



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2026 – 08:38 PM UTC

PDB ID : 4BFR / pdb_00004bfr
Title : Discovery and Optimization of Pyrimidone Indoline Amide PI3Kbeta Inhibitors for the Treatment of Phosphatase and TENsin homologue (PTEN)-Deficient Cancers
Authors : Certal, V.; Carry, J.C.; Halley, F.; Virone-Oddos, A.; Thompson, F.; Filoche-Romme, B.; El-Ahmad, Y.; Karlsson, A.; Charrier, V.; Delorme, C.; Rak, A.; Abecassis, P.Y.; Amara, C.; Vincent, L.; Bonnevaux, H.; Nicolas, J.P.; Mathieu, M.; Bertrand, T.; Marquette, J.P.; Michot, N.; Benard, T.; Perrin, M.A.; Perron, S.; Monget, S.; Gruss-Leleu, F.; Doerflinger, G.; Guizani, H.; Brollo, M.; Delbarre, L.; Bertin, L.; Richepin, P.; Loyau, V.; Garcia-Echeverria, C.; Lengauer, C.; Schio, L.
Deposited on : 2013-03-22
Resolution : 2.80 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:

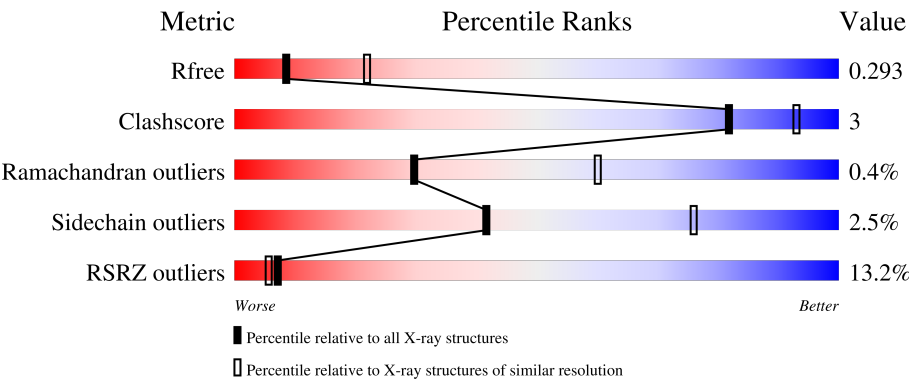
MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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}	180053	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

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	952	14% 81% 9% 10%

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Buster-report

Percentile statistics

CCP4

Density-Fitness

Ideal geometry (proteins)

Ideal geometry (DNA, RNA)

Validation Pipeline (wwPDB-VP)

:

wwPDB partial adaption of 1.1.7 (2018)

: 20250101.v01 (using entries in the PDB archive January 1st 2025)

: 9.0.010 (Gargrove)

: 1.0.12

: Engh & Huber (2001)

: Parkinson et al. (1996)

: 2.49

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Mol	Chain	Length	Quality of chain
1	B	952	

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 13777 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.

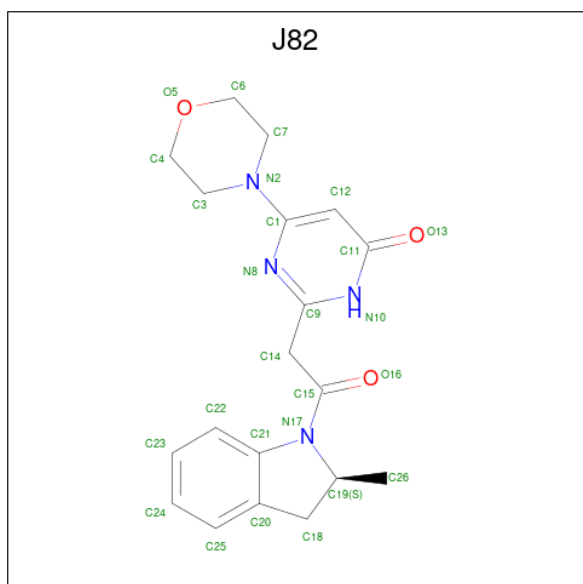
- Molecule 1 is a protein called PHOSPHATIDYLINOSITOL 4,5-BISPHOSPHATE 3-KINASE CATALYTIC S SUBUNIT BETA ISOFORM.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	855	Total	C	N	O	S	0	0	0
			6902	4436	1165	1259	42			
1	B	836	Total	C	N	O	S	0	0	0
			6743	4339	1138	1225	41			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	113	GLY	-	expression tag	UNP Q8BTI9
B	113	GLY	-	expression tag	UNP Q8BTI9

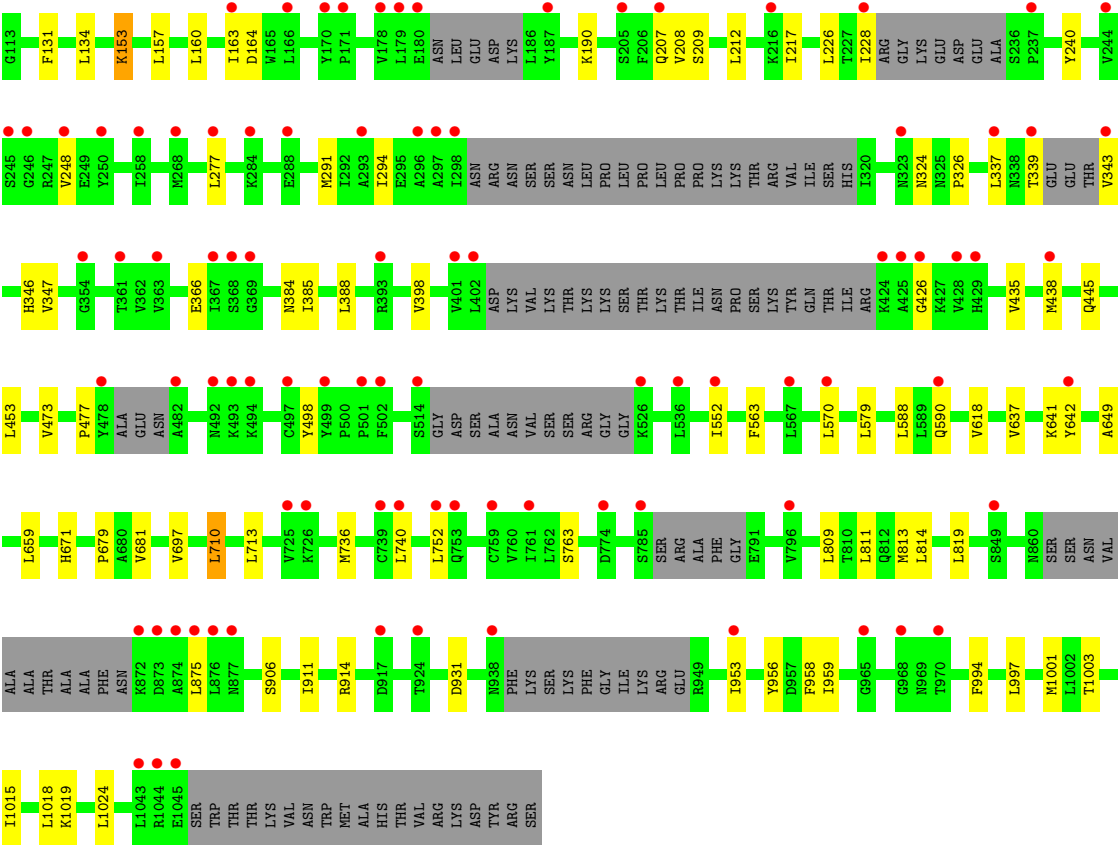
- Molecule 2 is 2-[2-(2-METHYL-2,3-DIHYDRO-INDOL-1-YL)-2-OXO-ETHYL]-6-MORPHOLIN-4-YL-3H-PYRIMIDIN-4-ONE (CCD ID: J82) (formula: $C_{19}H_{22}N_4O_3$).



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	33	Total	O	0	0
			33	33		
3	B	47	Total	O	0	0
			47	47		



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	122.31Å 129.03Å 154.90Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	56.00 – 2.80 56.00 – 2.80	Depositor EDS
% Data completeness (in resolution range)	99.7 (56.00-2.80) 99.7 (56.00-2.80)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.83 (at 2.82Å)	Xtriage
Refinement program	BUSTER 2.11.4	Depositor
R, R_{free}	0.260 , 0.275 0.280 , 0.293	Depositor DCC
R_{free} test set	3084 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å ²)	68.0	Xtriage
Anisotropy	0.278	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 48.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	13777	wwPDB-VP
Average B, all atoms (Å ²)	76.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.30% 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 [i](#)

5.1 Standard geometry [i](#)

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	0.71	0/7047	1.28	6/9524 (0.1%)
1	B	0.71	0/6879	1.26	1/9287 (0.0%)
All	All	0.71	0/13926	1.27	7/18811 (0.0%)

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	958	PHE	CA-CB-CG	5.34	119.14	113.80
1	B	958	PHE	CA-CB-CG	5.34	119.14	113.80
1	A	503	ASP	CA-CB-CG	5.26	117.86	112.60
1	A	766	TYR	CA-C-N	5.09	127.71	120.53
1	A	766	TYR	C-N-CA	5.09	127.71	120.53
1	A	120	ILE	CA-C-N	5.03	125.67	119.99
1	A	120	ILE	C-N-CA	5.03	125.67	119.99

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	6902	0	6937	33	0
1	B	6743	0	6808	34	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	26	0	22	1	0
2	B	26	0	22	1	0
3	A	33	0	0	0	0
3	B	47	0	0	0	0
All	All	13777	0	13789	69	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 3.

All (69) 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:153:LYS:HD2	1:B:659:LEU:HB3	1.61	0.82
1:A:153:LYS:HD2	1:A:659:LEU:HB3	1.60	0.82
1:A:868:ALA:N	1:A:869:ALA:HA	1.94	0.81
1:A:868:ALA:H	1:A:869:ALA:HA	1.50	0.71
1:B:914:ARG:HB2	1:B:953:ILE:HD13	1.80	0.63
1:B:911:ILE:HG22	1:B:914:ARG:HD3	1.83	0.59
1:B:618:VAL:HG21	1:B:649:ALA:HB1	1.87	0.57
1:A:208:VAL:HG21	1:A:217:ILE:HG12	1.90	0.54
1:A:320:ILE:HG12	1:A:500:PRO:HD3	1.89	0.54
1:B:208:VAL:HG21	1:B:217:ILE:HG12	1.89	0.54
1:B:641:LYS:HG2	1:B:681:VAL:HG11	1.91	0.53
1:A:641:LYS:HG2	1:A:681:VAL:HG11	1.92	0.52
1:B:385:ILE:HA	1:B:388:LEU:HD12	1.91	0.52
1:A:477:PRO:HG2	1:A:679:PRO:HB2	1.92	0.52
1:B:240:TYR:HB3	1:B:277:LEU:HD22	1.92	0.52
1:B:994:PHE:HB3	1:B:1018:LEU:HD21	1.91	0.52
1:A:385:ILE:HA	1:A:388:LEU:HD12	1.91	0.51
1:A:994:PHE:HB3	1:A:1018:LEU:HD21	1.91	0.51
1:B:477:PRO:HG2	1:B:679:PRO:HB2	1.92	0.50
1:B:160:LEU:HG	1:B:164:ASP:HB3	1.94	0.49
1:A:1019:LYS:HA	1:A:1024:LEU:HD12	1.94	0.49
1:B:339:THR:HG23	1:B:343:VAL:HG22	1.95	0.49
1:B:813:MET:HE1	1:B:997:LEU:HB3	1.95	0.48
1:A:637:VAL:HG11	1:A:671:HIS:HB3	1.96	0.48
1:B:1019:LYS:HA	1:B:1024:LEU:HD12	1.95	0.48
1:A:813:MET:HE1	1:A:997:LEU:HB3	1.96	0.47
1:B:291:MET:HA	1:B:294:ILE:HD12	1.96	0.47
1:A:151:GLU:HA	1:A:154:ILE:HD12	1.97	0.47
1:A:326:PRO:HA	1:A:384:ASN:HA	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:196:HIS:HB3	1:A:203:VAL:HG12	1.97	0.46
1:B:346:HIS:HB3	1:B:366:GLU:HG2	1.98	0.46
1:B:956:TYR:HA	1:B:959:ILE:HD12	1.97	0.46
1:A:195:VAL:HG22	1:A:275:PHE:HB2	1.97	0.46
1:B:326:PRO:HA	1:B:384:ASN:HA	1.96	0.46
1:B:294:ILE:HG12	1:B:697:VAL:HB	1.98	0.45
1:A:209:SER:HB3	1:A:212:LEU:HD12	1.99	0.45
2:B:2000:J82:H19	2:B:2000:J82:H142	1.88	0.45
1:A:809:LEU:HD13	1:A:1001:MET:HE2	1.99	0.45
1:B:809:LEU:HD13	1:B:1001:MET:HE2	1.99	0.45
1:A:642:TYR:HB2	1:A:1003:THR:HG21	1.98	0.44
1:A:811:LEU:HA	1:A:814:LEU:HD12	1.98	0.44
1:B:811:LEU:HA	1:B:814:LEU:HD12	1.98	0.44
1:A:336:LYS:HB2	1:A:483:THR:HA	1.99	0.44
1:B:642:TYR:HB2	1:B:1003:THR:HG21	1.98	0.44
1:B:736:MET:HE2	1:B:740:LEU:HD11	1.99	0.44
1:B:435:VAL:HG21	1:B:453:LEU:HB3	2.00	0.43
1:A:190:LYS:HD3	1:A:207:GLN:HB3	2.01	0.43
1:B:209:SER:HB3	1:B:212:LEU:HD12	2.00	0.43
1:A:320:ILE:HG23	1:A:321:TRP:H	1.83	0.43
1:B:347:VAL:HG22	1:B:398:VAL:HG22	2.01	0.43
1:B:190:LYS:HD3	1:B:207:GLN:HB3	2.01	0.42
1:B:906:SER:HA	1:B:911:ILE:HD12	2.00	0.42
1:A:347:VAL:HG22	1:A:398:VAL:HG22	2.01	0.42
1:A:806:GLN:HE21	1:A:1006:LEU:HG	1.85	0.42
2:A:2000:J82:H19	2:A:2000:J82:H142	1.90	0.42
1:A:956:TYR:HB3	1:A:1050:LYS:HD2	2.02	0.42
1:A:552:ILE:HG22	1:A:570:LEU:HD12	2.03	0.41
1:A:773:MET:HB3	1:A:779:PRO:HD2	2.03	0.41
1:B:710:LEU:HA	1:B:713:LEU:HD12	2.03	0.41
1:A:906:SER:HA	1:A:911:ILE:HD12	2.02	0.41
1:B:552:ILE:HG22	1:B:570:LEU:HD12	2.03	0.41
1:B:637:VAL:HG11	1:B:671:HIS:HB3	2.03	0.41
1:B:438:MET:HE2	1:B:473:VAL:HG11	2.02	0.40
1:A:131:PHE:HA	1:A:134:LEU:HD12	2.03	0.40
1:A:674:SER:HA	1:A:839:GLY:HA2	2.03	0.40
1:A:710:LEU:HA	1:A:713:LEU:HD12	2.03	0.40
1:A:779:PRO:HB3	1:A:799:LYS:HG2	2.03	0.40
1:B:131:PHE:HA	1:B:134:LEU:HD12	2.04	0.40
1:B:445:GLN:HA	1:B:498:TYR:HA	2.02	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	839/952 (88%)	813 (97%)	23 (3%)	3 (0%)	30	60
1	B	814/952 (86%)	787 (97%)	24 (3%)	3 (0%)	30	60
All	All	1653/1904 (87%)	1600 (97%)	47 (3%)	6 (0%)	30	60

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	867	THR
1	A	763	SER
1	B	763	SER
1	B	931	ASP
1	A	335	ASN
1	B	426	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	763/849 (90%)	743 (97%)	20 (3%)	40	75
1	B	747/849 (88%)	730 (98%)	17 (2%)	44	78
All	All	1510/1698 (89%)	1473 (98%)	37 (2%)	42	76

All (37) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	153	LYS
1	A	226	LEU
1	A	320	ILE
1	A	487	ILE
1	A	503	ASP
1	A	563	PHE
1	A	579	LEU
1	A	588	LEU
1	A	627	GLU
1	A	710	LEU
1	A	722	LEU
1	A	752	LEU
1	A	819	LEU
1	A	875	LEU
1	A	935	ILE
1	A	939	PHE
1	A	954	LEU
1	A	987	LEU
1	A	1015	ILE
1	A	1040	ASP
1	B	153	LYS
1	B	157	LEU
1	B	163	ILE
1	B	226	LEU
1	B	228	ILE
1	B	248	VAL
1	B	324	ASN
1	B	337	LEU
1	B	563	PHE
1	B	579	LEU
1	B	588	LEU
1	B	590	GLN
1	B	710	LEU
1	B	752	LEU
1	B	819	LEU
1	B	875	LEU
1	B	1015	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (44) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	129	HIS
1	A	181	ASN

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Mol	Chain	Res	Type
1	A	243	GLN
1	A	261	GLN
1	A	274	HIS
1	A	289	GLN
1	A	376	ASN
1	A	384	ASN
1	A	436	ASN
1	A	445	GLN
1	A	481	ASN
1	A	607	ASN
1	A	635	GLN
1	A	661	ASN
1	A	711	ASN
1	A	742	GLN
1	A	757	ASN
1	A	800	ASN
1	A	806	GLN
1	A	877	ASN
1	A	926	GLN
1	A	929	HIS
1	A	969	ASN
1	A	992	ASN
1	A	1052	ASN
1	B	129	HIS
1	B	243	GLN
1	B	335	ASN
1	B	384	ASN
1	B	429	HIS
1	B	436	ASN
1	B	445	GLN
1	B	590	GLN
1	B	607	ASN
1	B	635	GLN
1	B	684	GLN
1	B	711	ASN
1	B	742	GLN
1	B	757	ASN
1	B	860	ASN
1	B	877	ASN
1	B	926	GLN
1	B	938	ASN
1	B	992	ASN

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 oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

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	B	2000	-	27,29,29	1.08	2 (7%)	33,41,41	1.41	4 (12%)
2	J82	A	2000	-	27,29,29	1.09	2 (7%)	33,41,41	1.37	4 (12%)

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	B	2000	-	-	4/10/32/32	0/4/4/4
2	J82	A	2000	-	-	4/10/32/32	0/4/4/4

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	2000	J82	C19-N17	4.65	1.53	1.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	2000	J82	C19-N17	4.59	1.53	1.48
2	B	2000	J82	C12-C1	2.46	1.42	1.38
2	A	2000	J82	C12-C1	2.34	1.42	1.38

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	2000	J82	C12-C1-N8	-5.24	119.33	122.86
2	A	2000	J82	C12-C1-N8	-4.89	119.57	122.86
2	B	2000	J82	C11-C12-C1	4.34	122.01	119.28
2	A	2000	J82	C11-C12-C1	4.19	121.91	119.28
2	A	2000	J82	C26-C19-C18	-2.54	109.53	114.84
2	A	2000	J82	C11-N10-C9	-2.54	121.33	123.42
2	B	2000	J82	C26-C19-C18	-2.49	109.64	114.84
2	B	2000	J82	C11-N10-C9	-2.45	121.41	123.42

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	2000	J82	C9-C14-C15-O16
2	A	2000	J82	C9-C14-C15-N17
2	B	2000	J82	C9-C14-C15-O16
2	B	2000	J82	C9-C14-C15-N17
2	A	2000	J82	C14-C15-N17-C19
2	B	2000	J82	C14-C15-N17-C19
2	B	2000	J82	O16-C15-N17-C19
2	A	2000	J82	O16-C15-N17-C19

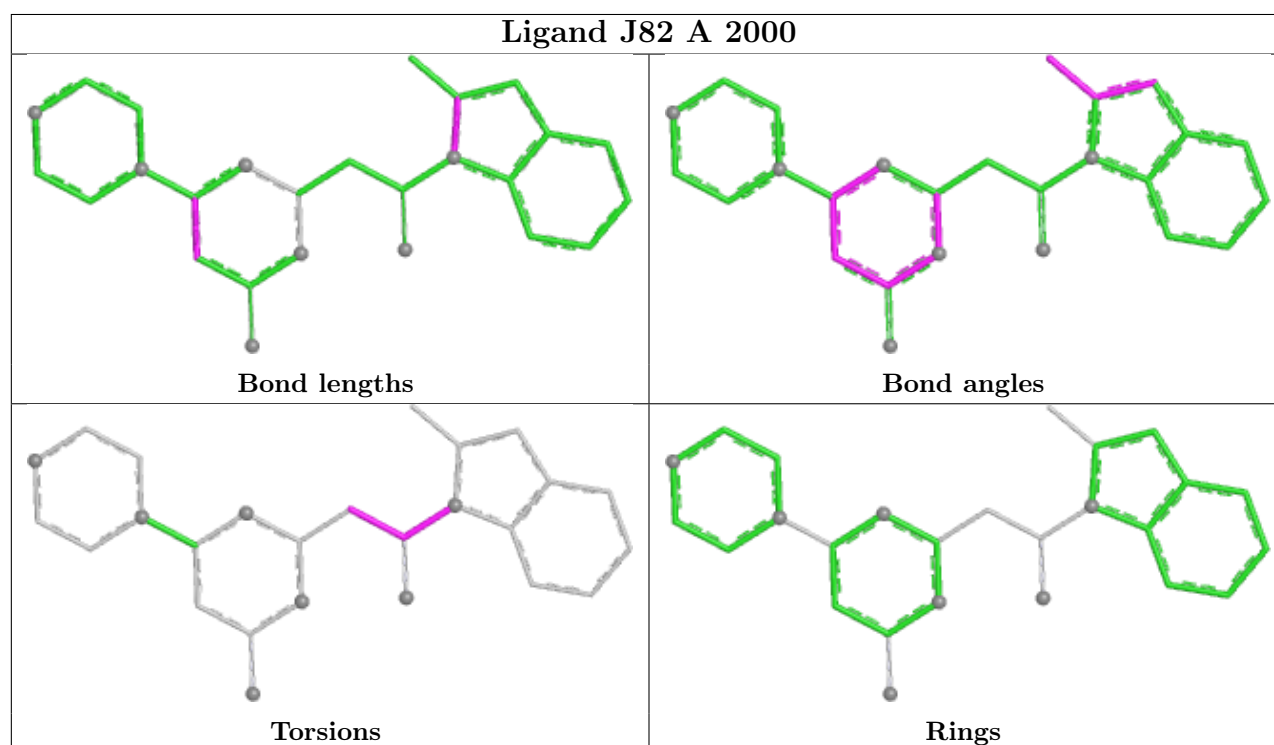
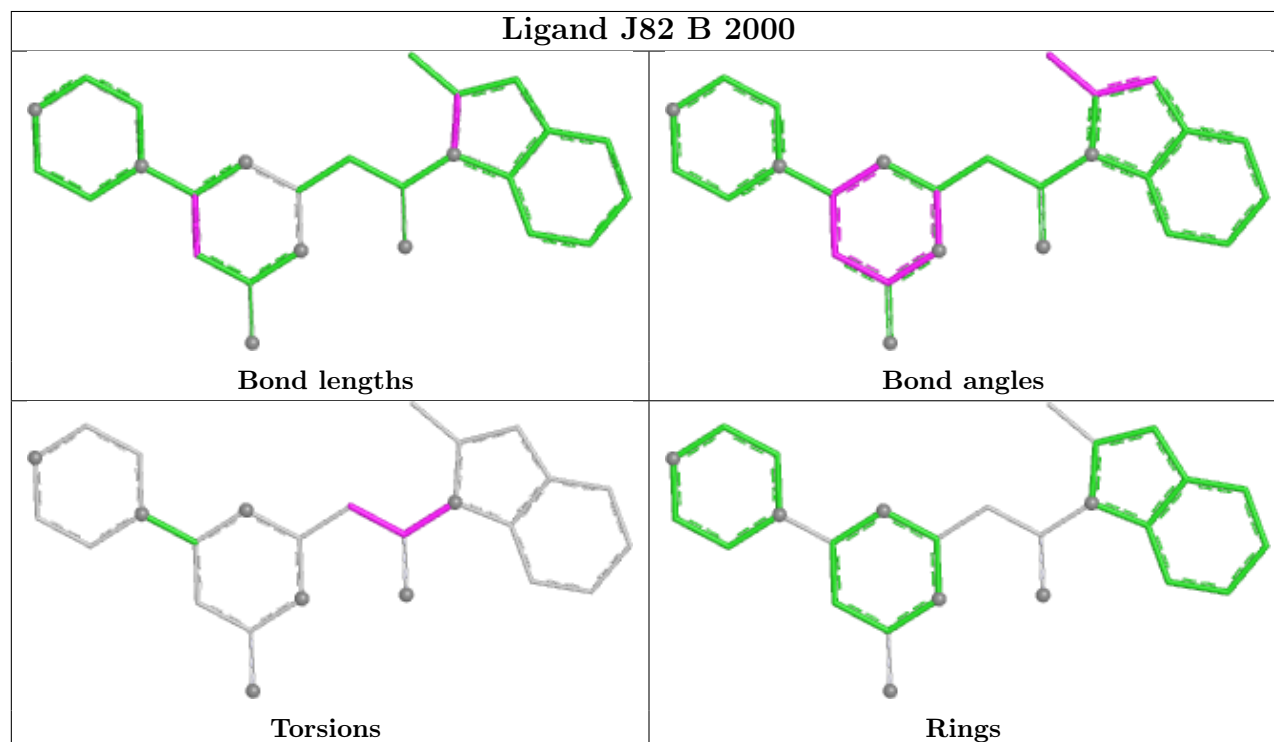
There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	2000	J82	1	0
2	A	2000	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 [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, 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	855/952 (89%)	1.15	133 (15%) 5 4	46, 81, 113, 138	0
1	B	836/952 (87%)	0.94	91 (10%) 10 8	49, 70, 95, 138	0
All	All	1691/1904 (88%)	1.05	224 (13%) 7 6	46, 74, 109, 138	0

All (224) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	399	TYR	5.0
1	B	246	GLY	4.9
1	A	939	PHE	4.9
1	A	868	ALA	4.9
1	A	298	ILE	4.7
1	B	339	THR	4.7
1	A	162	TRP	4.4
1	A	228	ILE	4.3
1	A	154	ILE	4.2
1	B	785	SER	4.0
1	A	430	TYR	3.9
1	A	374	ILE	3.9
1	B	739	CYS	3.8
1	B	753	GLN	3.8
1	A	320	ILE	3.7
1	A	492	ASN	3.7
1	B	478	TYR	3.7
1	B	514	SER	3.7
1	A	924	THR	3.6
1	B	1044	ARG	3.6
1	B	482	ALA	3.5
1	B	298	ILE	3.5
1	B	297	ALA	3.5
1	A	685	PHE	3.4

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Mol	Chain	Res	Type	RSRZ
1	A	292	ILE	3.4
1	B	428	VAL	3.4
1	A	245	SER	3.4
1	B	228	ILE	3.4
1	B	968	GLY	3.3
1	A	968	GLY	3.3
1	A	432	VAL	3.3
1	B	244	VAL	3.2
1	A	867	THR	3.2
1	B	938	ASN	3.2
1	A	160	LEU	3.2
1	A	337	LEU	3.2
1	A	479	ALA	3.1
1	B	499	TYR	3.1
1	A	297	ALA	3.1
1	A	149	PHE	3.1
1	A	863	ASN	3.1
1	A	117	ASP	3.0
1	A	118	SER	3.0
1	A	862	SER	3.0
1	B	402	LEU	3.0
1	B	970	THR	3.0
1	A	367	ILE	3.0
1	B	361	THR	3.0
1	A	459	PHE	3.0
1	A	790	GLY	2.9
1	B	179	LEU	2.9
1	B	752	LEU	2.9
1	A	728	SER	2.9
1	A	244	VAL	2.9
1	A	193	VAL	2.9
1	B	876	LEU	2.9
1	A	864	VAL	2.8
1	B	296	ALA	2.8
1	A	493	LYS	2.8
1	B	493	LYS	2.8
1	A	514	SER	2.8
1	B	1043	LEU	2.8
1	A	396	PHE	2.7
1	B	425	ALA	2.7
1	B	268	MET	2.7
1	A	969	ASN	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	119	LYS	2.7
1	B	180	GLU	2.7
1	A	276	ILE	2.7
1	B	872	LYS	2.7
1	A	684	GLN	2.7
1	A	752	LEU	2.7
1	B	367	ILE	2.6
1	A	275	PHE	2.6
1	A	877	ASN	2.6
1	A	529	LEU	2.6
1	A	861	SER	2.6
1	A	866	ALA	2.6
1	A	526	LYS	2.6
1	A	379	LEU	2.6
1	A	762	LEU	2.6
1	B	953	ILE	2.6
1	B	1045	GLU	2.6
1	B	170	TYR	2.6
1	B	965	GLY	2.6
1	A	220	LEU	2.6
1	A	376	ASN	2.6
1	B	873	ASP	2.6
1	B	245	SER	2.6
1	A	226	LEU	2.6
1	B	166	LEU	2.6
1	B	761	ILE	2.6
1	B	424	LYS	2.5
1	A	178	VAL	2.5
1	B	163	ILE	2.5
1	B	248	VAL	2.5
1	B	293	ALA	2.5
1	A	210	PRO	2.5
1	A	363	VAL	2.5
1	A	473	VAL	2.5
1	A	478	TYR	2.5
1	B	178	VAL	2.5
1	A	289	GLN	2.5
1	A	361	THR	2.5
1	A	935	ILE	2.5
1	A	199	ASN	2.5
1	A	731	LYS	2.5
1	B	494	LYS	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	200	SER	2.5
1	A	329	ILE	2.5
1	A	698	GLY	2.5
1	B	369	GLY	2.5
1	B	849	SER	2.5
1	A	248	VAL	2.5
1	A	590	GLN	2.5
1	B	429	HIS	2.5
1	A	202	ASP	2.4
1	B	570	LEU	2.4
1	B	426	GLY	2.4
1	B	536	LEU	2.4
1	A	679	PRO	2.4
1	A	375	TRP	2.4
1	A	789	PHE	2.4
1	A	742	GLN	2.4
1	B	590	GLN	2.4
1	A	214	PRO	2.4
1	B	501	PRO	2.4
1	A	195	VAL	2.4
1	A	131	PHE	2.4
1	A	151	GLU	2.4
1	A	768	GLU	2.4
1	B	288	GLU	2.4
1	B	337	LEU	2.4
1	A	338	ASN	2.4
1	B	492	ASN	2.4
1	A	352	PHE	2.4
1	A	235	ALA	2.4
1	B	368	SER	2.4
1	A	165	TRP	2.4
1	B	237	PRO	2.4
1	B	323	ASN	2.3
1	B	526	LYS	2.3
1	B	877	ASN	2.3
1	B	207	GLN	2.3
1	A	357	LEU	2.3
1	A	333	LYS	2.3
1	B	924	THR	2.3
1	A	769	LYS	2.3
1	A	547	ASN	2.3
1	A	242	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	294	ILE	2.3
1	A	733	LYS	2.3
1	A	958	PHE	2.3
1	A	865	ALA	2.3
1	A	128	LEU	2.3
1	A	227	THR	2.3
1	A	332	VAL	2.3
1	B	725	VAL	2.3
1	B	354	GLY	2.3
1	B	438	MET	2.2
1	A	1060	LYS	2.2
1	B	363	VAL	2.2
1	B	401	VAL	2.2
1	A	250	TYR	2.2
1	A	499	TYR	2.2
1	A	482	ALA	2.2
1	A	224	LYS	2.2
1	A	591	ILE	2.2
1	A	964	GLN	2.2
1	A	486	HIS	2.2
1	A	934	HIS	2.2
1	B	497	CYS	2.2
1	B	250	TYR	2.2
1	A	485	LEU	2.2
1	A	722	LEU	2.2
1	A	869	ALA	2.2
1	B	875	LEU	2.2
1	A	196	HIS	2.2
1	A	1061	ASP	2.2
1	B	642	TYR	2.2
1	A	206	PHE	2.2
1	B	502	PHE	2.2
1	A	191	LEU	2.2
1	B	277	LEU	2.2
1	B	567	LEU	2.2
1	B	393	ARG	2.2
1	A	192	VAL	2.2
1	B	917	ASP	2.2
1	A	701	LYS	2.2
1	B	759	CYS	2.2
1	A	179	LEU	2.2
1	A	754	SER	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	258	ILE	2.1
1	B	171	PRO	2.1
1	B	726	LYS	2.1
1	A	936	LEU	2.1
1	A	194	ALA	2.1
1	A	393	ARG	2.1
1	A	720	ILE	2.1
1	B	343	VAL	2.1
1	B	216	LYS	2.1
1	A	271	THR	2.1
1	B	740	LEU	2.1
1	B	187	TYR	2.1
1	A	124	ILE	2.1
1	A	394	LEU	2.1
1	B	774	ASP	2.1
1	A	498	TYR	2.1
1	B	796	VAL	2.1
1	A	358	LEU	2.1
1	A	729	ARG	2.1
1	A	120	ILE	2.1
1	A	730	ALA	2.1
1	B	205	SER	2.0
1	A	637	VAL	2.0
1	A	564	PRO	2.0
1	A	653	PHE	2.0
1	B	552	ILE	2.0
1	A	882	TYR	2.0
1	A	291	MET	2.0
1	A	123	LEU	2.0
1	B	874	ALA	2.0
1	B	284	LYS	2.0
1	A	642	TYR	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

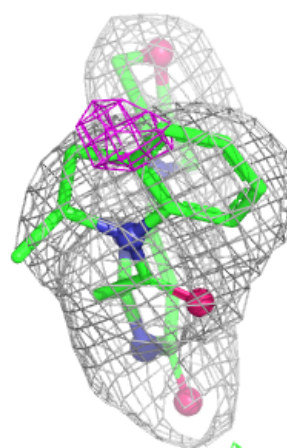
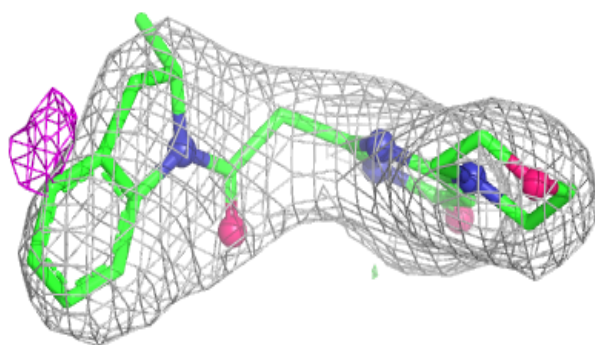
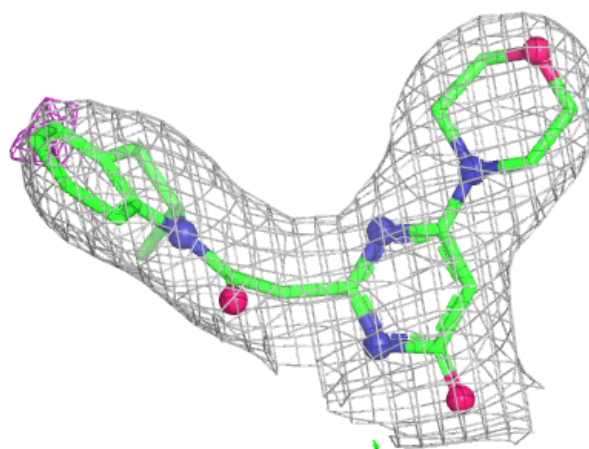
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

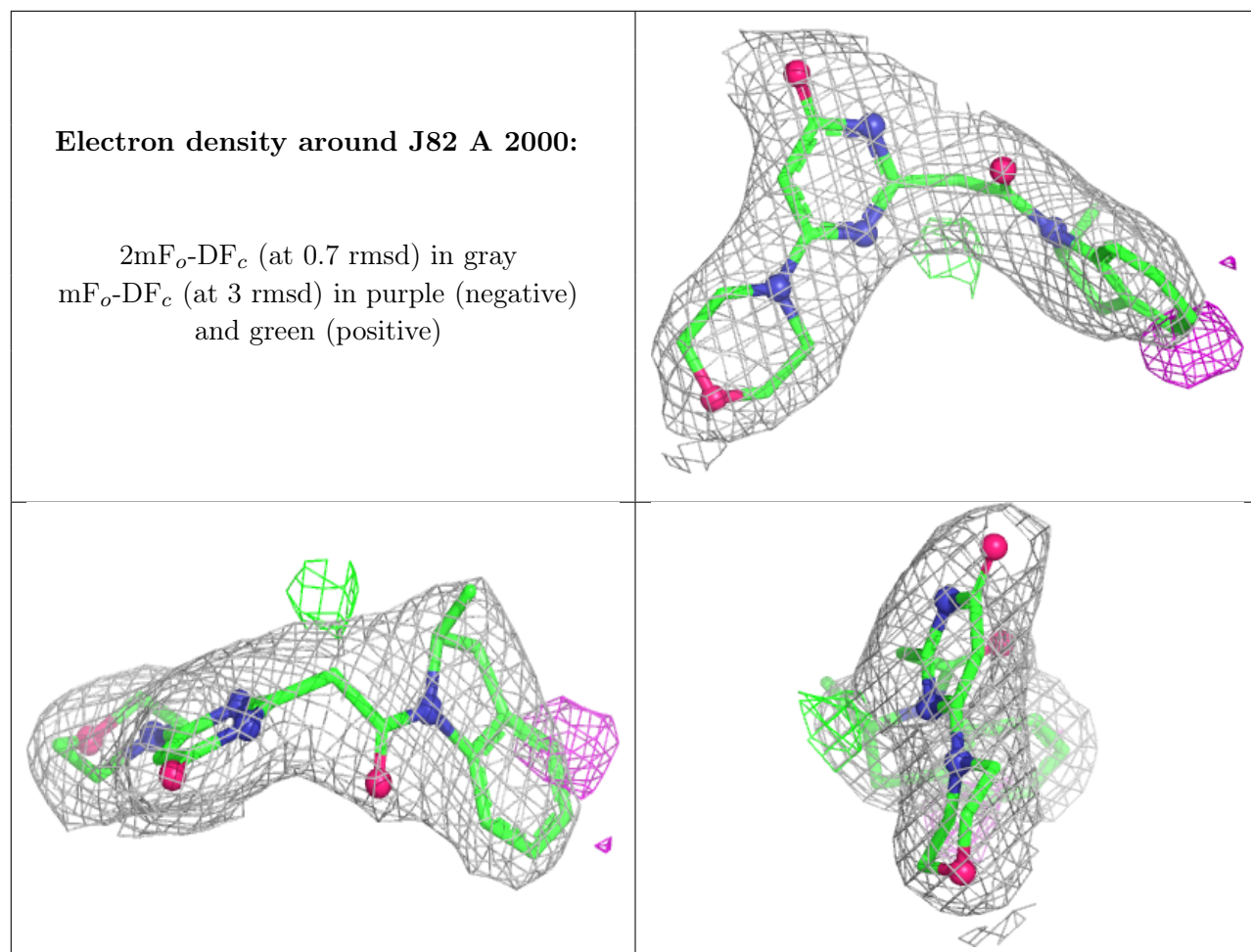
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	J82	B	2000	26/26	0.91	0.12	50,50,51,52	0
2	J82	A	2000	26/26	0.92	0.11	48,49,51,51	0

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 B 2000:

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.