHE	2.1
1	A	420	TRP	2.1
1	A	475	LEU	2.0
1	A	563	GLN	2.0

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

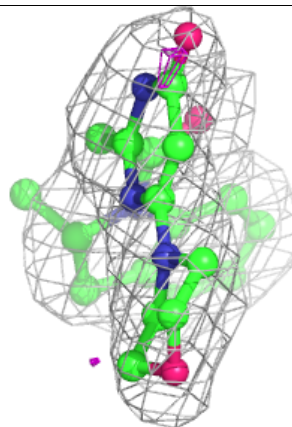
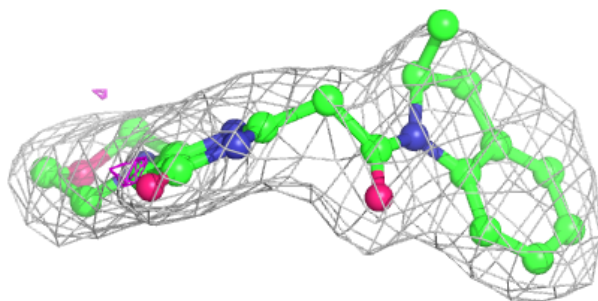
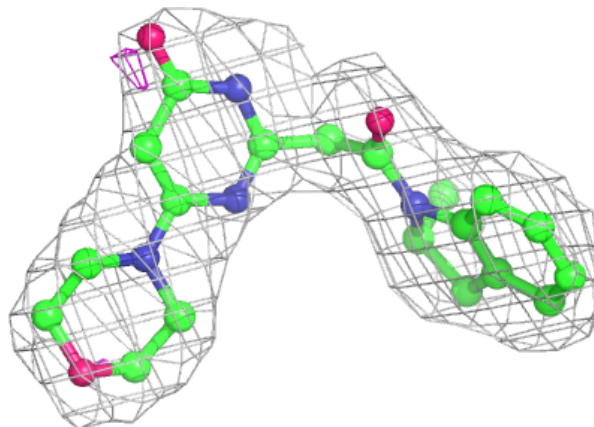
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q < 0.9' lists 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	J82	A	1500	26/26	0.93	0.19	26,30,31,33	0
2	J82	B	1500	26/26	0.97	0.17	27,31,32,33	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.

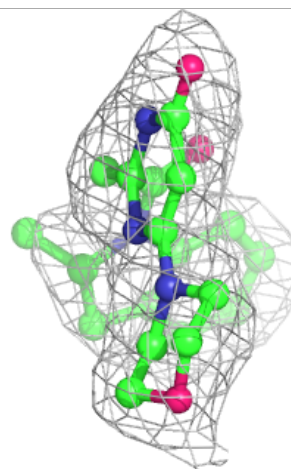
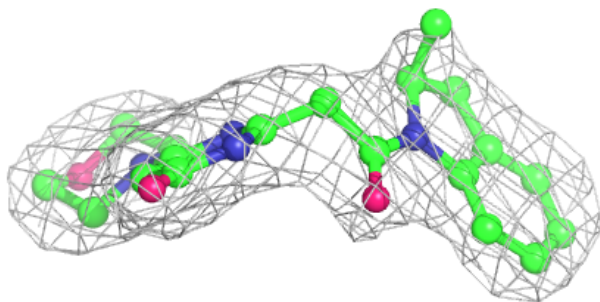
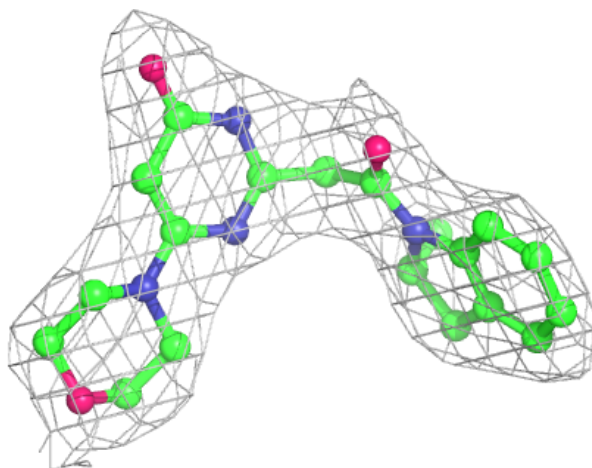
Electron density around J82 A 1500:

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 J82 B 1500:

$2mF_o-DF_c$ (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.