



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 06:33 AM UTC

PDB ID : 3QRI / pdb_00003qri
Title : The crystal structure of human abl1 kinase domain in complex with DCC-2036
Authors : Chan, W.W.; Wise, S.C.; Kaufman, M.D.; Ahn, Y.M.; Ensinger, C.L.; Haack, T.; Hood, M.M.; Jones, J.; Lord, J.W.; Lu, W.P.; Miller, D.; Patt, W.C.; Smith, B.D.; Petillo, P.A.; Rutkoski, T.J.; Telikepalli, H.; Vogeti, L.; Yao, T.; Chun, L.; Clark, R.; Evangelista, P.; Gavrilescu, L.C.; Lazarides, K.; Zaleskas, V.M.; Stewart, L.J.; Van Etten, R.A.; Flynn, D.L.
Deposited on : 2011-02-18
Resolution : 2.10 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)

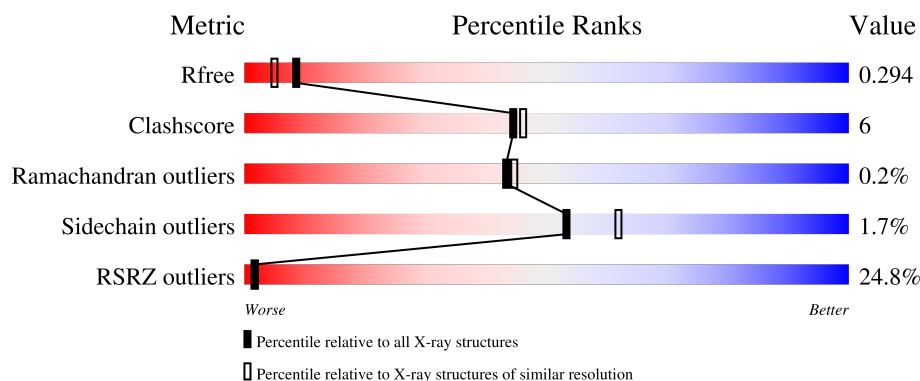
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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	6658 (2.10-2.10)
Clashscore	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)
RSRZ outliers	180081	6662 (2.10-2.10)

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	277	22% 87% 12% .
1	B	277	26% 83% 11% 5%

Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 4863 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 Tyrosine-protein kinase ABL1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	275	Total	C	N	O	S	0	6	0
			2254	1454	365	414	21			
1	B	262	Total	C	N	O	S	0	4	0
			2125	1376	344	387	18			

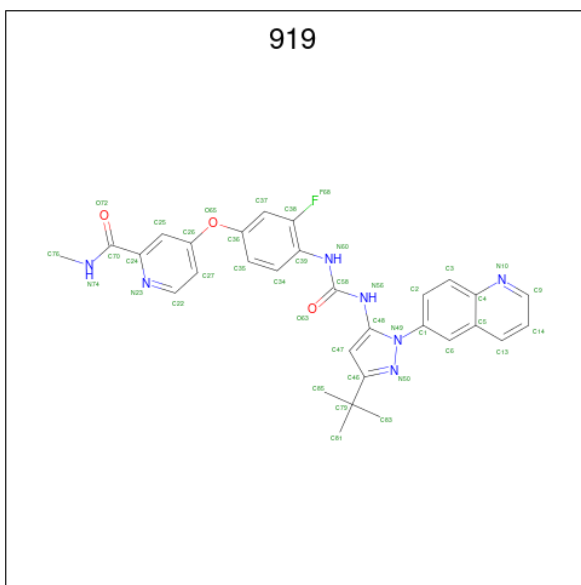
There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	223	THR	-	expression tag	UNP P00519
A	224	SER	-	expression tag	UNP P00519
A	225	MET	-	expression tag	UNP P00519
A	226	ASP	-	expression tag	UNP P00519
A	227	PRO	-	expression tag	UNP P00519
A	228	SER	-	expression tag	UNP P00519
B	223	THR	-	expression tag	UNP P00519
B	224	SER	-	expression tag	UNP P00519
B	225	MET	-	expression tag	UNP P00519
B	226	ASP	-	expression tag	UNP P00519
B	227	PRO	-	expression tag	UNP P00519
B	228	SER	-	expression tag	UNP P00519

- Molecule 2 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total	Na	0	0
			2	2		

- Molecule 3 is 4-[4-({[3-tert-butyl-1-(quinolin-6-yl)-1H-pyrazol-5-yl]carbamoyl}amino)-3-fluorophenoxy]-N-methylpyridine-2-carboxamide (CCD ID: 919) (formula: C₃₀H₂₈FN₇O₃).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total 41	C 30	F 1	N 7	O 3	0	0
3	B	1	Total 41	C 30	F 1	N 7	O 3	0	0

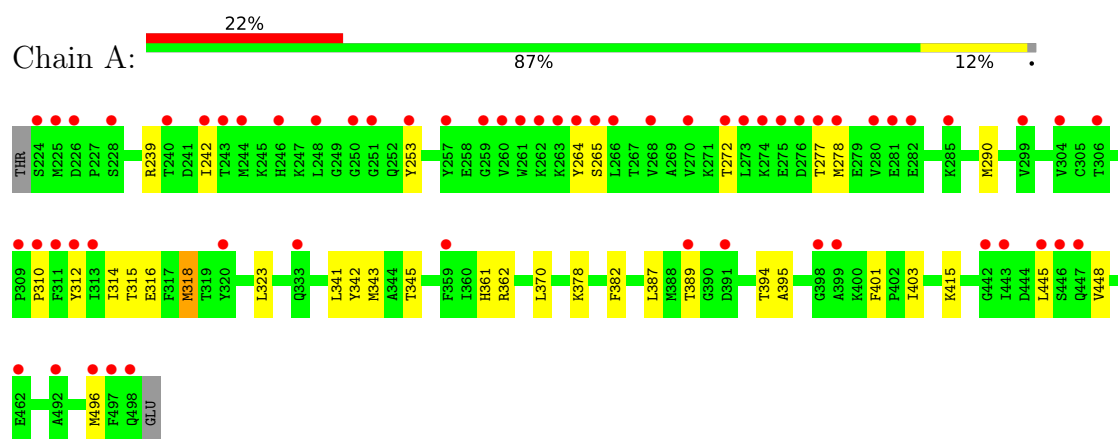
- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	207	Total O 207 207	0	0
4	B	193	Total O 193 193	0	0

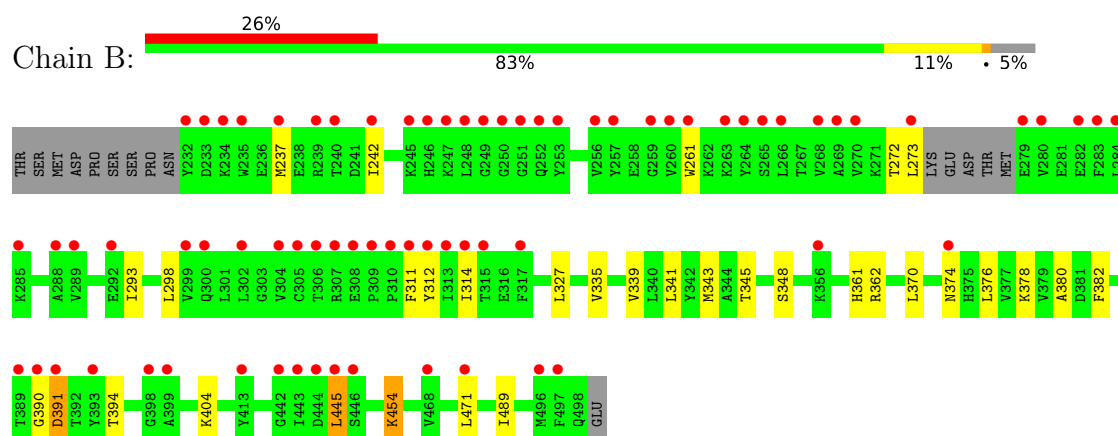
3 Residue-property plots

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: Tyrosine-protein kinase ABL1



• Molecule 1: Tyrosine-protein kinase ABL1



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	60.26Å 59.70Å 79.43Å 90.00° 108.71° 90.00°	Depositor
Resolution (Å)	57.08 – 2.10 57.08 – 2.10	Depositor EDS
% Data completeness (in resolution range)	(Not available) (57.08-2.10) 97.2 (57.08-2.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.11	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.67 (at 2.10Å)	Xtriage
Refinement program	REFMAC 5.5.0088	Depositor
R, R_{free}	0.213 , 0.272 (Not available) , 0.294	Depositor DCC
R_{free} test set	1540 reflections (4.90%)	wwPDB-VP
Wilson B-factor (Å ²)	18.0	Xtriage
Anisotropy	0.184	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 45.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	4863	wwPDB-VP
Average B, all atoms (Å ²)	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 20.80 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 8.0354e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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: NA, 919

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	0.59	0/2330	0.84	1/3154 (0.0%)
1	B	0.58	0/2191	0.82	0/2968
All	All	0.59	0/4521	0.83	1/6122 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	448	VAL	N-CA-C	6.34	117.01	110.36

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	2254	0	2217	28	0
1	B	2125	0	2077	24	0
2	A	2	0	0	0	0
3	A	41	0	28	0	0
3	B	41	0	28	2	0
4	A	207	0	0	1	0
4	B	193	0	0	2	0
All	All	4863	0	4350	53	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 6.

All (53) 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:A:318[A]:MET:HA	1:A:318[A]:MET:HE2	1.46	0.95
1:A:242:ILE:HD11	1:A:314:ILE:HD13	1.49	0.94
1:A:341:LEU:HD11	1:A:496:MET:HE1	1.60	0.84
1:A:318[A]:MET:HA	1:A:318[A]:MET:CE	2.12	0.79
1:B:374:ASN:HB3	4:B:578:HOH:O	1.84	0.76
1:B:339:VAL:HG12	1:B:343[B]:MET:HE3	1.71	0.70
1:B:376:LEU:HD21	1:B:378:LYS:NZ	2.09	0.68
1:A:242:ILE:HD11	1:A:314:ILE:CD1	2.24	0.67
1:A:242:ILE:CD1	1:A:314:ILE:HD13	2.23	0.66
1:A:316:GLU:OE2	1:A:378:LYS:NZ	2.30	0.63
1:A:242:ILE:CD1	1:A:314:ILE:CD1	2.77	0.63
1:A:401:PHE:HB2	1:A:403:ILE:HD13	1.79	0.62
1:B:404:LYS:HE3	1:B:445:LEU:HD12	1.82	0.61
1:B:341:LEU:O	1:B:345[B]:THR:HG23	2.02	0.59
1:B:327:LEU:HD21	1:B:343[A]:MET:HE1	1.84	0.59
1:A:239:ARG:NH1	1:A:310:PRO:O	2.34	0.58
1:B:314:ILE:HD12	1:B:314:ILE:N	2.18	0.58
1:B:339:VAL:CG1	1:B:343[B]:MET:HE3	2.35	0.57
1:A:342:TYR:O	1:A:345[B]:THR:HG22	2.04	0.57
1:A:361:HIS:O	1:A:362:ARG:HB2	2.05	0.56
1:B:376:LEU:HD21	1:B:378:LYS:HZ1	1.70	0.56
1:B:272:THR:HG22	1:B:312:TYR:CD2	2.41	0.56
1:A:394:THR:HG21	1:A:445:LEU:HD23	1.89	0.54
1:A:272:THR:HG22	1:A:312:TYR:CD2	2.44	0.52
1:A:394:THR:CG2	1:A:445:LEU:HD23	2.39	0.52
1:B:390:GLY:CA	1:B:391:ASP:CB	2.89	0.51
1:A:394:THR:OG1	1:A:395:ALA:N	2.44	0.51
1:B:361:HIS:O	1:B:362:ARG:HB2	2.10	0.51
1:A:362:ARG:NH2	4:A:503:HOH:O	2.44	0.50
1:B:471:LEU:HD11	1:B:489:ILE:HD13	1.94	0.49
1:A:323:LEU:CD1	1:A:343[A]:MET:HE2	2.42	0.48
1:B:454:LYS:NZ	4:B:568:HOH:O	2.45	0.48
3:B:2:919:O63	3:B:2:919:H34	2.15	0.47
1:A:370:LEU:HD21	1:A:382:PHE:CZ	2.50	0.46
1:B:380:ALA:HB1	3:B:2:919:H34	1.98	0.46
1:B:242:ILE:CD1	1:B:314:ILE:HG12	2.46	0.45
1:A:277:THR:O	1:A:277:THR:HG22	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:293:ILE:CG2	1:B:298:LEU:HD13	2.47	0.45
1:B:272:THR:HG22	1:B:312:TYR:CE2	2.52	0.45
1:A:370:LEU:HD21	1:A:382:PHE:HZ	1.81	0.45
1:B:293:ILE:HG23	1:B:298:LEU:HD13	2.00	0.43
1:B:335:VAL:HG13	1:B:343[B]:MET:HE1	2.00	0.43
1:A:323:LEU:HD11	1:A:343[A]:MET:HE2	2.01	0.43
1:B:327:LEU:HD21	1:B:343[A]:MET:CE	2.49	0.42
1:A:264:TYR:O	1:A:265:SER:C	2.63	0.42
1:B:370:LEU:HD21	1:B:382:PHE:HZ	1.84	0.42
1:A:253:TYR:C	1:A:387:LEU:HD13	2.45	0.42
1:B:273:LEU:HD23	1:B:311:PHE:HD2	1.86	0.41
1:A:242:ILE:CD1	1:A:314:ILE:HD11	2.51	0.41
1:A:290:MET:HE1	1:A:315:THR:CG2	2.50	0.41
1:A:323:LEU:CD1	1:A:343[A]:MET:CE	2.97	0.41
1:A:290:MET:HE1	1:A:315:THR:HG21	2.02	0.41
1:B:237:MET:HE1	1:B:261:TRP:CE2	2.55	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	279/277 (101%)	265 (95%)	14 (5%)	0	100	100
1	B	262/277 (95%)	254 (97%)	7 (3%)	1 (0%)	30	28
All	All	541/554 (98%)	519 (96%)	21 (4%)	1 (0%)	43	44

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	391	ASP

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	244/243 (100%)	239 (98%)	5 (2%)	48	56
1	B	225/243 (93%)	221 (98%)	4 (2%)	51	60
All	All	469/486 (96%)	460 (98%)	9 (2%)	53	58

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	278	MET
1	A	318[A]	MET
1	A	318[B]	MET
1	A	389	THR
1	A	415	LYS
1	B	348	SER
1	B	394	THR
1	B	445	LEU
1	B	454	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	447	GLN
1	B	252	GLN
1	B	375	HIS

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 [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 for Mogul analysis.

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	919	A	500	-	45,45,45	1.12	3 (6%)	64,65,65	1.87	14 (21%)
3	919	B	2	-	45,45,45	1.16	2 (4%)	64,65,65	2.08	13 (20%)

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	919	A	500	-	-	0/28/28/28	0/5/5/5
3	919	B	2	-	-	1/28/28/28	0/5/5/5

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	2	919	C1-N49	-4.26	1.35	1.43
3	A	500	919	C1-N49	-4.23	1.35	1.43
3	B	2	919	C39-N60	-2.55	1.36	1.41
3	A	500	919	C39-N60	-2.37	1.37	1.41
3	A	500	919	C5-C4	-2.24	1.38	1.42

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	2	919	C24-C70-N74	7.09	120.42	115.56
3	B	2	919	C6-C1-N49	6.93	126.83	119.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	2	919	C1-N49-C48	-6.55	123.36	129.78
3	A	500	919	C6-C1-N49	6.30	126.16	119.45
3	A	500	919	C24-C70-N74	5.03	119.01	115.56
3	A	500	919	C36-O65-C26	4.73	129.58	118.78
3	B	2	919	C79-C46-C47	-4.52	122.25	128.66
3	A	500	919	C79-C46-C47	-3.68	123.44	128.66
3	A	500	919	C22-N23-C24	3.67	121.66	116.93
3	B	2	919	C36-O65-C26	3.59	127.00	118.78
3	A	500	919	C14-C9-N10	-3.43	118.94	123.97
3	B	2	919	C22-N23-C24	3.29	121.17	116.93
3	A	500	919	C25-C24-N23	-3.10	119.55	123.27
3	A	500	919	C9-N10-C4	2.80	121.16	116.93
3	B	2	919	C9-N10-C4	2.74	121.08	116.93
3	A	500	919	C27-C22-N23	-2.73	120.62	123.97
3	B	2	919	C14-C9-N10	-2.73	119.96	123.97
3	B	2	919	C25-C24-N23	-2.73	120.00	123.27
3	A	500	919	C46-N50-N49	-2.71	101.99	104.27
3	A	500	919	F68-C38-C39	2.69	120.94	117.59
3	B	2	919	C46-N50-N49	-2.45	102.21	104.27
3	B	2	919	C1-N49-N50	-2.39	115.21	118.67
3	B	2	919	C27-C22-N23	-2.38	121.05	123.97
3	A	500	919	C2-C1-C6	-2.35	114.89	119.17
3	B	2	919	C2-C1-C6	-2.31	114.95	119.17
3	A	500	919	C1-N49-C48	-2.28	127.54	129.78
3	A	500	919	C81-C79-C46	-2.15	105.97	109.63

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	2	919	O72-C70-N74-C76

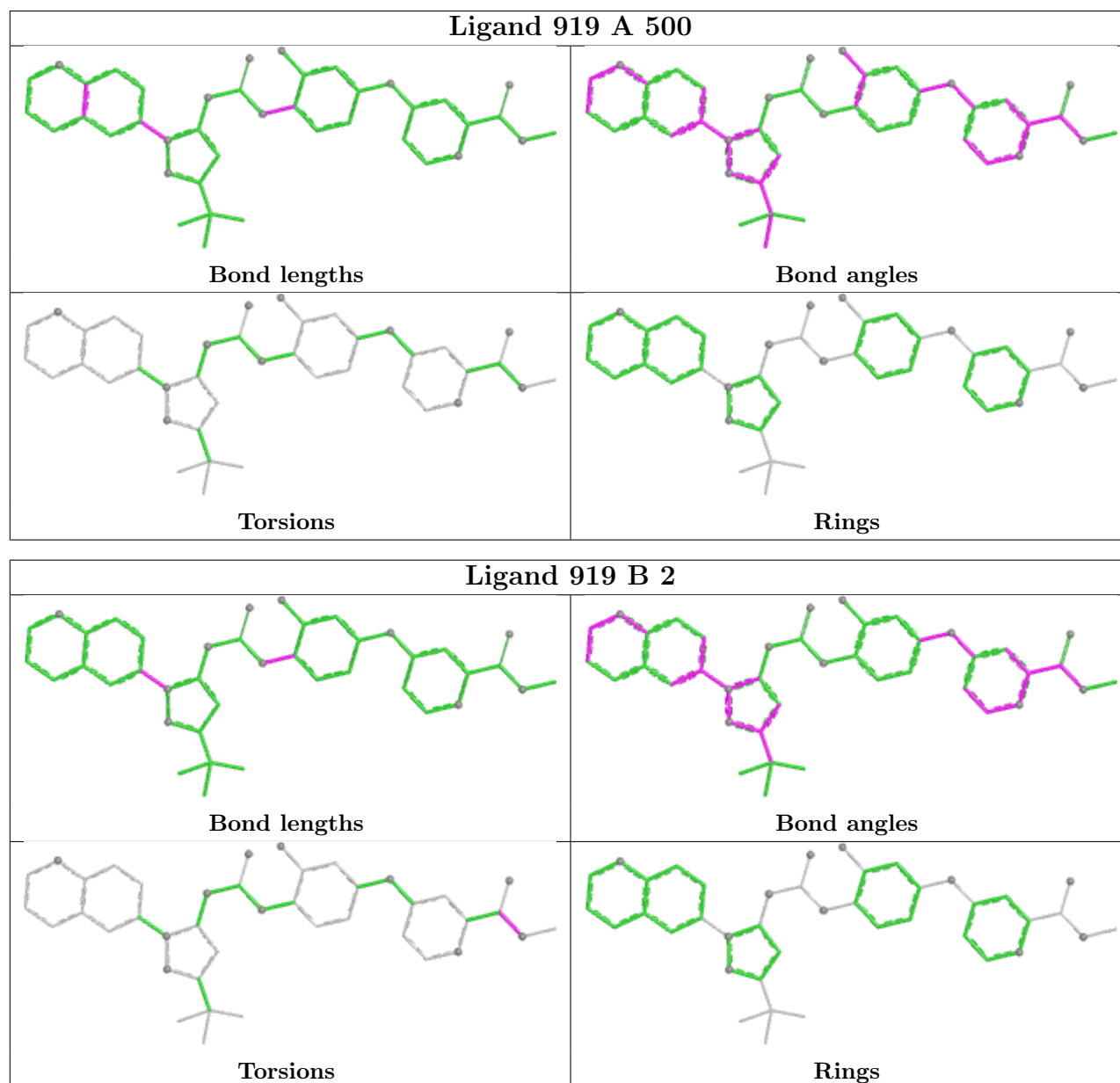
There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	2	919	2	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	275/277 (99%)	1.22	60 (21%) 2 2	14, 31, 48, 57	6 (2%)
1	B	262/277 (94%)	1.42	73 (27%) 1 1	15, 32, 52, 57	4 (1%)
All	All	537/554 (96%)	1.32	133 (24%) 2 2	14, 31, 51, 57	10 (1%)

All (133) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	389	THR	6.3
1	A	389	THR	6.0
1	B	232	TYR	5.7
1	A	497	PHE	5.6
1	A	442	GLY	5.4
1	A	276	ASP	5.1
1	A	278	MET	4.9
1	B	311	PHE	4.8
1	B	308	GLU	4.5
1	A	311	PHE	4.2
1	B	242	ILE	4.2
1	A	265	SER	4.2
1	A	277	THR	4.0
1	B	261	TRP	4.0
1	B	260	VAL	4.0
1	A	248	LEU	3.9
1	A	280	VAL	3.9
1	B	312	TYR	3.9
1	B	264	TYR	3.8
1	B	266	LEU	3.8
1	A	274	LYS	3.8
1	B	235	TRP	3.7
1	B	253	TYR	3.7
1	A	264	TYR	3.7

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Mol	Chain	Res	Type	RSRZ
1	A	242	ILE	3.7
1	B	263	LYS	3.7
1	B	250	GLY	3.7
1	A	498	GLN	3.7
1	B	248	LEU	3.6
1	B	305	CYS	3.6
1	A	246	HIS	3.6
1	B	246	HIS	3.6
1	A	266	LEU	3.6
1	B	233	ASP	3.5
1	B	442	GLY	3.5
1	B	391	ASP	3.5
1	B	300	GLN	3.4
1	B	280	VAL	3.4
1	B	310	PRO	3.4
1	B	443	ILE	3.4
1	A	251	GLY	3.3
1	A	260	VAL	3.3
1	B	237	MET	3.3
1	B	306	THR	3.3
1	A	250	GLY	3.3
1	A	445	LEU	3.2
1	B	445	LEU	3.2
1	B	496	MET	3.2
1	A	253	TYR	3.2
1	B	240	THR	3.2
1	A	262	LYS	3.2
1	A	261	TRP	3.1
1	B	283	PHE	3.1
1	B	292	GLU	3.1
1	A	275	GLU	3.0
1	B	265	SER	2.9
1	B	444	ASP	2.9
1	A	257	TYR	2.9
1	B	273	LEU	2.9
1	B	239	ARG	2.9
1	A	281	GLU	2.9
1	B	302	LEU	2.9
1	A	391	ASP	2.9
1	B	307	ARG	2.9
1	A	359	PHE	2.9
1	B	252	GLN	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	446	SER	2.8
1	B	268	VAL	2.8
1	A	443	ILE	2.8
1	B	413	TYR	2.8
1	A	309	PRO	2.8
1	B	234	LYS	2.8
1	A	263	LYS	2.7
1	A	243	THR	2.7
1	A	496	MET	2.7
1	B	304	VAL	2.7
1	A	273	LEU	2.7
1	B	315	THR	2.7
1	B	471	LEU	2.7
1	B	279	GLU	2.6
1	B	313	ILE	2.6
1	B	282	GLU	2.6
1	B	393	TYR	2.6
1	B	299	VAL	2.5
1	B	314	ILE	2.5
1	A	259	GLY	2.5
1	B	390	GLY	2.5
1	B	446	SER	2.5
1	A	447	GLN	2.5
1	A	226	ASP	2.5
1	A	224	SER	2.5
1	A	228	SER	2.5
1	B	288	ALA	2.4
1	B	249	GLY	2.4
1	A	492	ALA	2.4
1	B	259	GLY	2.4
1	A	268	VAL	2.4
1	B	245	LYS	2.4
1	B	269	ALA	2.4
1	B	399	ALA	2.4
1	B	289	VAL	2.4
1	B	284	LEU	2.3
1	B	309	PRO	2.3
1	A	282	GLU	2.3
1	A	244	MET	2.3
1	A	270	VAL	2.2
1	A	299	VAL	2.2
1	A	310	PRO	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	256	VAL	2.2
1	A	398	GLY	2.2
1	B	398	GLY	2.2
1	A	312	TYR	2.2
1	A	285	LYS	2.2
1	B	468	VAL	2.2
1	A	313	ILE	2.1
1	B	497	PHE	2.1
1	B	374	ASN	2.1
1	A	306	THR	2.1
1	B	317	PHE	2.1
1	A	304	VAL	2.1
1	B	270	VAL	2.1
1	B	356	LYS	2.1
1	A	225	MET	2.1
1	B	257	TYR	2.1
1	A	272	THR	2.1
1	A	333	GLN	2.1
1	A	240	THR	2.1
1	B	251	GLY	2.1
1	B	247	LYS	2.1
1	A	462	GLU	2.0
1	B	285	LYS	2.0
1	A	399	ALA	2.0
1	A	320	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 ⓘ

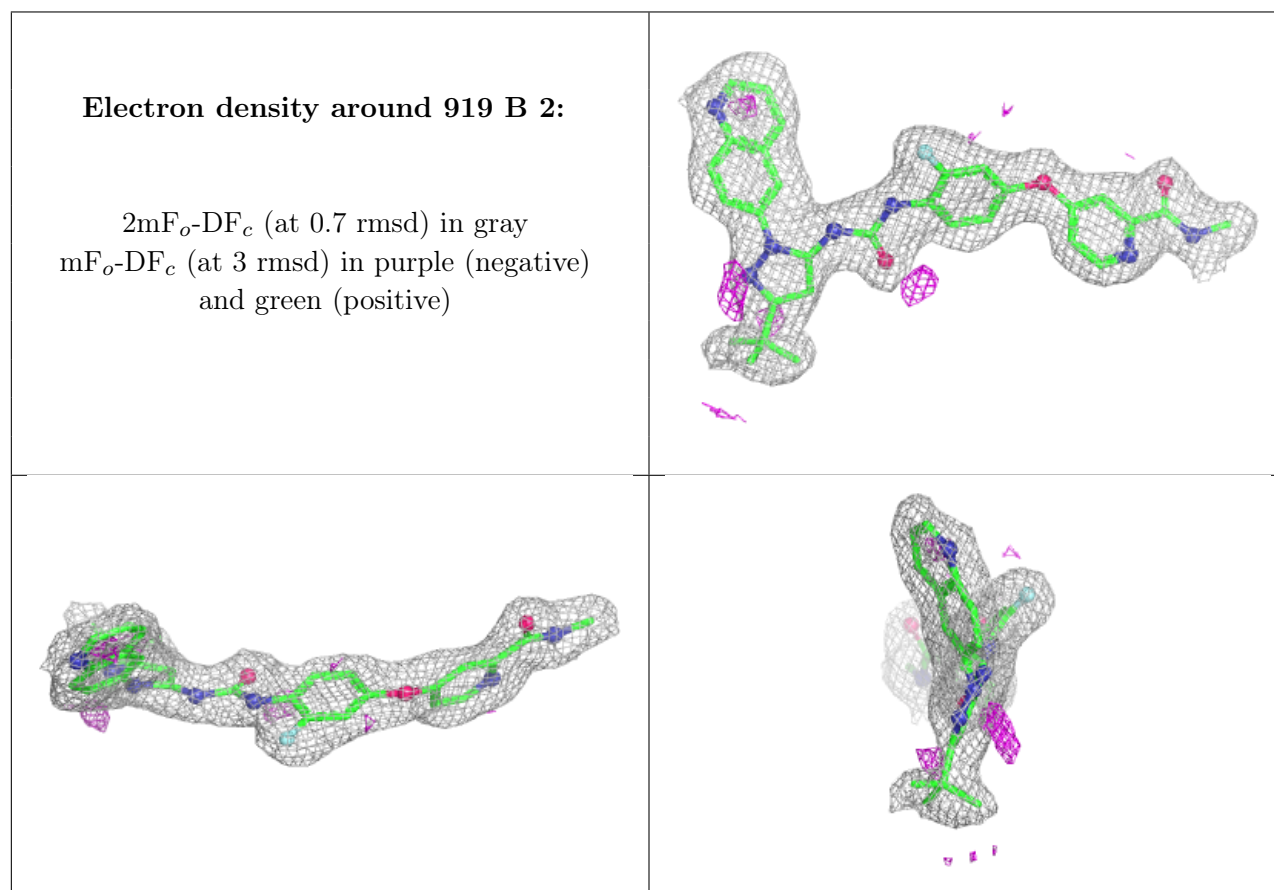
There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

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.

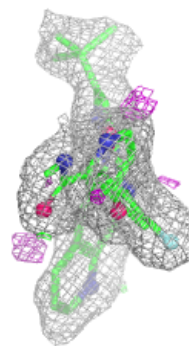
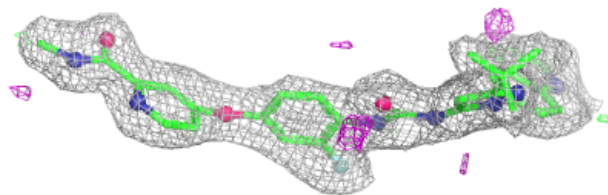
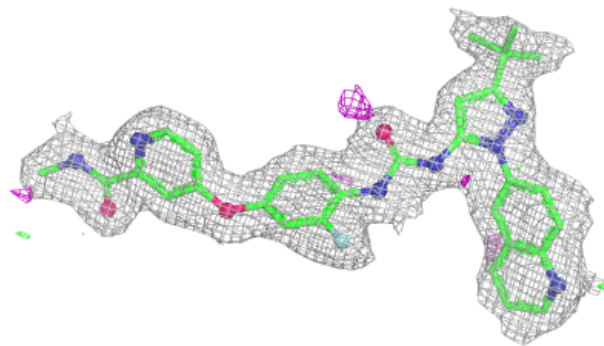
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	NA	A	2	1/1	0.84	0.19	59,59,59,59	0
2	NA	A	1	1/1	0.87	0.23	52,52,52,52	0
3	919	B	2	41/41	0.89	0.12	28,32,34,35	0
3	919	A	500	41/41	0.90	0.11	25,28,30,32	0

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 919 A 500:

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



6.5 Other polymers ⓘ

There are no such residues in this entry.