Full wwPDB X-ray Structure Validation Report (i)

May 4, 2024 – 06:25 pm BST

PDB ID	:	6HD6
Title	:	ABL1 IN COMPLEX WITH COMPOUND6 AND IMATINIB (STI-571)
Authors	:	Cowan-Jacob, S.W.
Deposited on	:	2018-08-17
Resolution	:	2.30 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*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) 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 (i)) were used in the production of this report:

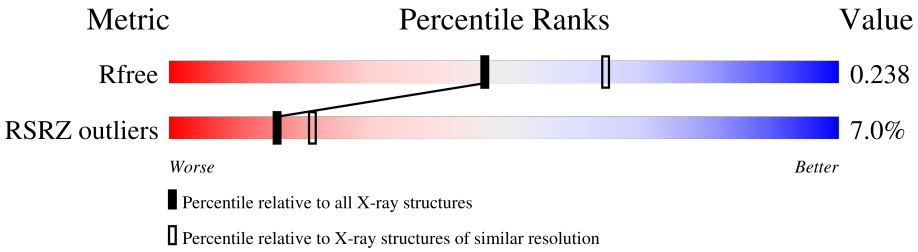
MolProbity	:	FAILED
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36.2
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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}	130704	5042 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

MolProbity failed to run properly - the sequence quality summary graphics cannot be shown.

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 5135 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 Tyrosine-protein kinase ABL1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	285	Total	C	N	O	S	0	2	0
			2322	1492	375	437	18			
1	B	283	Total	C	N	O	S	0	0	0
			2299	1478	372	431	18			

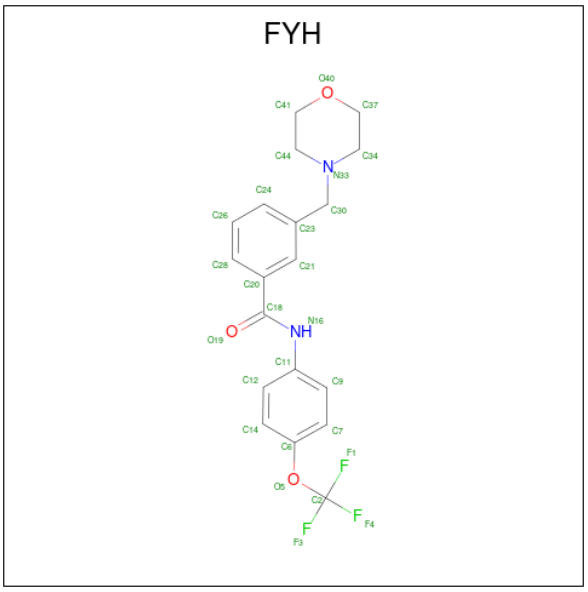
There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	242	GLY	-	expression tag	UNP P00520
A	243	ALA	-	expression tag	UNP P00520
A	244	MET	-	expression tag	UNP P00520
A	245	ASP	-	expression tag	UNP P00520
A	246	PRO	-	expression tag	UNP P00520
A	247	SER	-	expression tag	UNP P00520
B	242	GLY	-	expression tag	UNP P00520
B	243	ALA	-	expression tag	UNP P00520
B	244	MET	-	expression tag	UNP P00520
B	245	ASP	-	expression tag	UNP P00520
B	246	PRO	-	expression tag	UNP P00520
B	247	SER	-	expression tag	UNP P00520

- Molecule 2 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

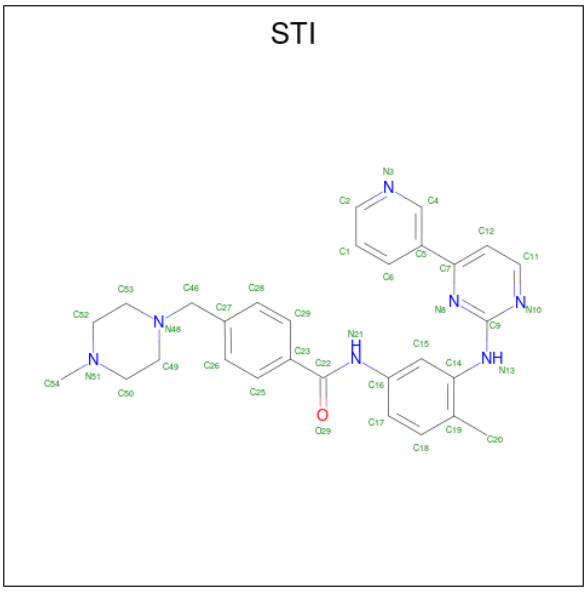
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Cl	0	0
			1	1		

- Molecule 3 is 3-(morpholin-4-ylmethyl)- {N}-[4-(trifluoromethyloxy)phenyl]benzamide (three-letter code: FYH) (formula: $C_{19}H_{19}F_3N_2O_3$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	F	N	O	0	1
			54	38	6	4	6		

- Molecule 4 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: $C_{29}H_{31}N_7O$).



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

- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	258	Total O 258 258	0	0
5	B	127	Total O 127 127	0	0

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3 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	42.08Å 65.20Å 66.35Å 73.30° 79.82° 84.54°	Depositor
Resolution (Å)	35.25 – 2.30 33.75 – 2.30	Depositor EDS
% Data completeness (in resolution range)	94.6 (35.25-2.30) 94.6 (33.75-2.30)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.13 (at 2.29Å)	Xtriage
Refinement program	REFMAC 5.3.0040	Depositor
R, R_{free}	0.175 , 0.238 0.174 , 0.238	Depositor DCC
R_{free} test set	1397 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	28.9	Xtriage
Anisotropy	0.153	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 62.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	5135	wwPDB-VP
Average B, all atoms (Å^2)	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.83% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

4 Model quality

4.1 Standard geometry

MolProbity failed to run properly - this section is therefore empty.

4.2 Too-close contacts

MolProbity failed to run properly - this section is therefore empty.

4.3 Torsion angles

4.3.1 Protein backbone

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4.3.2 Protein sidechains

MolProbity failed to run properly - this section is therefore empty.

4.3.3 RNA

MolProbity failed to run properly - this section is therefore empty.

4.4 Non-standard residues in protein, DNA, RNA chains

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

4.5 Carbohydrates

There are no monosaccharides in this entry.

4.6 Ligand geometry

Of 5 ligands modelled in this entry, 1 is monoatomic - leaving 4 for Mogul analysis.

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	$\#\|Z\| > 2$
3	FYH	A	602[B]	-	29,29,29	1.00	1 (3%)	40,40,40	1.09	3 (7%)
4	STI	B	601	-	40,41,41	0.98	2 (5%)	51,56,56	2.12	10 (19%)
3	FYH	A	602[A]	-	29,29,29	1.12	2 (6%)	40,40,40	1.23	5 (12%)
4	STI	A	603	-	40,41,41	1.12	2 (5%)	51,56,56	2.01	10 (19%)

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
3	FYH	A	602[B]	-	-	6/17/25/25	0/3/3/3
4	STI	B	601	-	-	1/16/30/30	0/5/5/5
3	FYH	A	602[A]	-	-	2/17/25/25	0/3/3/3
4	STI	A	603	-	-	2/16/30/30	0/5/5/5

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	603	STI	C7-N8	-2.40	1.33	1.37
3	A	602[A]	FYH	O5-C2	2.30	1.44	1.31
3	A	602[B]	FYH	O5-C2	2.29	1.44	1.31
3	A	602[A]	FYH	C30-C23	2.25	1.55	1.51
4	B	601	STI	C46-C27	2.09	1.55	1.51
4	A	603	STI	C4-N3	2.07	1.36	1.32
4	B	601	STI	C12-C11	2.04	1.39	1.36

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	B	601	STI	N10-C9-N8	-7.59	119.19	126.52
4	B	601	STI	C11-N10-C9	7.24	121.87	115.45
4	A	603	STI	C11-N10-C9	6.86	121.54	115.45
4	A	603	STI	N10-C9-N8	-6.81	119.94	126.52
4	A	603	STI	C12-C11-N10	-5.21	118.67	123.81
4	B	601	STI	C12-C11-N10	-4.70	119.17	123.81
3	A	602[A]	FYH	O19-C18-C20	-3.54	114.63	120.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	B	601	STI	O29-C22-C23	-3.48	114.73	120.94
4	B	601	STI	C9-N8-C7	3.45	121.22	115.60
4	B	601	STI	C54-N51-C50	3.32	115.62	110.66
4	A	603	STI	C9-N8-C7	3.06	120.59	115.60
3	A	602[A]	FYH	C30-N33-C34	2.82	117.33	111.06
3	A	602[B]	FYH	C34-N33-C44	2.79	115.11	108.83
3	A	602[B]	FYH	C30-N33-C44	2.70	117.07	111.06
3	A	602[A]	FYH	C20-C18-N16	2.68	121.82	115.92
4	A	603	STI	C46-N48-C53	2.62	116.90	111.06
3	A	602[A]	FYH	C23-C30-N33	2.61	118.18	113.12
3	A	602[A]	FYH	C34-N33-C44	2.58	114.64	108.83
4	A	603	STI	C18-C19-C14	2.47	119.77	117.44
4	B	601	STI	C18-C19-C14	2.38	119.68	117.44
3	A	602[B]	FYH	O19-C18-C20	-2.35	116.75	120.94
4	B	601	STI	C50-N51-C52	2.29	112.73	109.52
4	A	603	STI	N13-C9-N10	2.13	122.88	116.28
4	B	601	STI	C14-N13-C9	-2.08	123.34	129.60
4	A	603	STI	C25-C26-C27	-2.07	118.19	121.03
4	A	603	STI	C5-C4-N3	-2.04	118.26	123.86
4	B	601	STI	C19-C14-N13	2.03	122.54	118.70
4	A	603	STI	C2-N3-C4	2.03	121.57	117.25

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	603	STI	C15-C14-N13-C9
3	A	602[A]	FYH	C23-C30-N33-C44
3	A	602[A]	FYH	C23-C30-N33-C34
3	A	602[B]	FYH	C23-C30-N33-C44
3	A	602[B]	FYH	N16-C18-C20-C28
3	A	602[B]	FYH	O19-C18-C20-C28
3	A	602[B]	FYH	N16-C18-C20-C21
3	A	602[B]	FYH	O19-C18-C20-C21
3	A	602[B]	FYH	C23-C30-N33-C34
4	B	601	STI	C15-C14-N13-C9
4	A	603	STI	C19-C14-N13-C9

There are no ring outliers.

No monomer is involved in short contacts.

4.7 Other polymers (i)

There are no such residues in this entry.

4.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

5 Fit of model and data

5.1 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^{th} 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	285/293 (97%)	-0.06	5 (1%) 68 74	10, 24, 49, 68	0
1	B	283/293 (96%)	0.52	35 (12%) 4 5	20, 41, 69, 80	0
All	All	568/586 (96%)	0.22	40 (7%) 16 21	10, 33, 66, 80	0

All (40) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	297	MET	7.2
1	B	407	MET	7.1
1	B	416	ALA	5.9
1	B	414	ALA	5.8
1	B	408	THR	4.5
1	B	409	GLY	4.1
1	B	299	VAL	3.8
1	B	406	LEU	3.8
1	B	518	GLU	3.7
1	B	327	GLU	3.6
1	A	408	THR	3.5
1	A	299	VAL	3.3
1	B	282	LYS	3.1
1	B	298	GLU	3.1
1	B	293	LYS	3.1
1	B	353	GLU	3.1
1	B	329	PRO	3.0
1	B	521	ILE	2.9
1	B	519	SER	2.9
1	B	269	GLY	2.7
1	B	418	ALA	2.7
1	B	516	PHE	2.6
1	B	486	LYS	2.6
1	B	292	LEU	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	265	HIS	2.5
1	B	261	ILE	2.4
1	B	352	GLN	2.4
1	A	409	GLY	2.3
1	B	404	SER	2.3
1	B	410	ASP	2.3
1	B	265	HIS	2.3
1	B	514	THR	2.3
1	B	259	THR	2.2
1	B	280	TRP	2.2
1	B	517	GLN	2.2
1	B	262	THR	2.2
1	B	405	ARG	2.2
1	B	417	GLY	2.2
1	B	284	SER	2.1
1	B	328	PRO	2.1

5.2 Non-standard residues in protein, DNA, RNA chains (i)

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

5.3 Carbohydrates (i)

There are no monosaccharides in this entry.

5.4 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^{th} 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.

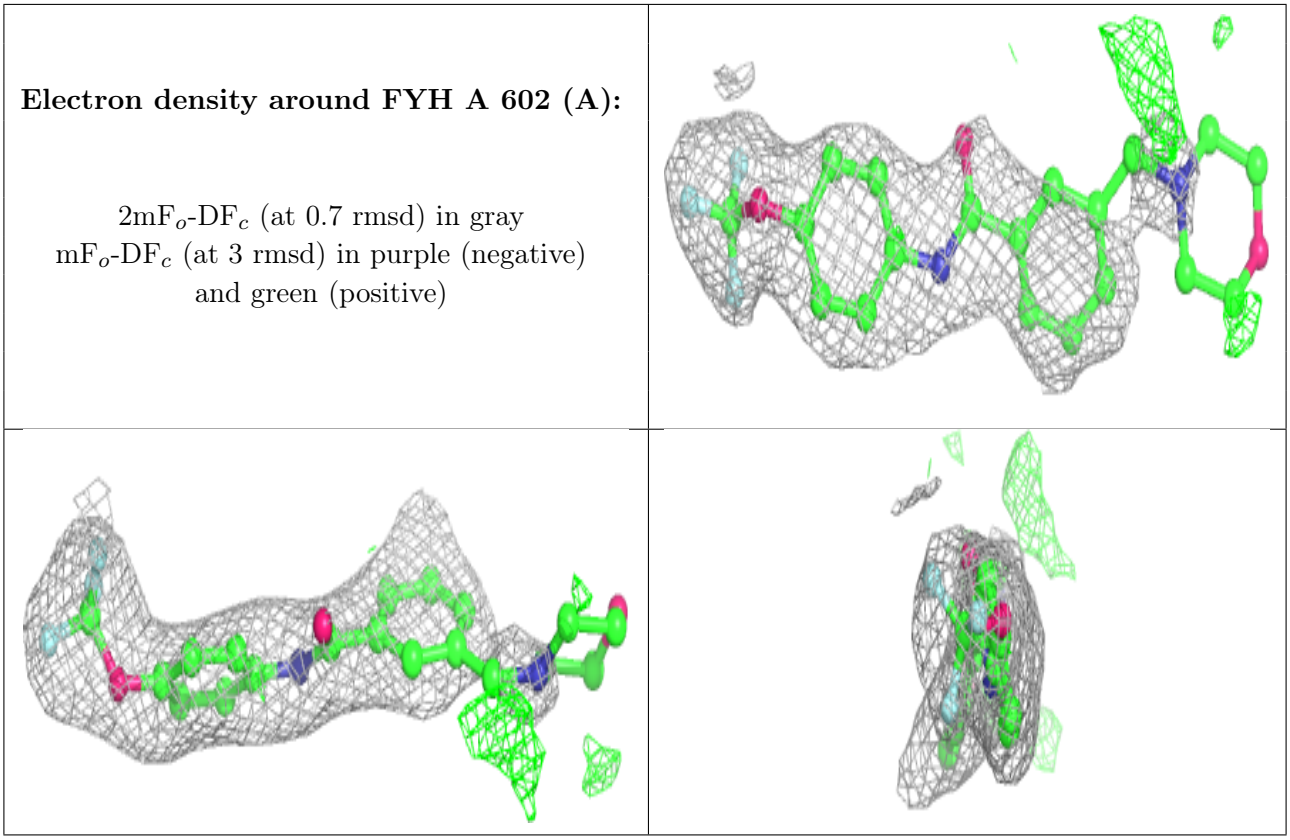
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	FYH	A	602[A]	27/27	0.94	0.29	32,40,51,52	27
3	FYH	A	602[B]	27/27	0.94	0.29	23,28,30,31	27
4	STI	A	603	37/37	0.96	0.14	13,16,20,20	0
4	STI	B	601	37/37	0.96	0.12	24,30,37,37	0
2	CL	A	601	1/1	0.99	0.07	30,30,30,30	0

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.

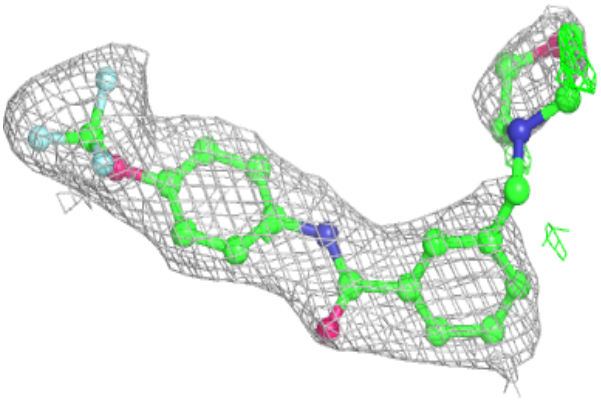
Electron density around FYH A 602 (A):

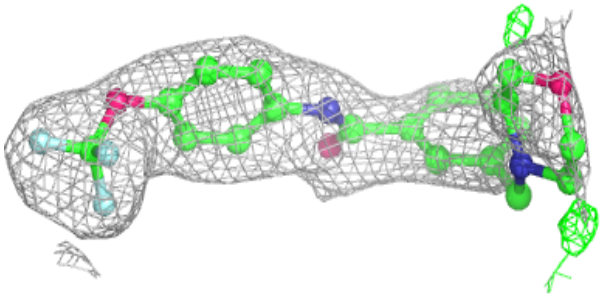
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

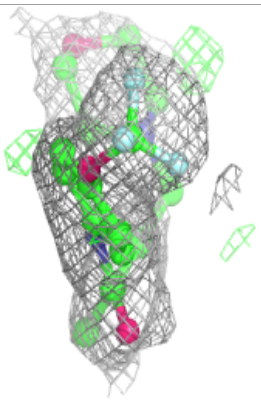


Electron density around FYH A 602 (B):

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

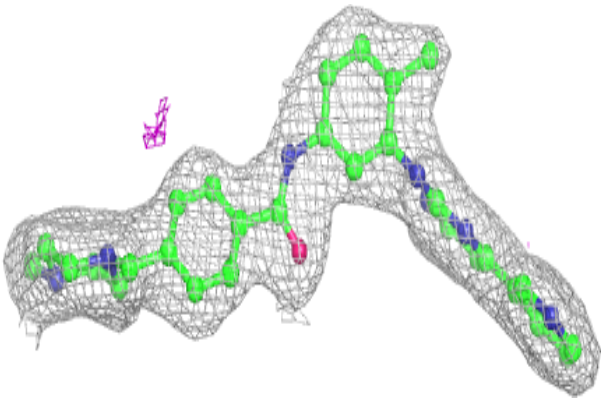


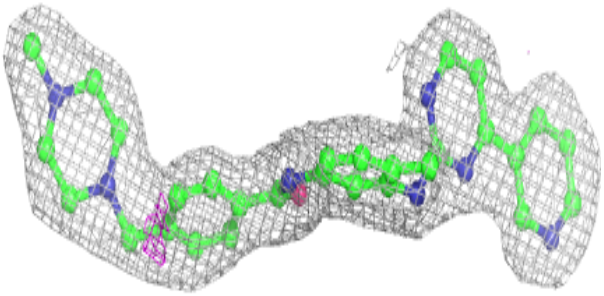


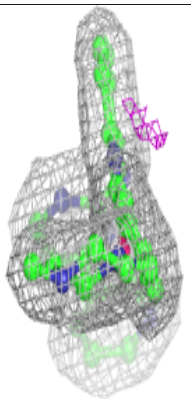


Electron density around STI A 603:

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

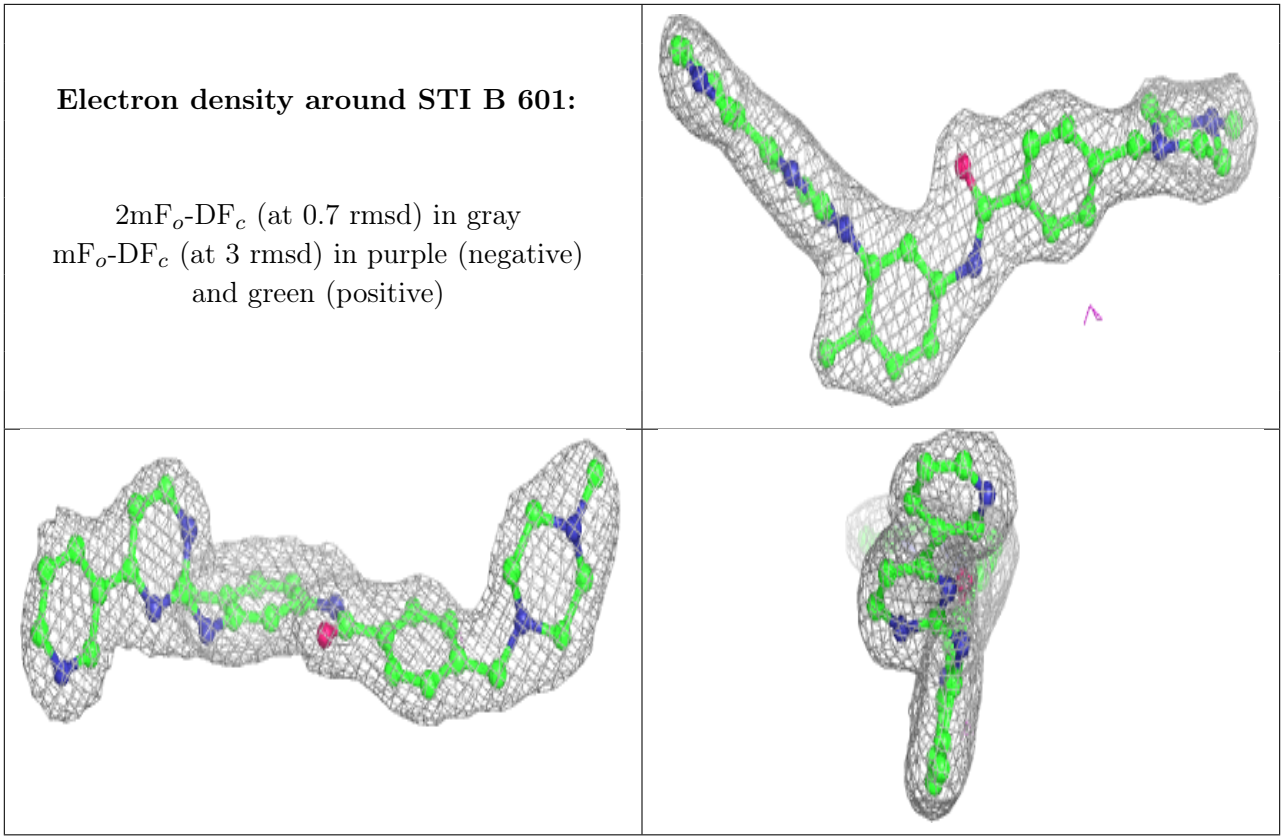






Electron density around STI B 601:

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



5.5 Other polymers (i)

There are no such residues in this entry.