



# Full wwPDB X-ray Structure Validation Report ⓘ

May 22, 2020 – 04:24 pm BST

PDB ID : 4MXY  
Title : Src M314L T338M double mutant bound to kinase inhibitor bosutinib  
Authors : Levinson, N.M.; Boxer, S.G.  
Deposited on : 2013-09-26  
Resolution : 2.58 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.

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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

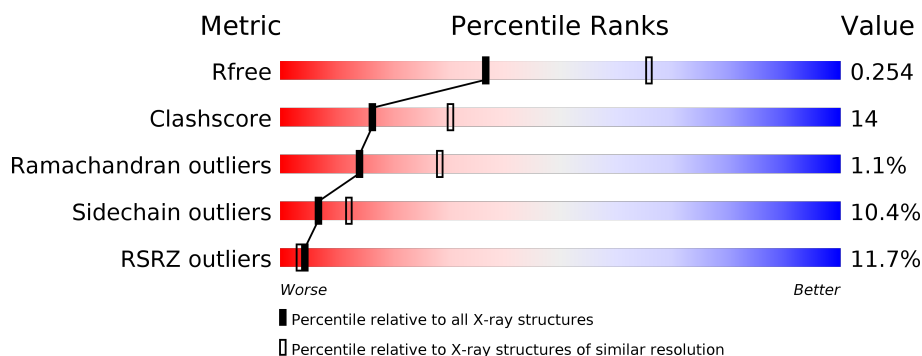
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.58 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	3676 (2.60-2.56)
Clashscore	141614	4049 (2.60-2.56)
Ramachandran outliers	138981	3979 (2.60-2.56)
Sidechain outliers	138945	3979 (2.60-2.56)
RSRZ outliers	127900	3614 (2.60-2.56)

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	286	<div> <div>14%</div> <div> <div></div> <div>59%</div> <div>29%</div> <div>5%</div> <div>7%</div> </div> </div>
1	B	286	<div> <div>8%</div> <div> <div></div> <div>65%</div> <div>25%</div> <div>• 8%</div> </div> </div>

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 4410 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.

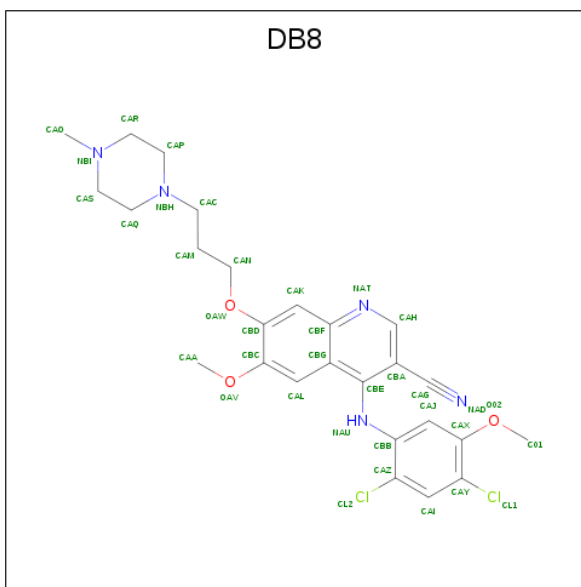
- Molecule 1 is a protein called Proto-oncogene tyrosine-protein kinase Src.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	266	Total	C	N	O	S	0	0	0
			2145	1379	358	392	16			
1	B	264	Total	C	N	O	S	0	0	0
			2127	1368	355	388	16			

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	248	GLY	-	EXPRESSION TAG	UNP P12931
A	249	HIS	-	EXPRESSION TAG	UNP P12931
A	250	MET	-	EXPRESSION TAG	UNP P12931
A	314	LEU	MET	ENGINEERED MUTATION	UNP P12931
A	338	MET	THR	ENGINEERED MUTATION	UNP P12931
B	248	GLY	-	EXPRESSION TAG	UNP P12931
B	249	HIS	-	EXPRESSION TAG	UNP P12931
B	250	MET	-	EXPRESSION TAG	UNP P12931
B	314	LEU	MET	ENGINEERED MUTATION	UNP P12931
B	338	MET	THR	ENGINEERED MUTATION	UNP P12931

- Molecule 2 is 4-[(2,4-dichloro-5-methoxyphenyl)amino]-6-methoxy-7-[3-(4-methylpiperazin-1-yl)propoxy]quinoline-3-carbonitrile (three-letter code: DB8) (formula: C<sub>26</sub>H<sub>29</sub>Cl<sub>2</sub>N<sub>5</sub>O<sub>3</sub>).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total 36	C 26	Cl 2	N 5	O 3	0	0
2	B	1	Total 36	C 26	Cl 2	N 5	O 3	0	0

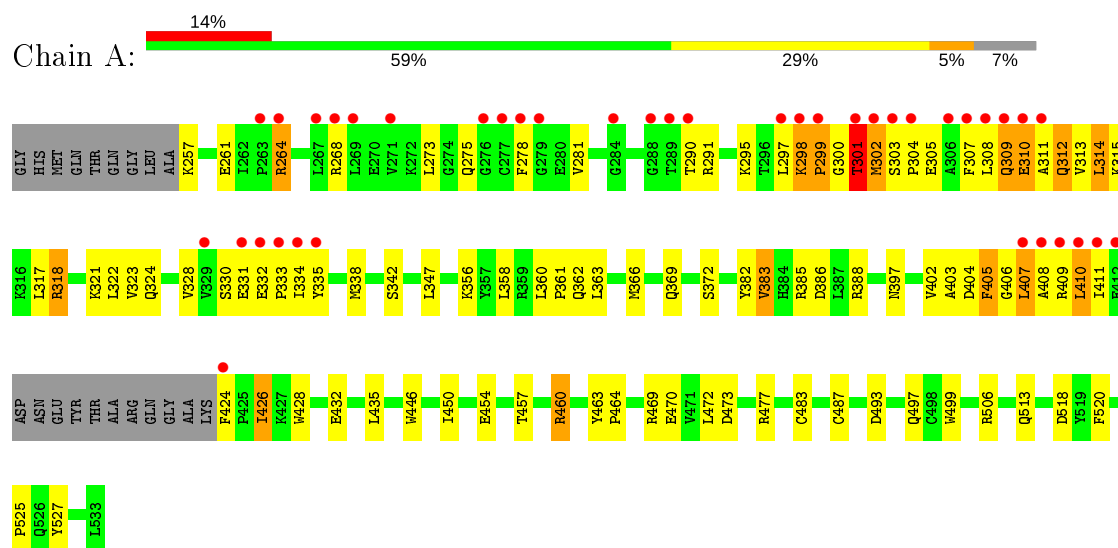
- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	39	Total O 39 39	0	0
3	B	27	Total O 27 27	0	0

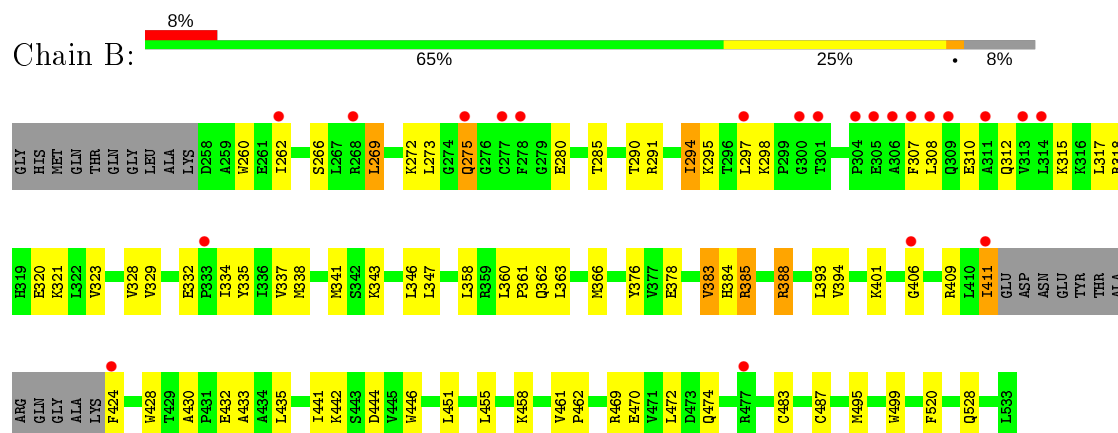
### 3 Residue-property plots [i](#)

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: 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, $\alpha$ , $\beta$ , $\gamma$	41.87Å 63.05Å 73.96Å 79.03° 87.82° 89.91°	Depositor
Resolution (Å)	61.89 – 2.58 61.89 – 2.58	Depositor EDS
% Data completeness (in resolution range)	94.1 (61.89-2.58) 94.1 (61.89-2.58)	Depositor EDS
$R_{merge}$	0.20	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.80 (at 2.58Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7_650)	Depositor
R, $R_{free}$	0.208 , 0.266 0.196 , 0.254	Depositor DCC
$R_{free}$ test set	1108 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	31.7	Xtriage
Anisotropy	0.519	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 40.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.038 for h,-k,-l	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	4410	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.43% 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: DB8

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	0.44	0/2197	0.58	0/2974
1	B	0.43	0/2179	0.54	0/2951
All	All	0.44	0/4376	0.56	0/5925

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.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	298	LYS	Peptide

### 5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2145	0	2139	66	0
1	B	2127	0	2120	56	0
2	A	36	0	29	5	0
2	B	36	0	29	7	0
3	A	39	0	0	2	0
3	B	27	0	0	0	0
All	All	4410	0	4317	124	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 14.

All (124) 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:385:ARG:HD2	1:A:409:ARG:HD3	1.45	0.95
1:A:383:VAL:HG12	1:A:411:ILE:HG12	1.62	0.81
1:A:309:GLN:HA	1:A:312:GLN:HG2	1.64	0.79
1:B:363:LEU:HD23	1:B:366:MET:CE	2.13	0.79
1:A:435:LEU:HD21	1:A:472:LEU:HD21	1.67	0.76
1:B:363:LEU:HD23	1:B:366:MET:HE3	1.69	0.74
1:A:323:VAL:HG12	1:A:338:MET:HE2	1.72	0.71
1:B:383:VAL:HG13	1:B:409:ARG:HG3	1.73	0.71
1:B:295:LYS:HB2	2:B:601:DB8:O02	1.91	0.69
1:A:257:LYS:HD2	1:A:261:GLU:HG3	1.74	0.69
1:B:269:LEU:HD22	1:B:294:ILE:HD12	1.75	0.67
1:B:320:GLU:O	1:B:401:LYS:HE3	1.95	0.66
1:B:385:ARG:HD2	1:B:409:ARG:HG2	1.79	0.65
1:A:332:GLU:HA	1:A:333:PRO:C	2.19	0.63
1:B:260:TRP:CD1	1:B:315:LYS:HE2	2.33	0.62
1:B:432:GLU:HG2	1:B:433:ALA:N	2.13	0.62
1:B:346:LEU:HD21	1:B:455:LEU:HD21	1.82	0.61
1:A:388:ARG:HB3	1:A:428:TRP:CD1	2.36	0.61
1:A:264:ARG:HG3	1:A:264:ARG:HH11	1.65	0.60
1:A:332:GLU:HG3	1:A:333:PRO:HA	1.83	0.60
1:B:409:ARG:HH21	1:B:411:ILE:HG23	1.67	0.60
1:A:323:VAL:HG12	1:A:338:MET:CE	2.32	0.59
1:B:343:LYS:HB2	1:B:394:VAL:HB	1.85	0.59
1:A:310:GLU:O	1:A:310:GLU:HG3	2.04	0.58
1:A:342:SER:O	2:A:601:DB8:HAMA	2.03	0.58
1:A:295:LYS:HB2	2:A:601:DB8:O02	2.05	0.57
1:A:322:LEU:HD22	1:A:402:VAL:HB	1.88	0.56
1:A:318:ARG:HH12	1:A:324:GLN:NE2	2.04	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:297:LEU:HB2	1:B:307:PHE:CE2	2.41	0.55
1:B:384:HIS:O	1:B:385:ARG:HB2	2.07	0.55
1:A:383:VAL:HG22	1:A:385:ARG:HG3	1.89	0.55
1:A:310:GLU:OE2	2:A:601:DB8:CL1	2.62	0.55
1:B:275:GLN:HB2	1:B:280:GLU:HG2	1.89	0.55
1:A:323:VAL:HG21	1:A:403:ALA:HB2	1.89	0.54
1:A:460:ARG:O	3:A:706:HOH:O	2.18	0.54
1:B:308:LEU:HB3	1:B:312:GLN:HE21	1.73	0.54
1:B:435:LEU:HD21	1:B:472:LEU:HD21	1.90	0.54
1:B:262:ILE:HD11	1:B:337:VAL:HG21	1.91	0.52
1:B:363:LEU:HA	1:B:366:MET:HE3	1.92	0.52
1:B:297:LEU:HD13	1:B:307:PHE:CD1	2.44	0.52
1:A:363:LEU:HD23	1:A:366:MET:CE	2.40	0.52
1:A:383:VAL:CG1	1:A:411:ILE:HG12	2.35	0.52
1:A:369:GLN:O	1:A:372:SER:HB3	2.10	0.51
1:A:297:LEU:HG	1:A:299:PRO:O	2.11	0.51
1:B:358:LEU:HD13	1:B:366:MET:HE1	1.93	0.51
1:A:386:ASP:HB2	1:A:407:LEU:HD12	1.91	0.51
1:A:323:VAL:CG1	1:A:338:MET:HE2	2.40	0.50
2:A:601:DB8:CAG	2:A:601:DB8:CAJ	2.89	0.50
1:A:360:LEU:HB3	1:A:361:PRO:HD3	1.94	0.50
1:B:273:LEU:HD13	2:B:601:DB8:CBD	2.42	0.50
1:B:383:VAL:HG12	1:B:411:ILE:HG12	1.93	0.50
1:B:362:GLN:O	1:B:366:MET:HG3	2.11	0.49
2:A:601:DB8:CAG	2:A:601:DB8:CBB	2.91	0.49
1:B:317:LEU:HB3	1:B:376:TYR:HE2	1.78	0.48
1:A:309:GLN:HA	1:A:312:GLN:CG	2.38	0.48
1:B:338:MET:CG	2:B:601:DB8:H01B	2.44	0.48
1:A:428:TRP:HE1	1:A:454:GLU:CD	2.17	0.48
1:A:460:ARG:NH2	3:A:713:HOH:O	2.47	0.47
1:B:358:LEU:HD13	1:B:366:MET:CE	2.44	0.47
1:A:273:LEU:HB2	1:A:281:VAL:HG12	1.96	0.47
1:A:264:ARG:HH11	1:A:264:ARG:CG	2.28	0.47
1:B:388:ARG:HB3	1:B:428:TRP:CD1	2.50	0.47
1:A:297:LEU:HD12	1:A:301:THR:OG1	2.15	0.47
1:A:520:PHE:O	1:A:525:PRO:HA	2.14	0.47
1:B:323:VAL:HG21	1:B:393:LEU:HD12	1.97	0.47
1:A:311:ALA:O	1:A:315:LYS:HG3	2.15	0.46
1:A:302:MET:HE2	1:A:303:SER:H	1.80	0.46
1:B:338:MET:HG3	2:B:601:DB8:H01B	1.96	0.46
1:A:330:SER:HA	1:A:334:ILE:HG12	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:601:DB8:CAG	2:B:601:DB8:CBB	2.94	0.46
1:A:426:ILE:HD13	1:A:472:LEU:HD13	1.98	0.46
1:A:404:ASP:C	1:A:406:GLY:H	2.19	0.45
1:A:463:TYR:N	1:A:464:PRO:HD3	2.32	0.45
1:A:483:CYS:SG	1:A:487:CYS:O	2.75	0.45
1:A:313:VAL:HG12	1:A:317:LEU:HD12	1.99	0.45
1:B:269:LEU:HD23	1:B:269:LEU:N	2.31	0.45
1:A:310:GLU:O	1:A:314:LEU:HB2	2.17	0.44
1:A:382:TYR:CE2	1:A:410:LEU:HD22	2.52	0.44
1:A:473:ASP:O	1:A:477:ARG:HG3	2.17	0.44
1:A:385:ARG:CD	1:A:409:ARG:HD3	2.33	0.44
1:B:341:MET:O	2:B:601:DB8:HAK	2.18	0.44
1:B:451:LEU:HD12	1:B:451:LEU:O	2.17	0.44
1:B:297:LEU:HD22	1:B:307:PHE:CD2	2.53	0.44
1:A:457:THR:OG1	1:A:460:ARG:HB2	2.18	0.44
1:B:361:PRO:HA	1:B:520:PHE:CE2	2.54	0.43
1:B:383:VAL:HG22	1:B:385:ARG:HG3	1.99	0.43
1:A:432:GLU:OE2	1:A:506:ARG:NH2	2.52	0.43
1:A:385:ARG:HD3	1:A:407:LEU:O	2.19	0.43
1:B:308:LEU:HB3	1:B:312:GLN:NE2	2.34	0.43
1:B:385:ARG:HB3	1:B:424:PHE:HE2	1.84	0.43
1:B:378:GLU:HA	1:B:441:ILE:HD13	2.00	0.43
1:B:321:LYS:HA	1:B:401:LYS:HG3	2.01	0.42
1:B:441:ILE:O	1:B:444:ASP:HB2	2.19	0.42
1:A:321:LYS:HE3	1:A:369:GLN:HG2	2.02	0.42
1:A:372:SER:HA	1:A:513:GLN:NE2	2.35	0.42
1:A:450:ILE:HD13	1:A:499:TRP:CZ2	2.54	0.42
1:A:323:VAL:CG2	1:A:403:ALA:HB2	2.49	0.42
1:A:518:ASP:CG	1:B:461:VAL:HG23	2.39	0.42
1:B:329:VAL:HB	1:B:335:TYR:HB2	2.02	0.42
1:B:442:LYS:HA	1:B:442:LYS:HD3	1.70	0.42
1:A:309:GLN:O	1:A:313:VAL:HG23	2.20	0.42
1:B:430:ALA:HB2	1:B:446:TRP:HB3	2.00	0.42
1:B:446:TRP:CD1	1:B:446:TRP:C	2.92	0.42
1:A:446:TRP:CE3	1:A:499:TRP:HA	2.55	0.42
1:B:295:LYS:HB2	2:B:601:DB8:C01	2.49	0.42
1:A:300:GLY:O	1:A:302:MET:N	2.53	0.42
1:B:269:LEU:CD2	1:B:294:ILE:HD12	2.47	0.42
1:A:405:PHE:HB3	1:A:408:ALA:HB3	2.02	0.41
1:A:435:LEU:CD2	1:A:472:LEU:HD21	2.43	0.41
1:B:461:VAL:HA	1:B:462:PRO:HD3	1.89	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:446:TRP:CZ3	1:A:499:TRP:O	2.73	0.41
1:B:358:LEU:O	1:B:458:LYS:HE2	2.20	0.41
1:A:308:LEU:HD23	1:A:308:LEU:HA	1.79	0.41
1:B:483:CYS:SG	1:B:487:CYS:O	2.78	0.41
1:B:495:MET:HB3	1:B:499:TRP:CH2	2.56	0.41
1:A:358:LEU:HD23	1:A:358:LEU:HA	1.85	0.41
1:A:264:ARG:NH1	1:A:264:ARG:CG	2.84	0.41
1:B:360:LEU:HD12	1:B:360:LEU:HA	1.91	0.41
1:B:310:GLU:HB2	1:B:406:GLY:HA2	2.03	0.41
1:A:493:ASP:O	1:A:497:GLN:HG3	2.20	0.41
1:A:264:ARG:HG3	1:A:335:TYR:HE2	1.86	0.40
1:B:260:TRP:HB3	1:B:328:VAL:HG23	2.01	0.40
1:B:308:LEU:HD21	1:B:334:ILE:HG21	2.02	0.40
1:A:362:GLN:O	1:A:366:MET:HG3	2.21	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	262/286 (92%)	240 (92%)	17 (6%)	5 (2%)	8	14
1	B	260/286 (91%)	247 (95%)	12 (5%)	1 (0%)	34	55
All	All	522/572 (91%)	487 (93%)	29 (6%)	6 (1%)	14	28

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	299	PRO
1	A	301	THR
1	A	304	PRO
1	B	385	ARG

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Mol	Chain	Res	Type
1	A	331	GLU
1	A	405	PHE

### 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	231/245 (94%)	202 (87%)	29 (13%)	4	8
1	B	229/245 (94%)	210 (92%)	19 (8%)	11	21
All	All	460/490 (94%)	412 (90%)	48 (10%)	7	12

All (48) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	264	ARG
1	A	268	ARG
1	A	275	GLN
1	A	278	PHE
1	A	290	THR
1	A	291	ARG
1	A	298	LYS
1	A	301	THR
1	A	302	MET
1	A	305	GLU
1	A	307	PHE
1	A	309	GLN
1	A	310	GLU
1	A	312	GLN
1	A	314	LEU
1	A	318	ARG
1	A	328	VAL
1	A	347	LEU
1	A	356	LYS
1	A	383	VAL
1	A	397	ASN

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Mol	Chain	Res	Type
1	A	407	LEU
1	A	410	LEU
1	A	424	PHE
1	A	426	ILE
1	A	460	ARG
1	A	469	ARG
1	A	470	GLU
1	A	527	TYR
1	B	266	SER
1	B	269	LEU
1	B	272	LYS
1	B	275	GLN
1	B	285	THR
1	B	290	THR
1	B	291	ARG
1	B	294	ILE
1	B	298	LYS
1	B	318	ARG
1	B	332	GLU
1	B	347	LEU
1	B	383	VAL
1	B	388	ARG
1	B	411	ILE
1	B	469	ARG
1	B	470	GLU
1	B	474	GLN
1	B	528	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	275	GLN
1	A	312	GLN
1	A	324	GLN
1	A	391	ASN
1	A	397	ASN
1	A	513	GLN
1	B	275	GLN
1	B	312	GLN
1	B	391	ASN
1	B	397	ASN
1	B	474	GLN

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Mol	Chain	Res	Type
1	B	513	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 carbohydrates 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	DB8	B	601	-	38,39,39	4.48	19 (50%)	51,54,54	2.47	17 (33%)
2	DB8	A	601	-	38,39,39	4.24	19 (50%)	51,54,54	2.50	17 (33%)

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	DB8	B	601	-	-	9/17/27/27	0/4/4/4
2	DB8	A	601	-	-	9/17/27/27	0/4/4/4

All (38) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	601	DB8	CAH-CBA	8.49	1.51	1.40
2	B	601	DB8	CAK-CBD	8.32	1.51	1.36
2	B	601	DB8	CAH-NAT	8.16	1.45	1.31
2	B	601	DB8	CAL-CBC	7.80	1.50	1.36
2	A	601	DB8	CAH-CBA	7.77	1.50	1.40
2	A	601	DB8	CAL-CBC	7.69	1.50	1.36
2	A	601	DB8	CAK-CBD	7.67	1.50	1.36
2	B	601	DB8	CAI-CAZ	7.30	1.50	1.38
2	A	601	DB8	CAJ-CBB	7.26	1.50	1.39
2	B	601	DB8	CAI-CAY	7.18	1.50	1.38
2	B	601	DB8	CAJ-CBB	7.16	1.50	1.39
2	B	601	DB8	CAK-CBF	7.02	1.52	1.41
2	A	601	DB8	CAH-NAT	6.95	1.43	1.31
2	A	601	DB8	CAK-CBF	6.67	1.52	1.41
2	A	601	DB8	CAI-CAZ	6.65	1.49	1.38
2	B	601	DB8	CAX-CAY	6.57	1.51	1.39
2	A	601	DB8	CAX-CAY	6.57	1.51	1.39
2	B	601	DB8	CBE-CBG	6.41	1.54	1.43
2	B	601	DB8	CBG-CBF	6.36	1.53	1.42
2	A	601	DB8	CAI-CAY	6.35	1.48	1.38
2	A	601	DB8	CBG-CBF	6.15	1.52	1.42
2	B	601	DB8	CAJ-CAX	6.11	1.49	1.38
2	A	601	DB8	CAJ-CAX	6.08	1.49	1.38
2	A	601	DB8	CBE-CBG	6.08	1.54	1.43
2	B	601	DB8	CBB-CAZ	5.47	1.52	1.39
2	A	601	DB8	CBB-CAZ	5.04	1.51	1.39
2	B	601	DB8	CAL-CBG	4.37	1.50	1.42
2	A	601	DB8	CAL-CBG	4.36	1.50	1.42
2	A	601	DB8	CBD-CBC	4.36	1.50	1.40
2	B	601	DB8	CBF-NAT	4.36	1.45	1.37
2	B	601	DB8	CBD-CBC	4.11	1.49	1.40
2	A	601	DB8	CBA-CAG	3.94	1.50	1.44
2	B	601	DB8	CBA-CAG	3.88	1.50	1.44
2	A	601	DB8	CBF-NAT	3.82	1.44	1.37
2	A	601	DB8	CBE-NAU	3.06	1.48	1.38
2	B	601	DB8	CBE-NAU	3.00	1.48	1.38
2	B	601	DB8	CBB-NAU	2.33	1.46	1.39
2	A	601	DB8	CBB-NAU	2.17	1.45	1.39

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	601	DB8	CAO-NBI-CAS	6.97	121.09	110.66
2	A	601	DB8	CAO-NBI-CAS	6.96	121.08	110.66
2	A	601	DB8	OAV-CBC-CAL	-6.62	116.68	125.24
2	B	601	DB8	O02-CAX-CAY	5.83	122.27	116.60
2	A	601	DB8	O02-CAX-CAY	5.37	121.82	116.60
2	A	601	DB8	OAV-CBC-CBD	5.01	122.39	115.41
2	B	601	DB8	OAV-CBC-CAL	-4.94	118.86	125.24
2	B	601	DB8	CBA-CAH-NAT	-4.88	122.05	125.68
2	A	601	DB8	CAC-NBH-CAP	4.61	123.02	111.23
2	B	601	DB8	CAC-NBH-CAP	4.41	122.52	111.23
2	B	601	DB8	O02-CAX-CAJ	-4.36	116.62	124.12
2	A	601	DB8	OAW-CBD-CAK	-4.31	117.90	125.19
2	A	601	DB8	CBA-CAH-NAT	-4.14	122.60	125.68
2	B	601	DB8	CAH-NAT-CBF	3.81	121.50	116.91
2	B	601	DB8	OAV-CBC-CBD	3.80	120.70	115.41
2	A	601	DB8	O02-CAX-CAJ	-3.72	117.72	124.12
2	A	601	DB8	CAO-NBI-CAR	3.64	116.11	110.66
2	B	601	DB8	CAO-NBI-CAR	3.58	116.01	110.66
2	A	601	DB8	CBB-CAZ-CL2	3.37	123.37	119.54
2	B	601	DB8	CAL-CBG-CBE	-3.36	119.09	123.22
2	B	601	DB8	OAW-CBD-CAK	-3.26	119.67	125.19
2	A	601	DB8	CAH-NAT-CBF	3.23	120.81	116.91
2	B	601	DB8	CAK-CBF-NAT	3.19	121.60	117.97
2	A	601	DB8	CAL-CBG-CBE	-3.12	119.38	123.22
2	B	601	DB8	CBB-CAZ-CL2	2.86	122.79	119.54
2	A	601	DB8	OAW-CBD-CBC	2.85	121.61	115.73
2	B	601	DB8	CBG-CBF-NAT	-2.55	120.12	122.83
2	A	601	DB8	CAX-CAY-CL1	2.43	122.29	119.43
2	B	601	DB8	CAJ-CBB-NAU	-2.21	116.48	121.05
2	B	601	DB8	CAS-NBI-CAR	2.19	112.59	109.52
2	B	601	DB8	CAI-CAZ-CBB	-2.10	120.00	121.72
2	A	601	DB8	CBG-CBF-NAT	-2.05	120.65	122.83
2	A	601	DB8	CAI-CAZ-CBB	-2.01	120.07	121.72
2	A	601	DB8	CBE-CBG-CBF	2.01	120.23	117.30

There are no chirality outliers.

All (18) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	601	DB8	CAM-CAC-NBH-CAQ
2	A	601	DB8	CAC-CAM-CAN-OAW
2	B	601	DB8	NBH-CAC-CAM-CAN
2	A	601	DB8	CAM-CAC-NBH-CAP

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Mol	Chain	Res	Type	Atoms
2	B	601	DB8	CAY-CAX-O02-C01
2	A	601	DB8	CAY-CAX-O02-C01
2	B	601	DB8	CAM-CAC-NBH-CAQ
2	B	601	DB8	CAM-CAC-NBH-CAP
2	A	601	DB8	CBA-CBE-NAU-CBB
2	A	601	DB8	CAJ-CAX-O02-C01
2	B	601	DB8	CBA-CBE-NAU-CBB
2	B	601	DB8	CAJ-CAX-O02-C01
2	B	601	DB8	CAZ-CBB-NAU-CBE
2	A	601	DB8	CAZ-CBB-NAU-CBE
2	B	601	DB8	CAJ-CBB-NAU-CBE
2	A	601	DB8	CAJ-CBB-NAU-CBE
2	B	601	DB8	CBD-CBC-OAV-CAA
2	A	601	DB8	CAM-CAN-OAW-CBD

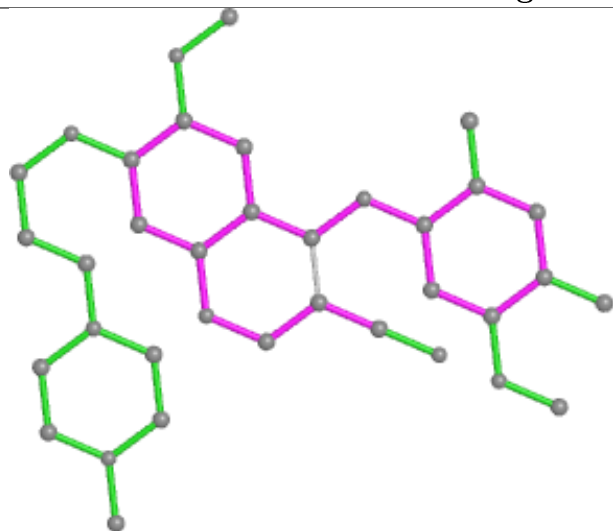
There are no ring outliers.

2 monomers are involved in 12 short contacts:

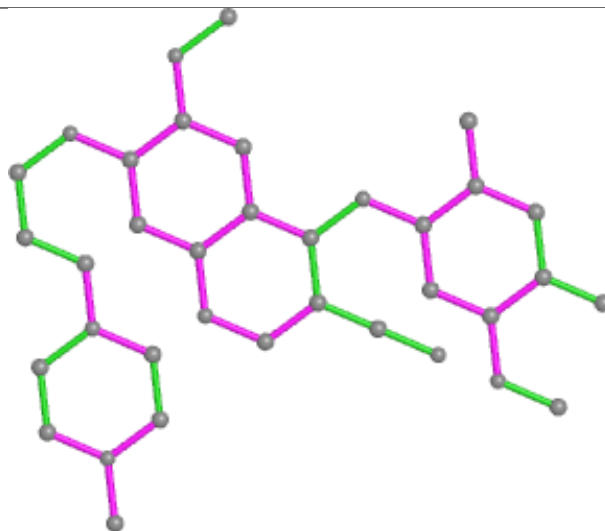
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	601	DB8	7	0
2	A	601	DB8	5	0

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.

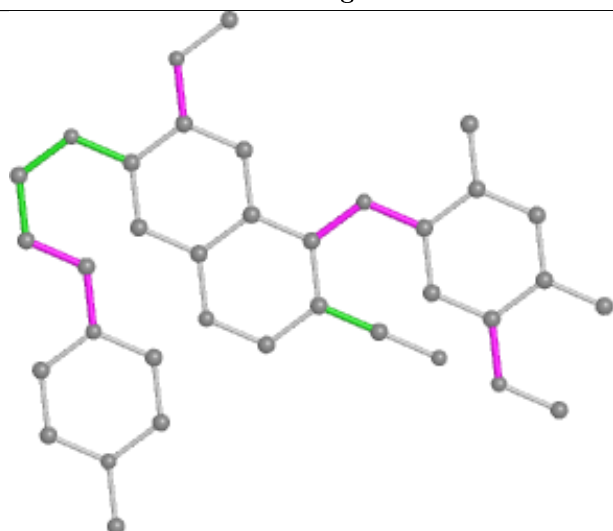
## Ligand DB8 B 601



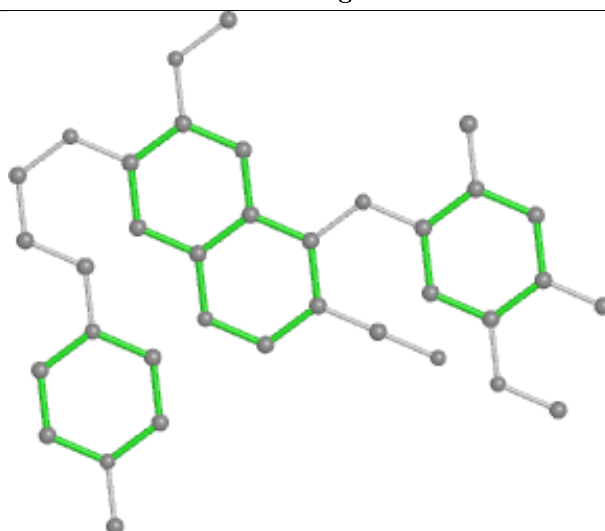
Bond lengths



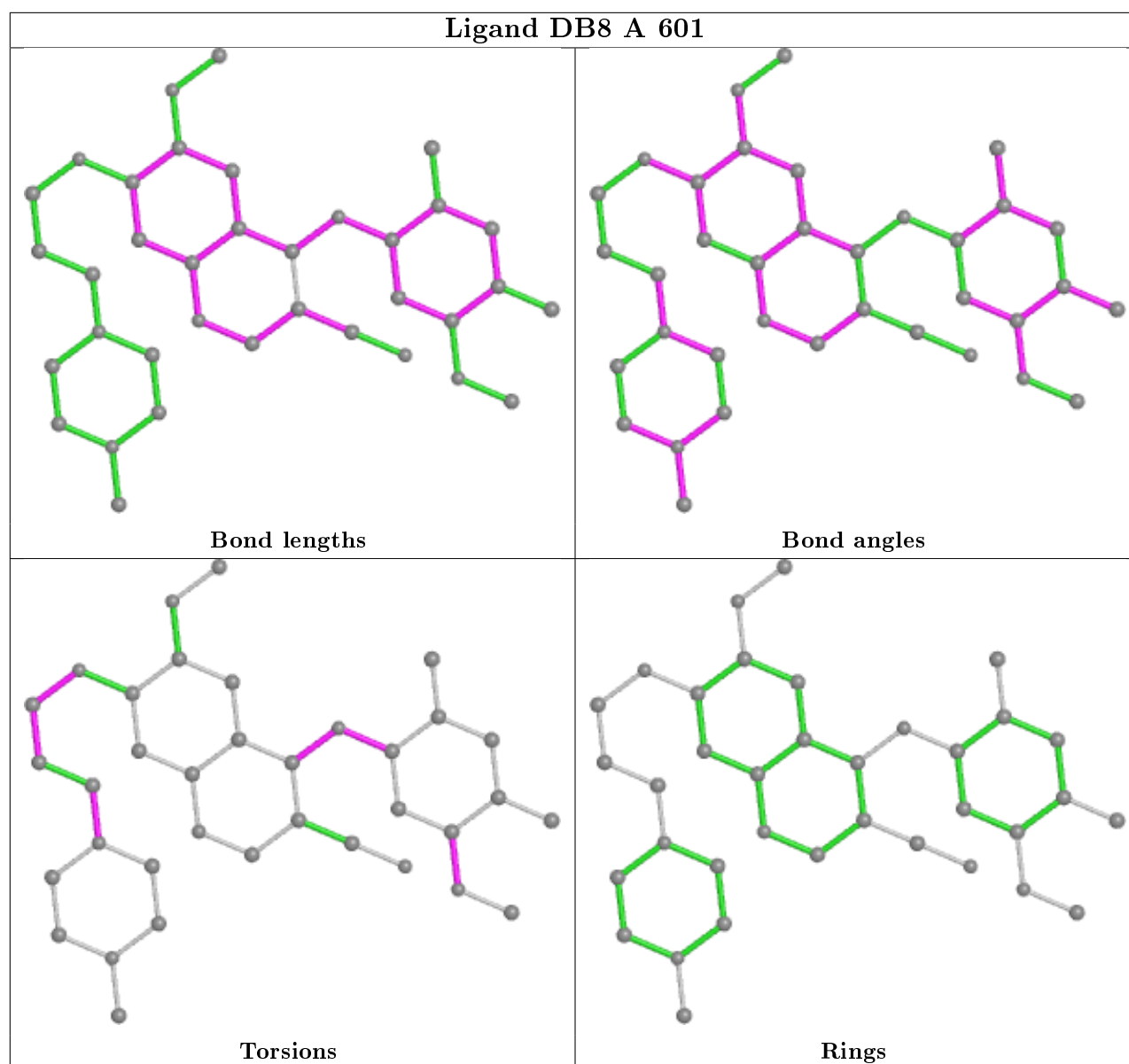
Bond angles



Torsions



Rings



## 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	266/286 (93%)	0.90	40 (15%) <b>2</b> <b>1</b>	19, 35, 85, 99	0
1	B	264/286 (92%)	0.68	22 (8%) <b>11</b> <b>9</b>	19, 36, 75, 89	0
All	All	530/572 (92%)	0.79	62 (11%) <b>4</b> <b>3</b>	19, 36, 83, 99	0

All (62) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	297	LEU	7.4
1	B	277	CYS	6.9
1	B	311	ALA	6.4
1	A	307	PHE	6.2
1	A	331	GLU	6.2
1	A	333	PRO	5.8
1	A	299	PRO	5.7
1	B	301	THR	5.4
1	A	306	ALA	5.0
1	B	411	ILE	4.9
1	A	303	SER	4.9
1	A	302	MET	4.8
1	B	308	LEU	4.7
1	B	313	VAL	4.6
1	A	311	ALA	4.5
1	A	271	VAL	4.4
1	A	268	ARG	4.3
1	A	277	CYS	4.3
1	A	424	PHE	4.3
1	B	306	ALA	4.2
1	A	332	GLU	4.1
1	A	308	LEU	4.0
1	A	408	ALA	4.0
1	A	301	THR	3.9

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Mol	Chain	Res	Type	RSRZ
1	A	309	GLN	3.8
1	B	278	PHE	3.8
1	B	307	PHE	3.7
1	A	411	ILE	3.7
1	B	297	LEU	3.7
1	B	300	GLY	3.6
1	B	309	GLN	3.6
1	A	407	LEU	3.6
1	A	267	LEU	3.5
1	A	298	LYS	3.2
1	A	410	LEU	3.2
1	A	278	PHE	3.1
1	B	268	ARG	3.1
1	B	304	PRO	3.0
1	A	412	GLU	2.9
1	B	424	PHE	2.9
1	A	409	ARG	2.8
1	A	334	ILE	2.8
1	A	329	VAL	2.7
1	A	335	TYR	2.7
1	A	289	THR	2.6
1	B	275	GLN	2.6
1	A	279	GLY	2.6
1	A	288	GLY	2.5
1	A	269	LEU	2.5
1	A	310	GLU	2.5
1	A	284	GLY	2.5
1	B	333	PRO	2.4
1	B	305	GLU	2.3
1	A	290	THR	2.3
1	B	262	ILE	2.3
1	B	314	LEU	2.2
1	B	477	ARG	2.1
1	A	276	GLY	2.1
1	B	406	GLY	2.1
1	A	264	ARG	2.1
1	A	263	PRO	2.1
1	A	304	PRO	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

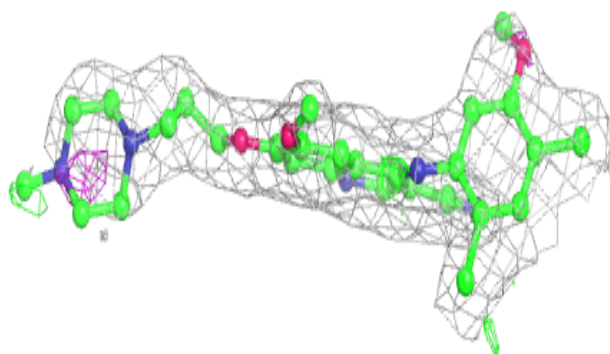
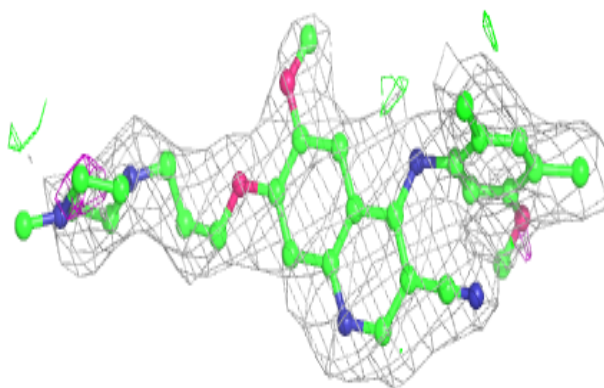
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

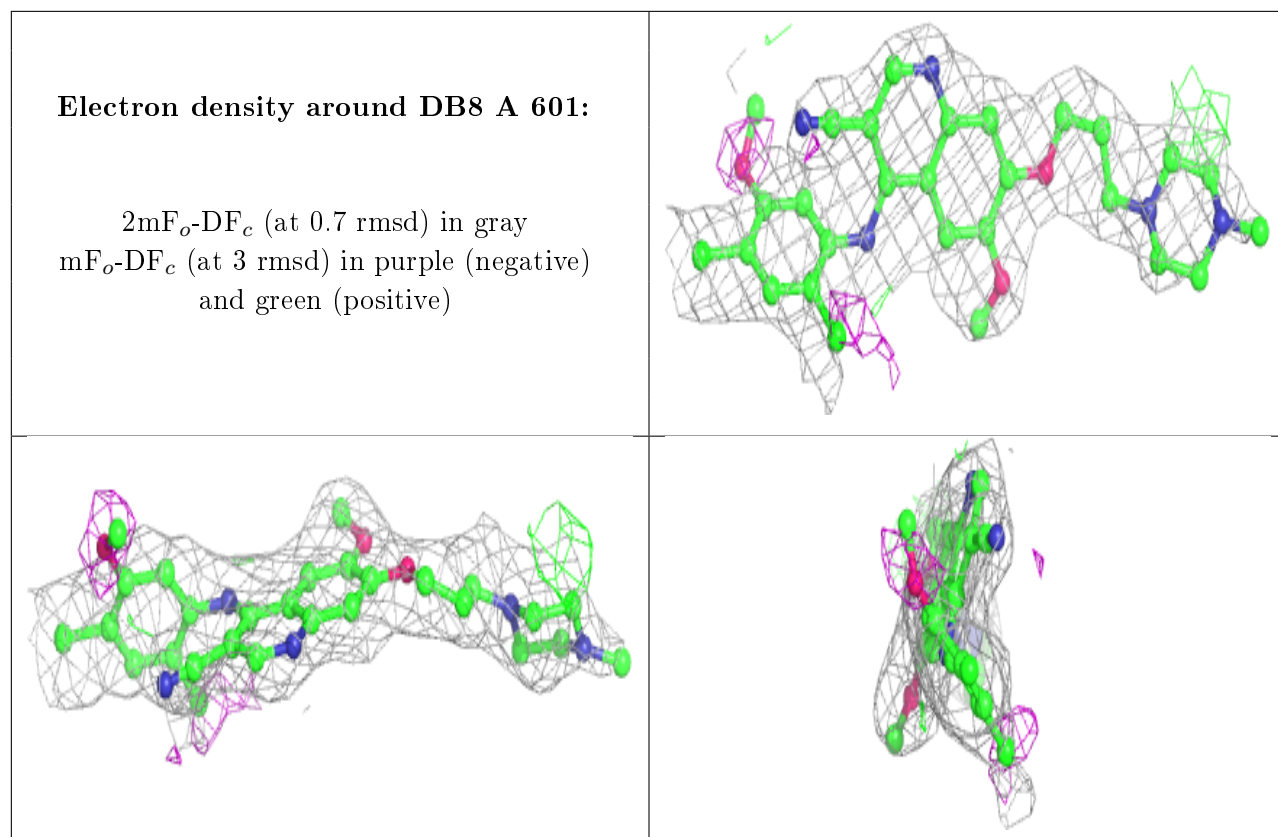
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	DB8	B	601	36/36	0.85	0.27	36,50,73,76	0
2	DB8	A	601	36/36	0.86	0.25	43,54,70,88	0

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 DB8 B 601:

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)





## 6.5 Other polymers [i](#)

There are no such residues in this entry.