



# Full wwPDB X-ray Structure Validation Report ⓘ

May 25, 2020 – 07:08 pm BST

PDB ID : 3OEZ  
Title : crystal structure of the L317I mutant of the chicken c-Src tyrosine kinase domain complexed with imatinib  
Authors : Boubeva, R.; Pernot, L.; Perozzo, R.; Scapozza, L.  
Deposited on : 2010-08-13  
Resolution : 2.40 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

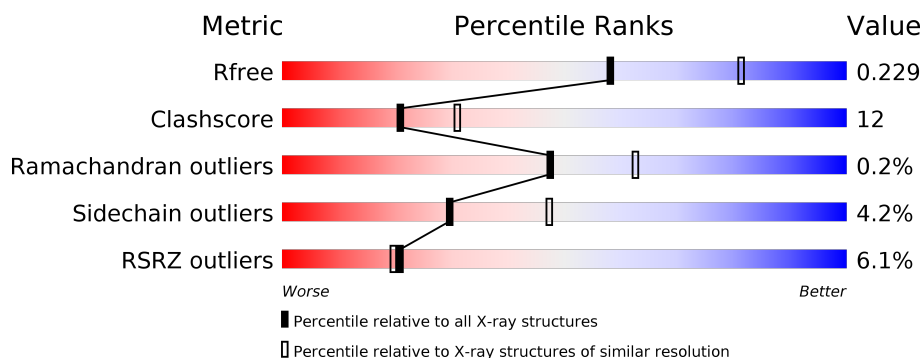
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.40 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	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (2.40-2.40)

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>2%</div> <div> <div></div> <div>69%</div> <div>20%</div> <div>• 9%</div> </div> </div>
1	B	286	<div> <div>9%</div> <div> <div></div> <div>68%</div> <div>22%</div> <div>• 9%</div> </div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	ACT	A	1	-	-	X	-

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 4576 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.

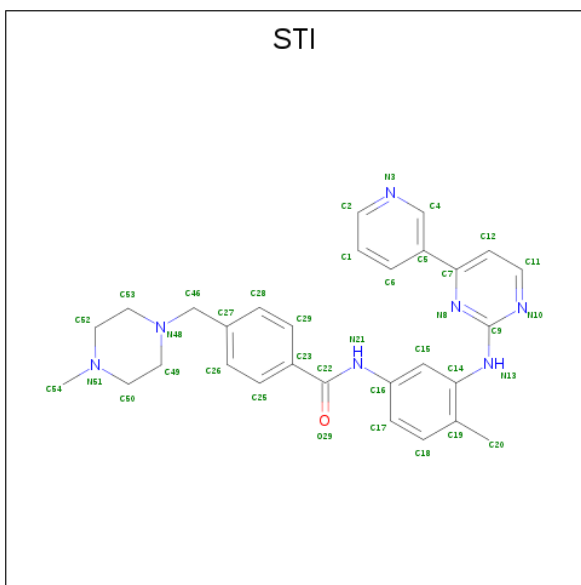
- Molecule 1 is a protein called Proto-oncogene tyrosine-protein kinase Src.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	261	Total	C	N	O	S	0	0	0
			2103	1351	350	385	17			
1	B	261	Total	C	N	O	S	0	0	0
			2100	1348	350	385	17			

There are 8 discrepancies between the modelled and reference sequences:

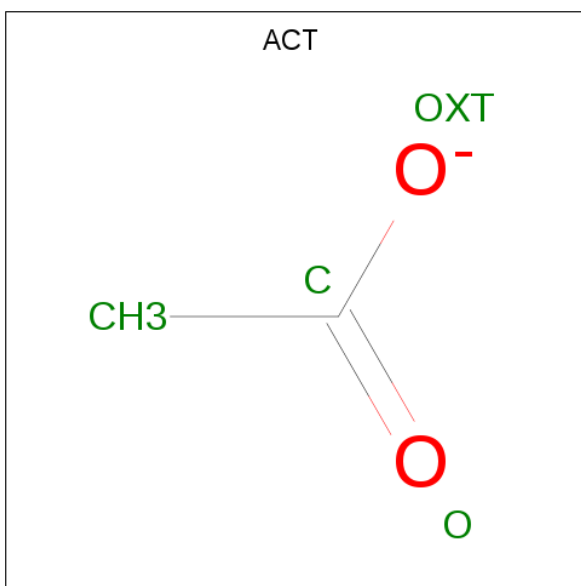
Chain	Residue	Modelled	Actual	Comment	Reference
A	248	GLY	-	EXPRESSION TAG	UNP P00523
A	249	HIS	-	EXPRESSION TAG	UNP P00523
A	250	MET	-	EXPRESSION TAG	UNP P00523
A	317	ILE	LEU	ENGINEERED MUTATION	UNP P00523
B	248	GLY	-	EXPRESSION TAG	UNP P00523
B	249	HIS	-	EXPRESSION TAG	UNP P00523
B	250	MET	-	EXPRESSION TAG	UNP P00523
B	317	ILE	LEU	ENGINEERED MUTATION	UNP P00523

- Molecule 2 is 4-(4-METHYL-PIPERAZIN-1-YLMETHYL)-N-[4-METHYL-3-(4-PYRIDIN-3-YL-PYRIMIDIN-2-YLAMINO)-PHENYL]-BENZAMIDE (three-letter code: STI) (formula: C<sub>29</sub>H<sub>31</sub>N<sub>7</sub>O).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total 37	C 29	N 7	O 1	0	0
2	B	1	Total 37	C 29	N 7	O 1	0	0

- Molecule 3 is ACETATE ION (three-letter code: ACT) (formula:  $\text{C}_2\text{H}_3\text{O}_2$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			4	2	2		

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula:  $\text{C}_3\text{H}_8\text{O}_3$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			6	3	3		

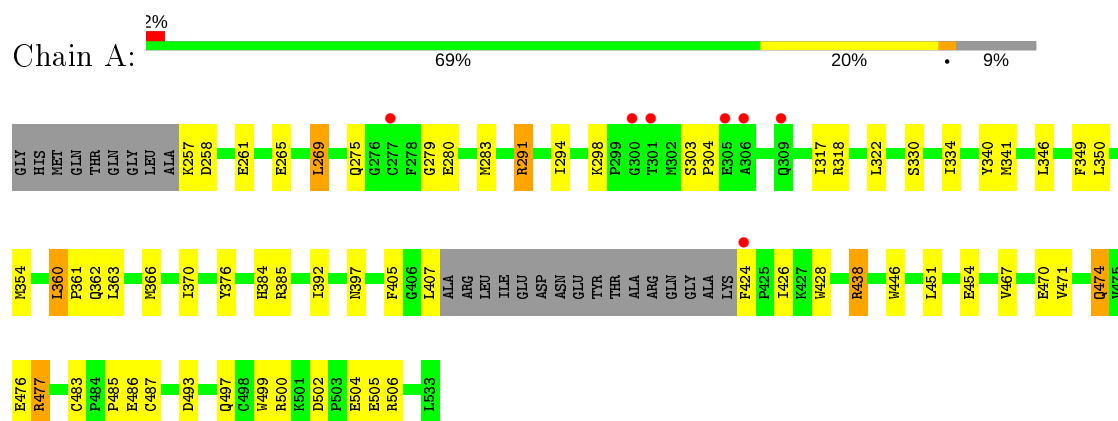
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	150	Total	O	0	0
			150	150		
5	B	139	Total	O	0	0
			139	139		

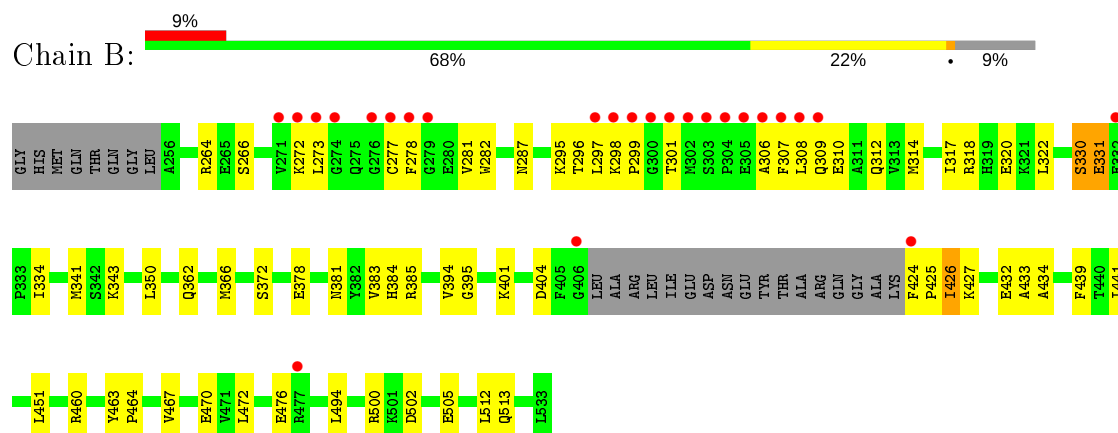
### 3 Residue-property plots [i](#)

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, $\alpha$ , $\beta$ , $\gamma$	41.90Å 63.43Å 74.14Å 79.16° 90.02° 90.19°	Depositor
Resolution (Å)	32.70 – 2.40 32.70 – 2.40	Depositor EDS
% Data completeness (in resolution range)	96.5 (32.70-2.40) 96.5 (32.70-2.40)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	0.06	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.08 (at 2.39Å)	Xtriage
Refinement program	PHENIX (phenix.refine)	Depositor
R, $R_{free}$	0.194 , 0.240 0.182 , 0.229	Depositor DCC
$R_{free}$ test set	1379 reflections (4.87%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	32.6	Xtriage
Anisotropy	0.395	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 42.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.019 for h,-k,-l	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	4576	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.22% 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 ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, STI, ACT

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	0.40	0/2155	0.54	0/2917
1	B	0.39	0/2152	0.52	0/2913
All	All	0.39	0/4307	0.53	0/5830

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2103	0	2089	48	0
1	B	2100	0	2083	56	0
2	A	37	0	31	2	0
2	B	37	0	31	7	0
3	A	4	0	3	3	0
4	A	6	0	8	0	0
5	A	150	0	0	0	0
5	B	139	0	0	2	0
All	All	4576	0	4245	104	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 12.

All (104) 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:291:ARG:HH11	1:A:291:ARG:HG3	1.33	0.93
1:A:257:LYS:HG2	1:A:258:ASP:H	1.33	0.91
1:A:500:ARG:HD3	1:A:505:GLU:HB3	1.53	0.90
1:A:257:LYS:HG2	1:A:258:ASP:N	1.84	0.90
1:B:295:LYS:HB2	2:B:601:STI:H201	1.59	0.83
1:B:500:ARG:HD3	1:B:505:GLU:HB3	1.63	0.80
1:B:295:LYS:HB2	2:B:601:STI:C20	2.12	0.79
1:A:291:ARG:HH11	1:A:291:ARG:CG	1.96	0.78
1:A:477:ARG:O	1:A:477:ARG:HG2	1.84	0.77
1:B:278:PHE:O	1:B:297:LEU:HA	1.90	0.72
1:A:500:ARG:CD	1:A:505:GLU:HB3	2.19	0.71
1:B:343:LYS:HD3	1:B:395:GLY:O	1.94	0.67
1:A:291:ARG:NH1	1:A:291:ARG:HG3	2.04	0.67
1:B:384:HIS:O	1:B:385:ARG:HB2	1.96	0.66
1:A:279:GLY:HA2	1:A:298:LYS:HG2	1.78	0.65
1:B:502:ASP:HB3	1:B:505:GLU:HG2	1.80	0.64
1:A:283:MET:HG3	1:A:340:TYR:CE1	2.33	0.63
1:A:275:GLN:HG2	1:A:280:GLU:HG2	1.80	0.62
1:A:384:HIS:O	1:A:385:ARG:HB2	2.00	0.62
1:B:467:VAL:HG22	1:B:470:GLU:HG2	1.79	0.62
1:A:349:PHE:CE1	1:A:354:MET:HG3	2.34	0.62
1:B:309:GLN:HA	1:B:312:GLN:HG2	1.81	0.62
1:A:363:LEU:HD23	1:A:366:MET:HE1	1.80	0.61
1:B:308:LEU:O	1:B:312:GLN:HG2	2.01	0.60
1:B:310:GLU:O	1:B:314:MET:HG3	2.00	0.60
1:B:460:ARG:NH2	5:B:10:HOH:O	2.35	0.60
1:B:297:LEU:HB3	1:B:334:ILE:HB	1.84	0.58
1:A:502:ASP:HB3	1:A:505:GLU:OE1	2.03	0.58
1:B:298:LYS:HB3	1:B:301:THR:OG1	2.04	0.58
1:A:363:LEU:HD23	1:A:366:MET:CE	2.34	0.57
1:B:309:GLN:HA	1:B:312:GLN:CG	2.33	0.57
1:A:397:ASN:ND2	3:A:1:ACT:H2	2.20	0.56
1:B:472:LEU:O	1:B:476:GLU:HB2	2.06	0.56
1:A:257:LYS:CG	1:A:258:ASP:H	2.11	0.55
1:B:331:GLU:HA	1:B:331:GLU:OE1	2.07	0.55
1:B:341:MET:O	2:B:601:STI:H21	2.07	0.55
1:A:362:GLN:O	1:A:366:MET:HG3	2.07	0.55
1:B:385:ARG:HG2	1:B:439:PHE:CD2	2.42	0.55
1:B:277:CYS:O	1:B:298:LYS:HB2	2.07	0.54
1:B:273:LEU:HD12	1:B:281:VAL:HG12	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:297:LEU:HB2	1:B:307:PHE:CE2	2.44	0.53
1:B:272:LYS:HG2	1:B:282:TRP:CH2	2.45	0.52
1:B:426:ILE:HD11	1:B:434:ALA:HB1	1.91	0.51
1:A:279:GLY:HA2	1:A:298:LYS:HE2	1.93	0.51
1:A:341:MET:O	2:A:601:STI:H21	2.09	0.51
1:A:446:TRP:CE3	1:A:499:TRP:HA	2.46	0.51
1:A:405:PHE:HB2	1:A:407:LEU:HG	1.93	0.50
1:B:295:LYS:CB	2:B:601:STI:H201	2.37	0.50
1:B:272:LYS:HG2	1:B:282:TRP:CZ3	2.49	0.48
1:B:306:ALA:C	1:B:308:LEU:H	2.17	0.47
1:B:372:SER:HA	1:B:513:GLN:OE1	2.15	0.47
1:B:383:VAL:O	2:B:601:STI:H492	2.15	0.47
1:A:451:LEU:HD23	1:A:451:LEU:O	2.15	0.46
1:A:467:VAL:O	1:A:471:VAL:HG23	2.14	0.46
1:B:381:ASN:ND2	5:B:120:HOH:O	2.46	0.46
1:A:283:MET:HG3	1:A:340:TYR:CZ	2.50	0.46
1:A:426:ILE:HD13	1:A:426:ILE:HA	1.77	0.46
1:B:424:PHE:CD2	1:B:425:PRO:HD3	2.51	0.46
1:A:360:LEU:HB3	1:A:361:PRO:HD3	1.97	0.46
1:B:320:GLU:O	1:B:401:LYS:HE2	2.16	0.46
1:B:277:CYS:O	1:B:298:LYS:HD2	2.15	0.46
1:B:317:ILE:HG21	1:B:322:LEU:HD22	1.97	0.45
1:A:397:ASN:HD22	3:A:1:ACT:CH3	2.30	0.45
1:A:476:GLU:OE1	1:A:476:GLU:HA	2.16	0.45
1:B:273:LEU:HB2	1:B:281:VAL:O	2.17	0.45
1:B:385:ARG:HD3	2:B:601:STI:H542	1.99	0.44
1:A:330:SER:HA	1:A:334:ILE:HD12	1.99	0.44
1:B:378:GLU:HG3	1:B:441:ILE:HG12	1.99	0.44
1:A:317:ILE:HG23	1:A:376:TYR:HE2	1.83	0.44
1:B:264:ARG:NH2	1:B:331:GLU:O	2.49	0.44
1:B:432:GLU:HG2	1:B:433:ALA:N	2.32	0.44
1:A:279:GLY:CA	1:A:298:LYS:HG2	2.47	0.43
1:B:308:LEU:HD21	1:B:334:ILE:CG2	2.48	0.43
1:B:463:TYR:N	1:B:464:PRO:HD3	2.33	0.43
1:A:483:CYS:SG	1:A:487:CYS:O	2.76	0.43
1:B:451:LEU:HD23	1:B:451:LEU:O	2.19	0.43
1:A:257:LYS:CD	1:A:261:GLU:HG3	2.49	0.43
1:B:297:LEU:HD23	1:B:334:ILE:HG13	2.01	0.43
1:A:346:LEU:CB	1:A:392:ILE:HB	2.49	0.43
1:A:385:ARG:HD2	2:A:601:STI:H542	2.01	0.43
1:A:397:ASN:ND2	3:A:1:ACT:CH3	2.80	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:306:ALA:C	1:B:308:LEU:N	2.73	0.42
1:B:297:LEU:HD23	1:B:334:ILE:CG1	2.50	0.42
1:B:343:LYS:HE2	1:B:394:VAL:CG1	2.50	0.42
1:A:346:LEU:HB3	1:A:392:ILE:HB	2.01	0.42
1:B:308:LEU:HD13	1:B:330:SER:HB3	2.02	0.42
1:B:362:GLN:O	1:B:366:MET:HG3	2.20	0.42
1:B:424:PHE:HD2	1:B:425:PRO:HD3	1.83	0.42
1:A:428:TRP:HE1	1:A:454:GLU:CD	2.23	0.41
1:B:266:SER:HB2	1:B:287:ASN:OD1	2.19	0.41
1:B:426:ILE:HD12	1:B:472:LEU:HD21	2.03	0.41
1:A:438:ARG:HA	1:A:438:ARG:HD3	1.57	0.41
1:B:281:VAL:HG22	1:B:295:LYS:HG3	2.01	0.41
1:A:474:GLN:HE22	1:A:477:ARG:NH1	2.19	0.41
1:B:296:THR:HG22	1:B:297:LEU:N	2.35	0.41
1:A:303:SER:HA	1:A:304:PRO:HD3	1.97	0.41
1:A:269:LEU:HD22	1:A:294:ILE:HD13	2.02	0.41
1:A:485:PRO:O	1:A:486:GLU:HB2	2.20	0.41
1:B:494:LEU:HD11	1:B:512:LEU:HD23	2.03	0.41
1:B:404:ASP:HB3	2:B:601:STI:C23	2.51	0.40
1:A:504:GLU:HA	1:A:504:GLU:OE1	2.21	0.40
1:A:497:GLN:O	1:A:506:ARG:HG3	2.21	0.40
1:A:366:MET:O	1:A:370:ILE:HG13	2.21	0.40
1:B:343:LYS:HE2	1:B:394:VAL:HG12	2.04	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	257/286 (90%)	251 (98%)	6 (2%)	0	100	100
1	B	257/286 (90%)	243 (95%)	13 (5%)	1 (0%)	34	48

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	514/572 (90%)	494 (96%)	19 (4%)	1 (0%)	47 62

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	299	PRO

### 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	227/245 (93%)	214 (94%)	13 (6%)	20 33
1	B	226/245 (92%)	220 (97%)	6 (3%)	44 65
All	All	453/490 (92%)	434 (96%)	19 (4%)	30 47

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	265	GLU
1	A	269	LEU
1	A	291	ARG
1	A	318	ARG
1	A	322	LEU
1	A	350	LEU
1	A	360	LEU
1	A	424	PHE
1	A	438	ARG
1	A	470	GLU
1	A	474	GLN
1	A	477	ARG
1	A	493	ASP
1	B	318	ARG
1	B	330	SER
1	B	331	GLU
1	B	350	LEU

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Mol	Chain	Res	Type
1	B	426	ILE
1	B	427	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	397	ASN
1	A	474	GLN
1	B	381	ASN
1	B	397	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 carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

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	STI	A	601	-	41,41,41	2.31	22 (53%)	56,56,56	1.93	10 (17%)
2	STI	B	601	-	41,41,41	2.42	23 (56%)	56,56,56	1.98	9 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	ACT	A	1	-	1,3,3	1.80	0	0,3,3	0.00	-
4	GOL	A	534	-	5,5,5	0.75	0	5,5,5	0.84	0

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	STI	A	601	-	-	2/20/30/30	0/5/5/5
2	STI	B	601	-	-	2/20/30/30	0/5/5/5
4	GOL	A	534	-	-	2/4/4/4	-

All (45) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	601	STI	C25-C23	4.65	1.47	1.39
2	A	601	STI	C25-C23	4.28	1.46	1.39
2	B	601	STI	C15-C16	4.17	1.46	1.39
2	A	601	STI	C15-C16	4.11	1.46	1.39
2	A	601	STI	C14-C19	3.90	1.48	1.40
2	B	601	STI	C4-C5	3.70	1.46	1.39
2	B	601	STI	C14-C19	3.63	1.47	1.40
2	B	601	STI	C17-C18	3.46	1.45	1.38
2	B	601	STI	C26-C25	3.44	1.45	1.38
2	B	601	STI	C6-C5	3.43	1.46	1.39
2	A	601	STI	C4-C5	3.42	1.45	1.39
2	B	601	STI	C50-N51	3.37	1.53	1.46
2	A	601	STI	C26-C27	3.36	1.46	1.38
2	A	601	STI	C50-N51	3.29	1.53	1.46
2	B	601	STI	C26-C27	3.25	1.45	1.38
2	A	601	STI	C6-C5	3.25	1.46	1.39
2	A	601	STI	C26-C25	3.20	1.44	1.38
2	B	601	STI	C29-C23	3.17	1.44	1.39
2	A	601	STI	C17-C18	3.13	1.44	1.38
2	A	601	STI	C28-C27	3.13	1.45	1.38
2	B	601	STI	C28-C27	3.08	1.45	1.38
2	A	601	STI	C9-N10	3.05	1.38	1.34
2	A	601	STI	C29-C23	2.99	1.44	1.39
2	B	601	STI	C17-C16	2.90	1.44	1.39
2	B	601	STI	C52-N51	2.76	1.52	1.46
2	B	601	STI	C9-N10	2.67	1.38	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	601	STI	C52-N51	2.56	1.51	1.46
2	B	601	STI	C2-N3	2.54	1.41	1.33
2	B	601	STI	C1-C6	2.43	1.44	1.38
2	A	601	STI	C2-N3	2.42	1.40	1.33
2	B	601	STI	C12-C7	2.38	1.44	1.38
2	A	601	STI	C12-C7	2.35	1.44	1.38
2	B	601	STI	C7-N8	2.32	1.38	1.34
2	A	601	STI	C17-C16	2.26	1.43	1.39
2	B	601	STI	C20-C19	2.25	1.55	1.51
2	B	601	STI	C1-C2	2.20	1.44	1.37
2	A	601	STI	C11-N10	2.16	1.39	1.34
2	A	601	STI	C12-C11	2.16	1.42	1.38
2	A	601	STI	C20-C19	2.16	1.55	1.51
2	B	601	STI	C49-N48	2.14	1.52	1.46
2	A	601	STI	C4-N3	2.14	1.38	1.34
2	B	601	STI	C18-C19	2.13	1.44	1.39
2	A	601	STI	C1-C6	2.13	1.43	1.38
2	A	601	STI	C1-C2	2.04	1.43	1.37
2	B	601	STI	C12-C11	2.04	1.42	1.38

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	601	STI	C7-N8-C9	6.20	121.80	116.69
2	A	601	STI	N10-C9-N8	-5.81	121.05	126.55
2	B	601	STI	N10-C9-N8	-5.79	121.06	126.55
2	B	601	STI	C7-N8-C9	5.72	121.40	116.69
2	B	601	STI	C11-N10-C9	5.67	120.48	115.45
2	A	601	STI	C50-N51-C52	5.06	116.61	109.52
2	A	601	STI	C11-N10-C9	4.92	119.81	115.45
2	B	601	STI	C50-N51-C52	4.61	115.97	109.52
2	B	601	STI	C14-N13-C9	-3.92	117.78	129.60
2	A	601	STI	C2-N3-C4	3.40	122.74	116.85
2	B	601	STI	C12-C11-N10	-3.18	120.00	123.96
2	B	601	STI	C2-N3-C4	3.07	122.16	116.85
2	B	601	STI	O29-C22-C23	-3.05	115.49	120.94
2	A	601	STI	C12-C11-N10	-3.01	120.22	123.96
2	B	601	STI	C54-N51-C52	2.71	114.71	110.66
2	A	601	STI	C54-N51-C52	2.47	114.36	110.66
2	A	601	STI	C14-N13-C9	-2.45	122.21	129.60
2	A	601	STI	C20-C19-C14	2.39	123.95	121.25
2	A	601	STI	C12-C7-N8	-2.18	119.14	121.97



There are no chirality outliers.

All (6) torsion outliers are listed below:

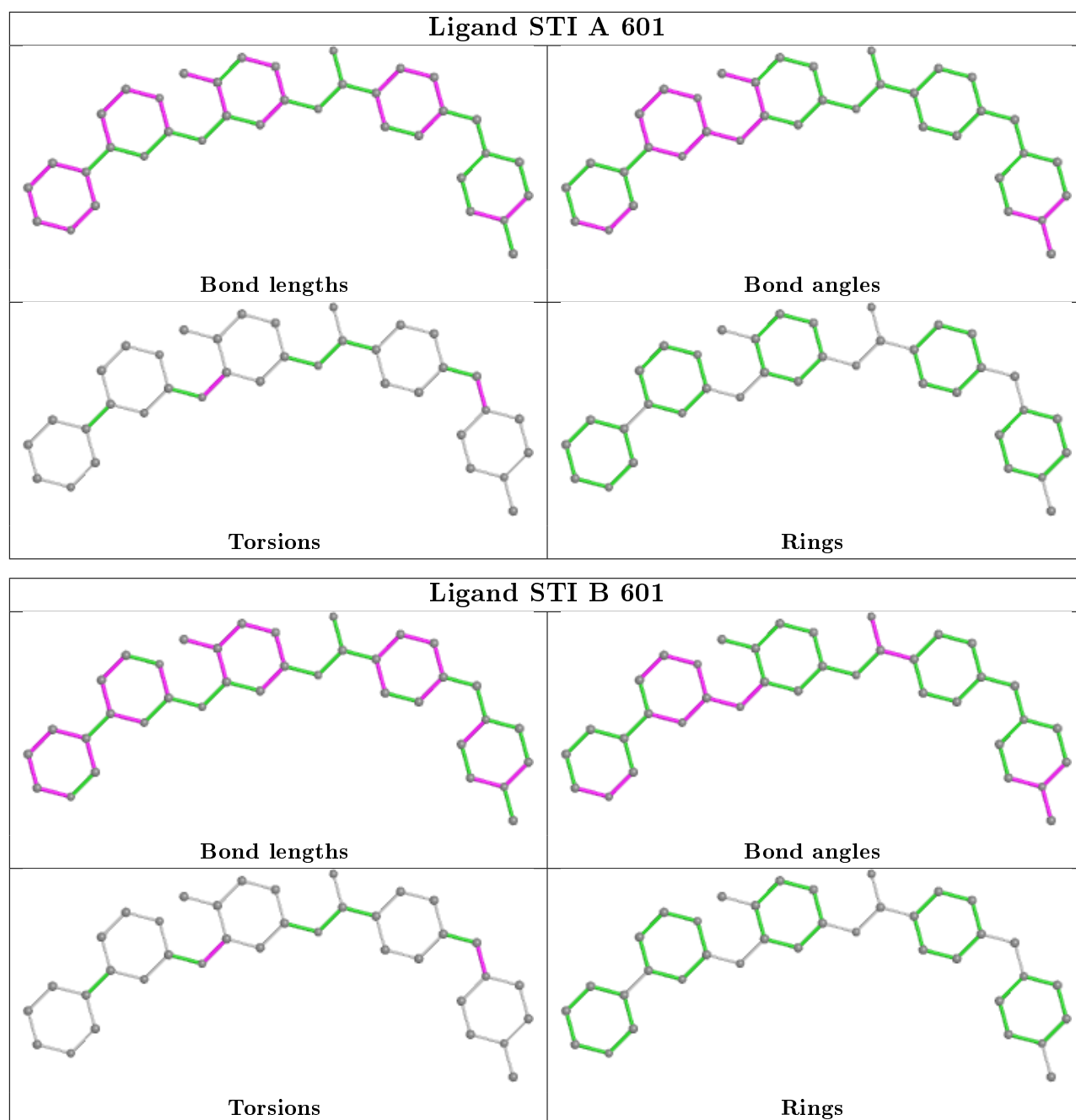
Mol	Chain	Res	Type	Atoms
2	A	601	STI	C15-C14-N13-C9
2	A	601	STI	C27-C46-N48-C53
2	B	601	STI	C15-C14-N13-C9
4	A	534	GOL	O1-C1-C2-O2
2	B	601	STI	C27-C46-N48-C53
4	A	534	GOL	O1-C1-C2-C3

There are no ring outliers.

3 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	601	STI	2	0
2	B	601	STI	7	0
3	A	1	ACT	3	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 ⓘ

### 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	261/286 (91%)	-0.15	7 (2%) 54 52	20, 34, 62, 89	0
1	B	261/286 (91%)	0.32	25 (9%) 8 7	20, 36, 99, 119	0
All	All	522/572 (91%)	0.09	32 (6%) 21 20	20, 35, 83, 119	0

All (32) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	277	CYS	7.8
1	B	301	THR	7.5
1	B	278	PHE	7.2
1	B	300	GLY	7.1
1	B	299	PRO	6.9
1	B	302	MET	5.2
1	B	306	ALA	4.9
1	B	297	LEU	4.6
1	B	279	GLY	4.1
1	B	304	PRO	4.0
1	B	309	GLN	3.9
1	A	277	CYS	3.9
1	B	424	PHE	3.8
1	A	305	GLU	3.8
1	B	406	GLY	3.8
1	A	424	PHE	3.6
1	B	477	ARG	3.6
1	A	300	GLY	3.6
1	B	305	GLU	3.3
1	B	308	LEU	3.2
1	A	306	ALA	3.0
1	B	272	LYS	2.9
1	A	309	GLN	2.8
1	B	273	LEU	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	274	GLY	2.5
1	B	332	GLU	2.5
1	B	276	GLY	2.5
1	A	301	THR	2.4
1	B	298	LYS	2.3
1	B	303	SER	2.2
1	B	271	VAL	2.2
1	B	307	PHE	2.2

## 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](#)

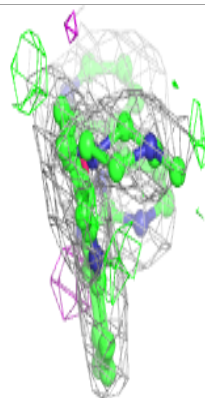
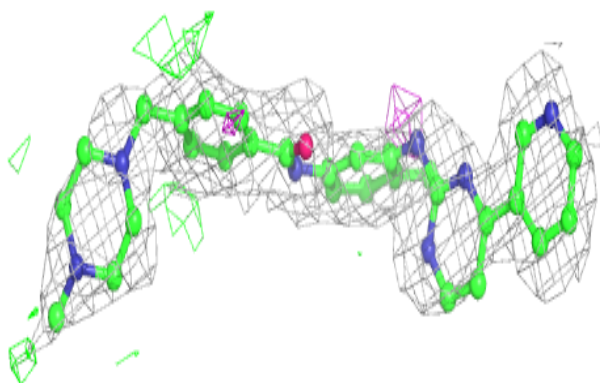
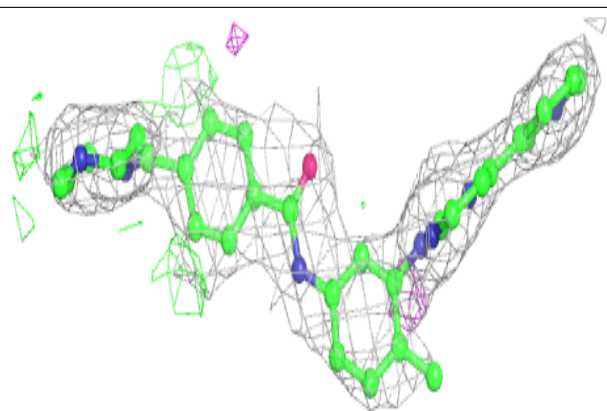
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 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	STI	B	601	37/37	0.85	0.22	38,55,61,62	0
3	ACT	A	1	4/4	0.95	0.09	39,41,45,46	0
2	STI	A	601	37/37	0.96	0.12	22,31,41,44	0
4	GOL	A	534	6/6	0.97	0.13	31,37,43,45	0

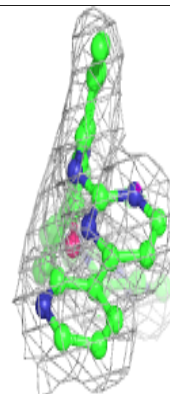
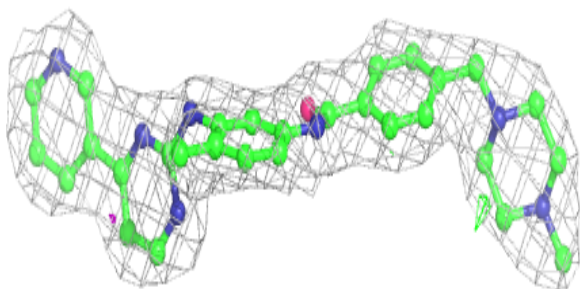
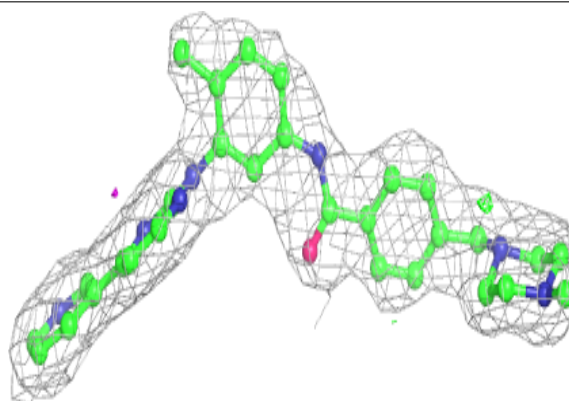
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

**Electron density around STI B 601:**

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

**Electron density around STI A 601:**

$2mF_o-DF_c$  (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.