



# wwPDB X-ray Structure Validation Summary Report ⓘ

May 15, 2020 – 01:51 pm BST

PDB ID : 4JVG  
Title : B-Raf Kinase in Complex with Birb796  
Authors : Lavoie, H.; Thevakumaran, N.; Gavory, G.; Li, J.; Padeganeh, A.; Guiral, S.;  
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Deposited on : 2013-03-25  
Resolution : 3.09 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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.

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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

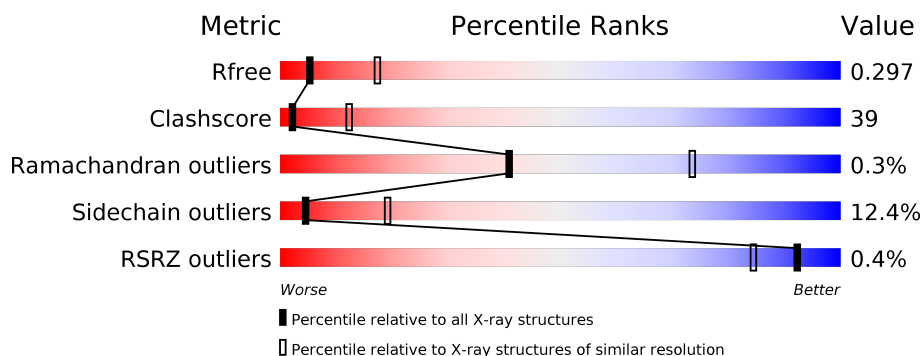
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 3.09 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	1094 (3.10-3.10)
Clashscore	141614	1184 (3.10-3.10)
Ramachandran outliers	138981	1141 (3.10-3.10)
Sidechain outliers	138945	1141 (3.10-3.10)
RSRZ outliers	127900	1067 (3.10-3.10)

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 on 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	284	
1	B	284	
1	C	284	
1	D	284	

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 8481 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 Serine/threonine-protein kinase B-raf.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	259	Total	C	N	O	S	34	0	0
			2072	1312	368	379	13			
1	A	262	Total	C	N	O	S	25	0	0
			2094	1326	372	383	13			
1	C	258	Total	C	N	O	S	5	0	0
			2065	1308	367	377	13			
1	D	262	Total	C	N	O	S	19	0	0
			2094	1326	372	383	13			

There are 80 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	440	GLY	-	EXPRESSION TAG	UNP P15056
B	441	ALA	-	EXPRESSION TAG	UNP P15056
B	442	MET	-	EXPRESSION TAG	UNP P15056
B	443	ASP	-	EXPRESSION TAG	UNP P15056
B	543	ALA	ILE	ENGINEERED MUTATION	UNP P15056
B	544	SER	ILE	ENGINEERED MUTATION	UNP P15056
B	551	LYS	ILE	ENGINEERED MUTATION	UNP P15056
B	562	ARG	GLN	ENGINEERED MUTATION	UNP P15056
B	588	ASN	LEU	ENGINEERED MUTATION	UNP P15056
B	630	SER	LYS	ENGINEERED MUTATION	UNP P15056
B	667	GLU	PHE	ENGINEERED MUTATION	UNP P15056
B	673	SER	TYR	ENGINEERED MUTATION	UNP P15056
B	688	ARG	ALA	ENGINEERED MUTATION	UNP P15056
B	706	SER	LEU	ENGINEERED MUTATION	UNP P15056
B	709	ARG	GLN	ENGINEERED MUTATION	UNP P15056
B	713	GLU	SER	ENGINEERED MUTATION	UNP P15056
B	716	GLU	LEU	ENGINEERED MUTATION	UNP P15056
B	720	GLU	SER	ENGINEERED MUTATION	UNP P15056
B	722	SER	PRO	ENGINEERED MUTATION	UNP P15056
B	723	GLY	LYS	ENGINEERED MUTATION	UNP P15056
A	440	GLY	-	EXPRESSION TAG	UNP P15056

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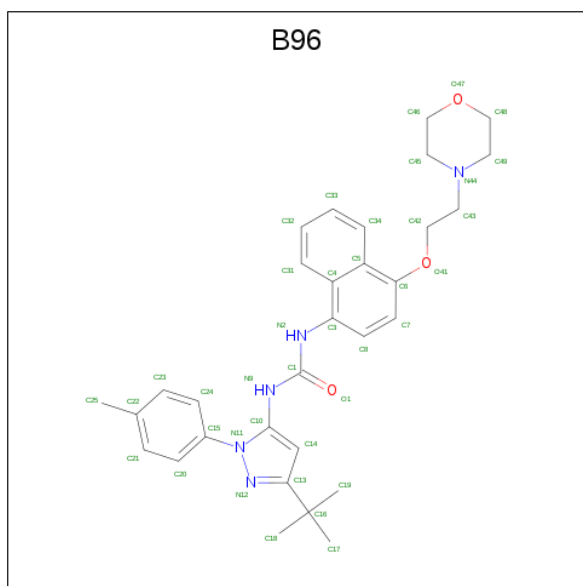
Chain	Residue	Modelled	Actual	Comment	Reference
A	441	ALA	-	EXPRESSION TAG	UNP P15056
A	442	MET	-	EXPRESSION TAG	UNP P15056
A	443	ASP	-	EXPRESSION TAG	UNP P15056
A	543	ALA	ILE	ENGINEERED MUTATION	UNP P15056
A	544	SER	ILE	ENGINEERED MUTATION	UNP P15056
A	551	LYS	ILE	ENGINEERED MUTATION	UNP P15056
A	562	ARG	GLN	ENGINEERED MUTATION	UNP P15056
A	588	ASN	LEU	ENGINEERED MUTATION	UNP P15056
A	630	SER	LYS	ENGINEERED MUTATION	UNP P15056
A	667	GLU	PHE	ENGINEERED MUTATION	UNP P15056
A	673	SER	TYR	ENGINEERED MUTATION	UNP P15056
A	688	ARG	ALA	ENGINEERED MUTATION	UNP P15056
A	706	SER	LEU	ENGINEERED MUTATION	UNP P15056
A	709	ARG	GLN	ENGINEERED MUTATION	UNP P15056
A	713	GLU	SER	ENGINEERED MUTATION	UNP P15056
A	716	GLU	LEU	ENGINEERED MUTATION	UNP P15056
A	720	GLU	SER	ENGINEERED MUTATION	UNP P15056
A	722	SER	PRO	ENGINEERED MUTATION	UNP P15056
A	723	GLY	LYS	ENGINEERED MUTATION	UNP P15056
C	440	GLY	-	EXPRESSION TAG	UNP P15056
C	441	ALA	-	EXPRESSION TAG	UNP P15056
C	442	MET	-	EXPRESSION TAG	UNP P15056
C	443	ASP	-	EXPRESSION TAG	UNP P15056
C	543	ALA	ILE	ENGINEERED MUTATION	UNP P15056
C	544	SER	ILE	ENGINEERED MUTATION	UNP P15056
C	551	LYS	ILE	ENGINEERED MUTATION	UNP P15056
C	562	ARG	GLN	ENGINEERED MUTATION	UNP P15056
C	588	ASN	LEU	ENGINEERED MUTATION	UNP P15056
C	630	SER	LYS	ENGINEERED MUTATION	UNP P15056
C	667	GLU	PHE	ENGINEERED MUTATION	UNP P15056
C	673	SER	TYR	ENGINEERED MUTATION	UNP P15056
C	688	ARG	ALA	ENGINEERED MUTATION	UNP P15056
C	706	SER	LEU	ENGINEERED MUTATION	UNP P15056
C	709	ARG	GLN	ENGINEERED MUTATION	UNP P15056
C	713	GLU	SER	ENGINEERED MUTATION	UNP P15056
C	716	GLU	LEU	ENGINEERED MUTATION	UNP P15056
C	720	GLU	SER	ENGINEERED MUTATION	UNP P15056
C	722	SER	PRO	ENGINEERED MUTATION	UNP P15056
C	723	GLY	LYS	ENGINEERED MUTATION	UNP P15056
D	440	GLY	-	EXPRESSION TAG	UNP P15056
D	441	ALA	-	EXPRESSION TAG	UNP P15056
D	442	MET	-	EXPRESSION TAG	UNP P15056

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Chain	Residue	Modelled	Actual	Comment	Reference
D	443	ASP	-	EXPRESSION TAG	UNP P15056
D	543	ALA	ILE	ENGINEERED MUTATION	UNP P15056
D	544	SER	ILE	ENGINEERED MUTATION	UNP P15056
D	551	LYS	ILE	ENGINEERED MUTATION	UNP P15056
D	562	ARG	GLN	ENGINEERED MUTATION	UNP P15056
D	588	ASN	LEU	ENGINEERED MUTATION	UNP P15056
D	630	SER	LYS	ENGINEERED MUTATION	UNP P15056
D	667	GLU	PHE	ENGINEERED MUTATION	UNP P15056
D	673	SER	TYR	ENGINEERED MUTATION	UNP P15056
D	688	ARG	ALA	ENGINEERED MUTATION	UNP P15056
D	706	SER	LEU	ENGINEERED MUTATION	UNP P15056
D	709	ARG	GLN	ENGINEERED MUTATION	UNP P15056
D	713	GLU	SER	ENGINEERED MUTATION	UNP P15056
D	716	GLU	LEU	ENGINEERED MUTATION	UNP P15056
D	720	GLU	SER	ENGINEERED MUTATION	UNP P15056
D	722	SER	PRO	ENGINEERED MUTATION	UNP P15056
D	723	GLY	LYS	ENGINEERED MUTATION	UNP P15056

- Molecule 2 is 1-(5-TERT-BUTYL-2-P-TOLYL-2H-PYRAZOL-3-YL)-3-[4-(2-MORPHOLIN-4-YL-ETHOXY)-NAPHTHALEN-1-YL]-UREA (three-letter code: B96) (formula:  $C_{31}H_{37}N_5O_3$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	B	1	Total	C	N	O	0	0
			39	31	5	3		
2	A	1	Total	C	N	O	0	0
			39	31	5	3		

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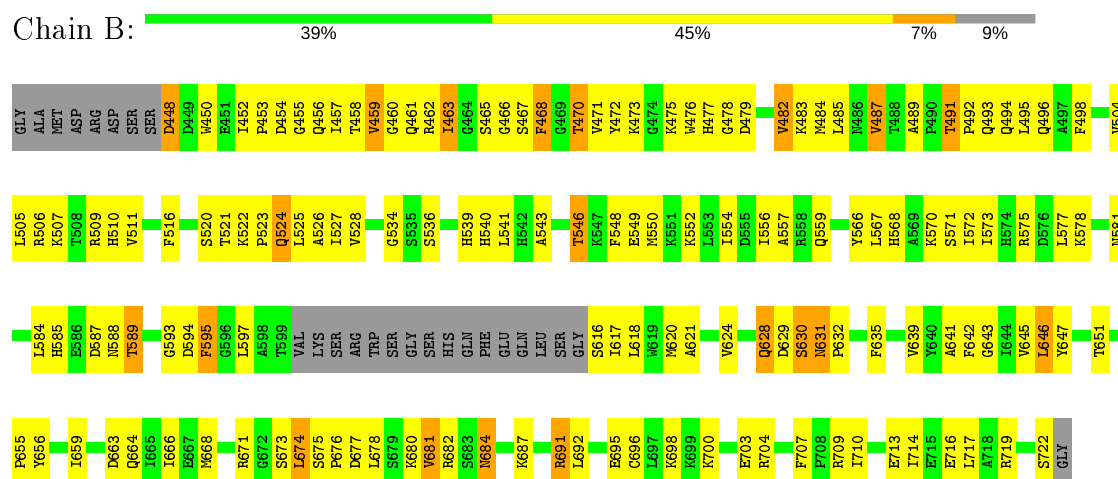
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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	C	1	Total	C	N	O	0	0
			39	31	5	3		
2	D	1	Total	C	N	O	0	0
			39	31	5	3		

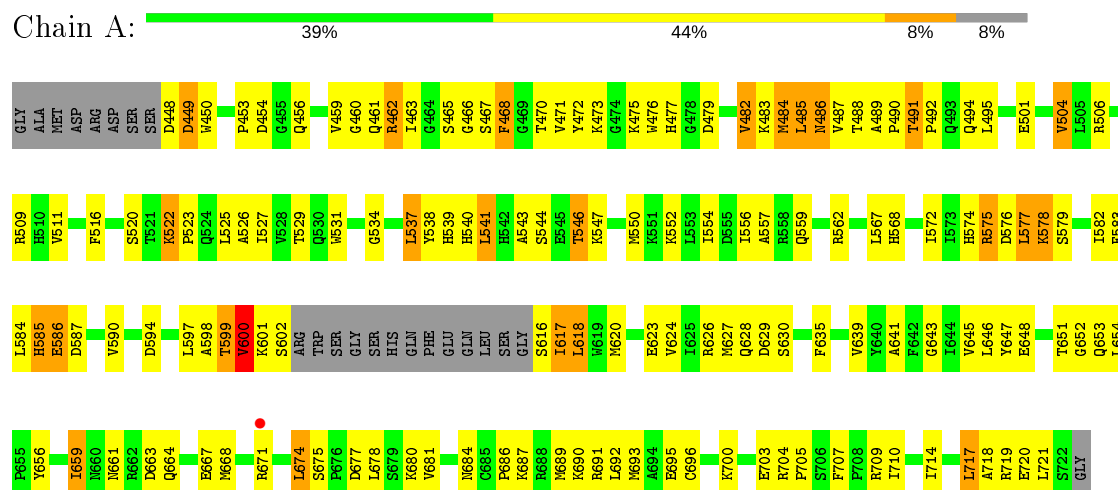
### 3 Residue-property plots

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: Serine/threonine-protein kinase B-raf

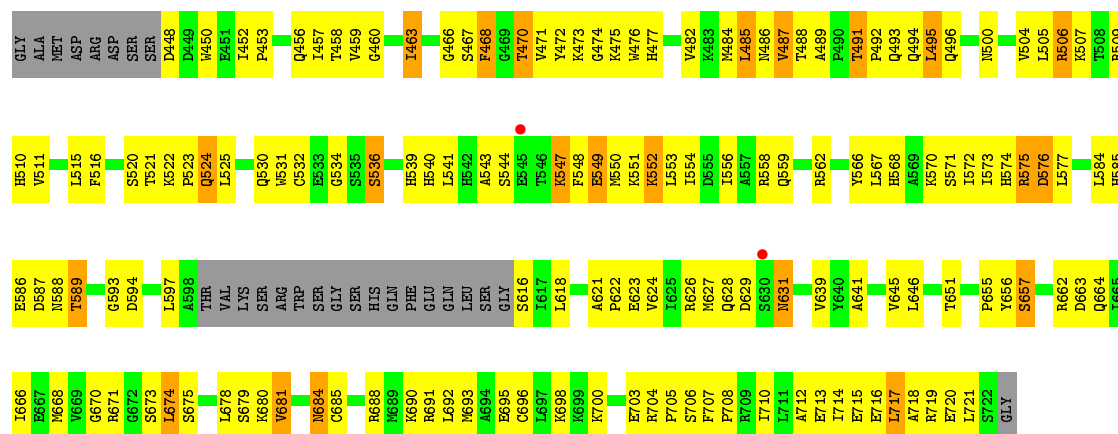


- Molecule 1: Serine/threonine-protein kinase B-raf



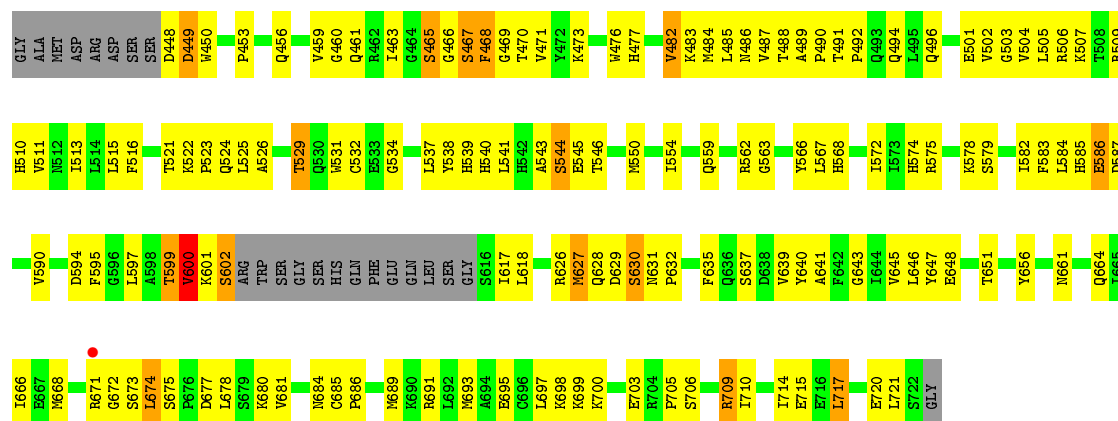
- Molecule 1: Serine/threonine-protein kinase B-raf





● Molecule 1: Serine/threonine-protein kinase B-raf

Chain D: 41% 46% 5% 8%





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	55.00Å 120.61Å 81.71Å 90.00° 90.44° 90.00°	Depositor
Resolution (Å)	42.54 – 3.09 48.52 – 3.09	Depositor EDS
% Data completeness (in resolution range)	89.5 (42.54-3.09) 90.9 (48.52-3.09)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.10	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.02 (at 3.07Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.1_743)	Depositor
R, $R_{free}$	0.232 , 0.295 0.233 , 0.297	Depositor DCC
$R_{free}$ test set	911 reflections (5.14%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	68.5	Xtriage
Anisotropy	0.176	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 67.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.37$ , $\langle L^2 \rangle = 0.21$	Xtriage
Estimated twinning fraction	0.049 for h,-k,-l	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	8481	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	71.0	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 95.25 % 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 1.5845e-09. 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 [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: B96

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	0.43	0/2136	0.65	0/2878
1	B	0.43	0/2114	0.60	0/2849
1	C	0.45	0/2107	0.65	0/2839
1	D	0.42	0/2136	0.64	0/2878
All	All	0.43	0/8493	0.64	0/11444

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	C	0	1
1	D	0	3
All	All	0	5

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	600	VAL	Peptide
1	C	485	LEU	Peptide
1	D	465	SER	Peptide
1	D	467	SER	Peptide
1	D	600	VAL	Peptide

## 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	2094	0	2113	177	2
1	B	2072	0	2087	169	1
1	C	2065	0	2080	189	1
1	D	2094	0	2114	147	1
2	A	39	0	37	9	0
2	B	39	0	37	9	0
2	C	39	0	37	8	0
2	D	39	0	37	7	0
All	All	8481	0	8542	664	3

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 39.

The worst 5 of 664 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:C:585:HIS:ND1	1:C:586:GLU:HG3	1.59	1.17
1:C:575:ARG:HH11	1:C:575:ARG:CG	1.61	1.13
1:A:575:ARG:NH2	1:A:602:SER:HB3	1.66	1.10
1:C:713:GLU:HG3	1:C:717:LEU:HD21	1.33	1.09
1:C:585:HIS:CE1	1:C:586:GLU:HG3	1.90	1.07

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:461:GLN:OE1	1:D:691:ARG:NH2[1_454]	1.83	0.37
1:B:549:GLU:OE1	1:C:493:GLN:NE2[1_554]	2.05	0.15
1:A:454:ASP:OD2	1:A:547:LYS:NZ[1_455]	2.12	0.08

## 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	258/284 (91%)	233 (90%)	24 (9%)	1 (0%)	34	69
1	B	255/284 (90%)	238 (93%)	17 (7%)	0	100	100
1	C	254/284 (89%)	234 (92%)	19 (8%)	1 (0%)	34	69
1	D	258/284 (91%)	232 (90%)	25 (10%)	1 (0%)	34	69
All	All	1025/1136 (90%)	937 (91%)	85 (8%)	3 (0%)	41	73

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	600	VAL
1	C	487	VAL
1	A	600	VAL

### 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	231/248 (93%)	196 (85%)	35 (15%)	3	12
1	B	228/248 (92%)	197 (86%)	31 (14%)	3	16
1	C	227/248 (92%)	199 (88%)	28 (12%)	4	19
1	D	231/248 (93%)	211 (91%)	20 (9%)	10	36
All	All	917/992 (92%)	803 (88%)	114 (12%)	4	19

5 of 114 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	585	HIS
1	A	677	ASP
1	D	600	VAL
1	A	599	THR
1	A	618	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 14 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	524	GLN
1	C	530	GLN
1	D	461	GLN
1	C	512	ASN
1	C	585	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 ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

4 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	B96	C	801	-	43,43,43	2.36	7 (16%)	55,61,61	2.12	10 (18%)
2	B96	B	801	-	43,43,43	2.48	7 (16%)	55,61,61	2.05	10 (18%)
2	B96	D	801	-	43,43,43	2.45	8 (18%)	55,61,61	2.38	9 (16%)
2	B96	A	801	-	43,43,43	2.60	9 (20%)	55,61,61	2.34	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	B96	C	801	-	-	2/22/32/32	0/5/5/5
2	B96	B	801	-	-	2/22/32/32	0/5/5/5
2	B96	D	801	-	-	2/22/32/32	0/5/5/5
2	B96	A	801	-	-	2/22/32/32	0/5/5/5

The worst 5 of 31 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	801	B96	N12-N11	-12.61	1.14	1.39
2	A	801	B96	N12-N11	-12.56	1.14	1.39
2	D	801	B96	N12-N11	-11.95	1.16	1.39
2	C	801	B96	N12-N11	-11.32	1.17	1.39
2	A	801	B96	C10-N11	-5.72	1.31	1.37

The worst 5 of 38 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	801	B96	C15-N11-C10	-13.45	113.12	129.11
2	A	801	B96	C15-N11-C10	-12.84	113.84	129.11
2	C	801	B96	C15-N11-C10	-11.67	115.24	129.11
2	B	801	B96	C15-N11-C10	-11.30	115.67	129.11
2	A	801	B96	C42-O41-C6	-5.23	102.09	117.74

There are no chirality outliers.

5 of 8 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	801	B96	C20-C15-N11-C10
2	C	801	B96	C24-C15-N11-C10

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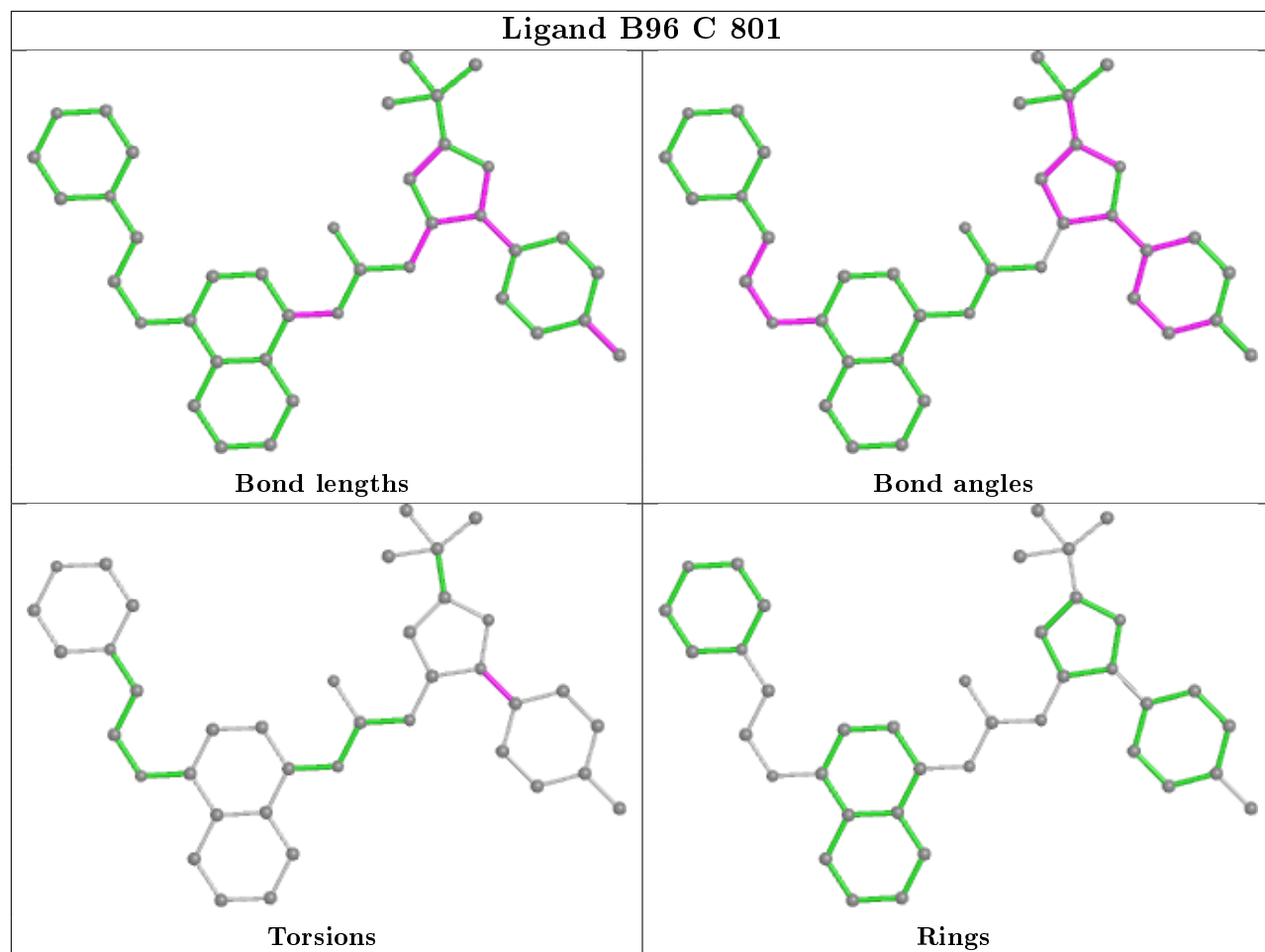
Mol	Chain	Res	Type	Atoms
2	B	801	B96	C20-C15-N11-C10
2	B	801	B96	C24-C15-N11-C10
2	D	801	B96	C20-C15-N11-C10

There are no ring outliers.

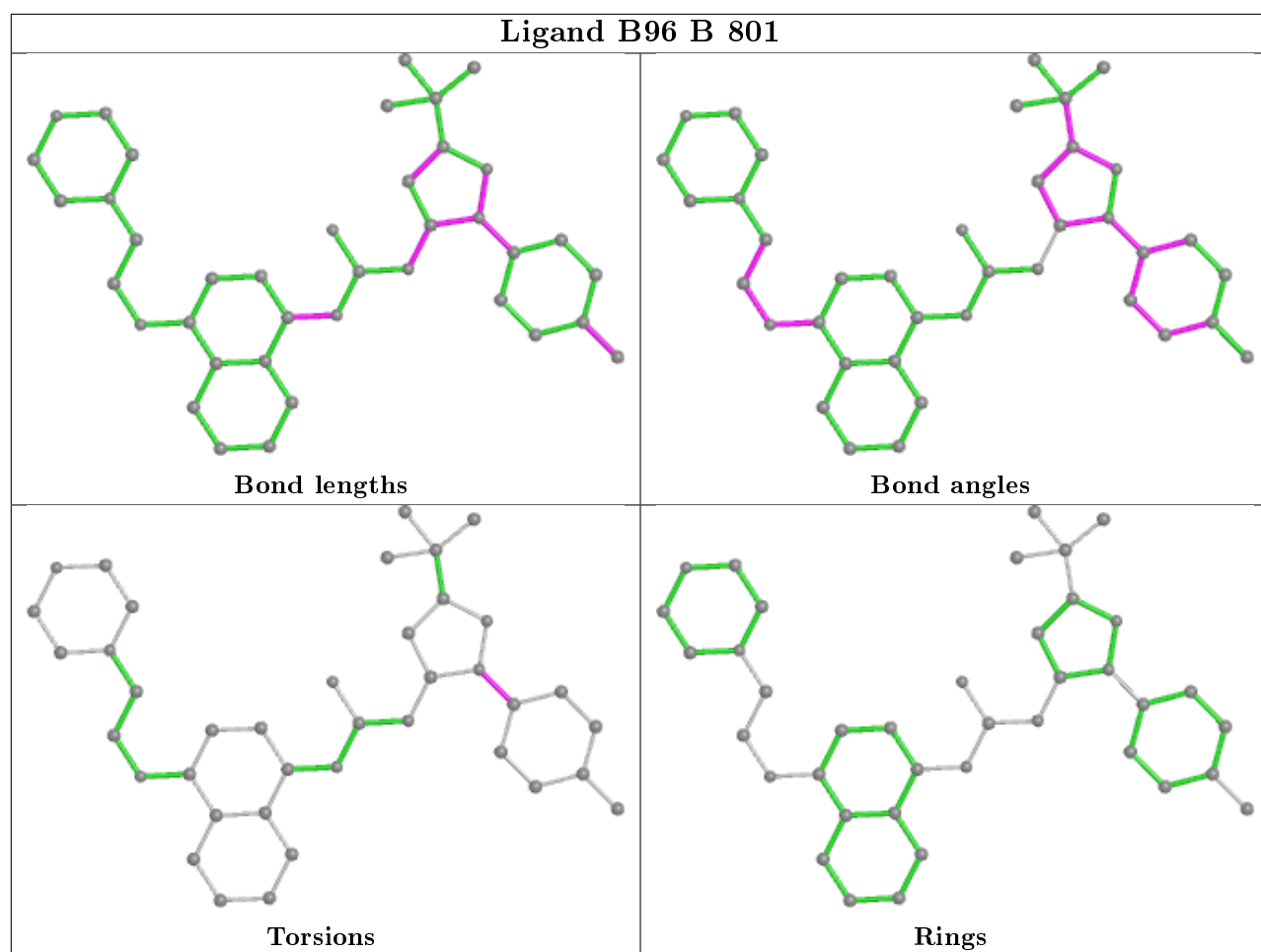
4 monomers are involved in 33 short contacts:

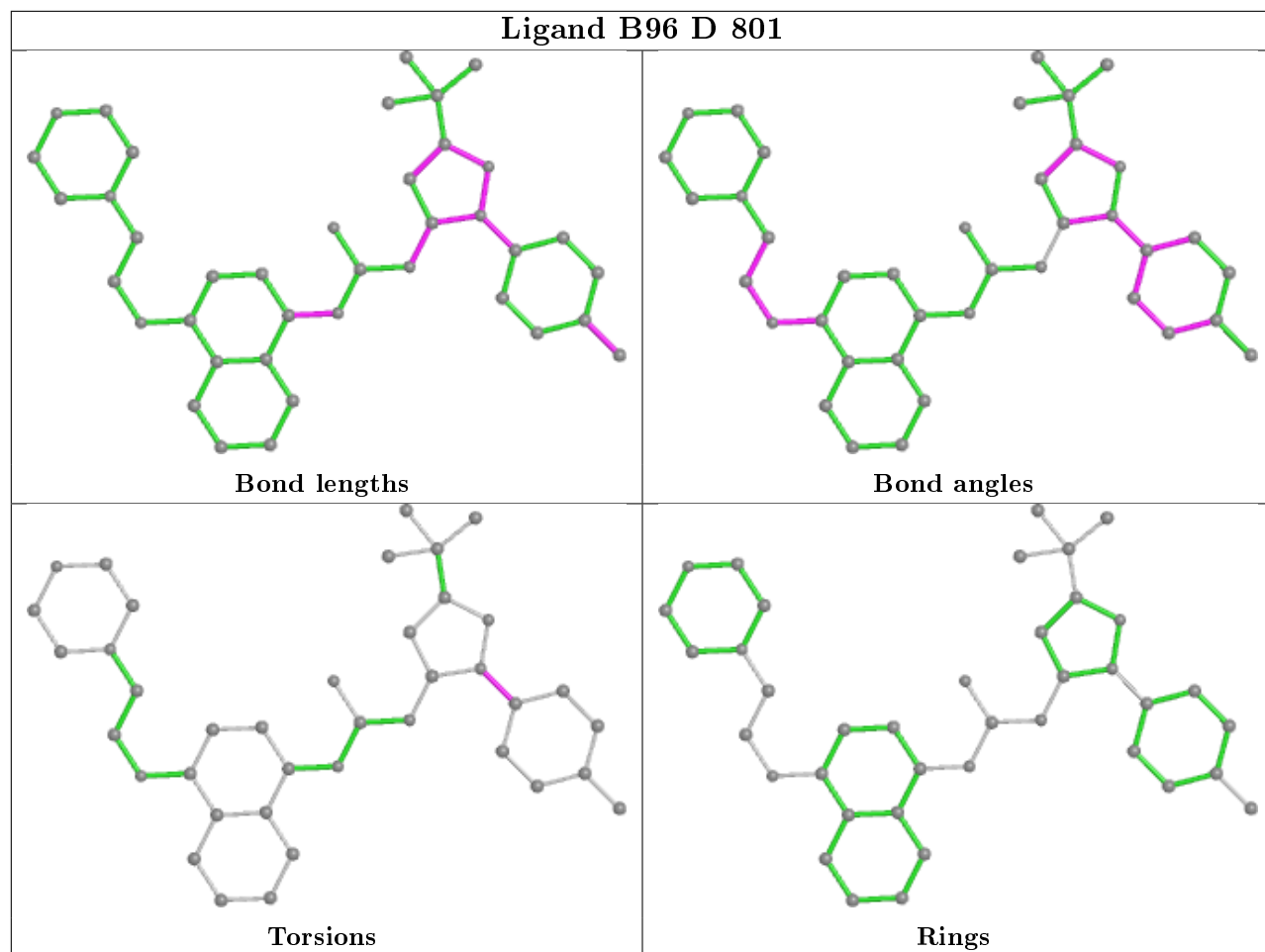
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	801	B96	8	0
2	B	801	B96	9	0
2	D	801	B96	7	0
2	A	801	B96	9	0

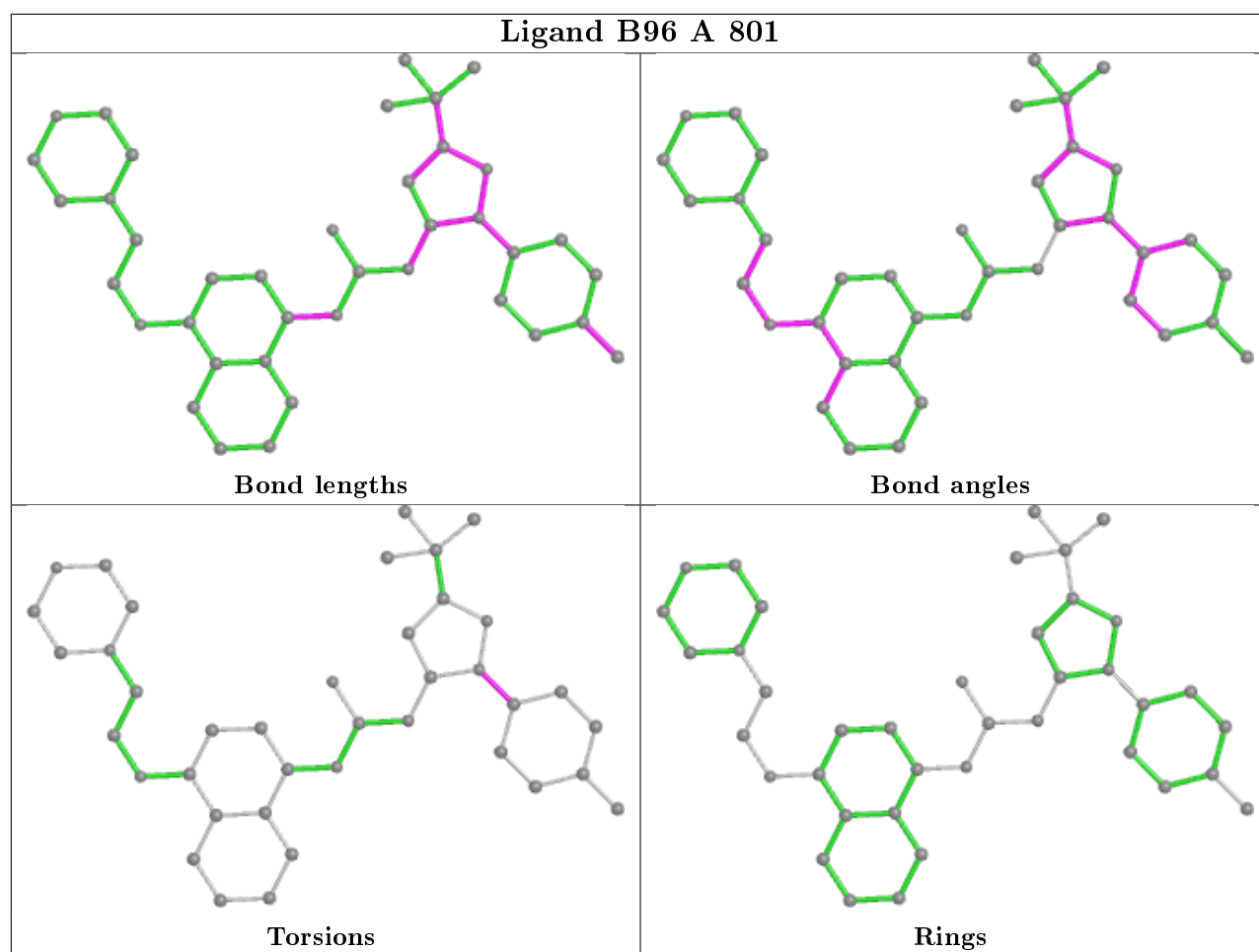
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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 [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	262/284 (92%)	-0.45	1 (0%) 92 84	30, 69, 111, 126	23 (8%)
1	B	259/284 (91%)	-0.45	0 100 100	27, 63, 105, 146	36 (13%)
1	C	258/284 (90%)	-0.33	2 (0%) 86 72	44, 67, 121, 168	3 (1%)
1	D	262/284 (92%)	-0.48	1 (0%) 92 84	33, 70, 116, 165	18 (6%)
All	All	1041/1136 (91%)	-0.43	4 (0%) 92 84	27, 68, 114, 168	80 (7%)

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	671	ARG	3.8
1	C	545	GLU	3.8
1	D	671	ARG	3.8
1	C	630	SER	3.4

### 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 carbohydrates in this entry.

### 6.4 Ligands [i](#)

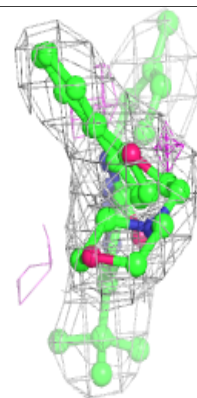
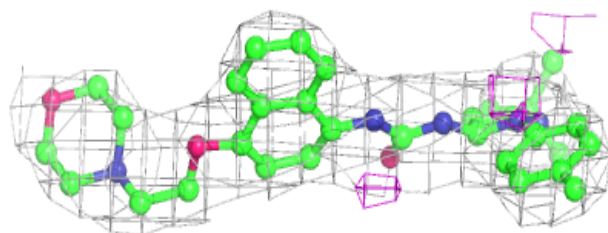
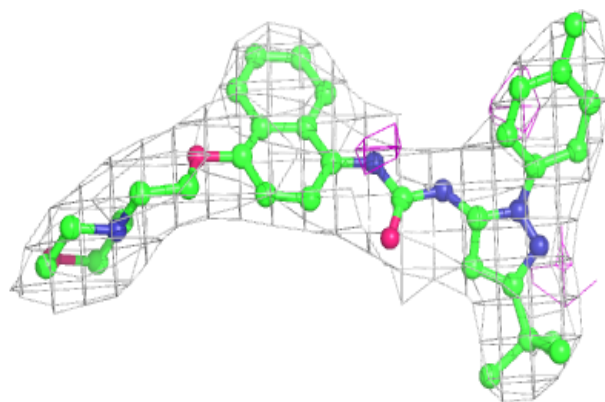
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 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	B96	B	801	39/39	0.96	0.21	33,48,59,62	0
2	B96	D	801	39/39	0.96	0.21	34,49,55,60	0
2	B96	A	801	39/39	0.96	0.20	27,50,56,58	0
2	B96	C	801	39/39	0.97	0.21	36,45,58,61	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.

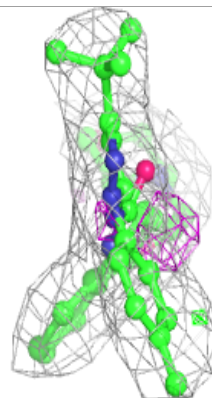
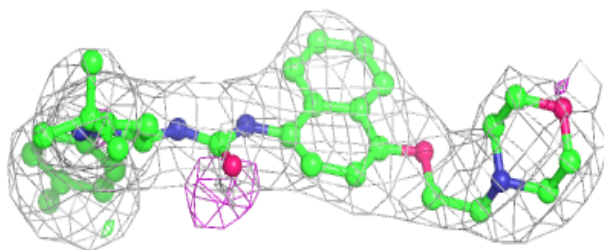
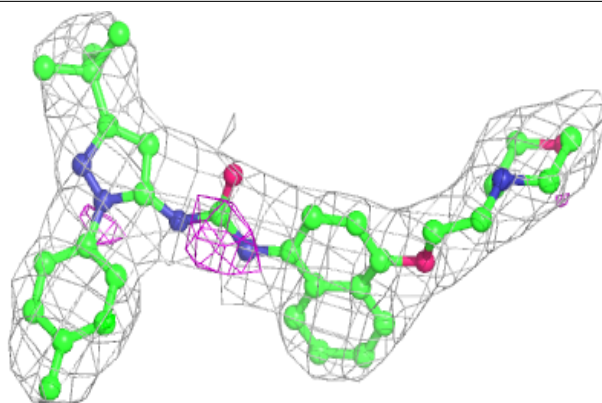
**Electron density around B96 B 801:**

2mF<sub>o</sub>-DF<sub>c</sub> (at 0.7 rmsd) in gray  
mF<sub>o</sub>-DF<sub>c</sub> (at 3 rmsd) in purple (negative)  
and green (positive)

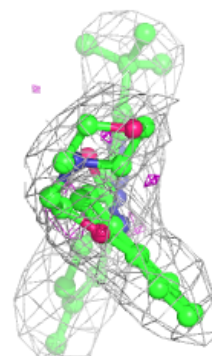
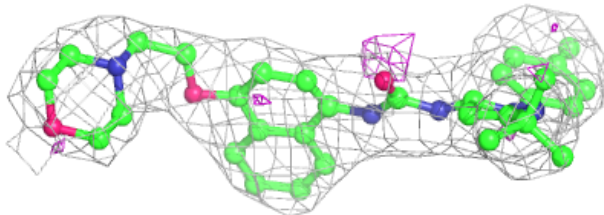
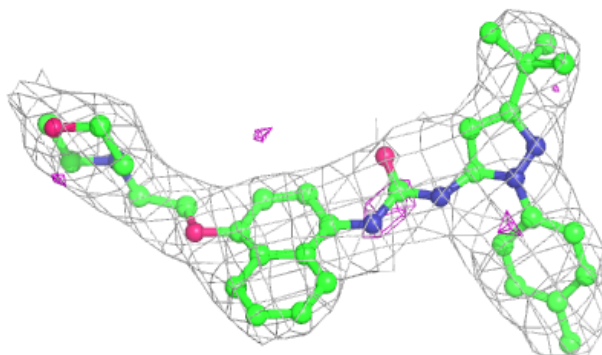


**Electron density around B96 D 801:**

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

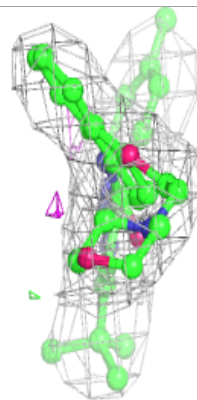
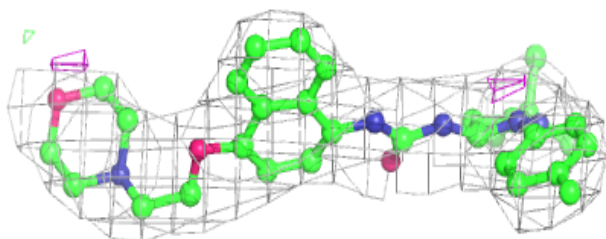
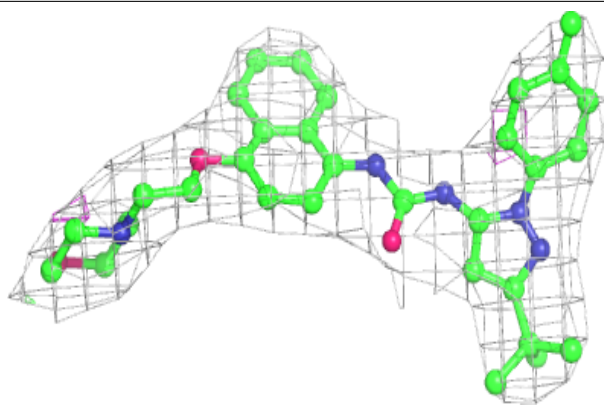
**Electron density around B96 A 801:**

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



**Electron density around B96 C 801:**

$2mF_o-DF_c$  (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.