Full wwPDB X-ray Structure Validation Report ⓘ

May 9, 2022 – 11:30 am BST

PDB ID	:	7QIE
Title	:	Crystal Structure of Phosphatidylinositol 5-Phosphate 4-Kinase (PI5P4K2C) bound to an allosteric inhibitor
Authors	:	Howard, T.D.; Ogg, D.T.
Deposited on	:	2021-12-14
Resolution	:	2.39 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see references ⓘ) were used in the production of this report:

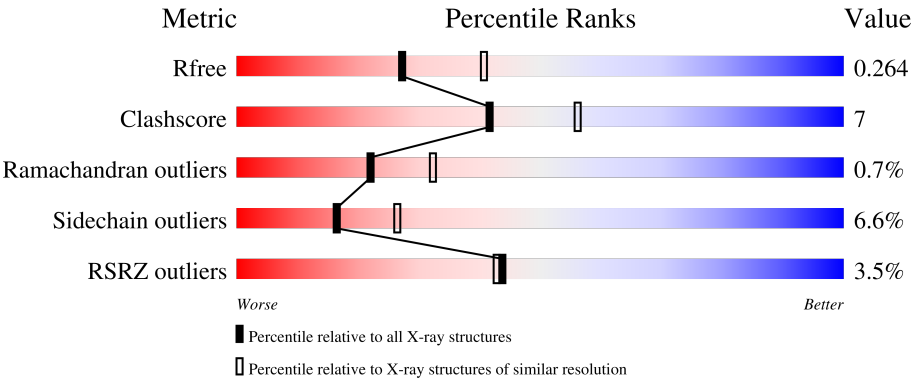
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.28.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0267
CCP4	:	7.1.010 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.28.1

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 2.39 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 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	363	64% 15% 19%
1	B	363	65% 13% 20%
1	C	363	6% 64% 15% 19%
1	D	363	2% 67% 17% 14%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 10055 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 Phosphatidylinositol 5-phosphate 4-kinase type-2 gamma.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	294	Total	C	N	O	S	0	0	0
			2417	1555	408	443	11			
1	B	292	Total	C	N	O	S	0	0	0
			2395	1537	407	440	11			
1	C	294	Total	C	N	O	S	0	0	0
			2398	1539	403	445	11			
1	D	311	Total	C	N	O	S	0	0	0
			2538	1632	427	468	11			

There are 228 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	17	MET	-	initiating methionine	UNP Q8TBX8
A	18	GLY	-	expression tag	UNP Q8TBX8
A	19	HIS	-	expression tag	UNP Q8TBX8
A	20	HIS	-	expression tag	UNP Q8TBX8
A	21	HIS	-	expression tag	UNP Q8TBX8
A	22	HIS	-	expression tag	UNP Q8TBX8
A	23	HIS	-	expression tag	UNP Q8TBX8
A	24	HIS	-	expression tag	UNP Q8TBX8
A	25	GLU	-	expression tag	UNP Q8TBX8
A	26	ASN	-	expression tag	UNP Q8TBX8
A	27	LEU	-	expression tag	UNP Q8TBX8
A	28	TYR	-	expression tag	UNP Q8TBX8
A	29	PHE	-	expression tag	UNP Q8TBX8
A	30	GLN	-	expression tag	UNP Q8TBX8
A	31	GLY	-	expression tag	UNP Q8TBX8
A	?	-	ALA	deletion	UNP Q8TBX8
A	?	-	PRO	deletion	UNP Q8TBX8
A	?	-	VAL	deletion	UNP Q8TBX8
A	?	-	ARG	deletion	UNP Q8TBX8
A	?	-	GLU	deletion	UNP Q8TBX8
A	?	-	ASP	deletion	UNP Q8TBX8

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	GLU	deletion	UNP Q8TBX8
A	?	-	SER	deletion	UNP Q8TBX8
A	?	-	GLU	deletion	UNP Q8TBX8
A	?	-	VAL	deletion	UNP Q8TBX8
A	?	-	ASP	deletion	UNP Q8TBX8
A	?	-	GLY	deletion	UNP Q8TBX8
A	?	-	ASP	deletion	UNP Q8TBX8
A	?	-	CYS	deletion	UNP Q8TBX8
A	?	-	SER	deletion	UNP Q8TBX8
A	?	-	LEU	deletion	UNP Q8TBX8
A	?	-	THR	deletion	UNP Q8TBX8
A	?	-	GLY	deletion	UNP Q8TBX8
A	?	-	PRO	deletion	UNP Q8TBX8
A	?	-	PRO	deletion	UNP Q8TBX8
A	?	-	ALA	deletion	UNP Q8TBX8
A	?	-	LEU	deletion	UNP Q8TBX8
A	?	-	VAL	deletion	UNP Q8TBX8
A	?	-	GLY	deletion	UNP Q8TBX8
A	?	-	SER	deletion	UNP Q8TBX8
A	?	-	TYR	deletion	UNP Q8TBX8
A	?	-	GLY	deletion	UNP Q8TBX8
A	?	-	THR	deletion	UNP Q8TBX8
A	?	-	SER	deletion	UNP Q8TBX8
A	?	-	PRO	deletion	UNP Q8TBX8
A	?	-	GLU	deletion	UNP Q8TBX8
A	?	-	GLY	deletion	UNP Q8TBX8
A	?	-	ILE	deletion	UNP Q8TBX8
A	?	-	GLY	deletion	UNP Q8TBX8
A	?	-	GLY	deletion	UNP Q8TBX8
A	?	-	TYR	deletion	UNP Q8TBX8
A	?	-	ILE	deletion	UNP Q8TBX8
A	?	-	HIS	deletion	UNP Q8TBX8
A	?	-	SER	deletion	UNP Q8TBX8
A	?	-	HIS	deletion	UNP Q8TBX8
A	?	-	ARG	deletion	UNP Q8TBX8
A	?	-	PRO	deletion	UNP Q8TBX8
B	17	MET	-	initiating methionine	UNP Q8TBX8
B	18	GLY	-	expression tag	UNP Q8TBX8
B	19	HIS	-	expression tag	UNP Q8TBX8
B	20	HIS	-	expression tag	UNP Q8TBX8
B	21	HIS	-	expression tag	UNP Q8TBX8
B	22	HIS	-	expression tag	UNP Q8TBX8

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	23	HIS	-	expression tag	UNP Q8TBX8
B	24	HIS	-	expression tag	UNP Q8TBX8
B	25	GLU	-	expression tag	UNP Q8TBX8
B	26	ASN	-	expression tag	UNP Q8TBX8
B	27	LEU	-	expression tag	UNP Q8TBX8
B	28	TYR	-	expression tag	UNP Q8TBX8
B	29	PHE	-	expression tag	UNP Q8TBX8
B	30	GLN	-	expression tag	UNP Q8TBX8
B	31	GLY	-	expression tag	UNP Q8TBX8
B	?	-	ALA	deletion	UNP Q8TBX8
B	?	-	PRO	deletion	UNP Q8TBX8
B	?	-	VAL	deletion	UNP Q8TBX8
B	?	-	ARG	deletion	UNP Q8TBX8
B	?	-	GLU	deletion	UNP Q8TBX8
B	?	-	ASP	deletion	UNP Q8TBX8
B	?	-	GLU	deletion	UNP Q8TBX8
B	?	-	SER	deletion	UNP Q8TBX8
B	?	-	GLU	deletion	UNP Q8TBX8
B	?	-	VAL	deletion	UNP Q8TBX8
B	?	-	ASP	deletion	UNP Q8TBX8
B	?	-	GLY	deletion	UNP Q8TBX8
B	?	-	ASP	deletion	UNP Q8TBX8
B	?	-	CYS	deletion	UNP Q8TBX8
B	?	-	SER	deletion	UNP Q8TBX8
B	?	-	LEU	deletion	UNP Q8TBX8
B	?	-	THR	deletion	UNP Q8TBX8
B	?	-	GLY	deletion	UNP Q8TBX8
B	?	-	PRO	deletion	UNP Q8TBX8
B	?	-	PRO	deletion	UNP Q8TBX8
B	?	-	ALA	deletion	UNP Q8TBX8
B	?	-	LEU	deletion	UNP Q8TBX8
B	?	-	VAL	deletion	UNP Q8TBX8
B	?	-	GLY	deletion	UNP Q8TBX8
B	?	-	SER	deletion	UNP Q8TBX8
B	?	-	TYR	deletion	UNP Q8TBX8
B	?	-	GLY	deletion	UNP Q8TBX8
B	?	-	THR	deletion	UNP Q8TBX8
B	?	-	SER	deletion	UNP Q8TBX8
B	?	-	PRO	deletion	UNP Q8TBX8
B	?	-	GLU	deletion	UNP Q8TBX8
B	?	-	GLY	deletion	UNP Q8TBX8
B	?	-	ILE	deletion	UNP Q8TBX8

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	?	-	GLY	deletion	UNP Q8TBX8
B	?	-	GLY	deletion	UNP Q8TBX8
B	?	-	TYR	deletion	UNP Q8TBX8
B	?	-	ILE	deletion	UNP Q8TBX8
B	?	-	HIS	deletion	UNP Q8TBX8
B	?	-	SER	deletion	UNP Q8TBX8
B	?	-	HIS	deletion	UNP Q8TBX8
B	?	-	ARG	deletion	UNP Q8TBX8
B	?	-	PRO	deletion	UNP Q8TBX8
C	17	MET	-	initiating methionine	UNP Q8TBX8
C	18	GLY	-	expression tag	UNP Q8TBX8
C	19	HIS	-	expression tag	UNP Q8TBX8
C	20	HIS	-	expression tag	UNP Q8TBX8
C	21	HIS	-	expression tag	UNP Q8TBX8
C	22	HIS	-	expression tag	UNP Q8TBX8
C	23	HIS	-	expression tag	UNP Q8TBX8
C	24	HIS	-	expression tag	UNP Q8TBX8
C	25	GLU	-	expression tag	UNP Q8TBX8
C	26	ASN	-	expression tag	UNP Q8TBX8
C	27	LEU	-	expression tag	UNP Q8TBX8
C	28	TYR	-	expression tag	UNP Q8TBX8
C	29	PHE	-	expression tag	UNP Q8TBX8
C	30	GLN	-	expression tag	UNP Q8TBX8
C	31	GLY	-	expression tag	UNP Q8TBX8
C	?	-	ALA	deletion	UNP Q8TBX8
C	?	-	PRO	deletion	UNP Q8TBX8
C	?	-	VAL	deletion	UNP Q8TBX8
C	?	-	ARG	deletion	UNP Q8TBX8
C	?	-	GLU	deletion	UNP Q8TBX8
C	?	-	ASP	deletion	UNP Q8TBX8
C	?	-	GLU	deletion	UNP Q8TBX8
C	?	-	SER	deletion	UNP Q8TBX8
C	?	-	GLU	deletion	UNP Q8TBX8
C	?	-	VAL	deletion	UNP Q8TBX8
C	?	-	ASP	deletion	UNP Q8TBX8
C	?	-	GLY	deletion	UNP Q8TBX8
C	?	-	ASP	deletion	UNP Q8TBX8
C	?	-	CYS	deletion	UNP Q8TBX8
C	?	-	SER	deletion	UNP Q8TBX8
C	?	-	LEU	deletion	UNP Q8TBX8
C	?	-	THR	deletion	UNP Q8TBX8
C	?	-	GLY	deletion	UNP Q8TBX8

Continued on next page...

Continued from previous page...

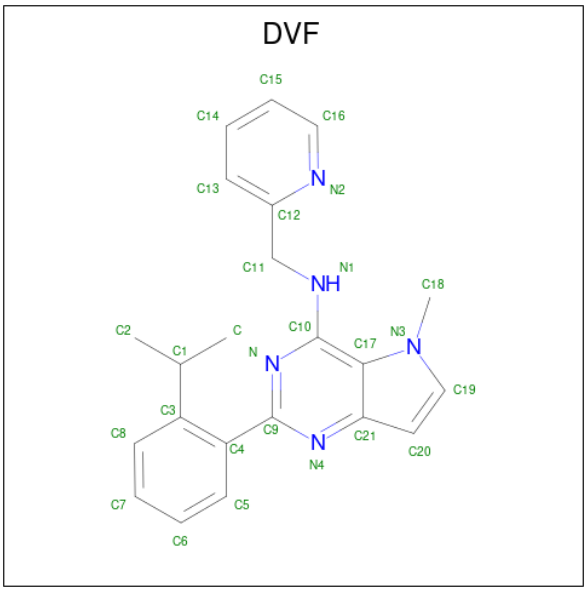
Chain	Residue	Modelled	Actual	Comment	Reference
C	?	-	PRO	deletion	UNP Q8TBX8
C	?	-	PRO	deletion	UNP Q8TBX8
C	?	-	ALA	deletion	UNP Q8TBX8
C	?	-	LEU	deletion	UNP Q8TBX8
C	?	-	VAL	deletion	UNP Q8TBX8
C	?	-	GLY	deletion	UNP Q8TBX8
C	?	-	SER	deletion	UNP Q8TBX8
C	?	-	TYR	deletion	UNP Q8TBX8
C	?	-	GLY	deletion	UNP Q8TBX8
C	?	-	THR	deletion	UNP Q8TBX8
C	?	-	SER	deletion	UNP Q8TBX8
C	?	-	PRO	deletion	UNP Q8TBX8
C	?	-	GLU	deletion	UNP Q8TBX8
C	?	-	GLY	deletion	UNP Q8TBX8
C	?	-	ILE	deletion	UNP Q8TBX8
C	?	-	GLY	deletion	UNP Q8TBX8
C	?	-	GLY	deletion	UNP Q8TBX8
C	?	-	TYR	deletion	UNP Q8TBX8
C	?	-	ILE	deletion	UNP Q8TBX8
C	?	-	HIS	deletion	UNP Q8TBX8
C	?	-	SER	deletion	UNP Q8TBX8
C	?	-	HIS	deletion	UNP Q8TBX8
C	?	-	ARG	deletion	UNP Q8TBX8
C	?	-	PRO	deletion	UNP Q8TBX8
D	17	MET	-	initiating methionine	UNP Q8TBX8
D	18	GLY	-	expression tag	UNP Q8TBX8
D	19	HIS	-	expression tag	UNP Q8TBX8
D	20	HIS	-	expression tag	UNP Q8TBX8
D	21	HIS	-	expression tag	UNP Q8TBX8
D	22	HIS	-	expression tag	UNP Q8TBX8
D	23	HIS	-	expression tag	UNP Q8TBX8
D	24	HIS	-	expression tag	UNP Q8TBX8
D	25	GLU	-	expression tag	UNP Q8TBX8
D	26	ASN	-	expression tag	UNP Q8TBX8
D	27	LEU	-	expression tag	UNP Q8TBX8
D	28	TYR	-	expression tag	UNP Q8TBX8
D	29	PHE	-	expression tag	UNP Q8TBX8
D	30	GLN	-	expression tag	UNP Q8TBX8
D	31	GLY	-	expression tag	UNP Q8TBX8
D	?	-	ALA	deletion	UNP Q8TBX8
D	?	-	PRO	deletion	UNP Q8TBX8
D	?	-	VAL	deletion	UNP Q8TBX8

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
D	?	-	ARG	deletion	UNP Q8TBX8
D	?	-	GLU	deletion	UNP Q8TBX8
D	?	-	ASP	deletion	UNP Q8TBX8
D	?	-	GLU	deletion	UNP Q8TBX8
D	?	-	SER	deletion	UNP Q8TBX8
D	?	-	GLU	deletion	UNP Q8TBX8
D	?	-	VAL	deletion	UNP Q8TBX8
D	?	-	ASP	deletion	UNP Q8TBX8
D	?	-	GLY	deletion	UNP Q8TBX8
D	?	-	ASP	deletion	UNP Q8TBX8
D	?	-	CYS	deletion	UNP Q8TBX8
D	?	-	SER	deletion	UNP Q8TBX8
D	?	-	LEU	deletion	UNP Q8TBX8
D	?	-	THR	deletion	UNP Q8TBX8
D	?	-	GLY	deletion	UNP Q8TBX8
D	?	-	PRO	deletion	UNP Q8TBX8
D	?	-	PRO	deletion	UNP Q8TBX8
D	?	-	ALA	deletion	UNP Q8TBX8
D	?	-	LEU	deletion	UNP Q8TBX8
D	?	-	VAL	deletion	UNP Q8TBX8
D	?	-	GLY	deletion	UNP Q8TBX8
D	?	-	SER	deletion	UNP Q8TBX8
D	?	-	TYR	deletion	UNP Q8TBX8
D	?	-	GLY	deletion	UNP Q8TBX8
D	?	-	THR	deletion	UNP Q8TBX8
D	?	-	SER	deletion	UNP Q8TBX8
D	?	-	PRO	deletion	UNP Q8TBX8
D	?	-	GLU	deletion	UNP Q8TBX8
D	?	-	GLY	deletion	UNP Q8TBX8
D	?	-	ILE	deletion	UNP Q8TBX8
D	?	-	GLY	deletion	UNP Q8TBX8
D	?	-	GLY	deletion	UNP Q8TBX8
D	?	-	TYR	deletion	UNP Q8TBX8
D	?	-	ILE	deletion	UNP Q8TBX8
D	?	-	HIS	deletion	UNP Q8TBX8
D	?	-	SER	deletion	UNP Q8TBX8
D	?	-	HIS	deletion	UNP Q8TBX8
D	?	-	ARG	deletion	UNP Q8TBX8
D	?	-	PRO	deletion	UNP Q8TBX8

- Molecule 2 is 5-methyl-2-(2-propan-2-ylphenyl)- {N}-(pyridin-2-ylmethyl)pyrrolo[3,2-d]pyrimidin-4-amine (three-letter code: DVF) (formula: $C_{22}H_{23}N_5$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C N 27 22 5	0	0
2	B	1	Total C N 27 22 5	0	0
2	C	1	Total C N 27 22 5	0	0
2	D	1	Total C N 27 22 5	0	0

- Molecule 3 is water.

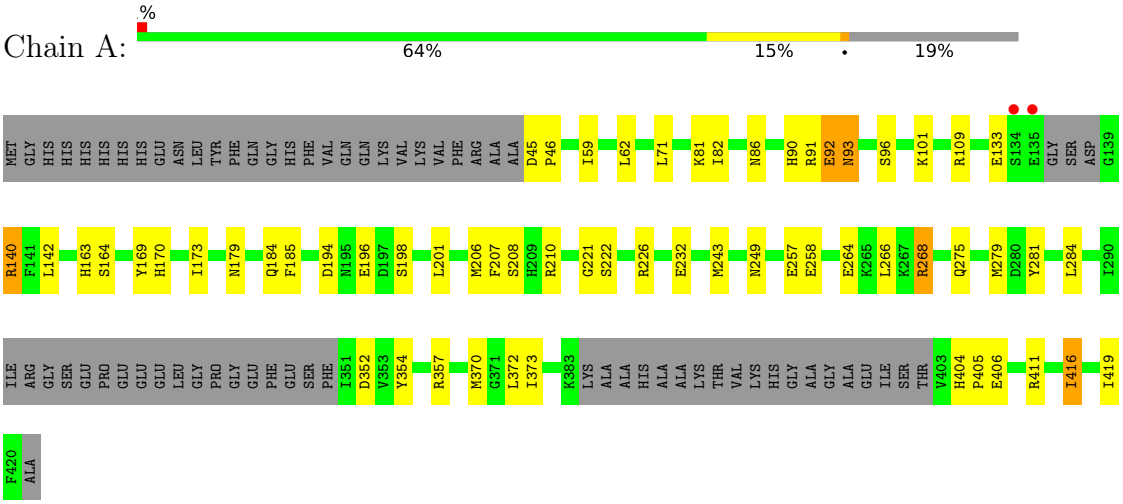
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	56	Total O 56 56	0	0
3	B	69	Total O 69 69	0	0
3	C	37	Total O 37 37	0	0
3	D	37	Total O 37 37	0	0

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.

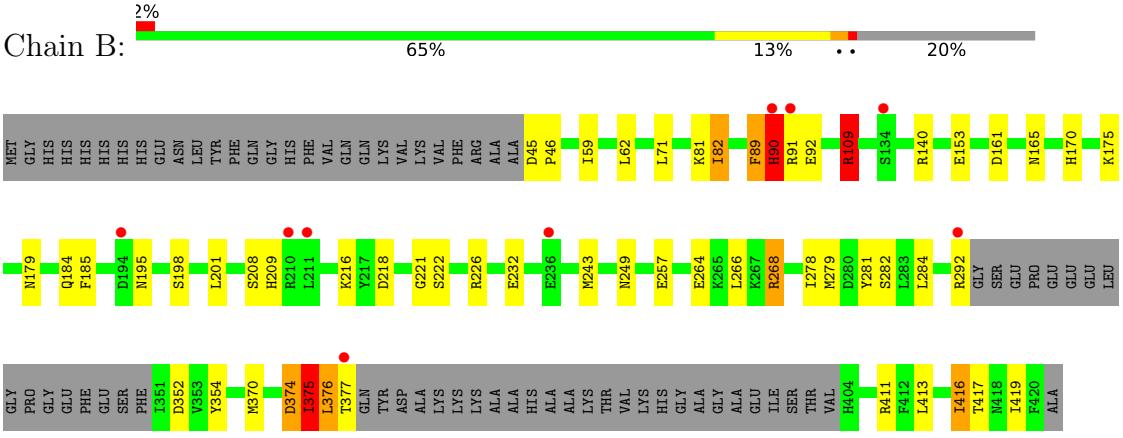
• Molecule 1: Phosphatidylinositol 5-phosphate 4-kinase type-2 gamma

Chain A:



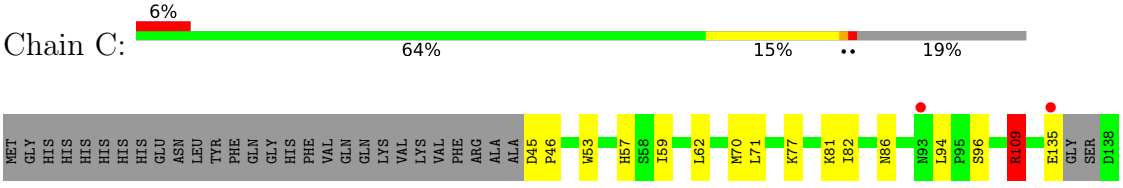
• Molecule 1: Phosphatidylinositol 5-phosphate 4-kinase type-2 gamma

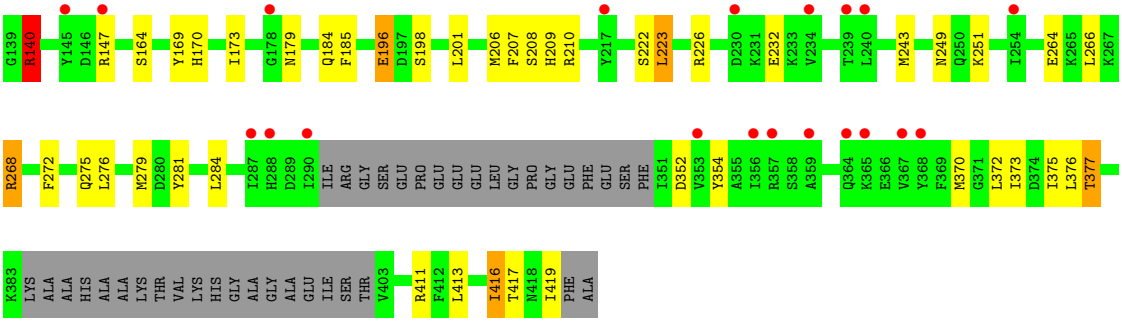
Chain B:



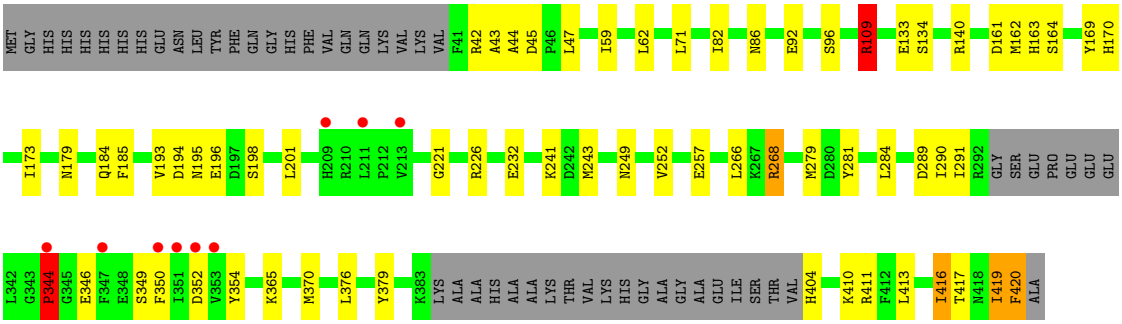
• Molecule 1: Phosphatidylinositol 5-phosphate 4-kinase type-2 gamma

Chain C:





• Molecule 1: Phosphatidylinositol 5-phosphate 4-kinase type-2 gamma



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	49.41Å 114.79Å 146.85Å 90.00° 95.51° 90.00°	Depositor
Resolution (Å)	146.17 – 2.39 146.17 – 2.39	Depositor EDS
% Data completeness (in resolution range)	56.4 (146.17-2.39) 56.4 (146.17-2.39)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.65 (at 2.40Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.211 , 0.266 0.213 , 0.264	Depositor DCC
R_{free} test set	1799 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å^2)	46.6	Xtriage
Anisotropy	0.338	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	(Not available) , (Not available)	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	10055	wwPDB-VP
Average B, all atoms (Å^2)	61.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.38% 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.

5 Model quality

5.1 Standard geometry

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

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	0.71	0/2471	0.89	0/3332
1	B	0.73	0/2449	0.91	2/3302 (0.1%)
1	C	0.70	0/2451	0.87	3/3309 (0.1%)
1	D	0.71	0/2597	0.91	2/3504 (0.1%)
All	All	0.72	0/9968	0.90	7/13447 (0.1%)

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
1	B	0	3
1	D	0	2
All	All	0	6

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	420	PHE	CA-C-O	9.25	139.53	120.10
1	C	109	ARG	NE-CZ-NH2	-5.89	117.35	120.30
1	B	374	ASP	CB-CA-C	5.55	121.49	110.40
1	C	140	ARG	NE-CZ-NH1	-5.37	117.61	120.30
1	D	109	ARG	NE-CZ-NH2	-5.32	117.64	120.30
1	C	140	ARG	CG-CD-NE	-5.28	100.71	111.80
1	B	109	ARG	NE-CZ-NH2	-5.27	117.67	120.30

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	92	GLU	Peptide
1	B	374	ASP	Peptide
1	B	375	ILE	Peptide
1	B	89	PHE	Peptide
1	D	419	ILE	Peptide
1	D	43	ALA	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	2417	0	2399	33	0
1	B	2395	0	2376	35	0
1	C	2398	0	2355	36	0
1	D	2538	0	2496	34	0
2	A	27	0	0	0	0
2	B	27	0	0	1	0
2	C	27	0	0	0	0
2	D	27	0	0	1	0
3	A	56	0	0	1	0
3	B	69	0	0	0	0
3	C	37	0	0	2	0
3	D	37	0	0	3	0
All	All	10055	0	9626	137	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 7.

All (137) 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:D:226:ARG:NH1	3:D:601:HOH:O	1.68	1.20
1:B:376:LEU:O	1:B:377:THR:HG22	1.42	1.17
1:D:226:ARG:HG2	1:D:241:LYS:HB3	1.48	0.93
1:D:252:VAL:O	1:D:420:PHE:HB2	1.76	0.85

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:372:LEU:O	1:C:373:ILE:HD12	1.80	0.81
1:A:372:LEU:O	1:A:373:ILE:HD12	1.80	0.81
1:A:404:HIS:CD2	1:A:405:PRO:HD2	2.19	0.77
1:A:221:GLY:O	1:A:411:ARG:HD3	1.89	0.73
1:B:266:LEU:HD22	1:B:416:ILE:HD11	1.71	0.72
1:B:376:LEU:O	1:B:377:THR:CG2	2.30	0.72
1:B:161:ASP:HB3	1:B:377:THR:HG23	1.73	0.70
1:A:90:HIS:O	1:A:92:GLU:N	2.24	0.70
1:B:90:HIS:O	1:B:92:GLU:N	2.24	0.70
1:A:266:LEU:HD22	1:A:416:ILE:HD11	1.74	0.69
1:C:206:MET:SD	1:C:373:ILE:HD11	2.33	0.69
1:D:42:ARG:HB3	1:D:44:ALA:O	1.97	0.64
1:D:266:LEU:HD22	1:D:416:ILE:HD11	1.79	0.64
1:B:90:HIS:O	1:B:90:HIS:ND1	2.31	0.63
1:A:179:ASN:O	1:A:268:ARG:NH2	2.32	0.63
1:C:179:ASN:O	1:C:268:ARG:NH2	2.31	0.63
1:D:179:ASN:O	1:D:268:ARG:NH2	2.33	0.61
1:B:221:GLY:O	1:B:411:ARG:NH1	2.35	0.60
1:D:290:ILE:HG12	1:D:365:LYS:O	2.01	0.60
1:D:252:VAL:O	1:D:420:PHE:CB	2.50	0.60
1:B:179:ASN:O	1:B:268:ARG:NH2	2.35	0.59
1:D:133:GLU:OE2	1:D:140:ARG:NH1	2.34	0.59
1:C:147:ARG:HB2	1:C:209:HIS:HA	1.86	0.58
1:D:221:GLY:O	1:D:411:ARG:CD	2.52	0.57
1:B:165:ASN:OD1	1:B:377:THR:HG21	2.04	0.57
1:B:89:PHE:CE2	1:B:90:HIS:HD2	2.23	0.57
1:B:413:LEU:O	1:B:417:THR:HG23	2.05	0.57
1:A:221:GLY:O	1:A:411:ARG:CD	2.53	0.56
1:A:194:ASP:O	1:A:194:ASP:OD1	2.23	0.56
1:C:373:ILE:HA	1:C:377:THR:HG22	1.88	0.56
1:B:195:ASN:O	1:B:195:ASN:OD1	2.25	0.55
1:B:416:ILE:O	1:B:419:ILE:HG12	2.08	0.54
1:D:352:ASP:HB2	3:D:629:HOH:O	2.08	0.54
1:A:206:MET:SD	1:A:373:ILE:HD11	2.48	0.53
1:A:45:ASP:OD2	1:A:140:ARG:NH1	2.41	0.53
1:C:206:MET:SD	1:C:373:ILE:CD1	2.96	0.53
1:A:416:ILE:O	1:A:419:ILE:HG12	2.09	0.52
1:B:218:ASP:O	1:B:226:ARG:NH2	2.41	0.52
1:D:413:LEU:O	1:D:417:THR:HG23	2.10	0.52
1:C:223:LEU:C	1:C:223:LEU:HD13	2.29	0.52
1:C:413:LEU:O	1:C:417:THR:HG23	2.10	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:45:ASP:CG	1:D:140:ARG:HH22	2.13	0.52
1:C:62:LEU:O	1:C:109:ARG:NH2	2.42	0.52
1:A:206:MET:SD	1:A:373:ILE:CD1	2.98	0.51
1:B:185:PHE:CD1	1:B:201:LEU:HD11	2.46	0.51
1:B:278:ILE:CD1	1:B:377:THR:HB	2.40	0.51
1:C:266:LEU:HD22	1:C:416:ILE:HD11	1.93	0.51
1:D:416:ILE:O	1:D:419:ILE:HG12	2.10	0.51
1:A:81:LYS:O	1:A:82:ILE:HD13	2.10	0.51
1:A:62:LEU:O	1:A:109:ARG:NH2	2.44	0.51
1:C:416:ILE:O	1:C:419:ILE:HG12	2.11	0.51
1:C:45:ASP:OD1	1:C:46:PRO:HD2	2.10	0.50
1:B:185:PHE:CE2	1:B:376:LEU:HD22	2.46	0.50
1:D:185:PHE:CD1	1:D:201:LEU:HD11	2.47	0.50
1:B:375:ILE:C	1:B:377:THR:H	2.15	0.50
1:A:90:HIS:O	1:A:90:HIS:ND1	2.44	0.49
1:A:185:PHE:CD1	1:A:201:LEU:HD11	2.48	0.49
1:D:62:LEU:O	1:D:109:ARG:NH2	2.46	0.49
1:C:86:ASN:O	1:C:96:SER:HB2	2.13	0.49
1:C:185:PHE:CD1	1:C:201:LEU:HD11	2.48	0.48
1:B:81:LYS:O	1:B:82:ILE:HD13	2.13	0.48
1:B:222:SER:HA	1:B:411:ARG:HH12	1.78	0.48
1:B:62:LEU:O	1:B:109:ARG:NH2	2.47	0.48
1:A:71:LEU:HD12	1:A:170:HIS:CE1	2.49	0.48
1:A:86:ASN:O	1:A:96:SER:HB2	2.14	0.47
1:C:81:LYS:O	1:C:82:ILE:HD13	2.14	0.47
1:D:266:LEU:CD2	1:D:416:ILE:HD11	2.42	0.47
1:C:53:TRP:CD1	1:C:94:LEU:HD11	2.49	0.47
1:D:221:GLY:O	1:D:411:ARG:HD2	2.14	0.47
1:A:266:LEU:CD2	1:A:416:ILE:HD11	2.43	0.47
1:D:47:LEU:CD2	1:D:140:ARG:HG3	2.45	0.47
1:B:90:HIS:O	1:B:90:HIS:CG	2.68	0.46
1:D:226:ARG:O	1:D:243:MET:HB2	2.16	0.46
1:A:184:GLN:HG3	1:A:354:TYR:OH	2.16	0.46
1:A:45:ASP:OD1	1:A:46:PRO:HD2	2.15	0.46
1:B:216:LYS:HE3	2:B:501:DVF:C5	2.45	0.46
1:D:379:TYR:HB2	3:D:628:HOH:O	2.14	0.46
1:D:344:PRO:HD2	1:D:346:GLU:HG2	1.96	0.46
1:D:71:LEU:HD12	1:D:170:HIS:CE1	2.50	0.46
1:C:57:HIS:HE1	3:C:630:HOH:O	1.98	0.45
1:B:279:MET:HA	1:B:281:TYR:CE1	2.51	0.45
1:C:71:LEU:HD12	1:C:170:HIS:CE1	2.52	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:284:LEU:O	1:A:370:MET:HA	2.17	0.45
1:B:208:SER:HA	1:B:352:ASP:OD1	2.17	0.45
1:C:184:GLN:HG3	1:C:354:TYR:OH	2.17	0.45
1:C:372:LEU:C	1:C:373:ILE:HD12	2.36	0.45
1:A:404:HIS:CE1	1:A:406:GLU:HB3	2.52	0.45
1:D:194:ASP:O	1:D:195:ASN:CG	2.54	0.45
1:A:208:SER:HA	1:A:352:ASP:OD1	2.17	0.45
1:C:223:LEU:N	1:C:411:ARG:HH11	2.15	0.45
1:A:279:MET:HA	1:A:281:TYR:CE1	2.52	0.45
1:B:184:GLN:HG3	1:B:354:TYR:OH	2.17	0.44
1:A:222:SER:HB2	1:A:226:ARG:HG3	1.99	0.44
1:B:266:LEU:CD2	1:B:416:ILE:HD11	2.45	0.44
1:B:284:LEU:O	1:B:370:MET:HA	2.17	0.44
1:C:284:LEU:O	1:C:370:MET:HA	2.18	0.44
1:C:266:LEU:CD2	1:C:416:ILE:HD11	2.48	0.44
1:D:162:MET:HE2	1:D:162:MET:HB3	1.83	0.44
1:C:196:GLU:O	1:C:196:GLU:HG3	2.16	0.44
1:C:208:SER:HA	1:C:352:ASP:OD1	2.17	0.44
1:D:184:GLN:HG3	1:D:354:TYR:OH	2.18	0.43
1:D:284:LEU:O	1:D:370:MET:HA	2.18	0.43
1:C:222:SER:HA	1:C:411:ARG:NH1	2.33	0.43
1:D:47:LEU:HD21	1:D:140:ARG:HG3	2.00	0.43
1:B:45:ASP:OD1	1:B:46:PRO:HD2	2.18	0.43
1:B:226:ARG:O	1:B:243:MET:HB2	2.19	0.43
1:C:207:PHE:CZ	1:C:284:LEU:HD21	2.53	0.43
1:D:161:ASP:HB3	2:D:501:DVF:C20	2.48	0.43
1:B:222:SER:HB2	1:B:226:ARG:HG3	2.00	0.43
1:D:86:ASN:O	1:D:96:SER:HB2	2.18	0.43
1:A:90:HIS:C	1:A:92:GLU:N	2.71	0.43
1:B:71:LEU:HD12	1:B:170:HIS:CE1	2.54	0.43
1:C:45:ASP:OD2	1:C:140:ARG:NH1	2.53	0.42
1:C:226:ARG:O	1:C:243:MET:HB2	2.20	0.42
1:A:169:TYR:O	1:A:173:ILE:HG12	2.20	0.42
1:D:169:TYR:O	1:D:173:ILE:HG12	2.19	0.42
1:C:223:LEU:H	1:C:411:ARG:HH11	1.67	0.42
1:D:279:MET:HA	1:D:281:TYR:CE1	2.54	0.42
1:C:169:TYR:O	1:C:173:ILE:HG12	2.19	0.42
1:A:207:PHE:CZ	1:A:284:LEU:HD21	2.54	0.42
1:C:222:SER:HB2	1:C:226:ARG:HG3	2.02	0.42
1:A:133:GLU:HG3	1:A:142:LEU:HD23	2.02	0.41
1:B:140:ARG:HG2	1:B:153:GLU:OE1	2.20	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:226:ARG:O	1:A:243:MET:HB2	2.21	0.41
1:A:45:ASP:CG	1:A:140:ARG:HH12	2.23	0.41
1:B:209:HIS:H	1:B:209:HIS:CD2	2.38	0.41
1:C:375:ILE:HG22	3:C:622:HOH:O	2.20	0.41
1:C:272:PHE:CZ	1:C:276:LEU:HD11	2.55	0.41
1:C:279:MET:HA	1:C:281:TYR:CE1	2.55	0.41
1:C:82:ILE:CG2	1:D:82:ILE:HD11	2.51	0.40
1:D:45:ASP:OD1	1:D:140:ARG:NH2	2.51	0.40
1:A:101:LYS:NZ	3:A:609:HOH:O	2.53	0.40
1:B:375:ILE:O	1:B:377:THR:N	2.53	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	286/363 (79%)	276 (96%)	8 (3%)	2 (1%)	22 32
1	B	286/363 (79%)	273 (96%)	9 (3%)	4 (1%)	11 15
1	C	286/363 (79%)	277 (97%)	9 (3%)	0	100 100
1	D	305/363 (84%)	289 (95%)	14 (5%)	2 (1%)	22 32
All	All	1163/1452 (80%)	1115 (96%)	40 (3%)	8 (1%)	22 32

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	91	ARG
1	B	91	ARG
1	B	376	LEU
1	D	291	ILE
1	A	93	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	375	ILE
1	D	344	PRO
1	B	90	HIS

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	272/326 (83%)	255 (94%)	17 (6%)	18	28
1	B	270/326 (83%)	256 (95%)	14 (5%)	23	38
1	C	268/326 (82%)	248 (92%)	20 (8%)	13	21
1	D	282/326 (86%)	261 (93%)	21 (7%)	13	22
All	All	1092/1304 (84%)	1020 (93%)	72 (7%)	16	26

All (72) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	59	ILE
1	A	93	ASN
1	A	140	ARG
1	A	163	HIS
1	A	164	SER
1	A	196	GLU
1	A	198	SER
1	A	210	ARG
1	A	232	GLU
1	A	249	ASN
1	A	257	GLU
1	A	258	GLU
1	A	264	GLU
1	A	268	ARG
1	A	275	GLN
1	A	357	ARG
1	A	416	ILE
1	B	59	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	82	ILE
1	B	90	HIS
1	B	109	ARG
1	B	175	LYS
1	B	198	SER
1	B	232	GLU
1	B	249	ASN
1	B	257	GLU
1	B	264	GLU
1	B	268	ARG
1	B	282	SER
1	B	292	ARG
1	B	416	ILE
1	C	59	ILE
1	C	70	MET
1	C	77	LYS
1	C	109	ARG
1	C	135	GLU
1	C	140	ARG
1	C	164	SER
1	C	196	GLU
1	C	198	SER
1	C	210	ARG
1	C	223	LEU
1	C	232	GLU
1	C	249	ASN
1	C	251	LYS
1	C	264	GLU
1	C	268	ARG
1	C	275	GLN
1	C	376	LEU
1	C	377	THR
1	C	416	ILE
1	D	59	ILE
1	D	92	GLU
1	D	109	ARG
1	D	134	SER
1	D	163	HIS
1	D	164	SER
1	D	193	VAL
1	D	196	GLU
1	D	198	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	232	GLU
1	D	249	ASN
1	D	257	GLU
1	D	268	ARG
1	D	289	ASP
1	D	344	PRO
1	D	349	SER
1	D	350	PHE
1	D	376	LEU
1	D	404	HIS
1	D	410	LYS
1	D	416	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	64	GLN
1	A	120	GLN
1	A	163	HIS
1	A	209	HIS
1	A	247	ASN
1	A	288	HIS
1	A	404	HIS
1	B	64	GLN
1	B	209	HIS
1	B	247	ASN
1	B	288	HIS
1	C	57	HIS
1	C	163	HIS
1	C	168	ASN
1	C	247	ASN
1	C	288	HIS
1	D	120	GLN
1	D	247	ASN
1	D	288	HIS

5.3.3 RNA

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)

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	DVF	A	501	-	27,30,30	0.49	0	28,42,42	0.62	0
2	DVF	B	501	-	27,30,30	0.74	1 (3%)	28,42,42	1.23	1 (3%)
2	DVF	D	501	-	27,30,30	0.47	0	28,42,42	0.75	1 (3%)
2	DVF	C	501	-	27,30,30	0.51	0	28,42,42	1.22	4 (14%)

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	DVF	A	501	-	-	0/13/13/13	0/4/4/4
2	DVF	B	501	-	-	6/13/13/13	0/4/4/4
2	DVF	D	501	-	-	0/13/13/13	0/4/4/4
2	DVF	C	501	-	-	1/13/13/13	0/4/4/4

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	501	DVF	C4-C9	2.33	1.54	1.48

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	501	DVF	C17-C10-N	5.62	124.71	117.72
2	C	501	DVF	C17-C10-N	3.15	121.64	117.72
2	C	501	DVF	C9-N4-C21	-2.93	114.52	116.50
2	D	501	DVF	C17-C10-N	2.43	120.74	117.72
2	C	501	DVF	C2-C1-C3	-2.22	107.89	111.76
2	C	501	DVF	C4-C3-C1	-2.07	118.66	121.80

There are no chirality outliers.

All (7) torsion outliers are listed below:

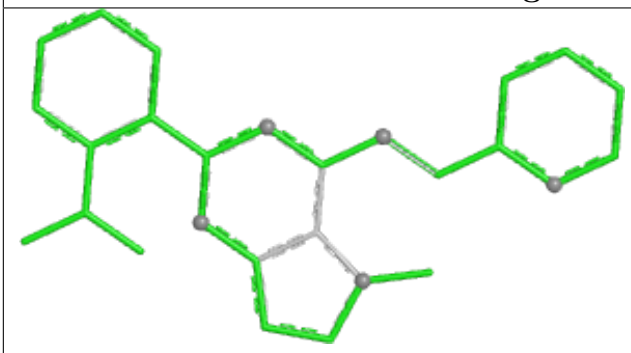
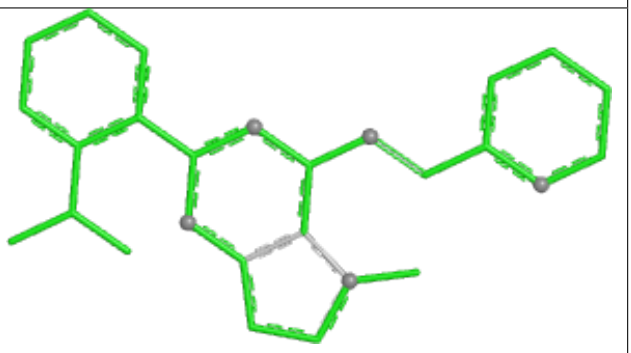
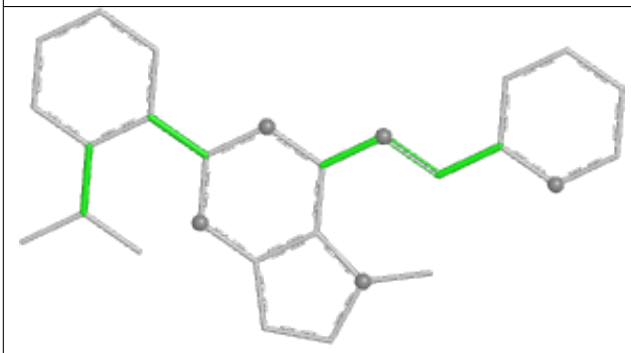
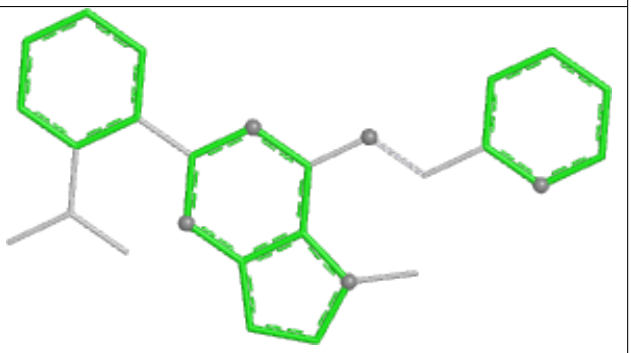
Mol	Chain	Res	Type	Atoms
2	B	501	DVF	C5-C4-C9-N4
2	B	501	DVF	C5-C4-C9-N
2	B	501	DVF	C3-C4-C9-N4
2	B	501	DVF	C3-C4-C9-N
2	C	501	DVF	C5-C4-C9-N
2	B	501	DVF	N1-C11-C12-C13
2	B	501	DVF	N1-C11-C12-N2

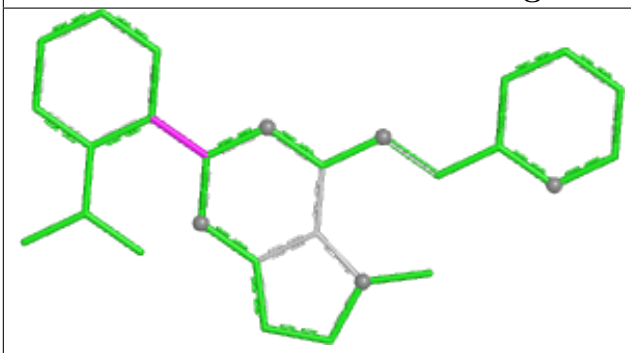
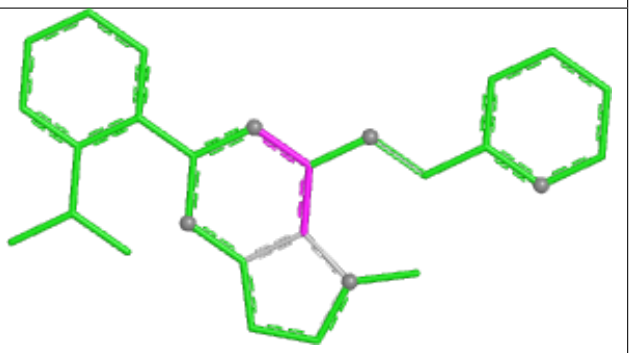
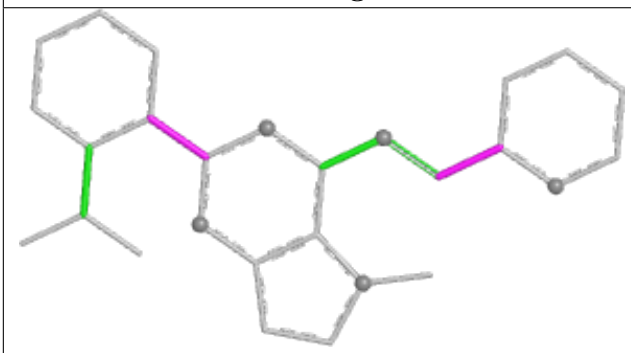
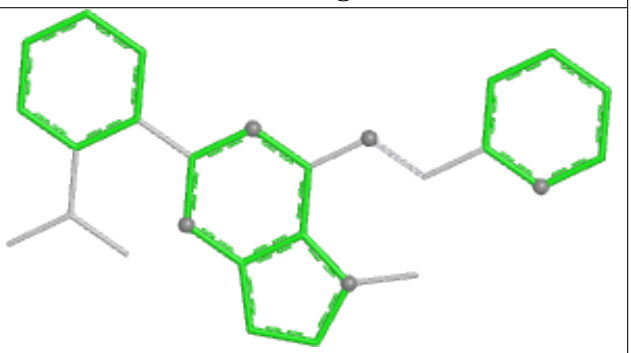
There are no ring outliers.

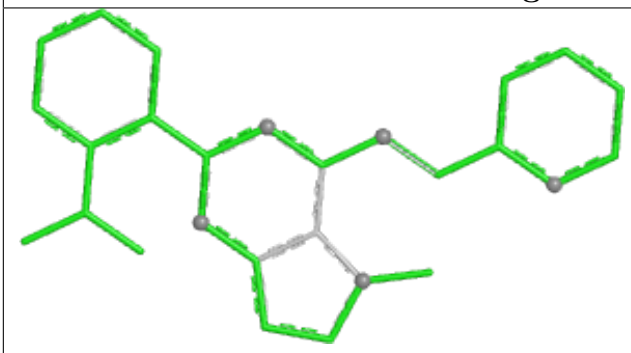
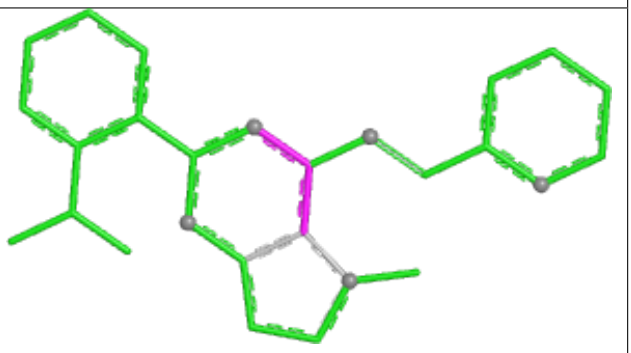
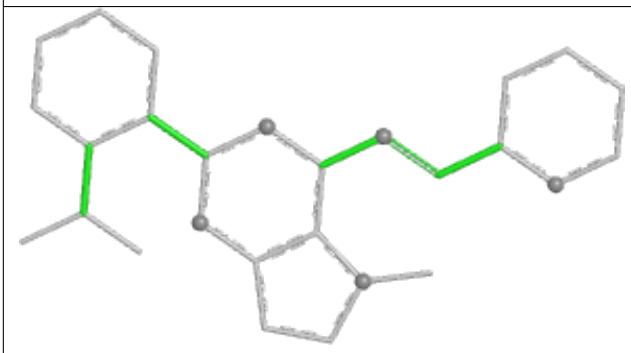
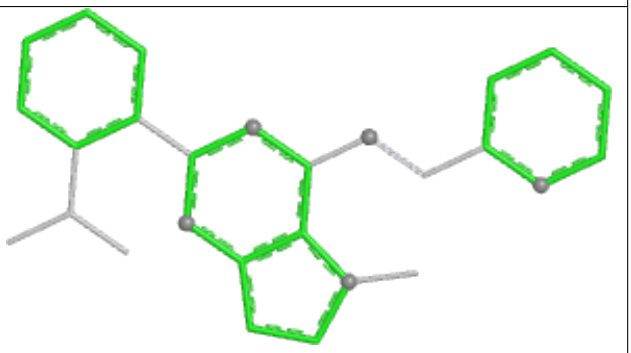
2 monomers are involved in 2 short contacts:

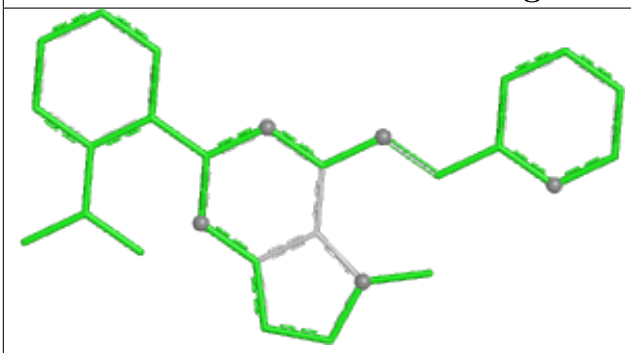
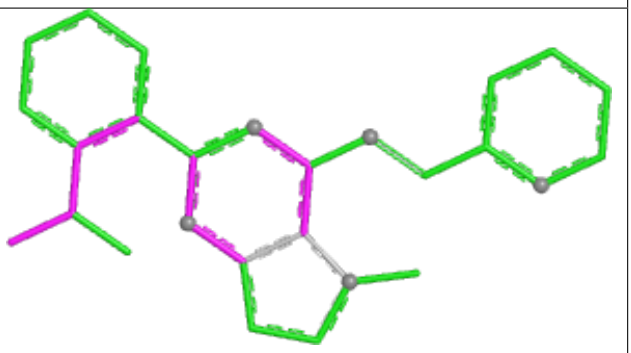
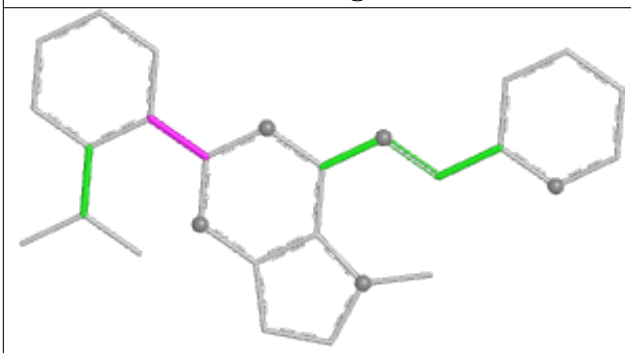
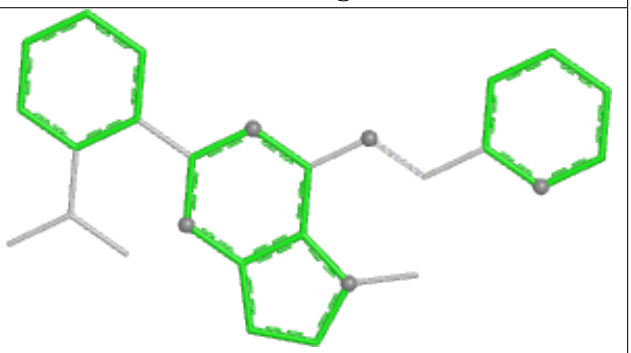
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	501	DVF	1	0
2	D	501	DVF	1	0

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.

Ligand DVF A 501	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand DVF B 501	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand DVF D 501	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand DVF C 501	
 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^{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	294/363 (80%)	0.11	2 (0%)	87	86	30, 56, 95, 128	0
1	B	292/363 (80%)	0.21	9 (3%)	49	47	25, 50, 99, 141	0
1	C	294/363 (80%)	0.42	22 (7%)	14	13	30, 67, 131, 153	0
1	D	311/363 (85%)	0.26	9 (2%)	51	50	28, 54, 108, 139	0
All	All	1191/1452 (82%)	0.25	42 (3%)	44	43	25, 57, 113, 153	0

All (42) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	353	VAL	5.6
1	D	351	ILE	5.1
1	C	367	VAL	4.9
1	C	239	THR	4.9
1	D	350	PHE	4.8
1	C	234	VAL	4.7
1	B	236	GLU	4.5
1	C	288	HIS	4.5
1	C	359	ALA	4.3
1	C	353	VAL	4.1
1	C	240	LEU	3.9
1	B	377	THR	3.8
1	A	134	SER	3.6
1	D	209	HIS	3.5
1	B	211	LEU	3.5
1	B	210	ARG	3.4
1	D	347	PHE	3.4
1	D	211	LEU	3.2
1	C	287	ILE	3.2
1	C	364	GLN	3.2
1	C	217	TYR	3.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	135	GLU	3.1
1	C	365	LYS	3.1
1	B	134	SER	2.7
1	D	344	PRO	2.7
1	C	356	ILE	2.6
1	C	93	ASN	2.5
1	B	91	ARG	2.3
1	C	178	GLY	2.3
1	C	145	TYR	2.3
1	C	147	ARG	2.3
1	C	230	ASP	2.3
1	B	90	HIS	2.3
1	C	254	ILE	2.3
1	C	290	ILE	2.3
1	B	194	ASP	2.2
1	A	135	GLU	2.2
1	C	357	ARG	2.1
1	C	368	TYR	2.1
1	D	213	VAL	2.1
1	B	292	ARG	2.1
1	D	352	ASP	2.0

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

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

6.3 Carbohydrates (i)

There are no 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	B-factors(Å^2)	Q<0.9
2	DVF	B	501	27/27	0.91	0.23	42,62,73,75	0
2	DVF	D	501	27/27	0.94	0.13	32,39,45,48	0

Continued on next page...

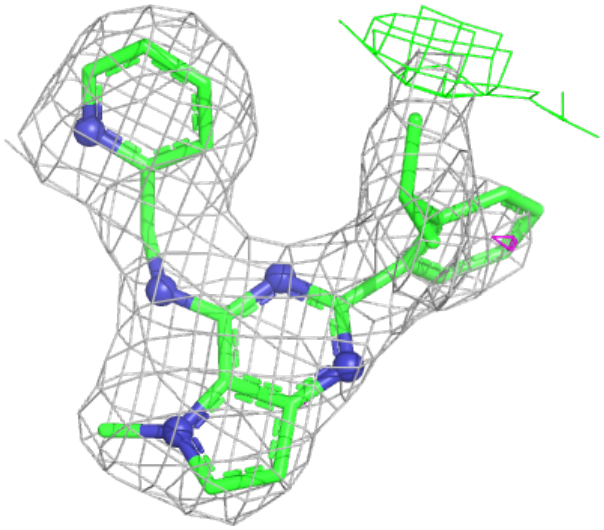
Continued from previous page...

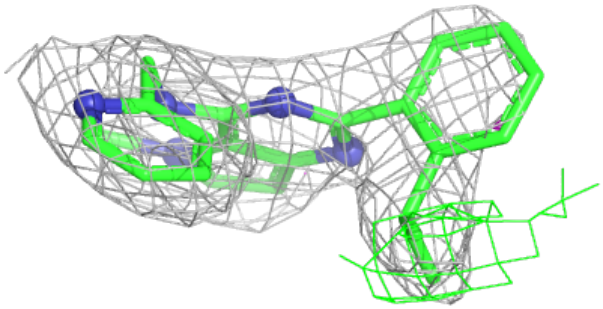
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	DVF	A	501	27/27	0.97	0.13	32,37,40,41	0
2	DVF	C	501	27/27	0.98	0.15	37,43,48,49	0

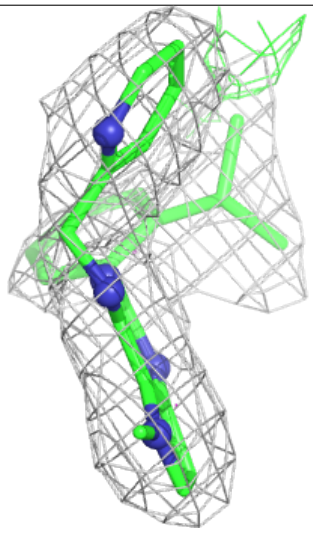
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around DVF B 501:

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

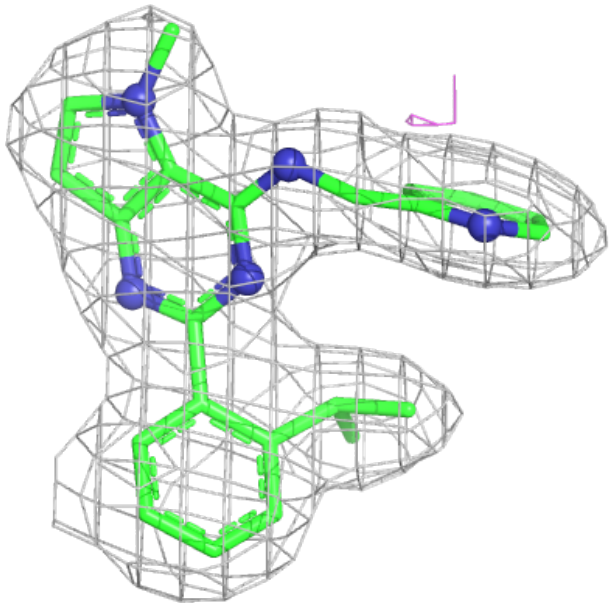


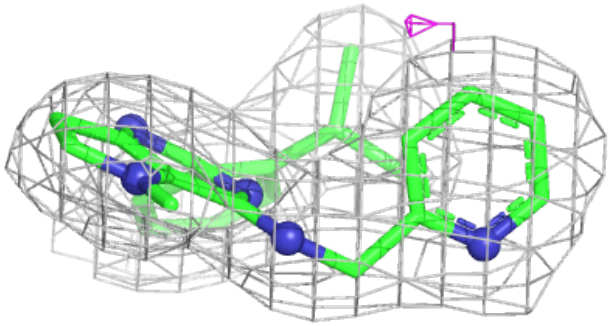


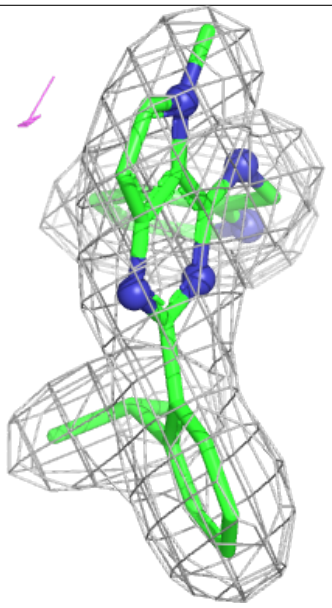


Electron density around DVF D 501:

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

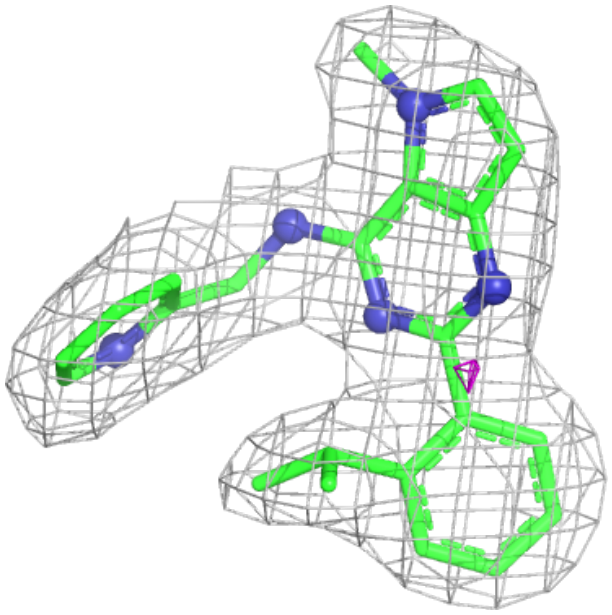


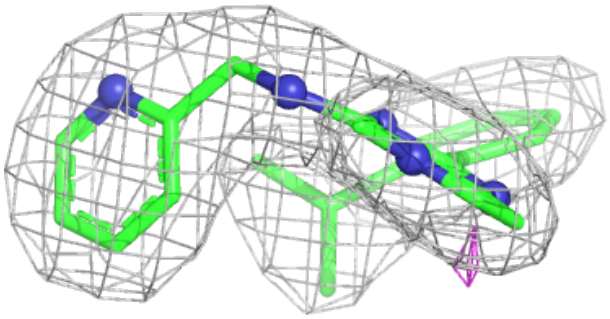


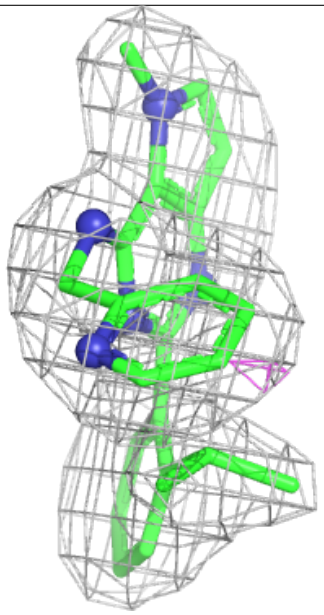


Electron density around DVF A 501:

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

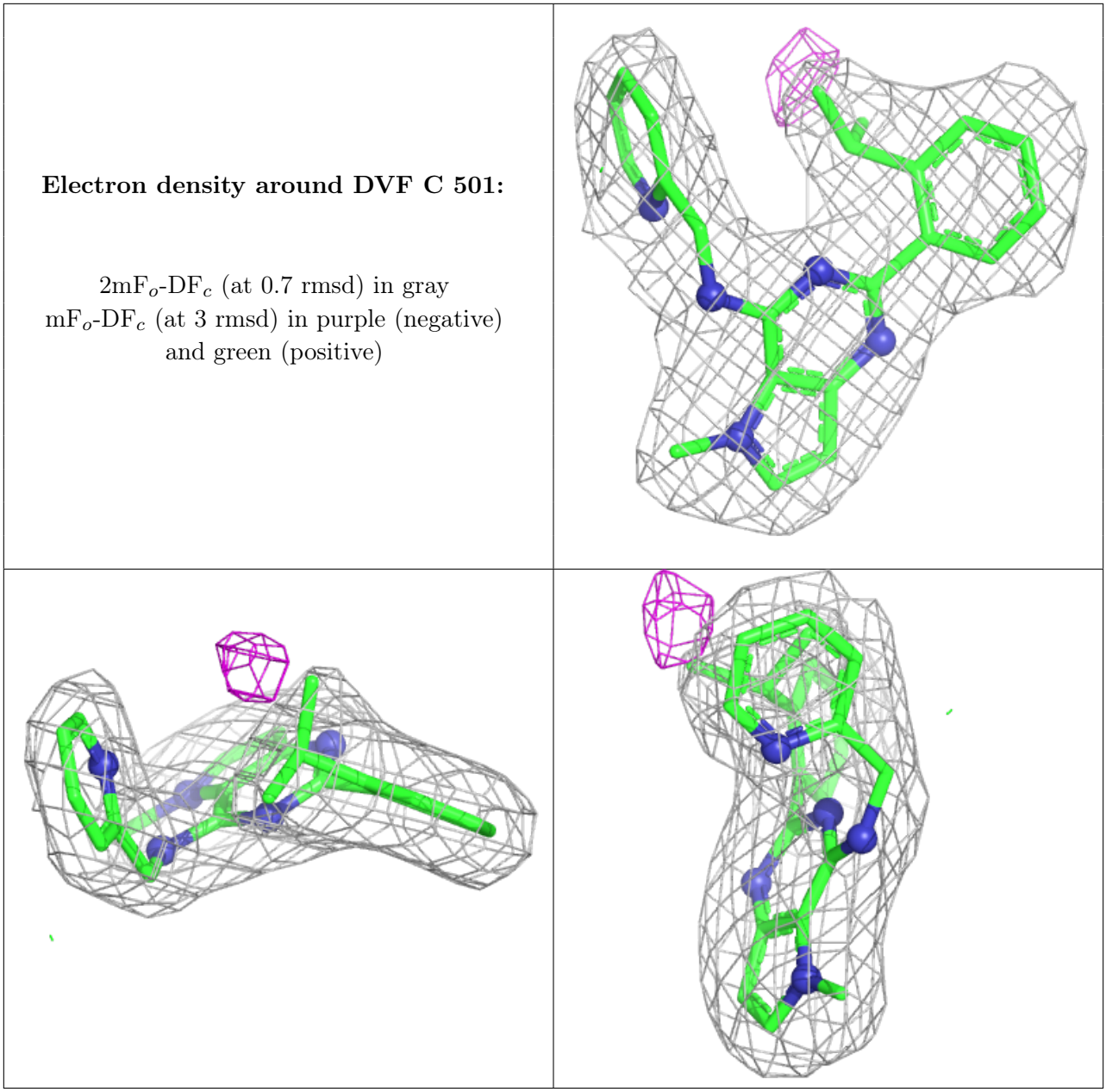






Electron density around DVF C 501:

$2mF_o$-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

There are no such residues in this entry.