



# wwPDB X-ray Structure Validation Summary Report ⓘ

May 26, 2020 – 05:56 am BST

PDB ID : 3FBV  
Title : Crystal structure of the oligomer formed by the kinase-ribonuclease domain of Ire1  
Authors : Korennykh, A.V.; Egea, P.F.; Korostelev, A.A.; Finer-Moore, J.; Zhang, C.; Shokat, K.M.; Stroud, R.M.; Walter, P.  
Deposited on : 2008-11-19  
Resolution : 3.20 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](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.11

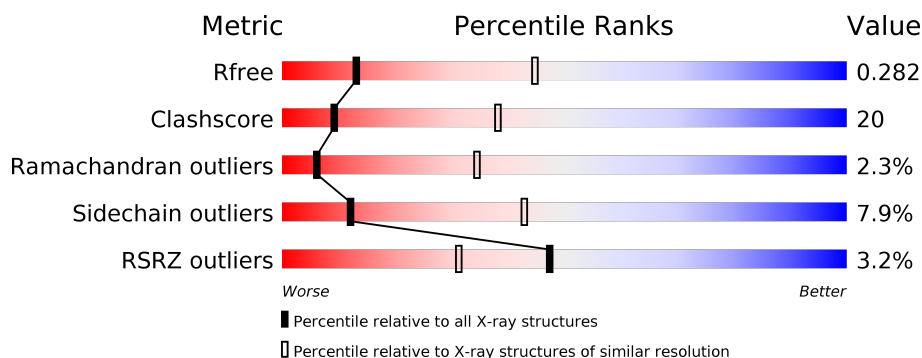
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 3.20 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	1133 (3.20-3.20)
Clashscore	141614	1253 (3.20-3.20)
Ramachandran outliers	138981	1234 (3.20-3.20)
Sidechain outliers	138945	1233 (3.20-3.20)
RSRZ outliers	127900	1095 (3.20-3.20)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	448	<div> <div>%</div> <div> <div></div> <div>56%</div> <div>32%</div> <div>• • 7%</div> </div> </div>
1	B	448	<div> <div>58%</div> <div>30%</div> <div>5%</div> <div>7%</div> </div>
1	C	448	<div> <div>%</div> <div> <div></div> <div>54%</div> <div>34%</div> <div>5%</div> <div>7%</div> </div> </div>
1	D	448	<div> <div>55%</div> <div>33%</div> <div>6%</div> <div>5%</div> </div>
1	E	448	<div> <div>2%</div> <div> <div></div> <div>57%</div> <div>31%</div> <div>5%</div> <div>7%</div> </div> </div>
1	F	448	<div> <div>%</div> <div> <div></div> <div>54%</div> <div>33%</div> <div>5%</div> <div>7%</div> </div> </div>

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Mol	Chain	Length	Quality of chain
1	G	448	
1	H	448	
1	I	448	
1	J	448	
1	K	448	
1	L	448	
1	M	448	
1	N	448	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
1	TPO	I	844	-	-	-	X
1	TPO	L	844	-	-	-	X
2	APJ	J	1999	-	-	-	X

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 48018 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 Serine/threonine-protein kinase/endoribonuclease IRE1.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	418	Total	C	N	O	P	S	0	0	0
			3399	2162	580	636	3	18			
1	B	418	Total	C	N	O	P	S	0	0	0
			3399	2162	580	636	3	18			
1	C	418	Total	C	N	O	P	S	0	0	0
			3399	2162	580	636	3	18			
1	D	425	Total	C	N	O	P	S	0	0	0
			3457	2199	589	648	3	18			
1	E	418	Total	C	N	O	P	S	0	0	0
			3399	2162	580	636	3	18			
1	F	418	Total	C	N	O	P	S	0	0	0
			3399	2162	580	636	3	18			
1	G	418	Total	C	N	O	P	S	0	0	0
			3399	2162	580	636	3	18			
1	H	418	Total	C	N	O	P	S	0	0	0
			3399	2162	580	636	3	18			
1	I	416	Total	C	N	O	P	S	0	0	0
			3382	2150	577	634	3	18			
1	J	416	Total	C	N	O	P	S	0	0	0
			3382	2150	577	634	3	18			
1	K	425	Total	C	N	O	P	S	0	0	0
			3457	2199	589	648	3	18			
1	L	418	Total	C	N	O	P	S	0	0	0
			3399	2162	580	636	3	18			
1	M	418	Total	C	N	O	P	S	0	0	0
			3399	2162	580	636	3	18			
1	N	418	Total	C	N	O	P	S	0	0	0
			3399	2162	580	636	3	18			

There are 406 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	640	PRO	-	EXPRESSION TAG	UNP P32361

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Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	ASN	DELETION	UNP P32361
A	?	-	ASN	DELETION	UNP P32361
A	?	-	LEU	DELETION	UNP P32361
A	?	-	GLN	DELETION	UNP P32361
A	?	-	CYS	DELETION	UNP P32361
A	?	-	GLN	DELETION	UNP P32361
A	?	-	VAL	DELETION	UNP P32361
A	?	-	GLU	DELETION	UNP P32361
A	?	-	THR	DELETION	UNP P32361
A	?	-	GLU	DELETION	UNP P32361
A	?	-	HIS	DELETION	UNP P32361
A	?	-	SER	DELETION	UNP P32361
A	?	-	SER	DELETION	UNP P32361
A	?	-	SER	DELETION	UNP P32361
A	?	-	ARG	DELETION	UNP P32361
A	?	-	HIS	DELETION	UNP P32361
A	?	-	THR	DELETION	UNP P32361
A	?	-	VAL	DELETION	UNP P32361
A	?	-	VAL	DELETION	UNP P32361
A	?	-	SER	DELETION	UNP P32361
A	?	-	SER	DELETION	UNP P32361
A	?	-	ASP	DELETION	UNP P32361
A	?	-	SER	DELETION	UNP P32361
A	?	-	PHE	DELETION	UNP P32361
A	?	-	TYR	DELETION	UNP P32361
A	?	-	ASP	DELETION	UNP P32361
A	?	-	PRO	DELETION	UNP P32361
A	?	-	PHE	DELETION	UNP P32361
B	640	PRO	-	EXPRESSION TAG	UNP P32361
B	?	-	ASN	DELETION	UNP P32361
B	?	-	ASN	DELETION	UNP P32361
B	?	-	LEU	DELETION	UNP P32361
B	?	-	GLN	DELETION	UNP P32361
B	?	-	CYS	DELETION	UNP P32361
B	?	-	GLN	DELETION	UNP P32361
B	?	-	VAL	DELETION	UNP P32361
B	?	-	GLU	DELETION	UNP P32361
B	?	-	THR	DELETION	UNP P32361
B	?	-	GLU	DELETION	UNP P32361
B	?	-	HIS	DELETION	UNP P32361
B	?	-	SER	DELETION	UNP P32361
B	?	-	SER	DELETION	UNP P32361

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Chain	Residue	Modelled	Actual	Comment	Reference
B	?	-	SER	DELETION	UNP P32361
B	?	-	ARG	DELETION	UNP P32361
B	?	-	HIS	DELETION	UNP P32361
B	?	-	THR	DELETION	UNP P32361
B	?	-	VAL	DELETION	UNP P32361
B	?	-	VAL	DELETION	UNP P32361
B	?	-	SER	DELETION	UNP P32361
B	?	-	SER	DELETION	UNP P32361
B	?	-	ASP	DELETION	UNP P32361
B	?	-	SER	DELETION	UNP P32361
B	?	-	PHE	DELETION	UNP P32361
B	?	-	TYR	DELETION	UNP P32361
B	?	-	ASP	DELETION	UNP P32361
B	?	-	PRO	DELETION	UNP P32361
B	?	-	PHE	DELETION	UNP P32361
C	640	PRO	-	EXPRESSION TAG	UNP P32361
C	?	-	ASN	DELETION	UNP P32361
C	?	-	ASN	DELETION	UNP P32361
C	?	-	LEU	DELETION	UNP P32361
C	?	-	GLN	DELETION	UNP P32361
C	?	-	CYS	DELETION	UNP P32361
C	?	-	GLN	DELETION	UNP P32361
C	?	-	VAL	DELETION	UNP P32361
C	?	-	GLU	DELETION	UNP P32361
C	?	-	THR	DELETION	UNP P32361
C	?	-	GLU	DELETION	UNP P32361
C	?	-	HIS	DELETION	UNP P32361
C	?	-	SER	DELETION	UNP P32361
C	?	-	SER	DELETION	UNP P32361
C	?	-	SER	DELETION	UNP P32361
C	?	-	ARG	DELETION	UNP P32361
C	?	-	HIS	DELETION	UNP P32361
C	?	-	THR	DELETION	UNP P32361
C	?	-	VAL	DELETION	UNP P32361
C	?	-	VAL	DELETION	UNP P32361
C	?	-	SER	DELETION	UNP P32361
C	?	-	SER	DELETION	UNP P32361
C	?	-	ASP	DELETION	UNP P32361
C	?	-	SER	DELETION	UNP P32361
C	?	-	PHE	DELETION	UNP P32361
C	?	-	TYR	DELETION	UNP P32361
C	?	-	ASP	DELETION	UNP P32361

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Chain	Residue	Modelled	Actual	Comment	Reference
C	?	-	PRO	DELETION	UNP P32361
C	?	-	PHE	DELETION	UNP P32361
D	640	PRO	-	EXPRESSION TAG	UNP P32361
D	?	-	ASN	DELETION	UNP P32361
D	?	-	ASN	DELETION	UNP P32361
D	?	-	LEU	DELETION	UNP P32361
D	?	-	GLN	DELETION	UNP P32361
D	?	-	CYS	DELETION	UNP P32361
D	?	-	GLN	DELETION	UNP P32361
D	?	-	VAL	DELETION	UNP P32361
D	?	-	GLU	DELETION	UNP P32361
D	?	-	THR	DELETION	UNP P32361
D	?	-	GLU	DELETION	UNP P32361
D	?	-	HIS	DELETION	UNP P32361
D	?	-	SER	DELETION	UNP P32361
D	?	-	SER	DELETION	UNP P32361
D	?	-	SER	DELETION	UNP P32361
D	?	-	ARG	DELETION	UNP P32361
D	?	-	HIS	DELETION	UNP P32361
D	?	-	THR	DELETION	UNP P32361
D	?	-	VAL	DELETION	UNP P32361
D	?	-	VAL	DELETION	UNP P32361
D	?	-	SER	DELETION	UNP P32361
D	?	-	SER	DELETION	UNP P32361
D	?	-	ASP	DELETION	UNP P32361
D	?	-	SER	DELETION	UNP P32361
D	?	-	PHE	DELETION	UNP P32361
D	?	-	TYR	DELETION	UNP P32361
D	?	-	ASP	DELETION	UNP P32361
D	?	-	PRO	DELETION	UNP P32361
D	?	-	PHE	DELETION	UNP P32361
E	640	PRO	-	EXPRESSION TAG	UNP P32361
E	?	-	ASN	DELETION	UNP P32361
E	?	-	ASN	DELETION	UNP P32361
E	?	-	LEU	DELETION	UNP P32361
E	?	-	GLN	DELETION	UNP P32361
E	?	-	CYS	DELETION	UNP P32361
E	?	-	GLN	DELETION	UNP P32361
E	?	-	VAL	DELETION	UNP P32361
E	?	-	GLU	DELETION	UNP P32361
E	?	-	THR	DELETION	UNP P32361
E	?	-	GLU	DELETION	UNP P32361

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Chain	Residue	Modelled	Actual	Comment	Reference
E	?	-	HIS	DELETION	UNP P32361
E	?	-	SER	DELETION	UNP P32361
E	?	-	SER	DELETION	UNP P32361
E	?	-	SER	DELETION	UNP P32361
E	?	-	ARG	DELETION	UNP P32361
E	?	-	HIS	DELETION	UNP P32361
E	?	-	THR	DELETION	UNP P32361
E	?	-	VAL	DELETION	UNP P32361
E	?	-	VAL	DELETION	UNP P32361
E	?	-	SER	DELETION	UNP P32361
E	?	-	SER	DELETION	UNP P32361
E	?	-	ASP	DELETION	UNP P32361
E	?	-	SER	DELETION	UNP P32361
E	?	-	PHE	DELETION	UNP P32361
E	?	-	TYR	DELETION	UNP P32361
E	?	-	ASP	DELETION	UNP P32361
E	?	-	PRO	DELETION	UNP P32361
E	?	-	PHE	DELETION	UNP P32361
F	640	PRO	-	EXPRESSION TAG	UNP P32361
F	?	-	ASN	DELETION	UNP P32361
F	?	-	ASN	DELETION	UNP P32361
F	?	-	LEU	DELETION	UNP P32361
F	?	-	GLN	DELETION	UNP P32361
F	?	-	CYS	DELETION	UNP P32361
F	?	-	GLN	DELETION	UNP P32361
F	?	-	VAL	DELETION	UNP P32361
F	?	-	GLU	DELETION	UNP P32361
F	?	-	THR	DELETION	UNP P32361
F	?	-	GLU	DELETION	UNP P32361
F	?	-	HIS	DELETION	UNP P32361
F	?	-	SER	DELETION	UNP P32361
F	?	-	SER	DELETION	UNP P32361
F	?	-	SER	DELETION	UNP P32361
F	?	-	ARG	DELETION	UNP P32361
F	?	-	HIS	DELETION	UNP P32361
F	?	-	THR	DELETION	UNP P32361
F	?	-	VAL	DELETION	UNP P32361
F	?	-	VAL	DELETION	UNP P32361
F	?	-	SER	DELETION	UNP P32361
F	?	-	SER	DELETION	UNP P32361
F	?	-	ASP	DELETION	UNP P32361
F	?	-	SER	DELETION	UNP P32361

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Chain	Residue	Modelled	Actual	Comment	Reference
F	?	-	PHE	DELETION	UNP P32361
F	?	-	TYR	DELETION	UNP P32361
F	?	-	ASP	DELETION	UNP P32361
F	?	-	PRO	DELETION	UNP P32361
F	?	-	PHE	DELETION	UNP P32361
G	640	PRO	-	EXPRESSION TAG	UNP P32361
G	?	-	ASN	DELETION	UNP P32361
G	?	-	ASN	DELETION	UNP P32361
G	?	-	LEU	DELETION	UNP P32361
G	?	-	GLN	DELETION	UNP P32361
G	?	-	CYS	DELETION	UNP P32361
G	?	-	GLN	DELETION	UNP P32361
G	?	-	VAL	DELETION	UNP P32361
G	?	-	GLU	DELETION	UNP P32361
G	?	-	THR	DELETION	UNP P32361
G	?	-	GLU	DELETION	UNP P32361
G	?	-	HIS	DELETION	UNP P32361
G	?	-	SER	DELETION	UNP P32361
G	?	-	SER	DELETION	UNP P32361
G	?	-	SER	DELETION	UNP P32361
G	?	-	ARG	DELETION	UNP P32361
G	?	-	HIS	DELETION	UNP P32361
G	?	-	THR	DELETION	UNP P32361
G	?	-	VAL	DELETION	UNP P32361
G	?	-	VAL	DELETION	UNP P32361
G	?	-	SER	DELETION	UNP P32361
G	?	-	SER	DELETION	UNP P32361
G	?	-	ASP	DELETION	UNP P32361
G	?	-	SER	DELETION	UNP P32361
G	?	-	PHE	DELETION	UNP P32361
G	?	-	TYR	DELETION	UNP P32361
G	?	-	ASP	DELETION	UNP P32361
G	?	-	PRO	DELETION	UNP P32361
G	?	-	PHE	DELETION	UNP P32361
H	640	PRO	-	EXPRESSION TAG	UNP P32361
H	?	-	ASN	DELETION	UNP P32361
H	?	-	ASN	DELETION	UNP P32361
H	?	-	LEU	DELETION	UNP P32361
H	?	-	GLN	DELETION	UNP P32361
H	?	-	CYS	DELETION	UNP P32361
H	?	-	GLN	DELETION	UNP P32361
H	?	-	VAL	DELETION	UNP P32361

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Chain	Residue	Modelled	Actual	Comment	Reference
H	?	-	GLU	DELETION	UNP P32361
H	?	-	THR	DELETION	UNP P32361
H	?	-	GLU	DELETION	UNP P32361
H	?	-	HIS	DELETION	UNP P32361
H	?	-	SER	DELETION	UNP P32361
H	?	-	SER	DELETION	UNP P32361
H	?	-	SER	DELETION	UNP P32361
H	?	-	ARG	DELETION	UNP P32361
H	?	-	HIS	DELETION	UNP P32361
H	?	-	THR	DELETION	UNP P32361
H	?	-	VAL	DELETION	UNP P32361
H	?	-	VAL	DELETION	UNP P32361
H	?	-	SER	DELETION	UNP P32361
H	?	-	SER	DELETION	UNP P32361
H	?	-	ASP	DELETION	UNP P32361
H	?	-	SER	DELETION	UNP P32361
H	?	-	PHE	DELETION	UNP P32361
H	?	-	TYR	DELETION	UNP P32361
H	?	-	ASP	DELETION	UNP P32361
H	?	-	PRO	DELETION	UNP P32361
H	?	-	PHE	DELETION	UNP P32361
I	640	PRO	-	EXPRESSION TAG	UNP P32361
I	?	-	ASN	DELETION	UNP P32361
I	?	-	ASN	DELETION	UNP P32361
I	?	-	LEU	DELETION	UNP P32361
I	?	-	GLN	DELETION	UNP P32361
I	?	-	CYS	DELETION	UNP P32361
I	?	-	GLN	DELETION	UNP P32361
I	?	-	VAL	DELETION	UNP P32361
I	?	-	GLU	DELETION	UNP P32361
I	?	-	THR	DELETION	UNP P32361
I	?	-	GLU	DELETION	UNP P32361
I	?	-	HIS	DELETION	UNP P32361
I	?	-	SER	DELETION	UNP P32361
I	?	-	SER	DELETION	UNP P32361
I	?	-	SER	DELETION	UNP P32361
I	?	-	ARG	DELETION	UNP P32361
I	?	-	HIS	DELETION	UNP P32361
I	?	-	THR	DELETION	UNP P32361
I	?	-	VAL	DELETION	UNP P32361
I	?	-	VAL	DELETION	UNP P32361
I	?	-	SER	DELETION	UNP P32361

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Chain	Residue	Modelled	Actual	Comment	Reference
I	?	-	SER	DELETION	UNP P32361
I	?	-	ASP	DELETION	UNP P32361
I	?	-	SER	DELETION	UNP P32361
I	?	-	PHE	DELETION	UNP P32361
I	?	-	TYR	DELETION	UNP P32361
I	?	-	ASP	DELETION	UNP P32361
I	?	-	PRO	DELETION	UNP P32361
I	?	-	PHE	DELETION	UNP P32361
J	640	PRO	-	EXPRESSION TAG	UNP P32361
J	?	-	ASN	DELETION	UNP P32361
J	?	-	ASN	DELETION	UNP P32361
J	?	-	LEU	DELETION	UNP P32361
J	?	-	GLN	DELETION	UNP P32361
J	?	-	CYS	DELETION	UNP P32361
J	?	-	GLN	DELETION	UNP P32361
J	?	-	VAL	DELETION	UNP P32361
J	?	-	GLU	DELETION	UNP P32361
J	?	-	THR	DELETION	UNP P32361
J	?	-	GLU	DELETION	UNP P32361
J	?	-	HIS	DELETION	UNP P32361
J	?	-	SER	DELETION	UNP P32361
J	?	-	SER	DELETION	UNP P32361
J	?	-	SER	DELETION	UNP P32361
J	?	-	ARG	DELETION	UNP P32361
J	?	-	HIS	DELETION	UNP P32361
J	?	-	THR	DELETION	UNP P32361
J	?	-	VAL	DELETION	UNP P32361
J	?	-	VAL	DELETION	UNP P32361
J	?	-	SER	DELETION	UNP P32361
J	?	-	SER	DELETION	UNP P32361
J	?	-	ASP	DELETION	UNP P32361
J	?	-	SER	DELETION	UNP P32361
J	?	-	PHE	DELETION	UNP P32361
J	?	-	TYR	DELETION	UNP P32361
J	?	-	ASP	DELETION	UNP P32361
J	?	-	PRO	DELETION	UNP P32361
J	?	-	PHE	DELETION	UNP P32361
K	640	PRO	-	EXPRESSION TAG	UNP P32361
K	?	-	ASN	DELETION	UNP P32361
K	?	-	ASN	DELETION	UNP P32361
K	?	-	LEU	DELETION	UNP P32361
K	?	-	GLN	DELETION	UNP P32361

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Chain	Residue	Modelled	Actual	Comment	Reference
K	?	-	CYS	DELETION	UNP P32361
K	?	-	GLN	DELETION	UNP P32361
K	?	-	VAL	DELETION	UNP P32361
K	?	-	GLU	DELETION	UNP P32361
K	?	-	THR	DELETION	UNP P32361
K	?	-	GLU	DELETION	UNP P32361
K	?	-	HIS	DELETION	UNP P32361
K	?	-	SER	DELETION	UNP P32361
K	?	-	SER	DELETION	UNP P32361
K	?	-	SER	DELETION	UNP P32361
K	?	-	ARG	DELETION	UNP P32361
K	?	-	HIS	DELETION	UNP P32361
K	?	-	THR	DELETION	UNP P32361
K	?	-	VAL	DELETION	UNP P32361
K	?	-	VAL	DELETION	UNP P32361
K	?	-	SER	DELETION	UNP P32361
K	?	-	SER	DELETION	UNP P32361
K	?	-	ASP	DELETION	UNP P32361
K	?	-	SER	DELETION	UNP P32361
K	?	-	PHE	DELETION	UNP P32361
K	?	-	TYR	DELETION	UNP P32361
K	?	-	ASP	DELETION	UNP P32361
K	?	-	PRO	DELETION	UNP P32361
K	?	-	PHE	DELETION	UNP P32361
L	640	PRO	-	EXPRESSION TAG	UNP P32361
L	?	-	ASN	DELETION	UNP P32361
L	?	-	ASN	DELETION	UNP P32361
L	?	-	LEU	DELETION	UNP P32361
L	?	-	GLN	DELETION	UNP P32361
L	?	-	CYS	DELETION	UNP P32361
L	?	-	GLN	DELETION	UNP P32361
L	?	-	VAL	DELETION	UNP P32361
L	?	-	GLU	DELETION	UNP P32361
L	?	-	THR	DELETION	UNP P32361
L	?	-	GLU	DELETION	UNP P32361
L	?	-	HIS	DELETION	UNP P32361
L	?	-	SER	DELETION	UNP P32361
L	?	-	SER	DELETION	UNP P32361
L	?	-	SER	DELETION	UNP P32361
L	?	-	ARG	DELETION	UNP P32361
L	?	-	HIS	DELETION	UNP P32361
L	?	-	THR	DELETION	UNP P32361

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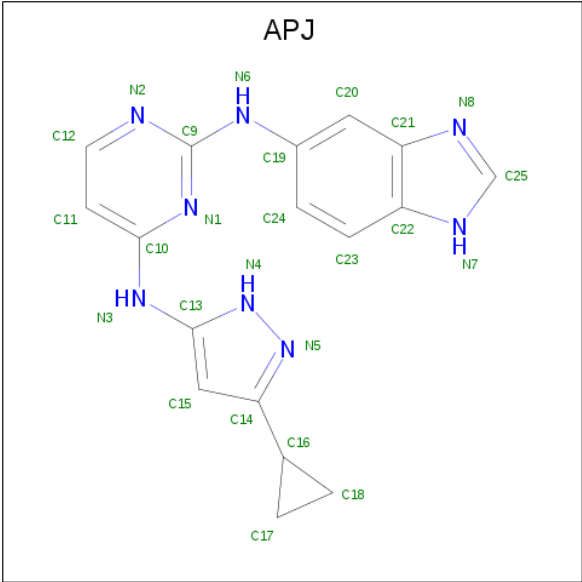
Chain	Residue	Modelled	Actual	Comment	Reference
L	?	-	VAL	DELETION	UNP P32361
L	?	-	VAL	DELETION	UNP P32361
L	?	-	SER	DELETION	UNP P32361
L	?	-	SER	DELETION	UNP P32361
L	?	-	ASP	DELETION	UNP P32361
L	?	-	SER	DELETION	UNP P32361
L	?	-	PHE	DELETION	UNP P32361
L	?	-	TYR	DELETION	UNP P32361
L	?	-	ASP	DELETION	UNP P32361
L	?	-	PRO	DELETION	UNP P32361
L	?	-	PHE	DELETION	UNP P32361
M	640	PRO	-	EXPRESSION TAG	UNP P32361
M	?	-	ASN	DELETION	UNP P32361
M	?	-	ASN	DELETION	UNP P32361
M	?	-	LEU	DELETION	UNP P32361
M	?	-	GLN	DELETION	UNP P32361
M	?	-	CYS	DELETION	UNP P32361
M	?	-	GLN	DELETION	UNP P32361
M	?	-	VAL	DELETION	UNP P32361
M	?	-	GLU	DELETION	UNP P32361
M	?	-	THR	DELETION	UNP P32361
M	?	-	GLU	DELETION	UNP P32361
M	?	-	HIS	DELETION	UNP P32361
M	?	-	SER	DELETION	UNP P32361
M	?	-	SER	DELETION	UNP P32361
M	?	-	SER	DELETION	UNP P32361
M	?	-	ARG	DELETION	UNP P32361
M	?	-	HIS	DELETION	UNP P32361
M	?	-	THR	DELETION	UNP P32361
M	?	-	VAL	DELETION	UNP P32361
M	?	-	VAL	DELETION	UNP P32361
M	?	-	SER	DELETION	UNP P32361
M	?	-	SER	DELETION	UNP P32361
M	?	-	ASP	DELETION	UNP P32361
M	?	-	SER	DELETION	UNP P32361
M	?	-	PHE	DELETION	UNP P32361
M	?	-	TYR	DELETION	UNP P32361
M	?	-	ASP	DELETION	UNP P32361
M	?	-	PRO	DELETION	UNP P32361
M	?	-	PHE	DELETION	UNP P32361
N	640	PRO	-	EXPRESSION TAG	UNP P32361
N	?	-	ASN	DELETION	UNP P32361

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Chain	Residue	Modelled	Actual	Comment	Reference
N	?	-	ASN	DELETION	UNP P32361
N	?	-	LEU	DELETION	UNP P32361
N	?	-	GLN	DELETION	UNP P32361
N	?	-	CYS	DELETION	UNP P32361
N	?	-	GLN	DELETION	UNP P32361
N	?	-	VAL	DELETION	UNP P32361
N	?	-	GLU	DELETION	UNP P32361
N	?	-	THR	DELETION	UNP P32361
N	?	-	GLU	DELETION	UNP P32361
N	?	-	HIS	DELETION	UNP P32361
N	?	-	SER	DELETION	UNP P32361
N	?	-	SER	DELETION	UNP P32361
N	?	-	SER	DELETION	UNP P32361
N	?	-	ARG	DELETION	UNP P32361
N	?	-	HIS	DELETION	UNP P32361
N	?	-	THR	DELETION	UNP P32361
N	?	-	VAL	DELETION	UNP P32361
N	?	-	VAL	DELETION	UNP P32361
N	?	-	SER	DELETION	UNP P32361
N	?	-	SER	DELETION	UNP P32361
N	?	-	ASP	DELETION	UNP P32361
N	?	-	SER	DELETION	UNP P32361
N	?	-	PHE	DELETION	UNP P32361
N	?	-	TYR	DELETION	UNP P32361
N	?	-	ASP	DELETION	UNP P32361
N	?	-	PRO	DELETION	UNP P32361
N	?	-	PHE	DELETION	UNP P32361

- Molecule 2 is N 2 -1H-benzimidazol-5-yl-N 4 -(3-cyclopropyl-1H-pyrazol-5-yl)pyrimidine-2,4 -diamine (three-letter code: APJ) (formula: C<sub>17</sub>H<sub>16</sub>N<sub>8</sub>).

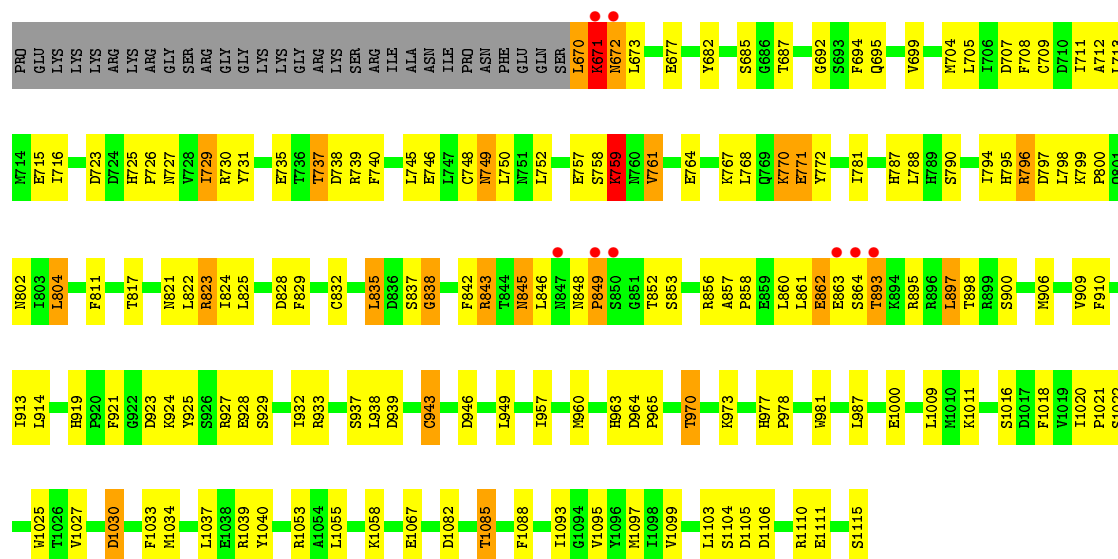


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	N	0	0
			25	17	8		
2	B	1	Total	C	N	0	0
			25	17	8		
2	C	1	Total	C	N	0	0
			25	17	8		
2	D	1	Total	C	N	0	0
			25	17	8		
2	E	1	Total	C	N	0	0
			25	17	8		
2	F	1	Total	C	N	0	0
			25	17	8		
2	G	1	Total	C	N	0	0
			25	17	8		
2	H	1	Total	C	N	0	0
			25	17	8		
2	I	1	Total	C	N	0	0
			25	17	8		
2	J	1	Total	C	N	0	0
			25	17	8		
2	K	1	Total	C	N	0	0
			25	17	8		
2	L	1	Total	C	N	0	0
			25	17	8		
2	M	1	Total	C	N	0	0
			25	17	8		
2	N	1	Total	C	N	0	0
			25	17	8		

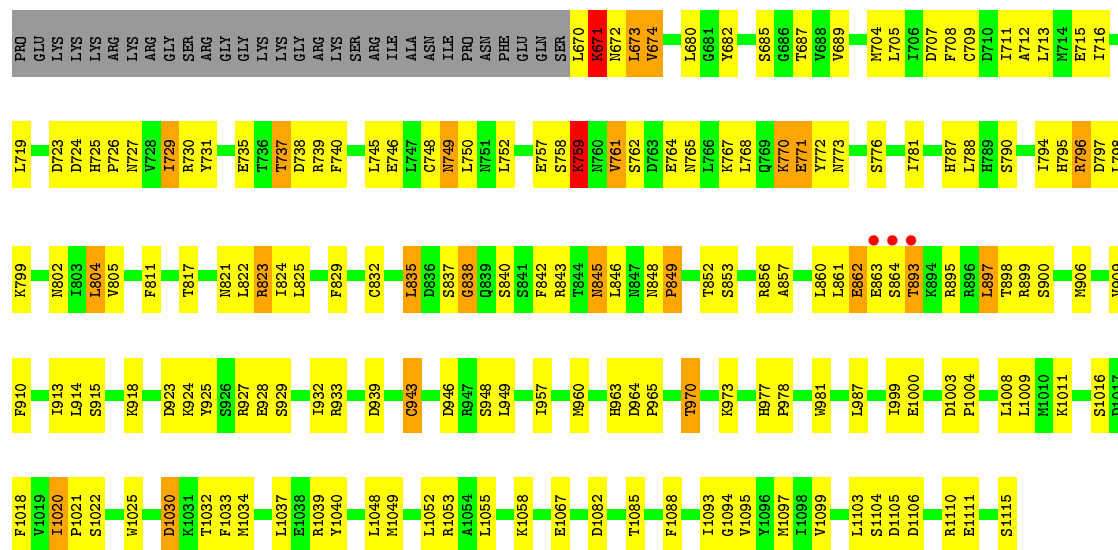




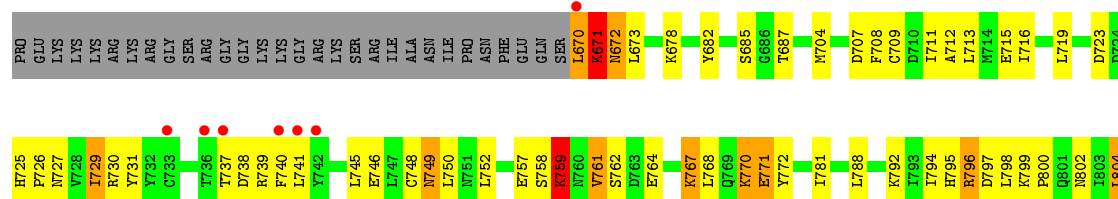


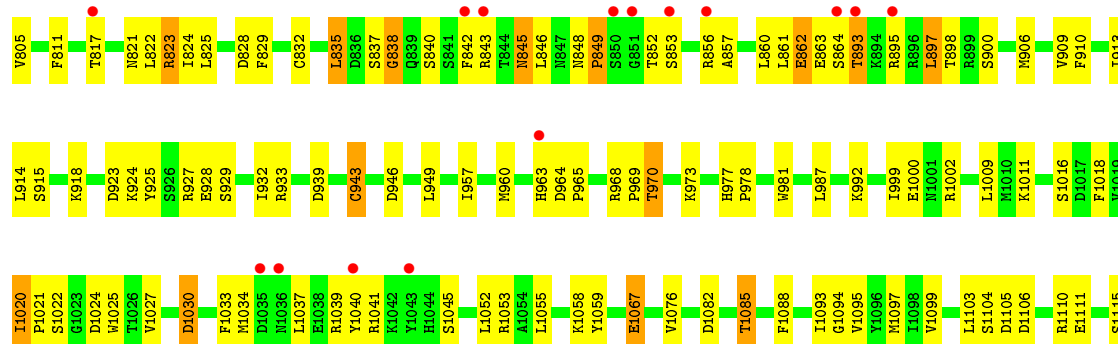


• Molecule 1: Serine/threonine-protein kinase/endoribonuclease IRE1

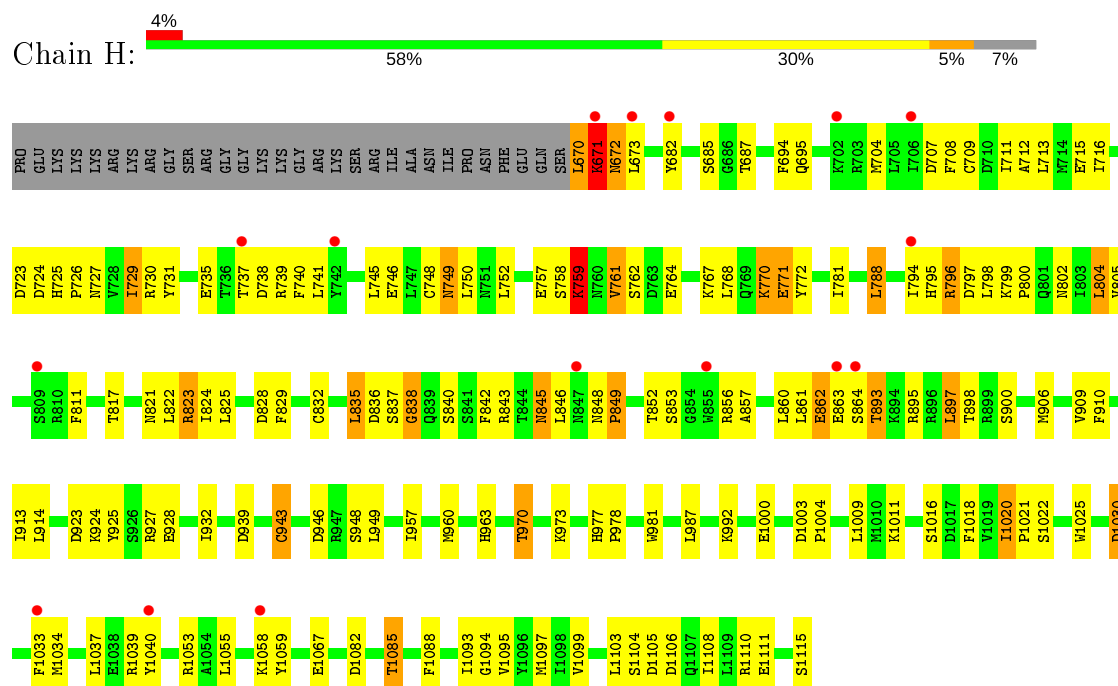


• Molecule 1: Serine/threonine-protein kinase/endoribonuclease IRE1

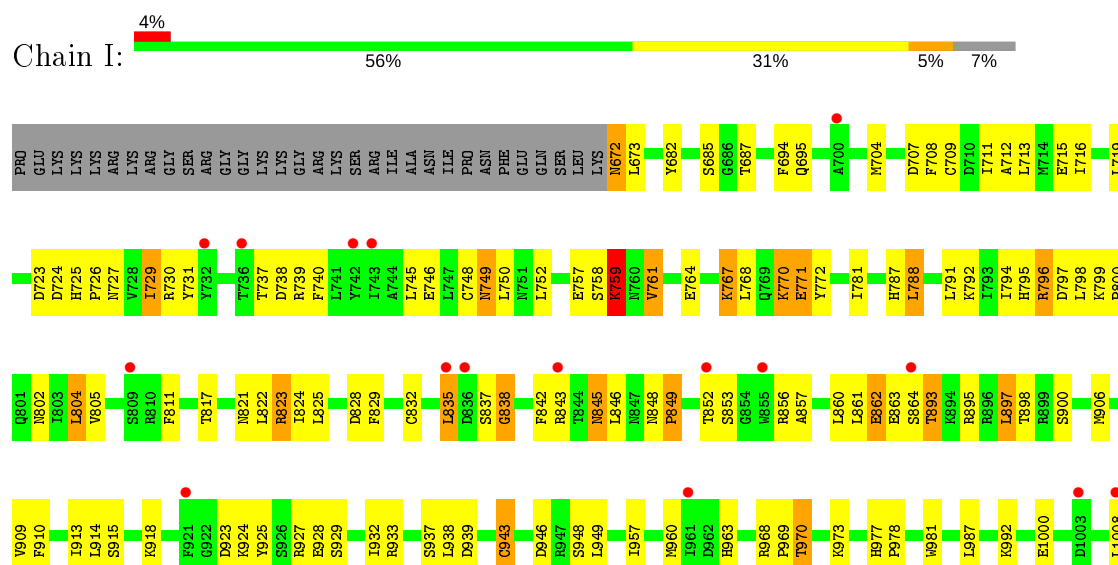


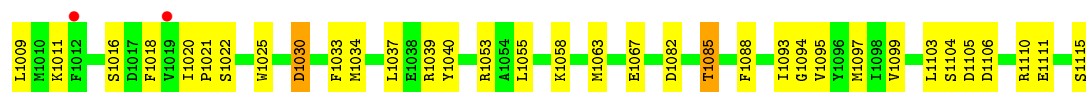


• Molecule 1: Serine/threonine-protein kinase/endoribonuclease IRE1

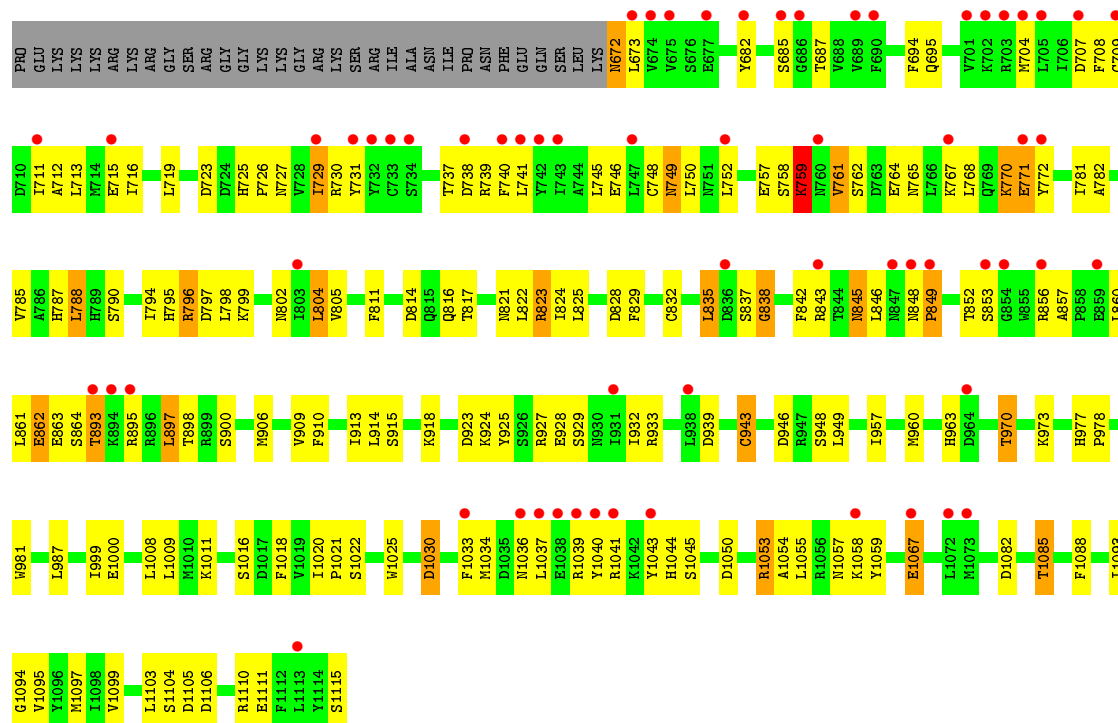


• Molecule 1: Serine/threonine-protein kinase/endoribonuclease IRE1

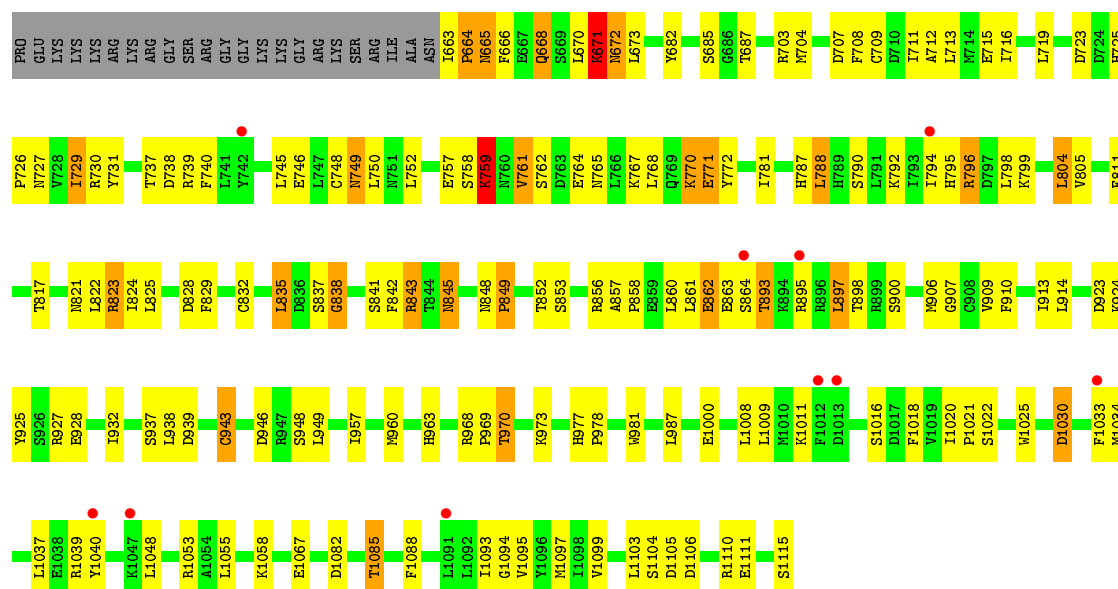




• Molecule 1: Serine/threonine-protein kinase/endoribonuclease IRE1



• Molecule 1: Serine/threonine-protein kinase/endoribonuclease IRE1



[illegible]

Chain M:

2% 55% 33% 5% 7%

PRO GLU LYS LYS LYS ARG ARG GLY SER ARG GLY LYS LYS ARG GLY LYS SER ARG GLY LYS SER ARG GLU GLN SER L670 K671 N672 L673 L678 Y682 S685 G686 T687 F694 Q695 M704 D707 F708 C709 D710 I711 A712 L713 M714 E715 I716 V719

D723 D724 H725 P726 N727 V728 T737 D738 R739 F740 L741 Y742 L745 E746 L747 C748 M749 L750 F751 L752 E757 S758 K759 H760 V761 S762 D763 E764 K767 L768 Q769 K770 E886 E771 Y772 M773 S776 I781 L788 I794 H795 R796 D797 L798 K799 N802 T803 L804

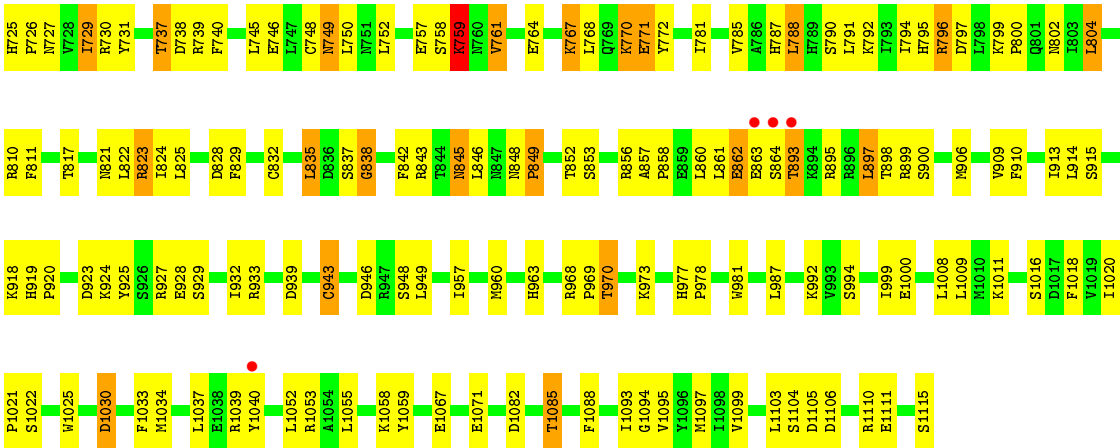
Y805 F811 T817 N821 R823 L822 R824 L825 D828 F829 C832 L835 R836 S837 G838 F842 R843 T844 N845 L846 N847 R848 P849 T852 S853 R856 A857 L860 L861 E862 E863 S864 T893 K894 R895 R896 L897 T898 R899 S900 N906 G907 C908 V909 F910 I913 L914

D923 K924 Y925 S926 R927 E928 S929 I932 R933 R937 L938 D939 C943 D946 R947 S948 L949 I957 M960 R963 D964 P965 R968 P969 T970 K973 R977 P978 W981 L987 K992 E1000 H1001 R1002 L1008 L1009 H1010 K1011 S1016 D1017 F1018 V1019 I1020 P1021

S1022 W1025 T1026 V1027 D1030 F1033 M1034 L1037 E1038 R1039 Y1040 R1041 K1042 L1048 L1052 R1053 A1054 L1055 K1058 Y1059 E1067 D1082 T1085 F1088 I1093 G1094 V1095 Y1096 M1097 I1098 V1099 L1103 S1104 D1105 D1106 R1110 E1111 S1115

Chain N:

Residue	Percentage
PRO	55%
GLY	55%
LVS	55%
LVS	55%
ARG	55%
LVS	55%
ARG	55%
GLY	55%
SER	55%
ARG	55%
GLY	55%
LVS	55%
GLY	55%
ARG	55%
LVS	55%
SER	55%
ARG	55%
ILE	55%
ALA	55%
ASN	55%
ILE	55%
PRO	55%
ASN	55%
PHE	55%
GLU	55%
GLN	55%
SER	55%
L670	55%
K671	55%
N672	55%
L673	55%
V674	55%
Y682	55%
S685	55%
G686	55%
T687	55%
F694	55%
Q695	55%
M704	55%
L705	55%
I706	55%
D707	55%
F708	55%
C709	55%
I710	55%
D711	55%
M712	55%
L713	55%
M714	55%
E715	55%
D723	55%
D724	55%



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	156.82Å 163.47Å 292.83Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.98 – 3.20 48.95 – 3.11	Depositor EDS
% Data completeness (in resolution range)	100.0 (19.98-3.20) 99.0 (48.95-3.11)	Depositor EDS
$R_{merge}$	0.05	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.92 (at 3.12Å)	Xtriage
Refinement program	ELVES, PHENIX	Depositor
R, $R_{free}$	0.235 , 0.283 0.239 , 0.282	Depositor DCC
$R_{free}$ test set	6993 reflections (5.20%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	82.4	Xtriage
Anisotropy	0.094	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.26 , 81.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.40$ , $\langle L^2 \rangle = 0.23$	Xtriage
Estimated twinning fraction	0.075 for k,h,-l	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	48018	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	147.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.58% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: TPO, APJ, SEP

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	0.35	0/3437	0.51	1/4629 (0.0%)
1	B	0.35	0/3437	0.49	0/4629
1	C	0.37	0/3437	0.51	0/4629
1	D	0.37	0/3497	0.51	0/4711
1	E	0.33	0/3437	0.48	0/4629
1	F	0.34	0/3437	0.49	0/4629
1	G	0.29	0/3437	0.47	0/4629
1	H	0.28	0/3437	0.47	0/4629
1	I	0.27	0/3420	0.45	0/4607
1	J	0.27	0/3420	0.45	0/4607
1	K	0.28	0/3497	0.47	0/4711
1	L	0.28	0/3437	0.47	0/4629
1	M	0.32	0/3437	0.48	0/4629
1	N	0.34	0/3437	0.50	0/4629
All	All	0.32	0/48204	0.48	1/64926 (0.0%)

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	1
1	C	0	1
1	D	0	2
1	E	0	1
1	F	0	1
1	G	0	2
1	H	0	1
1	K	0	2

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Mol	Chain	#Chirality outliers	#Planarity outliers
1	L	0	2
1	M	0	2
1	N	0	1
All	All	0	17

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1039	ARG	N-CA-C	-5.47	96.22	111.00

There are no chirality outliers.

5 of 17 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	671	LYS	Peptide
1	B	671	LYS	Peptide
1	C	671	LYS	Peptide
1	D	670	LEU	Peptide
1	D	671	LYS	Peptide

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

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3399	0	3409	136	1
1	B	3399	0	3409	132	0
1	C	3399	0	3409	151	1
1	D	3457	0	3461	158	0
1	E	3399	0	3409	135	0
1	F	3399	0	3409	141	0
1	G	3399	0	3409	145	0
1	H	3399	0	3409	130	0
1	I	3382	0	3385	136	2
1	J	3382	0	3385	148	2
1	K	3457	0	3461	141	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	L	3399	0	3409	123	0
1	M	3399	0	3409	147	0
1	N	3399	0	3409	138	0
2	A	25	0	16	7	0
2	B	25	0	16	8	0
2	C	25	0	16	7	0
2	D	25	0	16	8	0
2	E	25	0	16	7	0
2	F	25	0	16	7	0
2	G	25	0	16	7	0
2	H	25	0	16	7	0
2	I	25	0	16	7	0
2	J	25	0	16	7	0
2	K	25	0	16	8	0
2	L	25	0	16	7	0
2	M	25	0	16	7	0
2	N	25	0	16	7	0
All	All	48018	0	48006	1914	3

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 20.

The worst 5 of 1914 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:668:GLN:HG3	1:D:739:ARG:HE	0.93	1.07
1:K:668:GLN:HG3	1:K:739:ARG:HE	1.19	1.02
1:F:848:ASN:HB3	1:F:849:PRO:HA	1.42	1.02
1:I:848:ASN:HB3	1:I:849:PRO:HA	1.42	1.01
1:A:848:ASN:HB3	1:A:849:PRO:HA	1.43	1.01

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:848:ASN:OD1	1:J:1045:SER:OG[4_457]	1.97	0.23
1:I:848:ASN:CG	1:J:1045:SER:OG[4_457]	2.05	0.15
1:A:1021:PRO:O	1:C:739:ARG:NH1[4_456]	2.10	0.10

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	413/448 (92%)	351 (85%)	50 (12%)	12 (3%)	4	28
1	B	413/448 (92%)	352 (85%)	52 (13%)	9 (2%)	6	35
1	C	413/448 (92%)	348 (84%)	56 (14%)	9 (2%)	6	35
1	D	420/448 (94%)	353 (84%)	57 (14%)	10 (2%)	6	34
1	E	413/448 (92%)	354 (86%)	50 (12%)	9 (2%)	6	35
1	F	413/448 (92%)	352 (85%)	52 (13%)	9 (2%)	6	35
1	G	413/448 (92%)	351 (85%)	53 (13%)	9 (2%)	6	35
1	H	413/448 (92%)	352 (85%)	52 (13%)	9 (2%)	6	35
1	I	411/448 (92%)	353 (86%)	49 (12%)	9 (2%)	6	35
1	J	411/448 (92%)	350 (85%)	52 (13%)	9 (2%)	6	35
1	K	420/448 (94%)	349 (83%)	61 (14%)	10 (2%)	6	34
1	L	413/448 (92%)	352 (85%)	52 (13%)	9 (2%)	6	35
1	M	413/448 (92%)	353 (86%)	51 (12%)	9 (2%)	6	35
1	N	413/448 (92%)	353 (86%)	51 (12%)	9 (2%)	6	35
All	All	5792/6272 (92%)	4923 (85%)	738 (13%)	131 (2%)	6	34

5 of 131 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	759	LYS
1	A	770	LYS
1	A	771	GLU
1	A	862	GLU
1	A	1039	ARG

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	380/405 (94%)	351 (92%)	29 (8%)	13	45
1	B	380/405 (94%)	352 (93%)	28 (7%)	13	46
1	C	380/405 (94%)	350 (92%)	30 (8%)	12	43
1	D	387/405 (96%)	353 (91%)	34 (9%)	10	36
1	E	380/405 (94%)	349 (92%)	31 (8%)	11	41
1	F	380/405 (94%)	349 (92%)	31 (8%)	11	41
1	G	380/405 (94%)	350 (92%)	30 (8%)	12	43
1	H	380/405 (94%)	350 (92%)	30 (8%)	12	43
1	I	378/405 (93%)	351 (93%)	27 (7%)	14	47
1	J	378/405 (93%)	351 (93%)	27 (7%)	14	47
1	K	387/405 (96%)	356 (92%)	31 (8%)	12	42
1	L	380/405 (94%)	350 (92%)	30 (8%)	12	43
1	M	380/405 (94%)	352 (93%)	28 (7%)	13	46
1	N	380/405 (94%)	347 (91%)	33 (9%)	10	37
All	All	5330/5670 (94%)	4911 (92%)	419 (8%)	12	43

5 of 419 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	G	749	ASN
1	H	943	CYS
1	N	671	LYS
1	G	796	ARG
1	G	1085	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 150 such sidechains are listed below:

Mol	Chain	Res	Type
1	G	725	HIS

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Mol	Chain	Res	Type
1	H	845	ASN
1	M	1090	ASN
1	G	753	GLN
1	H	725	HIS

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

42 non-standard protein/DNA/RNA residues 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
1	SEP	C	841	1	8,9,10	1.54	1 (12%)	8,12,14	1.47	1 (12%)
1	SEP	H	840	1	8,9,10	1.60	1 (12%)	8,12,14	1.77	2 (25%)
1	TPO	M	844	1	8,10,11	3.00	5 (62%)	10,14,16	1.60	2 (20%)
1	SEP	K	841	1	8,9,10	1.53	1 (12%)	8,12,14	1.41	1 (12%)
1	SEP	H	841	1	8,9,10	1.54	1 (12%)	8,12,14	1.47	1 (12%)
1	TPO	E	844	1	8,10,11	2.98	5 (62%)	10,14,16	1.61	2 (20%)
1	SEP	I	840	1	8,9,10	1.58	1 (12%)	8,12,14	1.81	2 (25%)
1	TPO	N	844	1	8,10,11	2.97	5 (62%)	10,14,16	1.59	2 (20%)
1	SEP	F	840	1	8,9,10	1.56	1 (12%)	8,12,14	1.79	2 (25%)
1	TPO	L	844	1	8,10,11	2.98	5 (62%)	10,14,16	1.59	2 (20%)
1	SEP	N	840	1	8,9,10	1.60	1 (12%)	8,12,14	1.81	2 (25%)
1	SEP	L	840	1	8,9,10	1.58	1 (12%)	8,12,14	1.79	2 (25%)
1	TPO	A	844	1	8,10,11	2.99	5 (62%)	10,14,16	1.59	2 (20%)
1	SEP	G	840	1	8,9,10	1.58	1 (12%)	8,12,14	1.82	2 (25%)
1	SEP	E	840	1	8,9,10	1.56	1 (12%)	8,12,14	1.82	2 (25%)
1	SEP	B	841	1	8,9,10	1.51	1 (12%)	8,12,14	1.46	1 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
1	TPO	J	844	1	8,10,11	2.97	5 (62%)	10,14,16	1.59	2 (20%)
1	SEP	J	841	1	8,9,10	1.53	1 (12%)	8,12,14	1.45	1 (12%)
1	TPO	B	844	1	8,10,11	2.98	5 (62%)	10,14,16	1.58	2 (20%)
1	SEP	D	840	1	8,9,10	1.60	1 (12%)	8,12,14	1.83	2 (25%)
1	TPO	F	844	1	8,10,11	3.00	5 (62%)	10,14,16	1.58	2 (20%)
1	SEP	J	840	1	8,9,10	1.58	1 (12%)	8,12,14	1.83	2 (25%)
1	SEP	A	841	1	8,9,10	1.52	1 (12%)	8,12,14	1.43	1 (12%)
1	TPO	K	844	1	8,10,11	3.00	5 (62%)	10,14,16	1.58	2 (20%)
1	SEP	A	840	1	8,9,10	1.57	1 (12%)	8,12,14	1.83	2 (25%)
1	SEP	I	841	1	8,9,10	1.55	1 (12%)	8,12,14	1.44	1 (12%)
1	TPO	C	844	1	8,10,11	2.96	5 (62%)	10,14,16	1.61	2 (20%)
1	TPO	H	844	1	8,10,11	2.98	5 (62%)	10,14,16	1.59	2 (20%)
1	SEP	M	840	1	8,9,10	1.57	1 (12%)	8,12,14	1.78	2 (25%)
1	SEP	B	840	1	8,9,10	1.58	1 (12%)	8,12,14	1.81	2 (25%)
1	TPO	D	844	1	8,10,11	2.99	5 (62%)	10,14,16	1.59	2 (20%)
1	SEP	K	840	1	8,9,10	1.58	1 (12%)	8,12,14	1.85	2 (25%)
1	TPO	G	844	1	8,10,11	2.99	5 (62%)	10,14,16	1.57	2 (20%)
1	TPO	I	844	1	8,10,11	3.00	5 (62%)	10,14,16	1.56	2 (20%)
1	SEP	F	841	1	8,9,10	1.62	1 (12%)	8,12,14	1.47	1 (12%)
1	SEP	G	841	1	8,9,10	1.53	1 (12%)	8,12,14	1.45	1 (12%)
1	SEP	D	841	1	8,9,10	1.50	1 (12%)	8,12,14	1.39	1 (12%)
1	SEP	E	841	1	8,9,10	1.52	1 (12%)	8,12,14	1.48	2 (25%)
1	SEP	N	841	1	8,9,10	1.56	1 (12%)	8,12,14	1.48	1 (12%)
1	SEP	L	841	1	8,9,10	1.54	1 (12%)	8,12,14	1.44	1 (12%)
1	SEP	M	841	1	8,9,10	1.49	1 (12%)	8,12,14	1.40	1 (12%)
1	SEP	C	840	1	8,9,10	1.58	1 (12%)	8,12,14	1.81	2 (25%)

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
1	SEP	C	841	1	-	1/5/8/10	-
1	SEP	H	840	1	-	4/5/8/10	-
1	TPO	M	844	1	-	4/9/11/13	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	SEP	K	841	1	-	1/5/8/10	-
1	SEP	H	841	1	-	1/5/8/10	-
1	TPO	E	844	1	-	4/9/11/13	-
1	SEP	I	840	1	-	4/5/8/10	-
1	TPO	N	844	1	-	4/9/11/13	-
1	SEP	F	840	1	-	4/5/8/10	-
1	TPO	L	844	1	-	4/9/11/13	-
1	SEP	N	840	1	-	4/5/8/10	-
1	SEP	L	840	1	-	4/5/8/10	-
1	TPO	A	844	1	-	4/9/11/13	-
1	SEP	G	840	1	-	4/5/8/10	-
1	SEP	E	840	1	-	3/5/8/10	-
1	SEP	B	841	1	-	1/5/8/10	-
1	TPO	J	844	1	-	4/9/11/13	-
1	SEP	J	841	1	-	1/5/8/10	-
1	TPO	B	844	1	-	4/9/11/13	-
1	SEP	D	840	1	-	4/5/8/10	-
1	TPO	F	844	1	-	4/9/11/13	-
1	SEP	J	840	1	-	4/5/8/10	-
1	SEP	A	841	1	-	1/5/8/10	-
1	TPO	K	844	1	-	4/9/11/13	-
1	SEP	A	840	1	-	4/5/8/10	-
1	SEP	I	841	1	-	1/5/8/10	-
1	TPO	C	844	1	-	4/9/11/13	-
1	TPO	H	844	1	-	4/9/11/13	-
1	SEP	M	840	1	-	4/5/8/10	-
1	SEP	B	840	1	-	4/5/8/10	-
1	TPO	D	844	1	-	4/9/11/13	-
1	SEP	K	840	1	-	4/5/8/10	-
1	TPO	G	844	1	-	4/9/11/13	-
1	TPO	I	844	1	-	4/9/11/13	-
1	SEP	F	841	1	-	1/5/8/10	-
1	SEP	G	841	1	-	1/5/8/10	-
1	SEP	D	841	1	-	1/5/8/10	-
1	SEP	E	841	1	-	1/5/8/10	-
1	SEP	N	841	1	-	1/5/8/10	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	SEP	L	841	1	-	1/5/8/10	-
1	SEP	M	841	1	-	1/5/8/10	-
1	SEP	C	840	1	-	4/5/8/10	-

The worst 5 of 98 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	844	TPO	O-C	5.30	1.41	1.19
1	F	844	TPO	O-C	5.18	1.40	1.19
1	I	844	TPO	O-C	5.17	1.40	1.19
1	M	844	TPO	O-C	5.17	1.40	1.19
1	K	844	TPO	O-C	5.16	1.40	1.19

The worst 5 of 71 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	844	TPO	O-C-CA	-4.13	113.95	124.78
1	N	844	TPO	O-C-CA	-4.12	113.99	124.78
1	E	844	TPO	O-C-CA	-4.11	114.00	124.78
1	M	844	TPO	O-C-CA	-4.11	114.00	124.78
1	J	844	TPO	O-C-CA	-4.10	114.04	124.78

There are no chirality outliers.

5 of 125 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	H	840	SEP	CB-OG-P-O2P
1	H	840	SEP	CB-OG-P-O3P
1	M	844	TPO	N-CA-CB-CG2
1	M	844	TPO	N-CA-CB-OG1
1	M	844	TPO	O-C-CA-CB

There are no ring outliers.

4 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	H	840	SEP	3	0
1	K	841	SEP	2	0
1	F	840	SEP	3	0
1	G	840	SEP	1	0



## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

14 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	APJ	K	1999	-	26,29,29	1.80	5 (19%)	30,41,41	2.76	11 (36%)
2	APJ	J	1999	-	26,29,29	1.82	6 (23%)	30,41,41	2.74	11 (36%)
2	APJ	I	1999	-	26,29,29	1.81	6 (23%)	30,41,41	2.77	12 (40%)
2	APJ	H	1999	-	26,29,29	1.78	6 (23%)	30,41,41	2.76	12 (40%)
2	APJ	N	1999	-	26,29,29	1.77	5 (19%)	30,41,41	2.79	11 (36%)
2	APJ	M	1999	-	26,29,29	1.80	6 (23%)	30,41,41	2.77	11 (36%)
2	APJ	L	1999	-	26,29,29	1.79	5 (19%)	30,41,41	2.77	11 (36%)
2	APJ	C	1999	-	26,29,29	1.78	6 (23%)	30,41,41	2.88	11 (36%)
2	APJ	B	1999	-	26,29,29	1.80	6 (23%)	30,41,41	2.77	11 (36%)
2	APJ	A	1999	-	26,29,29	1.88	6 (23%)	30,41,41	2.78	12 (40%)
2	APJ	G	1999	-	26,29,29	1.84	6 (23%)	30,41,41	2.77	11 (36%)
2	APJ	F	1999	-	26,29,29	1.77	6 (23%)	30,41,41	2.76	12 (40%)
2	APJ	E	1999	-	26,29,29	1.76	5 (19%)	30,41,41	2.77	11 (36%)
2	APJ	D	1999	-	26,29,29	1.79	5 (19%)	30,41,41	2.77	12 (40%)

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	APJ	K	1999	-	-	2/10/14/14	0/5/5/5
2	APJ	J	1999	-	-	2/10/14/14	0/5/5/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	APJ	I	1999	-	-	2/10/14/14	0/5/5/5
2	APJ	H	1999	-	-	2/10/14/14	0/5/5/5
2	APJ	N	1999	-	-	2/10/14/14	0/5/5/5
2	APJ	M	1999	-	-	2/10/14/14	0/5/5/5
2	APJ	L	1999	-	-	2/10/14/14	0/5/5/5
2	APJ	C	1999	-	-	2/10/14/14	0/5/5/5
2	APJ	B	1999	-	-	2/10/14/14	0/5/5/5
2	APJ	A	1999	-	-	2/10/14/14	0/5/5/5
2	APJ	G	1999	-	-	2/10/14/14	0/5/5/5
2	APJ	F	1999	-	-	2/10/14/14	0/5/5/5
2	APJ	E	1999	-	-	2/10/14/14	0/5/5/5
2	APJ	D	1999	-	-	2/10/14/14	0/5/5/5

The worst 5 of 79 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1999	APJ	N5-N4	-5.81	1.26	1.37
2	C	1999	APJ	N5-N4	-5.72	1.26	1.37
2	G	1999	APJ	N5-N4	-5.72	1.26	1.37
2	D	1999	APJ	N5-N4	-5.64	1.26	1.37
2	H	1999	APJ	N5-N4	-5.64	1.26	1.37

The worst 5 of 159 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	J	1999	APJ	N2-C9-N1	-7.48	119.46	126.55
2	I	1999	APJ	N2-C9-N1	-7.18	119.74	126.55
2	M	1999	APJ	N2-C9-N1	-7.11	119.81	126.55
2	G	1999	APJ	N2-C9-N1	-7.10	119.82	126.55
2	L	1999	APJ	N2-C9-N1	-7.09	119.83	126.55

There are no chirality outliers.

5 of 28 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	K	1999	APJ	N5-C14-C16-C18
2	K	1999	APJ	C15-C14-C16-C18
2	J	1999	APJ	N5-C14-C16-C18
2	J	1999	APJ	C15-C14-C16-C18

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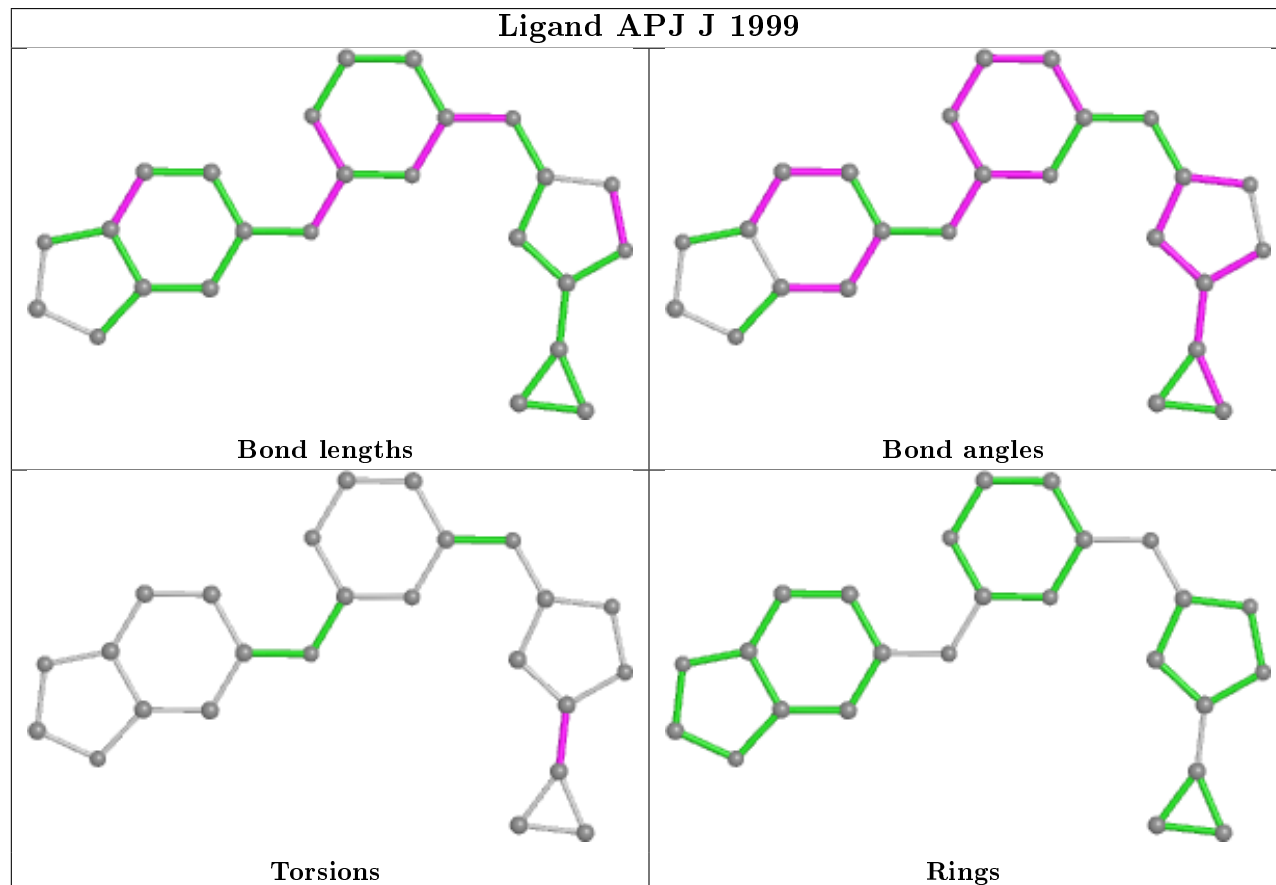
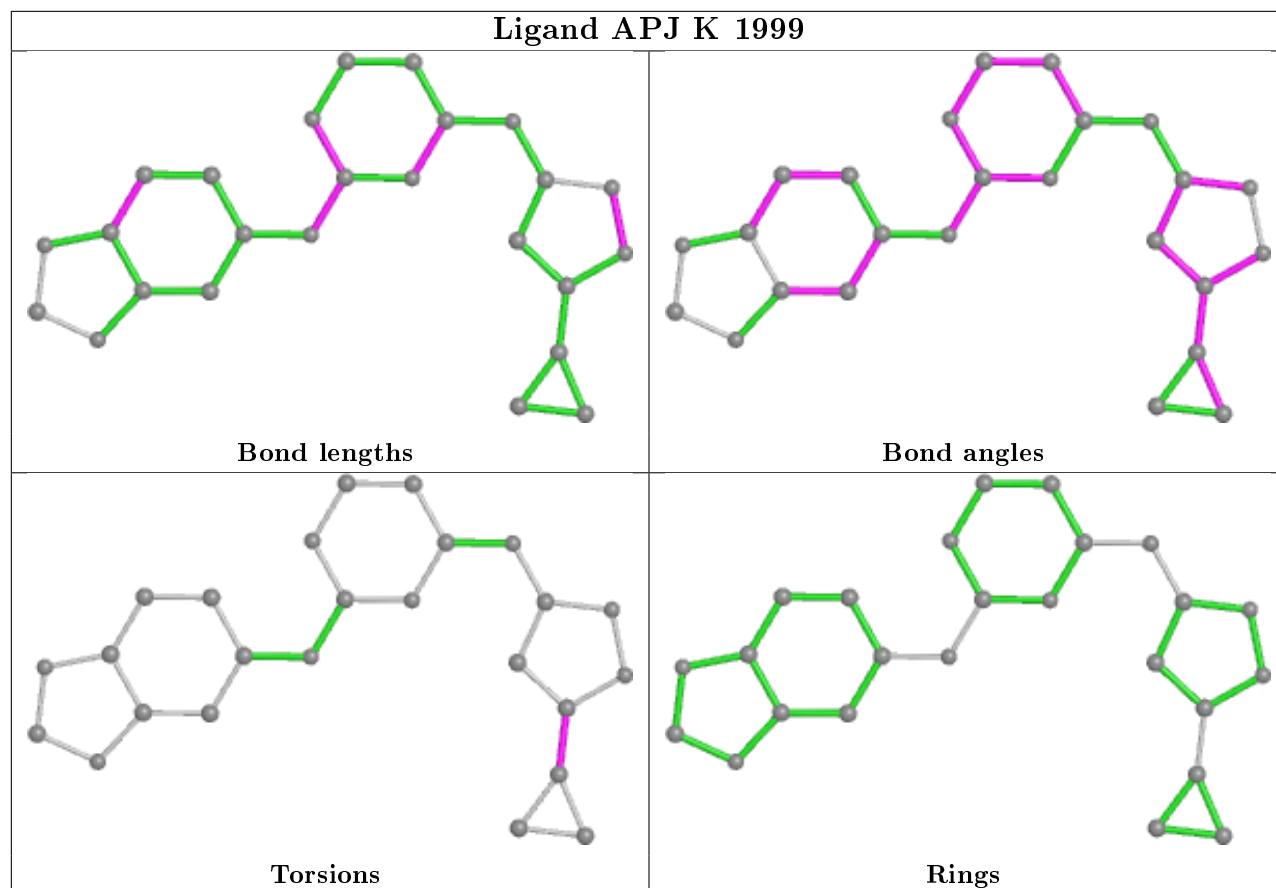
Mol	Chain	Res	Type	Atoms
2	I	1999	APJ	N5-C14-C16-C18

There are no ring outliers.

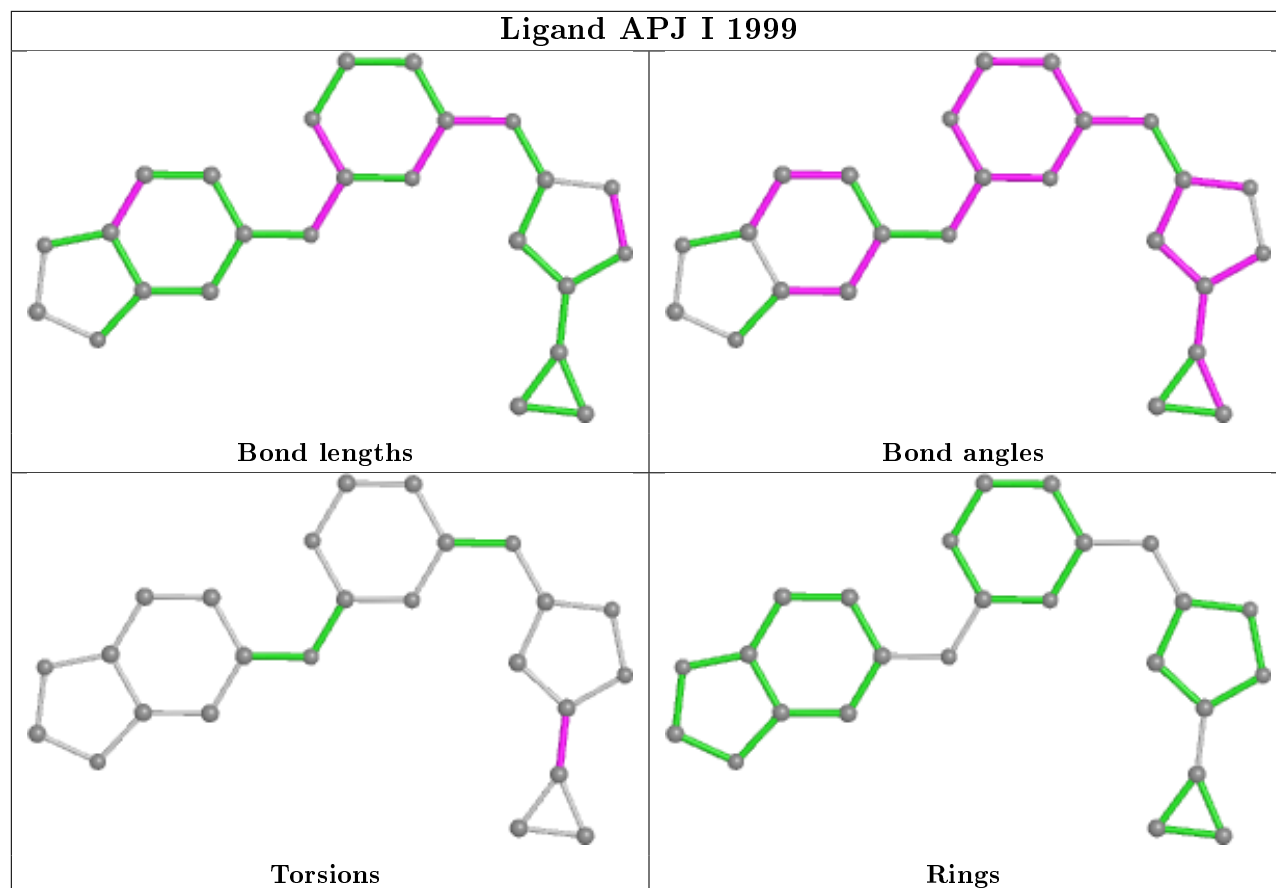
14 monomers are involved in 101 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	K	1999	APJ	8	0
2	J	1999	APJ	7	0
2	I	1999	APJ	7	0
2	H	1999	APJ	7	0
2	N	1999	APJ	7	0
2	M	1999	APJ	7	0
2	L	1999	APJ	7	0
2	C	1999	APJ	7	0
2	B	1999	APJ	8	0
2	A	1999	APJ	7	0
2	G	1999	APJ	7	0
2	F	1999	APJ	7	0
2	E	1999	APJ	7	0
2	D	1999	APJ	8	0

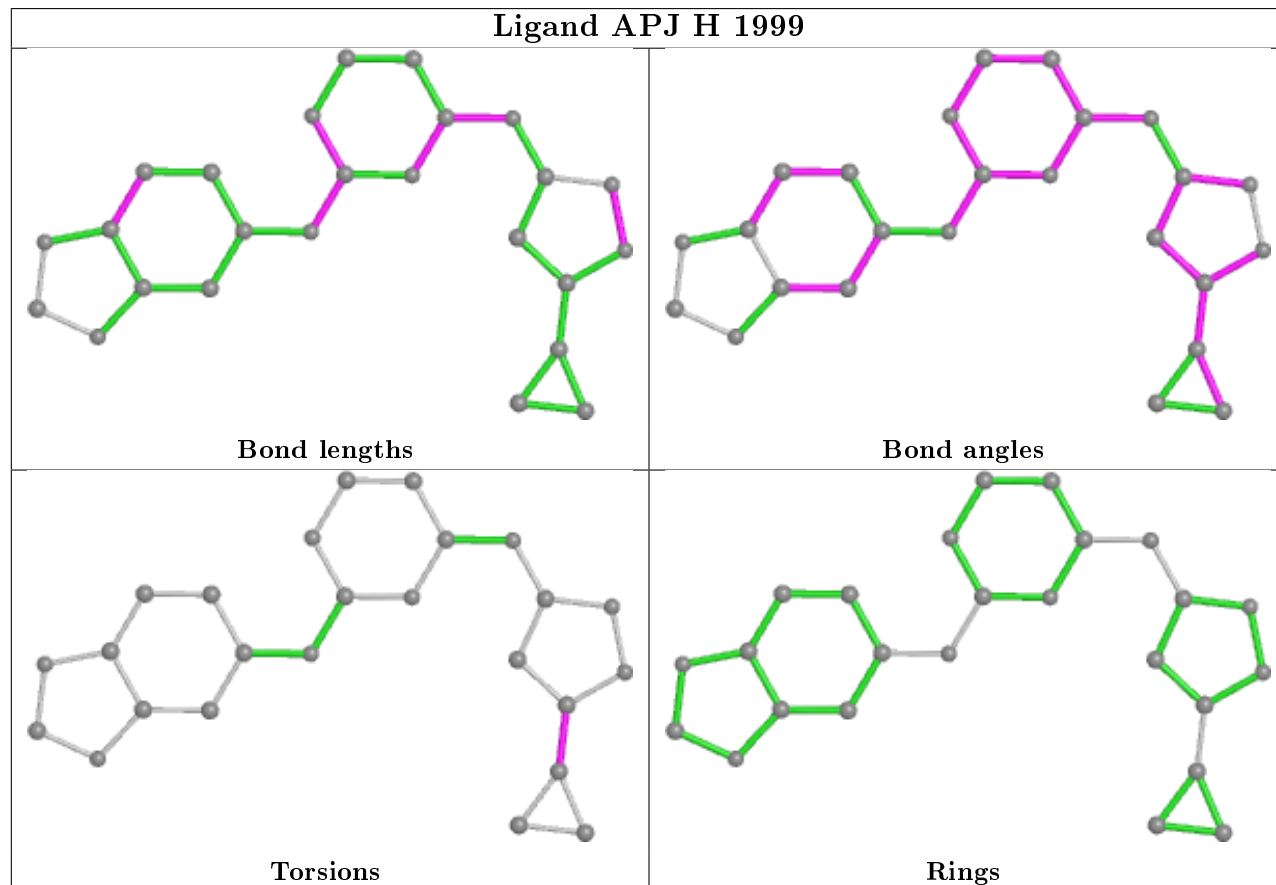
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

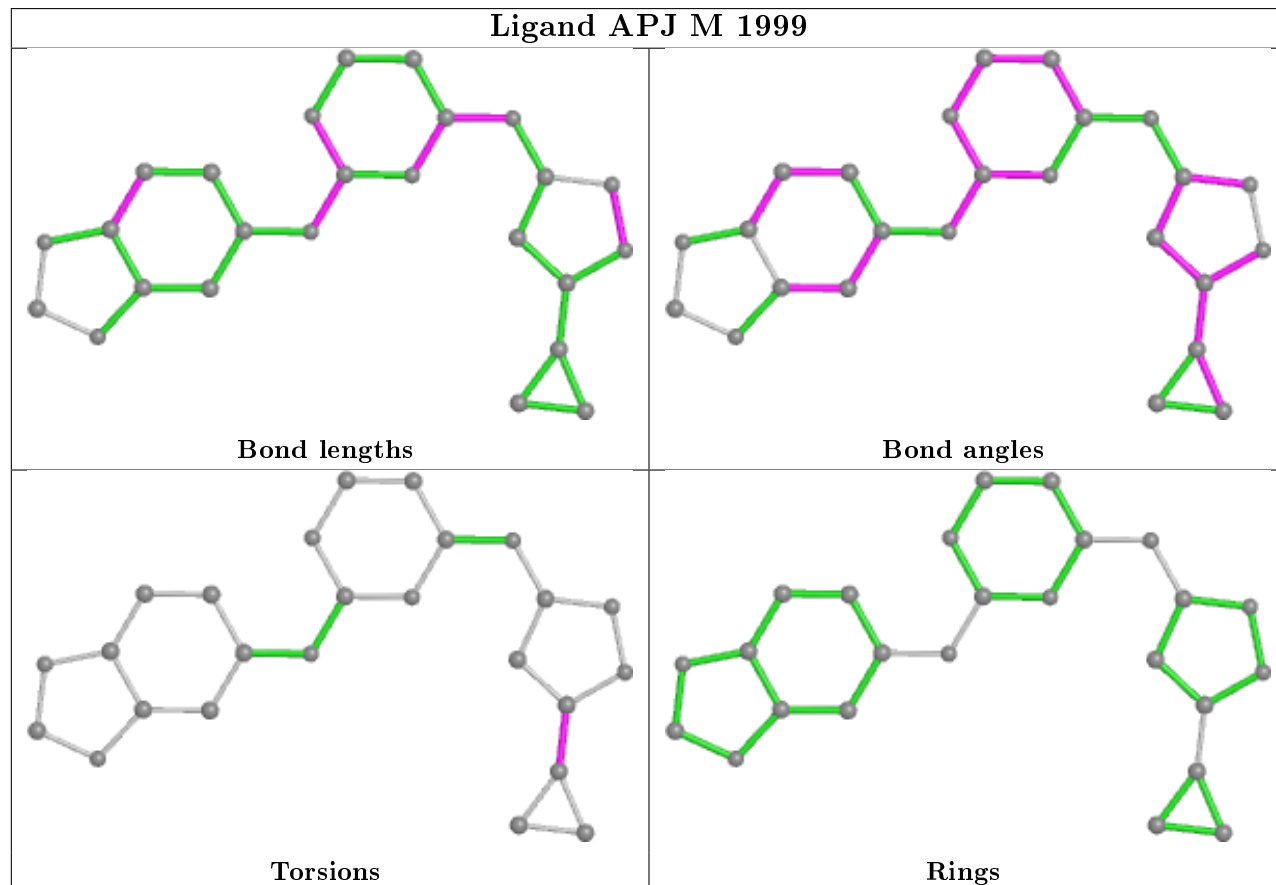
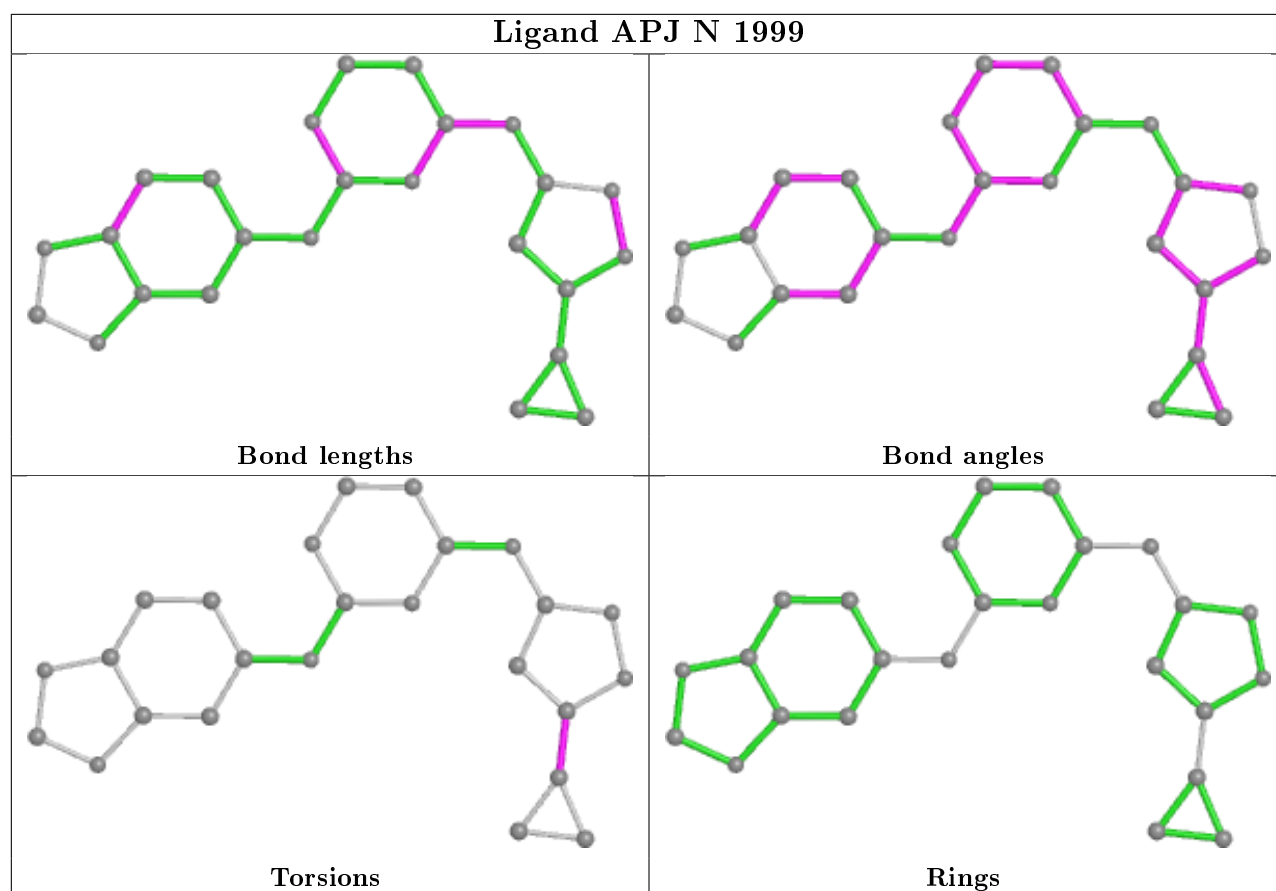


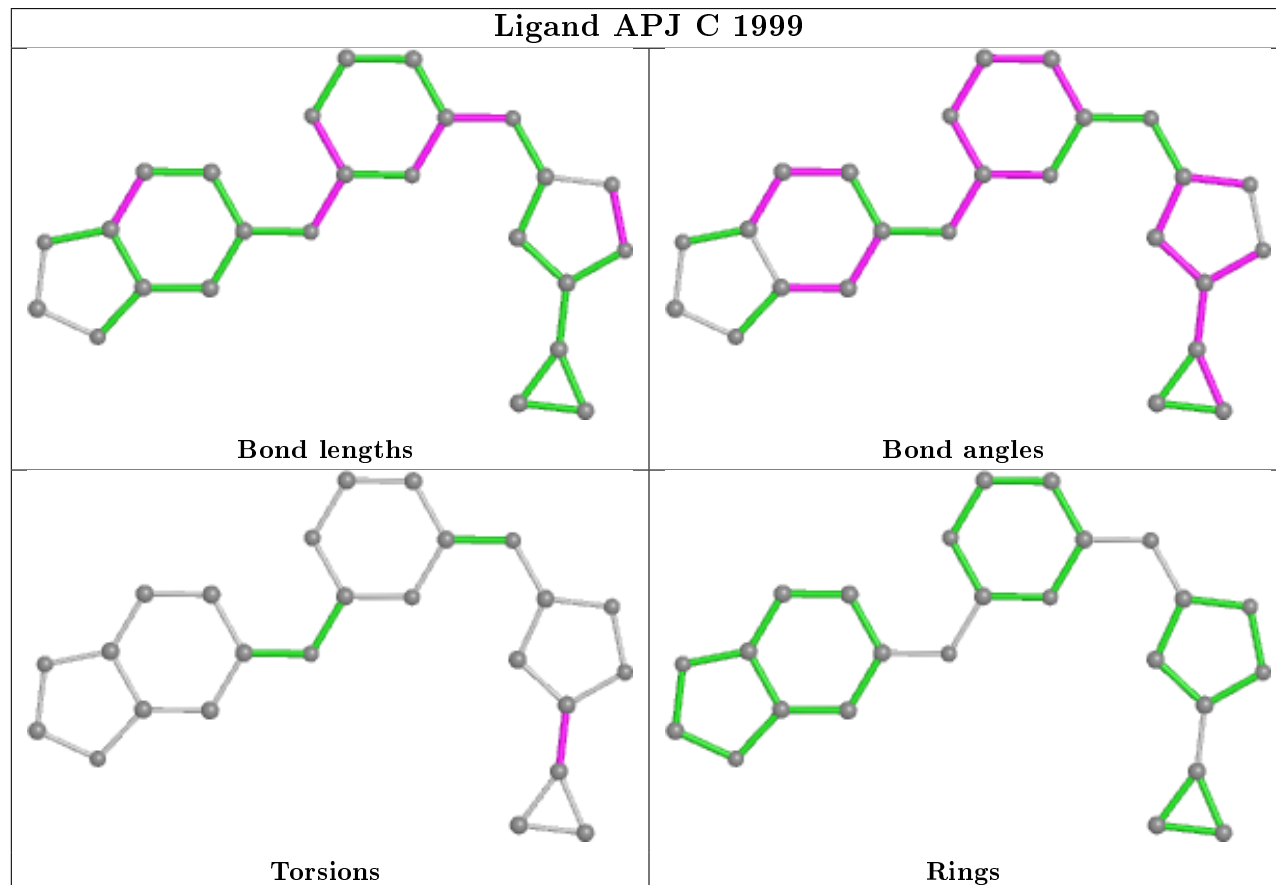
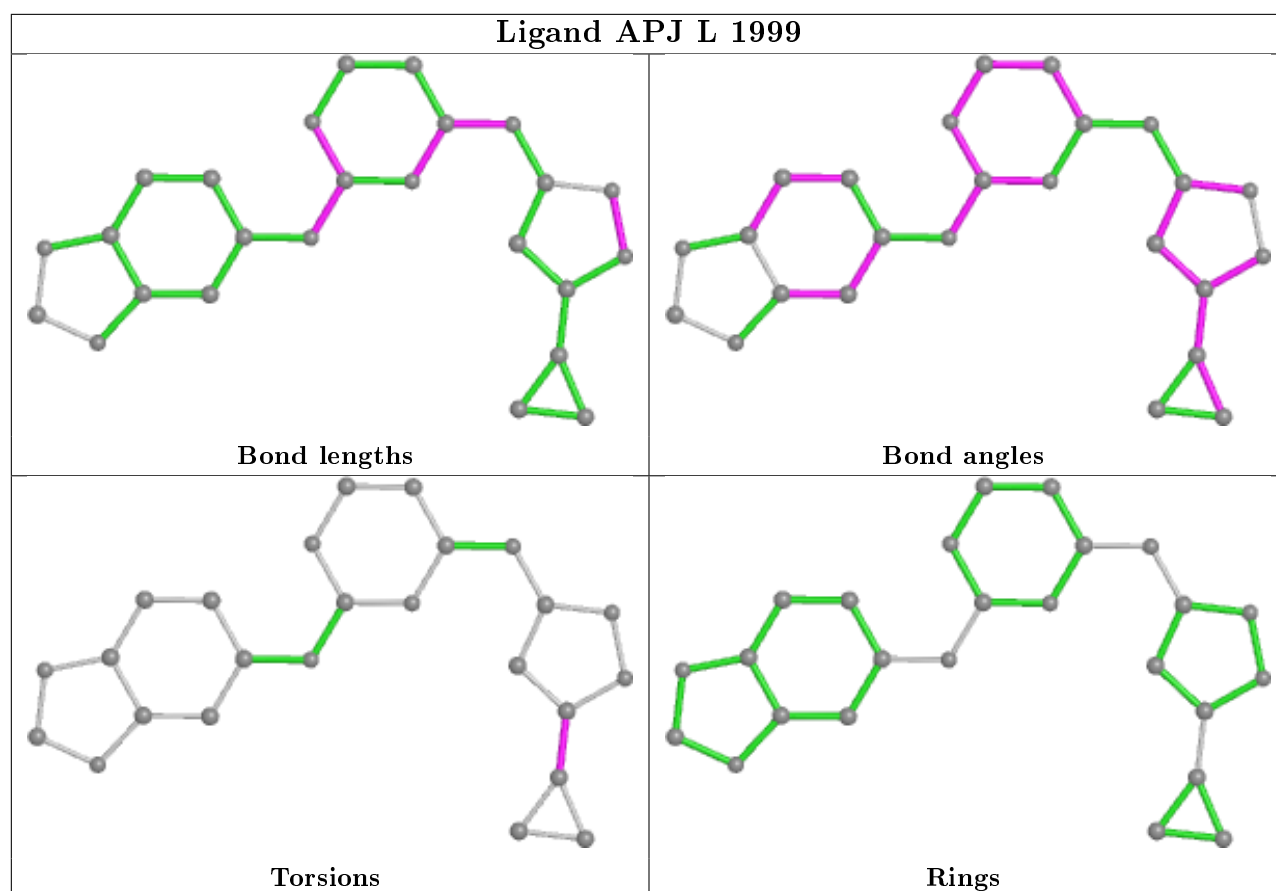
## Ligand APJ I 1999

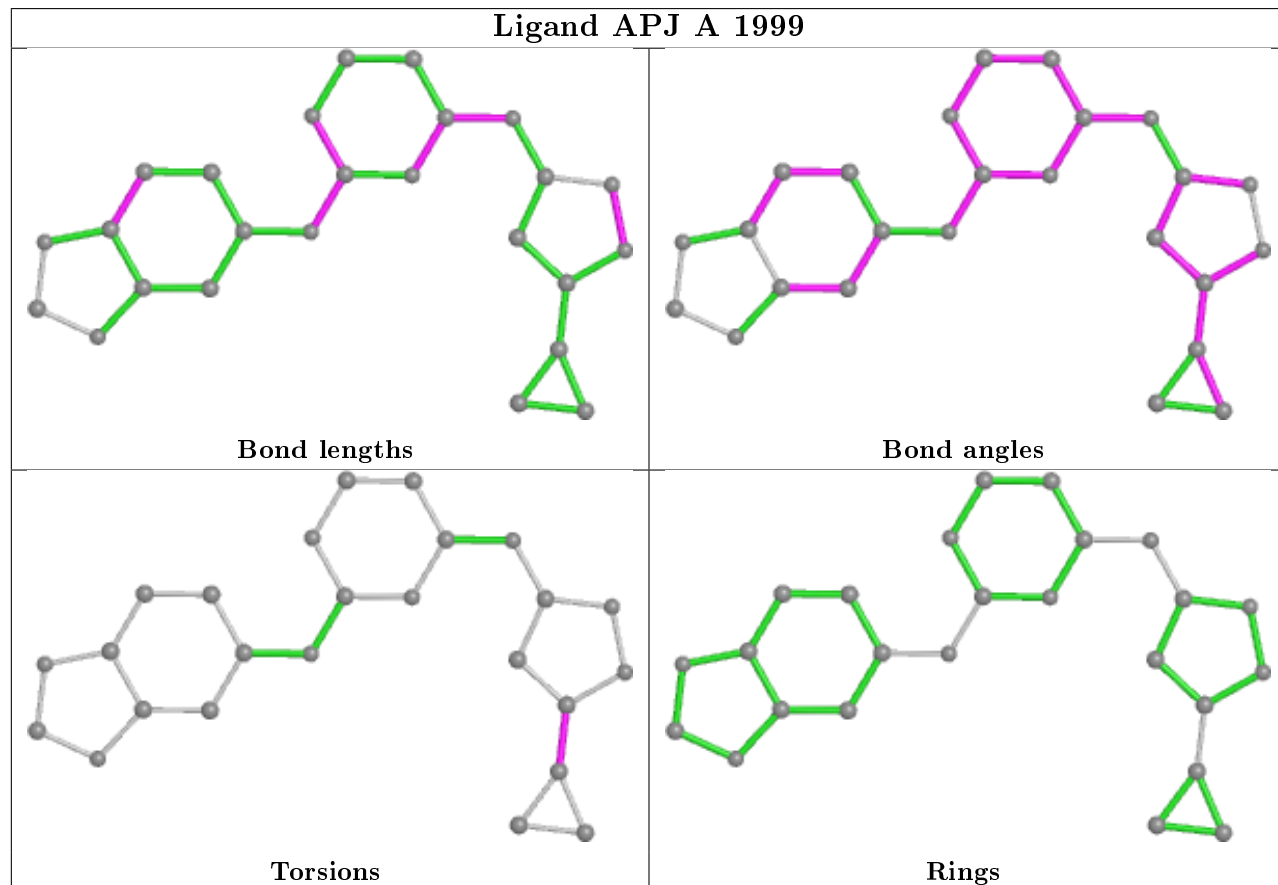
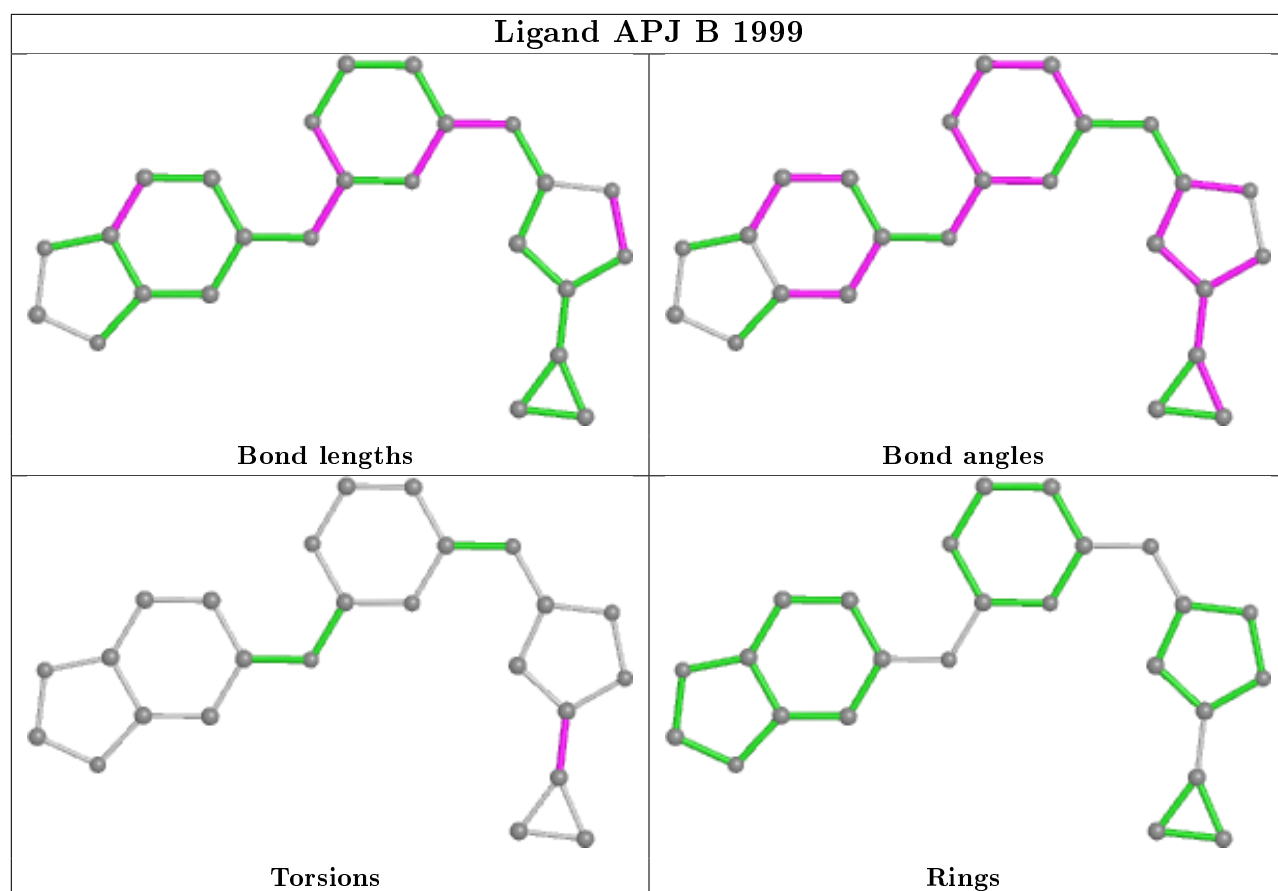


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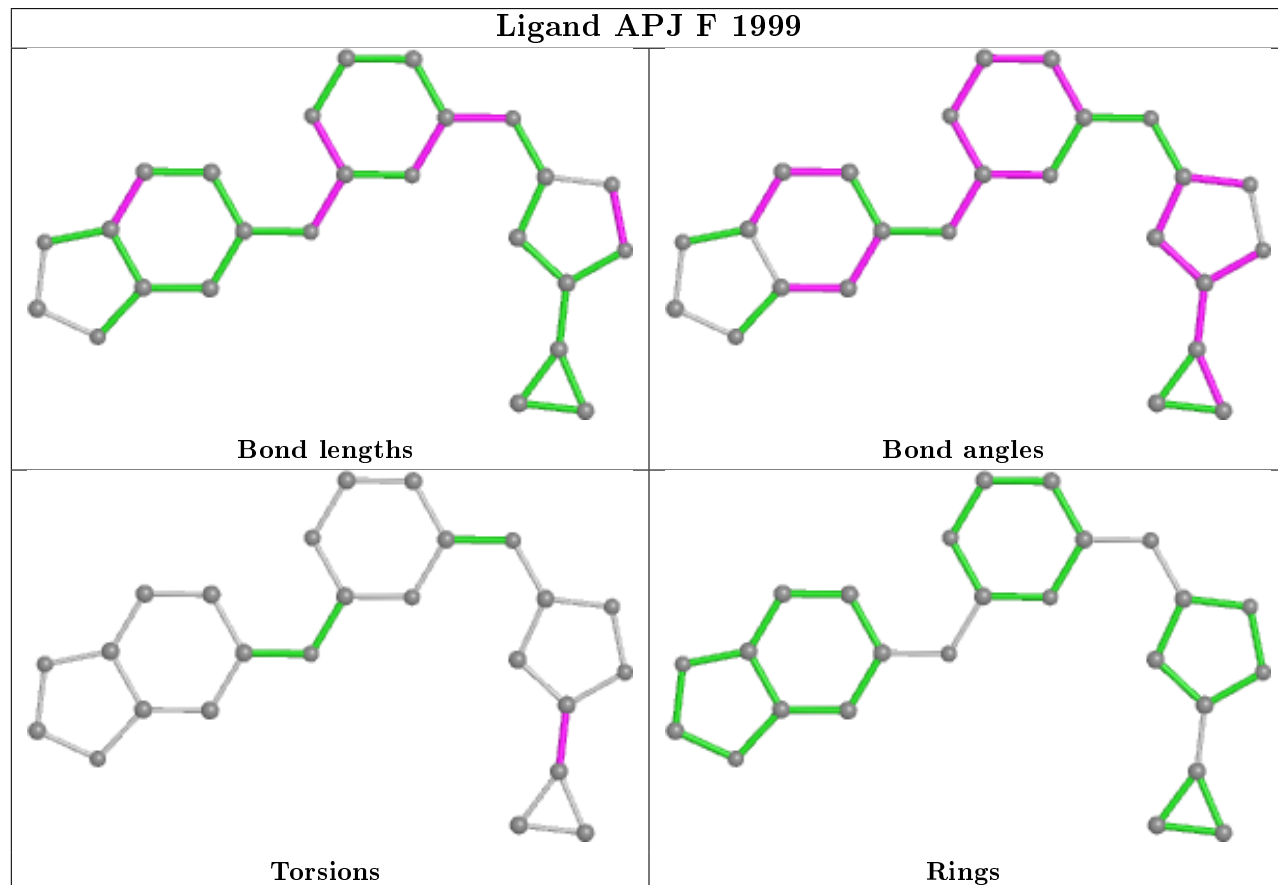
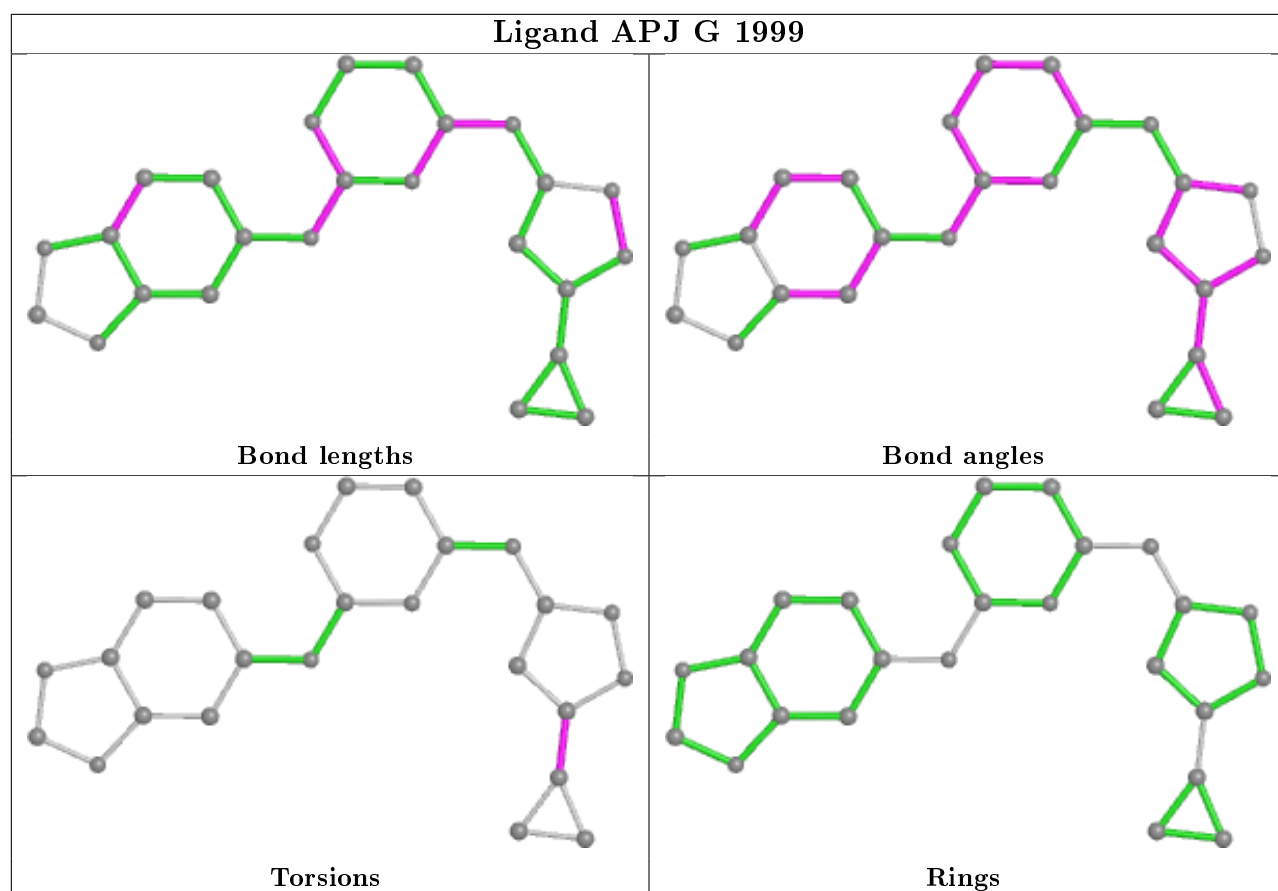


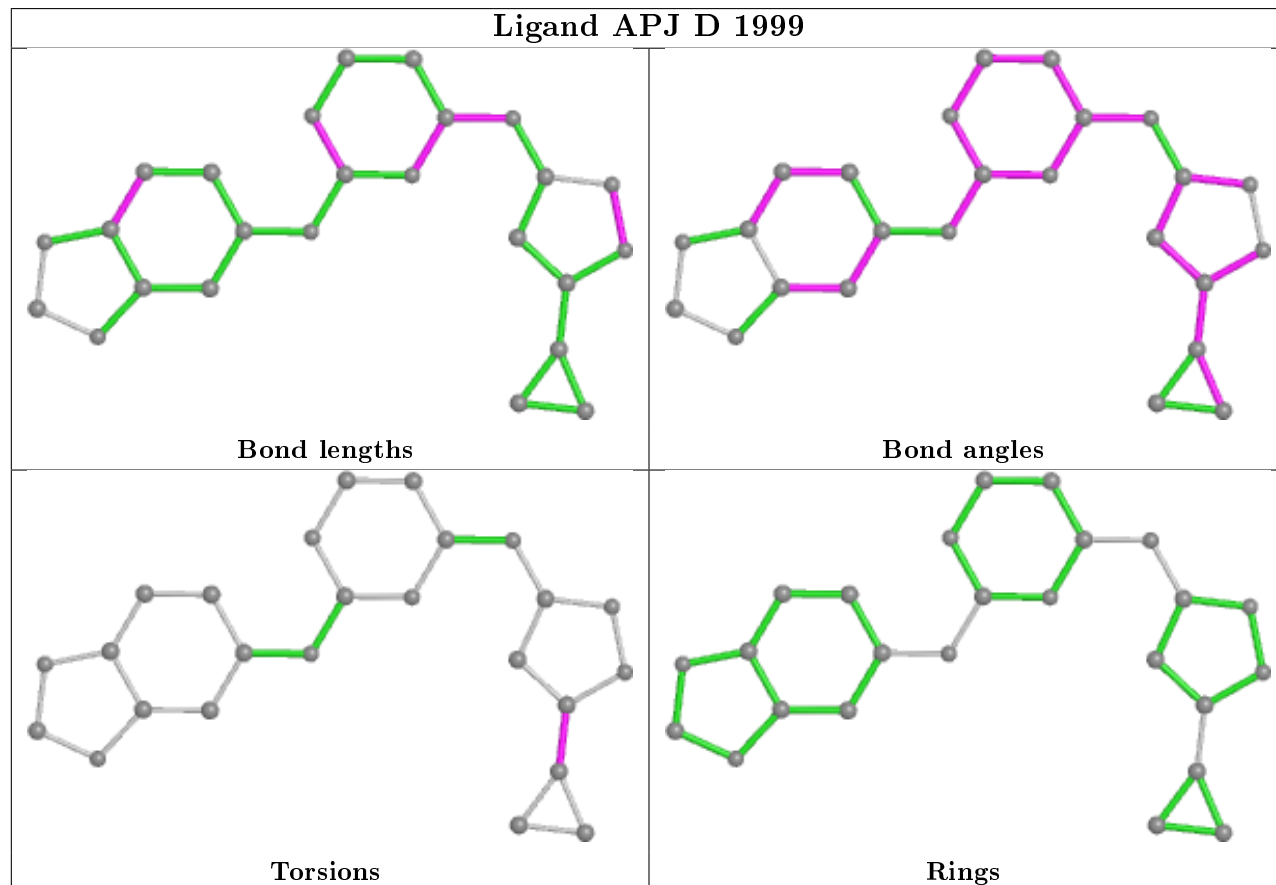
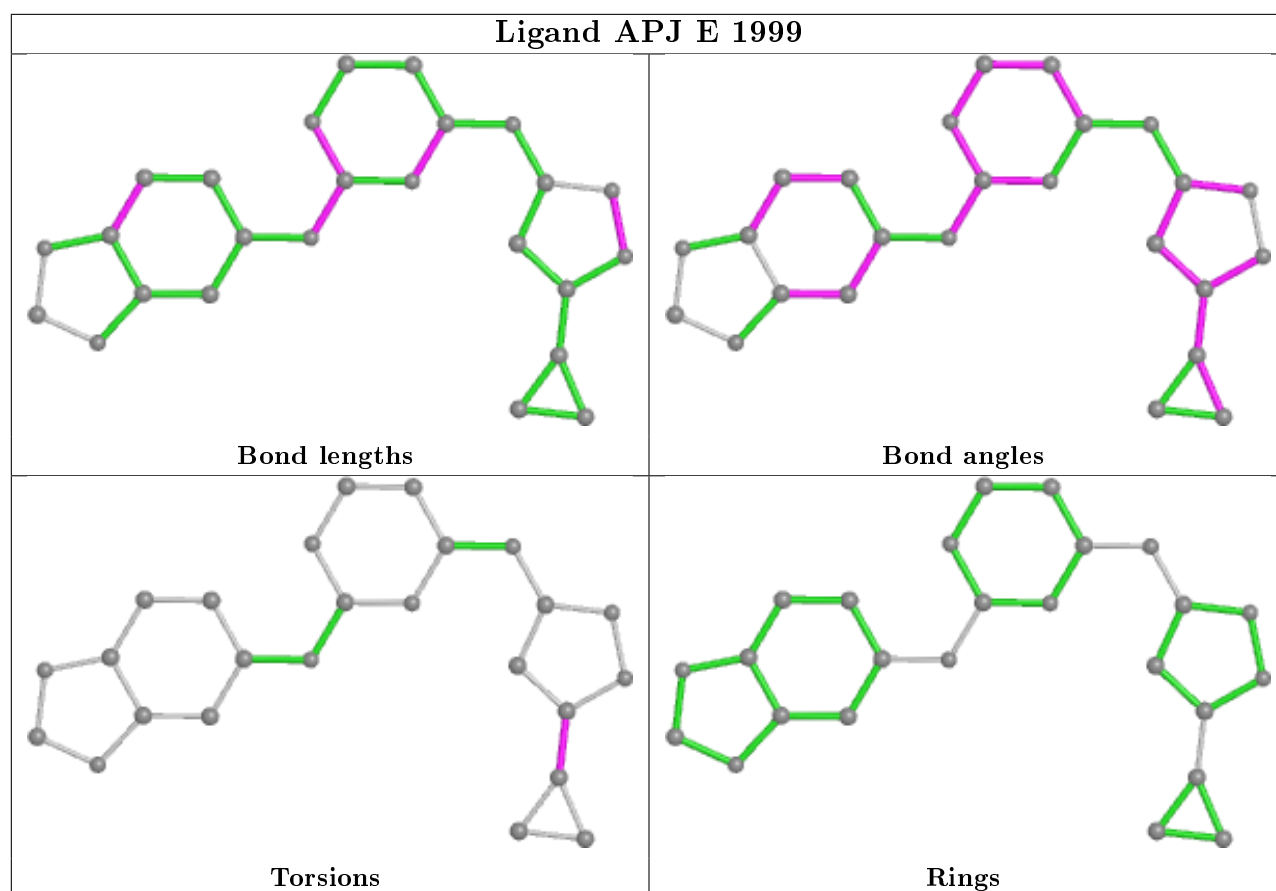












## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	415/448 (92%)	-0.16	6 (1%) 75 63	53, 111, 203, 287	0
1	B	415/448 (92%)	-0.17	2 (0%) 91 86	53, 108, 202, 287	0
1	C	415/448 (92%)	-0.19	5 (1%) 79 67	41, 102, 208, 268	0
1	D	422/448 (94%)	-0.27	2 (0%) 91 86	44, 99, 190, 261	0
1	E	415/448 (92%)	-0.19	8 (1%) 66 53	70, 119, 208, 308	0
1	F	415/448 (92%)	-0.19	3 (0%) 87 81	65, 107, 200, 259	0
1	G	415/448 (92%)	0.20	22 (5%) 26 14	99, 161, 256, 323	0
1	H	415/448 (92%)	0.16	16 (3%) 39 25	109, 166, 248, 312	0
1	I	413/448 (92%)	0.19	18 (4%) 34 21	123, 185, 259, 322	0
1	J	413/448 (92%)	0.68	63 (15%) 2 1	145, 210, 301, 366	0
1	K	422/448 (94%)	0.10	10 (2%) 59 44	108, 173, 258, 302	0
1	L	415/448 (92%)	0.28	20 (4%) 30 18	122, 177, 242, 319	0
1	M	415/448 (92%)	-0.10	7 (1%) 70 57	74, 123, 209, 271	0
1	N	415/448 (92%)	-0.15	4 (0%) 82 72	70, 106, 198, 296	0
All	All	5820/6272 (92%)	0.01	186 (3%) 47 31	41, 141, 246, 366	0

The worst 5 of 186 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	L	864	SER	12.5
1	L	863	GLU	8.7
1	N	893	THR	7.4
1	F	864	SER	5.8
1	N	864	SER	5.8

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
1	SEP	L	840	10/11	0.50	0.32	244,256,269,270	0
1	SEP	L	841	10/11	0.54	0.23	213,235,255,263	0
1	SEP	A	840	10/11	0.66	0.28	202,208,216,216	0
1	TPO	I	844	11/12	0.69	0.48	258,270,291,301	0
1	TPO	J	844	11/12	0.70	0.22	253,261,280,285	0
1	TPO	L	844	11/12	0.71	0.44	306,329,351,352	0
1	TPO	F	844	11/12	0.73	0.30	232,250,267,271	0
1	SEP	H	840	10/11	0.73	0.21	179,184,191,192	0
1	TPO	N	844	11/12	0.76	0.22	235,252,274,280	0
1	TPO	H	844	11/12	0.76	0.23	260,273,298,309	0
1	TPO	E	844	11/12	0.79	0.23	238,260,293,298	0
1	SEP	J	840	10/11	0.79	0.25	210,217,231,232	0
1	TPO	D	844	11/12	0.80	0.20	216,242,266,272	0
1	SEP	K	840	10/11	0.80	0.27	184,186,190,191	0
1	TPO	G	844	11/12	0.81	0.37	280,298,330,346	0
1	TPO	K	844	11/12	0.82	0.36	261,276,304,315	0
1	SEP	G	840	10/11	0.83	0.22	187,192,200,202	0
1	SEP	I	840	10/11	0.83	0.23	216,220,226,226	0
1	SEP	M	840	10/11	0.84	0.27	146,150,158,160	0
1	SEP	F	840	10/11	0.84	0.17	138,142,146,152	0
1	SEP	N	840	10/11	0.85	0.15	172,174,179,183	0
1	SEP	K	841	10/11	0.85	0.15	148,161,173,180	0
1	SEP	A	841	10/11	0.85	0.13	117,131,144,148	0
1	TPO	C	844	11/12	0.86	0.23	199,232,261,263	0
1	TPO	M	844	11/12	0.86	0.22	228,257,285,285	0
1	SEP	B	840	10/11	0.87	0.22	147,153,162,164	0
1	TPO	B	844	11/12	0.87	0.23	166,194,212,216	0
1	SEP	C	840	10/11	0.87	0.20	151,156,164,164	0
1	SEP	E	840	10/11	0.89	0.28	184,188,196,198	0
1	TPO	A	844	11/12	0.90	0.17	256,286,315,317	0
1	SEP	G	841	10/11	0.90	0.11	141,156,172,175	0
1	SEP	B	841	10/11	0.90	0.17	111,133,156,162	0
1	SEP	D	840	10/11	0.90	0.22	134,138,146,146	0
1	SEP	F	841	10/11	0.91	0.13	110,119,130,131	0
1	SEP	H	841	10/11	0.91	0.13	145,157,165,172	0
1	SEP	J	841	10/11	0.92	0.14	175,183,188,193	0
1	SEP	E	841	10/11	0.92	0.12	117,136,158,163	0

*Continued on next page...*

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
1	SEP	C	841	10/11	0.92	0.15	90,114,135,145	0
1	SEP	I	841	10/11	0.92	0.12	171,181,192,193	0
1	SEP	N	841	10/11	0.93	0.10	120,133,149,152	0
1	SEP	M	841	10/11	0.94	0.10	103,112,132,137	0
1	SEP	D	841	10/11	0.95	0.12	82,92,114,119	0

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

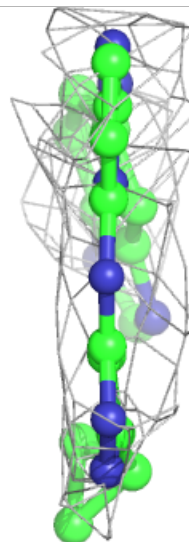
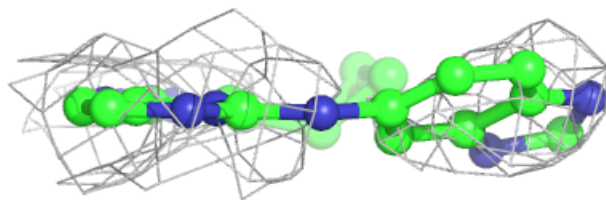
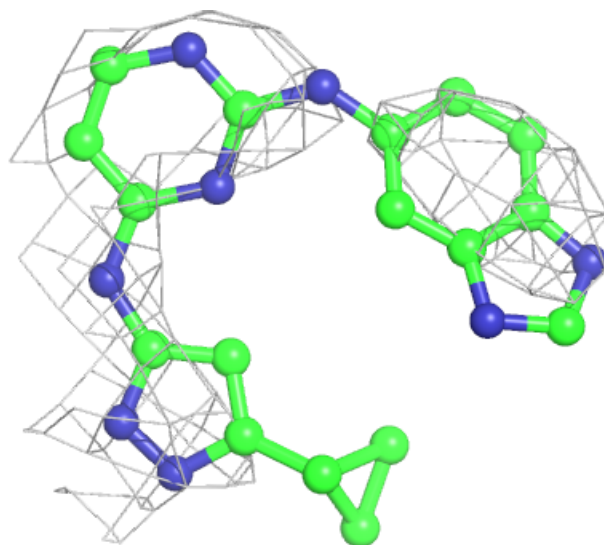
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	APJ	J	1999	25/25	0.76	0.68	197,197,197,197	0
2	APJ	H	1999	25/25	0.81	0.49	170,170,170,170	0
2	APJ	I	1999	25/25	0.83	0.29	171,171,171,171	0
2	APJ	L	1999	25/25	0.84	0.34	142,142,142,142	0
2	APJ	K	1999	25/25	0.88	0.40	135,135,135,135	0
2	APJ	M	1999	25/25	0.92	0.24	113,113,113,113	0
2	APJ	G	1999	25/25	0.92	0.31	145,145,145,145	0
2	APJ	D	1999	25/25	0.92	0.24	78,78,78,78	0
2	APJ	C	1999	25/25	0.93	0.26	66,66,66,66	0
2	APJ	F	1999	25/25	0.93	0.23	93,93,93,93	0
2	APJ	A	1999	25/25	0.93	0.22	93,93,93,93	0
2	APJ	N	1999	25/25	0.94	0.21	87,87,87,87	0
2	APJ	B	1999	25/25	0.94	0.21	96,96,96,96	0
2	APJ	E	1999	25/25	0.95	0.22	101,101,101,101	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.

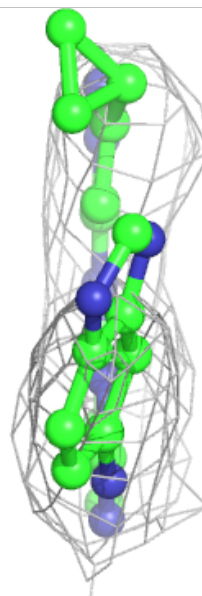
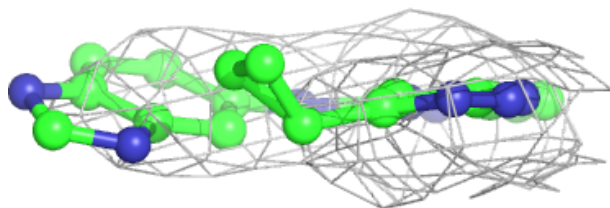
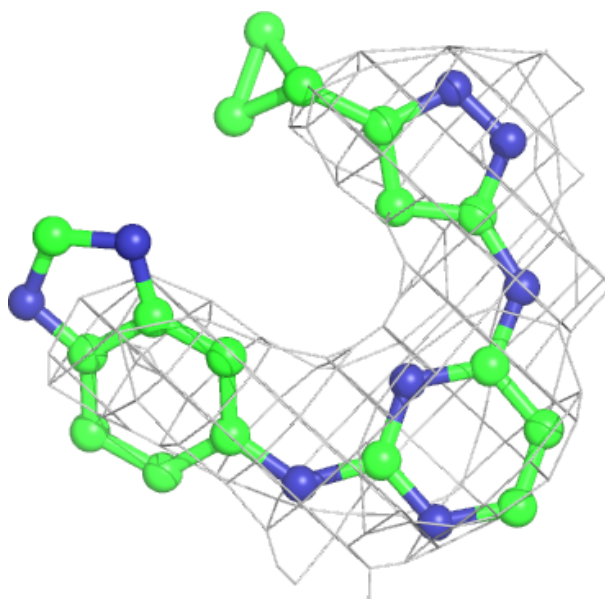
**Electron density around APJ J 1999:**

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and green (positive)



**Electron density around APJ H 1999:**

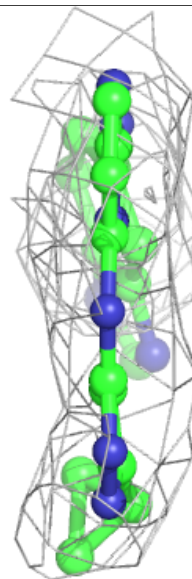
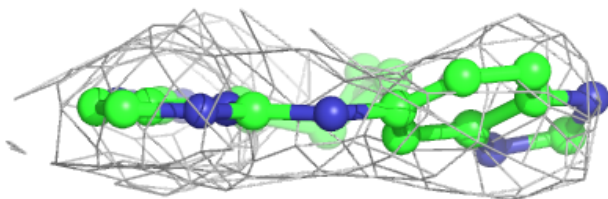
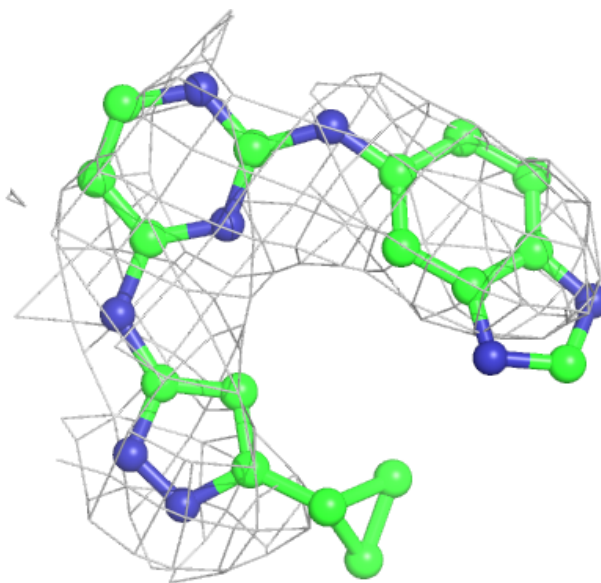
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





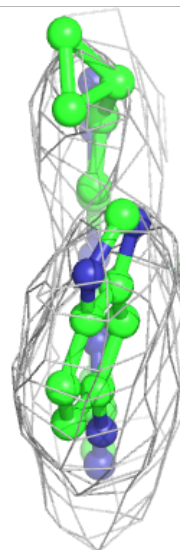
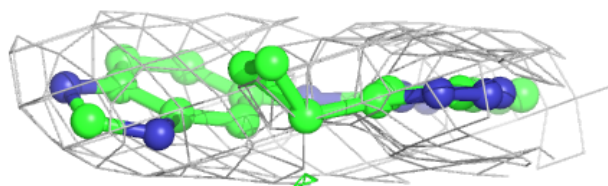
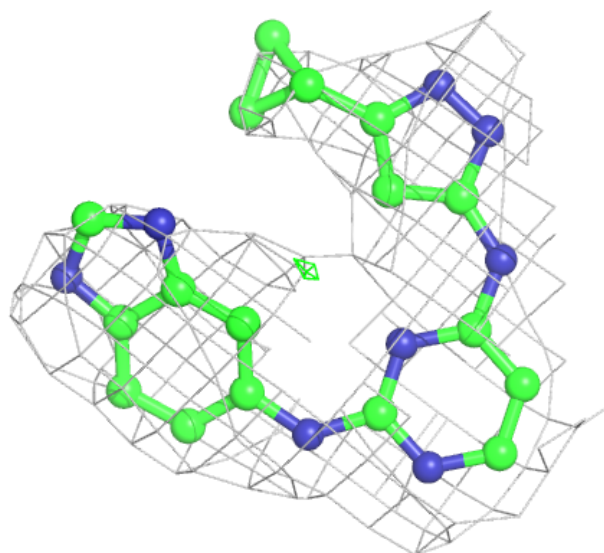
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and green (positive)



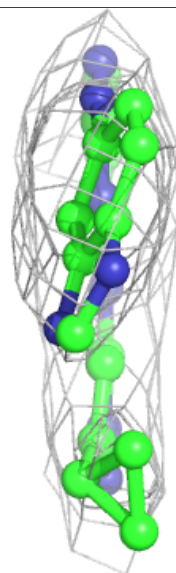
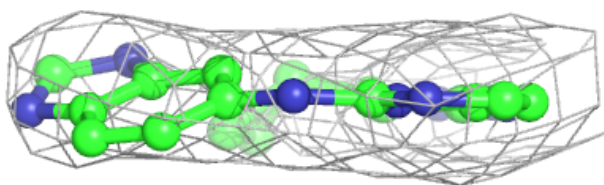
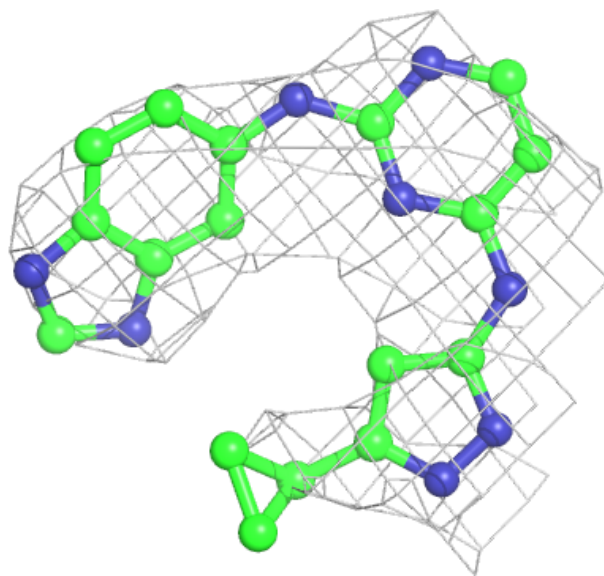
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 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



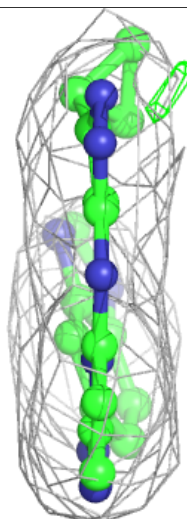
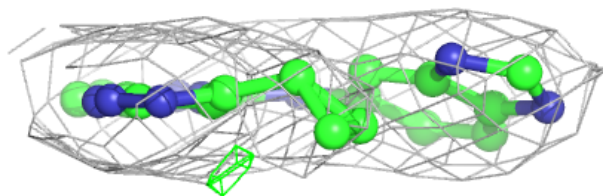
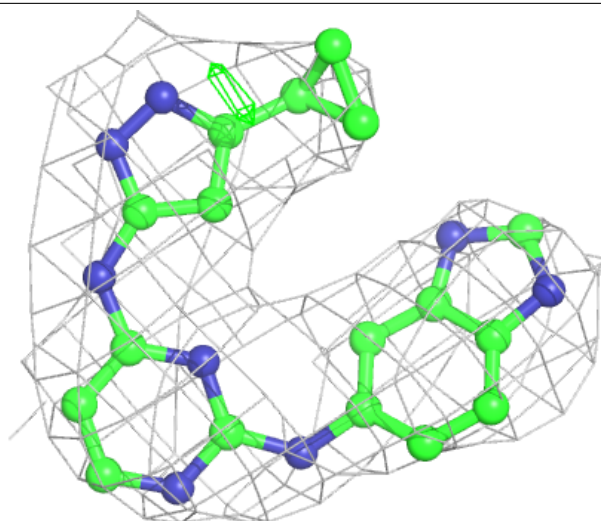
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and green (positive)



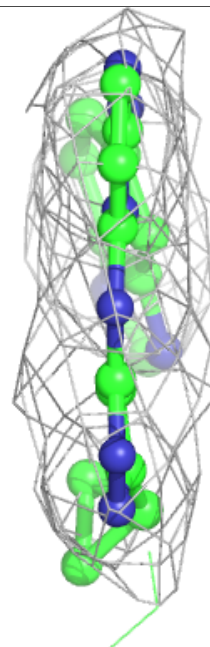
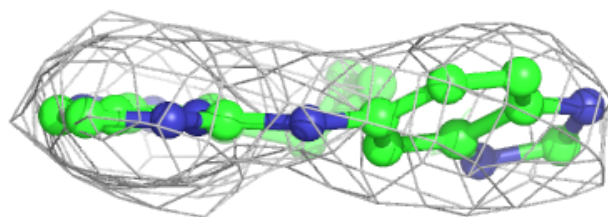
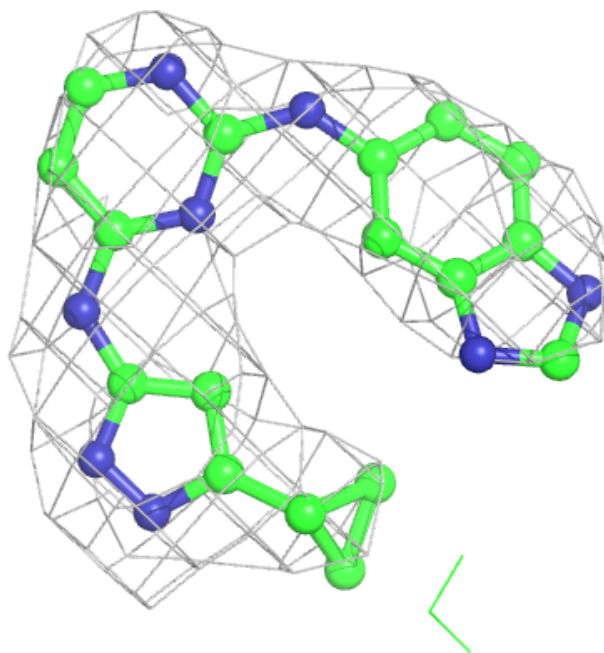
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and green (positive)



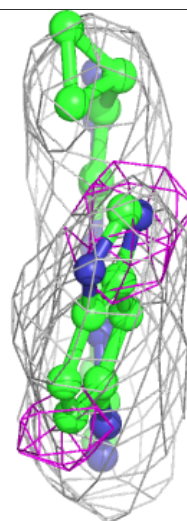
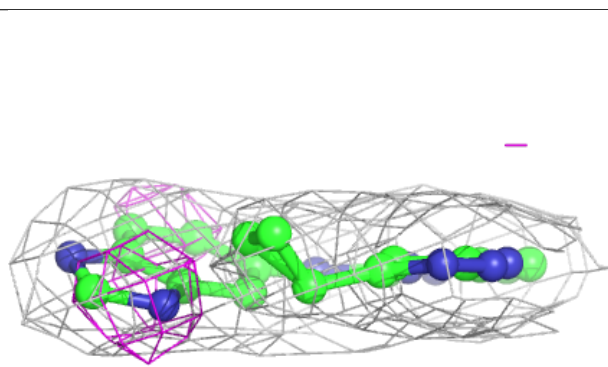
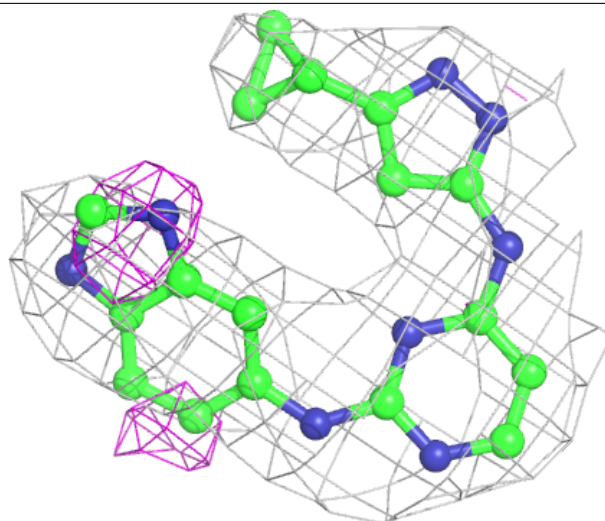
**Electron density around APJ G 1999:**

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and green (positive)



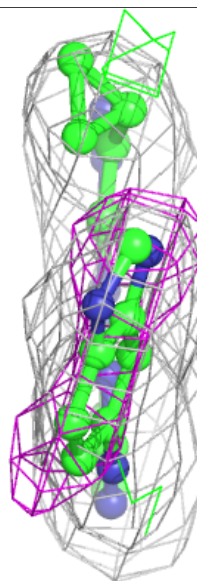
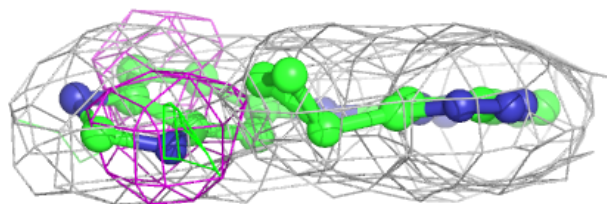
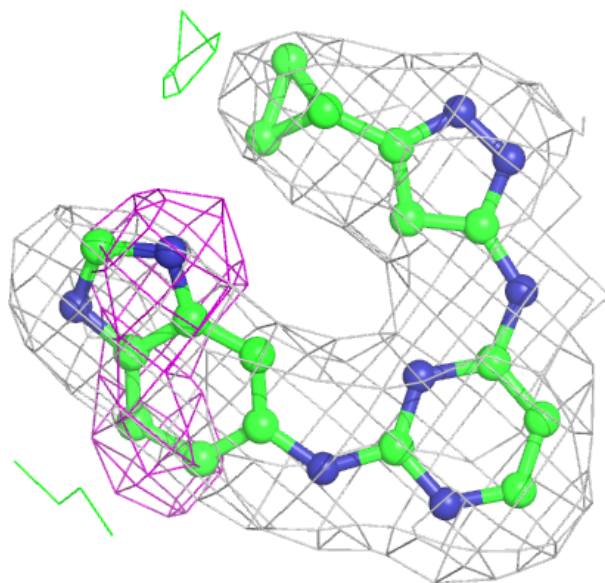
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and green (positive)



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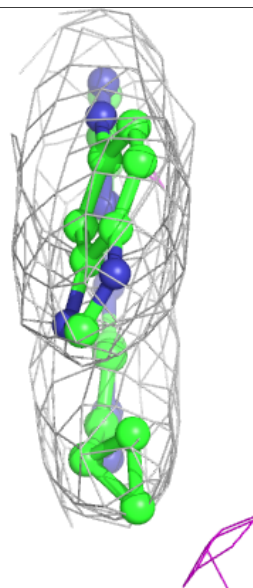
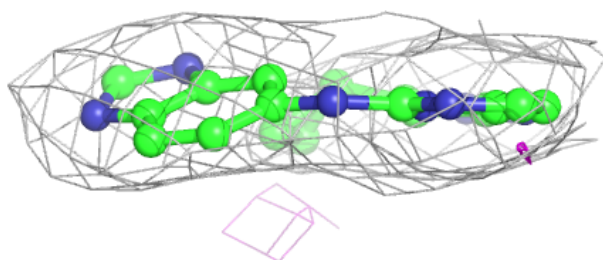
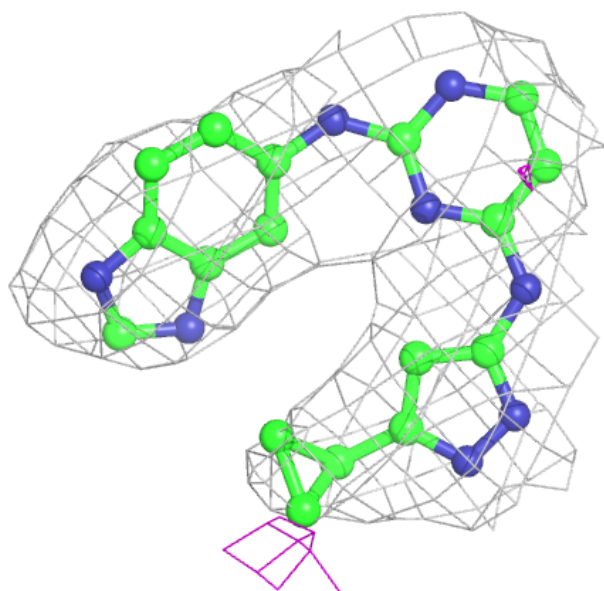
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and green (positive)





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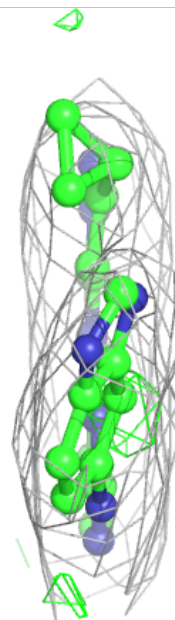
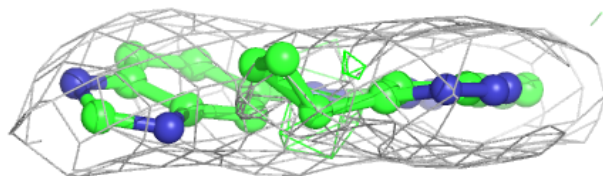
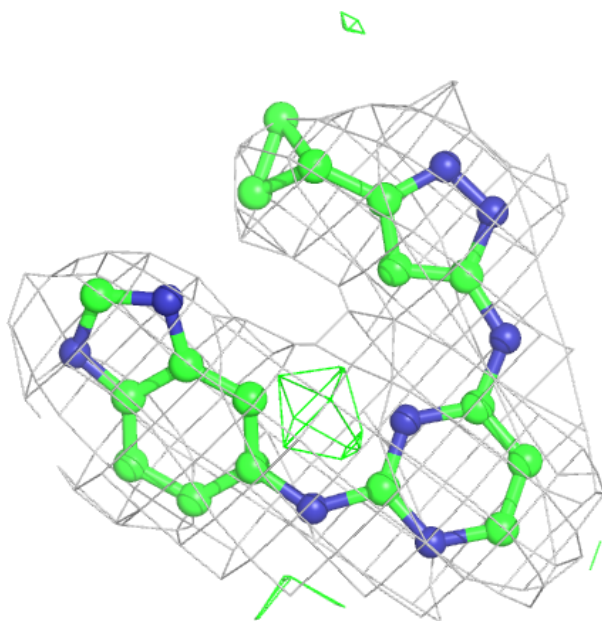
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and green (positive)





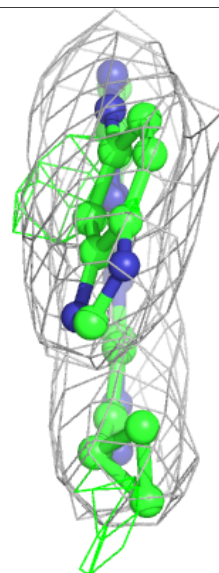
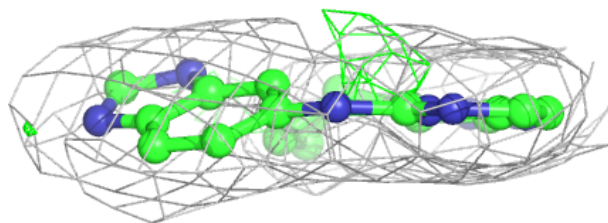
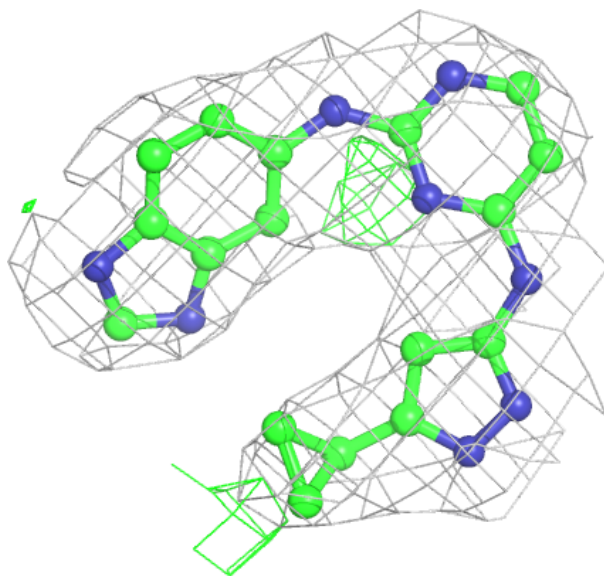
**Electron density around APJ A 1999:**

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and green (positive)



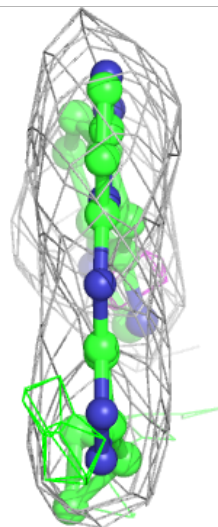
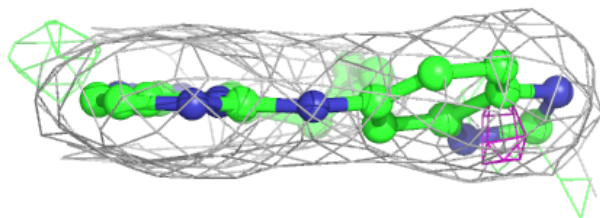
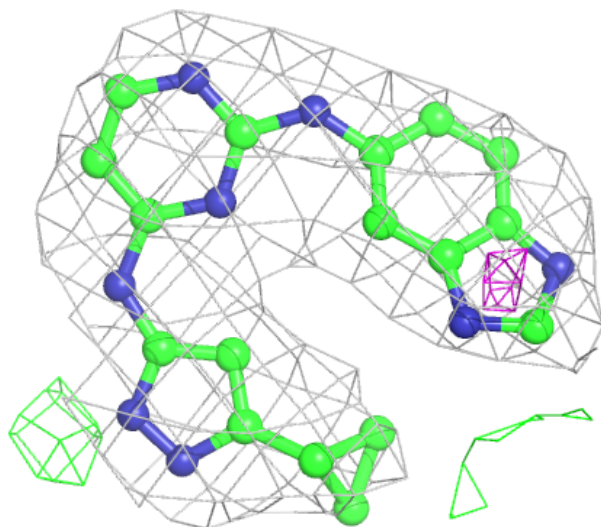
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and green (positive)



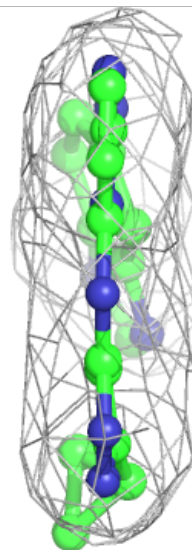
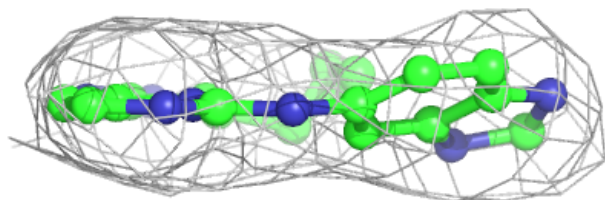
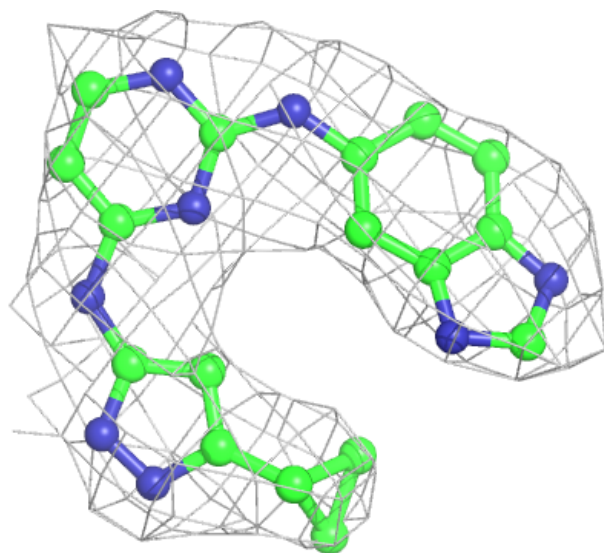
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and green (positive)



**Electron density around APJ E 1999:**

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



## 6.5 Other polymers [i](#)

There are no such residues in this entry.