



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 4, 2025 – 10:05 AM EDT

PDB ID : 9EJR / pdb\_00009ejr  
Title : Bruton's tyrosine kinase in complex with compound PTI52  
Authors : Lin, D.Y.; Andreotti, A.H.; Tonge, P.J.; Bravo, E.; Li, X.  
Deposited on : 2024-11-28  
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](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4-5-2 with Phenix2.0rc1  
Mogul : 2022.3.0, CSD as543be (2022)  
Xtriage (Phenix) : 2.0rc1  
EDS : 3.0  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
CCP4 : 9.0.006 (Gargrove)  
Density-Fitness : 1.0.12  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.45.1

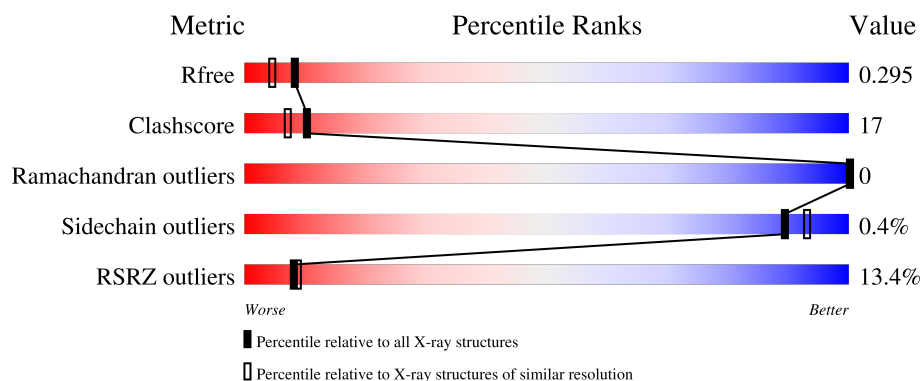
# 1 Overall quality at a glance

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))
$R_{free}$	164625	6234 (2.10-2.10)
Clashscore	180529	6893 (2.10-2.10)
Ramachandran outliers	177936	6839 (2.10-2.10)
Sidechain outliers	177891	6840 (2.10-2.10)
RSRZ outliers	164620	6234 (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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	279	<div> <div>6%</div> <div>66%</div> <div>27%</div> <div>7%</div> </div>
1	B	279	<div> <div>18%</div> <div>64%</div> <div>28%</div> <div>8%</div> </div>

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 4703 atoms, of which 60 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.

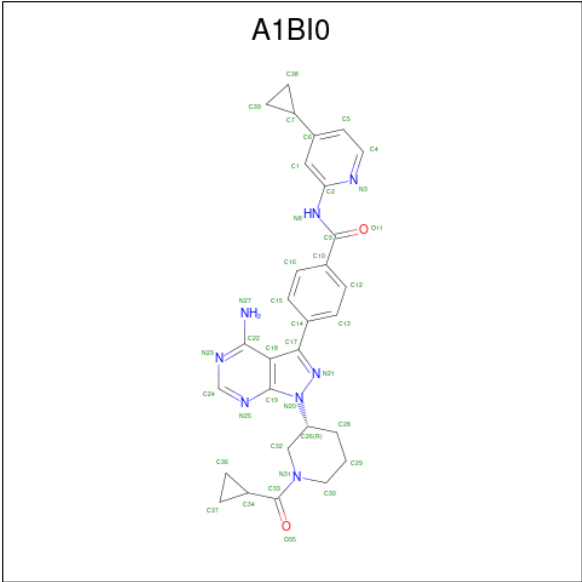
- Molecule 1 is a protein called Tyrosine-protein kinase BTK.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	260	Total	C	N	O	S	0	3	0
			2128	1364	354	391	19			
1	B	256	Total	C	N	O	S	0	1	0
			2043	1316	338	370	19			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	381	MET	-	initiating methionine	UNP P35991
A	390	GLY	LEU	engineered mutation	UNP P35991
A	551	GLU	TYR	engineered mutation	UNP P35991
A	617	PRO	TYR	engineered mutation	UNP P35991
B	381	MET	-	initiating methionine	UNP P35991
B	390	GLY	LEU	engineered mutation	UNP P35991
B	551	GLU	TYR	engineered mutation	UNP P35991
B	617	PRO	TYR	engineered mutation	UNP P35991

- Molecule 2 is 4-{4-amino-1-[(3R)-1-(cyclopropanecarbonyl)piperidin-3-yl]-1H-pyrazolo[3,4-d]pyrimidin-3-yl}-N-(4-cyclopropylpyridin-2-yl)benzamide (CCD ID: A1BI0) (formula: C<sub>29</sub>H<sub>30</sub>N<sub>8</sub>O<sub>2</sub>) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	H	N	O	0	0
			69	29	30	8	2		
2	B	1	Total	C	H	N	O	0	0
			69	29	30	8	2		

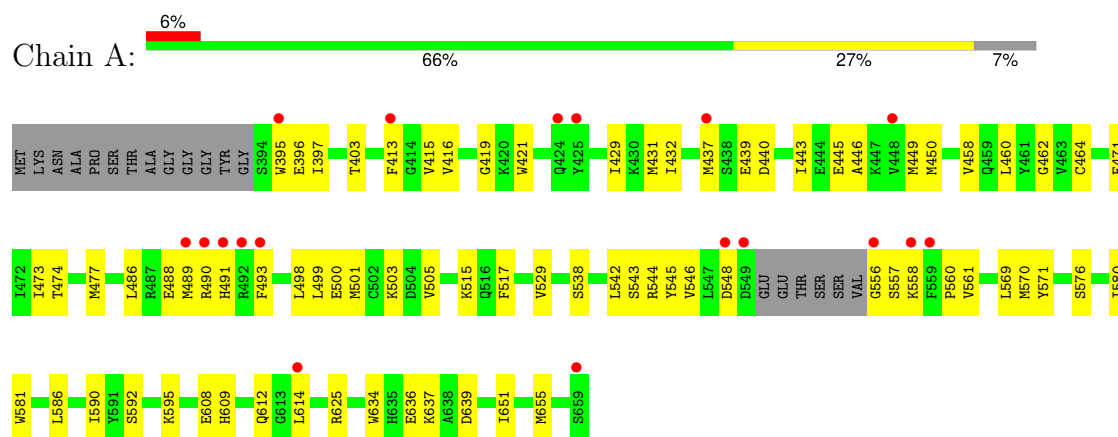
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	237	Total	O	0	0
			237	237		
3	B	157	Total	O	0	0
			157	157		

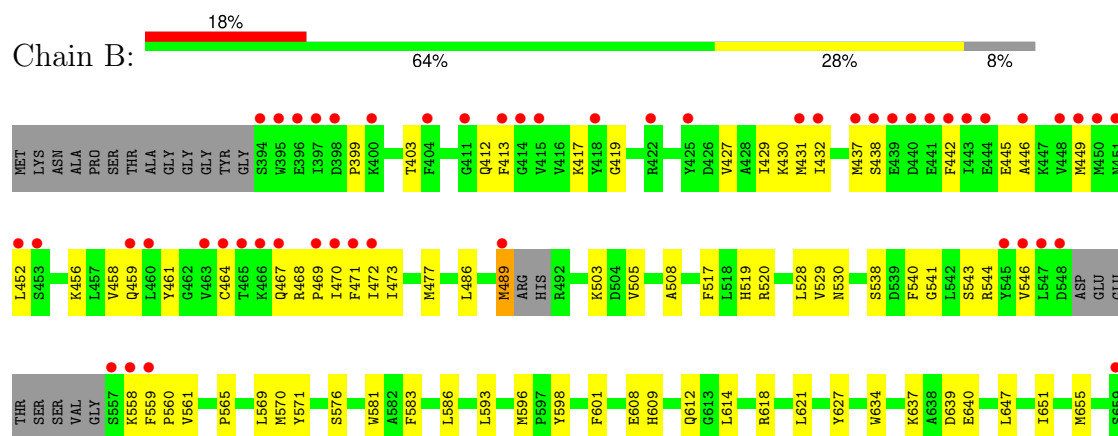
### 3 Residue-property plots

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 BTK



#### • Molecule 1: Tyrosine-protein kinase BTK



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	44.85Å 108.66Å 122.26Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.97 – 2.10 19.97 – 2.10	Depositor EDS
% Data completeness (in resolution range)	88.2 (19.97-2.10) 79.8 (19.97-2.10)	Depositor EDS
$R_{merge}$	0.53	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.69 (at 2.03Å)	Xtriage
Refinement program	PHENIX 1.21.2_5419	Depositor
R, $R_{free}$	0.247 , 0.295 0.248 , 0.295	Depositor DCC
$R_{free}$ test set	1592 reflections (4.07%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	10.4	Xtriage
Anisotropy	0.085	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 46.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.54$ , $\langle L^2 \rangle = 0.38$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.90	EDS
Total number of atoms	4703	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	23.0	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 60.61 % 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 1.4828e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: A1BI0

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	0.07	0/2183	0.21	0/2942
1	B	0.07	0/2093	0.22	0/2827
All	All	0.07	0/4276	0.21	0/5769

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	2128	0	2083	72	0
1	B	2043	0	1979	68	0
2	A	39	30	0	0	0
2	B	39	30	0	1	0
3	A	237	0	0	12	0
3	B	157	0	0	11	0
All	All	4643	60	4062	140	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 17.

All (140) 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:558:LYS:HG3	1:A:560:PRO:HD2	1.46	0.95
1:A:449:MET:HE2	1:A:517:PHE:HZ	1.38	0.89
1:B:432:ILE:HD13	1:B:437:MET:HE1	1.52	0.88
1:B:593:LEU:HD21	1:B:621:LEU:HD12	1.58	0.85
1:A:432:ILE:HG21	1:A:437:MET:HE2	1.61	0.83
1:A:464:CYS:HB2	1:A:471:PHE:HB2	1.59	0.82
1:A:501:MET:HE3	1:A:590:ILE:HG23	1.62	0.79
1:A:446:ALA:O	1:A:450:MET:HG2	1.82	0.78
1:A:503:LYS:HD3	1:A:655:MET:SD	2.26	0.75
1:B:413:PHE:O	1:B:432:ILE:HA	1.86	0.73
1:A:558:LYS:CG	1:A:560:PRO:HD2	2.20	0.71
1:A:498:LEU:HA	1:A:501:MET:HE2	1.73	0.71
1:A:445:GLU:HG3	1:A:449:MET:HE3	1.72	0.71
1:A:413:PHE:CE1	1:A:546:VAL:HG22	2.26	0.69
1:A:449:MET:HE2	1:A:517:PHE:CZ	2.26	0.69
1:A:413:PHE:HE1	1:A:546:VAL:HG22	1.56	0.69
1:A:395:TRP:CE3	1:A:450:MET:HE3	2.28	0.68
1:B:432:ILE:HD12	1:B:470:ILE:HG23	1.75	0.68
1:B:558:LYS:HB3	1:B:560:PRO:HD2	1.75	0.67
1:A:445:GLU:CG	1:A:449:MET:HE3	2.26	0.66
1:B:637:LYS:HD2	1:B:639:ASP:OD1	1.94	0.65
1:B:593:LEU:HD21	1:B:621:LEU:CD1	2.27	0.64
1:A:561:VAL:HG13	1:A:569:LEU:CD2	2.29	0.63
1:B:403:THR:O	1:B:419:GLY:HA3	1.99	0.63
1:B:576:SER:HB2	3:B:896:HOH:O	1.97	0.63
1:A:395:TRP:HB3	1:A:450:MET:HE2	1.79	0.63
1:A:440:ASP:HB2	3:A:805:HOH:O	1.97	0.63
1:B:505:VAL:HG11	1:B:586:LEU:HD23	1.80	0.62
1:B:432:ILE:HG21	1:B:437:MET:HE2	1.82	0.61
1:A:403:THR:O	1:A:419:GLY:HA3	2.00	0.61
1:A:505:VAL:HG11	1:A:586:LEU:HD23	1.84	0.60
1:A:432:ILE:CG2	1:A:437:MET:HE2	2.31	0.60
1:A:548:ASP:HB2	3:A:854:HOH:O	2.02	0.59
1:B:432:ILE:HD13	1:B:437:MET:CE	2.28	0.58
1:A:561:VAL:HG13	1:A:569:LEU:HD21	1.85	0.58
1:A:501:MET:CE	1:A:590:ILE:HG23	2.33	0.58
1:B:442:PHE:O	1:B:446:ALA:HB2	2.04	0.58
1:A:543:SER:HA	1:A:546:VAL:HG23	1.86	0.58
1:B:438:SER:O	1:B:442:PHE:HB3	2.04	0.57
1:A:515:LYS:HE2	3:A:923:HOH:O	2.03	0.57
1:B:561:VAL:HG13	1:B:569:LEU:HD21	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:505:VAL:HG11	1:B:586:LEU:CD2	2.34	0.57
1:A:609:HIS:ND1	1:A:614:LEU:HD22	2.19	0.57
1:A:505:VAL:HG11	1:A:586:LEU:CD2	2.35	0.57
1:A:413:PHE:O	1:A:432:ILE:HA	2.05	0.56
1:A:558:LYS:HE2	1:A:560:PRO:HG2	1.87	0.56
1:A:486:LEU:HA	1:A:493:PHE:HE2	1.71	0.56
1:A:609:HIS:HB3	1:A:614:LEU:HD23	1.87	0.55
1:A:576:SER:HB3	3:A:939:HOH:O	2.06	0.55
1:B:432:ILE:HD12	1:B:470:ILE:CG2	2.37	0.55
1:A:608:GLU:O	1:A:612:GLN:HG3	2.06	0.54
1:B:412:GLN:HG2	1:B:413:PHE:CD2	2.43	0.54
1:B:432:ILE:HD11	1:B:472:ILE:HD11	1.88	0.53
1:B:544:ARG:HB3	3:B:886:HOH:O	2.07	0.53
1:A:397:ILE:HD12	1:A:421:TRP:CZ2	2.43	0.53
1:A:397:ILE:HG12	1:A:462:GLY:HA3	1.91	0.53
1:B:477:MET:HE3	1:B:529:VAL:C	2.34	0.53
1:B:544:ARG:HG3	3:B:891:HOH:O	2.08	0.53
1:B:559:PHE:HZ	1:B:596[B]:MET:HE1	1.74	0.53
1:B:431:MET:HG2	1:B:471:PHE:CE1	2.45	0.52
1:B:503:LYS:HD3	1:B:655:MET:SD	2.49	0.52
1:A:458:VAL:HG21	1:A:538:SER:HB2	1.92	0.52
1:A:498:LEU:HD23	1:A:501:MET:HE2	1.91	0.52
1:A:576:SER:O	1:A:580:ILE:HG12	2.10	0.52
1:B:459:GLN:HG3	3:B:841:HOH:O	2.10	0.52
1:A:396:GLU:HB2	3:A:889:HOH:O	2.10	0.51
1:A:625:ARG:HA	3:A:899:HOH:O	2.10	0.51
1:A:557:SER:HB3	1:A:561:VAL:HG21	1.92	0.51
1:B:651:ILE:O	1:B:655:MET:HG3	2.11	0.51
1:B:449:MET:O	1:B:452:LEU:HB2	2.11	0.51
1:B:565:PRO:HD3	3:B:810:HOH:O	2.10	0.50
1:B:445:GLU:HG3	1:B:449:MET:HE2	1.94	0.50
1:A:609:HIS:HB3	1:A:614:LEU:CD2	2.42	0.50
1:A:439:GLU:O	1:A:443:ILE:HG13	2.12	0.49
1:B:427:VAL:HG12	1:B:461:TYR:CE2	2.47	0.49
1:B:473:ILE:HD12	1:B:473:ILE:N	2.27	0.49
1:B:543:SER:HA	1:B:546:VAL:HG23	1.94	0.49
1:A:501:MET:HE3	1:A:590:ILE:CG2	2.36	0.49
1:A:544:ARG:HH21	1:A:545:TYR:HE1	1.61	0.49
1:B:399:PRO:HB3	1:B:467:GLN:OE1	2.13	0.49
1:A:431:MET:HG2	1:A:471:PHE:CE1	2.48	0.49
1:A:473:ILE:HD12	1:A:473:ILE:N	2.27	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:595:LYS:HD3	3:A:920:HOH:O	2.13	0.48
1:A:488:GLU:HG2	1:A:491:HIS:CE1	2.48	0.48
1:A:503:LYS:HE2	3:B:864:HOH:O	2.12	0.48
1:B:570:MET:HG2	1:B:571:TYR:CE1	2.48	0.48
1:B:559:PHE:CZ	1:B:596[B]:MET:HE1	2.48	0.48
1:B:561:VAL:HG13	1:B:569:LEU:CD2	2.43	0.48
1:A:561:VAL:HG13	1:A:569:LEU:HD22	1.95	0.47
1:B:637:LYS:HD3	3:B:880:HOH:O	2.13	0.47
1:B:429:ILE:HD12	1:B:429:ILE:N	2.29	0.47
1:B:538:SER:HB3	3:B:889:HOH:O	2.15	0.47
1:A:581:TRP:CE3	1:A:634:TRP:HA	2.50	0.47
1:B:417:LYS:HD2	1:B:431:MET:HE3	1.95	0.47
1:B:445:GLU:HB2	3:B:835:HOH:O	2.13	0.47
1:B:456:LYS:HB3	1:B:508:ALA:HB2	1.97	0.46
1:B:413:PHE:CZ	1:B:546:VAL:HG22	2.50	0.46
1:B:608:GLU:O	1:B:612:GLN:HG3	2.15	0.46
1:B:609:HIS:HB3	1:B:614:LEU:HD23	1.98	0.46
1:A:543:SER:HB3	3:A:850:HOH:O	2.16	0.46
1:B:432:ILE:HB	1:B:470:ILE:HG23	1.98	0.45
1:A:460:LEU:HD23	1:A:474:THR:HG22	1.98	0.45
1:A:489:MET:HA	3:A:819:HOH:O	2.16	0.45
1:A:570:MET:HG2	1:A:571:TYR:CE1	2.52	0.45
1:B:468:ARG:HA	1:B:469:PRO:C	2.40	0.45
1:B:477:MET:HE3	1:B:530:ASN:N	2.32	0.45
1:B:520:ARG:HD2	3:B:891:HOH:O	2.16	0.45
1:A:556:GLY:HA3	3:A:917:HOH:O	2.15	0.45
1:A:651:ILE:O	1:A:655:MET:HG3	2.16	0.44
1:B:517:PHE:HE1	1:B:540:PHE:HB2	1.83	0.44
1:B:427:VAL:HG12	1:B:461:TYR:HE2	1.81	0.44
1:B:519:HIS:O	1:B:520:ARG:HB2	2.18	0.44
1:B:593:LEU:HD22	1:B:593:LEU:N	2.34	0.43
1:A:499:LEU:HD23	1:A:655:MET:HG2	1.99	0.43
1:B:413:PHE:HZ	1:B:546:VAL:HG22	1.84	0.43
1:B:464:CYS:O	1:B:470:ILE:HG13	2.19	0.43
1:A:413:PHE:CE2	1:A:542:LEU:HB3	2.54	0.43
1:B:637:LYS:HB3	1:B:640:GLU:HG3	2.00	0.43
1:B:430:LYS:HE2	2:B:701:A1BI0:C12	2.49	0.42
1:A:429:ILE:HD12	1:A:429:ILE:N	2.34	0.42
1:A:592:SER:HB3	1:A:595:LYS:HB3	2.02	0.42
1:B:598:TYR:HB3	1:B:601:PHE:HD2	1.85	0.42
1:B:464:CYS:HB2	1:B:471:PHE:HB2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:570:MET:HG2	1:B:571:TYR:CD1	2.55	0.42
1:A:464:CYS:CB	1:A:471:PHE:HB2	2.41	0.41
1:B:583:PHE:CD2	1:B:647:LEU:HD13	2.54	0.41
1:A:490:ARG:HA	3:A:840:HOH:O	2.20	0.41
1:B:417:LYS:HD2	1:B:431:MET:CE	2.50	0.41
1:B:618:ARG:HA	1:B:627:TYR:CE1	2.55	0.41
1:A:637[B]:LYS:HB3	1:A:639:ASP:OD1	2.20	0.41
1:B:541:GLY:HA2	3:B:891:HOH:O	2.21	0.41
1:A:500[A]:GLU:HB3	3:A:838:HOH:O	2.21	0.41
1:A:558:LYS:HE2	1:A:560:PRO:CG	2.48	0.41
1:A:543:SER:HA	1:A:546:VAL:CG2	2.50	0.40
1:A:477:MET:HE3	1:A:529:VAL:C	2.47	0.40
1:A:415:VAL:CG1	1:A:416:VAL:N	2.84	0.40
1:B:458:VAL:HG21	1:B:528:LEU:HD12	2.02	0.40
1:A:450:MET:CE	1:A:462:GLY:HA2	2.52	0.40
1:B:486:LEU:O	1:B:489:MET:HG3	2.22	0.40
1:B:581:TRP:CE3	1:B:634:TRP:HA	2.57	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	259/279 (93%)	251 (97%)	8 (3%)	0	100	100
1	B	251/279 (90%)	244 (97%)	7 (3%)	0	100	100
All	All	510/558 (91%)	495 (97%)	15 (3%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	232/248 (94%)	231 (100%)	1 (0%)	89	93
1	B	217/248 (88%)	216 (100%)	1 (0%)	86	91
All	All	449/496 (90%)	447 (100%)	2 (0%)	89	93

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	636	GLU
1	B	489	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	650	ASN
1	B	650	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

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	A1BI0	B	701	-	43,45,45	2.28	8 (18%)	54,66,66	1.93	10 (18%)
2	A1BI0	A	701	-	43,45,45	2.27	8 (18%)	54,66,66	1.90	9 (16%)

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	A1BI0	B	701	-	-	14/28/42/42	0/7/7/7
2	A1BI0	A	701	-	-	7/28/42/42	0/7/7/7

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	701	A1BI0	C33-N31	9.39	1.48	1.35
2	B	701	A1BI0	C33-N31	9.35	1.48	1.35
2	B	701	A1BI0	N21-N20	-4.96	1.31	1.37
2	A	701	A1BI0	N21-N20	-4.77	1.31	1.37
2	A	701	A1BI0	C9-N8	4.04	1.47	1.35
2	B	701	A1BI0	C9-N8	3.98	1.47	1.35
2	A	701	A1BI0	C14-C17	3.94	1.55	1.49
2	B	701	A1BI0	C14-C17	3.93	1.55	1.49
2	A	701	A1BI0	C22-N27	3.52	1.46	1.34
2	B	701	A1BI0	C22-N27	3.47	1.46	1.34
2	A	701	A1BI0	C2-N8	3.12	1.47	1.40
2	B	701	A1BI0	C2-N8	3.07	1.47	1.40
2	B	701	A1BI0	C34-C33	2.30	1.55	1.51
2	A	701	A1BI0	C34-C33	2.16	1.54	1.51
2	A	701	A1BI0	C10-C9	2.09	1.54	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	701	A1BI0	C10-C9	2.05	1.54	1.50

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	701	A1BI0	C39-C7-C6	8.00	132.21	121.28
2	A	701	A1BI0	C39-C7-C6	7.68	131.78	121.28
2	A	701	A1BI0	C38-C7-C6	6.38	130.00	121.28
2	B	701	A1BI0	C38-C7-C6	6.34	129.95	121.28
2	B	701	A1BI0	C5-C4-N3	-3.41	119.79	123.97
2	A	701	A1BI0	C5-C4-N3	-3.34	119.88	123.97
2	A	701	A1BI0	C30-N31-C32	3.25	119.33	113.07
2	A	701	A1BI0	C34-C33-N31	3.23	121.84	118.80
2	B	701	A1BI0	C34-C33-N31	2.99	121.62	118.80
2	A	701	A1BI0	C14-C17-N21	2.93	125.80	120.78
2	A	701	A1BI0	C17-N21-N20	2.82	107.42	105.17
2	B	701	A1BI0	C30-N31-C32	2.79	118.45	113.07
2	B	701	A1BI0	C14-C17-N21	2.59	125.22	120.78
2	B	701	A1BI0	C17-N21-N20	2.55	107.20	105.17
2	A	701	A1BI0	C1-C2-N3	-2.43	119.73	122.92
2	B	701	A1BI0	C1-C2-N3	-2.31	119.89	122.92
2	A	701	A1BI0	C4-N3-C2	2.30	120.50	117.21
2	B	701	A1BI0	C4-N3-C2	2.28	120.47	117.21
2	B	701	A1BI0	C2-N8-C9	-2.23	121.94	128.21

There are no chirality outliers.

All (21) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	701	A1BI0	C13-C14-C17-N21
2	A	701	A1BI0	C15-C14-C17-N21
2	A	701	A1BI0	C28-C26-N20-C19
2	A	701	A1BI0	C28-C26-N20-N21
2	B	701	A1BI0	C13-C14-C17-N21
2	B	701	A1BI0	C15-C14-C17-N21
2	B	701	A1BI0	C28-C26-N20-C19
2	B	701	A1BI0	C28-C26-N20-N21
2	B	701	A1BI0	N31-C33-C34-C36
2	B	701	A1BI0	O35-C33-C34-C36
2	B	701	A1BI0	C12-C10-C9-O11
2	B	701	A1BI0	C12-C10-C9-N8
2	B	701	A1BI0	C16-C10-C9-O11

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Mol	Chain	Res	Type	Atoms
2	B	701	A1BI0	C16-C10-C9-N8
2	B	701	A1BI0	N3-C2-N8-C9
2	B	701	A1BI0	C1-C6-C7-C39
2	B	701	A1BI0	C1-C2-N8-C9
2	A	701	A1BI0	O35-C33-C34-C36
2	A	701	A1BI0	N31-C33-C34-C36
2	B	701	A1BI0	C5-C6-C7-C39
2	A	701	A1BI0	C12-C10-C9-O11

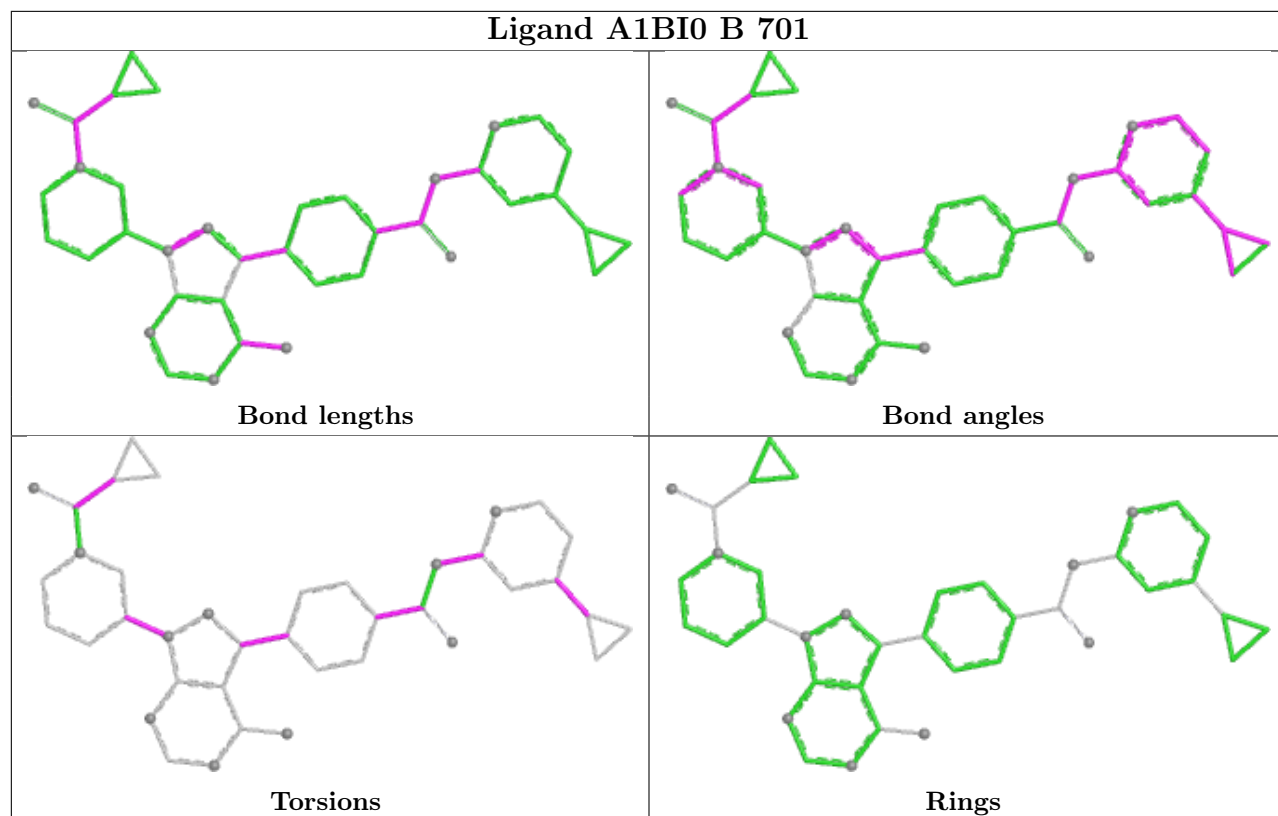
There are no ring outliers.

1 monomer is involved in 1 short contact:

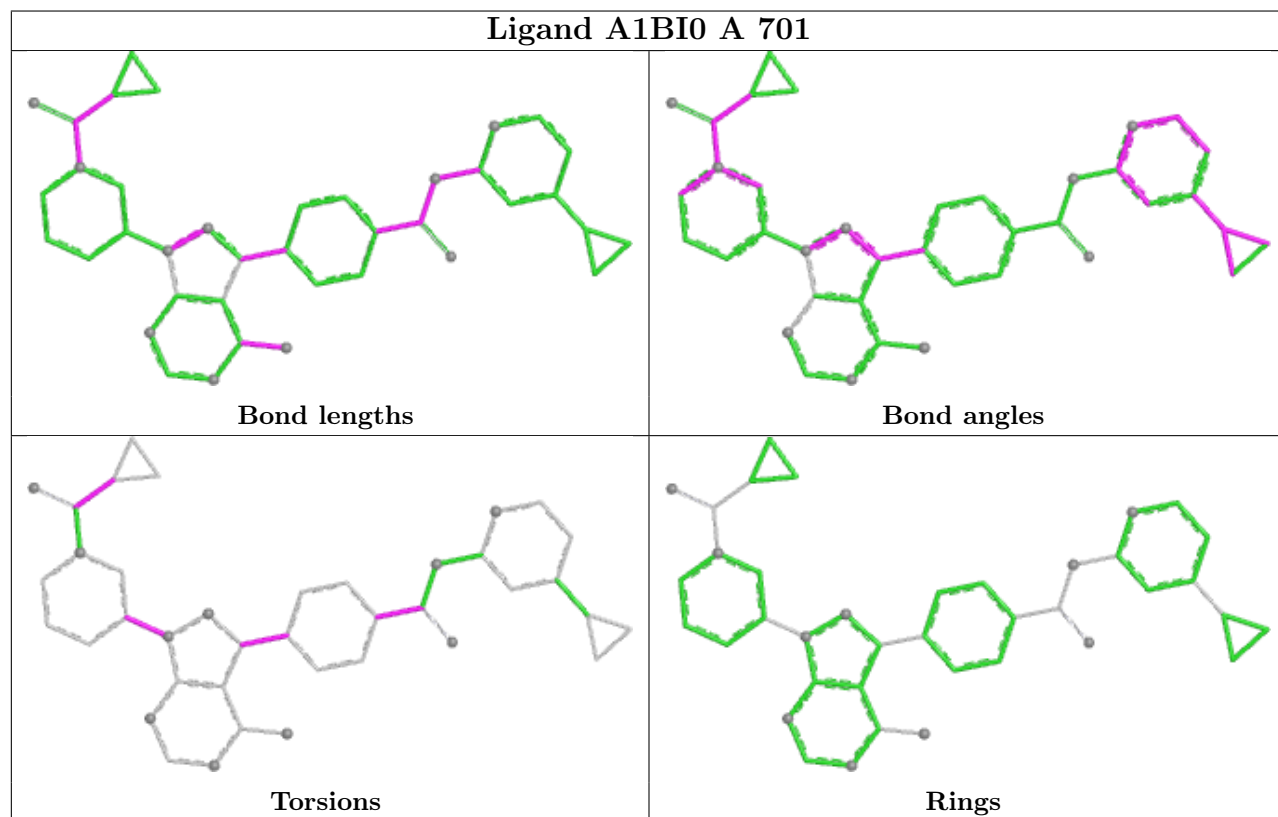
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	701	A1BI0	1	0

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.

## Ligand A1BI0 B 701



## Ligand A1BI0 A 701





## 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, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	260/279 (93%)	0.43	18 (6%) 24 26	7, 19, 37, 52	3 (1%)
1	B	256/279 (91%)	0.90	51 (19%) 3 4	8, 20, 51, 57	1 (0%)
All	All	516/558 (92%)	0.66	69 (13%) 8 9	7, 20, 48, 57	4 (0%)

All (69) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	440	ASP	5.2
1	B	442	PHE	4.8
1	B	466	LYS	4.7
1	A	489	MET	4.4
1	A	413	PHE	4.0
1	A	490	ARG	3.9
1	B	450	MET	3.8
1	B	425	TYR	3.7
1	A	424	GLN	3.6
1	A	549	ASP	3.5
1	A	491	HIS	3.5
1	B	446	ALA	3.4
1	B	438	SER	3.4
1	B	464	CYS	3.4
1	B	548	ASP	3.4
1	B	439	GLU	3.3
1	B	546	VAL	3.2
1	B	465	THR	3.1
1	B	451	ASN	3.0
1	B	394	SER	3.0
1	B	404	PHE	2.9
1	B	396	GLU	2.9
1	B	443	ILE	2.9
1	B	469	PRO	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	659	SER	2.8
1	A	556	GLY	2.8
1	B	448	VAL	2.8
1	B	400	LYS	2.7
1	B	431	MET	2.7
1	B	449	MET	2.7
1	B	659	SER	2.7
1	B	437	MET	2.7
1	B	413	PHE	2.7
1	B	489	MET	2.7
1	B	467	GLN	2.7
1	B	418	TYR	2.6
1	A	448	VAL	2.6
1	B	463	VAL	2.6
1	B	444	GLU	2.6
1	A	559	PHE	2.6
1	B	460	LEU	2.6
1	B	415	VAL	2.6
1	B	558	LYS	2.6
1	A	548	ASP	2.5
1	B	432	ILE	2.5
1	B	395	TRP	2.5
1	B	559	PHE	2.5
1	A	614	LEU	2.5
1	B	557	SER	2.4
1	B	547	LEU	2.4
1	A	425	TYR	2.4
1	B	397	ILE	2.4
1	A	558	LYS	2.4
1	B	441	GLU	2.3
1	B	414	GLY	2.3
1	A	492	ARG	2.3
1	A	493	PHE	2.2
1	B	398	ASP	2.2
1	B	453	SER	2.2
1	B	470	ILE	2.1
1	B	471	PHE	2.1
1	B	472	ILE	2.1
1	B	411	GLY	2.1
1	A	395	TRP	2.1
1	B	545	TYR	2.1
1	A	437	MET	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	452	LEU	2.0
1	B	459	GLN	2.0
1	B	422	ARG	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 6.4 Ligands [i](#)

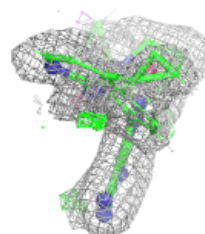
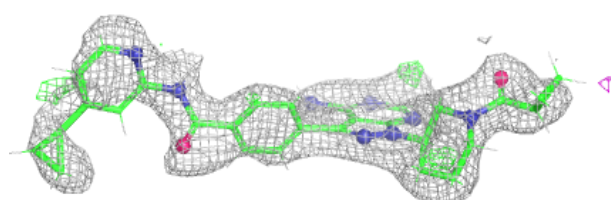
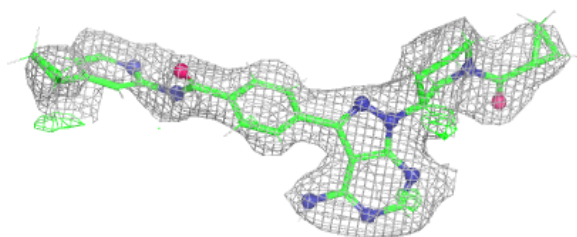
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	A1BI0	B	701	39/39	0.85	0.14	20,34,47,55	0
2	A1BI0	A	701	39/39	0.91	0.09	13,19,35,42	0

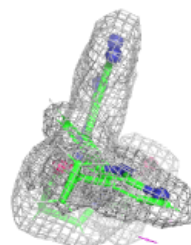
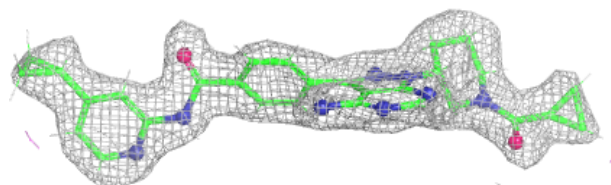
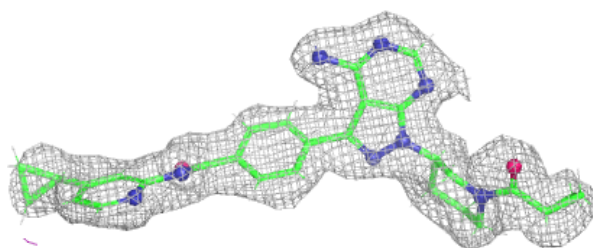
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

**Electron density around A1BI0 B 701:**

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

**Electron density around A1BI0 A 701:**

$2mF_o-DF_c$  (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.