



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 18, 2026 – 04:31 AM UTC

PDB ID : 3F3W / pdb_00003f3w
Title : Drug resistant cSrc kinase domain in complex with inhibitor RL45 (Type II)
Authors : Grutter, C.; Kluter, S.; Getlik, M.; Rauh, D.
Deposited on : 2008-10-31
Resolution : 2.60 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)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

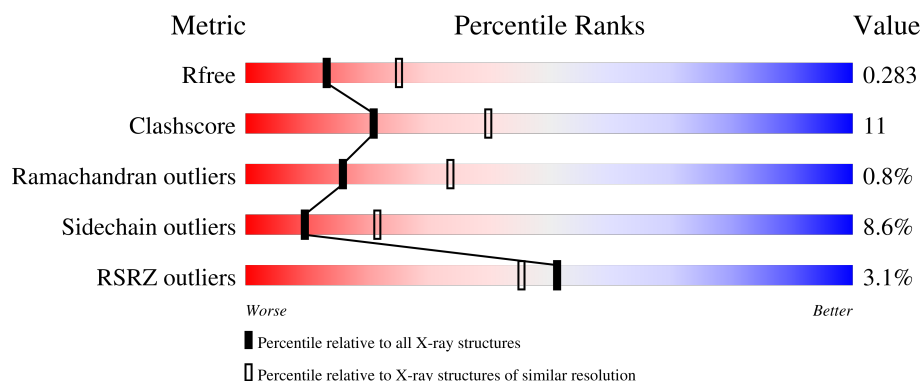
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (2.60-2.60)

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	286	
1	B	286	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 4308 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.

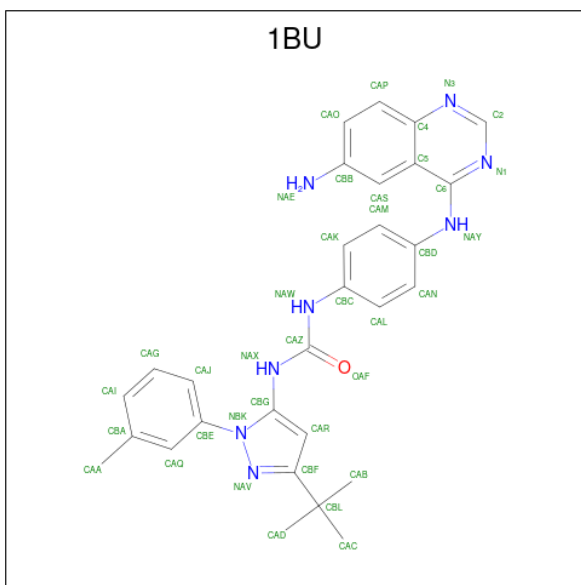
- Molecule 1 is a protein called Proto-oncogene tyrosine-protein kinase Src.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	261	Total	C	N	O	S	0	0	0
			2070	1334	337	380	19			
1	B	260	Total	C	N	O	S	0	0	0
			2089	1343	347	380	19			

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	248	GLY	-	expression tag	UNP P00523
A	249	HIS	-	expression tag	UNP P00523
A	250	MET	-	expression tag	UNP P00523
A	338	MET	THR	engineered mutation	UNP P00523
A	345	CYS	SER	engineered mutation	UNP P00523
B	248	GLY	-	expression tag	UNP P00523
B	249	HIS	-	expression tag	UNP P00523
B	250	MET	-	expression tag	UNP P00523
B	338	MET	THR	engineered mutation	UNP P00523
B	345	CYS	SER	engineered mutation	UNP P00523

- Molecule 2 is 1-{4-[(6-aminoquinazolin-4-yl)amino]phenyl}-3-[3-tert-butyl-1-(3-methylphenyl)-1H-pyrazol-5-yl]urea (CCD ID: 1BU) (formula: C₂₉H₃₀N₈O).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total 38	C 29	N 8	O 1	0	0
2	B	1	Total 38	C 29	N 8	O 1	0	0

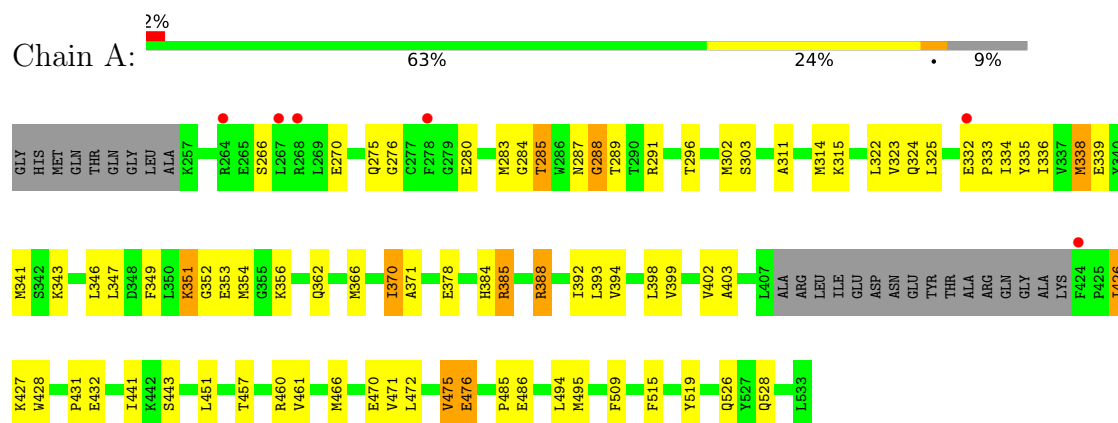
- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	37	Total O 37 37	0	0
3	B	36	Total O 36 36	0	0

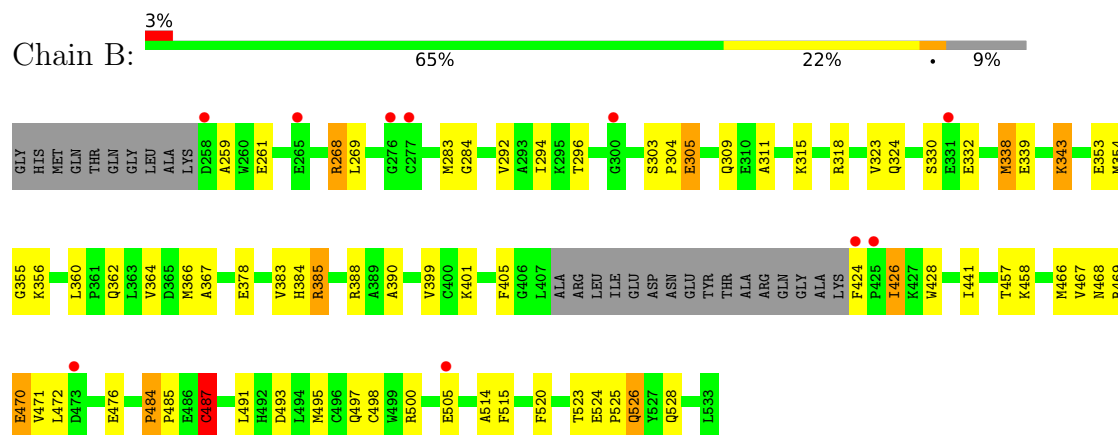
3 Residue-property plots [i](#)

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: Proto-oncogene tyrosine-protein kinase Src



- Molecule 1: Proto-oncogene tyrosine-protein kinase Src



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	42.06Å 63.69Å 75.12Å 78.70° 87.02° 89.96°	Depositor
Resolution (Å)	40.00 – 2.60 40.00 – 2.60	Depositor EDS
% Data completeness (in resolution range)	100.0 (40.00-2.60) 98.2 (40.00-2.60)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.47 (at 2.61Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.221 , 0.277 0.232 , 0.283	Depositor DCC
R_{free} test set	923 reflections (4.00%)	wwPDB-VP
Wilson B-factor (Å ²)	33.4	Xtriage
Anisotropy	0.415	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 26.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	4308	wwPDB-VP
Average B, all atoms (Å ²)	17.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 10.00% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: 1BU

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	1.07	2/2122 (0.1%)	1.21	9/2878 (0.3%)
1	B	1.06	2/2141 (0.1%)	1.20	6/2899 (0.2%)
All	All	1.06	4/4263 (0.1%)	1.21	15/5777 (0.3%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	457	THR	CA-CB	6.15	1.61	1.53
1	B	484	PRO	CA-C	6.10	1.55	1.51
1	A	475	VAL	CA-CB	5.54	1.62	1.54
1	A	457	THR	CA-CB	5.10	1.61	1.53

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	356	LYS	N-CA-C	-7.62	103.06	111.36
1	B	487	CYS	CA-C-N	-6.90	112.86	119.76
1	B	487	CYS	C-N-CA	-6.90	112.86	119.76
1	A	370	ILE	N-CA-C	-6.78	104.16	110.53
1	B	360	LEU	CA-C-N	-6.45	112.19	119.28
1	B	360	LEU	C-N-CA	-6.45	112.19	119.28
1	A	509	PHE	N-CA-C	-6.26	104.35	112.23
1	B	524	GLU	CA-C-N	5.73	125.41	119.56
1	B	524	GLU	C-N-CA	5.73	125.41	119.56
1	A	276	GLY	N-CA-C	-5.63	104.85	112.57
1	A	461	VAL	N-CA-C	5.47	114.92	108.96
1	A	352	GLY	CA-C-N	5.30	127.64	120.38
1	A	352	GLY	C-N-CA	5.30	127.64	120.38
1	A	495	MET	N-CA-C	-5.02	105.70	111.07
1	A	519	TYR	N-CA-C	5.01	117.14	111.02

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	2070	0	2023	47	0
1	B	2089	0	2067	43	0
2	A	38	0	30	2	0
2	B	38	0	30	3	0
3	A	37	0	0	1	0
3	B	36	0	0	4	0
All	All	4308	0	4150	92	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 11.

All (92) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:355:GLY:HA3	3:B:47:HOH:O	1.40	1.19
1:A:314:MET:HE2	1:A:325:LEU:HB2	1.42	0.99
1:A:427:LYS:HE3	3:B:34:HOH:O	1.69	0.93
1:A:384:HIS:O	1:A:385:ARG:HB2	1.70	0.92
1:B:424:PHE:HD1	1:B:426:ILE:HG22	1.37	0.89
1:A:280:GLU:H	1:A:296:THR:HB	1.43	0.82
1:A:388:ARG:HB3	1:A:428:TRP:CD1	2.14	0.82
1:B:520:PHE:O	1:B:525:PRO:HA	1.83	0.79
1:A:323:VAL:HG21	1:A:403:ALA:HB2	1.66	0.76
1:A:426:ILE:HD13	1:A:472:LEU:HG	1.71	0.72
1:B:466:MET:HE2	1:B:471:VAL:HG22	1.69	0.71
1:B:343:LYS:O	3:B:62:HOH:O	2.07	0.71
1:A:485:PRO:O	3:A:54:HOH:O	2.08	0.70
1:B:526:GLN:H	1:B:526:GLN:CD	1.99	0.70
1:B:383:VAL:HG12	1:B:385:ARG:HG3	1.73	0.69
1:A:485:PRO:O	1:A:486:GLU:HB2	1.94	0.68
1:A:270:GLU:HG3	1:A:284:GLY:HA2	1.80	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:314:MET:CE	1:A:325:LEU:HB2	2.25	0.61
1:A:347:LEU:O	1:A:351:LYS:HG2	2.00	0.61
1:B:500:ARG:HD3	1:B:505:GLU:HB3	1.84	0.59
1:B:526:GLN:NE2	1:B:526:GLN:C	2.59	0.59
1:B:526:GLN:C	1:B:526:GLN:HE21	2.10	0.59
1:A:370:ILE:HG12	1:A:392:ILE:HD12	1.84	0.58
1:A:426:ILE:CD1	1:A:472:LEU:HG	2.33	0.58
1:A:322:LEU:HD22	1:A:402:VAL:HB	1.85	0.58
1:A:349:PHE:CE1	1:A:354:MET:HG3	2.39	0.57
1:B:324:GLN:O	1:B:338:MET:HB2	2.04	0.56
1:B:493:ASP:O	1:B:497:GLN:HG3	2.07	0.55
1:A:388:ARG:CB	1:A:428:TRP:CD1	2.89	0.55
1:B:384:HIS:O	1:B:385:ARG:HB2	2.07	0.55
1:B:424:PHE:CD1	1:B:426:ILE:HG22	2.29	0.55
1:A:460:ARG:NE	1:B:514:ALA:HB1	2.22	0.54
1:B:495:MET:O	1:B:498:CYS:HB2	2.07	0.54
1:A:332:GLU:HA	1:A:333:PRO:C	2.32	0.54
2:B:1:1BU:HAM	2:B:1:1BU:N1	2.21	0.54
1:A:472:LEU:O	1:A:476:GLU:HB2	2.07	0.54
1:A:334:ILE:C	1:A:335:TYR:HD1	2.15	0.53
1:A:343:LYS:HE2	1:A:394:VAL:HG12	1.91	0.53
1:A:283:MET:HG3	1:A:284:GLY:N	2.23	0.52
1:B:388:ARG:HB3	1:B:428:TRP:CD1	2.44	0.52
1:A:362:GLN:O	1:A:366:MET:HG3	2.09	0.52
1:B:484:PRO:O	1:B:485:PRO:C	2.51	0.52
1:A:275:GLN:HG2	1:A:280:GLU:HG2	1.91	0.52
1:A:341:MET:HG3	1:A:393:LEU:HD13	1.92	0.52
1:A:324:GLN:O	1:A:338:MET:HB2	2.11	0.51
1:A:324:GLN:O	1:A:338:MET:CB	2.58	0.51
1:B:526:GLN:CD	1:B:526:GLN:N	2.66	0.50
1:A:323:VAL:CG2	1:A:403:ALA:HB2	2.39	0.50
1:A:431:PRO:O	1:A:432:GLU:C	2.54	0.50
1:A:311:ALA:HB2	1:A:336:ILE:HD13	1.92	0.50
1:B:515:PHE:HD2	3:B:40:HOH:O	1.93	0.49
1:A:287:ASN:O	1:A:289:THR:N	2.44	0.49
1:A:494:LEU:HD13	1:A:515:PHE:CE1	2.47	0.49
1:A:322:LEU:HD13	2:A:1:1BU:HAB	1.94	0.49
1:B:269:LEU:HG	1:B:294:ILE:HD13	1.94	0.48
1:A:466:MET:HE2	1:A:471:VAL:HG22	1.95	0.48
1:B:304:PRO:HG3	1:B:332:GLU:OE1	2.14	0.47
1:B:305:GLU:O	1:B:309:GLN:HG3	2.14	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:424:PHE:HB3	1:B:426:ILE:HG23	1.95	0.47
2:A:1:1BU:HAM	2:A:1:1BU:N1	2.28	0.47
1:B:476:GLU:OE2	1:B:476:GLU:HA	2.14	0.47
1:A:285:THR:CG2	1:A:288:GLY:HA2	2.45	0.46
1:B:261:GLU:OE2	1:B:330:SER:OG	2.25	0.46
1:B:378:GLU:HG3	1:B:441:ILE:HG12	1.98	0.46
1:B:466:MET:HE2	1:B:471:VAL:CG2	2.42	0.46
1:A:384:HIS:O	1:A:385:ARG:CB	2.49	0.46
1:A:346:LEU:N	1:A:392:ILE:O	2.48	0.45
1:B:390:ALA:O	1:B:405:PHE:CE2	2.70	0.45
1:B:426:ILE:HD13	1:B:472:LEU:HG	1.99	0.45
1:B:354:MET:O	1:B:355:GLY:C	2.60	0.45
1:A:302:MET:HG2	1:A:303:SER:N	2.32	0.44
1:B:466:MET:HA	1:B:470:GLU:OE1	2.17	0.44
1:A:378:GLU:HG3	1:A:441:ILE:HG12	1.99	0.44
1:B:324:GLN:O	1:B:338:MET:CB	2.65	0.44
1:B:339:GLU:OE1	1:B:401:LYS:NZ	2.44	0.44
1:A:280:GLU:N	1:A:296:THR:HB	2.23	0.44
1:B:311:ALA:O	1:B:315:LYS:HG3	2.17	0.44
1:A:287:ASN:C	1:A:289:THR:H	2.26	0.44
1:B:324:GLN:HG2	1:B:339:GLU:OE1	2.18	0.43
2:B:1:1BU:N1	2:B:1:1BU:CAM	2.81	0.43
1:A:311:ALA:O	1:A:315:LYS:HG3	2.19	0.43
1:A:370:ILE:O	1:A:371:ALA:C	2.61	0.43
1:B:390:ALA:O	1:B:405:PHE:HE2	2.02	0.43
1:B:487:CYS:SG	1:B:491:LEU:HB3	2.59	0.42
1:B:339:GLU:O	2:B:1:1BU:H2	2.20	0.42
1:B:364:VAL:O	1:B:367:ALA:HB3	2.20	0.42
1:B:467:VAL:O	1:B:468:ASN:C	2.63	0.42
1:A:314:MET:HE1	1:A:338:MET:SD	2.60	0.41
1:B:362:GLN:O	1:B:366:MET:HG3	2.20	0.41
1:A:366:MET:HE3	1:A:398:LEU:HD22	2.03	0.41
1:B:268:ARG:O	1:B:284:GLY:HA3	2.21	0.41
1:A:398:LEU:HA	1:A:398:LEU:HD23	1.88	0.41

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	257/286 (90%)	241 (94%)	14 (5%)	2 (1%)	16	34
1	B	256/286 (90%)	227 (89%)	27 (10%)	2 (1%)	16	34
All	All	513/572 (90%)	468 (91%)	41 (8%)	4 (1%)	16	34

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	288	GLY
1	B	385	ARG
1	A	385	ARG
1	B	259	ALA

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	219/245 (89%)	202 (92%)	17 (8%)	11	26
1	B	224/245 (91%)	203 (91%)	21 (9%)	8	18
All	All	443/490 (90%)	405 (91%)	38 (9%)	10	22

All (38) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	266	SER
1	A	285	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	291	ARG
1	A	338	MET
1	A	339	GLU
1	A	351	LYS
1	A	353	GLU
1	A	388	ARG
1	A	399	VAL
1	A	426	ILE
1	A	443	SER
1	A	451	LEU
1	A	470	GLU
1	A	475	VAL
1	A	476	GLU
1	A	526	GLN
1	A	528	GLN
1	B	268	ARG
1	B	283	MET
1	B	292	VAL
1	B	296	THR
1	B	303	SER
1	B	305	GLU
1	B	318	ARG
1	B	323	VAL
1	B	338	MET
1	B	343	LYS
1	B	353	GLU
1	B	356	LYS
1	B	399	VAL
1	B	426	ILE
1	B	458	LYS
1	B	469	ARG
1	B	470	GLU
1	B	487	CYS
1	B	523	THR
1	B	526	GLN
1	B	528	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	287	ASN
1	A	309	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	397	ASN
1	B	324	GLN
1	B	526	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

2 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	1BU	B	1	-	42,42,42	1.87	9 (21%)	59,61,61	2.32	15 (25%)
2	1BU	A	1	-	42,42,42	1.91	11 (26%)	59,61,61	2.42	16 (27%)

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	1BU	B	1	-	-	2/22/22/22	0/5/5/5

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	1BU	A	1	-	-	2/22/22/22	0/5/5/5

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1	1BU	NBK-NAV	-6.67	1.24	1.39
2	B	1	1BU	NBK-NAV	-6.40	1.25	1.39
2	A	1	1BU	CBE-NBK	-4.31	1.35	1.43
2	A	1	1BU	CBG-NAX	-4.19	1.33	1.39
2	B	1	1BU	CBE-NBK	-4.01	1.35	1.43
2	B	1	1BU	CBG-NAX	-3.54	1.34	1.39
2	B	1	1BU	CAR-CBF	-3.23	1.34	1.39
2	A	1	1BU	CAR-CBG	-3.11	1.33	1.37
2	B	1	1BU	C6-C5	-2.77	1.41	1.44
2	B	1	1BU	CBC-NAW	-2.77	1.36	1.41
2	B	1	1BU	C6-N1	2.57	1.37	1.34
2	A	1	1BU	C6-C5	-2.49	1.41	1.44
2	A	1	1BU	CBC-NAW	-2.47	1.36	1.41
2	A	1	1BU	C6-N1	2.47	1.37	1.34
2	A	1	1BU	CAR-CBF	-2.41	1.35	1.39
2	A	1	1BU	CAZ-NAX	-2.25	1.34	1.39
2	B	1	1BU	CBL-CBF	2.22	1.56	1.52
2	A	1	1BU	CAA-CBA	2.12	1.57	1.51
2	A	1	1BU	CBD-NAY	-2.06	1.36	1.40
2	B	1	1BU	CAR-CBG	-2.04	1.34	1.37

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1	1BU	C2-N1-C6	9.10	123.67	116.60
2	B	1	1BU	C2-N1-C6	7.08	122.10	116.60
2	A	1	1BU	C5-C6-N1	-6.71	116.38	121.35
2	B	1	1BU	CBF-NAV-NBK	5.78	109.11	104.27
2	B	1	1BU	C5-C6-N1	-5.77	117.08	121.35
2	A	1	1BU	N3-C2-N1	-5.67	120.98	128.67
2	B	1	1BU	N3-C2-N1	-5.51	121.19	128.67
2	A	1	1BU	C6-C5-C4	4.76	118.67	115.86
2	B	1	1BU	C6-C5-C4	4.74	118.66	115.86
2	B	1	1BU	C2-N3-C4	4.51	120.56	115.43
2	B	1	1BU	CAR-CBG-NAX	-4.20	125.73	132.60
2	A	1	1BU	C2-N3-C4	4.14	120.14	115.43
2	B	1	1BU	NAX-CBG-NBK	4.08	127.00	120.11

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1	1BU	CAR-CBG-NAX	-3.92	126.19	132.60
2	A	1	1BU	CAS-C5-C6	-3.70	121.83	124.84
2	B	1	1BU	CAS-C5-C6	-3.60	121.91	124.84
2	A	1	1BU	NAX-CBG-NBK	3.50	126.03	120.11
2	A	1	1BU	CBF-NAV-NBK	3.40	107.12	104.27
2	B	1	1BU	CAR-CBF-NAV	-3.25	108.02	111.86
2	A	1	1BU	CBE-NBK-CBG	-3.10	126.74	129.78
2	A	1	1BU	C5-C6-NAY	2.77	122.57	119.77
2	A	1	1BU	CBE-NBK-NAV	2.58	122.42	118.67
2	A	1	1BU	C5-C4-N3	-2.53	120.14	122.82
2	A	1	1BU	CBL-CBF-NAV	2.47	123.69	120.42
2	B	1	1BU	NAY-C6-N1	2.45	121.47	118.71
2	B	1	1BU	CBL-CBF-NAV	2.36	123.54	120.42
2	B	1	1BU	CBG-NBK-NAV	-2.33	109.80	111.82
2	B	1	1BU	C5-C4-N3	-2.28	120.40	122.82
2	A	1	1BU	CAP-C4-C5	2.19	121.49	119.13
2	B	1	1BU	CAQ-CBE-NBK	2.12	122.34	119.27
2	A	1	1BU	NAY-C6-N1	2.08	121.05	118.71

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1	1BU	C5-C6-NAY-CBD
2	A	1	1BU	N1-C6-NAY-CBD
2	B	1	1BU	N1-C6-NAY-CBD
2	B	1	1BU	C5-C6-NAY-CBD

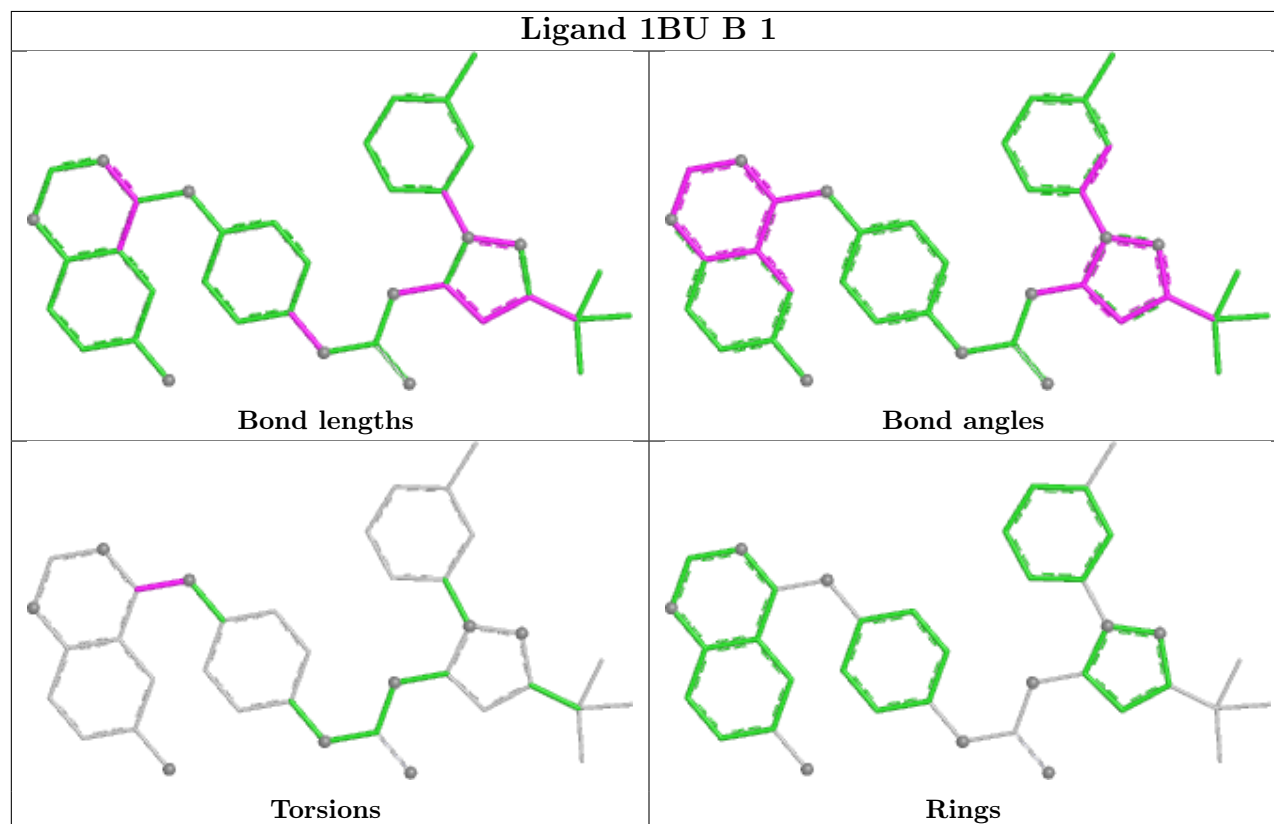
There are no ring outliers.

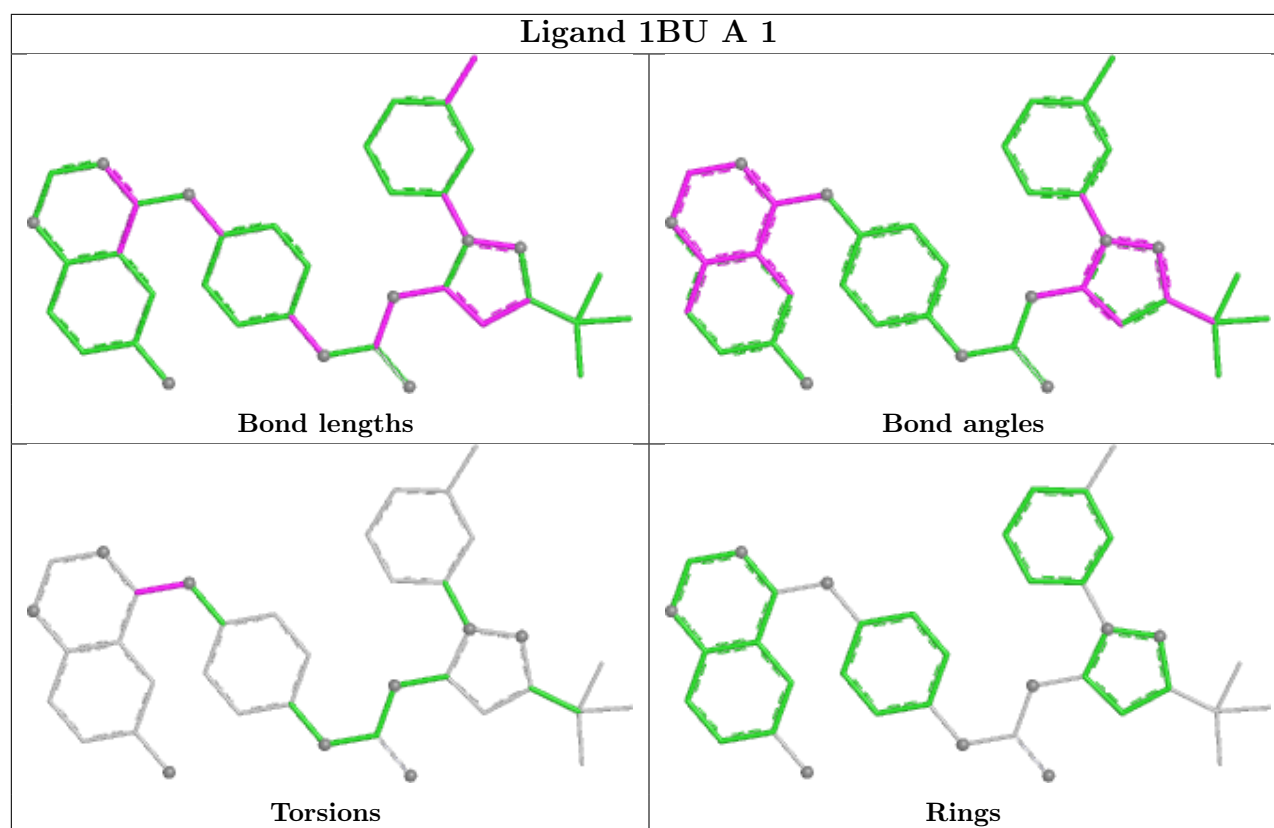
2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	1	1BU	3	0
2	A	1	1BU	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 [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, 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	261/286 (91%)	0.23	6 (2%) 61 55	2, 14, 49, 61	0
1	B	260/286 (90%)	0.16	10 (3%) 44 38	3, 13, 37, 48	0
All	All	521/572 (91%)	0.19	16 (3%) 51 45	2, 14, 46, 61	0

All (16) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	267	LEU	3.9
1	A	278	PHE	3.4
1	B	473	ASP	3.2
1	A	424	PHE	2.8
1	B	277	CYS	2.6
1	B	300	GLY	2.4
1	A	332	GLU	2.4
1	B	331	GLU	2.4
1	A	268	ARG	2.4
1	A	264	ARG	2.3
1	B	258	ASP	2.2
1	B	425	PRO	2.1
1	B	505	GLU	2.1
1	B	276	GLY	2.1
1	B	265	GLU	2.1
1	B	424	PHE	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](#)

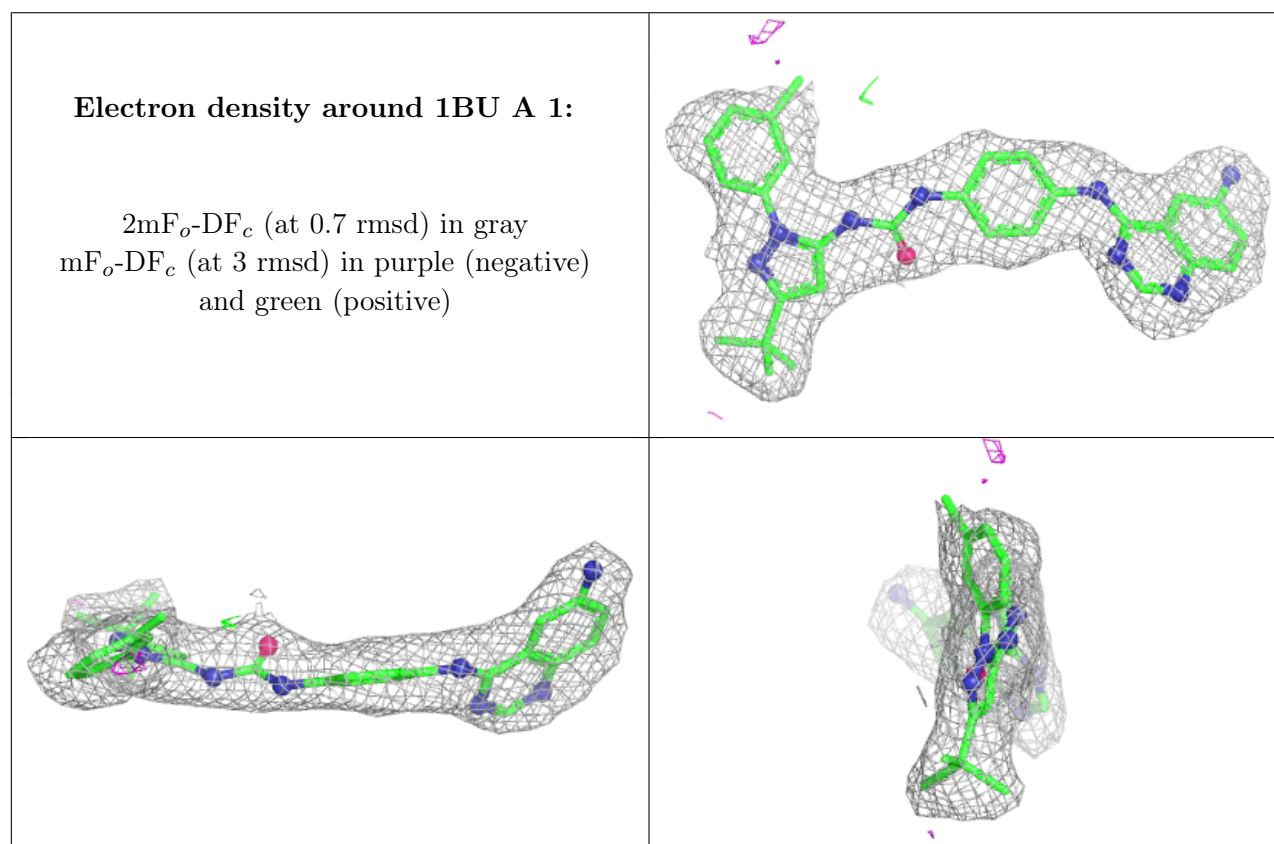
There are no oligosaccharides in this entry.

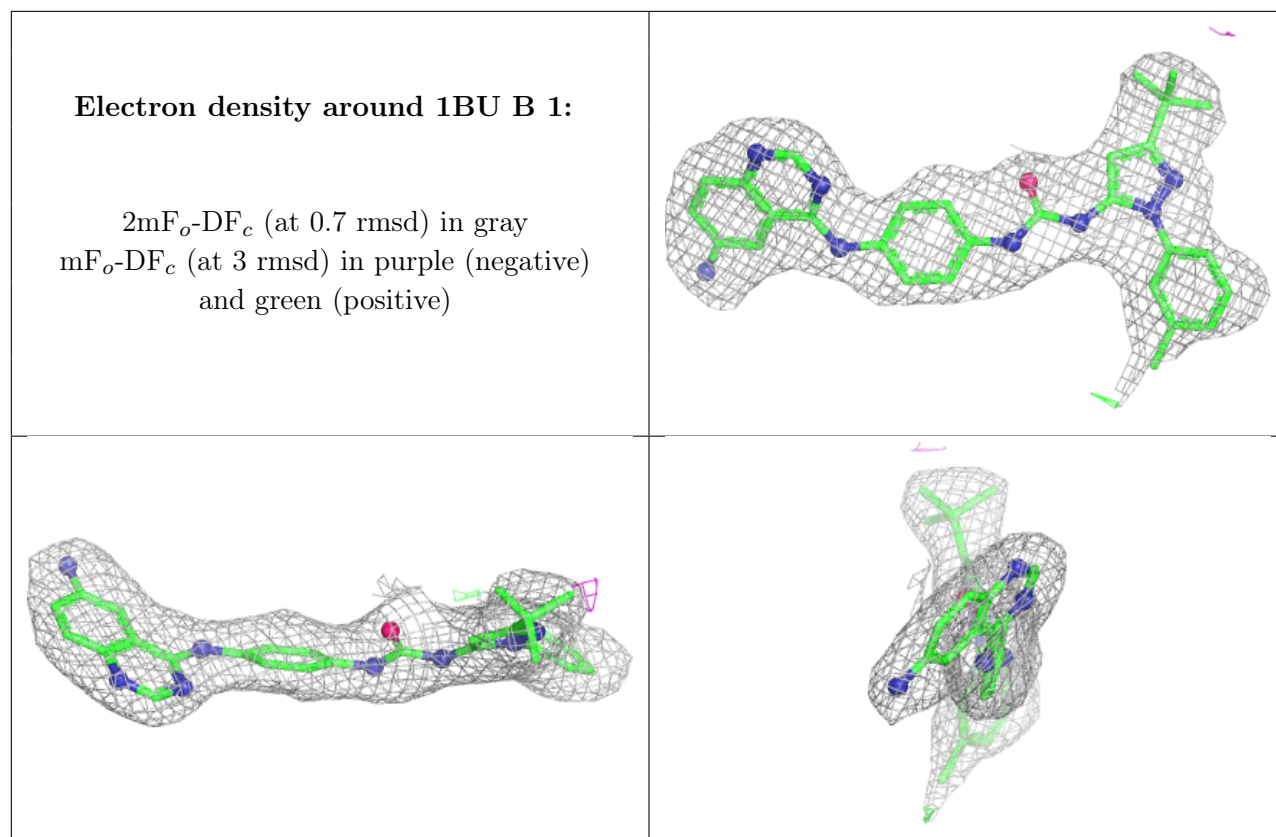
6.4 Ligands [i](#)

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, 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	1BU	A	1	38/38	0.92	0.10	13,21,28,28	0
2	1BU	B	1	38/38	0.93	0.09	17,23,25,26	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.