

# wwPDB X-ray Structure Validation Summary Report (i)

### Oct 16, 2023 – 01:02 AM EDT

PDB ID : 8FJZ

Title : Crystal structure of HPK1 kinase domain T165E,S171E phosphomimetic mu-

tant in complex with 3-{4-[(3R,5S)-3-Amino-5-methylpiperidin-1-yl]-6-chloro-

7H-pyrrolo[2,3-d]pyrimidin-5-yl}benzonitrile

Authors : McTigue, M.; Johnson, E.; Cronin, C.

Deposited on : 2022-12-20

Resolution : 1.90 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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: 4.02b-467

Mogul: 1.8.5 (274361), CSD as541be (2020)

Xtriage (Phenix) : 1.13

EDS : 2.36

buster-report : 1.1.7 (2018)

Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)

 $Refmac \quad : \quad 5.8.0158$ 

CCP4 : 7.0.044 (Gargrove)

Ideal geometry (proteins) : Engh & Huber (2001) Ideal geometry (DNA, RNA) : Parkinson et al. (1996)

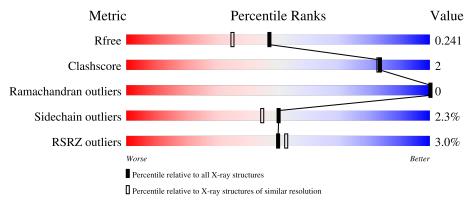
Validation Pipeline (wwPDB-VP) : 2.36

# 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 1.90 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	Similar resolution
Metric	$(\# \mathrm{Entries})$	$(\#  ext{Entries},  ext{ resolution range}( ext{Å}))$
$R_{free}$	130704	6207 (1.90-1.90)
Clashscore	141614	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)
RSRZ outliers	127900	6082 (1.90-1.90)

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 <=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	331	80%	7%	13%
1	В	331	79%	5%	14%
1	С	331	80%	7%	13%
1	D	331	79%	%	16%



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Mol	Chain	Length	Quality of chain						
1	Е	331	81%	•	15%				
1	F	331	74%	<b>%</b>	17%				



# 2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 14170 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 Mitogen-activated protein kinase kinase kinase kinase 1.

Mol	Chain	Residues		${f Atoms}$					AltConf	Trace
1	A	288	Total	С	N	О	S	0	0	0
1	A	200	2246	1447	384	404	11	U	0	
1	В	284	Total	С	N	О	S	0	0	0
1	Б	204	2220	1427	384	398	11	U	0	
1	С	288	Total	С	N	О	S	0	0	0
1		200	2246	1441	388	406	11	U		
1	D	279	Total	С	N	О	S	0	0	0
1	D	219	2181	1403	377	390	11	U		
1	Е	283	Total	С	N	О	S	0	0	0
1		200	2209	1418	385	396	10	U	0	
1	1 F	276	Total	С	N	О	S	0	0	0
1		276	2072	1326	360	376	10	U		

There are 156 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-23	MET	-	expression tag	UNP Q92918
A	-22	ALA	-	expression tag	UNP Q92918
A	-21	SER	-	expression tag	UNP Q92918
A	-20	HIS	-	expression tag	UNP Q92918
A	-19	HIS	-	expression tag	UNP Q92918
A	-18	HIS	-	expression tag	UNP Q92918
A	-17	HIS	-	expression tag	UNP Q92918
A	-16	HIS	-	expression tag	UNP Q92918
A	-15	HIS	-	expression tag	UNP Q92918
A	-14	ASP	-	expression tag	UNP Q92918
A	-13	TYR	-	expression tag	UNP Q92918
A	-12	ASP	-	expression tag	UNP Q92918
A	-11	GLY	-	expression tag	UNP Q92918
A	-10	ALA	-	expression tag	UNP Q92918
A	-9	THR	-	expression tag	UNP Q92918
A	-8	THR	-	expression tag	UNP Q92918
A	-7	GLU	-	expression tag	UNP Q92918



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Chain	Residue	Modelled	Actual	Comment	Reference
A	-6	ASN	-	expression tag	UNP Q92918
A	-5	LEU	-	expression tag	UNP Q92918
A	-4	TYR	_	expression tag	UNP Q92918
A	-3	PHE	-	expression tag	UNP Q92918
A	-2	GLN	-	expression tag	UNP Q92918
A	-1	GLY	-	expression tag	UNP Q92918
A	0	SER	-	expression tag	UNP Q92918
A	165	GLU	THR	engineered mutation	UNP Q92918
A	171	GLU	SER	engineered mutation	UNP Q92918
В	-23	MET	-	expression tag	UNP Q92918
В	-22	ALA	-	expression tag	UNP Q92918
В	-21	SER	-	expression tag	UNP Q92918
В	-20	HIS	-	expression tag	UNP Q92918
В	-19	HIS	-	expression tag	UNP Q92918
В	-18	HIS	-	expression tag	UNP Q92918
В	-17	HIS	-	expression tag	UNP Q92918
В	-16	HIS	_	expression tag	UNP Q92918
В	-15	HIS	-	expression tag	UNP Q92918
В	-14	ASP	-	expression tag	UNP Q92918
В	-13	TYR	-	expression tag	UNP Q92918
В	-12	ASP	-	expression tag	UNP Q92918
В	-11	GLY	-	expression tag	UNP Q92918
В	-10	ALA	-	expression tag	UNP Q92918
В	-9	THR	-	expression tag	UNP Q92918
В	-8	THR	-	expression tag	UNP Q92918
В	-7	GLU	-	expression tag	UNP Q92918
В	-6	ASN	-	expression tag	UNP Q92918
В	-5	LEU	-	expression tag	UNP Q92918
В	-4	TYR	-	expression tag	UNP Q92918
В	-3	PHE	-	expression tag	UNP Q92918
В	-2	GLN	-	expression tag	UNP Q92918
В	-1	GLY	-	expression tag	UNP Q92918
В	0	SER	-	expression tag	UNP Q92918
В	165	GLU	THR	engineered mutation	UNP Q92918
В	171	GLU	SER	engineered mutation	UNP Q92918
С	-23	MET	-	expression tag	UNP Q92918
С	-22	ALA	-	expression tag	UNP Q92918
С	-21	SER	-	expression tag	UNP Q92918
С	-20	HIS	-	expression tag	UNP Q92918
С	-19	HIS	-	expression tag	UNP Q92918
С	-18	HIS	-	expression tag	UNP Q92918
С	-17	HIS	-	expression tag	UNP Q92918



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Chain	Residue	Modelled  Modelled	Actual	Comment	Reference
С	-16	HIS	-	expression tag	UNP Q92918
С	-15	HIS	-	expression tag	UNP Q92918
С	-14	ASP	-	expression tag	UNP Q92918
С	-13	TYR	-	expression tag	UNP Q92918
С	-12	ASP	-	expression tag	UNP Q92918
С	-11	GLY	-	expression tag	UNP Q92918
С	-10	ALA	-	expression tag	UNP Q92918
С	-9	THR	-	expression tag	UNP Q92918
С	-8	THR	-	expression tag	UNP Q92918
С	-7	GLU	-	expression tag	UNP Q92918
С	-6	ASN	-	expression tag	UNP Q92918
С	-5	LEU	-	expression tag	UNP Q92918
С	-4	TYR	-	expression tag	UNP Q92918
С	-3	PHE	-	expression tag	UNP Q92918
С	-2	GLN	-	expression tag	UNP Q92918
С	-1	GLY	-	expression tag	UNP Q92918
С	0	SER	-	expression tag	UNP Q92918
С	165	GLU	THR	engineered mutation	UNP Q92918
С	171	GLU	SER	engineered mutation	UNP Q92918
D	-23	MET	-	expression tag	UNP Q92918
D	-22	ALA	-	expression tag	UNP Q92918
D	-21	SER	-	expression tag	UNP Q92918
D	-20	HIS	-	expression tag	UNP Q92918
D	-19	HIS	-	expression tag	UNP Q92918
D	-18	HIS	-	expression tag	UNP Q92918
D	-17	HIS	-	expression tag	UNP Q92918
D	-16	HIS	-	expression tag	UNP Q92918
D	-15	HIS	-	expression tag	UNP Q92918
D	-14	ASP	-	expression tag	UNP Q92918
D	-13	TYR	-	expression tag	UNP Q92918
D	-12	ASP	-	expression tag	UNP Q92918
D	-11	GLY	-	expression tag	UNP Q92918
D	-10	ALA	-	expression tag	UNP Q92918
D	-9	THR	-	expression tag	UNP Q92918
D	-8	THR	-	expression tag	UNP Q92918
D	-7	GLU	-	expression tag	UNP Q92918
D	-6	ASN		expression tag	UNP Q92918
D	-5	LEU	-	expression tag	UNP Q92918
D	-4	TYR	-	expression tag	UNP Q92918
D	-3	PHE	-	expression tag	UNP Q92918
D	-2	GLN	-	expression tag	UNP Q92918
D	-1	GLY	-	expression tag	UNP Q92918



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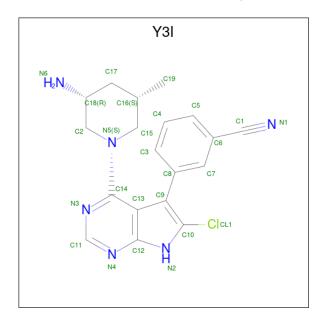
D	Chain	Residue	Modelled	Actual	Comment	Reference
D	D	0	SER	-	expression tag	UNP Q92918
E -23 MET - expression tag UNP Q92918 E -22 ALA - expression tag UNP Q92918 E -21 SER - expression tag UNP Q92918 E -20 HIS - expression tag UNP Q92918 E -19 HIS - expression tag UNP Q92918 E -19 HIS - expression tag UNP Q92918 E -18 HIS - expression tag UNP Q92918 E -18 HIS - expression tag UNP Q92918 E -16 HIS - expression tag UNP Q92918 E -16 HIS - expression tag UNP Q92918 E -11 HIS - expression tag UNP Q92918 E -12 ASP - expression tag UNP Q92918 E -13 TYR - expression tag UNP Q92918 E -11 GLY - expression tag UNP Q92918 E -11 GLY - expression tag UNP Q92918 E -10 ALA - expression tag UNP Q92918 E -3 THR - expression tag UNP Q92918 E -3 THR - expression tag UNP Q92918 E -4 TYR - expression tag UNP Q92918 E -5 LEU - expression tag UNP Q92918 E -6 ASN - expression tag UNP Q92918 E -1 GLY - expression tag UNP Q92918 E -2 GLN - expression tag UNP Q92918 E -1 GLY - expression tag UNP Q92918 F -22 ALA - expression tag UNP Q92918 F -23 MET - expression tag UNP Q92918 F -21 SER - expression tag UNP Q92918 F -21 SER - expression tag UNP Q92918 F -21 SER - expression tag UNP Q92918 F -18 HIS - expression tag UNP Q92918 F -19 HIS - expression tag UNP Q92918 F -16 HIS - expression tag UNP Q92918 F -16 HIS - expression tag UNP Q92918 F -17 HIS - expression tag UNP Q92918 F -18 HIS - expression tag UNP Q92918 F -11 GHUS - expression tag UNP Q92918 F -11 HIS - expression tag UNP Q92918 F -11	D	165	GLU	THR	engineered mutation	UNP Q92918
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E 0 SER - expression tag UNP Q92918 E 165 GLU THR engineered mutation UNP Q92918 E 171 GLU SER engineered mutation UNP Q92918 F -23 MET - expression tag UNP Q92918 F -22 ALA - expression tag UNP Q92918 F -21 SER - expression tag UNP Q92918 F -20 HIS - expression tag UNP Q92918 F -19 HIS - expression tag UNP Q92918 F -18 HIS - expression tag UNP Q92918 F -18 HIS - expression tag UNP Q92918 F -17 HIS - expression tag UNP Q92918 F -17 HIS - expression tag UNP Q92918 F -16 HIS - expression tag UNP Q92918 F -15 HIS - expression tag UNP Q92918 F -15 HIS - expression tag UNP Q92918 F -14 ASP - expression tag UNP Q92918 F -13 TYR - expression tag UNP Q92918 F -13 TYR - expression tag UNP Q92918	Е	-2	GLN	-	expression tag	UNP Q92918
E         165         GLU         THR         engineered mutation         UNP Q92918           E         171         GLU         SER         engineered mutation         UNP Q92918           F         -23         MET         -         expression tag         UNP Q92918           F         -22         ALA         -         expression tag         UNP Q92918           F         -21         SER         -         expression tag         UNP Q92918           F         -20         HIS         -         expression tag         UNP Q92918           F         -19         HIS         -         expression tag         UNP Q92918           F         -18         HIS         -         expression tag         UNP Q92918           F         -16         HIS         -         expression tag         UNP Q92918           F         -15         HIS         -         expression tag         UNP Q92918           F         -14         ASP         -         expression tag         UNP Q92918           F         -13         TYR         -         expression tag         UNP Q92918           F         -12         ASP         -         expression tag	Е	-1	GLY	_	expression tag	UNP Q92918
E         171         GLU         SER         engineered mutation         UNP Q92918           F         -23         MET         -         expression tag         UNP Q92918           F         -22         ALA         -         expression tag         UNP Q92918           F         -21         SER         -         expression tag         UNP Q92918           F         -20         HIS         -         expression tag         UNP Q92918           F         -19         HIS         -         expression tag         UNP Q92918           F         -18         HIS         -         expression tag         UNP Q92918           F         -16         HIS         -         expression tag         UNP Q92918           F         -16         HIS         -         expression tag         UNP Q92918           F         -15         HIS         -         expression tag         UNP Q92918           F         -14         ASP         -         expression tag         UNP Q92918           F         -13         TYR         -         expression tag         UNP Q92918           F         -12         ASP         -         expression tag	Е	0	SER	_	expression tag	UNP Q92918
F -23 MET - expression tag UNP Q92918 F -22 ALA - expression tag UNP Q92918 F -21 SER - expression tag UNP Q92918 F -20 HIS - expression tag UNP Q92918 F -19 HIS - expression tag UNP Q92918 F -18 HIS - expression tag UNP Q92918 F -17 HIS - expression tag UNP Q92918 F -16 HIS - expression tag UNP Q92918 F -15 HIS - expression tag UNP Q92918 F -15 HIS - expression tag UNP Q92918 F -14 ASP - expression tag UNP Q92918 F -13 TYR - expression tag UNP Q92918 F -13 TYR - expression tag UNP Q92918 F -13 TYR - expression tag UNP Q92918	Е	165	GLU	THR	engineered mutation	UNP Q92918
F         -22         ALA         -         expression tag         UNP Q92918           F         -21         SER         -         expression tag         UNP Q92918           F         -20         HIS         -         expression tag         UNP Q92918           F         -19         HIS         -         expression tag         UNP Q92918           F         -18         HIS         -         expression tag         UNP Q92918           F         -16         HIS         -         expression tag         UNP Q92918           F         -15         HIS         -         expression tag         UNP Q92918           F         -14         ASP         -         expression tag         UNP Q92918           F         -13         TYR         -         expression tag         UNP Q92918           F         -12         ASP         -         expression tag         UNP Q92918	Е	171	GLU	SER	engineered mutation	UNP Q92918
F         -21         SER         -         expression tag         UNP Q92918           F         -20         HIS         -         expression tag         UNP Q92918           F         -19         HIS         -         expression tag         UNP Q92918           F         -18         HIS         -         expression tag         UNP Q92918           F         -16         HIS         -         expression tag         UNP Q92918           F         -15         HIS         -         expression tag         UNP Q92918           F         -14         ASP         -         expression tag         UNP Q92918           F         -13         TYR         -         expression tag         UNP Q92918           F         -12         ASP         -         expression tag         UNP Q92918	F	-23	MET	-	expression tag	UNP Q92918
F -20 HIS - expression tag UNP Q92918 F -19 HIS - expression tag UNP Q92918 F -18 HIS - expression tag UNP Q92918 F -17 HIS - expression tag UNP Q92918 F -16 HIS - expression tag UNP Q92918 F -15 HIS - expression tag UNP Q92918 F -14 ASP - expression tag UNP Q92918 F -13 TYR - expression tag UNP Q92918 F -13 ASP - expression tag UNP Q92918 F -12 ASP - expression tag UNP Q92918	F	-22	ALA	-	expression tag	UNP Q92918
F         -19         HIS         -         expression tag         UNP Q92918           F         -18         HIS         -         expression tag         UNP Q92918           F         -17         HIS         -         expression tag         UNP Q92918           F         -16         HIS         -         expression tag         UNP Q92918           F         -15         HIS         -         expression tag         UNP Q92918           F         -14         ASP         -         expression tag         UNP Q92918           F         -13         TYR         -         expression tag         UNP Q92918           F         -12         ASP         -         expression tag         UNP Q92918	F	-21	SER	-	expression tag	UNP Q92918
F         -18         HIS         -         expression tag         UNP Q92918           F         -17         HIS         -         expression tag         UNP Q92918           F         -16         HIS         -         expression tag         UNP Q92918           F         -15         HIS         -         expression tag         UNP Q92918           F         -14         ASP         -         expression tag         UNP Q92918           F         -13         TYR         -         expression tag         UNP Q92918           F         -12         ASP         -         expression tag         UNP Q92918	F	-20	HIS	-	expression tag	UNP Q92918
F         -17         HIS         -         expression tag         UNP Q92918           F         -16         HIS         -         expression tag         UNP Q92918           F         -15         HIS         -         expression tag         UNP Q92918           F         -14         ASP         -         expression tag         UNP Q92918           F         -13         TYR         -         expression tag         UNP Q92918           F         -12         ASP         -         expression tag         UNP Q92918	F	-19	HIS	-	expression tag	UNP Q92918
F         -16         HIS         -         expression tag         UNP Q92918           F         -15         HIS         -         expression tag         UNP Q92918           F         -14         ASP         -         expression tag         UNP Q92918           F         -13         TYR         -         expression tag         UNP Q92918           F         -12         ASP         -         expression tag         UNP Q92918	F	-18	HIS	-	expression tag	UNP Q92918
F         -15         HIS         -         expression tag         UNP Q92918           F         -14         ASP         -         expression tag         UNP Q92918           F         -13         TYR         -         expression tag         UNP Q92918           F         -12         ASP         -         expression tag         UNP Q92918	F	-17	HIS	-	expression tag	UNP Q92918
F         -14         ASP         -         expression tag         UNP Q92918           F         -13         TYR         -         expression tag         UNP Q92918           F         -12         ASP         -         expression tag         UNP Q92918	F	-16	HIS	-	expression tag	UNP Q92918
F         -13         TYR         -         expression tag         UNP Q92918           F         -12         ASP         -         expression tag         UNP Q92918	F	-15	HIS	-	expression tag	UNP Q92918
F -12 ASP - expression tag UNP Q92918	F	-14	ASP	-	expression tag	UNP Q92918
	F	-13	TYR	-	expression tag	UNP Q92918
	F	-12	ASP	-	expression tag	UNP Q92918
F -11 GLY - expression tag UNP Q92918	F	-11	GLY	-	expression tag	UNP Q92918



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Chain	Residue	Modelled	Actual	Actual Comment	
F	-10	ALA	-	expression tag	UNP Q92918
F	-9	THR	-	expression tag	UNP Q92918
F	-8	THR	-	expression tag	UNP Q92918
F	-7	GLU	-	expression tag	UNP Q92918
F	-6	ASN	-	expression tag	UNP Q92918
F	-5	LEU	-	expression tag	UNP Q92918
F	-4	TYR	-	expression tag	UNP Q92918
F	-3	PHE	-	expression tag	UNP Q92918
F	-2	GLN	-	expression tag	UNP Q92918
F	-1	GLY	-	expression tag	UNP Q92918
F	0	SER	-	expression tag	UNP Q92918
F	165	GLU	THR	engineered mutation	UNP Q92918
F	171	GLU	SER	engineered mutation	UNP Q92918

• Molecule 2 is (3P)-3- $\{4-[(3R,5S)-3-amino-5-methylpiperidin-1-yl]-6-chloro-7H-pyrrolo[2, 3-d]pyrimidin-5-yl\}benzonitrile (three-letter code: Y3I) (formula: <math>C_{19}H_{19}ClN_6$ ) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
2	Δ	1	Total	С	Cl	N	0	0	
	Λ	1	26	19	1	6	U	U	
2	R	1	Total	С	Cl	N	0	0	
	Ъ	1	26	19	1	6		U	
2	С	1	Total	С	Cl	N	0	0	
2		1	26	19	1	6	0	U	
2	9 D	1	Total	С	Cl	N	0	0	
	1	26	19	1	6	0	U		



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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
2	2 E 1	1	Total	С	Cl	N	0	0	
		1	26	19	1	6	U		
2	Г	1	Total	С	Cl	N	0	0	
	2 F	1	26	19	1	6	0	U	

### • Molecule 3 is water.

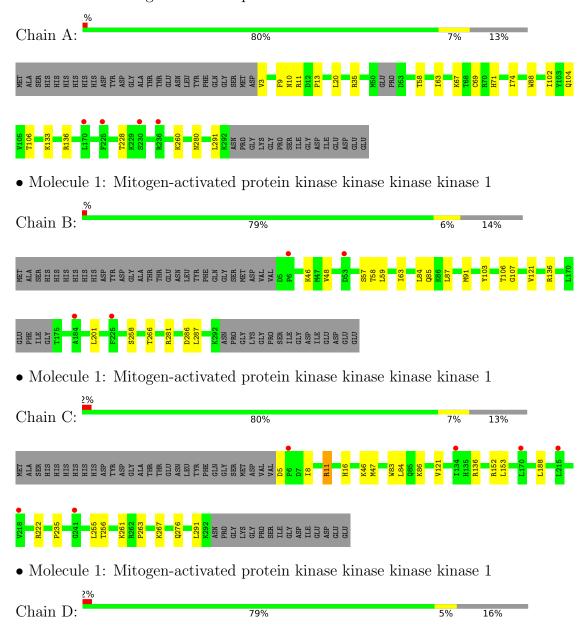
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	214	Total O 214 214	0	0
3	В	190	Total O 190 190	0	0
3	С	120	Total O 120 120	0	0
3	D	138	Total O 138 138	0	0
3	E	114	Total O 114 114	0	0
3	F	64	Total O 64 64	0	0



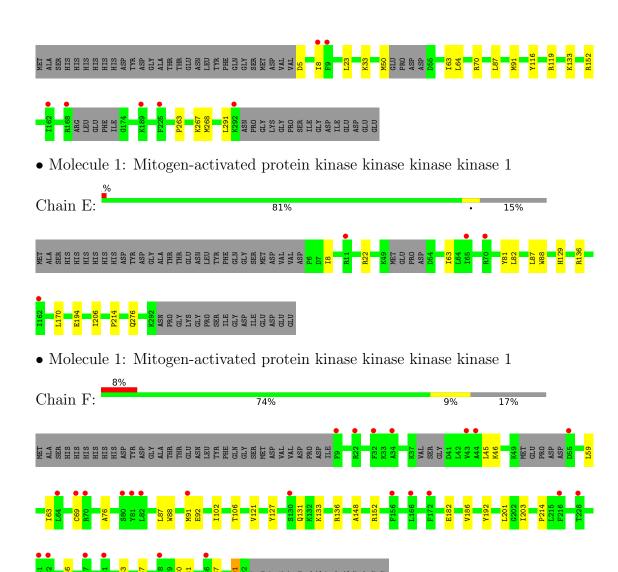
# 3 Residue-property plots (i)

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: Mitogen-activated protein kinase kinase kinase kinase 1









# 4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants	57.71Å 87.40Å 109.07Å	Donogitor
a, b, c, $\alpha$ , $\beta$ , $\gamma$	96.43° 99.99° 108.89°	Depositor
Resolution (Å)	81.34 - 1.90	Depositor
rtesolution (A)	81.34 - 1.90	EDS
% Data completeness	96.5 (81.34-1.90)	Depositor
(in resolution range)	96.5 (81.34-1.90)	EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$< I/\sigma(I) > 1$	2.18 (at 1.90Å)	Xtriage
Refinement program	BUSTER 2.11.8 (8-JUN-2022)	Depositor
P. P.	0.214 , 0.249	Depositor
$R, R_{free}$	0.206 , 0.241	DCC
$R_{free}$ test set	7448 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	33.7	Xtriage
Anisotropy	0.289	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$ , $B_{sol}(Å^2)$	0.34, 51.5	EDS
L-test for twinning <sup>2</sup>	$ < L > = 0.48, < L^2> = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	14170	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 15.59% of the height of the origin peak. No significant pseudotranslation is detected.

<sup>&</sup>lt;sup>2</sup>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.



<sup>&</sup>lt;sup>1</sup>Intensities estimated from amplitudes.

# 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: Y3I

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	
IVIOI	Chain	RMSZ	# Z  > 5	RMSZ	# Z  > 5
1	A	0.47	0/2293	0.60	0/3105
1	В	0.47	0/2267	0.59	0/3068
1	С	0.42	0/2294	0.56	0/3108
1	D	0.42	0/2226	0.55	0/3010
1	Е	0.38	0/2254	0.52	0/3048
1	F	0.33	0/2112	0.49	0/2865
All	All	0.42	0/13446	0.55	0/18204

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 (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	2246	0	2275	9	0
1	В	2220	0	2252	12	0
1	С	2246	0	2261	13	0
1	D	2181	0	2218	9	0
1	Е	2209	0	2249	5	0
1	F	2072	0	2027	18	0
2	A	26	0	0	0	0



n previous	paae
	n previous

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	В	26	0	0	2	0
2	С	26	0	0	1	0
2	D	26	0	0	1	0
2	Е	26	0	0	0	0
2	F	26	0	0	3	0
3	A	214	0	0	0	0
3	В	190	0	0	0	0
3	С	120	0	0	0	0
3	D	138	0	0	0	0
3	Ε	114	0	0	0	0
3	F	64	0	0	0	0
All	All	14170	0	13282	63	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 2.

The worst 5 of 63 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	$\begin{array}{c} {\rm Interatomic} \\ {\rm distance} \ ({\rm \AA}) \end{array}$	$\begin{array}{c} \text{Clash} \\ \text{overlap } (\text{\AA}) \end{array}$
1:F:76:ALA:HB3	1:F:92:GLU:HB2	1.75	0.69
1:E:8:ILE:HD11	1:E:82:LEU:HB2	1.80	0.63
1:B:103:TYR:HA	1:B:106:THR:HG22	1.81	0.61
1:D:116:TYR:HE1	1:D:119:ARG:NH1	1.99	0.61
1:F:91:MET:HE3	2:F:401:Y3I:CL1	2.40	0.59

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	284/331 (86%)	279 (98%)	5 (2%)	0	100 100



~ · · 1	c		
Continued	trom	nremous	naae.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Perce	ntiles
1	В	280/331 (85%)	274 (98%)	6 (2%)	0	100	100
1	C	286/331 (86%)	280 (98%)	6 (2%)	0	100	100
1	D	273/331 (82%)	265 (97%)	8 (3%)	0	100	100
1	E	279/331 (84%)	269 (96%)	10 (4%)	0	100	100
1	F	270/331 (82%)	263 (97%)	7 (3%)	0	100	100
All	All	1672/1986 (84%)	1630 (98%)	42 (2%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	239/281 (85%)	232 (97%)	7 (3%)	42 35
1	В	236/281 (84%)	231 (98%)	5 (2%)	53 48
1	С	237/281 (84%)	231 (98%)	6 (2%)	47 41
1	D	232/281 (83%)	226 (97%)	6 (3%)	46 39
1	E	234/281 (83%)	230 (98%)	4 (2%)	60 57
1	F	208/281 (74%)	204 (98%)	4 (2%)	57 53
All	All	1386/1686 (82%)	1354 (98%)	32 (2%)	50 45

5 of 32 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	F	152	ARG
1	F	236	ARG
1	С	11	ARG
1	В	281	ARG
1	F	280	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 10 such sidechains are listed below:



Mol	Chain	Res	Type
1	F	123	GLN
1	F	142	ASN
1	F	272	GLN
1	A	280	ASN
1	В	104	GLN

### 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 monosaccharides in this entry.

### 5.6 Ligand geometry (i)

6 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	Mol Type Chair		Res	Link	Вс	ond leng	ths	Bond angles		
MIOI	$Mol \mid Type \mid Chain \mid$	LIIIK		Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2	
2	Y3I	В	401	-	26,29,29	1.04	2 (7%)	28,42,42	0.70	0
2	Y3I	E	401	-	26,29,29	1.07	2 (7%)	28,42,42	0.90	2 (7%)
2	Y3I	С	401	-	26,29,29	1.21	4 (15%)	28,42,42	0.68	0
2	Y3I	D	401	-	26,29,29	1.02	2 (7%)	28,42,42	0.62	0
2	Y3I	F	401	-	26,29,29	1.03	1 (3%)	28,42,42	0.63	0
2	Y3I	A	401	-	26,29,29	1.09	1 (3%)	28,42,42	0.66	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	Y3I	В	401	-	-	0/10/22/22	0/4/4/4
2	Y3I	Е	401	-	-	0/10/22/22	0/4/4/4
2	Y3I	С	401	-	-	0/10/22/22	0/4/4/4
2	Y3I	D	401	-	-	0/10/22/22	0/4/4/4
2	Y3I	F	401	-	-	0/10/22/22	0/4/4/4
2	Y3I	A	401	-	-	0/10/22/22	0/4/4/4

The worst 5 of 12 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(A)	Ideal(A)
2	С	401	Y3I	C17-C18	3.26	1.60	1.53
2	F	401	Y3I	C9-C13	2.93	1.47	1.42
2	A	401	Y3I	C9-C13	2.69	1.46	1.42
2	Е	401	Y3I	C9-C13	2.58	1.46	1.42
2	D	401	Y3I	C9-C13	2.51	1.46	1.42

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Type Atoms		$Observed(^o)$	$\mathrm{Ideal}(^{o})$
2	Е	401	Y3I	C17-C18-C2	2.58	111.70	109.37
2	Е	401	Y3I	C9-C13-C12	-2.01	105.93	107.54

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

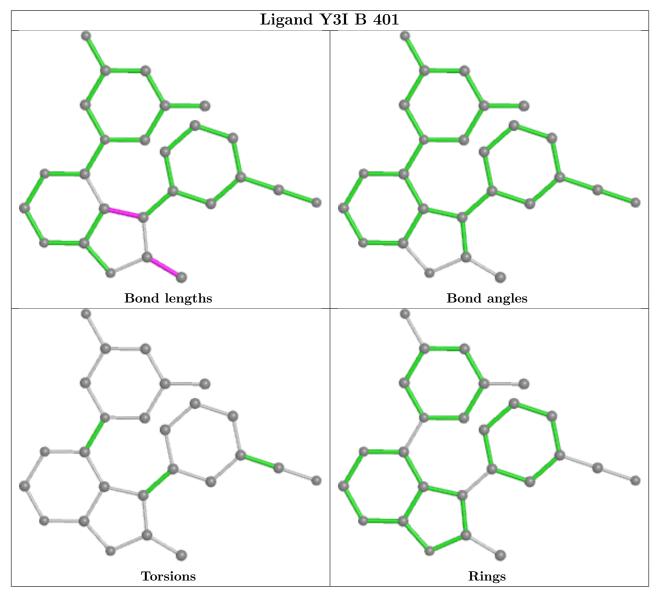
4 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	В	401	Y3I	2	0
2	С	401	Y3I	1	0
2	D	401	Y3I	1	0
2	F	401	Y3I	3	0

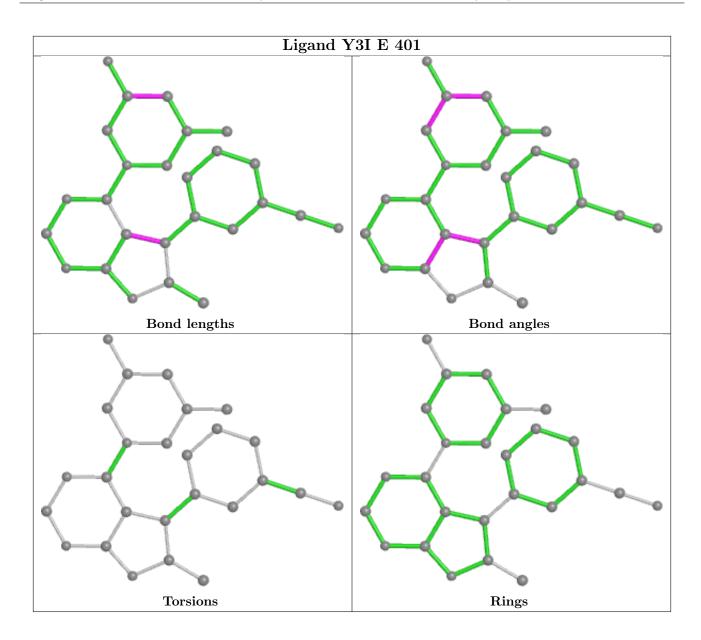
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier.



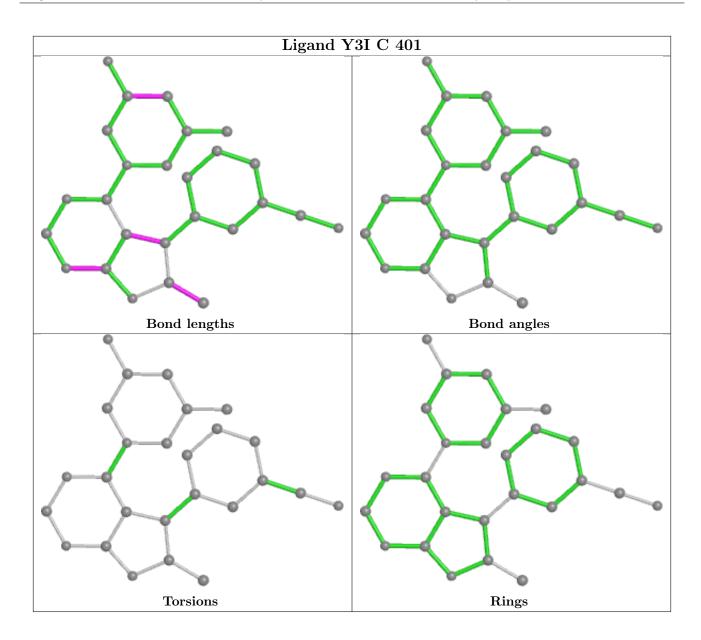
Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



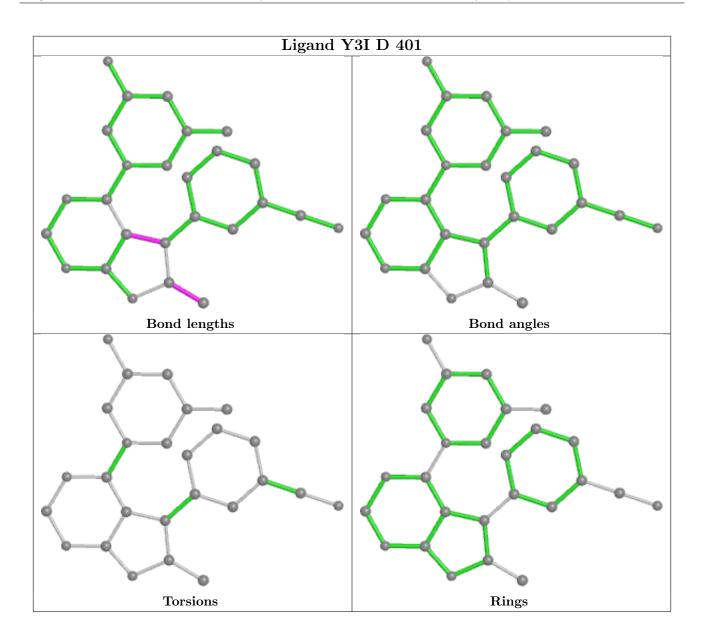




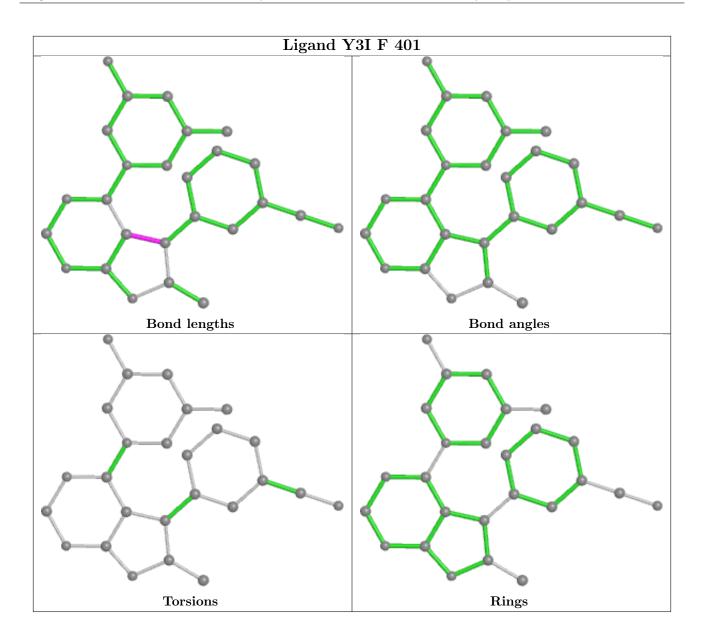




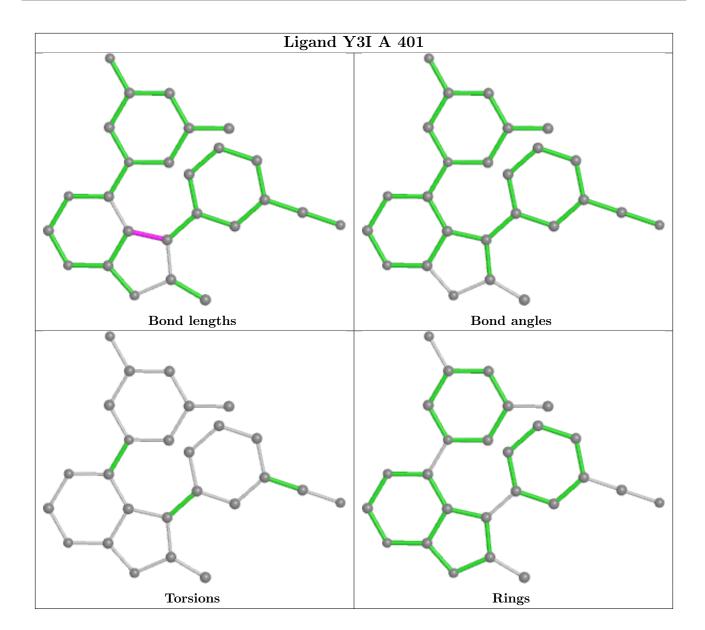












# 5.7 Other polymers (i)

There are no such residues in this entry.

# 5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.



# 6 Fit of model and data (i)

## 6.1 Protein, DNA and RNA chains (i)

In the following table, the column labelled '#RSRZ>2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median,  $95^{th}$  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>	$\# \mathrm{RSRZ}{>}2$	$OWAB(A^2)$	Q < 0.9
1	A	288/331 (87%)	-0.03	4 (1%) 75 77	21, 34, 56, 70	0
1	В	284/331 (85%)	-0.04	4 (1%) 75 77	22, 34, 59, 83	0
1	С	288/331 (87%)	0.11	6 (2%) 63 66	24, 42, 65, 73	0
1	D	279/331 (84%)	0.09	7 (2%) 57 60	22, 43, 69, 87	0
1	E	283/331 (85%)	0.12	4 (1%) 75 77	24, 45, 69, 84	0
1	F	276/331 (83%)	0.63	26 (9%) 8 9	25, 56, 82, 88	0
All	All	1698/1986 (85%)	0.14	51 (3%) 50 53	21, 42, 71, 88	0

The worst 5 of 51 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	43	VAL	4.9
1	F	64	LEU	4.5
1	F	81	TYR	4.5
1	F	32	PHE	4.3
1	F	231	GLY	4.3

# 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 monosaccharides 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,  $95^{th}$  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.

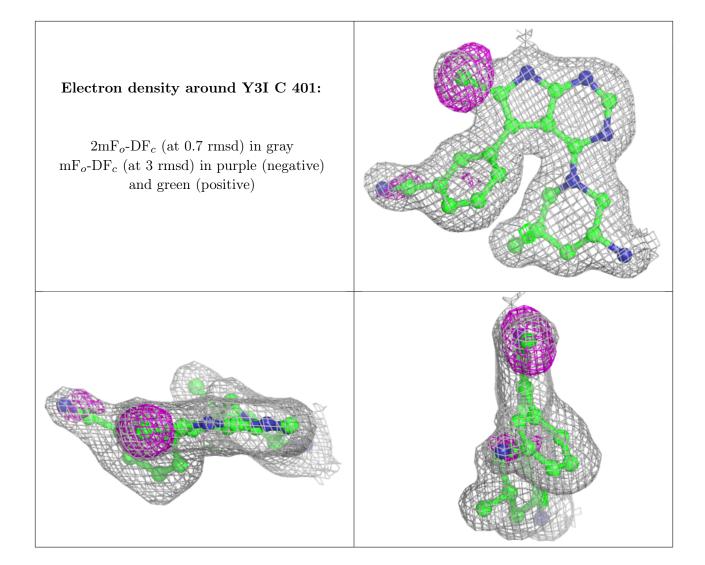
Mol	Type	Chain	Res	Atoms	RSCC	RSR	$\mathbf{B} ext{-}\mathbf{factors}(\mathbf{\mathring{A}}^2)$	Q<0.9
2	Y3I	F	401	26/26	0.78	0.14	56,57,59,62	0
2	Y3I	С	401	26/26	0.87	0.11	28,30,36,41	0
2	Y3I	A	401	26/26	0.88	0.11	25,27,31,41	0
2	Y3I	E	401	26/26	0.89	0.12	29,34,38,44	0
2	Y3I	В	401	26/26	0.89	0.12	24,28,34,42	0
2	Y3I	D	401	26/26	0.90	0.10	35,38,41,46	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.

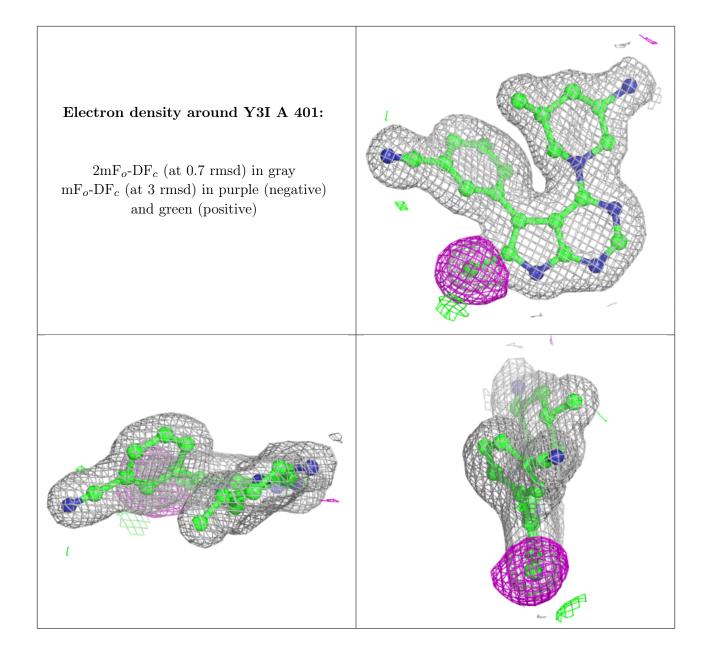


# Electron density around Y3I F 401: 2mF<sub>o</sub>-DF<sub>c</sub> (at 0.7 rmsd) in gray mF<sub>o</sub>-DF<sub>c</sub> (at 3 rmsd) in purple (negative) and green (positive)

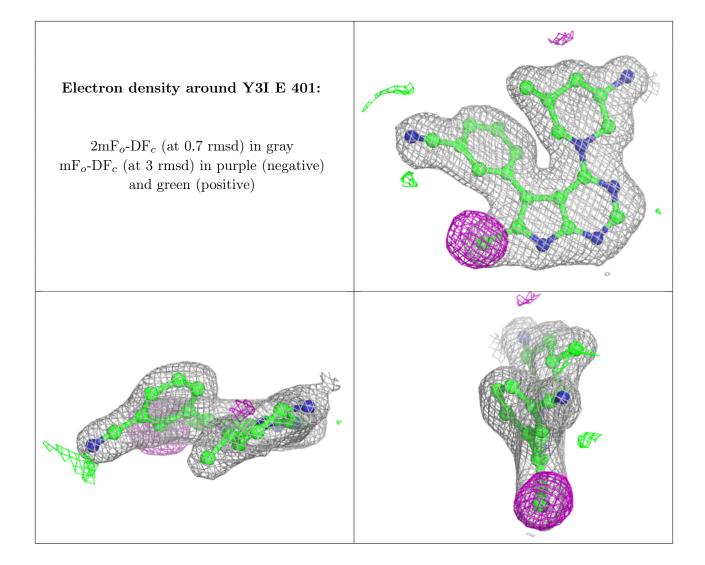




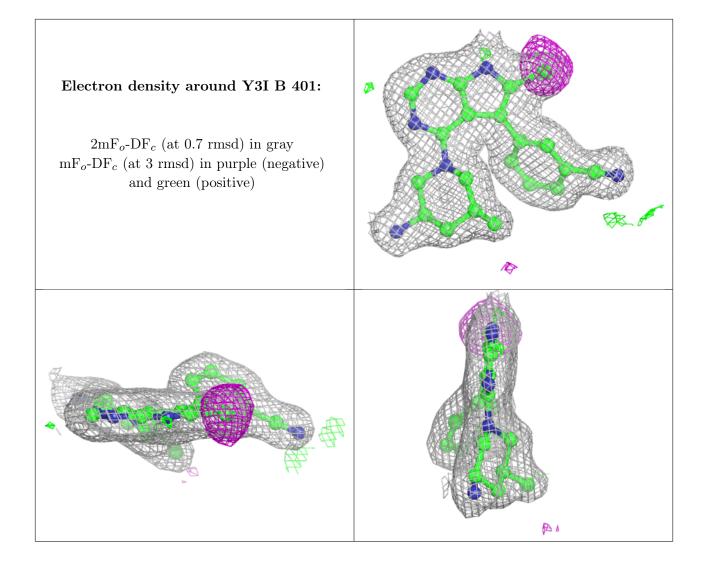




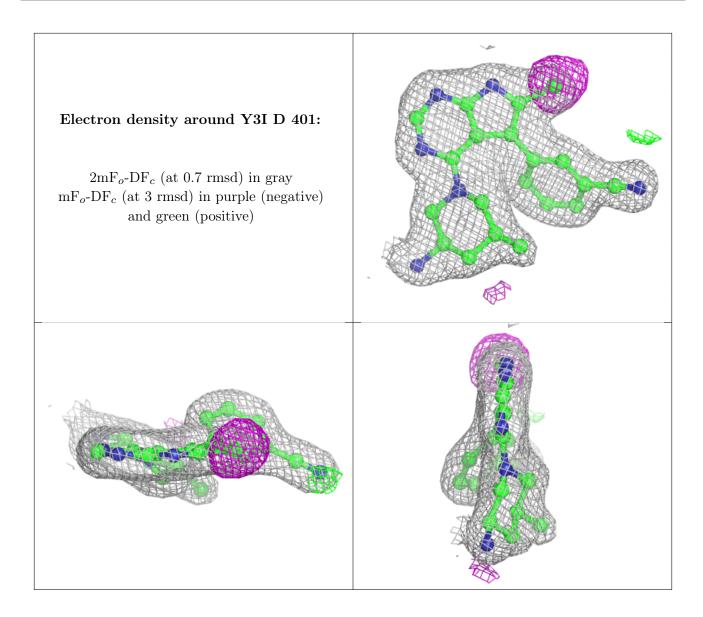












# 6.5 Other polymers (i)

There are no such residues in this entry.

