



wwPDB X-ray Structure Validation Summary Report ⓘ

Oct 29, 2024 – 07:34 AM EDT

PDB ID : 3SDJ
Title : Structure of RNase-inactive point mutant of oligomeric kinase/RNase Ire1
Authors : Korennykh, A.; Korostelev, A.; Egea, P.; Finer-Moore, J.; Zhang, C.; Stroud, R.; Shokat, K.; Walter, P.
Deposited on : 2011-06-09
Resolution : 3.65 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4.02b-467
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 1.20.1
EDS : 3.0
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4 : 9.0.003 (Gargrove)
Density-Fitness : 1.0.11
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.39

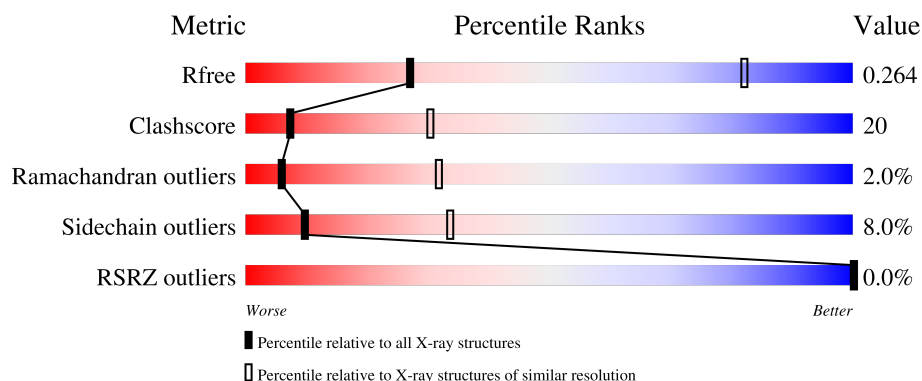
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.65 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}	164625	1261 (3.80-3.52)
Clashscore	180529	1328 (3.80-3.52)
Ramachandran outliers	177936	1306 (3.80-3.52)
Sidechain outliers	177891	1303 (3.80-3.52)
RSRZ outliers	164620	1260 (3.80-3.52)

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 $\leq 5\%$. 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	
1	B	448	
1	C	448	
1	D	448	
1	E	448	

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Mol	Chain	Length	Quality of chain
1	F	448	
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	SEP	G	840	-	-	X	-

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 47990 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
			3397	2160	579	637	3	18			
1	B	418	Total	C	N	O	P	S	0	0	0
			3397	2160	579	637	3	18			
1	C	418	Total	C	N	O	P	S	0	0	0
			3397	2160	579	637	3	18			
1	D	425	Total	C	N	O	P	S	0	0	0
			3455	2197	588	649	3	18			
1	E	418	Total	C	N	O	P	S	0	0	0
			3397	2160	579	637	3	18			
1	F	418	Total	C	N	O	P	S	0	0	0
			3397	2160	579	637	3	18			
1	G	418	Total	C	N	O	P	S	0	0	0
			3397	2160	579	637	3	18			
1	H	418	Total	C	N	O	P	S	0	0	0
			3397	2160	579	637	3	18			
1	I	416	Total	C	N	O	P	S	0	0	0
			3380	2148	576	635	3	18			
1	J	416	Total	C	N	O	P	S	0	0	0
			3380	2148	576	635	3	18			
1	K	425	Total	C	N	O	P	S	0	0	0
			3455	2197	588	649	3	18			
1	L	418	Total	C	N	O	P	S	0	0	0
			3397	2160	579	637	3	18			
1	M	418	Total	C	N	O	P	S	0	0	0
			3397	2160	579	637	3	18			
1	N	418	Total	C	N	O	P	S	0	0	0
			3397	2160	579	637	3	18			

There are 420 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
A	1061	ASN	HIS	engineered mutation	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

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Chain	Residue	Modelled	Actual	Comment	Reference
B	?	-	SER	deletion	UNP P32361
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
B	1061	ASN	HIS	engineered mutation	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

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Chain	Residue	Modelled	Actual	Comment	Reference
C	?	-	TYR	deletion	UNP P32361
C	?	-	ASP	deletion	UNP P32361
C	?	-	PRO	deletion	UNP P32361
C	?	-	PHE	deletion	UNP P32361
C	1061	ASN	HIS	engineered mutation	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
D	1061	ASN	HIS	engineered mutation	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

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Chain	Residue	Modelled	Actual	Comment	Reference
E	?	-	VAL	deletion	UNP P32361
E	?	-	GLU	deletion	UNP P32361
E	?	-	THR	deletion	UNP P32361
E	?	-	GLU	deletion	UNP P32361
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
E	1061	ASN	HIS	engineered mutation	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

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Chain	Residue	Modelled	Actual	Comment	Reference
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
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
F	1061	ASN	HIS	engineered mutation	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
G	1061	ASN	HIS	engineered mutation	UNP P32361
H	640	PRO	-	expression tag	UNP P32361

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Chain	Residue	Modelled	Actual	Comment	Reference
H	?	-	ASN	deletion	UNP P32361
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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
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
H	1061	ASN	HIS	engineered mutation	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

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Chain	Residue	Modelled	Actual	Comment	Reference
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
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
I	1061	ASN	HIS	engineered mutation	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

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Chain	Residue	Modelled	Actual	Comment	Reference
J	?	-	TYR	deletion	UNP P32361
J	?	-	ASP	deletion	UNP P32361
J	?	-	PRO	deletion	UNP P32361
J	?	-	PHE	deletion	UNP P32361
J	1061	ASN	HIS	engineered mutation	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
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
K	1061	ASN	HIS	engineered mutation	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

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Chain	Residue	Modelled	Actual	Comment	Reference
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
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
L	1061	ASN	HIS	engineered mutation	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

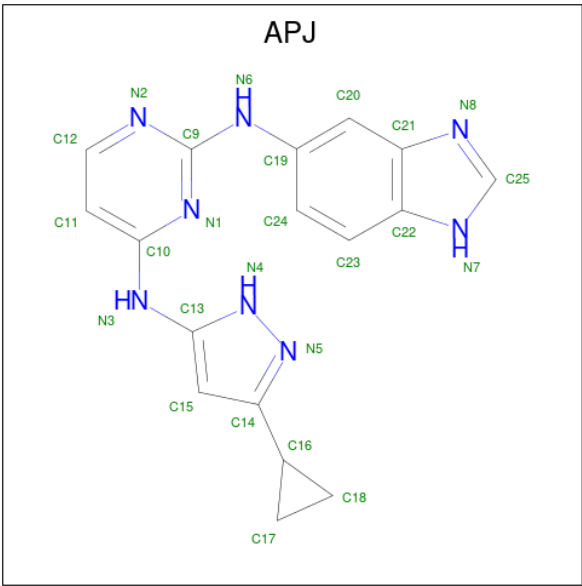
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Chain	Residue	Modelled	Actual	Comment	Reference
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M	?	-	SER	deletion	UNP P32361
M	?	-	SER	deletion	UNP P32361
M	?	-	ASP	deletion	UNP P32361
M	?	-	SER	deletion	UNP P32361
M	?	-	PHE	deletion	UNP P32361
M	?	-	TYR	deletion	UNP P32361
M	?	-	ASP	deletion	UNP P32361
M	?	-	PRO	deletion	UNP P32361
M	?	-	PHE	deletion	UNP P32361
M	1061	ASN	HIS	engineered mutation	UNP P32361
N	640	PRO	-	expression tag	UNP P32361
N	?	-	ASN	deletion	UNP P32361
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
N	1061	ASN	HIS	engineered mutation	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: C₁₇H₁₆N₈).

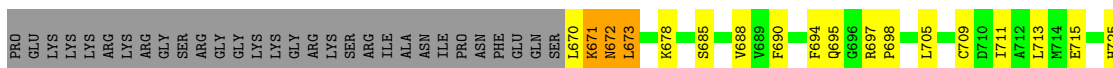


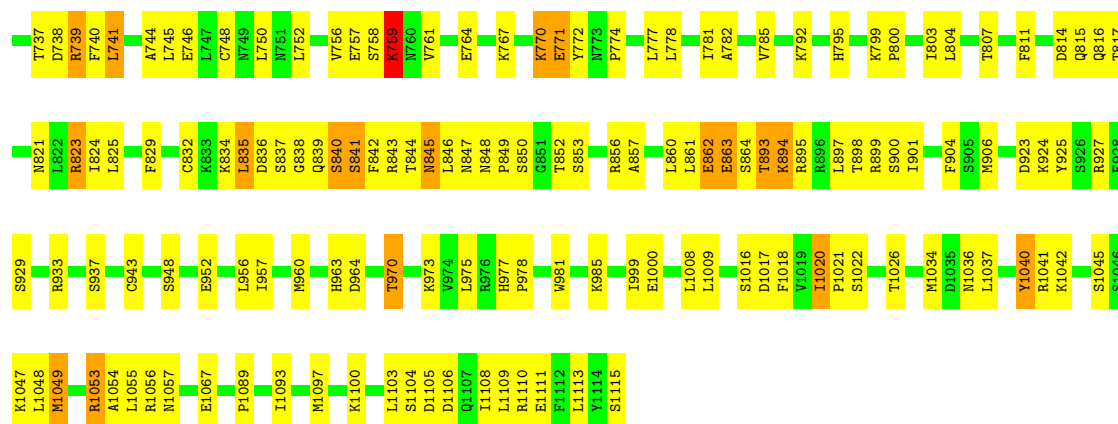
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	N	0	0
			25	17	8		
2	B	1	Total	C	N	0	0
			25	17	8		
2	C	1	Total	C	N	0	0
			25	17	8		
2	D	1	Total	C	N	0	0
			25	17	8		
2	E	1	Total	C	N	0	0
			25	17	8		
2	F	1	Total	C	N	0	0
			25	17	8		
2	G	1	Total	C	N	0	0
			25	17	8		
2	H	1	Total	C	N	0	0
			25	17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

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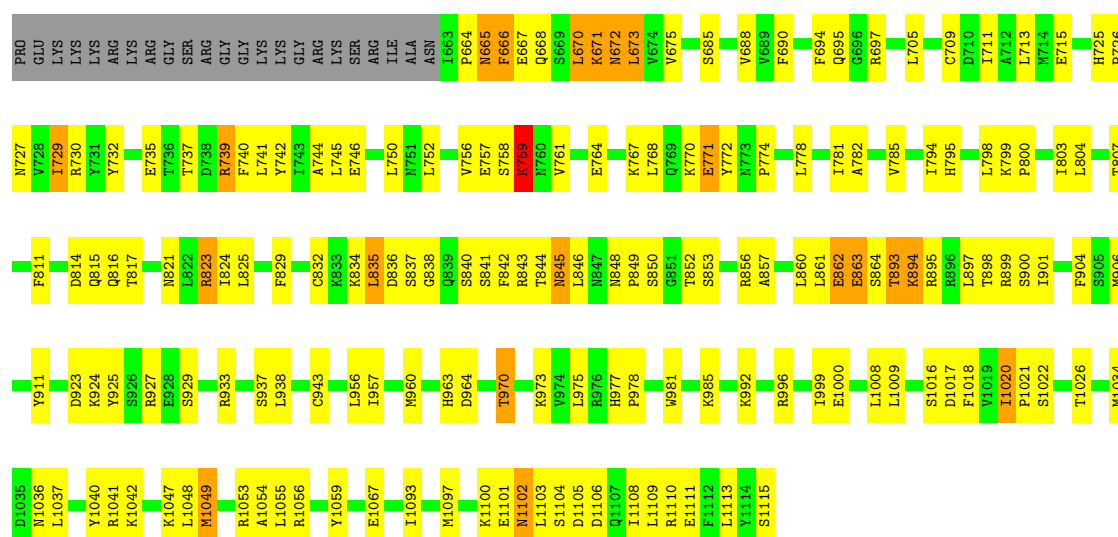
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	N		
2	N	1	25	17	8	0	0





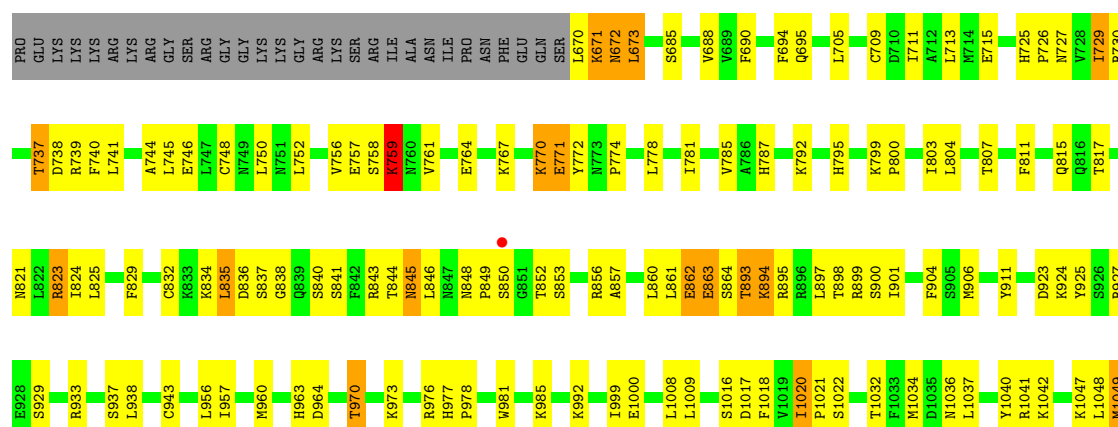
• Molecule 1: Serine/threonine-protein kinase/endoribonuclease IRE1

Chain K: 56% 34% 5%



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

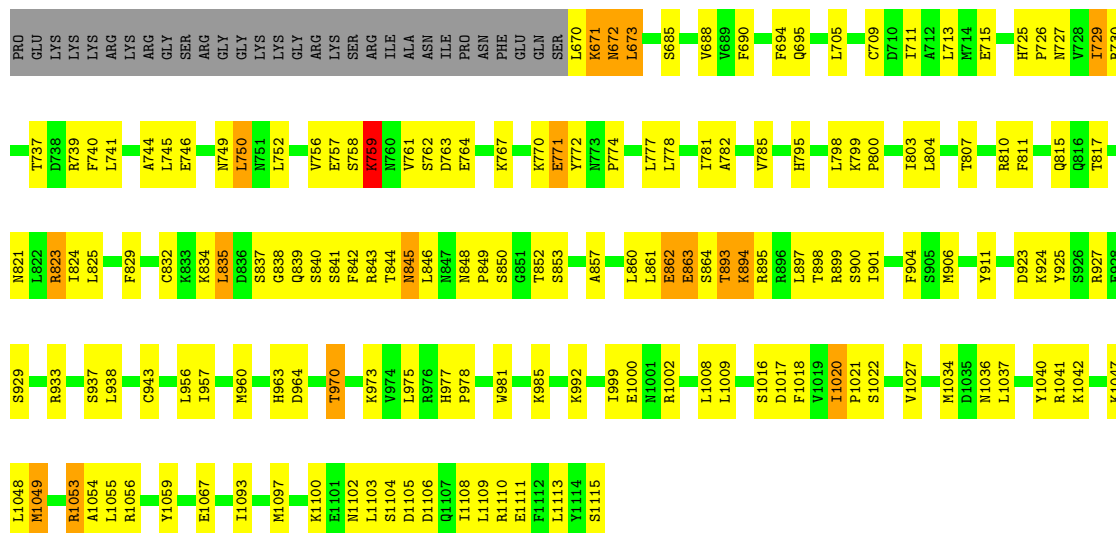
Chain L: 58% 31% 7%





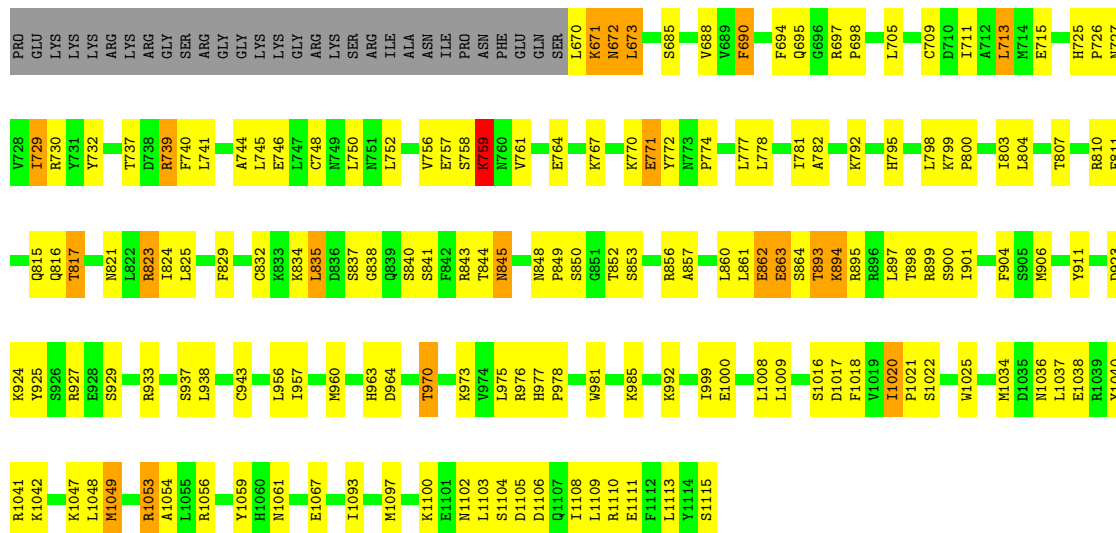
• Molecule 1: Serine/threonine-protein kinase/endoribonuclease IRE1

Chain M: 57% 32% 7%



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

Chain N: 57% 31% 7%



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	158.79Å 163.45Å 298.04Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.65 – 3.65 49.65 – 3.65	Depositor EDS
% Data completeness (in resolution range)	99.7 (49.65-3.65) 99.7 (49.65-3.65)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.68 (at 3.67Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.5_2)	Depositor
R, R_{free}	0.248 , 0.287 0.228 , 0.264	Depositor DCC
R_{free} test set	4331 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	101.7	Xtriage
Anisotropy	0.275	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 147.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	0.036 for k,h,-l	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	47990	wwPDB-VP
Average B, all atoms (Å ²)	147.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.90% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

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	0.34	0/3434	0.53	0/4625
1	B	0.33	0/3434	0.52	0/4625
1	C	0.33	0/3434	0.53	0/4625
1	D	0.33	0/3494	0.52	0/4707
1	E	0.32	0/3434	0.52	0/4625
1	F	0.34	0/3434	0.52	0/4625
1	G	0.32	0/3434	0.51	0/4625
1	H	0.32	0/3434	0.51	0/4625
1	I	0.33	0/3417	0.51	0/4603
1	J	0.33	0/3417	0.50	0/4603
1	K	0.34	0/3494	0.51	0/4707
1	L	0.35	0/3434	0.51	0/4625
1	M	0.32	0/3434	0.51	0/4625
1	N	0.33	0/3434	0.51	0/4625
All	All	0.33	0/48162	0.52	0/64870

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	1
1	E	0	1
1	F	0	1
1	G	0	1
1	H	0	1
1	K	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
1	L	0	1
1	M	0	1
1	N	0	1
All	All	0	12

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 12 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	671	LYS	Peptide
1	E	671	LYS	Peptide

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3397	0	3409	136	2
1	B	3397	0	3409	140	2
1	C	3397	0	3409	148	3
1	D	3455	0	3461	175	0
1	E	3397	0	3409	139	0
1	F	3397	0	3409	139	0
1	G	3397	0	3409	145	0
1	H	3397	0	3409	140	1
1	I	3380	0	3385	155	3
1	J	3380	0	3385	138	3
1	K	3455	0	3461	163	1
1	L	3397	0	3409	128	0
1	M	3397	0	3409	134	0
1	N	3397	0	3409	131	0
2	A	25	0	16	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	25	0	16	3	0
2	C	25	0	16	4	0
2	D	25	0	16	3	0
2	E	25	0	16	4	0
2	F	25	0	16	3	0
2	G	25	0	16	4	0
2	H	25	0	16	4	0
2	I	25	0	16	4	0
2	J	25	0	16	4	0
2	K	25	0	16	3	0
2	L	25	0	16	3	0
2	M	25	0	16	3	0
2	N	25	0	16	4	0
All	All	47990	0	48006	1941	8

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 1941 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:E:848:ASN:HB3	1:E:849:PRO:HA	1.46	0.97
1:D:848:ASN:HB3	1:D:849:PRO:HA	1.47	0.97
1:N:848:ASN:HB3	1:N:849:PRO:HA	1.46	0.97
1:B:848:ASN:HB3	1:B:849:PRO:HA	1.46	0.97
1:C:848:ASN:HB3	1:C:849:PRO:HA	1.45	0.97

The worst 5 of 8 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:H:739:ARG:NH1	1:K:863:GLU:OE2[3_556]	1.78	0.42
1:A:1021:PRO:O	1:C:739:ARG:NH1[4_456]	1.96	0.24
1:B:846:LEU:O	1:C:1042:LYS:NZ[4_556]	2.02	0.18
1:B:846:LEU:N	1:C:1042:LYS:NZ[4_556]	2.08	0.12
1:A:1038:GLU:O	1:A:1038:GLU:O[2_565]	2.11	0.09

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%)	355 (86%)	49 (12%)	9 (2%)	5	30
1	B	413/448 (92%)	356 (86%)	49 (12%)	8 (2%)	6	33
1	C	413/448 (92%)	359 (87%)	47 (11%)	7 (2%)	7	34
1	D	420/448 (94%)	361 (86%)	50 (12%)	9 (2%)	5	31
1	E	413/448 (92%)	359 (87%)	47 (11%)	7 (2%)	7	34
1	F	413/448 (92%)	356 (86%)	48 (12%)	9 (2%)	5	30
1	G	413/448 (92%)	357 (86%)	49 (12%)	7 (2%)	7	34
1	H	413/448 (92%)	357 (86%)	47 (11%)	9 (2%)	5	30
1	I	411/448 (92%)	357 (87%)	45 (11%)	9 (2%)	5	30
1	J	411/448 (92%)	356 (87%)	45 (11%)	10 (2%)	5	28
1	K	420/448 (94%)	365 (87%)	47 (11%)	8 (2%)	6	33
1	L	413/448 (92%)	358 (87%)	47 (11%)	8 (2%)	6	33
1	M	413/448 (92%)	358 (87%)	47 (11%)	8 (2%)	6	33
1	N	413/448 (92%)	356 (86%)	48 (12%)	9 (2%)	5	30
All	All	5792/6272 (92%)	5010 (86%)	665 (12%)	117 (2%)	6	32

5 of 117 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	893	THR

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%)	11	35
1	B	380/405 (94%)	349 (92%)	31 (8%)	9	33
1	C	380/405 (94%)	349 (92%)	31 (8%)	9	33
1	D	387/405 (96%)	356 (92%)	31 (8%)	10	34
1	E	380/405 (94%)	351 (92%)	29 (8%)	11	35
1	F	380/405 (94%)	348 (92%)	32 (8%)	9	32
1	G	380/405 (94%)	350 (92%)	30 (8%)	10	34
1	H	380/405 (94%)	349 (92%)	31 (8%)	9	33
1	I	378/405 (93%)	349 (92%)	29 (8%)	10	35
1	J	378/405 (93%)	349 (92%)	29 (8%)	10	35
1	K	387/405 (96%)	356 (92%)	31 (8%)	10	34
1	L	380/405 (94%)	350 (92%)	30 (8%)	10	34
1	M	380/405 (94%)	350 (92%)	30 (8%)	10	34
1	N	380/405 (94%)	348 (92%)	32 (8%)	9	32
All	All	5330/5670 (94%)	4905 (92%)	425 (8%)	10	34

5 of 425 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	H	863	GLU
1	J	823	ARG
1	N	713	LEU
1	H	1036	ASN
1	I	863	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 157 such sidechains are listed below:

Mol	Chain	Res	Type
1	K	725	HIS

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Mol	Chain	Res	Type
1	M	845	ASN
1	K	787	HIS
1	L	773	ASN
1	N	773	ASN

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	1.58	1 (12%)	7,12,14	1.33	1 (14%)
1	SEP	B	840	1	8,9,10	1.62	1 (12%)	7,12,14	1.47	1 (14%)
1	TPO	G	844	1	8,10,11	3.04	5 (62%)	10,14,16	1.72	2 (20%)
1	TPO	F	844	1	8,10,11	3.06	5 (62%)	10,14,16	1.69	2 (20%)
1	SEP	J	840	1	8,9,10	1.67	1 (12%)	7,12,14	1.41	1 (14%)
1	SEP	D	841	1	8,9,10	1.58	1 (12%)	7,12,14	1.28	1 (14%)
1	TPO	A	844	1	8,10,11	3.10	5 (62%)	10,14,16	1.72	2 (20%)
1	SEP	L	840	1	8,9,10	1.64	1 (12%)	7,12,14	1.33	1 (14%)
1	SEP	E	841	1	8,9,10	1.59	1 (12%)	7,12,14	1.28	1 (14%)
1	TPO	J	844	1	8,10,11	3.10	5 (62%)	10,14,16	1.72	2 (20%)
1	SEP	H	841	1	8,9,10	1.66	1 (12%)	7,12,14	1.34	1 (14%)
1	SEP	M	841	1	8,9,10	1.57	1 (12%)	7,12,14	1.12	1 (14%)
1	TPO	E	844	1	8,10,11	3.10	5 (62%)	10,14,16	1.72	2 (20%)
1	TPO	C	844	1	8,10,11	3.07	5 (62%)	10,14,16	1.73	2 (20%)
1	SEP	G	841	1	8,9,10	1.52	1 (12%)	7,12,14	1.32	1 (14%)
1	SEP	A	840	1	8,9,10	1.63	1 (12%)	7,12,14	1.55	1 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	SEP	M	840	1	8,9,10	1.64	1 (12%)	7,12,14	1.41	1 (14%)
1	TPO	H	844	1	8,10,11	3.14	5 (62%)	10,14,16	1.71	2 (20%)
1	SEP	L	841	1	8,9,10	1.73	1 (12%)	7,12,14	1.01	0
1	SEP	D	840	1	8,9,10	1.58	1 (12%)	7,12,14	1.64	1 (14%)
1	SEP	F	840	1	8,9,10	1.59	1 (12%)	7,12,14	1.31	1 (14%)
1	TPO	N	844	1	8,10,11	3.12	5 (62%)	10,14,16	1.69	2 (20%)
1	SEP	G	840	1	8,9,10	1.59	1 (12%)	7,12,14	1.36	1 (14%)
1	SEP	H	840	1	8,9,10	1.69	1 (12%)	7,12,14	1.38	1 (14%)
1	SEP	K	840	1	8,9,10	1.67	1 (12%)	7,12,14	1.42	1 (14%)
1	TPO	I	844	1	8,10,11	3.05	5 (62%)	10,14,16	1.69	2 (20%)
1	SEP	E	840	1	8,9,10	1.67	1 (12%)	7,12,14	1.68	1 (14%)
1	SEP	C	840	1	8,9,10	1.62	1 (12%)	7,12,14	1.42	1 (14%)
1	TPO	B	844	1	8,10,11	3.11	5 (62%)	10,14,16	1.66	2 (20%)
1	SEP	J	841	1	8,9,10	1.62	1 (12%)	7,12,14	1.09	1 (14%)
1	TPO	K	844	1	8,10,11	3.09	5 (62%)	10,14,16	1.68	2 (20%)
1	TPO	L	844	1	8,10,11	3.11	5 (62%)	10,14,16	1.66	2 (20%)
1	SEP	B	841	1	8,9,10	1.59	1 (12%)	7,12,14	1.46	1 (14%)
1	SEP	I	841	1	8,9,10	1.57	1 (12%)	7,12,14	1.37	1 (14%)
1	SEP	K	841	1	8,9,10	1.63	1 (12%)	7,12,14	1.23	1 (14%)
1	TPO	M	844	1	8,10,11	3.08	5 (62%)	10,14,16	1.72	2 (20%)
1	SEP	N	841	1	8,9,10	1.65	1 (12%)	7,12,14	1.22	1 (14%)
1	SEP	I	840	1	8,9,10	1.65	1 (12%)	7,12,14	1.26	1 (14%)
1	SEP	F	841	1	8,9,10	1.64	1 (12%)	7,12,14	1.05	0
1	SEP	N	840	1	8,9,10	1.64	1 (12%)	7,12,14	1.29	1 (14%)
1	SEP	A	841	1	8,9,10	1.63	1 (12%)	7,12,14	1.22	1 (14%)
1	TPO	D	844	1	8,10,11	3.11	5 (62%)	10,14,16	1.72	2 (20%)

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	-	0/6/8/10	-
1	SEP	B	840	1	-	0/6/8/10	-
1	TPO	G	844	1	-	4/9/11/13	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	TPO	F	844	1	-	4/9/11/13	-
1	SEP	J	840	1	-	0/6/8/10	-
1	SEP	D	841	1	-	0/6/8/10	-
1	TPO	A	844	1	-	4/9/11/13	-
1	SEP	L	840	1	-	0/6/8/10	-
1	SEP	E	841	1	-	0/6/8/10	-
1	TPO	J	844	1	-	4/9/11/13	-
1	SEP	H	841	1	-	0/6/8/10	-
1	SEP	M	841	1	-	0/6/8/10	-
1	TPO	E	844	1	-	4/9/11/13	-
1	TPO	C	844	1	-	4/9/11/13	-
1	SEP	G	841	1	-	0/6/8/10	-
1	SEP	A	840	1	-	0/6/8/10	-
1	SEP	M	840	1	-	0/6/8/10	-
1	TPO	H	844	1	-	4/9/11/13	-
1	SEP	L	841	1	-	0/6/8/10	-
1	SEP	D	840	1	-	0/6/8/10	-
1	SEP	F	840	1	-	0/6/8/10	-
1	TPO	N	844	1	-	4/9/11/13	-
1	SEP	G	840	1	-	0/6/8/10	-
1	SEP	H	840	1	-	0/6/8/10	-
1	SEP	K	840	1	-	0/6/8/10	-
1	TPO	I	844	1	-	5/9/11/13	-
1	SEP	E	840	1	-	0/6/8/10	-
1	SEP	C	840	1	-	0/6/8/10	-
1	TPO	B	844	1	-	5/9/11/13	-
1	SEP	J	841	1	-	0/6/8/10	-
1	TPO	K	844	1	-	4/9/11/13	-
1	TPO	L	844	1	-	4/9/11/13	-
1	SEP	B	841	1	-	0/6/8/10	-
1	SEP	I	841	1	-	0/6/8/10	-
1	SEP	K	841	1	-	0/6/8/10	-
1	TPO	M	844	1	-	4/9/11/13	-
1	SEP	N	841	1	-	0/6/8/10	-
1	SEP	I	840	1	-	0/6/8/10	-
1	SEP	F	841	1	-	0/6/8/10	-
1	SEP	N	840	1	-	0/6/8/10	-
1	SEP	A	841	1	-	0/6/8/10	-
1	TPO	D	844	1	-	4/9/11/13	-

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	5.56	1.41	1.20
1	I	844	TPO	O-C	5.48	1.40	1.20
1	M	844	TPO	O-C	5.42	1.40	1.20
1	L	844	TPO	O-C	5.42	1.40	1.20
1	H	844	TPO	O-C	5.41	1.40	1.20

The worst 5 of 54 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	844	TPO	O-C-CA	-4.32	113.65	124.77
1	C	844	TPO	O-C-CA	-4.30	113.70	124.77
1	M	844	TPO	O-C-CA	-4.27	113.80	124.77
1	H	844	TPO	O-C-CA	-4.24	113.87	124.77
1	E	844	TPO	O-C-CA	-4.23	113.89	124.77

There are no chirality outliers.

5 of 58 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	844	TPO	N-CA-CB-CG2
1	A	844	TPO	N-CA-CB-OG1
1	B	844	TPO	N-CA-CB-CG2
1	B	844	TPO	N-CA-CB-OG1
1	C	844	TPO	N-CA-CB-CG2

There are no ring outliers.

11 monomers are involved in 20 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	J	840	SEP	1	0
1	D	841	SEP	1	0
1	E	841	SEP	1	0
1	G	841	SEP	3	0
1	H	844	TPO	1	0
1	F	840	SEP	2	0
1	G	840	SEP	4	0
1	H	840	SEP	3	0
1	I	844	TPO	1	0
1	B	844	TPO	2	0
1	J	841	SEP	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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	-	25,29,29	1.97	7 (28%)	29,41,41	2.66	12 (41%)
2	APJ	F	1999	-	25,29,29	1.89	7 (28%)	29,41,41	2.67	13 (44%)
2	APJ	G	1999	-	25,29,29	1.97	7 (28%)	29,41,41	2.77	13 (44%)
2	APJ	M	1999	-	25,29,29	1.94	7 (28%)	29,41,41	2.76	12 (41%)
2	APJ	D	1999	-	25,29,29	1.93	7 (28%)	29,41,41	2.71	11 (37%)
2	APJ	A	1999	-	25,29,29	1.88	6 (24%)	29,41,41	2.57	12 (41%)
2	APJ	H	1999	-	25,29,29	1.93	7 (28%)	29,41,41	2.74	13 (44%)
2	APJ	L	1999	-	25,29,29	1.88	6 (24%)	29,41,41	2.63	11 (37%)
2	APJ	I	1999	-	25,29,29	1.94	7 (28%)	29,41,41	2.71	12 (41%)
2	APJ	B	1999	-	25,29,29	1.91	7 (28%)	29,41,41	2.63	11 (37%)
2	APJ	J	1999	-	25,29,29	1.91	6 (24%)	29,41,41	2.79	11 (37%)
2	APJ	N	1999	-	25,29,29	1.94	6 (24%)	29,41,41	2.68	11 (37%)
2	APJ	C	1999	-	25,29,29	1.93	7 (28%)	29,41,41	2.74	11 (37%)
2	APJ	E	1999	-	25,29,29	1.97	7 (28%)	29,41,41	2.78	12 (41%)

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	-	-	2/11/14/14	0/5/5/5
2	APJ	F	1999	-	-	2/11/14/14	0/5/5/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	APJ	G	1999	-	-	2/11/14/14	0/5/5/5
2	APJ	M	1999	-	-	2/11/14/14	0/5/5/5
2	APJ	D	1999	-	-	2/11/14/14	0/5/5/5
2	APJ	A	1999	-	-	2/11/14/14	0/5/5/5
2	APJ	H	1999	-	-	2/11/14/14	0/5/5/5
2	APJ	L	1999	-	-	2/11/14/14	0/5/5/5
2	APJ	I	1999	-	-	2/11/14/14	0/5/5/5
2	APJ	B	1999	-	-	2/11/14/14	0/5/5/5
2	APJ	J	1999	-	-	2/11/14/14	0/5/5/5
2	APJ	N	1999	-	-	2/11/14/14	0/5/5/5
2	APJ	C	1999	-	-	2/11/14/14	0/5/5/5
2	APJ	E	1999	-	-	2/11/14/14	0/5/5/5

The worst 5 of 94 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	1999	APJ	N5-N4	-5.96	1.26	1.37
2	N	1999	APJ	N5-N4	-5.92	1.26	1.37
2	D	1999	APJ	N5-N4	-5.81	1.26	1.37
2	M	1999	APJ	N5-N4	-5.78	1.26	1.37
2	I	1999	APJ	N5-N4	-5.74	1.26	1.37

The worst 5 of 165 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	J	1999	APJ	N2-C9-N1	-8.07	118.61	126.42
2	H	1999	APJ	N2-C9-N1	-7.96	118.72	126.42
2	G	1999	APJ	N2-C9-N1	-7.92	118.76	126.42
2	M	1999	APJ	N2-C9-N1	-7.79	118.89	126.42
2	E	1999	APJ	N2-C9-N1	-7.67	119.01	126.42

There are no chirality outliers.

5 of 28 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1999	APJ	N5-C14-C16-C18
2	A	1999	APJ	C15-C14-C16-C18
2	B	1999	APJ	N5-C14-C16-C18
2	B	1999	APJ	C15-C14-C16-C18

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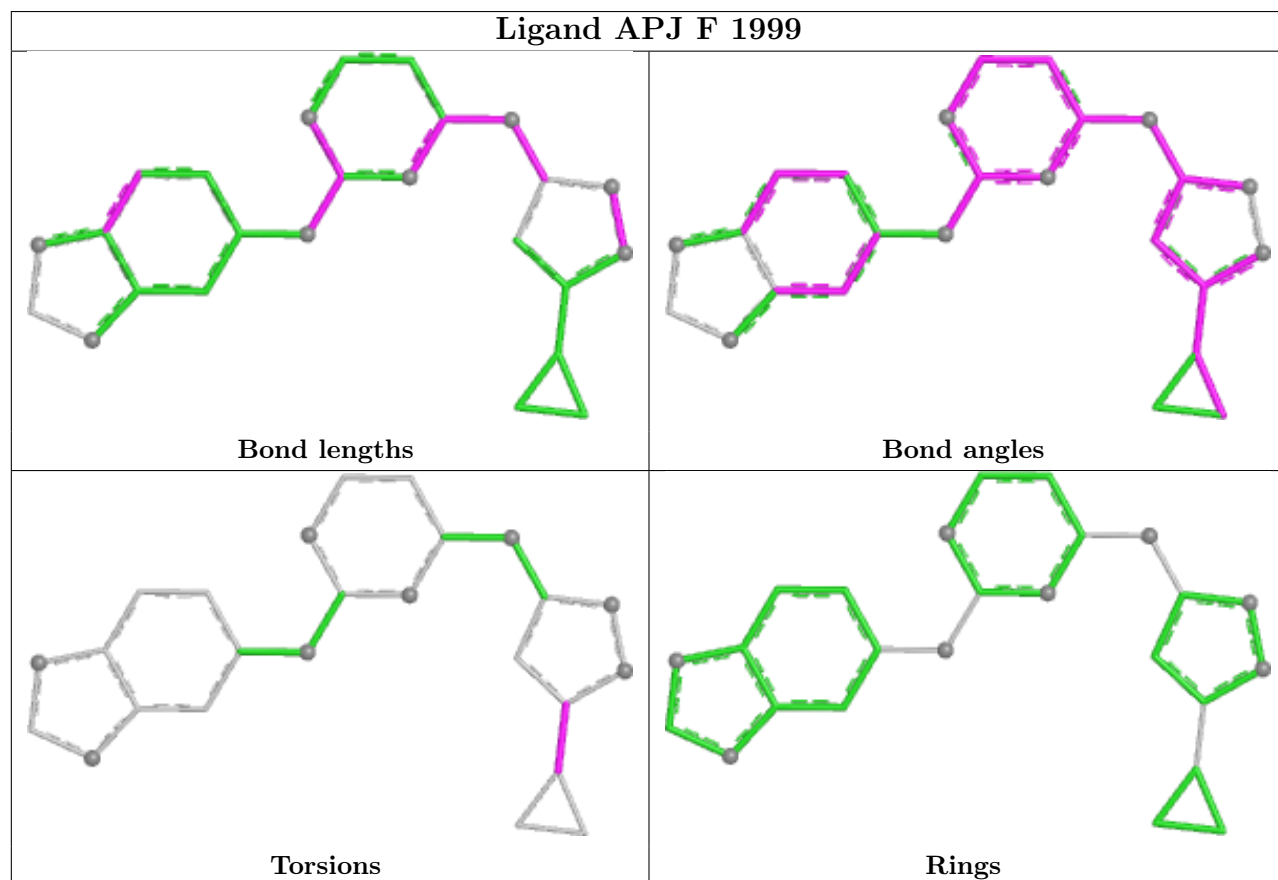
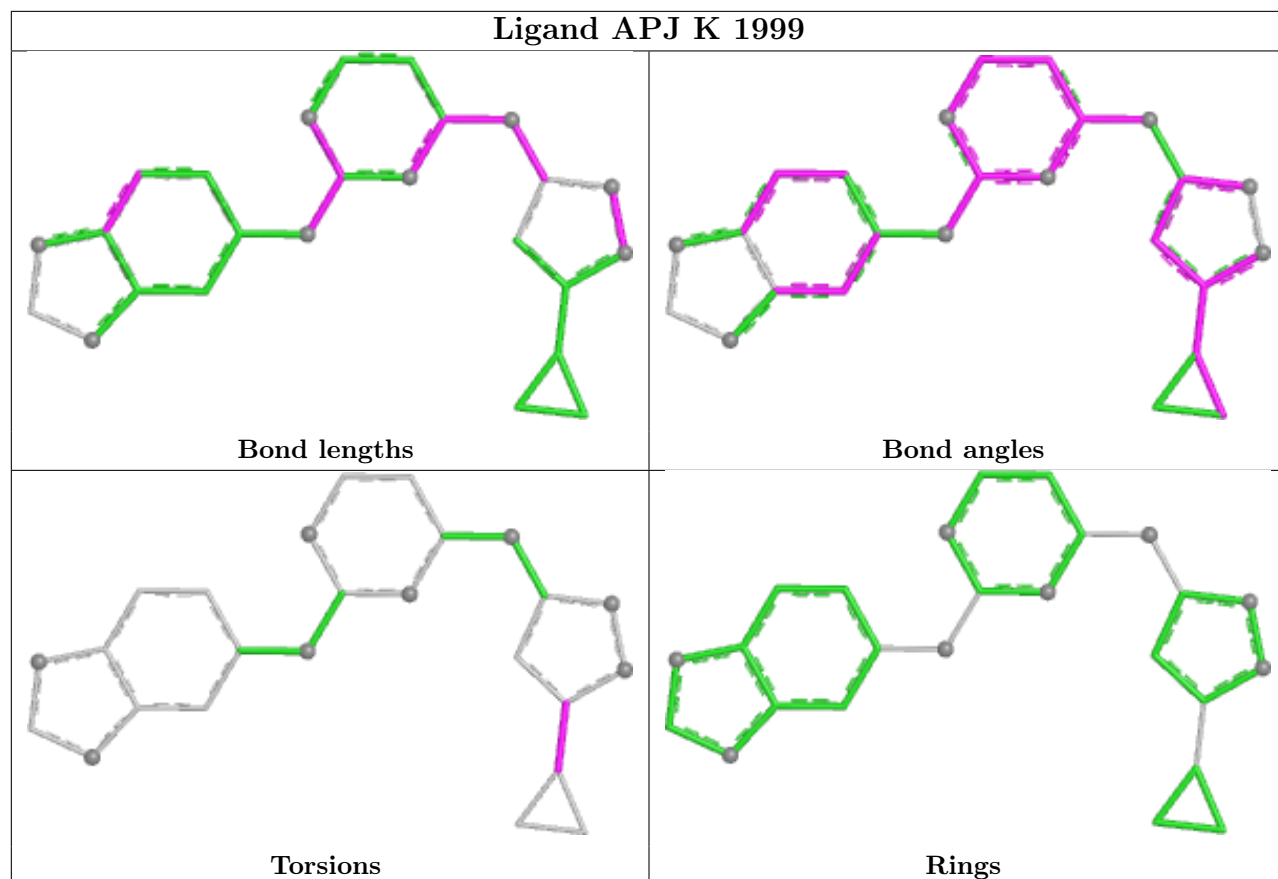
Mol	Chain	Res	Type	Atoms
2	C	1999	APJ	N5-C14-C16-C18

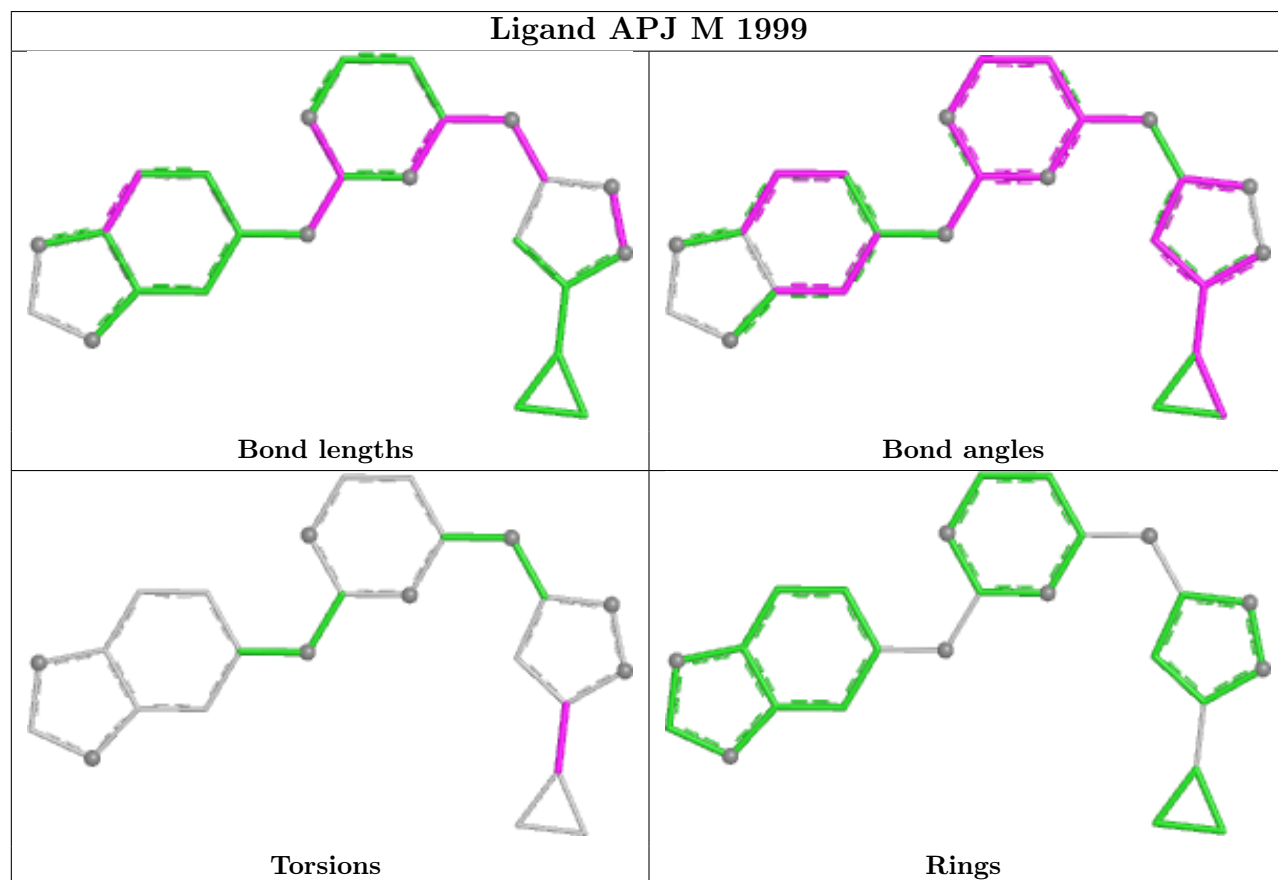
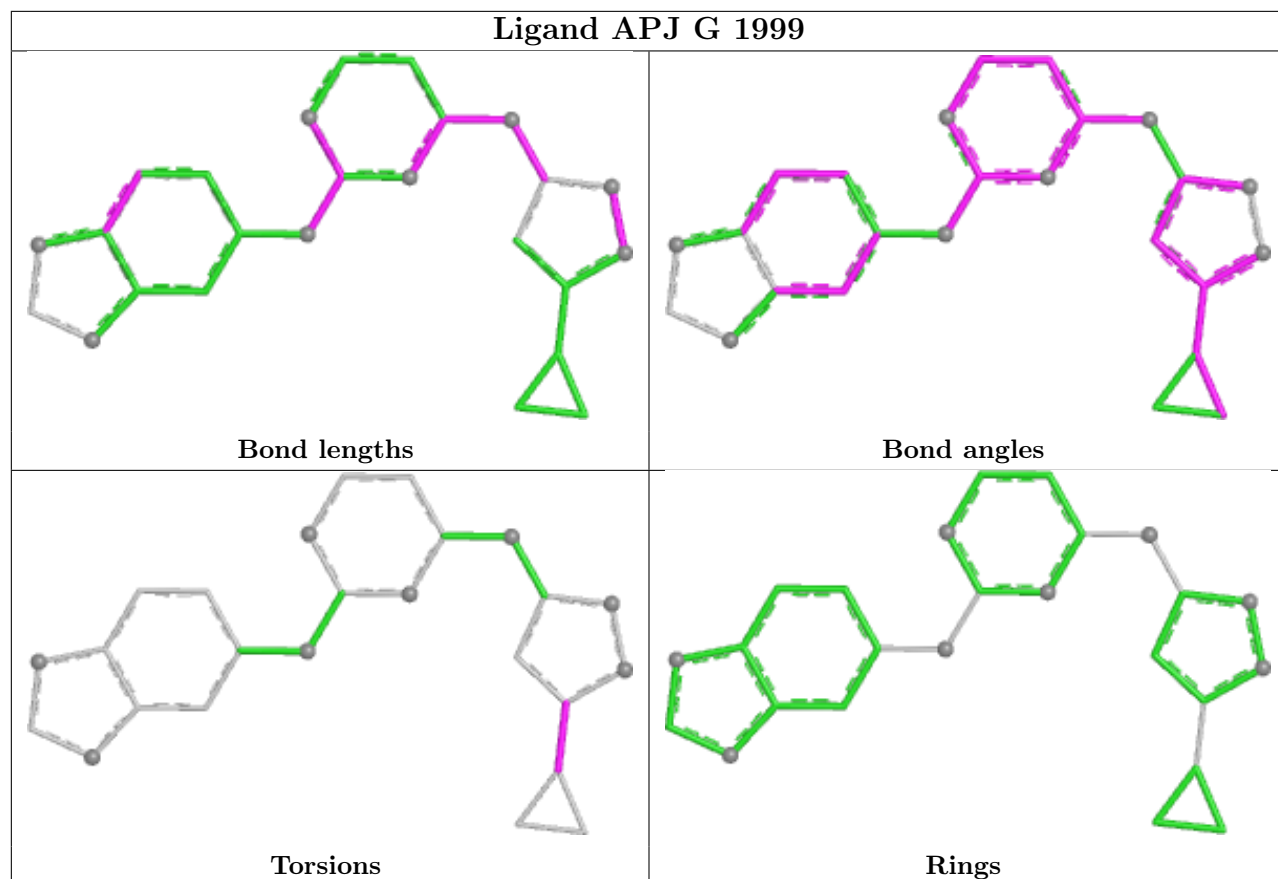
There are no ring outliers.

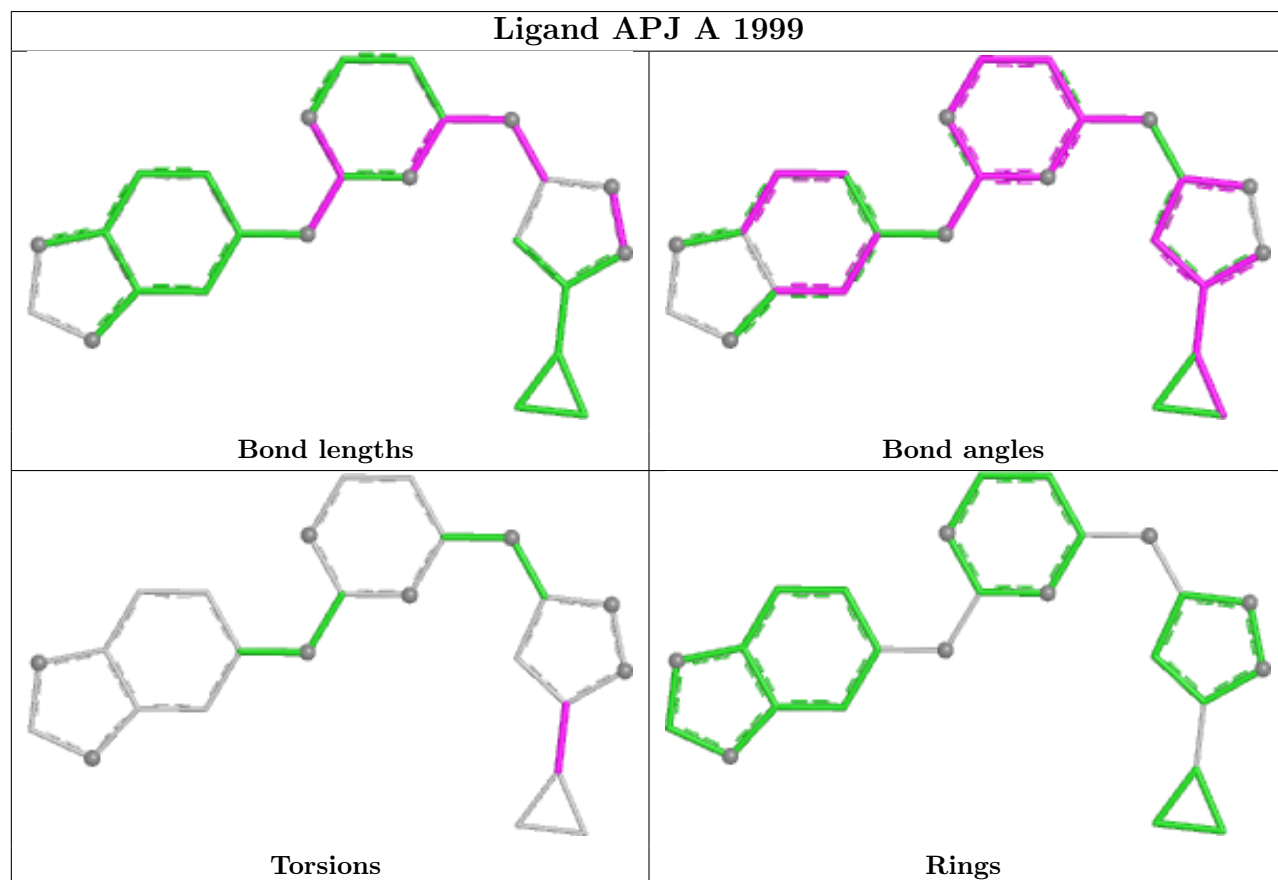
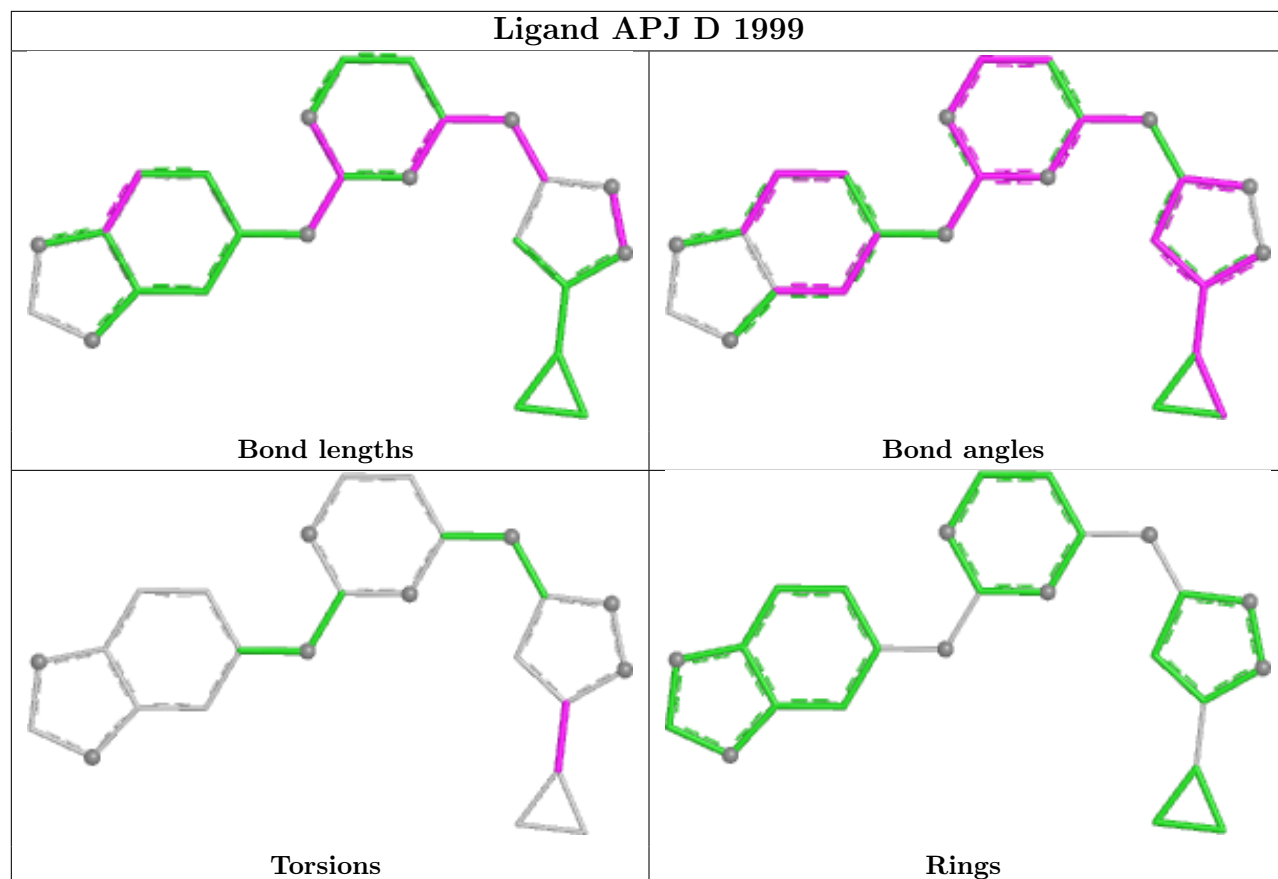
14 monomers are involved in 50 short contacts:

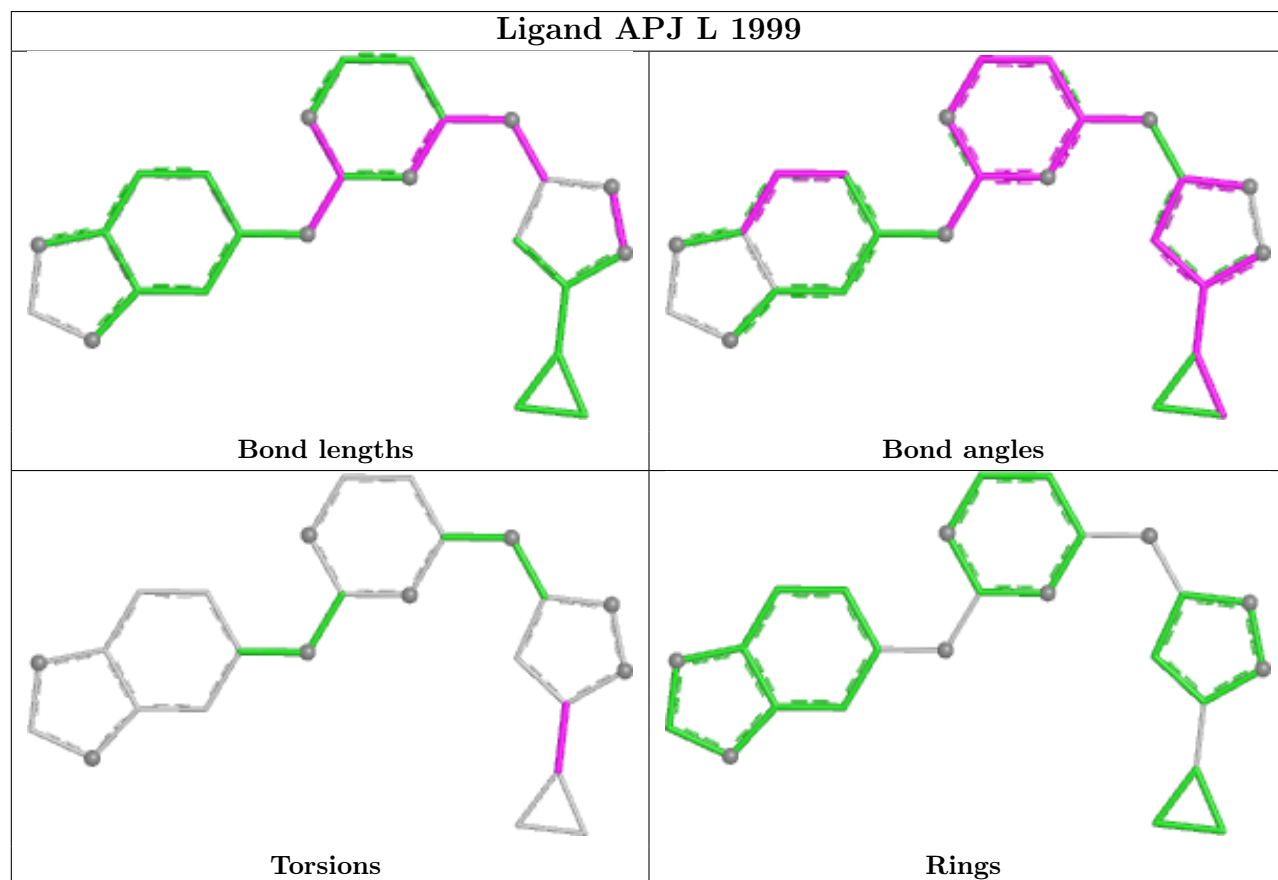
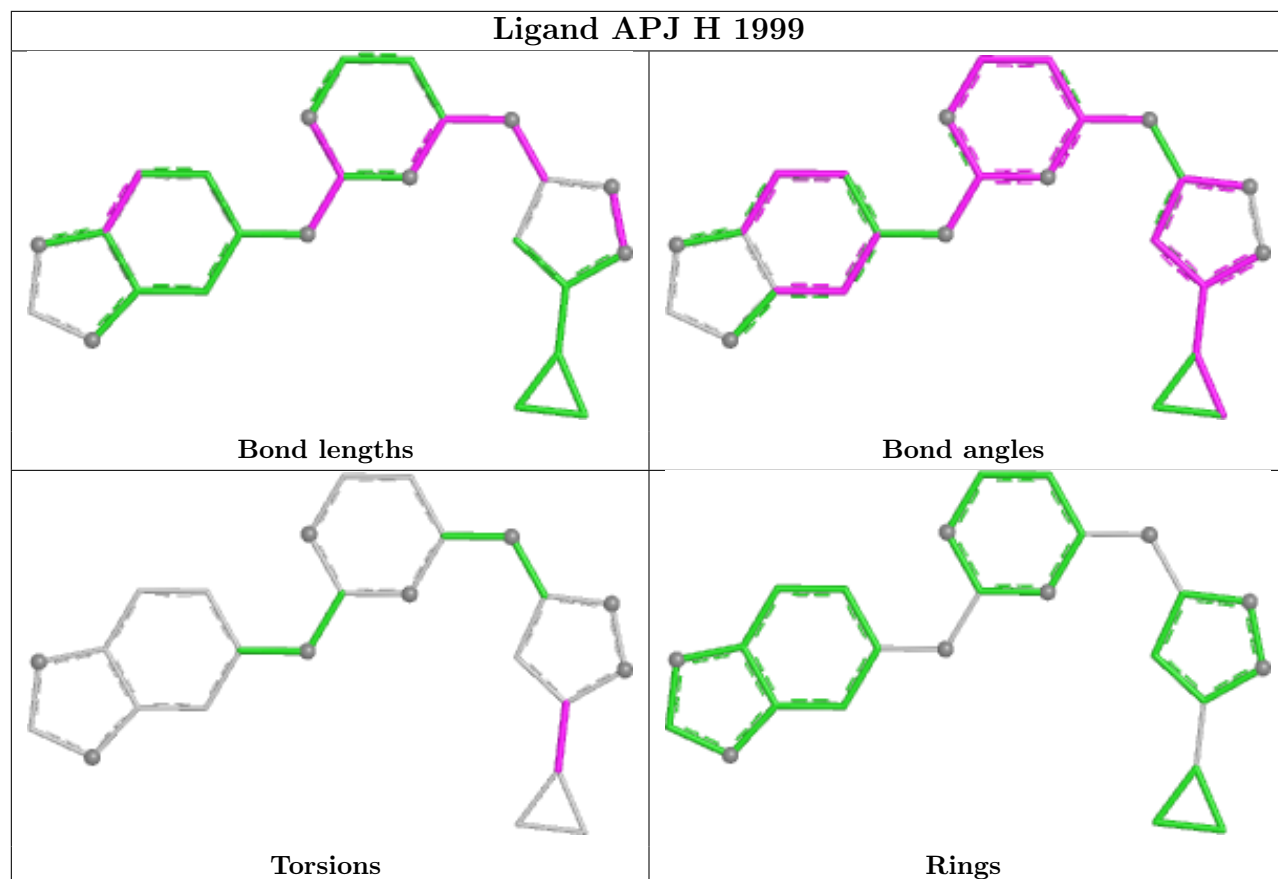
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	K	1999	APJ	3	0
2	F	1999	APJ	3	0
2	G	1999	APJ	4	0
2	M	1999	APJ	3	0
2	D	1999	APJ	3	0
2	A	1999	APJ	4	0
2	H	1999	APJ	4	0
2	L	1999	APJ	3	0
2	I	1999	APJ	4	0
2	B	1999	APJ	3	0
2	J	1999	APJ	4	0
2	N	1999	APJ	4	0
2	C	1999	APJ	4	0
2	E	1999	APJ	4	0

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.

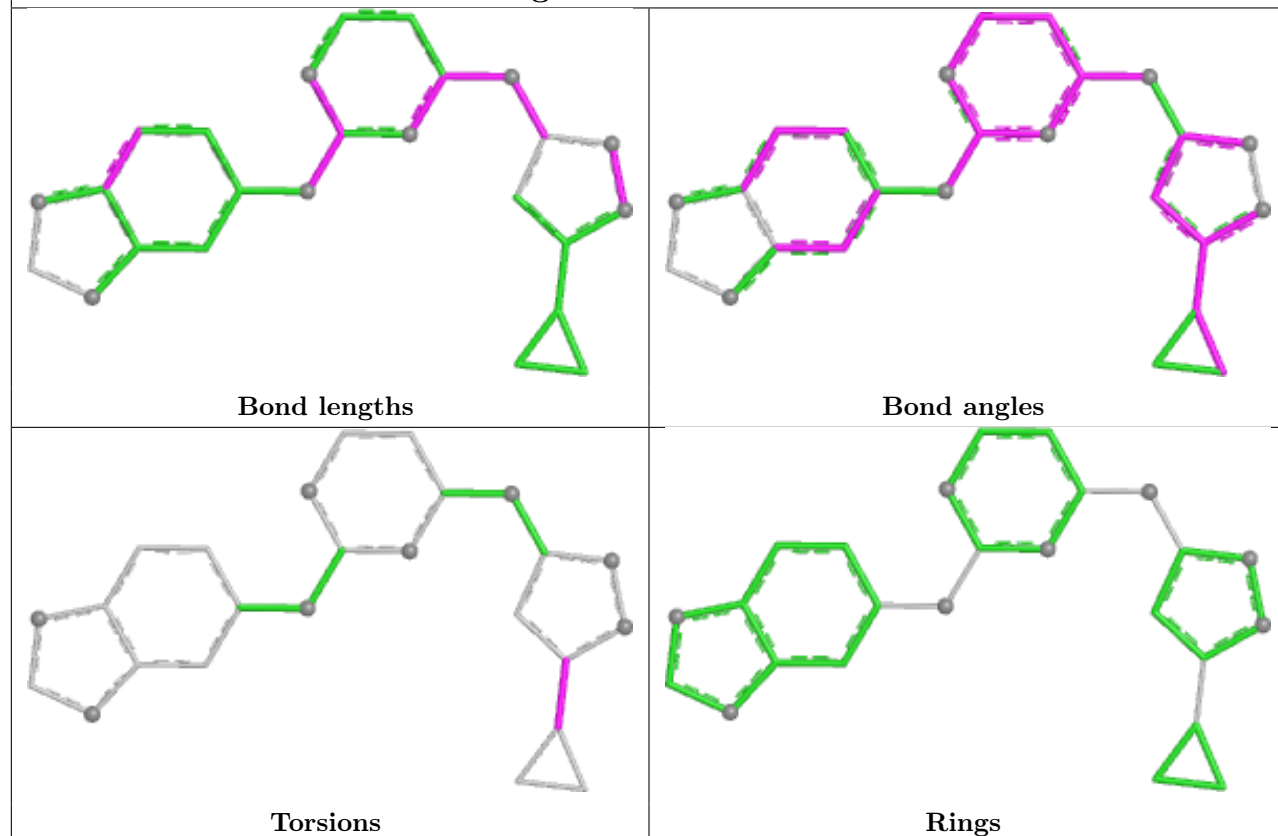




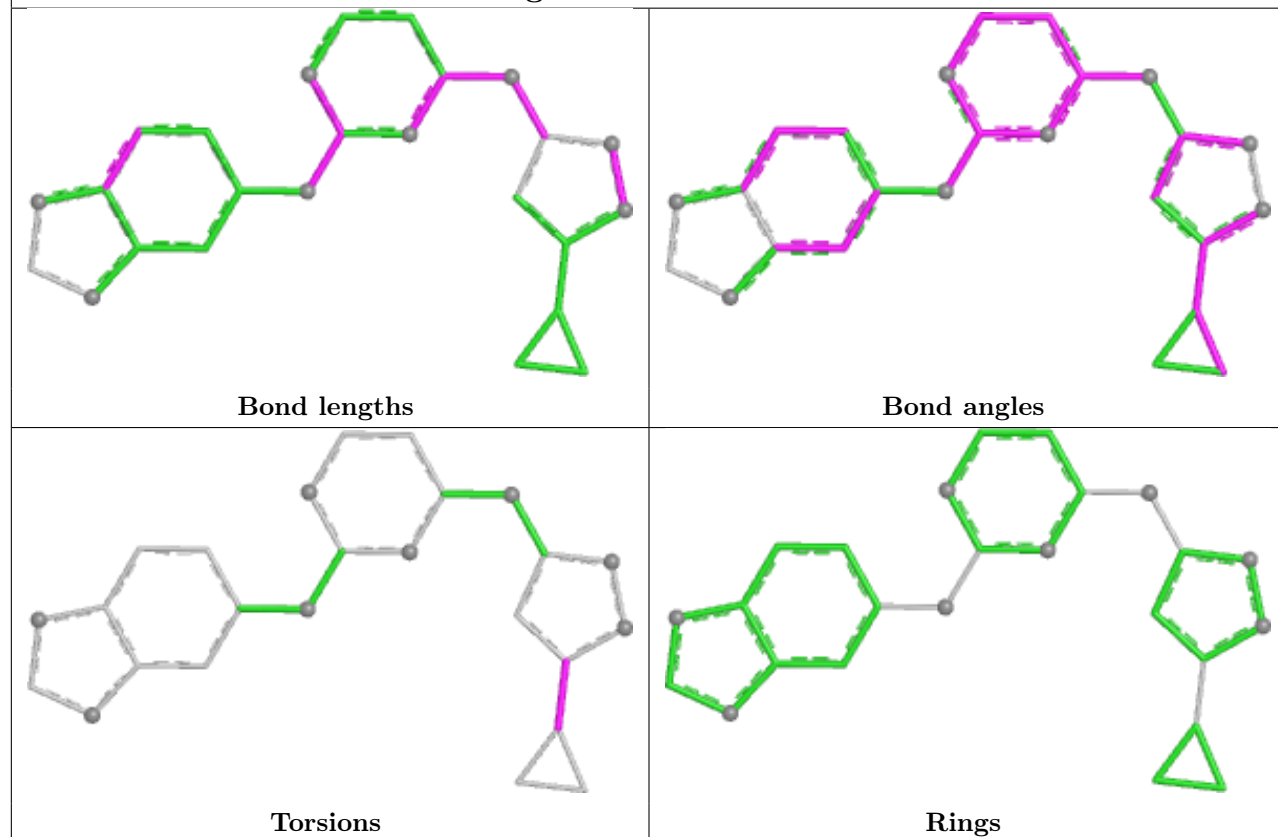


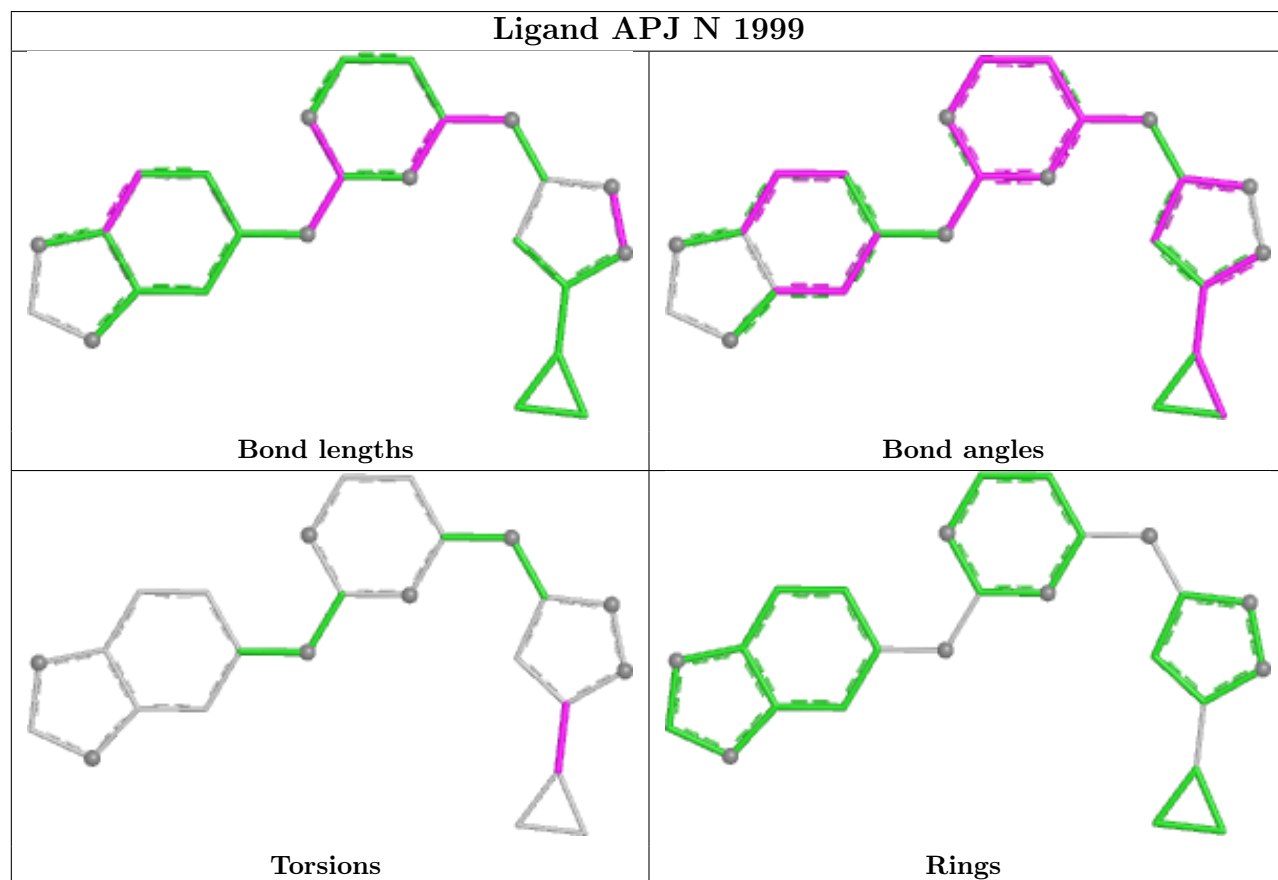
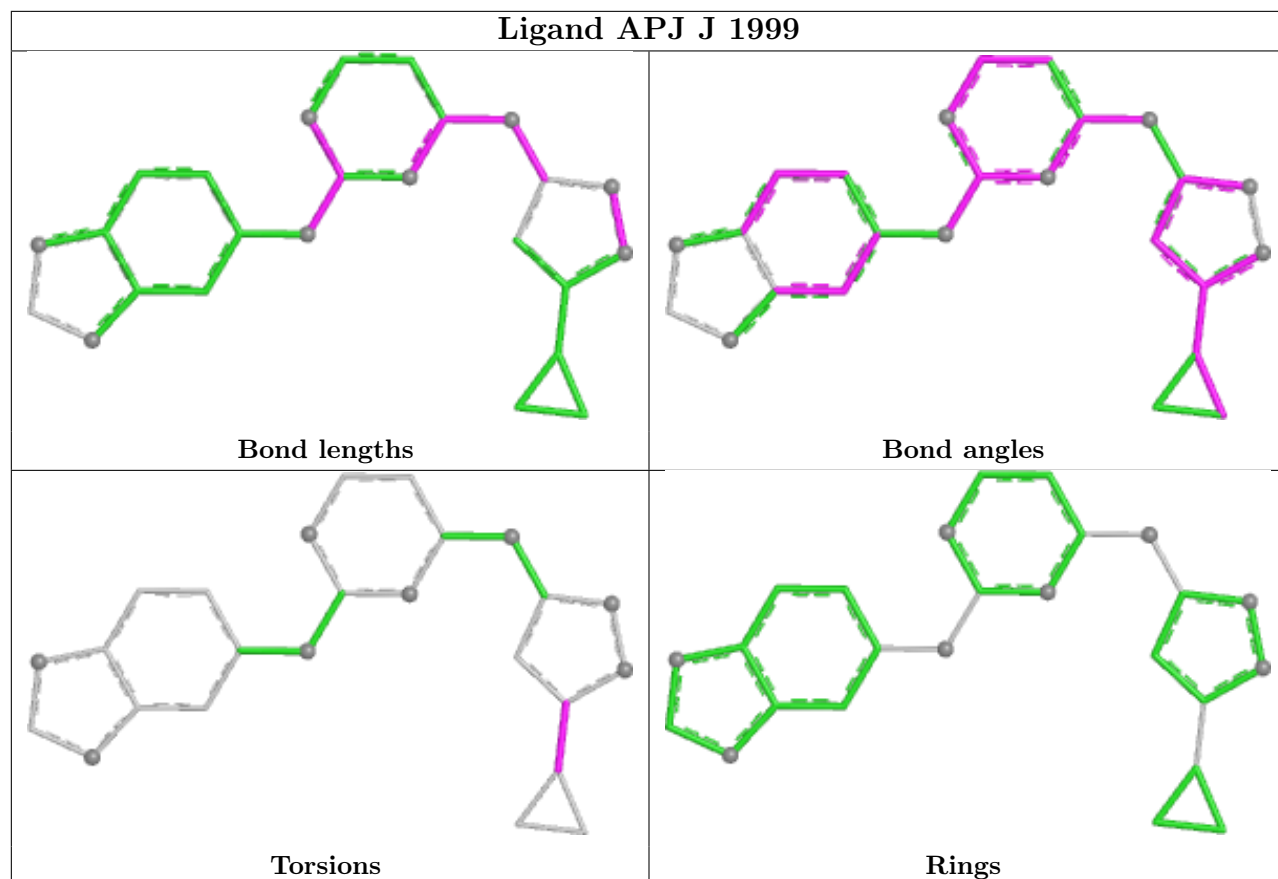


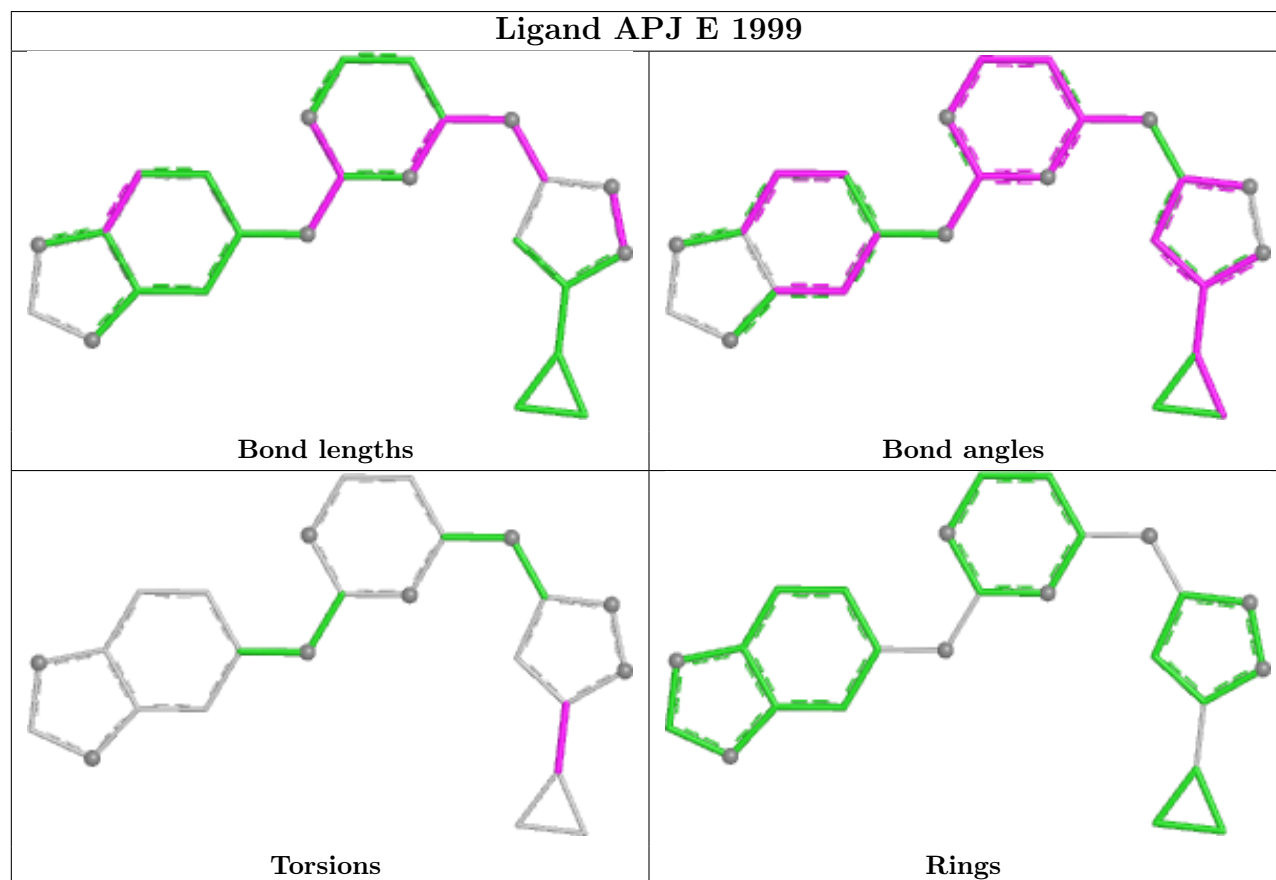
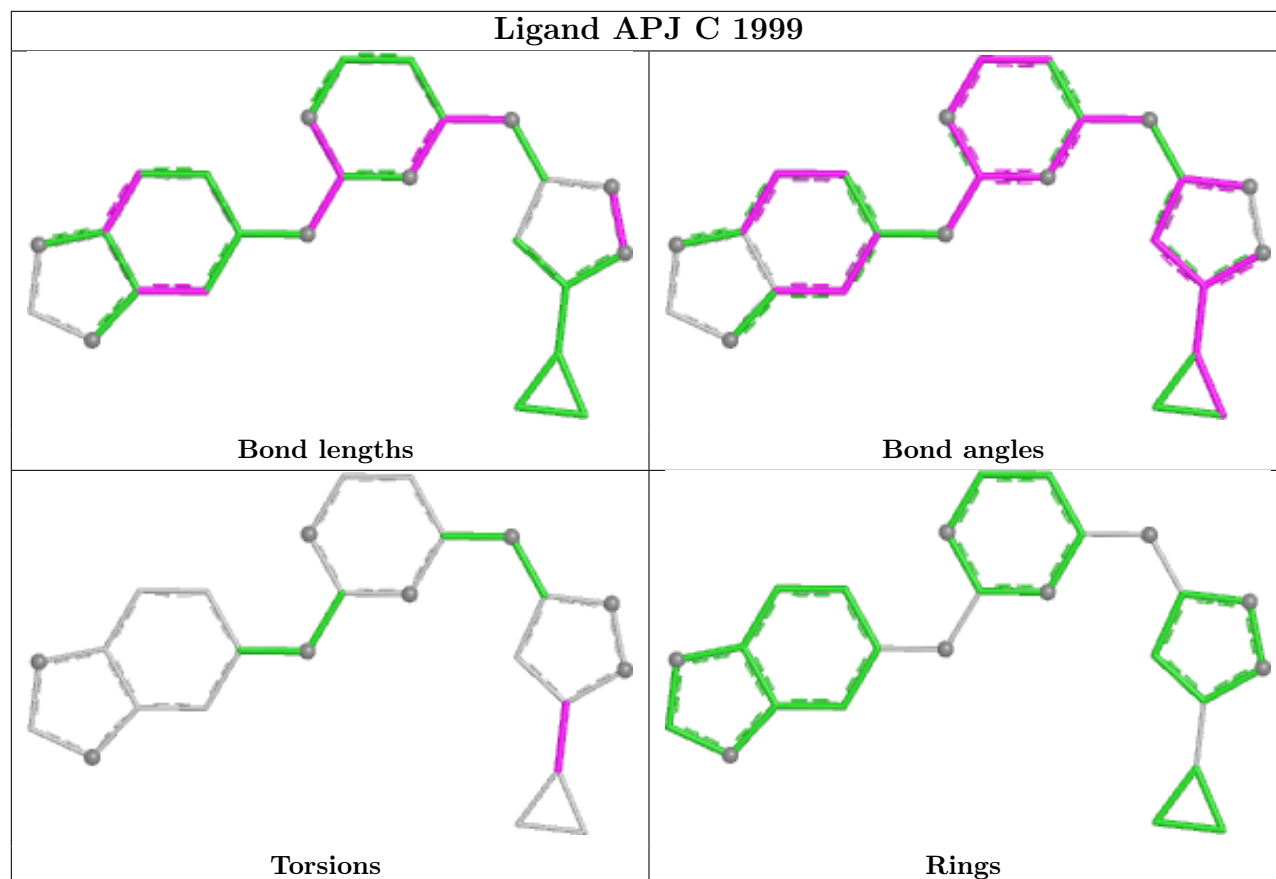
Ligand APJ I 1999



Ligand APJ B 1999







5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

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

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th 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	415/448 (92%)	-0.55	0 100 100	78, 139, 226, 317	0
1	B	415/448 (92%)	-0.57	0 100 100	81, 139, 217, 328	0
1	C	415/448 (92%)	-0.57	0 100 100	77, 139, 221, 317	0
1	D	422/448 (94%)	-0.57	0 100 100	74, 139, 217, 314	0
1	E	415/448 (92%)	-0.58	0 100 100	80, 139, 216, 317	0
1	F	415/448 (92%)	-0.51	0 100 100	77, 138, 220, 321	0
1	G	415/448 (92%)	-0.68	0 100 100	81, 141, 220, 315	0
1	H	415/448 (92%)	-0.72	0 100 100	82, 142, 215, 328	0
1	I	413/448 (92%)	-0.65	0 100 100	87, 141, 218, 314	0
1	J	413/448 (92%)	-0.68	0 100 100	88, 144, 222, 316	0
1	K	422/448 (94%)	-0.71	0 100 100	87, 142, 215, 317	0
1	L	415/448 (92%)	-0.63	1 (0%) 92 85	94, 146, 229, 320	0
1	M	415/448 (92%)	-0.64	0 100 100	74, 139, 221, 316	0
1	N	415/448 (92%)	-0.60	0 100 100	80, 140, 222, 316	0
All	All	5820/6272 (92%)	-0.62	1 (0%) 100 100	74, 141, 222, 328	0

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	L	850	SER	2.3

6.2 Non-standard residues in protein, DNA, RNA chains [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, 95th 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(\AA^2)	Q<0.9
1	TPO	G	844	11/12	0.19	0.10	236,257,277,288	0
1	TPO	K	844	11/12	0.47	0.11	233,255,276,276	0
1	TPO	D	844	11/12	0.55	0.09	237,258,279,286	0
1	TPO	J	844	11/12	0.56	0.09	247,288,304,312	0
1	TPO	L	844	11/12	0.57	0.10	236,272,293,294	0
1	TPO	I	844	11/12	0.59	0.11	231,259,282,291	0
1	TPO	N	844	11/12	0.60	0.10	261,293,306,316	0
1	TPO	C	844	11/12	0.62	0.10	237,258,278,286	0
1	TPO	A	844	11/12	0.62	0.10	234,256,276,285	0
1	TPO	F	844	11/12	0.66	0.09	240,258,277,289	0
1	TPO	H	844	11/12	0.69	0.07	230,258,277,282	0
1	TPO	M	844	11/12	0.73	0.07	231,259,278,290	0
1	TPO	B	844	11/12	0.73	0.09	229,257,278,285	0
1	TPO	E	844	11/12	0.75	0.07	234,254,281,286	0
1	SEP	L	841	10/11	0.82	0.09	134,147,196,197	0
1	SEP	E	840	10/11	0.82	0.08	158,189,203,206	0
1	SEP	I	840	10/11	0.84	0.08	160,186,200,209	0
1	SEP	M	840	10/11	0.85	0.08	154,187,197,203	0
1	SEP	F	841	10/11	0.85	0.10	116,138,197,198	0
1	SEP	L	840	10/11	0.85	0.07	207,220,237,239	0
1	SEP	J	840	10/11	0.86	0.07	155,184,194,203	0
1	SEP	C	840	10/11	0.88	0.08	159,179,200,201	0
1	SEP	A	840	10/11	0.89	0.06	169,189,198,203	0
1	SEP	N	840	10/11	0.89	0.07	148,189,198,207	0
1	SEP	I	841	10/11	0.89	0.07	127,141,173,189	0
1	SEP	E	841	10/11	0.90	0.06	131,138,180,181	0
1	SEP	C	841	10/11	0.90	0.07	126,141,180,190	0
1	SEP	H	840	10/11	0.90	0.07	152,186,199,207	0
1	SEP	F	840	10/11	0.90	0.08	151,184,195,208	0
1	SEP	K	840	10/11	0.90	0.07	150,189,200,205	0
1	SEP	K	841	10/11	0.90	0.07	120,145,183,194	0
1	SEP	D	840	10/11	0.90	0.10	153,182,197,198	0
1	SEP	B	840	10/11	0.91	0.07	162,186,197,200	0
1	SEP	N	841	10/11	0.91	0.08	126,139,192,195	0
1	SEP	B	841	10/11	0.91	0.07	128,139,178,183	0
1	SEP	G	840	10/11	0.92	0.08	152,182,195,202	0
1	SEP	A	841	10/11	0.92	0.06	127,137,181,195	0
1	SEP	J	841	10/11	0.94	0.05	126,144,188,190	0
1	SEP	H	841	10/11	0.94	0.05	129,143,187,192	0
1	SEP	D	841	10/11	0.94	0.06	113,140,178,195	0
1	SEP	M	841	10/11	0.94	0.05	121,141,182,183	0
1	SEP	G	841	10/11	0.95	0.06	96,144,182,190	0

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

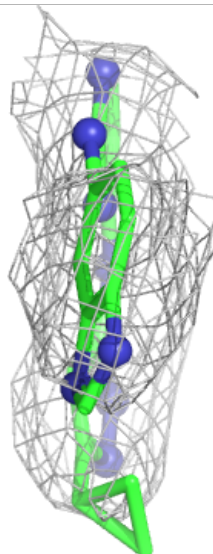
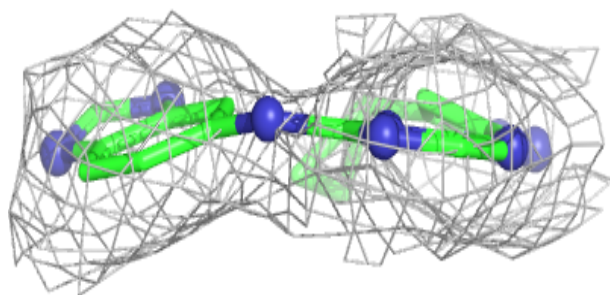
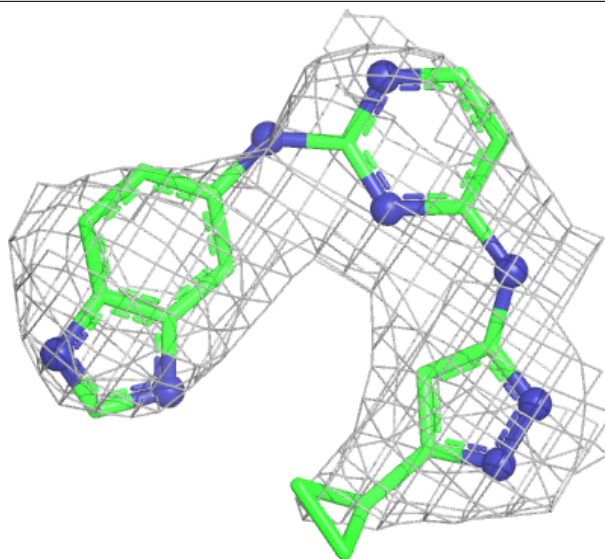
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	APJ	G	1999	25/25	0.91	0.11	141,161,194,202	0
2	APJ	J	1999	25/25	0.91	0.10	134,154,198,209	0
2	APJ	N	1999	25/25	0.91	0.14	114,158,189,205	0
2	APJ	H	1999	25/25	0.92	0.11	158,163,191,204	0
2	APJ	B	1999	25/25	0.93	0.10	123,154,195,205	0
2	APJ	K	1999	25/25	0.93	0.11	175,183,198,218	0
2	APJ	L	1999	25/25	0.93	0.11	148,172,198,209	0
2	APJ	E	1999	25/25	0.93	0.11	132,165,195,207	0
2	APJ	F	1999	25/25	0.94	0.13	121,155,184,208	0
2	APJ	I	1999	25/25	0.94	0.10	138,163,196,201	0
2	APJ	C	1999	25/25	0.94	0.11	126,146,182,205	0
2	APJ	M	1999	25/25	0.95	0.08	128,157,193,206	0
2	APJ	A	1999	25/25	0.95	0.10	132,162,192,211	0
2	APJ	D	1999	25/25	0.96	0.08	132,154,190,205	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.

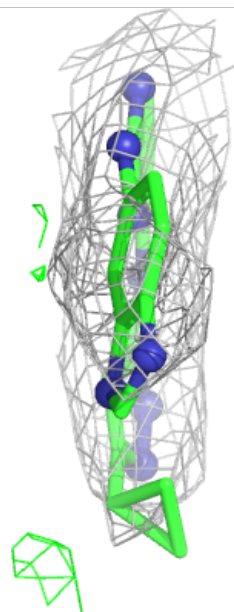
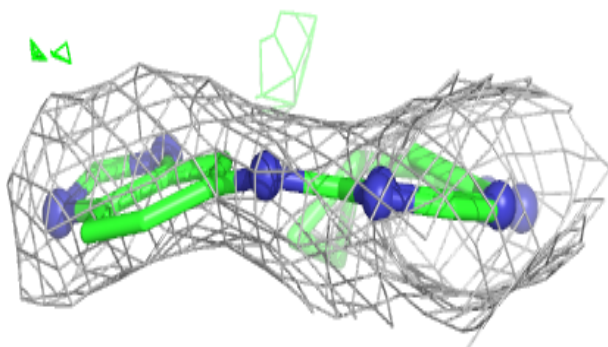
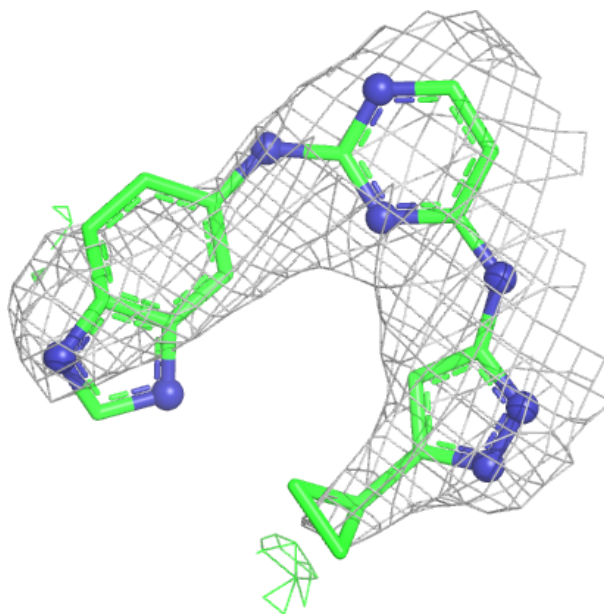
Electron density around APJ G 1999:

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



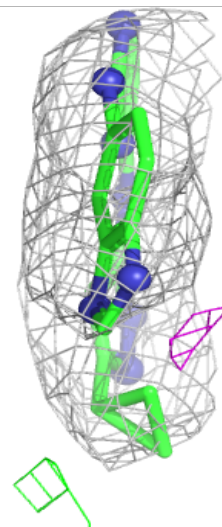
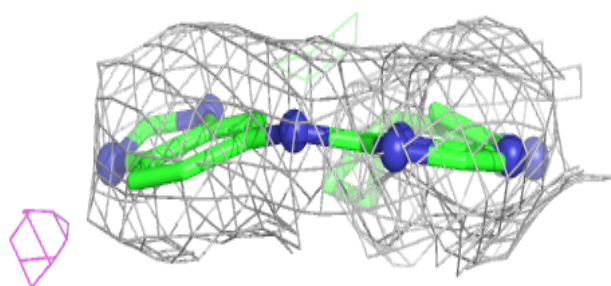
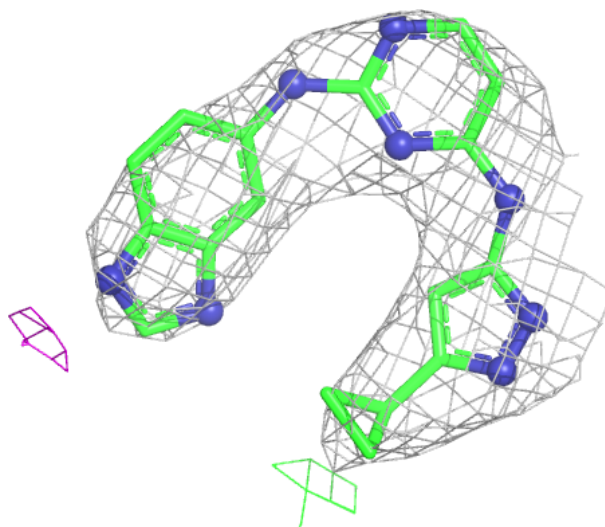
Electron density around APJ J 1999:

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



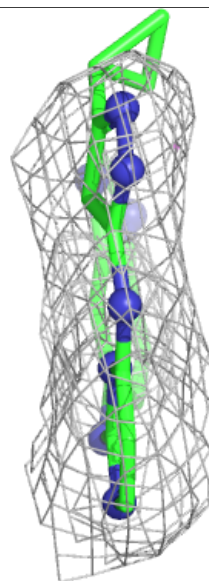
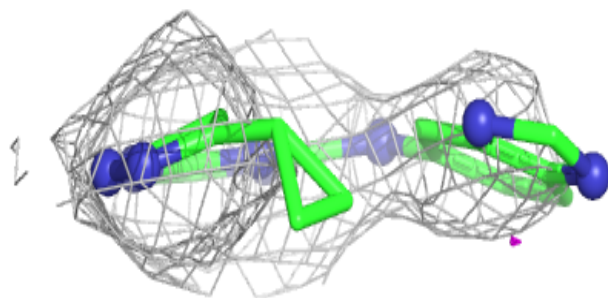
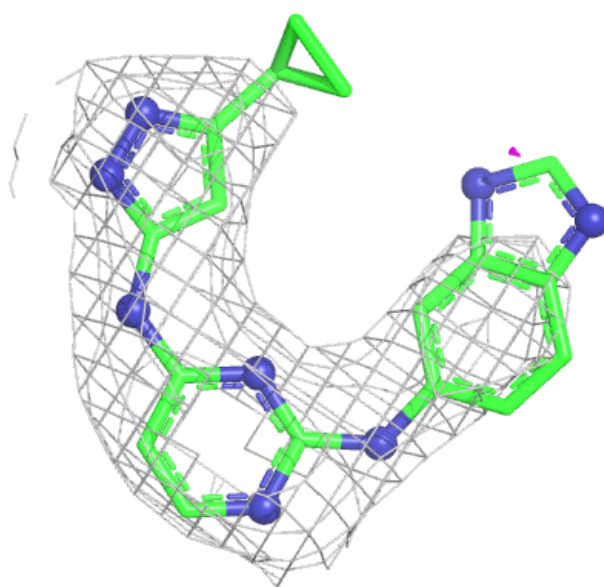
Electron density around APJ N 1999:

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



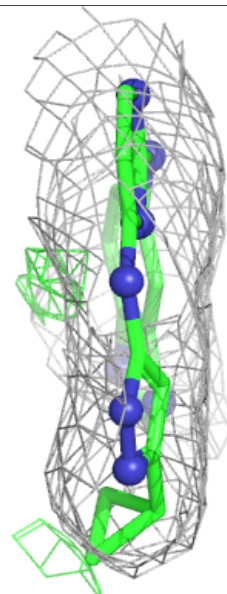
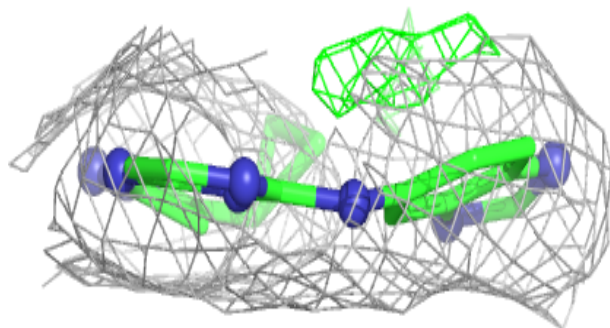
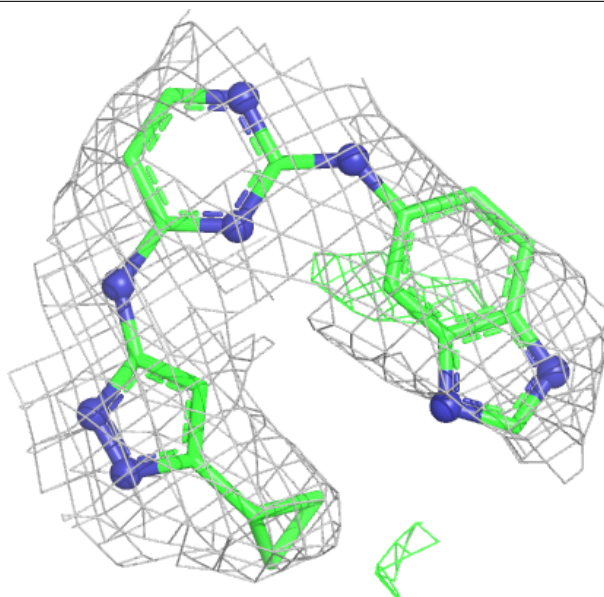
Electron density around APJ H 1999:

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



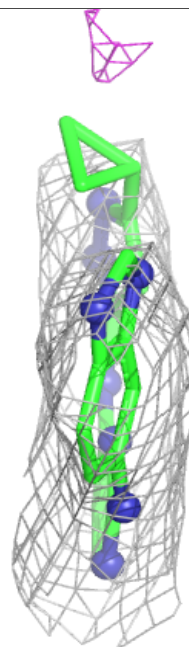
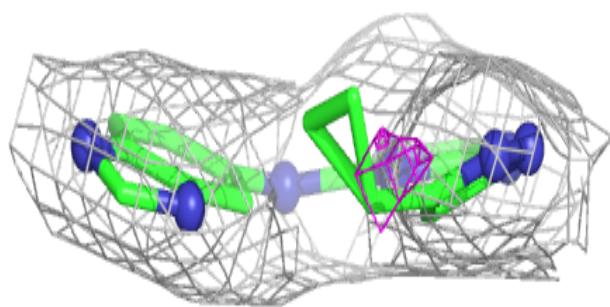
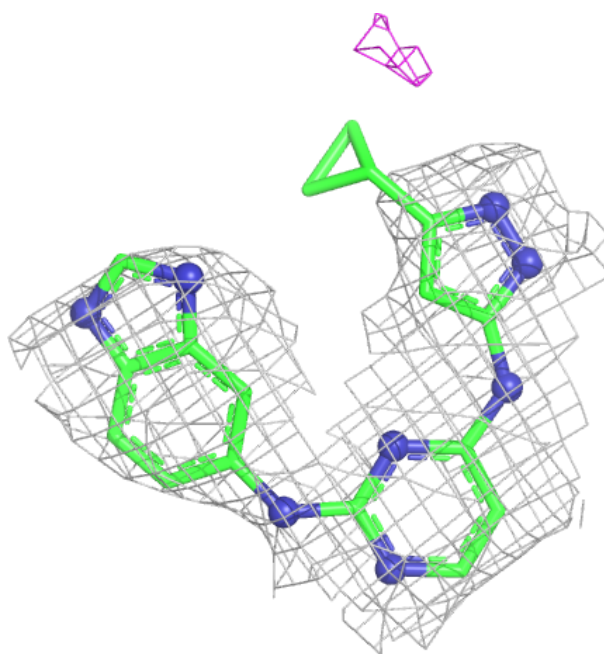
Electron density around APJ B 1999:

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



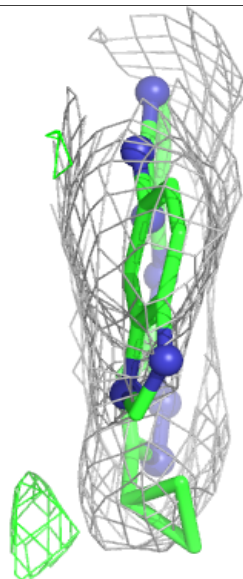
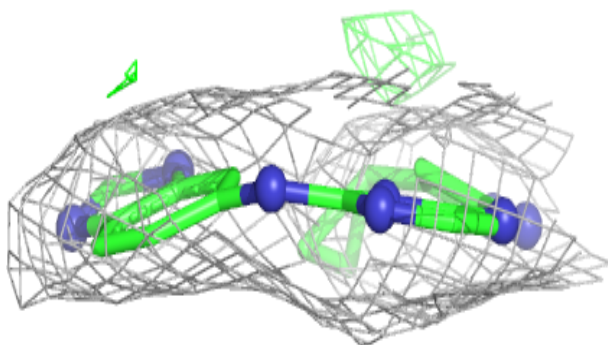
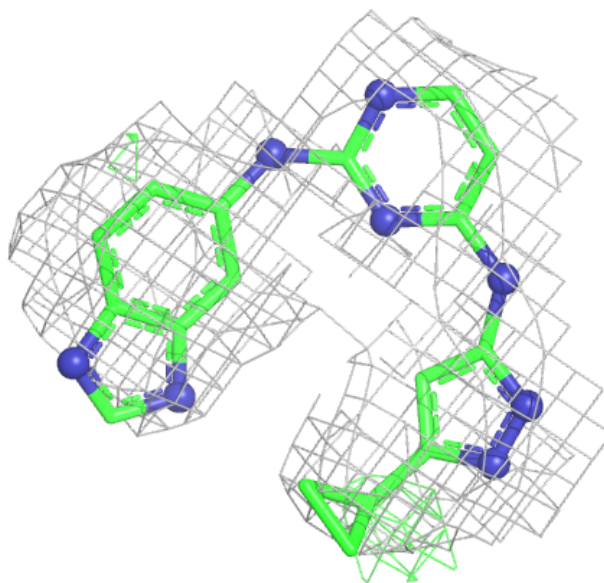
Electron density around APJ K 1999:

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



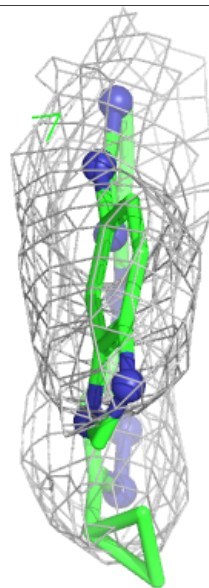
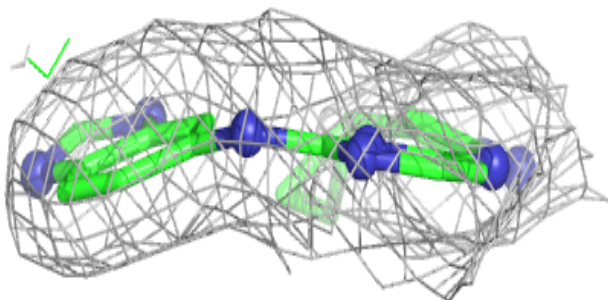
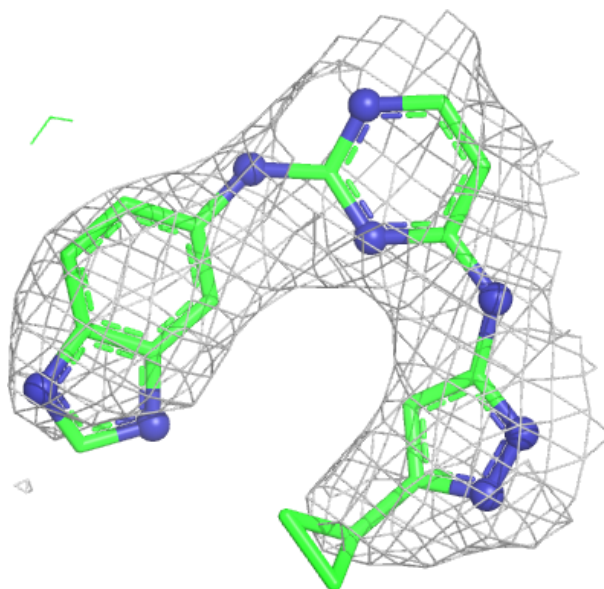
Electron density around APJ L 1999:

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



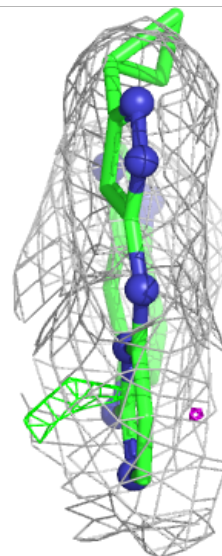
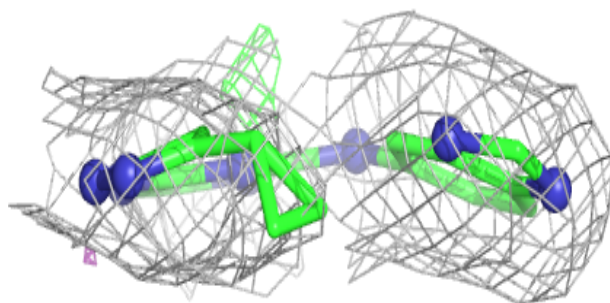
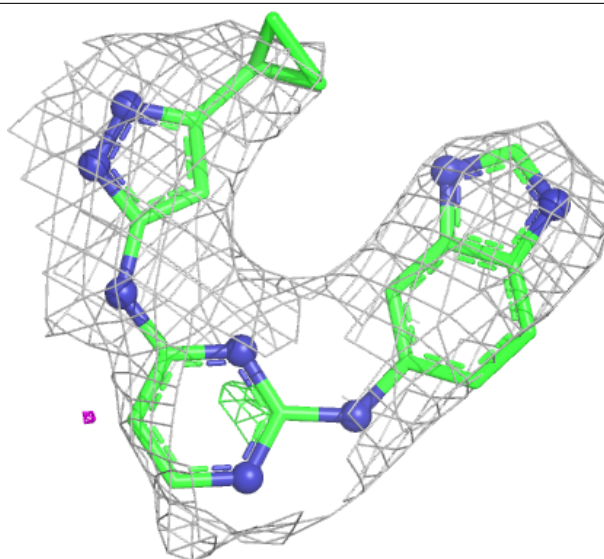
Electron density around APJ E 1999:

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



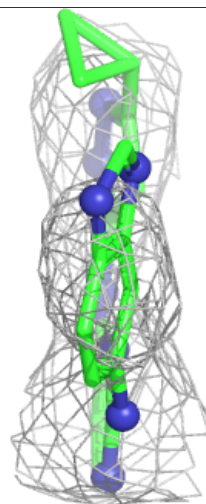
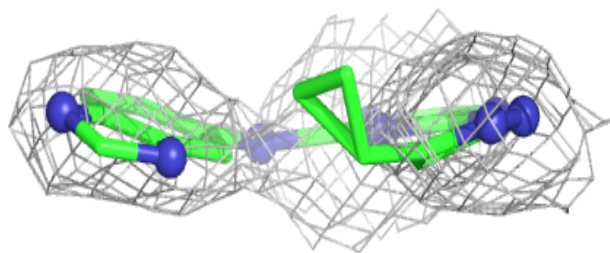
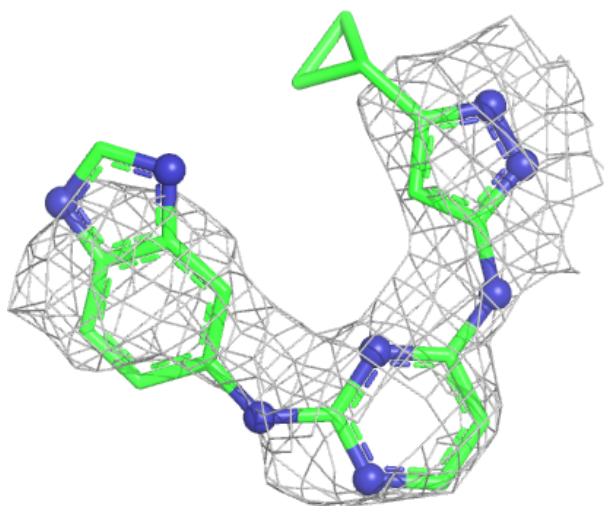
Electron density around APJ F 1999:

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



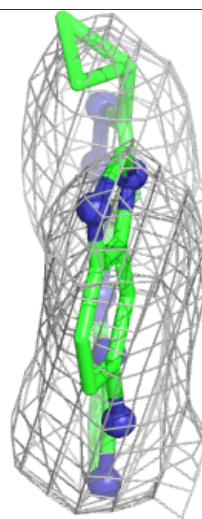
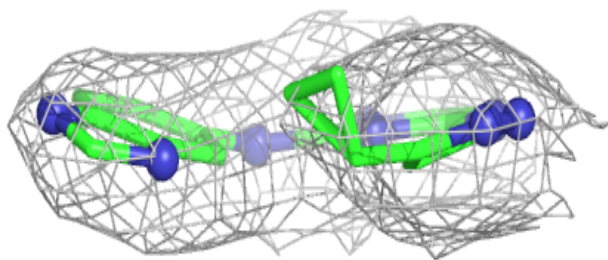
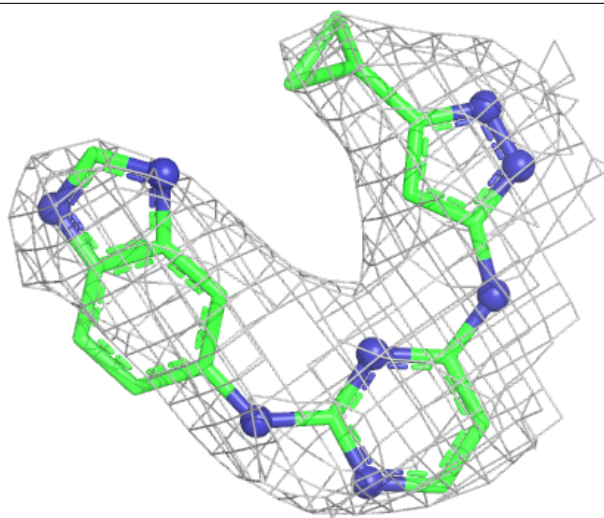
Electron density around APJ I 1999:

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



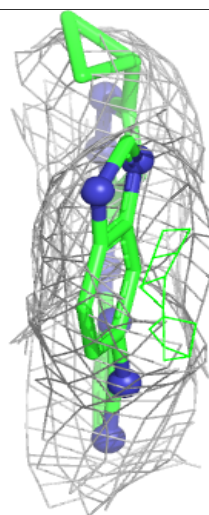
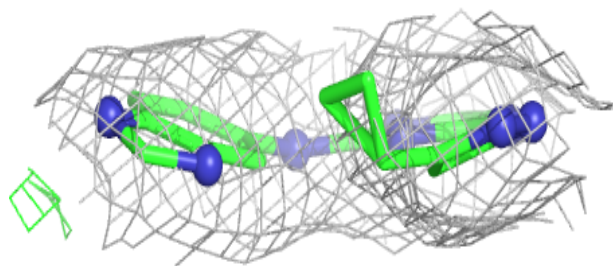
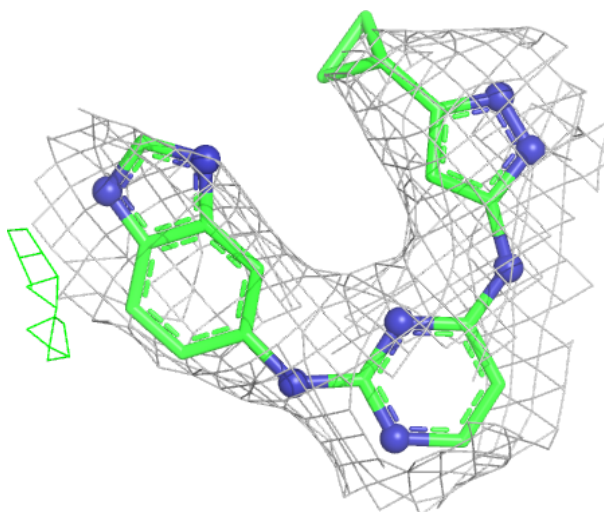
Electron density around APJ C 1999:

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



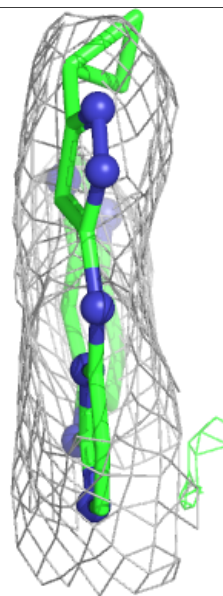
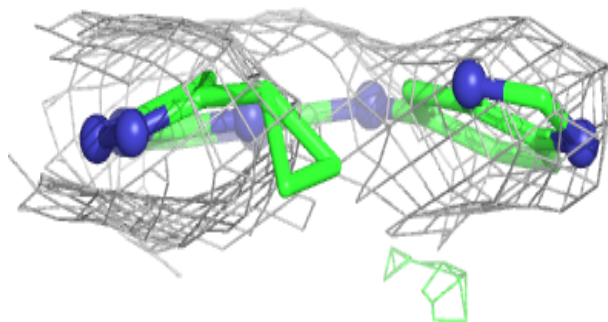
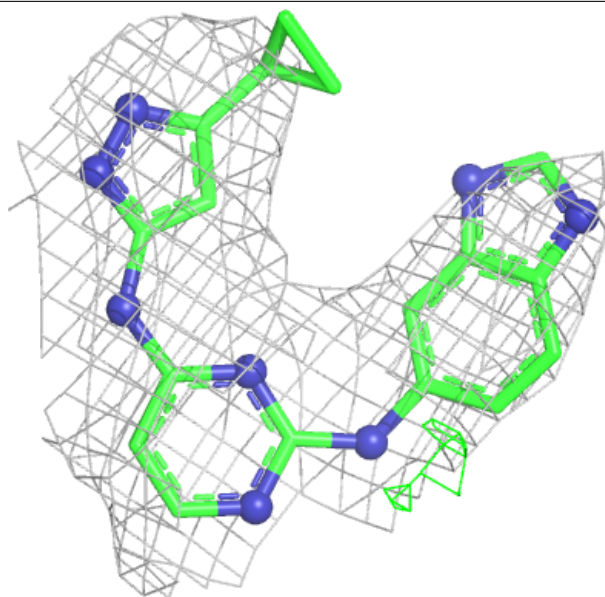
Electron density around APJ M 1999:

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



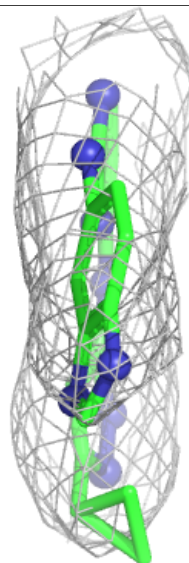
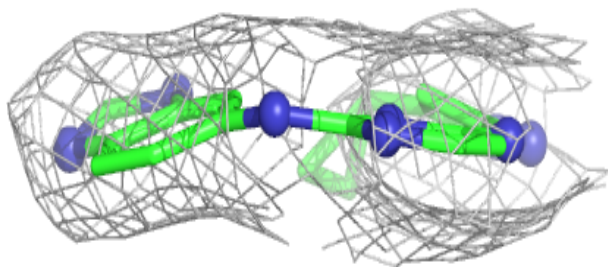
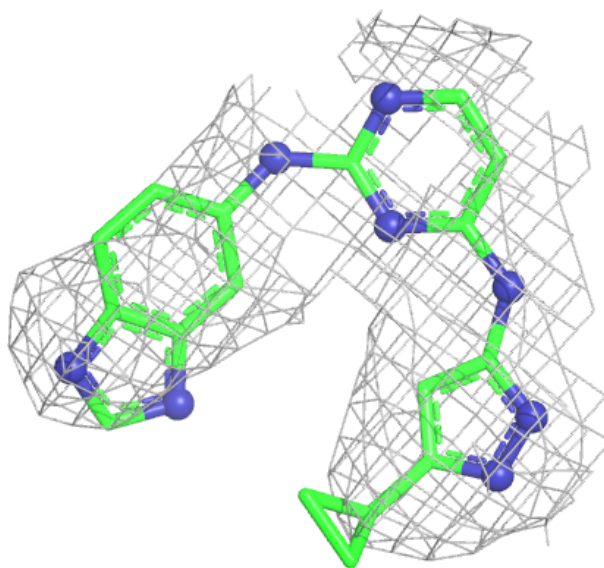
Electron density around APJ A 1999:

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



Electron density around APJ D 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.