



# Full wwPDB X-ray Structure Validation Report ⓘ

Apr 25, 2026 – 05:17 PM EDT

PDB ID : 4EHE / pdb\_00004ehe  
Title : B-Raf Kinase Domain in Complex with an Aminothienopyrimidine-based Inhibitor  
Authors : Voegtli, W.C.  
Deposited on : 2012-04-02  
Resolution : 3.30 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 Phenix2.0  
Mogul : 2022.3.0, CSD as543be (2022)  
Xtrriage (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)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.49

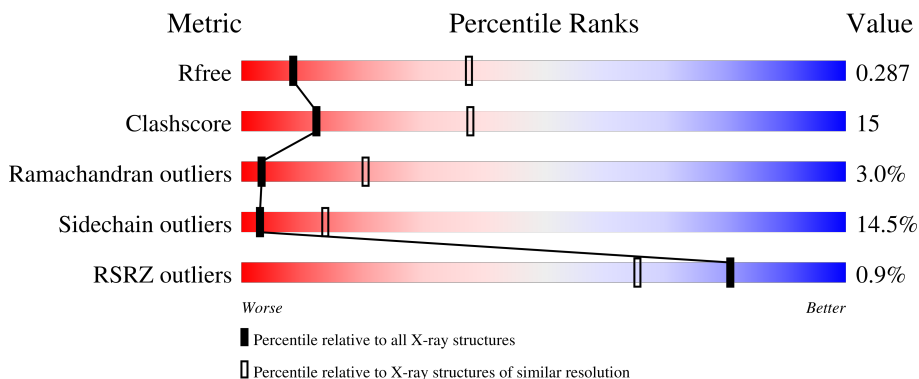
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.30 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	1169 (3.32-3.28)
Clashscore	190562	1209 (3.32-3.28)
Ramachandran outliers	187476	1188 (3.32-3.28)
Sidechain outliers	187428	1187 (3.32-3.28)
RSRZ outliers	180081	1169 (3.32-3.28)

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	307	
1	B	307	

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 4392 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.

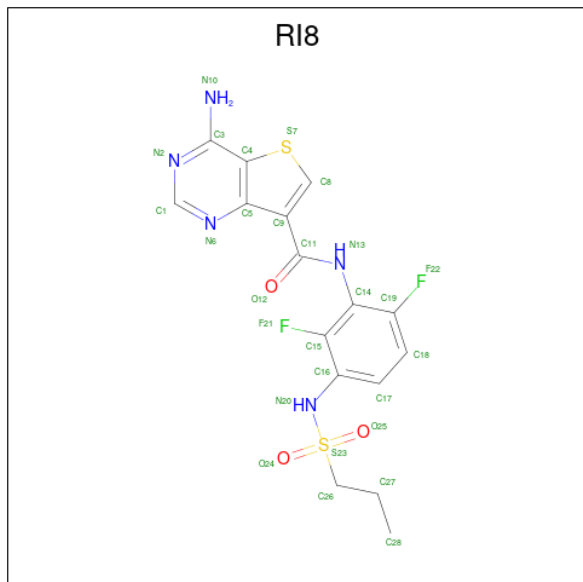
- Molecule 1 is a protein called Serine/threonine-protein kinase B-raf.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	266	Total	C	N	O	S	0	0	0
			2125	1361	372	379	13			
1	B	276	Total	C	N	O	S	0	0	0
			2211	1416	387	395	13			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	420	MET	-	expression tag	UNP P15056
A	421	ASP	-	expression tag	UNP P15056
A	422	ARG	-	expression tag	UNP P15056
A	423	GLY	-	expression tag	UNP P15056
A	424	SER	-	expression tag	UNP P15056
A	425	HIS	-	expression tag	UNP P15056
A	426	HIS	-	expression tag	UNP P15056
A	427	HIS	-	expression tag	UNP P15056
A	428	HIS	-	expression tag	UNP P15056
A	429	HIS	-	expression tag	UNP P15056
A	430	HIS	-	expression tag	UNP P15056
A	431	GLY	-	expression tag	UNP P15056
B	420	MET	-	expression tag	UNP P15056
B	421	ASP	-	expression tag	UNP P15056
B	422	ARG	-	expression tag	UNP P15056
B	423	GLY	-	expression tag	UNP P15056
B	424	SER	-	expression tag	UNP P15056
B	425	HIS	-	expression tag	UNP P15056
B	426	HIS	-	expression tag	UNP P15056
B	427	HIS	-	expression tag	UNP P15056
B	428	HIS	-	expression tag	UNP P15056
B	429	HIS	-	expression tag	UNP P15056
B	430	HIS	-	expression tag	UNP P15056
B	431	GLY	-	expression tag	UNP P15056

- Molecule 2 is 4-amino-N-{2,6-difluoro-3-[(propylsulfonyl)amino]phenyl}thieno[3,2-d]pyrimidine-7-carboxamide (CCD ID: RI8) (formula: C<sub>16</sub>H<sub>15</sub>F<sub>2</sub>N<sub>5</sub>O<sub>3</sub>S<sub>2</sub>).

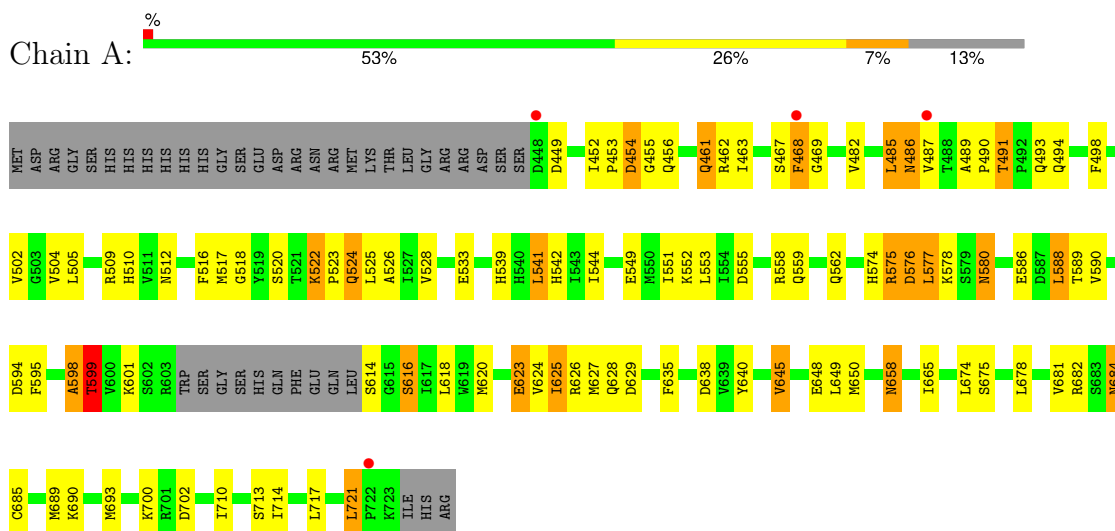


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
			Total	C	F	N	O			S
2	A	1	Total	16	2	5	3	2	0	0
2	B	1	Total	16	2	5	3	2	0	0

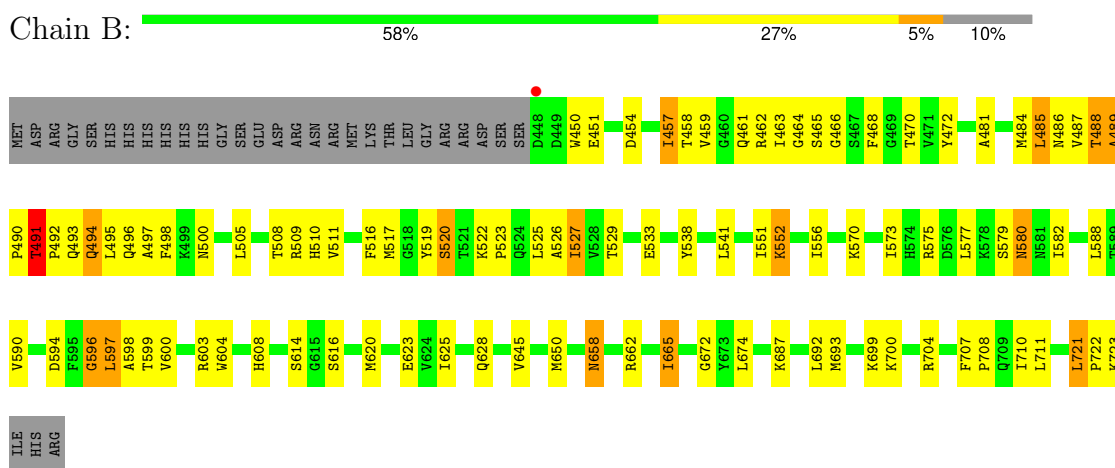
### 3 Residue-property plots [i](#)

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: Serine/threonine-protein kinase B-raf



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



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	108.20Å 108.20Å 153.10Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.46 – 3.30 29.46 – 3.30	Depositor EDS
% Data completeness (in resolution range)	100.0 (29.46-3.30) 98.2 (29.46-3.30)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.32 (at 3.31Å)	Xtrriage
Refinement program	REFMAC	Depositor
R, $R_{free}$	0.225 , 0.296 0.213 , 0.287	Depositor DCC
$R_{free}$ test set	698 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	72.0	Xtrriage
Anisotropy	0.134	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 14.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	4392	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	61.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.30% of the height of the origin peak. No significant pseudotranslation is detected.*

<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: RI8

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	0.67	0/2170	0.98	3/2927 (0.1%)
1	B	0.66	0/2261	1.02	3/3052 (0.1%)
All	All	0.67	0/4431	1.00	6/5979 (0.1%)

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

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
1	B	494	GLN	N-CA-C	-6.52	104.10	111.14
1	B	491	THR	CA-C-N	-5.49	113.90	119.83
1	B	491	THR	C-N-CA	-5.49	113.90	119.83
1	A	598	ALA	N-CA-C	-5.45	101.79	109.96
1	A	616	SER	N-CA-C	-5.34	104.04	110.88
1	A	599	THR	N-CA-CB	5.20	119.28	110.49

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	489	ALA	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	2125	0	2171	78	0
1	B	2211	0	2244	63	0
2	A	28	0	15	5	0
2	B	28	0	15	2	0
All	All	4392	0	4445	136	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 15.

All (136) 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:505:LEU:HD22	2:A:801:RI8:H26	1.43	0.97
1:A:580:ASN:H	1:A:580:ASN:HD22	1.05	0.96
1:B:580:ASN:H	1:B:580:ASN:HD22	1.16	0.94
1:B:580:ASN:HD22	1:B:580:ASN:N	1.73	0.86
1:B:454:ASP:H	1:B:522:LYS:HD3	1.42	0.84
1:A:628:GLN:HG3	1:A:629:ASP:H	1.41	0.83
1:A:505:LEU:CD2	2:A:801:RI8:H26	2.11	0.80
1:A:490:PRO:HA	1:A:491:THR:HB	1.65	0.78
1:B:658:ASN:HD22	1:B:658:ASN:H	1.29	0.78
1:A:574:HIS:CD2	1:A:595:PHE:HB3	2.18	0.77
1:B:594:ASP:H	2:B:801:RI8:HN20	1.33	0.77
1:A:580:ASN:HD22	1:A:580:ASN:N	1.81	0.76
1:A:594:ASP:H	2:A:801:RI8:HN20	1.31	0.76
1:A:580:ASN:H	1:A:580:ASN:ND2	1.83	0.76
1:A:578:LYS:NZ	1:A:616:SER:HB3	2.04	0.73
1:A:578:LYS:HZ2	1:A:616:SER:HB3	1.54	0.72
1:A:684:ASN:HD22	1:A:684:ASN:H	1.38	0.70
1:A:510:HIS:HA	1:B:517:MET:HE2	1.74	0.69
1:B:662:ARG:HA	1:B:665:ILE:HG13	1.75	0.68
1:B:462:ARG:HG2	1:B:472:TYR:HE2	1.60	0.67
1:A:516:PHE:O	1:B:509:ARG:HD3	1.94	0.67
1:B:457:ILE:HD12	1:B:457:ILE:H	1.61	0.66
1:B:580:ASN:N	1:B:580:ASN:ND2	2.37	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:522:LYS:HB2	1:A:523:PRO:HD3	1.79	0.65
1:B:454:ASP:N	1:B:522:LYS:HD3	2.11	0.64
1:B:551:ILE:HD12	1:B:551:ILE:H	1.64	0.63
1:B:582:ILE:HG23	1:B:590:VAL:HG13	1.82	0.62
1:B:462:ARG:HB3	1:B:462:ARG:CZ	2.30	0.61
1:A:520:SER:HB3	1:A:526:ALA:HB3	1.82	0.61
1:A:551:ILE:H	1:A:551:ILE:HD12	1.66	0.60
1:A:467:SER:C	1:A:469:GLY:H	2.09	0.60
1:A:658:ASN:H	1:A:658:ASN:HD22	1.48	0.59
1:A:620:MET:HE2	1:A:625:ILE:HA	1.84	0.59
1:B:464:GLY:O	1:B:470:THR:HG23	2.02	0.59
1:A:626:ARG:O	1:A:628:GLN:N	2.36	0.59
1:A:512:ASN:HA	1:A:590:VAL:O	2.04	0.58
1:A:689:MET:HG3	1:A:693:MET:HE2	1.85	0.57
1:B:462:ARG:HG2	1:B:472:TYR:CE2	2.40	0.57
1:B:650:MET:HG3	1:B:693:MET:HE1	1.87	0.57
1:A:452:ILE:HD11	1:A:518:GLY:HA3	1.87	0.55
1:B:573:ILE:HG22	1:B:575:ARG:HG3	1.88	0.55
1:A:682:ARG:O	1:A:685:CYS:HB3	2.06	0.55
1:B:468:PHE:HB2	1:B:608:HIS:CB	2.37	0.54
1:A:490:PRO:HA	1:A:491:THR:CB	2.37	0.54
1:A:575:ARG:O	1:A:576:ASP:HB2	2.07	0.54
1:A:586:GLU:O	1:A:588:LEU:HD13	2.08	0.54
1:A:628:GLN:HG3	1:A:629:ASP:N	2.13	0.53
1:B:603:ARG:O	1:B:604:TRP:HD1	1.92	0.53
1:A:578:LYS:HD2	1:A:580:ASN:ND2	2.23	0.53
1:A:580:ASN:N	1:A:580:ASN:ND2	2.45	0.53
1:B:603:ARG:O	1:B:604:TRP:CD1	2.62	0.53
1:B:707:PHE:O	1:B:708:PRO:C	2.51	0.53
1:A:551:ILE:HG13	1:A:721:LEU:HD21	1.91	0.52
1:B:658:ASN:HD22	1:B:658:ASN:N	2.04	0.52
1:A:468:PHE:HB3	1:A:601:LYS:NZ	2.25	0.52
1:B:527:ILE:HD13	1:B:597:LEU:HD21	1.91	0.52
1:A:690:LYS:HA	1:A:693:MET:HE3	1.91	0.51
1:A:468:PHE:HB3	1:A:601:LYS:HE3	1.92	0.51
1:A:553:LEU:HB3	1:A:650:MET:HE1	1.93	0.51
1:B:498:PHE:CE2	1:B:525:LEU:HB3	2.46	0.51
1:A:454:ASP:OD1	1:A:455:GLY:N	2.44	0.50
1:A:710:ILE:O	1:A:714:ILE:HG13	2.12	0.50
1:B:505:LEU:HD22	2:B:801:RI8:H26	1.94	0.50
1:A:509:ARG:HD2	1:B:450:TRP:CH2	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:681:VAL:HG11	1:A:693:MET:HE1	1.93	0.49
1:A:517:MET:HE2	1:B:510:HIS:HA	1.93	0.49
1:B:573:ILE:HG22	1:B:575:ARG:CG	2.43	0.49
1:B:650:MET:CG	1:B:693:MET:HE1	2.43	0.48
1:B:552:LYS:HD2	1:B:556:ILE:HD11	1.96	0.48
1:A:522:LYS:O	1:A:523:PRO:C	2.55	0.48
1:B:579:SER:HA	1:B:582:ILE:HD12	1.95	0.48
1:A:710:ILE:HG22	1:A:714:ILE:HD11	1.94	0.48
1:A:620:MET:HB2	1:A:625:ILE:HG12	1.94	0.48
1:A:490:PRO:HB3	1:A:494:GLN:OE1	2.14	0.47
1:B:520:SER:HB3	1:B:526:ALA:HB3	1.95	0.47
1:B:620:MET:HE2	1:B:625:ILE:HA	1.97	0.47
1:A:598:ALA:O	1:A:599:THR:OG1	2.30	0.47
1:A:485:LEU:HD23	1:A:525:LEU:HB3	1.96	0.47
1:A:517:MET:HG2	1:B:509:ARG:O	2.15	0.46
1:A:486:ASN:HA	1:A:524:GLN:OE1	2.16	0.46
1:A:555:ASP:OD1	1:A:558:ARG:NH1	2.49	0.46
1:B:494:GLN:HB3	1:B:604:TRP:CZ2	2.50	0.46
1:A:509:ARG:NH2	1:B:508:THR:O	2.45	0.46
1:B:538:TYR:N	1:B:579:SER:O	2.47	0.46
1:A:453:PRO:HB2	1:A:456:GLN:HE21	1.82	0.45
2:A:801:RI8:H17	2:A:801:RI8:O24	2.14	0.45
1:B:491:THR:HB	1:B:494:GLN:OE1	2.17	0.45
1:B:493:GLN:HB2	1:B:496:GLN:CB	2.46	0.45
1:A:485:LEU:HD21	1:A:498:PHE:HE1	1.81	0.45
1:B:489:ALA:HA	1:B:490:PRO:HD2	1.79	0.45
1:A:468:PHE:HB3	1:A:601:LYS:CE	2.46	0.45
1:A:620:MET:CB	1:A:625:ILE:HG12	2.47	0.45
1:B:672:GLY:O	1:B:699:LYS:HE2	2.16	0.45
1:B:487:VAL:HG21	1:B:604:TRP:CZ3	2.52	0.45
1:A:461:GLN:HE21	1:A:462:ARG:N	2.15	0.45
1:B:498:PHE:HE1	1:B:527:ILE:HD11	1.82	0.45
1:A:467:SER:C	1:A:469:GLY:N	2.75	0.44
1:B:623:GLU:OE1	1:B:704:ARG:NH2	2.49	0.44
1:B:492:PRO:HA	1:B:493:GLN:HA	1.50	0.44
1:B:497:ALA:O	1:B:500:ASN:HB2	2.17	0.44
1:B:658:ASN:H	1:B:658:ASN:ND2	2.05	0.44
1:B:519:TYR:CD1	1:B:519:TYR:C	2.95	0.44
1:B:454:ASP:HB2	1:B:522:LYS:NZ	2.33	0.44
1:A:467:SER:O	1:A:469:GLY:N	2.51	0.44
1:A:684:ASN:HD22	1:A:684:ASN:N	2.11	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:559:GLN:O	1:A:562:GLN:HB3	2.17	0.44
1:B:620:MET:HB3	1:B:625:ILE:HG12	1.99	0.44
1:B:468:PHE:HB2	1:B:608:HIS:HB2	2.00	0.44
1:B:481:ALA:HB3	1:B:529:THR:OG1	2.18	0.44
1:A:454:ASP:C	1:A:456:GLN:H	2.25	0.43
1:B:692:LEU:HD11	1:B:710:ILE:HG23	2.00	0.43
1:B:721:LEU:HB3	1:B:722:PRO:HD3	2.00	0.43
1:A:541:LEU:HB3	1:A:542:HIS:CE1	2.53	0.43
1:B:596:GLY:O	1:B:598:ALA:N	2.46	0.43
1:B:580:ASN:H	1:B:580:ASN:ND2	1.95	0.43
1:A:491:THR:O	1:A:494:GLN:HB2	2.18	0.43
1:A:539:HIS:CE1	1:A:544:ILE:HD13	2.54	0.43
1:A:626:ARG:O	1:A:626:ARG:HG3	2.20	0.42
1:A:623:GLU:HA	1:A:626:ARG:NH1	2.34	0.42
1:B:711:LEU:HD12	1:B:711:LEU:HA	1.87	0.42
1:A:640:TYR:CD2	1:A:640:TYR:C	2.97	0.42
1:A:485:LEU:C	1:A:487:VAL:H	2.26	0.42
1:A:678:LEU:O	1:A:690:LYS:HE3	2.20	0.42
1:A:649:LEU:HB2	1:A:650:MET:HE3	2.01	0.42
2:A:801:RI8:N6	2:A:801:RI8:N13	2.57	0.41
1:A:487:VAL:HG23	1:A:487:VAL:O	2.20	0.41
1:A:620:MET:HE3	1:A:624:VAL:HG12	2.02	0.41
1:A:509:ARG:HD3	1:B:516:PHE:O	2.21	0.41
1:A:577:LEU:HD23	1:A:577:LEU:HA	1.78	0.41
1:B:468:PHE:CE2	1:B:485:LEU:HD12	2.55	0.41
1:B:487:VAL:HG23	1:B:487:VAL:O	2.21	0.41
1:A:635:PHE:O	1:A:638:ASP:HB2	2.20	0.41
1:A:485:LEU:HD21	1:A:498:PHE:CE1	2.56	0.40
1:B:662:ARG:HE	1:B:662:ARG:HB3	1.71	0.40
1:A:645:VAL:O	1:A:648:GLU:HB2	2.21	0.40
1:A:574:HIS:C	1:A:575:ARG:HG3	2.46	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	262/307 (85%)	236 (90%)	18 (7%)	8 (3%)	3	20
1	B	274/307 (89%)	236 (86%)	30 (11%)	8 (3%)	3	21
All	All	536/614 (87%)	472 (88%)	48 (9%)	16 (3%)	3	20

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	468	PHE
1	A	486	ASN
1	A	576	ASP
1	A	599	THR
1	B	465	SER
1	B	466	GLY
1	B	486	ASN
1	A	627	MET
1	B	488	THR
1	B	523	PRO
1	B	721	LEU
1	A	454	ASP
1	B	489	ALA
1	A	522	LYS
1	B	596	GLY
1	A	491	THR

### 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	234/271 (86%)	199 (85%)	35 (15%)	3	13
1	B	243/271 (90%)	209 (86%)	34 (14%)	3	15
All	All	477/542 (88%)	408 (86%)	69 (14%)	3	14

All (69) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	449	ASP
1	A	461	GLN
1	A	463	ILE
1	A	482	VAL
1	A	485	LEU
1	A	493	GLN
1	A	502	VAL
1	A	504	VAL
1	A	524	GLN
1	A	528	VAL
1	A	533	GLU
1	A	541	LEU
1	A	549	GLU
1	A	552	LYS
1	A	575	ARG
1	A	577	LEU
1	A	580	ASN
1	A	588	LEU
1	A	589	THR
1	A	599	THR
1	A	614	SER
1	A	618	LEU
1	A	623	GLU
1	A	625	ILE
1	A	645	VAL
1	A	658	ASN
1	A	665	ILE
1	A	674	LEU
1	A	675	SER
1	A	684	ASN
1	A	700	LYS
1	A	702	ASP
1	A	713	SER
1	A	717	LEU
1	A	721	LEU
1	B	451	GLU
1	B	457	ILE
1	B	458	THR
1	B	459	VAL
1	B	461	GLN
1	B	463	ILE
1	B	484	MET
1	B	485	LEU

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	B	488	THR
1	B	491	THR
1	B	495	LEU
1	B	511	VAL
1	B	520	SER
1	B	527	ILE
1	B	533	GLU
1	B	541	LEU
1	B	552	LYS
1	B	570	LYS
1	B	577	LEU
1	B	580	ASN
1	B	588	LEU
1	B	597	LEU
1	B	599	THR
1	B	600	VAL
1	B	614	SER
1	B	616	SER
1	B	628	GLN
1	B	645	VAL
1	B	658	ASN
1	B	665	ILE
1	B	674	LEU
1	B	687	LYS
1	B	700	LYS
1	B	723	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	456	GLN
1	A	461	GLN
1	A	486	ASN
1	A	500	ASN
1	A	539	HIS
1	A	580	ASN
1	A	585	HIS
1	A	658	ASN
1	A	684	ASN
1	A	709	GLN
1	B	500	ASN
1	B	540	HIS

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Mol	Chain	Res	Type
1	B	580	ASN
1	B	585	HIS
1	B	628	GLN
1	B	653	GLN
1	B	658	ASN
1	B	684	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 [i](#)

2 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	RI8	B	801	-	28,30,30	2.00	5 (17%)	37,44,44	2.05	10 (27%)
2	RI8	A	801	-	28,30,30	1.92	5 (17%)	37,44,44	1.87	8 (21%)

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	RI8	B	801	-	-	2/17/17/17	0/3/3/3
2	RI8	A	801	-	-	2/17/17/17	0/3/3/3

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	801	RI8	C16-N20	-6.40	1.32	1.42
2	A	801	RI8	C16-N20	-5.74	1.33	1.42
2	A	801	RI8	S23-N20	4.74	1.72	1.62
2	B	801	RI8	S23-N20	4.69	1.72	1.62
2	B	801	RI8	O25-S23	3.10	1.47	1.43
2	A	801	RI8	O25-S23	2.93	1.47	1.43
2	B	801	RI8	O24-S23	2.85	1.47	1.43
2	A	801	RI8	O24-S23	2.68	1.47	1.43
2	B	801	RI8	C26-S23	2.28	1.85	1.78
2	A	801	RI8	C26-S23	2.02	1.84	1.78

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	801	RI8	C4-C5-N6	-5.38	118.63	123.24
2	A	801	RI8	C9-C8-S7	-5.32	110.59	114.16
2	B	801	RI8	C9-C8-S7	-4.54	111.11	114.16
2	B	801	RI8	C19-C14-C15	4.06	120.10	115.64
2	A	801	RI8	C19-C14-C15	4.06	120.09	115.64
2	B	801	RI8	O25-S23-O24	3.87	124.75	119.34
2	A	801	RI8	C4-C5-N6	-3.77	120.01	123.24
2	A	801	RI8	C9-C11-N13	-3.38	110.94	114.89
2	B	801	RI8	C9-C11-N13	-3.13	111.24	114.89
2	A	801	RI8	F21-C15-C16	2.98	123.02	118.28
2	A	801	RI8	C26-S23-N20	-2.84	102.69	106.72
2	B	801	RI8	C8-C9-C11	2.68	125.08	118.92
2	B	801	RI8	C16-C15-C14	-2.62	119.15	124.22
2	A	801	RI8	C8-C9-C11	2.62	124.94	118.92
2	B	801	RI8	C14-N13-C11	2.46	131.56	124.06
2	A	801	RI8	C16-C15-C14	-2.30	119.78	124.22
2	B	801	RI8	C1-N2-C3	-2.23	115.06	118.73
2	B	801	RI8	C17-C16-C15	2.22	120.80	117.72

There are no chirality outliers.

All (4) torsion outliers are listed below:

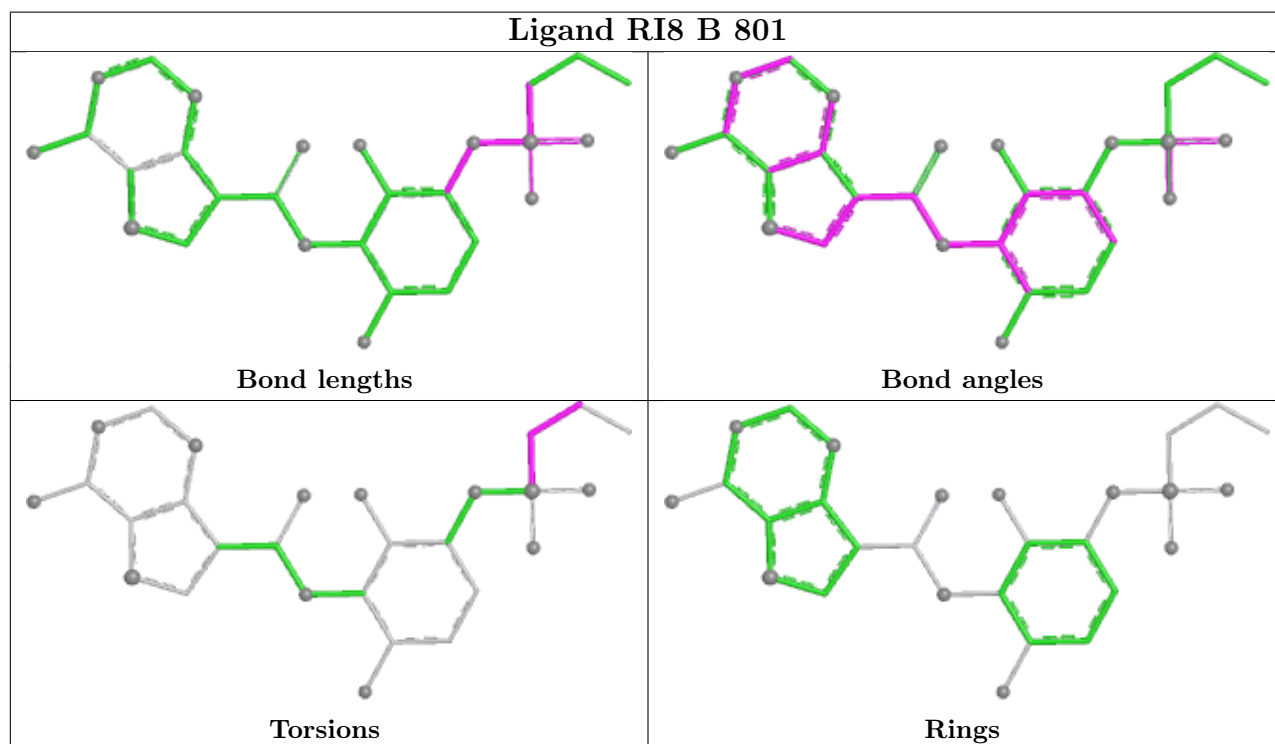
Mol	Chain	Res	Type	Atoms
2	A	801	RI8	C27-C26-S23-O24
2	B	801	RI8	S23-C26-C27-C28
2	B	801	RI8	C27-C26-S23-O24
2	A	801	RI8	N13-C11-C9-C5

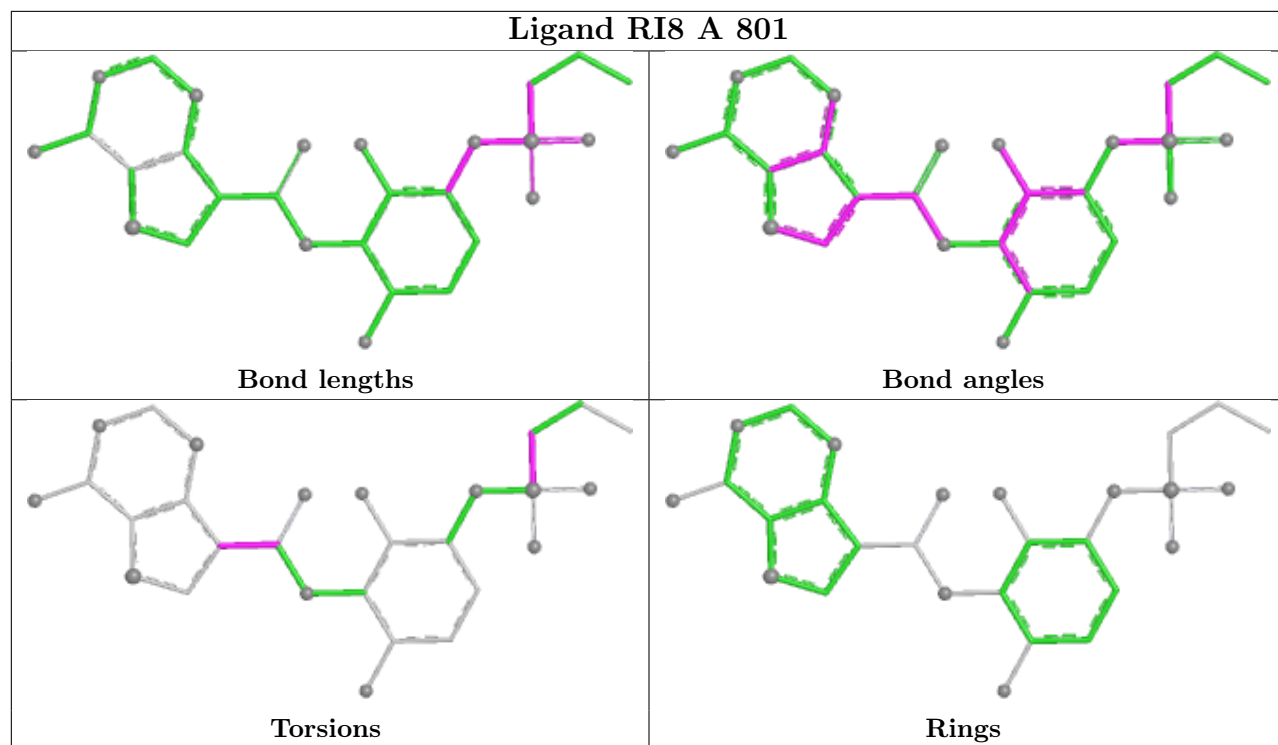
There are no ring outliers.

2 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	801	RI8	2	0
2	A	801	RI8	5	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	266/307 (86%)	-0.07	4 (1%) 72 53	43, 59, 94, 101	0
1	B	276/307 (89%)	-0.11	1 (0%) 88 79	38, 58, 83, 102	0
All	All	542/614 (88%)	-0.09	5 (0%) 81 65	38, 59, 91, 102	0

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	448	ASP	3.3
1	A	468	PHE	2.7
1	A	487	VAL	2.4
1	A	722	PRO	2.1
1	A	448	ASP	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](#)

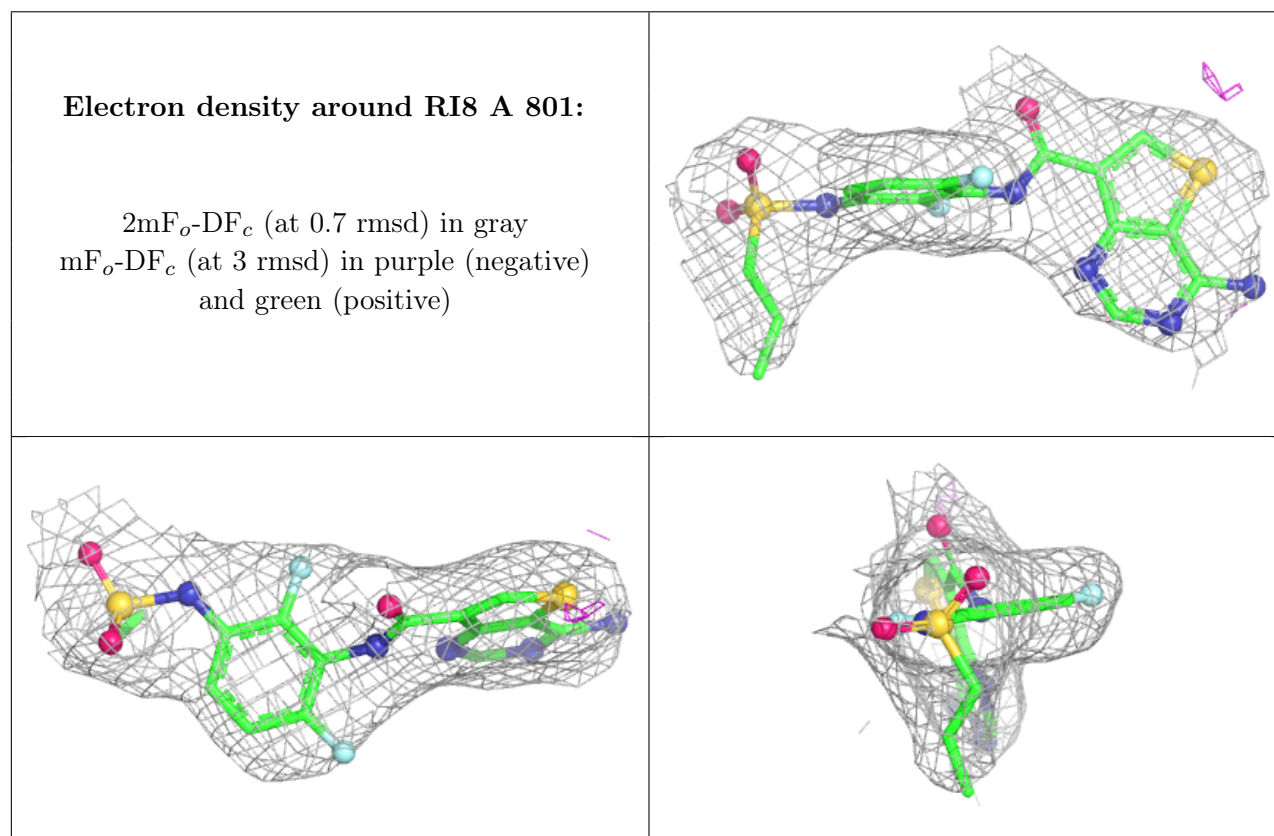
There are no oligosaccharides in this entry.

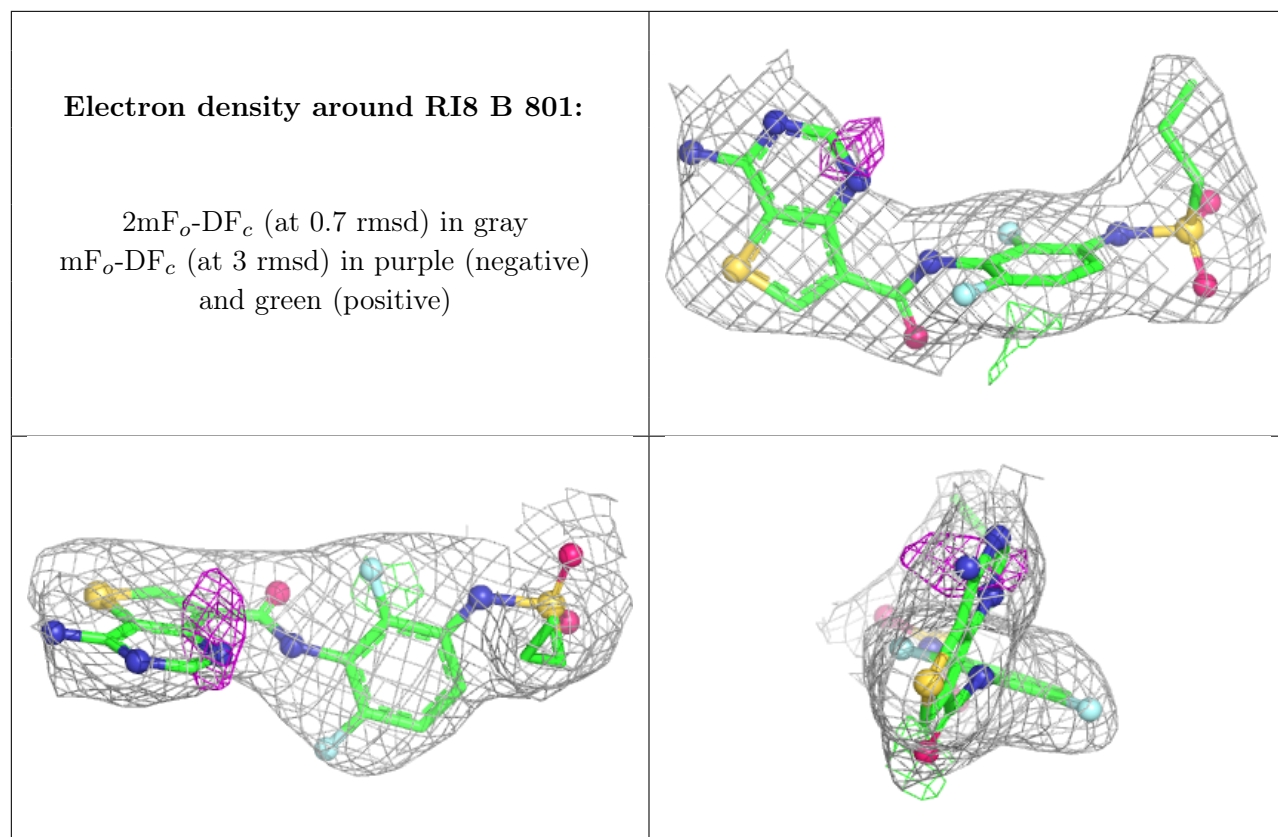
### 6.4 Ligands [i](#)

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	RI8	A	801	28/28	0.95	0.09	46,49,51,52	0
2	RI8	B	801	28/28	0.95	0.09	37,43,48,48	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.





## 6.5 Other polymers [i](#)

There are no such residues in this entry.