



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 20, 2020 – 12:59 PM BST

PDB ID : 5MU8
Title : HUMAN TNF-ALPHA IN COMPLEX WITH JNJ525
Authors : Blevitt, J.M.; Hack, M.D.; Herman, K.L.; Jackson, P.F.; Krawczuk, P.J.; Lebsack, A.D.; Liu, A.X.; Mirzadegan, T.; Nelen, M.I.; Patrick, A.P.; Steinbacher, S.; Milla, M.E.; Lumb, K.J.
Deposited on : 2017-01-12
Resolution : 3.00 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.13
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) : 2.13

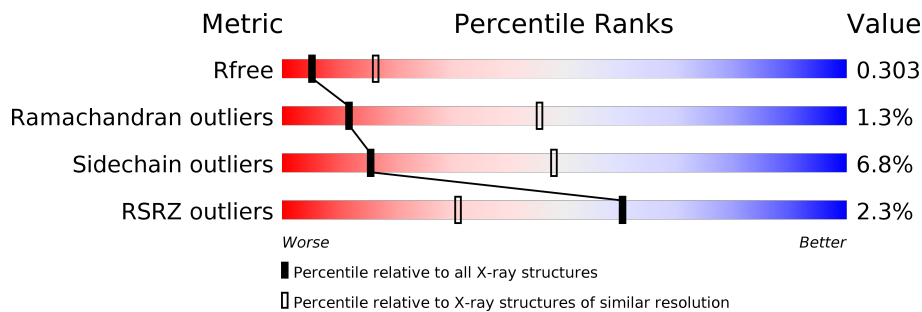
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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.








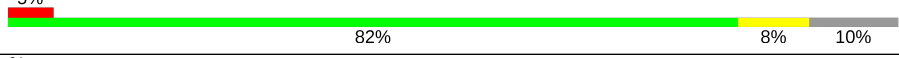

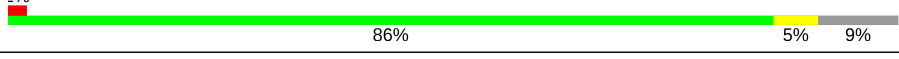



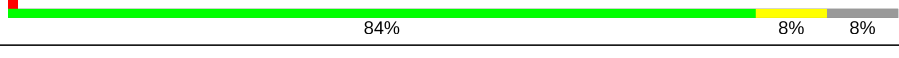
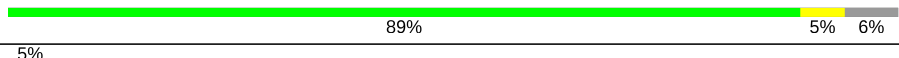


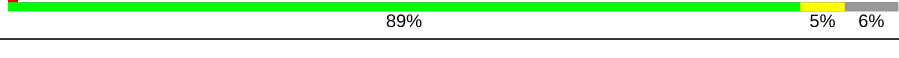



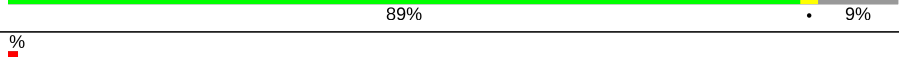
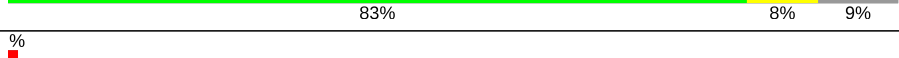
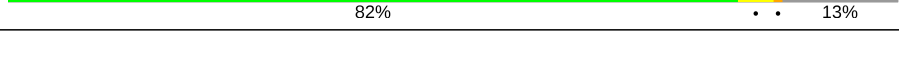

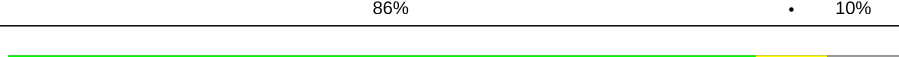

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	2092 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (3.00-3.00)

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 ≥ 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	159	83% 6% 11%
1	B	159	2% 86% 5% 9%
1	C	159	2% 83% 8% 8%
1	D	159	88% 6% 6%
1	F	159	% 82% 6% 12%
1	G	159	3% 84% 9% 6%
1	H	159	2% 87% 7% 6%

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Mol	Chain	Length	Quality of chain
1	I	159	 84% 5% 11%
1	J	159	 5% 81% 6% 13%
1	K	159	 4% 82% 11% 6%
1	L	159	 5% 86% 11%
1	M	159	 86% 8% 6%
1	N	159	 5% 82% 8% 10%
1	O	159	 85% 6% 9%
1	P	159	 2% 86% 5% 9%
1	Q	159	 87% 6% 6%
1	R	159	 82% 5% 13%
1	S	159	 3% 88% 6% 6%
1	T	159	 84% 8% 8%
1	U	159	 89% 5% 6%
1	V	159	 5% 82% 5% 13%
1	W	159	 82% 8% 10%
1	X	159	 89% 5% 6%
1	Y	159	 85% 9% 6%
1	Z	159	 3% 83% 7% 10%
1	a	159	 4% 86% 8% 6%
1	b	159	 89% 9%
1	c	159	 83% 8% 9%
1	d	159	 82% 13%
1	e	159	 88% 6%
1	f	159	 2% 86% 10%
1	g	159	 84% 8% 9%

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Mol	Chain	Length	Quality of chain
1	h	159	
1	i	159	
1	j	159	
1	k	159	
1	l	159	
1	m	159	
1	n	159	
1	o	159	
1	p	159	
1	q	159	
1	r	159	
1	s	159	
1	t	159	
1	u	159	
1	v	159	
1	w	159	

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
2	JNI	f	202	-	-	-	X

2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 56305 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 Tumor necrosis factor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	141	1105	709	186	208	2	0	0	0
1	B	145	1139	728	197	212	2	0	0	0
1	C	146	1145	733	198	212	2	0	0	0
1	D	149	1165	743	201	219	2	0	0	0
1	F	140	1099	707	184	206	2	0	0	0
1	G	149	1165	743	201	219	2	0	0	0
1	H	150	1172	748	202	220	2	0	0	0
1	I	141	1104	708	190	204	2	0	0	0
1	J	138	1085	699	182	202	2	0	0	0
1	K	149	1165	743	201	219	2	0	0	0
1	L	142	1111	713	191	205	2	0	0	0
1	M	149	1165	743	201	219	2	0	0	0
1	N	143	1117	717	187	211	2	0	0	0
1	O	145	1140	728	197	213	2	0	0	0
1	P	145	1140	729	196	213	2	0	0	0
1	Q	149	1165	743	201	219	2	0	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	R	138	1083	697	182	202	2	0	0	0
1	S	149	1165	743	201	219	2	0	0	0
1	T	146	1145	733	198	212	2	0	0	0
1	U	149	1165	743	201	219	2	0	0	0
1	V	138	1085	699	182	202	2	0	0	0
1	W	143	1126	720	195	209	2	0	0	0
1	X	150	1172	748	202	220	2	0	0	0
1	Y	149	1165	743	201	219	2	0	0	0
1	Z	143	1117	717	187	211	2	0	0	0
1	a	149	1165	743	201	219	2	0	0	0
1	b	144	1133	725	196	210	2	0	0	0
1	c	145	1140	728	197	213	2	0	0	0
1	d	138	1085	699	182	202	2	0	0	0
1	e	149	1165	743	201	219	2	0	0	0
1	f	143	1124	719	194	209	2	0	0	0
1	g	145	1138	728	197	211	2	0	0	0
1	h	137	1078	694	181	201	2	0	0	0
1	i	145	1138	728	197	211	2	0	0	0
1	j	150	1172	748	202	220	2	0	0	0
1	k	142	1119	716	194	207	2	0	0	0
1	l	143	1117	717	187	211	2	0	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	m	147	1152	736	199	215	2	0	0	0
1	n	147	1154	738	199	215	2	0	0	0
1	o	147	1151	735	199	215	2	0	0	0
1	p	139	1090	702	183	203	2	0	0	0
1	q	149	1165	743	201	219	2	0	0	0
1	r	144	1131	724	195	210	2	0	0	0
1	s	149	1165	743	201	219	2	0	0	0
1	t	143	1117	717	187	211	2	0	0	0
1	u	145	1138	728	197	211	2	0	0	0
1	v	144	1131	724	195	210	2	0	0	0
1	w	145	1138	728	197	211	2	0	0	0

There are 96 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	ALA	-	expression tag	UNP P01375
A	0	MET	-	expression tag	UNP P01375
B	-1	ALA	-	expression tag	UNP P01375
B	0	MET	-	expression tag	UNP P01375
C	-1	ALA	-	expression tag	UNP P01375
C	0	MET	-	expression tag	UNP P01375
D	-1	ALA	-	expression tag	UNP P01375
D	0	MET	-	expression tag	UNP P01375
F	-1	ALA	-	expression tag	UNP P01375
F	0	MET	-	expression tag	UNP P01375
G	-1	ALA	-	expression tag	UNP P01375
G	0	MET	-	expression tag	UNP P01375
H	-1	ALA	-	expression tag	UNP P01375
H	0	MET	-	expression tag	UNP P01375
I	-1	ALA	-	expression tag	UNP P01375
I	0	MET	-	expression tag	UNP P01375
J	-1	ALA	-	expression tag	UNP P01375

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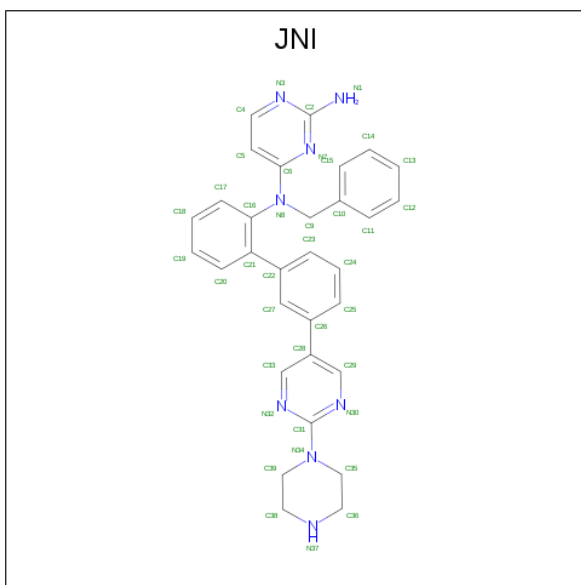
Chain	Residue	Modelled	Actual	Comment	Reference
J	0	MET	-	expression tag	UNP P01375
K	-1	ALA	-	expression tag	UNP P01375
K	0	MET	-	expression tag	UNP P01375
L	-1	ALA	-	expression tag	UNP P01375
L	0	MET	-	expression tag	UNP P01375
M	-1	ALA	-	expression tag	UNP P01375
M	0	MET	-	expression tag	UNP P01375
N	-1	ALA	-	expression tag	UNP P01375
N	0	MET	-	expression tag	UNP P01375
O	-1	ALA	-	expression tag	UNP P01375
O	0	MET	-	expression tag	UNP P01375
P	-1	ALA	-	expression tag	UNP P01375
P	0	MET	-	expression tag	UNP P01375
Q	-1	ALA	-	expression tag	UNP P01375
Q	0	MET	-	expression tag	UNP P01375
R	-1	ALA	-	expression tag	UNP P01375
R	0	MET	-	expression tag	UNP P01375
S	-1	ALA	-	expression tag	UNP P01375
S	0	MET	-	expression tag	UNP P01375
T	-1	ALA	-	expression tag	UNP P01375
T	0	MET	-	expression tag	UNP P01375
U	-1	ALA	-	expression tag	UNP P01375
U	0	MET	-	expression tag	UNP P01375
V	-1	ALA	-	expression tag	UNP P01375
V	0	MET	-	expression tag	UNP P01375
W	-1	ALA	-	expression tag	UNP P01375
W	0	MET	-	expression tag	UNP P01375
X	-1	ALA	-	expression tag	UNP P01375
X	0	MET	-	expression tag	UNP P01375
Y	-1	ALA	-	expression tag	UNP P01375
Y	0	MET	-	expression tag	UNP P01375
Z	-1	ALA	-	expression tag	UNP P01375
Z	0	MET	-	expression tag	UNP P01375
a	-1	ALA	-	expression tag	UNP P01375
a	0	MET	-	expression tag	UNP P01375
b	-1	ALA	-	expression tag	UNP P01375
b	0	MET	-	expression tag	UNP P01375
c	-1	ALA	-	expression tag	UNP P01375
c	0	MET	-	expression tag	UNP P01375
d	-1	ALA	-	expression tag	UNP P01375
d	0	MET	-	expression tag	UNP P01375
e	-1	ALA	-	expression tag	UNP P01375

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Chain	Residue	Modelled	Actual	Comment	Reference
e	0	MET	-	expression tag	UNP P01375
f	-1	ALA	-	expression tag	UNP P01375
f	0	MET	-	expression tag	UNP P01375
g	-1	ALA	-	expression tag	UNP P01375
g	0	MET	-	expression tag	UNP P01375
h	-1	ALA	-	expression tag	UNP P01375
h	0	MET	-	expression tag	UNP P01375
i	-1	ALA	-	expression tag	UNP P01375
i	0	MET	-	expression tag	UNP P01375
j	-1	ALA	-	expression tag	UNP P01375
j	0	MET	-	expression tag	UNP P01375
k	-1	ALA	-	expression tag	UNP P01375
k	0	MET	-	expression tag	UNP P01375
l	-1	ALA	-	expression tag	UNP P01375
l	0	MET	-	expression tag	UNP P01375
m	-1	ALA	-	expression tag	UNP P01375
m	0	MET	-	expression tag	UNP P01375
n	-1	ALA	-	expression tag	UNP P01375
n	0	MET	-	expression tag	UNP P01375
o	-1	ALA	-	expression tag	UNP P01375
o	0	MET	-	expression tag	UNP P01375
p	-1	ALA	-	expression tag	UNP P01375
p	0	MET	-	expression tag	UNP P01375
q	-1	ALA	-	expression tag	UNP P01375
q	0	MET	-	expression tag	UNP P01375
r	-1	ALA	-	expression tag	UNP P01375
r	0	MET	-	expression tag	UNP P01375
s	-1	ALA	-	expression tag	UNP P01375
s	0	MET	-	expression tag	UNP P01375
t	-1	ALA	-	expression tag	UNP P01375
t	0	MET	-	expression tag	UNP P01375
u	-1	ALA	-	expression tag	UNP P01375
u	0	MET	-	expression tag	UNP P01375
v	-1	ALA	-	expression tag	UNP P01375
v	0	MET	-	expression tag	UNP P01375
w	-1	ALA	-	expression tag	UNP P01375
w	0	MET	-	expression tag	UNP P01375

- Molecule 2 is {N}4-(phenylmethyl)- {N}4-[2-[3-(2-piperazin-1-ylpyrimidin-5-yl)phenyl]phenyl]pyrimidine-2,4-diamine (three-letter code: JNI) (formula: C₃₁H₃₀N₈).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	N	0	0
			39	31	8		
2	A	1	Total	C	N	0	0
			39	31	8		
2	C	1	Total	C	N	0	0
			39	31	8		
2	C	1	Total	C	N	0	0
			39	31	8		
2	D	1	Total	C	N	0	0
			39	31	8		
2	F	1	Total	C	N	0	0
			39	31	8		
2	F	1	Total	C	N	0	0
			39	31	8		
2	H	1	Total	C	N	0	0
			39	31	8		
2	H	1	Total	C	N	0	0
			39	31	8		
2	J	1	Total	C	N	0	0
			39	31	8		
2	J	1	Total	C	N	0	0
			39	31	8		
2	L	1	Total	C	N	0	0
			39	31	8		
2	M	1	Total	C	N	0	0
			39	31	8		
2	N	1	Total	C	N	0	0
			39	31	8		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	N		
2	P	1	39	31	8	0	0
2	P	1	39	31	8	0	0
2	Q	1	39	31	8	0	0
2	R	1	39	31	8	0	0
2	U	1	39	31	8	0	0
2	V	1	39	31	8	0	0
2	V	1	39	31	8	0	0
2	X	1	39	31	8	0	0
2	X	1	39	31	8	0	0
2	Z	1	39	31	8	0	0
2	Z	1	39	31	8	0	0
2	b	1	39	31	8	0	0
2	b	1	39	31	8	0	0
2	d	1	39	31	8	0	0
2	f	1	39	31	8	0	0
2	f	1	39	31	8	0	0
2	h	1	39	31	8	0	0
2	h	1	39	31	8	0	0
2	j	1	39	31	8	0	0
2	j	1	39	31	8	0	0
2	l	1	39	31	8	0	0

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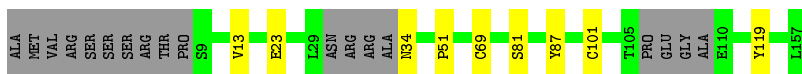
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	N		
2	n	1	Total 39	C 31	N 8	0	0
2	n	1	Total 39	C 31	N 8	0	0
2	o	1	Total 39	C 31	N 8	0	0
2	p	1	Total 39	C 31	N 8	0	0
2	p	1	Total 39	C 31	N 8	0	0
2	r	1	Total 39	C 31	N 8	0	0
2	r	1	Total 39	C 31	N 8	0	0
2	t	1	Total 39	C 31	N 8	0	0
2	t	1	Total 39	C 31	N 8	0	0
2	v	1	Total 39	C 31	N 8	0	0
2	v	1	Total 39	C 31	N 8	0	0

3 Residue-property plots [i](#)


These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Tumor necrosis factor

Chain A: 




- Molecule 1: Tumor necrosis factor

Chain B: 




- Molecule 1: Tumor necrosis factor

Chain C: 




- Molecule 1: Tumor necrosis factor

Chain D: 




- Molecule 1: Tumor necrosis factor

Chain F: 

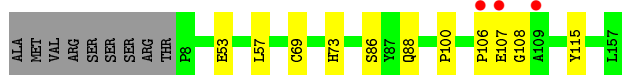
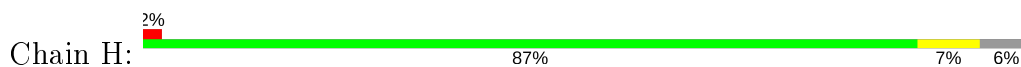


- Molecule 1: Tumor necrosis factor

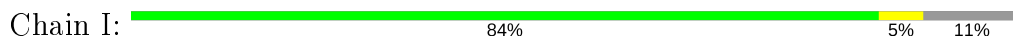
Chain G: 



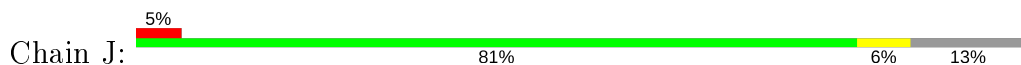
• Molecule 1: Tumor necrosis factor



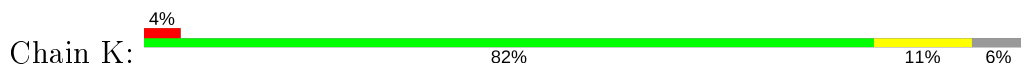
• Molecule 1: Tumor necrosis factor



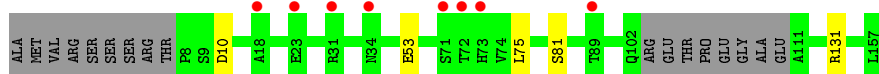
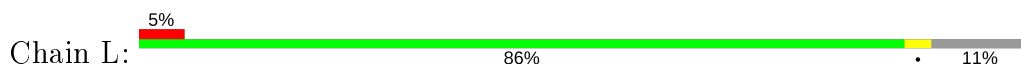
• Molecule 1: Tumor necrosis factor



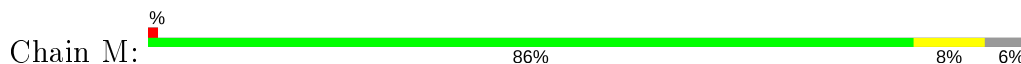
• Molecule 1: Tumor necrosis factor



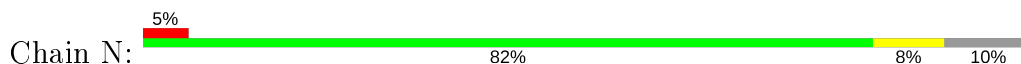
• Molecule 1: Tumor necrosis factor

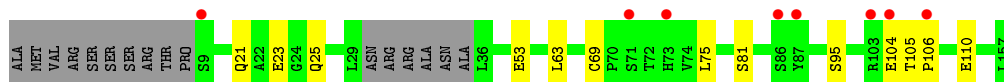


• Molecule 1: Tumor necrosis factor

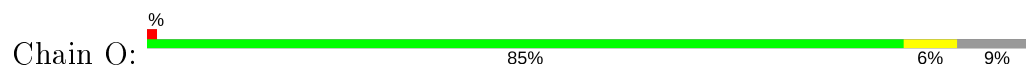


• Molecule 1: Tumor necrosis factor

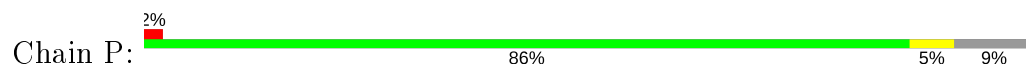




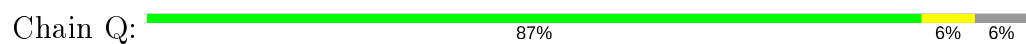
- Molecule 1: Tumor necrosis factor



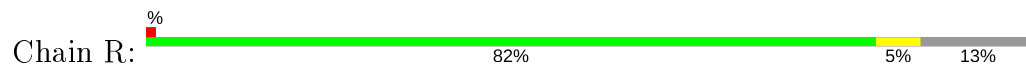
- Molecule 1: Tumor necrosis factor



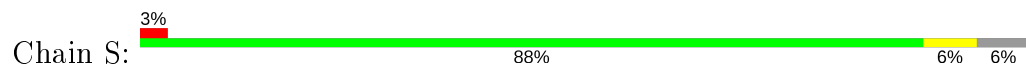
- Molecule 1: Tumor necrosis factor



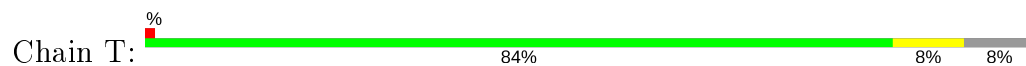
- Molecule 1: Tumor necrosis factor



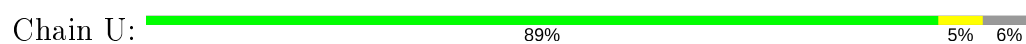
- Molecule 1: Tumor necrosis factor



- Molecule 1: Tumor necrosis factor

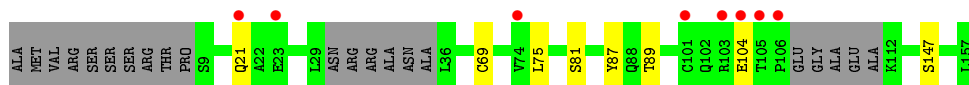
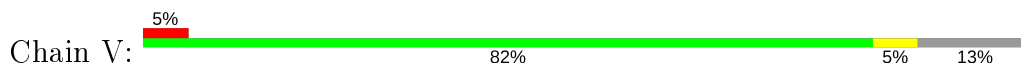


- Molecule 1: Tumor necrosis factor

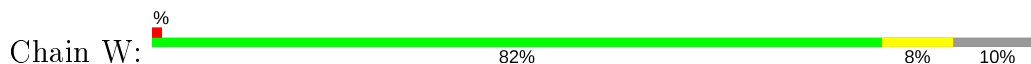




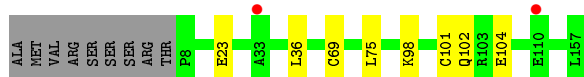
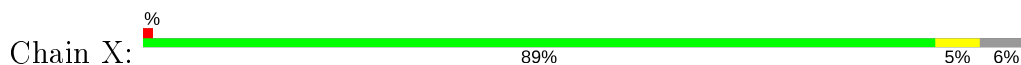
- Molecule 1: Tumor necrosis factor



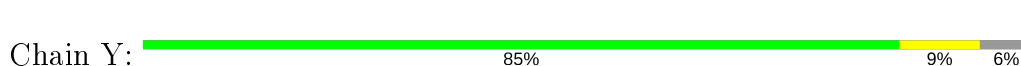
- Molecule 1: Tumor necrosis factor



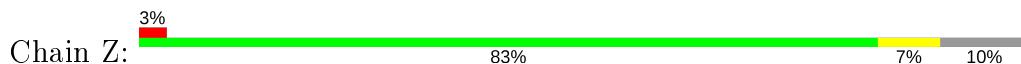
- Molecule 1: Tumor necrosis factor



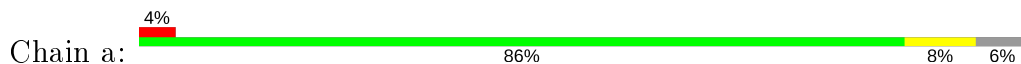
- Molecule 1: Tumor necrosis factor



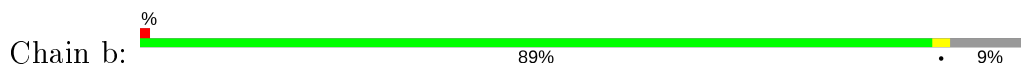
- Molecule 1: Tumor necrosis factor

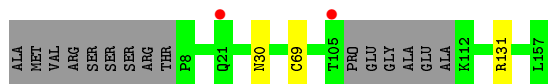


- Molecule 1: Tumor necrosis factor

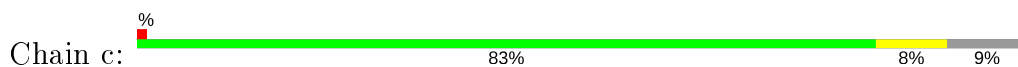


- Molecule 1: Tumor necrosis factor

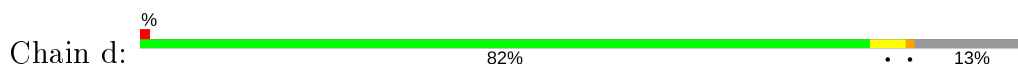




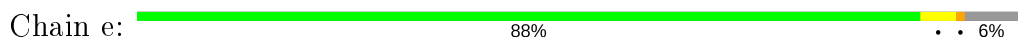
• Molecule 1: Tumor necrosis factor



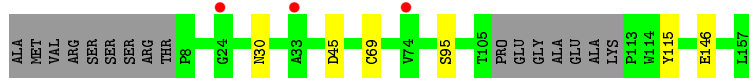
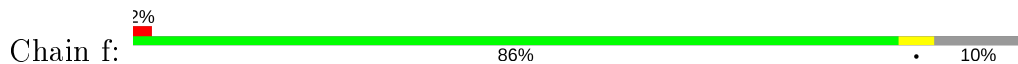
• Molecule 1: Tumor necrosis factor



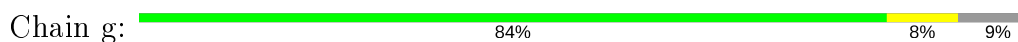
• Molecule 1: Tumor necrosis factor



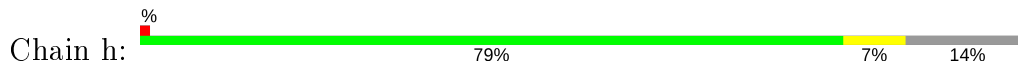
• Molecule 1: Tumor necrosis factor



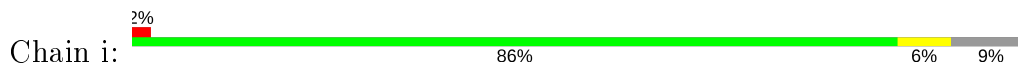
• Molecule 1: Tumor necrosis factor

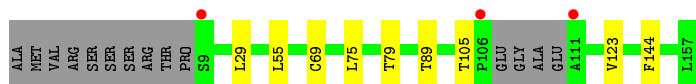


• Molecule 1: Tumor necrosis factor

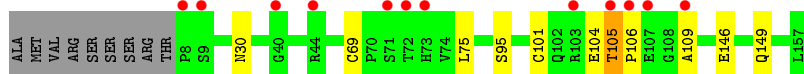
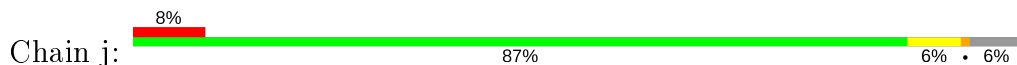


• Molecule 1: Tumor necrosis factor

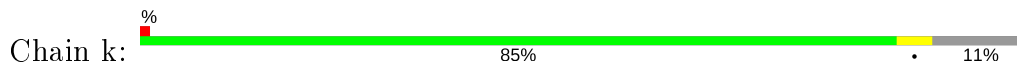




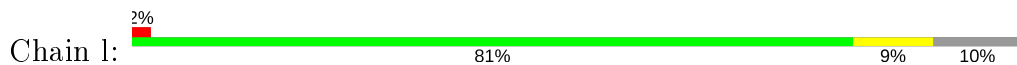
● Molecule 1: Tumor necrosis factor



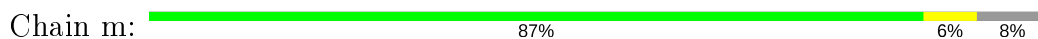
● Molecule 1: Tumor necrosis factor



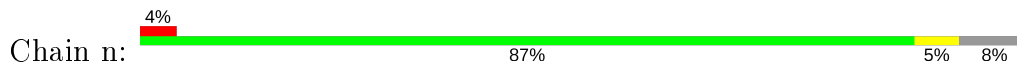
● Molecule 1: Tumor necrosis factor



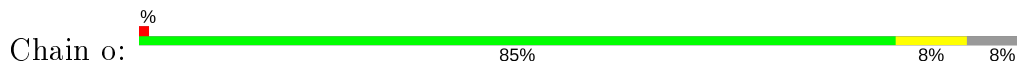
● Molecule 1: Tumor necrosis factor



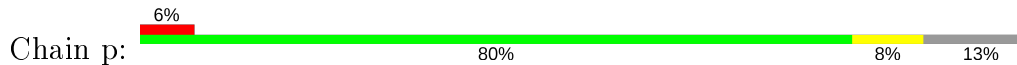
● Molecule 1: Tumor necrosis factor



● Molecule 1: Tumor necrosis factor

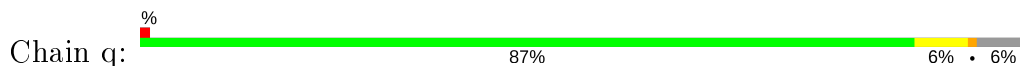


● Molecule 1: Tumor necrosis factor

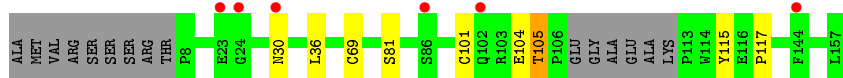
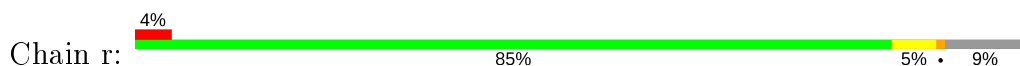




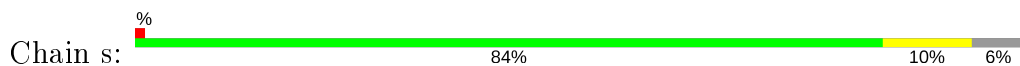
• Molecule 1: Tumor necrosis factor



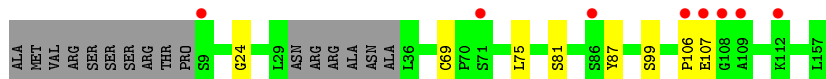
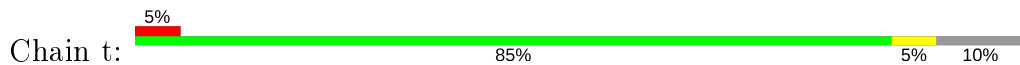
• Molecule 1: Tumor necrosis factor



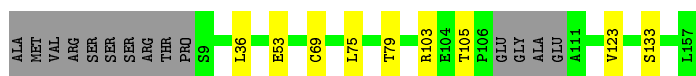
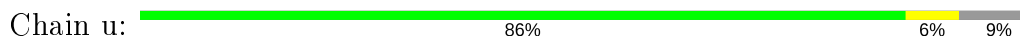
• Molecule 1: Tumor necrosis factor



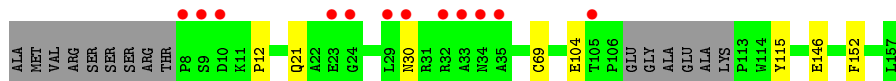
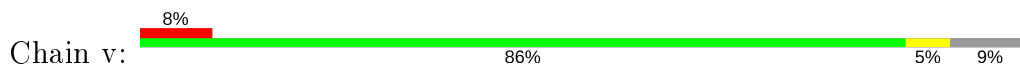
• Molecule 1: Tumor necrosis factor



• Molecule 1: Tumor necrosis factor

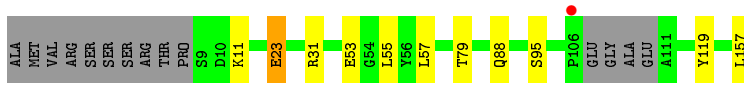


• Molecule 1: Tumor necrosis factor



● Molecule 1: Tumor necrosis factor

Chain w: %
84% 6% 9%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	104.89Å 118.35Å 186.75Å 97.57° 94.31° 98.75°	Depositor
Resolution (Å)	184.24 – 3.00 48.90 – 3.00	Depositor EDS
% Data completeness (in resolution range)	90.6 (184.24-3.00) 90.6 (48.90-3.00)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.39 (at 3.01Å)	Xtrriage
Refinement program	REFMAC 5.8.0049	Depositor
R, R_{free}	0.211 , 0.300 0.213 , 0.303	Depositor DCC
R_{free} test set	445 reflections (0.28%)	wwPDB-VP
Wilson B-factor (Å ²)	93.9	Xtrriage
Anisotropy	0.288	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 63.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	56305	wwPDB-VP
Average B, all atoms (Å ²)	114.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 16.62% 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 [i](#)

5.1 Standard geometry [i](#)

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

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	0.47	0/1128	0.69	0/1532
1	B	0.51	0/1163	0.77	0/1580
1	C	0.44	0/1171	0.67	0/1592
1	D	0.50	0/1191	0.76	1/1620 (0.1%)
1	F	0.44	0/1123	0.66	0/1526
1	G	0.47	0/1191	0.74	0/1620
1	H	0.41	0/1199	0.66	0/1631
1	I	0.44	0/1128	0.71	0/1533
1	J	0.44	0/1109	0.64	0/1507
1	K	0.47	0/1191	0.74	0/1620
1	L	0.42	0/1136	0.64	0/1544
1	M	0.46	0/1191	0.72	0/1620
1	N	0.46	0/1142	0.71	1/1553 (0.1%)
1	O	0.45	0/1164	0.72	0/1581
1	P	0.42	0/1166	0.66	0/1585
1	Q	0.45	0/1191	0.74	0/1620
1	R	0.43	0/1106	0.69	0/1502
1	S	0.50	0/1191	0.79	0/1620
1	T	0.48	0/1171	0.74	0/1592
1	U	0.48	0/1191	0.76	0/1620
1	V	0.43	0/1109	0.62	0/1507
1	W	0.49	0/1150	0.77	0/1562
1	X	0.45	0/1199	0.71	0/1631
1	Y	0.53	0/1191	0.80	1/1620 (0.1%)
1	Z	0.44	0/1142	0.67	0/1553
1	a	0.48	0/1191	0.74	0/1620
1	b	0.45	0/1158	0.71	0/1573
1	c	0.45	0/1164	0.72	0/1581
1	d	0.44	0/1109	0.68	0/1507
1	e	0.47	0/1191	0.75	0/1620
1	f	0.45	0/1149	0.64	0/1561
1	g	0.48	0/1163	0.72	0/1581

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	h	0.46	0/1101	0.68	0/1495
1	i	0.47	0/1163	0.76	0/1581
1	j	0.45	0/1199	0.65	0/1631
1	k	0.45	0/1143	0.72	0/1552
1	l	0.45	0/1142	0.72	0/1553
1	m	0.45	0/1177	0.72	0/1600
1	n	0.44	0/1180	0.64	0/1604
1	o	0.46	0/1176	0.69	0/1598
1	p	0.46	0/1114	0.70	0/1514
1	q	0.47	0/1191	0.70	0/1620
1	r	0.43	0/1157	0.64	0/1573
1	s	0.50	0/1191	0.73	0/1620
1	t	0.45	0/1142	0.65	0/1553
1	u	0.45	0/1163	0.71	0/1581
1	v	0.44	0/1157	0.65	0/1573
1	w	0.42	0/1163	0.67	0/1581
All	All	0.46	0/55718	0.71	3/75743 (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	W	0	1
1	e	0	1
All	All	0	2

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	Y	138	ARG	NE-CZ-NH1	5.36	122.98	120.30
1	D	131	ARG	NE-CZ-NH1	5.16	122.88	120.30
1	N	63	LEU	CA-CB-CG	5.00	126.80	115.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	W	100	PRO	Peptide

Continued on next page...

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Mol	Chain	Res	Type	Group
1	e	100	PRO	Peptide

5.2 Too-close contacts [i](#)

Due to software issues we are unable to calculate clashes - this section is therefore empty.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	135/159 (85%)	118 (87%)	15 (11%)	2 (2%)	10	42
1	B	141/159 (89%)	126 (89%)	14 (10%)	1 (1%)	22	60
1	C	142/159 (89%)	130 (92%)	10 (7%)	2 (1%)	11	43
1	D	147/159 (92%)	122 (83%)	21 (14%)	4 (3%)	5	26
1	F	134/159 (84%)	116 (87%)	18 (13%)	0	100	100
1	G	147/159 (92%)	136 (92%)	9 (6%)	2 (1%)	11	43
1	H	148/159 (93%)	136 (92%)	9 (6%)	3 (2%)	7	34
1	I	137/159 (86%)	126 (92%)	10 (7%)	1 (1%)	22	60
1	J	132/159 (83%)	121 (92%)	9 (7%)	2 (2%)	10	42
1	K	147/159 (92%)	128 (87%)	17 (12%)	2 (1%)	11	43
1	L	138/159 (87%)	131 (95%)	7 (5%)	0	100	100
1	M	147/159 (92%)	134 (91%)	10 (7%)	3 (2%)	7	34
1	N	139/159 (87%)	121 (87%)	16 (12%)	2 (1%)	11	43
1	O	141/159 (89%)	132 (94%)	9 (6%)	0	100	100
1	P	141/159 (89%)	129 (92%)	12 (8%)	0	100	100
1	Q	147/159 (92%)	131 (89%)	11 (8%)	5 (3%)	3	20
1	R	132/159 (83%)	123 (93%)	6 (4%)	3 (2%)	6	30

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	S	147/159 (92%)	137 (93%)	9 (6%)	1 (1%)	22	60
1	T	142/159 (89%)	135 (95%)	7 (5%)	0	100	100
1	U	147/159 (92%)	134 (91%)	12 (8%)	1 (1%)	22	60
1	V	132/159 (83%)	117 (89%)	15 (11%)	0	100	100
1	W	139/159 (87%)	133 (96%)	5 (4%)	1 (1%)	22	60
1	X	148/159 (93%)	140 (95%)	8 (5%)	0	100	100
1	Y	147/159 (92%)	131 (89%)	12 (8%)	4 (3%)	5	26
1	Z	139/159 (87%)	124 (89%)	12 (9%)	3 (2%)	6	31
1	a	147/159 (92%)	134 (91%)	13 (9%)	0	100	100
1	b	140/159 (88%)	129 (92%)	11 (8%)	0	100	100
1	c	141/159 (89%)	125 (89%)	13 (9%)	3 (2%)	7	33
1	d	132/159 (83%)	122 (92%)	9 (7%)	1 (1%)	19	57
1	e	147/159 (92%)	132 (90%)	12 (8%)	3 (2%)	7	34
1	f	139/159 (87%)	129 (93%)	10 (7%)	0	100	100
1	g	141/159 (89%)	132 (94%)	6 (4%)	3 (2%)	7	33
1	h	131/159 (82%)	121 (92%)	8 (6%)	2 (2%)	10	42
1	i	141/159 (89%)	130 (92%)	11 (8%)	0	100	100
1	j	148/159 (93%)	134 (90%)	11 (7%)	3 (2%)	7	34
1	k	138/159 (87%)	127 (92%)	9 (6%)	2 (1%)	11	43
1	l	139/159 (87%)	122 (88%)	12 (9%)	5 (4%)	3	19
1	m	143/159 (90%)	134 (94%)	8 (6%)	1 (1%)	22	60
1	n	143/159 (90%)	133 (93%)	9 (6%)	1 (1%)	22	60
1	o	143/159 (90%)	131 (92%)	8 (6%)	4 (3%)	5	25
1	p	133/159 (84%)	113 (85%)	18 (14%)	2 (2%)	10	42
1	q	147/159 (92%)	134 (91%)	10 (7%)	3 (2%)	7	34
1	r	140/159 (88%)	124 (89%)	14 (10%)	2 (1%)	11	43
1	s	147/159 (92%)	132 (90%)	9 (6%)	6 (4%)	3	16
1	t	139/159 (87%)	125 (90%)	12 (9%)	2 (1%)	11	43
1	u	141/159 (89%)	126 (89%)	15 (11%)	0	100	100
1	v	140/159 (88%)	126 (90%)	12 (9%)	2 (1%)	11	43
1	w	141/159 (89%)	124 (88%)	15 (11%)	2 (1%)	11	43

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	6777/7632 (89%)	6150 (91%)	538 (8%)	89 (1%)	12	45

All (89) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	110	GLU
1	M	105	THR
1	Q	105	THR
1	R	23	GLU
1	R	88	GLN
1	Y	105	THR
1	Y	109	ALA
1	e	107	GLU
1	e	145	ALA
1	h	21	GLN
1	k	145	ALA
1	l	147	SER
1	o	145	ALA
1	r	105	THR
1	t	24	GLY
1	t	106	PRO
1	C	144	PHE
1	J	22	ALA
1	J	51	PRO
1	M	104	GLU
1	S	23	GLU
1	U	109	ALA
1	Z	51	PRO
1	o	45	ASP
1	A	23	GLU
1	C	146	GLU
1	K	70	PRO
1	Y	11	LYS
1	c	11	LYS
1	e	110	GLU
1	j	105	THR
1	l	106	PRO
1	m	110	GLU
1	o	11	LYS
1	q	110	GLU
1	s	106	PRO
1	D	21	GLN

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Mol	Chain	Res	Type
1	D	105	THR
1	H	106	PRO
1	Y	45	ASP
1	Z	107	GLU
1	c	51	PRO
1	g	11	LYS
1	g	105	THR
1	j	106	PRO
1	j	109	ALA
1	k	11	LYS
1	l	107	GLU
1	o	105	THR
1	q	107	GLU
1	s	11	LYS
1	s	109	ALA
1	s	111	ALA
1	w	11	LYS
1	w	23	GLU
1	G	105	THR
1	G	142	LEU
1	H	108	GLY
1	I	11	LYS
1	M	11	LYS
1	N	110	GLU
1	Q	11	LYS
1	Q	106	PRO
1	c	60	SER
1	g	34	ASN
1	h	22	ALA
1	p	22	ALA
1	q	109	ALA
1	s	88	GLN
1	v	12	PRO
1	A	51	PRO
1	B	112	LYS
1	Q	88	GLN
1	W	74	VAL
1	v	146	GLU
1	N	106	PRO
1	d	105	THR
1	Z	24	GLY
1	n	106	PRO

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Mol	Chain	Res	Type
1	p	117	PRO
1	D	85	VAL
1	R	51	PRO
1	l	70	PRO
1	l	108	GLY
1	r	117	PRO
1	H	100	PRO
1	K	108	GLY
1	Q	113	PRO
1	s	108	GLY

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	120/134 (90%)	113 (94%)	7 (6%)	20 55
1	B	122/134 (91%)	115 (94%)	7 (6%)	20 56
1	C	124/134 (92%)	111 (90%)	13 (10%)	7 27
1	D	125/134 (93%)	122 (98%)	3 (2%)	49 79
1	F	120/134 (90%)	111 (92%)	9 (8%)	13 43
1	G	125/134 (93%)	112 (90%)	13 (10%)	7 27
1	H	126/134 (94%)	118 (94%)	8 (6%)	18 51
1	I	119/134 (89%)	112 (94%)	7 (6%)	19 54
1	J	119/134 (89%)	111 (93%)	8 (7%)	16 49
1	K	125/134 (93%)	109 (87%)	16 (13%)	4 19
1	L	120/134 (90%)	115 (96%)	5 (4%)	30 66
1	M	125/134 (93%)	115 (92%)	10 (8%)	12 40
1	N	121/134 (90%)	111 (92%)	10 (8%)	11 39
1	O	123/134 (92%)	113 (92%)	10 (8%)	11 40
1	P	124/134 (92%)	116 (94%)	8 (6%)	17 50
1	Q	125/134 (93%)	120 (96%)	5 (4%)	31 68

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	R	118/134 (88%)	113 (96%)	5 (4%)	30	66
1	S	125/134 (93%)	117 (94%)	8 (6%)	17	51
1	T	124/134 (92%)	112 (90%)	12 (10%)	8	31
1	U	125/134 (93%)	118 (94%)	7 (6%)	21	56
1	V	119/134 (89%)	111 (93%)	8 (7%)	16	49
1	W	122/134 (91%)	112 (92%)	10 (8%)	11	39
1	X	126/134 (94%)	118 (94%)	8 (6%)	18	51
1	Y	125/134 (93%)	116 (93%)	9 (7%)	14	45
1	Z	121/134 (90%)	113 (93%)	8 (7%)	16	49
1	a	125/134 (93%)	112 (90%)	13 (10%)	7	27
1	b	123/134 (92%)	120 (98%)	3 (2%)	49	79
1	c	123/134 (92%)	113 (92%)	10 (8%)	11	40
1	d	119/134 (89%)	112 (94%)	7 (6%)	19	54
1	e	125/134 (93%)	118 (94%)	7 (6%)	21	56
1	f	122/134 (91%)	116 (95%)	6 (5%)	25	61
1	g	123/134 (92%)	114 (93%)	9 (7%)	14	44
1	h	118/134 (88%)	109 (92%)	9 (8%)	13	43
1	i	123/134 (92%)	114 (93%)	9 (7%)	14	44
1	j	126/134 (94%)	117 (93%)	9 (7%)	14	46
1	k	121/134 (90%)	116 (96%)	5 (4%)	30	67
1	l	121/134 (90%)	111 (92%)	10 (8%)	11	39
1	m	124/134 (92%)	116 (94%)	8 (6%)	17	50
1	n	125/134 (93%)	118 (94%)	7 (6%)	21	56
1	o	124/134 (92%)	116 (94%)	8 (6%)	17	50
1	p	119/134 (89%)	109 (92%)	10 (8%)	11	38
1	q	125/134 (93%)	117 (94%)	8 (6%)	17	51
1	r	123/134 (92%)	115 (94%)	8 (6%)	17	50
1	s	125/134 (93%)	116 (93%)	9 (7%)	14	45
1	t	121/134 (90%)	115 (95%)	6 (5%)	24	60
1	u	123/134 (92%)	114 (93%)	9 (7%)	14	44
1	v	123/134 (92%)	117 (95%)	6 (5%)	25	61

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	w	123/134 (92%)	113 (92%)	10 (8%)	11	40
All	All	5892/6432 (92%)	5492 (93%)	400 (7%)	16	48

All (400) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	13	VAL
1	A	34	ASN
1	A	69	CYS
1	A	81	SER
1	A	87	TYR
1	A	101	CYS
1	A	119	TYR
1	B	39	ASN
1	B	57	LEU
1	B	104	GLU
1	B	119	TYR
1	B	133	SER
1	B	151	TYR
1	B	157	LEU
1	C	17	VAL
1	C	30	ASN
1	C	55	LEU
1	C	67	GLN
1	C	69	CYS
1	C	86	SER
1	C	89	THR
1	C	99	SER
1	C	102	GLN
1	C	104	GLU
1	C	144	PHE
1	C	147	SER
1	C	149	GLN
1	D	53	GLU
1	D	81	SER
1	D	83	ILE
1	F	21	GLN
1	F	36	LEU
1	F	63	LEU
1	F	69	CYS
1	F	75	LEU
1	F	81	SER

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Mol	Chain	Res	Type
1	F	101	CYS
1	F	104	GLU
1	F	110	GLU
1	G	10	ASP
1	G	55	LEU
1	G	57	LEU
1	G	69	CYS
1	G	75	LEU
1	G	79	THR
1	G	81	SER
1	G	89	THR
1	G	104	GLU
1	G	123	VAL
1	G	133	SER
1	G	135	GLU
1	G	144	PHE
1	H	53	GLU
1	H	57	LEU
1	H	69	CYS
1	H	73	HIS
1	H	86	SER
1	H	88	GLN
1	H	107	GLU
1	H	115	TYR
1	I	23	GLU
1	I	32	ARG
1	I	53	GLU
1	I	81	SER
1	I	119	TYR
1	I	123	VAL
1	I	144	PHE
1	J	36	LEU
1	J	53	GLU
1	J	69	CYS
1	J	75	LEU
1	J	87	TYR
1	J	89	THR
1	J	105	THR
1	J	147	SER
1	K	17	VAL
1	K	29	LEU
1	K	32	ARG

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Mol	Chain	Res	Type
1	K	36	LEU
1	K	53	GLU
1	K	55	LEU
1	K	57	LEU
1	K	69	CYS
1	K	75	LEU
1	K	81	SER
1	K	86	SER
1	K	101	CYS
1	K	103	ARG
1	K	123	VAL
1	K	133	SER
1	K	154	ILE
1	L	10	ASP
1	L	53	GLU
1	L	75	LEU
1	L	81	SER
1	L	131	ARG
1	M	19	ASN
1	M	29	LEU
1	M	32	ARG
1	M	53	GLU
1	M	79	THR
1	M	83	ILE
1	M	95	SER
1	M	123	VAL
1	M	142	LEU
1	M	144	PHE
1	N	21	GLN
1	N	23	GLU
1	N	25	GLN
1	N	53	GLU
1	N	69	CYS
1	N	75	LEU
1	N	81	SER
1	N	95	SER
1	N	104	GLU
1	N	105	THR
1	O	53	GLU
1	O	57	LEU
1	O	69	CYS
1	O	75	LEU

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Mol	Chain	Res	Type
1	O	79	THR
1	O	89	THR
1	O	95	SER
1	O	143	ASP
1	O	144	PHE
1	O	157	LEU
1	P	10	ASP
1	P	13	VAL
1	P	30	ASN
1	P	57	LEU
1	P	69	CYS
1	P	98	LYS
1	P	103	ARG
1	P	104	GLU
1	Q	9	SER
1	Q	32	ARG
1	Q	79	THR
1	Q	86	SER
1	Q	144	PHE
1	R	44	ARG
1	R	63	LEU
1	R	69	CYS
1	R	75	LEU
1	R	147	SER
1	S	53	GLU
1	S	57	LEU
1	S	69	CYS
1	S	75	LEU
1	S	81	SER
1	S	89	THR
1	S	107	GLU
1	S	157	LEU
1	T	30	ASN
1	T	34	ASN
1	T	36	LEU
1	T	63	LEU
1	T	69	CYS
1	T	75	LEU
1	T	87	TYR
1	T	98	LYS
1	T	101	CYS
1	T	104	GLU

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Mol	Chain	Res	Type
1	T	130	ASP
1	T	131	ARG
1	U	45	ASP
1	U	53	GLU
1	U	57	LEU
1	U	79	THR
1	U	95	SER
1	U	123	VAL
1	U	144	PHE
1	V	21	GLN
1	V	69	CYS
1	V	75	LEU
1	V	81	SER
1	V	87	TYR
1	V	89	THR
1	V	104	GLU
1	V	147	SER
1	W	17	VAL
1	W	21	GLN
1	W	36	LEU
1	W	53	GLU
1	W	57	LEU
1	W	72	THR
1	W	88	GLN
1	W	89	THR
1	W	133	SER
1	W	157	LEU
1	X	23	GLU
1	X	36	LEU
1	X	69	CYS
1	X	75	LEU
1	X	98	LYS
1	X	101	CYS
1	X	102	GLN
1	X	104	GLU
1	Y	31	ARG
1	Y	36	LEU
1	Y	43	LEU
1	Y	53	GLU
1	Y	75	LEU
1	Y	79	THR
1	Y	95	SER

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Mol	Chain	Res	Type
1	Y	119	TYR
1	Y	123	VAL
1	Z	16	VAL
1	Z	21	GLN
1	Z	36	LEU
1	Z	69	CYS
1	Z	86	SER
1	Z	89	THR
1	Z	99	SER
1	Z	104	GLU
1	a	13	VAL
1	a	21	GLN
1	a	36	LEU
1	a	57	LEU
1	a	75	LEU
1	a	89	THR
1	a	101	CYS
1	a	105	THR
1	a	119	TYR
1	a	123	VAL
1	a	133	SER
1	a	144	PHE
1	a	157	LEU
1	b	30	ASN
1	b	69	CYS
1	b	131	ARG
1	c	13	VAL
1	c	21	GLN
1	c	30	ASN
1	c	36	LEU
1	c	53	GLU
1	c	86	SER
1	c	88	GLN
1	c	95	SER
1	c	133	SER
1	c	144	PHE
1	d	53	GLU
1	d	65	LYS
1	d	69	CYS
1	d	75	LEU
1	d	81	SER
1	d	88	GLN

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Mol	Chain	Res	Type
1	d	105	THR
1	e	17	VAL
1	e	53	GLU
1	e	75	LEU
1	e	79	THR
1	e	89	THR
1	e	107	GLU
1	e	110	GLU
1	f	30	ASN
1	f	45	ASP
1	f	69	CYS
1	f	95	SER
1	f	115	TYR
1	f	146	GLU
1	g	31	ARG
1	g	53	GLU
1	g	57	LEU
1	g	75	LEU
1	g	79	THR
1	g	95	SER
1	g	123	VAL
1	g	144	PHE
1	g	147	SER
1	h	23	GLU
1	h	53	GLU
1	h	55	LEU
1	h	69	CYS
1	h	86	SER
1	h	101	CYS
1	h	102	GLN
1	h	104	GLU
1	h	135	GLU
1	i	29	LEU
1	i	55	LEU
1	i	69	CYS
1	i	75	LEU
1	i	79	THR
1	i	89	THR
1	i	105	THR
1	i	123	VAL
1	i	144	PHE
1	j	30	ASN

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Mol	Chain	Res	Type
1	j	69	CYS
1	j	75	LEU
1	j	95	SER
1	j	101	CYS
1	j	104	GLU
1	j	105	THR
1	j	146	GLU
1	j	149	GLN
1	k	17	VAL
1	k	31	ARG
1	k	79	THR
1	k	95	SER
1	k	119	TYR
1	l	23	GLU
1	l	36	LEU
1	l	63	LEU
1	l	75	LEU
1	l	89	THR
1	l	95	SER
1	l	99	SER
1	l	102	GLN
1	l	104	GLU
1	l	144	PHE
1	m	17	VAL
1	m	32	ARG
1	m	57	LEU
1	m	75	LEU
1	m	89	THR
1	m	101	CYS
1	m	104	GLU
1	m	123	VAL
1	n	10	ASP
1	n	57	LEU
1	n	69	CYS
1	n	75	LEU
1	n	95	SER
1	n	104	GLU
1	n	149	GLN
1	o	23	GLU
1	o	31	ARG
1	o	53	GLU
1	o	79	THR

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Mol	Chain	Res	Type
1	o	89	THR
1	o	107	GLU
1	o	119	TYR
1	o	125	GLN
1	p	53	GLU
1	p	67	GLN
1	p	69	CYS
1	p	75	LEU
1	p	88	GLN
1	p	89	THR
1	p	101	CYS
1	p	102	GLN
1	p	104	GLU
1	p	119	TYR
1	q	17	VAL
1	q	53	GLU
1	q	69	CYS
1	q	75	LEU
1	q	82	ARG
1	q	89	THR
1	q	104	GLU
1	q	107	GLU
1	r	30	ASN
1	r	36	LEU
1	r	69	CYS
1	r	81	SER
1	r	101	CYS
1	r	104	GLU
1	r	105	THR
1	r	115	TYR
1	s	10	ASP
1	s	17	VAL
1	s	27	GLN
1	s	30	ASN
1	s	57	LEU
1	s	95	SER
1	s	105	THR
1	s	112	LYS
1	s	144	PHE
1	t	69	CYS
1	t	75	LEU
1	t	81	SER

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Mol	Chain	Res	Type
1	t	87	TYR
1	t	99	SER
1	t	107	GLU
1	u	36	LEU
1	u	53	GLU
1	u	69	CYS
1	u	75	LEU
1	u	79	THR
1	u	103	ARG
1	u	105	THR
1	u	123	VAL
1	u	133	SER
1	v	21	GLN
1	v	30	ASN
1	v	69	CYS
1	v	104	GLU
1	v	115	TYR
1	v	152	PHE
1	w	23	GLU
1	w	31	ARG
1	w	53	GLU
1	w	55	LEU
1	w	57	LEU
1	w	79	THR
1	w	88	GLN
1	w	95	SER
1	w	119	TYR
1	w	157	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	L	125	GLN
1	T	39	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

46 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	JNI	v	201	-	44,44,44	0.91	2 (4%)	58,60,60	2.69	21 (36%)
2	JNI	Z	201	-	44,44,44	0.92	2 (4%)	58,60,60	2.46	18 (31%)
2	JNI	N	201	-	44,44,44	0.78	2 (4%)	58,60,60	2.29	17 (29%)
2	JNI	J	202	-	44,44,44	0.86	2 (4%)	58,60,60	2.41	17 (29%)
2	JNI	t	201	-	44,44,44	1.01	2 (4%)	58,60,60	2.61	20 (34%)
2	JNI	r	201	-	44,44,44	0.91	2 (4%)	58,60,60	2.53	21 (36%)
2	JNI	F	201	-	44,44,44	0.96	1 (2%)	58,60,60	2.44	18 (31%)
2	JNI	j	201	-	44,44,44	1.08	3 (6%)	58,60,60	3.02	22 (37%)
2	JNI	F	202	-	44,44,44	0.86	2 (4%)	58,60,60	2.39	19 (32%)
2	JNI	Z	202	-	44,44,44	0.96	2 (4%)	58,60,60	2.52	22 (37%)
2	JNI	C	202	-	44,44,44	0.80	2 (4%)	58,60,60	2.68	19 (32%)
2	JNI	P	202	-	44,44,44	0.79	2 (4%)	58,60,60	2.37	16 (27%)
2	JNI	t	202	-	44,44,44	0.98	2 (4%)	58,60,60	2.71	22 (37%)
2	JNI	V	202	-	44,44,44	1.00	2 (4%)	58,60,60	2.77	18 (31%)
2	JNI	H	202	-	44,44,44	1.36	6 (13%)	58,60,60	3.27	26 (44%)
2	JNI	n	201	-	44,44,44	1.03	2 (4%)	58,60,60	2.76	23 (39%)
2	JNI	j	202	-	44,44,44	1.13	2 (4%)	58,60,60	3.00	25 (43%)
2	JNI	f	201	-	44,44,44	1.04	4 (9%)	58,60,60	2.89	22 (37%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	JNI	b	202	-	44,44,44	1.41	8 (18%)	58,60,60	2.91	26 (44%)
2	JNI	f	202	-	44,44,44	0.91	2 (4%)	58,60,60	2.40	16 (27%)
2	JNI	C	201	-	44,44,44	0.83	2 (4%)	58,60,60	2.67	24 (41%)
2	JNI	b	201	-	44,44,44	1.09	5 (11%)	58,60,60	2.90	22 (37%)
2	JNI	p	202	-	44,44,44	0.91	2 (4%)	58,60,60	2.65	25 (43%)
2	JNI	r	202	-	44,44,44	1.25	5 (11%)	58,60,60	2.91	28 (48%)
2	JNI	v	202	-	44,44,44	1.15	3 (6%)	58,60,60	2.85	21 (36%)
2	JNI	P	201	-	44,44,44	0.81	1 (2%)	58,60,60	2.37	18 (31%)
2	JNI	h	202	-	44,44,44	1.11	4 (9%)	58,60,60	2.73	19 (32%)
2	JNI	Q	201	-	44,44,44	0.84	2 (4%)	58,60,60	2.62	16 (27%)
2	JNI	n	202	-	44,44,44	1.09	4 (9%)	58,60,60	2.89	25 (43%)
2	JNI	H	201	-	44,44,44	0.96	2 (4%)	58,60,60	2.58	15 (25%)
2	JNI	L	201	-	44,44,44	1.42	8 (18%)	58,60,60	3.33	28 (48%)
2	JNI	M	201	-	44,44,44	0.91	2 (4%)	58,60,60	2.77	18 (31%)
2	JNI	D	201	-	44,44,44	0.83	2 (4%)	58,60,60	2.57	17 (29%)
2	JNI	X	201	-	44,44,44	1.02	4 (9%)	58,60,60	2.94	22 (37%)
2	JNI	V	201	-	44,44,44	0.99	3 (6%)	58,60,60	2.41	17 (29%)
2	JNI	A	202	-	44,44,44	0.86	2 (4%)	58,60,60	2.48	20 (34%)
2	JNI	p	201	-	44,44,44	0.94	2 (4%)	58,60,60	2.46	15 (25%)
2	JNI	R	201	-	44,44,44	1.14	2 (4%)	58,60,60	2.80	22 (37%)
2	JNI	U	201	-	44,44,44	1.15	5 (11%)	58,60,60	2.94	21 (36%)
2	JNI	h	201	-	44,44,44	1.15	5 (11%)	58,60,60	2.93	23 (39%)
2	JNI	l	201	-	44,44,44	1.10	4 (9%)	58,60,60	2.61	23 (39%)
2	JNI	o	201	-	44,44,44	0.90	3 (6%)	58,60,60	2.77	18 (31%)
2	JNI	J	201	-	44,44,44	0.90	2 (4%)	58,60,60	2.41	16 (27%)
2	JNI	X	202	-	44,44,44	1.23	4 (9%)	58,60,60	2.96	26 (44%)
2	JNI	A	201	-	44,44,44	0.85	2 (4%)	58,60,60	2.42	17 (29%)
2	JNI	d	201	-	44,44,44	0.94	2 (4%)	58,60,60	2.63	21 (36%)

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	JNI	v	201	-	-	8/24/32/32	0/6/6/6

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	JNI	Z	201	-	-	2/24/32/32	0/6/6/6
2	JNI	N	201	-	-	1/24/32/32	0/6/6/6
2	JNI	J	202	-	-	11/24/32/32	0/6/6/6
2	JNI	t	201	-	-	2/24/32/32	0/6/6/6
2	JNI	r	201	-	-	8/24/32/32	0/6/6/6
2	JNI	F	201	-	-	4/24/32/32	0/6/6/6
2	JNI	j	201	-	-	3/24/32/32	0/6/6/6
2	JNI	F	202	-	-	11/24/32/32	0/6/6/6
2	JNI	Z	202	-	-	10/24/32/32	0/6/6/6
2	JNI	C	202	-	-	10/24/32/32	0/6/6/6
2	JNI	P	202	-	-	14/24/32/32	0/6/6/6
2	JNI	t	202	-	-	10/24/32/32	0/6/6/6
2	JNI	V	202	-	-	10/24/32/32	0/6/6/6
2	JNI	H	202	-	-	4/24/32/32	0/6/6/6
2	JNI	n	201	-	-	10/24/32/32	0/6/6/6
2	JNI	j	202	-	-	18/24/32/32	0/6/6/6
2	JNI	f	201	-	-	6/24/32/32	0/6/6/6
2	JNI	b	202	-	-	12/24/32/32	0/6/6/6
2	JNI	f	202	-	-	8/24/32/32	0/6/6/6
2	JNI	C	201	-	-	11/24/32/32	0/6/6/6
2	JNI	b	201	-	-	4/24/32/32	0/6/6/6
2	JNI	p	202	-	-	13/24/32/32	0/6/6/6
2	JNI	r	202	-	-	12/24/32/32	0/6/6/6
2	JNI	v	202	-	-	9/24/32/32	1/6/6/6
2	JNI	P	201	-	-	6/24/32/32	0/6/6/6
2	JNI	h	202	-	-	8/24/32/32	0/6/6/6
2	JNI	Q	201	-	-	5/24/32/32	0/6/6/6
2	JNI	n	202	-	-	16/24/32/32	0/6/6/6
2	JNI	H	201	-	-	6/24/32/32	0/6/6/6
2	JNI	L	201	-	-	4/24/32/32	0/6/6/6
2	JNI	M	201	-	-	5/24/32/32	0/6/6/6
2	JNI	D	201	-	-	2/24/32/32	0/6/6/6
2	JNI	X	201	-	-	5/24/32/32	0/6/6/6
2	JNI	V	201	-	-	7/24/32/32	0/6/6/6

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	JNI	A	202	-	-	8/24/32/32	0/6/6/6
2	JNI	p	201	-	-	6/24/32/32	0/6/6/6
2	JNI	R	201	-	-	2/24/32/32	0/6/6/6
2	JNI	U	201	-	-	6/24/32/32	0/6/6/6
2	JNI	h	201	-	-	2/24/32/32	0/6/6/6
2	JNI	l	201	-	-	4/24/32/32	0/6/6/6
2	JNI	o	201	-	-	8/24/32/32	0/6/6/6
2	JNI	J	201	-	-	2/24/32/32	0/6/6/6
2	JNI	X	202	-	-	11/24/32/32	0/6/6/6
2	JNI	A	201	-	-	2/24/32/32	0/6/6/6
2	JNI	d	201	-	-	4/24/32/32	0/6/6/6

All (134) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	L	201	JNI	C31-N34	4.08	1.43	1.35
2	j	202	JNI	C2-N1	3.57	1.41	1.33
2	V	202	JNI	C31-N34	3.44	1.42	1.35
2	t	202	JNI	C31-N34	3.34	1.41	1.35
2	r	202	JNI	C2-N1	3.31	1.40	1.33
2	b	202	JNI	C21-C16	3.30	1.45	1.41
2	H	202	JNI	C31-N34	3.27	1.41	1.35
2	j	202	JNI	C21-C16	3.25	1.45	1.41
2	h	202	JNI	C31-N34	3.21	1.41	1.35
2	b	202	JNI	C2-N1	3.17	1.40	1.33
2	n	201	JNI	C31-N34	3.13	1.41	1.35
2	Z	202	JNI	C31-N34	3.11	1.41	1.35
2	H	202	JNI	C21-C16	3.10	1.45	1.41
2	f	201	JNI	C31-N34	3.10	1.41	1.35
2	v	202	JNI	C31-N34	3.06	1.41	1.35
2	b	202	JNI	C21-C22	3.04	1.54	1.49
2	o	201	JNI	C2-N1	3.00	1.39	1.33
2	H	202	JNI	C2-N1	3.00	1.39	1.33
2	n	201	JNI	C2-N1	2.97	1.39	1.33
2	j	201	JNI	C21-C16	2.96	1.44	1.41
2	U	201	JNI	C31-N34	2.95	1.41	1.35
2	r	202	JNI	C21-C16	2.94	1.44	1.41
2	H	201	JNI	C31-N34	2.90	1.41	1.35
2	X	202	JNI	C2-N1	2.88	1.39	1.33
2	j	201	JNI	C2-N1	2.88	1.39	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	b	202	JNI	C31-N34	2.87	1.41	1.35
2	b	201	JNI	C2-N1	2.86	1.39	1.33
2	b	201	JNI	C21-C16	2.82	1.44	1.41
2	h	201	JNI	C31-N34	2.81	1.41	1.35
2	U	201	JNI	C39-N34	2.81	1.51	1.46
2	M	201	JNI	C2-N1	2.78	1.39	1.33
2	l	201	JNI	C31-N34	2.78	1.40	1.35
2	n	202	JNI	C2-N1	2.77	1.39	1.33
2	L	201	JNI	C21-C22	2.77	1.54	1.49
2	L	201	JNI	C21-C16	2.76	1.44	1.41
2	X	201	JNI	C2-N1	2.73	1.39	1.33
2	Q	201	JNI	C2-N1	2.72	1.39	1.33
2	v	202	JNI	C21-C16	2.69	1.44	1.41
2	X	202	JNI	C31-N34	2.69	1.40	1.35
2	v	202	JNI	C2-N1	2.68	1.39	1.33
2	h	201	JNI	C21-C16	2.68	1.44	1.41
2	t	201	JNI	C31-N34	2.66	1.40	1.35
2	p	202	JNI	C2-N1	2.64	1.39	1.33
2	h	202	JNI	C2-N1	2.63	1.39	1.33
2	p	201	JNI	C31-N34	2.63	1.40	1.35
2	J	201	JNI	C31-N34	2.62	1.40	1.35
2	U	201	JNI	C33-C28	2.58	1.44	1.39
2	F	202	JNI	C31-N34	2.58	1.40	1.35
2	R	201	JNI	C31-N34	2.58	1.40	1.35
2	b	201	JNI	C31-N34	2.57	1.40	1.35
2	l	201	JNI	C27-C22	2.56	1.44	1.39
2	d	201	JNI	C2-N1	2.55	1.39	1.33
2	D	201	JNI	C2-N1	2.55	1.39	1.33
2	X	202	JNI	C21-C16	2.54	1.44	1.41
2	X	201	JNI	C31-N34	2.53	1.40	1.35
2	Z	202	JNI	C2-N1	2.52	1.38	1.33
2	p	202	JNI	C31-N34	2.52	1.40	1.35
2	v	201	JNI	C2-N1	2.52	1.38	1.33
2	t	202	JNI	C2-N1	2.51	1.38	1.33
2	n	202	JNI	C21-C16	2.51	1.44	1.41
2	L	201	JNI	C27-C22	2.51	1.44	1.39
2	r	201	JNI	C2-N1	2.48	1.38	1.33
2	r	202	JNI	C31-N34	2.48	1.40	1.35
2	H	202	JNI	C27-C22	2.47	1.44	1.39
2	V	202	JNI	C2-N1	2.46	1.38	1.33
2	J	202	JNI	C2-N1	2.46	1.38	1.33
2	h	202	JNI	C21-C16	2.46	1.44	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	202	JNI	C31-N34	2.46	1.40	1.35
2	r	202	JNI	C21-C22	2.45	1.53	1.49
2	t	201	JNI	C39-N34	2.45	1.50	1.46
2	f	202	JNI	C2-N1	2.44	1.38	1.33
2	C	201	JNI	C2-N1	2.42	1.38	1.33
2	L	201	JNI	C27-C26	2.40	1.43	1.39
2	f	202	JNI	C31-N34	2.39	1.40	1.35
2	h	201	JNI	C39-N34	2.39	1.50	1.46
2	H	201	JNI	C2-N1	2.38	1.38	1.33
2	j	201	JNI	C31-N34	2.38	1.40	1.35
2	P	201	JNI	C2-N1	2.38	1.38	1.33
2	f	201	JNI	C21-C16	2.37	1.44	1.41
2	X	201	JNI	C39-N34	2.37	1.50	1.46
2	v	201	JNI	C21-C16	2.34	1.44	1.41
2	L	201	JNI	C2-N1	2.33	1.38	1.33
2	J	201	JNI	C2-N1	2.33	1.38	1.33
2	M	201	JNI	C31-N34	2.32	1.40	1.35
2	b	202	JNI	C27-C22	2.32	1.43	1.39
2	P	202	JNI	C2-N1	2.31	1.38	1.33
2	C	202	JNI	C2-N1	2.29	1.38	1.33
2	X	202	JNI	C27-C26	2.29	1.43	1.39
2	b	202	JNI	C20-C21	2.28	1.43	1.40
2	H	202	JNI	C27-C26	2.28	1.43	1.39
2	P	202	JNI	C2-N3	-2.28	1.32	1.35
2	A	202	JNI	C2-N3	-2.28	1.32	1.35
2	r	201	JNI	C31-N34	2.28	1.40	1.35
2	A	202	JNI	C2-N1	2.28	1.38	1.33
2	L	201	JNI	C35-C36	2.28	1.56	1.51
2	N	201	JNI	C2-N3	-2.28	1.32	1.35
2	J	202	JNI	C31-N34	2.27	1.40	1.35
2	U	201	JNI	C2-N1	2.26	1.38	1.33
2	R	201	JNI	C2-N1	2.25	1.38	1.33
2	V	201	JNI	C2-N1	2.24	1.38	1.33
2	V	201	JNI	C21-C16	2.23	1.43	1.41
2	A	201	JNI	C2-N1	2.22	1.38	1.33
2	h	201	JNI	C2-N1	2.21	1.38	1.33
2	p	201	JNI	C2-N1	2.19	1.38	1.33
2	h	201	JNI	C27-C22	2.17	1.43	1.39
2	r	202	JNI	C20-C21	2.16	1.43	1.40
2	n	202	JNI	C21-C22	2.16	1.53	1.49
2	A	201	JNI	C2-N3	-2.15	1.32	1.35
2	o	201	JNI	C31-N34	2.15	1.39	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	202	JNI	C2-N1	2.13	1.38	1.33
2	h	202	JNI	C35-N34	2.13	1.50	1.46
2	l	201	JNI	C2-N1	2.12	1.38	1.33
2	C	201	JNI	C2-N3	-2.12	1.32	1.35
2	b	202	JNI	C33-C28	2.11	1.43	1.39
2	b	201	JNI	C33-C28	2.11	1.43	1.39
2	L	201	JNI	C20-C21	2.10	1.43	1.40
2	n	202	JNI	C27-C26	2.09	1.43	1.39
2	b	201	JNI	C27-C26	2.09	1.43	1.39
2	Z	201	JNI	C2-N1	2.09	1.38	1.33
2	U	201	JNI	C21-C16	2.09	1.43	1.41
2	D	201	JNI	C2-N3	-2.07	1.32	1.35
2	o	201	JNI	C21-C16	2.07	1.43	1.41
2	H	202	JNI	C9-N8	2.07	1.50	1.47
2	b	202	JNI	C27-C26	2.06	1.43	1.39
2	f	201	JNI	C2-N1	2.06	1.38	1.33
2	V	201	JNI	C31-N34	2.06	1.39	1.35
2	d	201	JNI	C31-N34	2.06	1.39	1.35
2	F	201	JNI	C31-N34	2.05	1.39	1.35
2	X	201	JNI	C33-C28	2.04	1.43	1.39
2	Z	201	JNI	C31-N34	2.03	1.39	1.35
2	f	201	JNI	C2-N7	-2.03	1.31	1.35
2	l	201	JNI	C21-C22	2.02	1.53	1.49
2	N	201	JNI	C2-N1	2.01	1.37	1.33
2	Q	201	JNI	C2-N3	-2.01	1.32	1.35

All (945) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	M	201	JNI	C2-N7-C6	10.33	124.05	116.73
2	U	201	JNI	C2-N7-C6	10.29	124.02	116.73
2	j	201	JNI	C2-N7-C6	10.28	124.01	116.73
2	X	201	JNI	C2-N7-C6	9.84	123.70	116.73
2	b	201	JNI	C2-N7-C6	9.83	123.69	116.73
2	L	201	JNI	C33-N32-C31	9.77	124.30	115.64
2	v	201	JNI	C2-N7-C6	9.64	123.56	116.73
2	h	202	JNI	C2-N7-C6	9.63	123.55	116.73
2	o	201	JNI	C2-N7-C6	9.48	123.44	116.73
2	X	202	JNI	C2-N7-C6	9.01	123.11	116.73
2	H	202	JNI	C33-N32-C31	8.86	123.49	115.64
2	b	201	JNI	C29-N30-C31	8.83	123.47	115.64
2	U	201	JNI	C29-N30-C31	8.75	123.39	115.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L	201	JNI	C2-N7-C6	8.71	122.90	116.73
2	f	201	JNI	C2-N7-C6	8.65	122.86	116.73
2	t	201	JNI	C33-N32-C31	8.56	123.23	115.64
2	J	201	JNI	C33-N32-C31	8.51	123.19	115.64
2	h	201	JNI	C39-N34-C31	-8.42	107.73	121.69
2	v	202	JNI	C33-N32-C31	8.36	123.05	115.64
2	n	202	JNI	C2-N7-C6	8.34	122.64	116.73
2	F	201	JNI	C2-N7-C6	8.30	122.61	116.73
2	L	201	JNI	C29-N30-C31	8.19	122.90	115.64
2	X	201	JNI	C29-N30-C31	8.17	122.88	115.64
2	t	202	JNI	C29-N30-C31	8.15	122.86	115.64
2	r	201	JNI	C2-N7-C6	8.15	122.50	116.73
2	j	202	JNI	N7-C6-N8	8.13	123.51	115.77
2	v	202	JNI	C2-N7-C6	8.11	122.47	116.73
2	f	201	JNI	C29-N30-C31	8.10	122.82	115.64
2	R	201	JNI	C33-N32-C31	8.09	122.81	115.64
2	H	202	JNI	C29-N30-C31	8.08	122.80	115.64
2	d	201	JNI	C33-N32-C31	8.07	122.79	115.64
2	Q	201	JNI	C39-N34-C31	-8.06	108.33	121.69
2	H	201	JNI	C29-N30-C31	8.06	122.78	115.64
2	V	202	JNI	C29-N30-C31	8.03	122.75	115.64
2	h	201	JNI	C29-N30-C31	8.02	122.75	115.64
2	Z	202	JNI	C33-N32-C31	7.99	122.73	115.64
2	H	202	JNI	C2-N7-C6	7.90	122.33	116.73
2	V	202	JNI	C33-N32-C31	7.88	122.62	115.64
2	v	202	JNI	C29-N30-C31	7.86	122.61	115.64
2	h	202	JNI	C29-N30-C31	7.82	122.57	115.64
2	p	201	JNI	C2-N7-C6	7.82	122.27	116.73
2	r	202	JNI	C2-N7-C6	7.81	122.26	116.73
2	j	202	JNI	C2-N7-C6	7.80	122.25	116.73
2	Q	201	JNI	C29-N30-C31	7.79	122.54	115.64
2	n	201	JNI	C29-N30-C31	7.77	122.53	115.64
2	t	202	JNI	C33-N32-C31	7.76	122.52	115.64
2	F	201	JNI	C33-N32-C31	7.73	122.49	115.64
2	H	202	JNI	N30-C31-N34	7.72	125.26	116.90
2	D	201	JNI	C39-N34-C31	-7.69	108.95	121.69
2	n	201	JNI	C33-N32-C31	7.65	122.42	115.64
2	o	201	JNI	C29-N30-C31	7.65	122.42	115.64
2	Z	201	JNI	C2-N7-C6	7.60	122.11	116.73
2	b	202	JNI	C29-N30-C31	7.59	122.36	115.64
2	b	202	JNI	C2-N7-C6	7.57	122.09	116.73
2	j	201	JNI	C33-N32-C31	7.55	122.33	115.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	202	JNI	C33-N32-C31	7.55	122.33	115.64
2	f	201	JNI	C33-N32-C31	7.54	122.33	115.64
2	p	202	JNI	C29-N30-C31	7.54	122.33	115.64
2	V	201	JNI	C33-N32-C31	7.46	122.25	115.64
2	h	201	JNI	C2-N7-C6	7.46	122.01	116.73
2	H	202	JNI	C39-N34-C31	-7.45	109.34	121.69
2	h	202	JNI	C33-N32-C31	7.41	122.21	115.64
2	M	201	JNI	C29-N30-C31	7.39	122.19	115.64
2	H	201	JNI	C33-N32-C31	7.37	122.17	115.64
2	h	201	JNI	C33-N32-C31	7.35	122.16	115.64
2	V	202	JNI	N32-C31-N34	7.35	124.86	116.90
2	p	201	JNI	C33-N32-C31	7.34	122.15	115.64
2	J	201	JNI	C2-N7-C6	7.34	121.93	116.73
2	l	201	JNI	C33-N32-C31	7.34	122.14	115.64
2	Z	202	JNI	C29-N30-C31	7.33	122.14	115.64
2	L	201	JNI	N30-C31-N34	7.29	124.80	116.90
2	f	202	JNI	C33-N32-C31	7.29	122.10	115.64
2	l	201	JNI	C29-N30-C31	7.29	122.10	115.64
2	R	201	JNI	C2-N7-C6	7.28	121.89	116.73
2	F	202	JNI	C29-N30-C31	7.27	122.08	115.64
2	U	201	JNI	N32-C31-N34	7.27	124.77	116.90
2	r	202	JNI	C29-N30-C31	7.25	122.07	115.64
2	Z	201	JNI	C33-N32-C31	7.15	121.97	115.64
2	r	202	JNI	N7-C6-N8	7.09	122.52	115.77
2	j	201	JNI	C29-N30-C31	7.09	121.92	115.64
2	X	202	JNI	C33-N32-C31	7.09	121.92	115.64
2	Q	201	JNI	C2-N7-C6	7.05	121.73	116.73
2	A	201	JNI	C29-N30-C31	7.05	121.89	115.64
2	n	201	JNI	C2-N7-C6	7.04	121.72	116.73
2	C	201	JNI	C29-N30-C31	7.02	121.86	115.64
2	v	201	JNI	N32-C31-N34	7.02	124.50	116.90
2	d	201	JNI	C2-N7-C6	7.02	121.70	116.73
2	b	202	JNI	C33-N32-C31	7.01	121.86	115.64
2	X	202	JNI	C29-N30-C31	6.97	121.82	115.64
2	C	202	JNI	C29-N30-C31	6.92	121.77	115.64
2	D	201	JNI	C2-N7-C6	6.89	121.61	116.73
2	V	201	JNI	C2-N7-C6	6.89	121.61	116.73
2	v	201	JNI	C29-N30-C31	6.88	121.73	115.64
2	D	201	JNI	C29-N30-C31	6.86	121.72	115.64
2	J	202	JNI	C33-N32-C31	6.85	121.71	115.64
2	t	201	JNI	C2-N7-C6	6.81	121.55	116.73
2	l	201	JNI	C2-N7-C6	6.81	121.55	116.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	X	202	JNI	N32-C31-N34	6.79	124.25	116.90
2	N	201	JNI	C33-N32-C31	6.78	121.65	115.64
2	f	201	JNI	N1-C2-N3	6.75	124.29	117.44
2	f	202	JNI	C29-N30-C31	6.74	121.61	115.64
2	J	202	JNI	C29-N30-C31	6.73	121.61	115.64
2	R	201	JNI	C29-N30-C31	6.70	121.58	115.64
2	t	201	JNI	C29-N30-C31	6.65	121.53	115.64
2	P	201	JNI	C29-N30-C31	6.65	121.53	115.64
2	C	202	JNI	C39-N34-C31	-6.63	110.70	121.69
2	F	202	JNI	C33-N32-C31	6.62	121.51	115.64
2	P	202	JNI	C29-N30-C31	6.62	121.50	115.64
2	r	201	JNI	C29-N30-C31	6.61	121.50	115.64
2	v	202	JNI	N7-C6-N8	6.56	122.01	115.77
2	j	201	JNI	N32-C31-N34	6.55	123.99	116.90
2	P	202	JNI	C35-N34-C31	-6.54	110.84	121.69
2	p	201	JNI	C29-N30-C31	6.54	121.44	115.64
2	r	201	JNI	C33-N32-C31	6.54	121.44	115.64
2	A	201	JNI	C33-N32-C31	6.54	121.43	115.64
2	V	202	JNI	N7-C6-N8	6.50	121.96	115.77
2	p	202	JNI	C33-N32-C31	6.50	121.40	115.64
2	J	202	JNI	C2-N7-C6	6.47	121.31	116.73
2	D	201	JNI	C33-N32-C31	6.44	121.34	115.64
2	C	202	JNI	N7-C6-N8	6.43	121.89	115.77
2	Z	201	JNI	C29-N30-C31	6.42	121.33	115.64
2	t	202	JNI	C2-N7-C6	6.39	121.26	116.73
2	n	202	JNI	C33-N32-C31	6.38	121.29	115.64
2	n	202	JNI	C29-N30-C31	6.36	121.28	115.64
2	C	201	JNI	C33-N32-C31	6.31	121.23	115.64
2	A	202	JNI	C33-N32-C31	6.31	121.23	115.64
2	P	201	JNI	C33-N32-C31	6.30	121.22	115.64
2	V	201	JNI	C29-N30-C31	6.29	121.21	115.64
2	o	201	JNI	C33-N32-C31	6.28	121.21	115.64
2	o	201	JNI	C39-N34-C31	-6.27	111.29	121.69
2	H	201	JNI	C2-N7-C6	6.21	121.13	116.73
2	Z	202	JNI	C2-N7-C6	6.20	121.12	116.73
2	j	202	JNI	C29-N30-C31	6.17	121.11	115.64
2	d	201	JNI	N30-C31-N34	6.16	123.57	116.90
2	L	201	JNI	N32-C31-N30	-6.14	116.69	127.06
2	A	201	JNI	C35-N34-C31	-6.13	111.52	121.69
2	A	202	JNI	C29-N30-C31	6.13	121.07	115.64
2	r	202	JNI	C33-N32-C31	6.13	121.07	115.64
2	M	201	JNI	C33-N32-C31	6.13	121.07	115.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	U	201	JNI	C33-N32-C31	6.11	121.05	115.64
2	p	202	JNI	C2-N7-C6	6.11	121.06	116.73
2	H	201	JNI	N7-C6-N8	6.09	121.57	115.77
2	N	201	JNI	C29-N30-C31	6.09	121.03	115.64
2	M	201	JNI	C39-N34-C31	-6.08	111.60	121.69
2	X	201	JNI	C39-N34-C31	-6.02	111.71	121.69
2	V	202	JNI	C2-N7-C6	5.97	120.96	116.73
2	j	202	JNI	C33-N32-C31	5.96	120.93	115.64
2	J	201	JNI	C29-N30-C31	5.95	120.91	115.64
2	R	201	JNI	N30-C31-N34	5.94	123.33	116.90
2	R	201	JNI	C4-N3-C2	5.88	122.26	116.24
2	t	201	JNI	C35-N34-C31	-5.87	111.96	121.69
2	f	202	JNI	C2-N7-C6	5.85	120.88	116.73
2	V	201	JNI	C39-N34-C31	-5.83	112.02	121.69
2	P	202	JNI	C2-N7-C6	5.81	120.85	116.73
2	F	201	JNI	C29-N30-C31	5.78	120.76	115.64
2	X	201	JNI	C33-N32-C31	5.74	120.73	115.64
2	b	201	JNI	C33-N32-C31	5.73	120.72	115.64
2	d	201	JNI	C29-N30-C31	5.71	120.70	115.64
2	Q	201	JNI	C33-N32-C31	5.68	120.67	115.64
2	H	202	JNI	N32-C31-N30	-5.62	117.58	127.06
2	Q	201	JNI	N32-C31-N34	5.61	122.97	116.90
2	v	201	JNI	C33-N32-C31	5.61	120.61	115.64
2	b	201	JNI	C4-N3-C2	5.59	121.96	116.24
2	A	201	JNI	C2-N7-C6	5.58	120.69	116.73
2	L	201	JNI	C27-C22-C21	5.56	129.81	120.61
2	P	202	JNI	C39-N34-C31	-5.50	112.56	121.69
2	h	201	JNI	N30-C31-N34	5.46	122.81	116.90
2	j	202	JNI	C4-N3-C2	5.45	121.82	116.24
2	P	202	JNI	C33-N32-C31	5.45	120.47	115.64
2	j	202	JNI	N32-C31-N34	5.45	122.79	116.90
2	U	201	JNI	C39-N34-C31	-5.44	112.67	121.69
2	n	201	JNI	C35-N34-C31	-5.42	112.70	121.69
2	b	201	JNI	N3-C2-N7	-5.39	119.14	125.70
2	F	201	JNI	N30-C31-N34	5.38	122.73	116.90
2	p	202	JNI	N7-C6-N8	5.37	120.89	115.77
2	L	201	JNI	C17-C16-N8	-5.37	109.55	119.23
2	C	201	JNI	C2-N7-C6	5.35	120.52	116.73
2	b	202	JNI	C4-N3-C2	5.35	121.72	116.24
2	h	201	JNI	C35-N34-C31	-5.34	112.84	121.69
2	N	201	JNI	N7-C6-N8	5.33	120.85	115.77
2	C	201	JNI	C4-N3-C2	5.33	121.69	116.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	t	202	JNI	N7-C6-N8	5.29	120.81	115.77
2	H	201	JNI	N32-C31-N34	5.29	122.62	116.90
2	L	201	JNI	C16-N8-C6	5.27	127.07	121.20
2	A	202	JNI	C2-N7-C6	5.26	120.46	116.73
2	v	202	JNI	N32-C31-N34	5.25	122.58	116.90
2	N	201	JNI	C2-N7-C6	5.24	120.44	116.73
2	F	202	JNI	C2-N7-C6	5.22	120.43	116.73
2	X	202	JNI	C17-C16-N8	-5.22	109.83	119.23
2	X	201	JNI	N3-C2-N7	-5.21	119.36	125.70
2	n	202	JNI	C17-C16-N8	-5.18	109.90	119.23
2	P	201	JNI	C2-N7-C6	5.18	120.40	116.73
2	A	202	JNI	C39-N34-C31	-5.17	113.11	121.69
2	v	202	JNI	N32-C31-N30	-5.17	118.33	127.06
2	X	202	JNI	C4-N3-C2	5.16	121.52	116.24
2	p	202	JNI	C35-N34-C31	-5.16	113.14	121.69
2	t	202	JNI	N32-C31-N30	-5.11	118.42	127.06
2	J	202	JNI	C35-N34-C31	-5.10	113.23	121.69
2	n	202	JNI	C35-N34-C31	-5.10	113.23	121.69
2	j	202	JNI	C16-N8-C6	5.10	126.88	121.20
2	r	202	JNI	C4-N3-C2	5.09	121.45	116.24
2	t	202	JNI	C35-N34-C31	-5.09	113.25	121.69
2	X	202	JNI	N7-C6-N8	5.07	120.60	115.77
2	X	201	JNI	C35-N34-C31	-5.07	113.28	121.69
2	j	201	JNI	N3-C2-N7	-5.06	119.54	125.70
2	X	201	JNI	C4-N3-C2	5.05	121.40	116.24
2	f	201	JNI	N32-C31-N30	-5.04	118.55	127.06
2	A	202	JNI	C4-N3-C2	5.02	121.38	116.24
2	n	201	JNI	C4-N3-C2	5.02	121.38	116.24
2	C	202	JNI	N32-C31-N34	5.01	122.32	116.90
2	V	202	JNI	N32-C31-N30	-5.00	118.62	127.06
2	f	202	JNI	C35-N34-C31	-4.97	113.45	121.69
2	o	201	JNI	N32-C31-N34	4.94	122.25	116.90
2	o	201	JNI	N3-C2-N7	-4.93	119.69	125.70
2	n	202	JNI	C39-N34-C31	-4.93	113.51	121.69
2	L	201	JNI	C22-C21-C16	4.92	130.69	123.19
2	o	201	JNI	C4-N3-C2	4.90	121.26	116.24
2	Z	202	JNI	N32-C31-N30	-4.88	118.81	127.06
2	h	201	JNI	N32-C31-N30	-4.88	118.82	127.06
2	X	202	JNI	N3-C2-N7	-4.88	119.76	125.70
2	h	202	JNI	N32-C31-N30	-4.88	118.82	127.06
2	b	202	JNI	N32-C31-N34	4.88	122.18	116.90
2	H	202	JNI	C4-N3-C2	4.88	121.23	116.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	r	202	JNI	N32-C31-N34	4.85	122.15	116.90
2	H	201	JNI	C4-N3-C2	4.84	121.19	116.24
2	H	202	JNI	C27-C22-C21	4.83	128.61	120.61
2	n	201	JNI	N32-C31-N30	-4.83	118.90	127.06
2	b	201	JNI	N32-C31-N34	4.83	122.13	116.90
2	r	202	JNI	C17-C16-N8	-4.83	110.53	119.23
2	b	202	JNI	N3-C2-N7	-4.83	119.82	125.70
2	n	202	JNI	C25-C26-C28	-4.82	113.00	121.36
2	M	201	JNI	N3-C2-N7	-4.82	119.84	125.70
2	j	201	JNI	C35-N34-C31	-4.80	113.73	121.69
2	F	202	JNI	C4-N3-C2	4.79	121.14	116.24
2	p	202	JNI	C4-N3-C2	4.79	121.14	116.24
2	R	201	JNI	N3-C2-N7	-4.78	119.88	125.70
2	H	201	JNI	N32-C31-N30	-4.78	118.99	127.06
2	P	201	JNI	C4-N3-C2	4.77	121.12	116.24
2	b	202	JNI	C17-C16-N8	-4.76	110.64	119.23
2	j	201	JNI	C4-N3-C2	4.76	121.11	116.24
2	j	202	JNI	N3-C2-N7	-4.75	119.92	125.70
2	b	202	JNI	C20-C21-C16	-4.73	113.33	117.86
2	P	202	JNI	N7-C6-N8	4.73	120.27	115.77
2	b	201	JNI	N32-C31-N30	-4.72	119.08	127.06
2	r	201	JNI	C4-N3-C2	4.72	121.07	116.24
2	d	201	JNI	C4-N3-C2	4.71	121.06	116.24
2	f	202	JNI	C4-N3-C2	4.69	121.04	116.24
2	R	201	JNI	C39-N34-C31	-4.69	113.91	121.69
2	X	201	JNI	N32-C31-N34	4.69	121.97	116.90
2	n	201	JNI	N3-C2-N7	-4.67	120.02	125.70
2	Z	202	JNI	C10-C9-N8	-4.67	106.44	113.98
2	L	201	JNI	C20-C21-C16	-4.65	113.41	117.86
2	b	202	JNI	N32-C31-N30	-4.65	119.22	127.06
2	H	202	JNI	C23-C22-C21	-4.63	113.41	120.91
2	l	201	JNI	C27-C22-C21	4.63	128.28	120.61
2	U	201	JNI	N3-C2-N7	-4.62	120.08	125.70
2	f	202	JNI	N32-C31-N34	4.61	121.89	116.90
2	l	201	JNI	N32-C31-N30	-4.61	119.28	127.06
2	t	201	JNI	N32-C31-N30	-4.60	119.29	127.06
2	Q	201	JNI	C35-N34-C31	-4.60	114.06	121.69
2	p	201	JNI	C4-N3-C2	4.59	120.94	116.24
2	C	202	JNI	C4-N3-C2	4.59	120.94	116.24
2	n	202	JNI	C4-N3-C2	4.58	120.92	116.24
2	j	202	JNI	C35-N34-C31	-4.57	114.10	121.69
2	L	201	JNI	N3-C2-N7	-4.57	120.14	125.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	n	201	JNI	N32-C31-N34	4.57	121.84	116.90
2	D	201	JNI	N32-C31-N34	4.57	121.84	116.90
2	b	201	JNI	C39-N34-C31	-4.56	114.12	121.69
2	d	201	JNI	C39-N34-C31	-4.54	114.17	121.69
2	j	201	JNI	N32-C31-N30	-4.53	119.41	127.06
2	p	202	JNI	C39-N34-C31	-4.53	114.18	121.69
2	P	201	JNI	N7-C6-N8	4.52	120.08	115.77
2	v	202	JNI	C4-N3-C2	4.52	120.86	116.24
2	b	202	JNI	N7-C6-N8	4.52	120.07	115.77
2	J	202	JNI	C4-N3-C2	4.51	120.85	116.24
2	X	201	JNI	C16-N8-C6	4.50	126.22	121.20
2	U	201	JNI	N32-C31-N30	-4.49	119.48	127.06
2	C	201	JNI	C23-C22-C21	-4.47	113.66	120.91
2	r	202	JNI	N3-C2-N7	-4.46	120.27	125.70
2	D	201	JNI	C35-N34-C31	-4.46	114.30	121.69
2	Z	202	JNI	N30-C31-N34	4.45	121.72	116.90
2	H	202	JNI	N3-C2-N7	-4.44	120.29	125.70
2	f	201	JNI	C16-N8-C6	-4.44	116.26	121.20
2	U	201	JNI	C35-N34-C31	-4.42	114.37	121.69
2	C	201	JNI	N7-C6-N8	4.40	119.96	115.77
2	H	202	JNI	N7-C6-N8	4.39	119.95	115.77
2	R	201	JNI	N32-C31-N30	-4.38	119.66	127.06
2	A	202	JNI	C16-N8-C6	-4.38	116.32	121.20
2	j	201	JNI	N1-C2-N3	4.37	121.87	117.44
2	Z	202	JNI	C4-N3-C2	4.37	120.71	116.24
2	J	201	JNI	C4-N3-C2	4.36	120.70	116.24
2	o	201	JNI	N1-C2-N3	4.35	121.86	117.44
2	M	201	JNI	C4-N3-C2	4.35	120.69	116.24
2	r	202	JNI	C5-C6-N7	-4.35	116.44	123.53
2	o	201	JNI	C10-C9-N8	-4.34	106.96	113.98
2	C	202	JNI	C2-N7-C6	4.34	119.81	116.73
2	h	201	JNI	C4-N3-C2	4.32	120.66	116.24
2	v	202	JNI	C5-C6-N7	-4.32	116.48	123.53
2	p	201	JNI	C39-N34-C31	-4.32	114.53	121.69
2	t	202	JNI	C4-N3-C2	4.32	120.66	116.24
2	h	202	JNI	N3-C2-N7	-4.31	120.45	125.70
2	F	202	JNI	N30-C31-N34	4.31	121.56	116.90
2	A	201	JNI	C4-N3-C2	4.31	120.65	116.24
2	C	202	JNI	N32-C31-N30	-4.31	119.79	127.06
2	D	201	JNI	C4-N3-C2	4.28	120.62	116.24
2	X	202	JNI	N32-C31-N30	-4.28	119.84	127.06
2	j	202	JNI	C17-C16-N8	-4.27	111.53	119.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	201	JNI	C39-N34-C31	-4.27	114.61	121.69
2	f	202	JNI	C39-N34-C31	-4.27	114.61	121.69
2	f	202	JNI	N32-C31-N30	-4.26	119.87	127.06
2	v	201	JNI	N3-C2-N7	-4.26	120.51	125.70
2	t	202	JNI	N32-C31-N34	4.25	121.50	116.90
2	C	201	JNI	C27-C22-C21	4.25	127.65	120.61
2	V	201	JNI	C4-N3-C2	4.23	120.57	116.24
2	J	201	JNI	N32-C31-N30	-4.23	119.92	127.06
2	n	202	JNI	N7-C6-N8	4.22	119.79	115.77
2	A	202	JNI	N30-C31-N34	4.22	121.47	116.90
2	J	202	JNI	C39-N34-C31	-4.21	114.70	121.69
2	X	201	JNI	N32-C31-N30	-4.21	119.95	127.06
2	P	201	JNI	C16-N8-C6	-4.21	116.51	121.20
2	M	201	JNI	N32-C31-N34	4.20	121.45	116.90
2	A	202	JNI	C10-C9-N8	-4.19	107.20	113.98
2	V	202	JNI	C4-N3-C2	4.19	120.52	116.24
2	C	202	JNI	C5-C4-N3	-4.18	118.76	123.96
2	Z	201	JNI	N32-C31-N34	4.18	121.42	116.90
2	V	202	JNI	C29-C28-C26	-4.18	114.41	121.69
2	t	201	JNI	C23-C22-C21	-4.16	114.18	120.91
2	n	202	JNI	N3-C2-N7	-4.14	120.66	125.70
2	v	201	JNI	C5-C6-N7	-4.14	116.78	123.53
2	L	201	JNI	C4-N3-C2	4.13	120.47	116.24
2	F	202	JNI	N32-C31-N30	-4.13	120.08	127.06
2	o	201	JNI	N32-C31-N30	-4.13	120.08	127.06
2	A	201	JNI	N32-C31-N34	4.13	121.37	116.90
2	n	202	JNI	C20-C21-C16	-4.13	113.91	117.86
2	r	201	JNI	N3-C2-N7	-4.12	120.68	125.70
2	j	202	JNI	C5-C6-N7	-4.12	116.82	123.53
2	M	201	JNI	C35-N34-C31	-4.11	114.87	121.69
2	X	202	JNI	C20-C21-C16	-4.10	113.93	117.86
2	p	201	JNI	N32-C31-N30	-4.09	120.16	127.06
2	h	202	JNI	C35-N34-C31	-4.09	114.91	121.69
2	X	202	JNI	C5-C6-N7	-4.08	116.87	123.53
2	M	201	JNI	C5-C6-N7	-4.08	116.87	123.53
2	b	202	JNI	C27-C22-C21	4.08	127.36	120.61
2	U	201	JNI	N1-C2-N3	4.08	121.58	117.44
2	P	202	JNI	C4-N3-C2	4.07	120.41	116.24
2	N	201	JNI	C4-N3-C2	4.07	120.41	116.24
2	M	201	JNI	N1-C2-N3	4.07	121.57	117.44
2	Q	201	JNI	C4-N3-C2	4.07	120.40	116.24
2	t	201	JNI	C27-C22-C21	4.06	127.33	120.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	Z	201	JNI	C9-N8-C6	4.05	124.55	118.17
2	M	201	JNI	N32-C31-N30	-4.05	120.22	127.06
2	V	202	JNI	C28-C33-N32	-4.05	117.65	124.32
2	J	202	JNI	N32-C31-N30	-4.05	120.23	127.06
2	p	202	JNI	N32-C31-N30	-4.05	120.23	127.06
2	Q	201	JNI	N32-C31-N30	-4.05	120.23	127.06
2	d	201	JNI	C10-C9-N8	4.05	120.51	113.98
2	n	201	JNI	N7-C6-N8	4.04	119.62	115.77
2	r	202	JNI	N32-C31-N30	-4.04	120.23	127.06
2	N	201	JNI	C39-N34-C31	-4.04	115.00	121.69
2	C	201	JNI	N3-C2-N7	-4.04	120.79	125.70
2	D	201	JNI	C10-C9-N8	-4.03	107.46	113.98
2	C	202	JNI	C35-N34-C31	-4.03	115.00	121.69
2	h	202	JNI	C5-C6-N7	-4.03	116.95	123.53
2	v	201	JNI	C4-N3-C2	4.03	120.36	116.24
2	n	201	JNI	C39-N34-C31	-4.03	115.01	121.69
2	r	201	JNI	C10-C9-N8	-4.02	107.49	113.98
2	d	201	JNI	N32-C31-N30	-4.01	120.29	127.06
2	p	201	JNI	N3-C2-N7	-4.00	120.83	125.70
2	n	202	JNI	C5-C6-N7	-4.00	117.01	123.53
2	X	201	JNI	N1-C2-N3	4.00	121.49	117.44
2	h	202	JNI	C4-N3-C2	3.99	120.33	116.24
2	U	201	JNI	C4-N3-C2	3.99	120.32	116.24
2	j	201	JNI	C23-C22-C21	-3.98	114.45	120.91
2	f	201	JNI	C39-N34-C31	-3.98	115.08	121.69
2	f	201	JNI	C5-C6-N7	-3.97	117.05	123.53
2	v	202	JNI	N3-C2-N7	-3.97	120.86	125.70
2	j	201	JNI	C5-C6-N7	-3.97	117.05	123.53
2	H	201	JNI	C5-C4-N3	-3.96	119.04	123.96
2	Q	201	JNI	N7-C6-N8	3.95	119.53	115.77
2	D	201	JNI	N32-C31-N30	-3.93	120.42	127.06
2	C	201	JNI	C35-N34-C31	-3.93	115.17	121.69
2	C	202	JNI	C16-N8-C6	-3.93	116.83	121.20
2	l	201	JNI	C4-N3-C2	3.92	120.26	116.24
2	Z	201	JNI	C23-C22-C21	-3.91	114.57	120.91
2	d	201	JNI	N7-C6-N8	3.90	119.48	115.77
2	d	201	JNI	N3-C2-N7	-3.88	120.98	125.70
2	b	201	JNI	C5-C6-N7	-3.87	117.21	123.53
2	h	202	JNI	C39-N34-C31	-3.87	115.27	121.69
2	Z	201	JNI	C4-N3-C2	3.87	120.20	116.24
2	r	202	JNI	C20-C21-C16	-3.87	114.15	117.86
2	V	201	JNI	N32-C31-N30	-3.87	120.53	127.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	p	202	JNI	N3-C2-N7	-3.86	121.00	125.70
2	r	201	JNI	N32-C31-N30	-3.85	120.56	127.06
2	J	201	JNI	C28-C33-N32	-3.85	117.98	124.32
2	F	202	JNI	C39-N34-C31	-3.84	115.32	121.69
2	P	202	JNI	N3-C2-N7	-3.84	121.03	125.70
2	J	202	JNI	N3-C2-N7	-3.83	121.03	125.70
2	Z	201	JNI	N32-C31-N30	-3.82	120.61	127.06
2	Z	202	JNI	N3-C2-N7	-3.82	121.05	125.70
2	A	201	JNI	N32-C31-N30	-3.81	120.62	127.06
2	P	201	JNI	C39-N34-C31	-3.81	115.37	121.69
2	U	201	JNI	C5-C6-N7	-3.80	117.33	123.53
2	j	201	JNI	C27-C26-C28	3.80	127.14	120.86
2	F	201	JNI	N32-C31-N30	-3.79	120.66	127.06
2	j	202	JNI	N1-C2-N7	3.79	123.15	117.25
2	D	201	JNI	N3-C2-N7	-3.79	121.09	125.70
2	j	201	JNI	C25-C26-C28	-3.79	114.80	121.36
2	Q	201	JNI	N3-C2-N7	-3.78	121.09	125.70
2	C	201	JNI	C25-C26-C28	-3.78	114.81	121.36
2	l	201	JNI	C23-C22-C21	-3.77	114.80	120.91
2	f	202	JNI	C5-C4-N3	-3.77	119.28	123.96
2	R	201	JNI	N1-C2-N3	3.77	121.26	117.44
2	N	201	JNI	C5-C4-N3	-3.77	119.28	123.96
2	h	201	JNI	N3-C2-N7	-3.76	121.12	125.70
2	Z	201	JNI	C16-N8-C6	-3.76	117.02	121.20
2	n	202	JNI	C27-C22-C21	3.76	126.83	120.61
2	t	202	JNI	C39-N34-C31	-3.74	115.48	121.69
2	F	201	JNI	C4-N3-C2	3.74	120.06	116.24
2	P	201	JNI	C5-C4-N3	-3.74	119.32	123.96
2	C	201	JNI	N32-C31-N30	-3.73	120.75	127.06
2	p	202	JNI	C22-C21-C16	3.73	128.88	123.19
2	J	201	JNI	N3-C2-N7	-3.72	121.17	125.70
2	r	202	JNI	N1-C2-N7	3.71	123.02	117.25
2	A	202	JNI	N3-C2-N7	-3.71	121.19	125.70
2	H	202	JNI	C36-C35-N34	3.71	118.51	110.48
2	F	201	JNI	C9-N8-C6	3.70	123.99	118.17
2	t	201	JNI	C39-N34-C31	-3.69	115.56	121.69
2	b	202	JNI	C22-C21-C16	3.69	128.82	123.19
2	n	202	JNI	C27-C26-C28	3.69	126.96	120.86
2	N	201	JNI	C35-N34-C31	-3.68	115.58	121.69
2	t	202	JNI	N3-C2-N7	-3.67	121.23	125.70
2	j	201	JNI	C39-N34-C31	-3.67	115.61	121.69
2	J	201	JNI	C5-C6-N7	-3.66	117.56	123.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	l	201	JNI	C27-C26-C28	3.66	126.91	120.86
2	n	202	JNI	N32-C31-N30	-3.65	120.90	127.06
2	Z	201	JNI	C27-C22-C21	3.65	126.65	120.61
2	F	201	JNI	N3-C2-N7	-3.65	121.26	125.70
2	F	202	JNI	N3-C2-N7	-3.64	121.26	125.70
2	p	201	JNI	N30-C31-N34	3.64	120.83	116.90
2	o	201	JNI	C5-C6-N7	-3.63	117.60	123.53
2	F	202	JNI	C5-C4-N3	-3.63	119.44	123.96
2	d	201	JNI	C5-C4-N3	-3.63	119.44	123.96
2	C	201	JNI	C5-C4-N3	-3.63	119.45	123.96
2	Z	201	JNI	N3-C2-N7	-3.63	121.28	125.70
2	t	201	JNI	N30-C31-N34	3.63	120.83	116.90
2	C	201	JNI	N32-C31-N34	3.63	120.82	116.90
2	f	201	JNI	C35-N34-C31	-3.62	115.68	121.69
2	p	201	JNI	C35-N34-C31	-3.62	115.69	121.69
2	C	201	JNI	C22-C21-C16	3.62	128.70	123.19
2	t	202	JNI	C23-C22-C21	-3.61	115.06	120.91
2	t	201	JNI	C4-N3-C2	3.61	119.94	116.24
2	v	201	JNI	N7-C6-N8	3.61	119.21	115.77
2	A	202	JNI	C5-C4-N3	-3.61	119.47	123.96
2	A	201	JNI	N7-C6-N8	3.61	119.20	115.77
2	R	201	JNI	C5-C4-N3	-3.61	119.48	123.96
2	d	201	JNI	C5-C6-N7	-3.60	117.65	123.53
2	h	201	JNI	C25-C26-C28	-3.60	115.12	121.36
2	P	201	JNI	N32-C31-N30	-3.60	120.98	127.06
2	l	201	JNI	C5-C6-N7	-3.60	117.66	123.53
2	o	201	JNI	C35-N34-C31	-3.59	115.73	121.69
2	r	201	JNI	C5-C4-N3	-3.59	119.49	123.96
2	f	201	JNI	C17-C16-N8	-3.59	112.76	119.23
2	H	202	JNI	C5-C6-N7	-3.59	117.67	123.53
2	V	202	JNI	C5-C4-N3	-3.59	119.50	123.96
2	F	202	JNI	C28-C29-N30	-3.58	118.41	124.32
2	X	201	JNI	C5-C6-N7	-3.58	117.69	123.53
2	f	202	JNI	N7-C6-N8	3.57	119.17	115.77
2	H	202	JNI	C27-C26-C28	3.57	126.76	120.86
2	A	202	JNI	C35-N34-C31	-3.56	115.78	121.69
2	J	201	JNI	N7-C6-N8	3.56	119.16	115.77
2	F	202	JNI	N7-C6-N8	3.56	119.16	115.77
2	D	201	JNI	N7-C6-N8	3.56	119.16	115.77
2	R	201	JNI	C16-N8-C6	-3.56	117.24	121.20
2	R	201	JNI	C10-C9-N8	3.55	119.71	113.98
2	H	202	JNI	C22-C21-C16	3.54	128.59	123.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	N	201	JNI	N32-C31-N30	-3.54	121.08	127.06
2	j	202	JNI	C22-C21-C16	3.54	128.59	123.19
2	r	201	JNI	N1-C2-N3	3.53	121.02	117.44
2	f	201	JNI	N30-C31-N34	3.53	120.72	116.90
2	f	202	JNI	N3-C2-N7	-3.53	121.40	125.70
2	X	202	JNI	C22-C21-C16	3.53	128.57	123.19
2	f	201	JNI	N32-C31-N34	3.53	120.72	116.90
2	v	201	JNI	C39-N34-C31	-3.52	115.85	121.69
2	R	201	JNI	C35-N34-C31	-3.52	115.85	121.69
2	L	201	JNI	C36-C35-N34	3.52	118.11	110.48
2	A	202	JNI	N7-C6-N8	3.52	119.12	115.77
2	V	201	JNI	C5-C6-N7	-3.51	117.80	123.53
2	f	201	JNI	C22-C21-C16	3.51	128.54	123.19
2	F	201	JNI	C5-C6-N7	-3.51	117.81	123.53
2	Q	201	JNI	C10-C9-N8	-3.50	108.32	113.98
2	r	201	JNI	C5-C6-N7	-3.49	117.83	123.53
2	j	202	JNI	C5-C4-N3	-3.49	119.62	123.96
2	h	201	JNI	C22-C21-C16	3.49	128.51	123.19
2	P	201	JNI	N3-C2-N7	-3.49	121.45	125.70
2	v	201	JNI	N32-C31-N30	-3.48	121.19	127.06
2	Z	202	JNI	N7-C6-N8	3.47	119.08	115.77
2	P	201	JNI	C28-C29-N30	-3.47	118.59	124.32
2	p	202	JNI	C28-C29-N30	-3.47	118.60	124.32
2	C	201	JNI	C28-C29-N30	-3.47	118.60	124.32
2	l	201	JNI	C25-C26-C28	-3.47	115.35	121.36
2	h	202	JNI	N30-C31-N34	3.47	120.65	116.90
2	P	202	JNI	C28-C29-N30	-3.47	118.60	124.32
2	H	202	JNI	C38-N37-C36	3.47	120.30	110.34
2	p	202	JNI	C5-C4-N3	-3.46	119.66	123.96
2	A	201	JNI	C10-C9-N8	-3.45	108.40	113.98
2	H	201	JNI	C39-N34-C31	-3.45	115.97	121.69
2	f	201	JNI	C5-C4-N3	-3.45	119.68	123.96
2	J	202	JNI	C5-C4-N3	-3.44	119.68	123.96
2	n	202	JNI	C5-C4-N3	-3.44	119.69	123.96
2	p	201	JNI	C5-C4-N3	-3.44	119.69	123.96
2	b	202	JNI	C5-C6-N7	-3.43	117.93	123.53
2	n	202	JNI	C22-C21-C16	3.43	128.42	123.19
2	h	201	JNI	C9-N8-C6	3.43	123.56	118.17
2	A	202	JNI	C28-C29-N30	-3.42	118.68	124.32
2	H	201	JNI	N3-C2-N7	-3.42	121.53	125.70
2	r	202	JNI	C25-C26-C28	-3.42	115.43	121.36
2	V	201	JNI	C9-N8-C6	3.42	123.55	118.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	l	201	JNI	N30-C31-N34	3.41	120.59	116.90
2	j	202	JNI	C25-C26-C28	-3.41	115.45	121.36
2	V	201	JNI	N3-C2-N7	-3.40	121.56	125.70
2	H	201	JNI	C5-C6-N7	-3.39	118.00	123.53
2	L	201	JNI	N1-C2-N3	3.39	120.88	117.44
2	J	202	JNI	N32-C31-N34	3.39	120.57	116.90
2	R	201	JNI	C23-C22-C21	-3.38	115.43	120.91
2	F	202	JNI	C35-N34-C31	-3.38	116.08	121.69
2	R	201	JNI	C27-C22-C21	3.38	126.20	120.61
2	j	202	JNI	N32-C31-N30	-3.37	121.37	127.06
2	N	201	JNI	C28-C33-N32	-3.37	118.77	124.32
2	A	201	JNI	N3-C2-N7	-3.37	121.60	125.70
2	t	201	JNI	C5-C6-N7	-3.37	118.04	123.53
2	H	201	JNI	C35-N34-C31	-3.36	116.11	121.69
2	b	201	JNI	C5-C4-N3	-3.36	119.78	123.96
2	h	201	JNI	C5-C6-N7	-3.35	118.06	123.53
2	Z	201	JNI	C5-C6-N7	-3.35	118.06	123.53
2	r	201	JNI	N7-C6-N8	3.35	118.96	115.77
2	h	202	JNI	N32-C31-N34	3.35	120.52	116.90
2	b	201	JNI	N1-C2-N3	3.34	120.83	117.44
2	b	202	JNI	C25-C26-C28	-3.34	115.56	121.36
2	L	201	JNI	C23-C22-C21	-3.34	115.50	120.91
2	b	202	JNI	C39-N34-C31	-3.34	116.15	121.69
2	A	201	JNI	C5-C4-N3	-3.34	119.81	123.96
2	Q	201	JNI	C5-C4-N3	-3.33	119.82	123.96
2	U	201	JNI	C10-C9-N8	-3.33	108.59	113.98
2	R	201	JNI	C9-N8-C6	3.33	123.40	118.17
2	r	202	JNI	C5-C4-N3	-3.32	119.84	123.96
2	A	202	JNI	N32-C31-N30	-3.32	121.46	127.06
2	V	201	JNI	C5-C4-N3	-3.31	119.85	123.96
2	V	202	JNI	N3-C2-N7	-3.31	121.67	125.70
2	J	202	JNI	N1-C2-N3	3.30	120.79	117.44
2	l	201	JNI	C5-C4-N3	-3.30	119.86	123.96
2	C	201	JNI	C39-N34-C31	-3.30	116.21	121.69
2	A	202	JNI	C28-C33-N32	-3.30	118.89	124.32
2	f	201	JNI	C5-C6-N8	3.30	127.56	121.24
2	L	201	JNI	C5-C6-N7	-3.29	118.16	123.53
2	P	202	JNI	N32-C31-N30	-3.29	121.51	127.06
2	C	202	JNI	C28-C33-N32	-3.29	118.90	124.32
2	A	201	JNI	C28-C29-N30	-3.29	118.90	124.32
2	j	202	JNI	C28-C33-N32	-3.28	118.92	124.32
2	o	201	JNI	C5-C4-N3	-3.28	119.89	123.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	t	202	JNI	C5-C4-N3	-3.27	119.89	123.96
2	d	201	JNI	C9-C10-C11	-3.27	114.62	120.77
2	v	202	JNI	C5-C4-N3	-3.27	119.89	123.96
2	Q	201	JNI	C5-C6-N7	-3.27	118.20	123.53
2	p	201	JNI	C5-C6-N7	-3.26	118.21	123.53
2	V	202	JNI	C33-C28-C26	3.26	127.38	121.69
2	b	201	JNI	C16-N8-C6	3.26	124.83	121.20
2	b	202	JNI	C10-C9-N8	3.26	119.24	113.98
2	h	202	JNI	N7-C6-N8	3.26	118.87	115.77
2	r	201	JNI	C35-N34-C31	-3.25	116.29	121.69
2	r	201	JNI	C39-N34-C31	-3.25	116.30	121.69
2	D	201	JNI	C5-C4-N3	-3.25	119.92	123.96
2	j	201	JNI	C27-C22-C21	3.25	125.99	120.61
2	p	202	JNI	N32-C31-N34	3.24	120.41	116.90
2	C	201	JNI	C16-N8-C6	-3.24	117.59	121.20
2	p	201	JNI	C28-C33-N32	-3.24	118.98	124.32
2	X	202	JNI	C28-C33-N32	-3.23	118.99	124.32
2	M	201	JNI	C28-C29-N30	-3.23	118.99	124.32
2	N	201	JNI	C5-C6-N7	-3.22	118.27	123.53
2	P	201	JNI	C35-N34-C31	-3.22	116.35	121.69
2	Q	201	JNI	C28-C29-N30	-3.22	119.02	124.32
2	N	201	JNI	C28-C29-N30	-3.22	119.02	124.32
2	Z	202	JNI	C5-C4-N3	-3.21	119.97	123.96
2	t	201	JNI	N1-C2-N3	3.21	120.70	117.44
2	t	201	JNI	C5-C4-N3	-3.21	119.97	123.96
2	r	202	JNI	C35-N34-C31	-3.20	116.39	121.69
2	v	201	JNI	C28-C33-N32	-3.20	119.05	124.32
2	b	201	JNI	C23-C22-C21	-3.20	115.73	120.91
2	V	202	JNI	C5-C6-N7	-3.19	118.32	123.53
2	n	201	JNI	C23-C22-C21	-3.18	115.76	120.91
2	V	201	JNI	N32-C31-N34	3.18	120.34	116.90
2	r	202	JNI	C27-C22-C21	3.18	125.88	120.61
2	P	201	JNI	N30-C31-N34	3.17	120.33	116.90
2	D	201	JNI	C28-C29-N30	-3.17	119.09	124.32
2	h	201	JNI	C5-C4-N3	-3.17	120.02	123.96
2	d	201	JNI	C9-N8-C6	3.16	123.15	118.17
2	H	202	JNI	C5-C4-N3	-3.16	120.04	123.96
2	j	201	JNI	C5-C4-N3	-3.16	120.04	123.96
2	n	201	JNI	C5-C4-N3	-3.15	120.04	123.96
2	h	202	JNI	N1-C2-N3	3.15	120.64	117.44
2	p	201	JNI	N1-C2-N3	3.14	120.63	117.44
2	r	202	JNI	C9-N8-C6	3.14	123.11	118.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	201	JNI	C28-C33-N32	-3.14	119.14	124.32
2	v	201	JNI	N1-C2-N3	3.12	120.60	117.44
2	v	202	JNI	C17-C16-N8	-3.11	113.62	119.23
2	b	201	JNI	C10-C9-N8	-3.11	108.95	113.98
2	f	201	JNI	C4-N3-C2	3.11	119.42	116.24
2	H	202	JNI	C17-C16-N8	-3.11	113.63	119.23
2	P	201	JNI	C28-C33-N32	-3.09	119.23	124.32
2	b	202	JNI	C5-C4-N3	-3.08	120.13	123.96
2	V	202	JNI	C25-C26-C28	-3.08	116.02	121.36
2	F	201	JNI	C28-C33-N32	-3.06	119.28	124.32
2	b	201	JNI	C17-C16-N8	-3.06	113.72	119.23
2	l	201	JNI	N3-C2-N7	-3.04	121.99	125.70
2	t	201	JNI	C28-C33-N32	-3.04	119.31	124.32
2	C	201	JNI	C28-C33-N32	-3.03	119.32	124.32
2	H	201	JNI	C10-C9-N8	-3.03	109.08	113.98
2	N	201	JNI	C10-C9-N8	-3.03	109.09	113.98
2	D	201	JNI	C5-C6-N7	-3.02	118.60	123.53
2	v	202	JNI	C35-N34-C31	-3.02	116.68	121.69
2	h	202	JNI	C17-C16-N8	-3.02	113.79	119.23
2	J	201	JNI	C5-C4-N3	-3.02	120.21	123.96
2	t	202	JNI	C5-C6-N7	-3.02	118.61	123.53
2	A	202	JNI	C9-N8-C16	3.01	123.31	117.78
2	F	202	JNI	C39-N34-C35	3.01	118.15	111.52
2	r	201	JNI	C28-C33-N32	-3.00	119.37	124.32
2	M	201	JNI	C5-C4-N3	-3.00	120.23	123.96
2	r	201	JNI	N32-C31-N34	2.99	120.14	116.90
2	V	201	JNI	C28-C33-N32	-2.99	119.39	124.32
2	J	201	JNI	N30-C31-N34	2.99	120.13	116.90
2	b	201	JNI	C27-C22-C21	2.98	125.54	120.61
2	F	202	JNI	C28-C33-N32	-2.97	119.42	124.32
2	l	201	JNI	N32-C31-N34	2.97	120.12	116.90
2	J	202	JNI	C28-C29-N30	-2.97	119.42	124.32
2	n	202	JNI	N30-C31-N34	2.97	120.11	116.90
2	Z	201	JNI	C28-C33-N32	-2.97	119.43	124.32
2	Z	201	JNI	N1-C2-N3	2.97	120.45	117.44
2	X	201	JNI	C5-C4-N3	-2.96	120.28	123.96
2	X	202	JNI	C5-C4-N3	-2.96	120.28	123.96
2	p	202	JNI	C28-C33-N32	-2.96	119.44	124.32
2	v	201	JNI	C5-C4-N3	-2.96	120.28	123.96
2	H	202	JNI	C38-C39-N34	2.95	116.87	110.48
2	n	201	JNI	C28-C29-N30	-2.94	119.47	124.32
2	o	201	JNI	C28-C29-N30	-2.94	119.48	124.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	201	JNI	C27-C22-C21	2.93	125.47	120.61
2	X	201	JNI	C28-C29-N30	-2.93	119.48	124.32
2	t	202	JNI	N30-C31-N34	2.93	120.07	116.90
2	h	201	JNI	C27-C26-C28	2.93	125.70	120.86
2	j	201	JNI	C28-C33-N32	-2.92	119.50	124.32
2	v	202	JNI	C28-C33-N32	-2.92	119.50	124.32
2	n	201	JNI	C28-C33-N32	-2.92	119.51	124.32
2	n	201	JNI	C25-C26-C28	-2.91	116.31	121.36
2	r	201	JNI	C25-C26-C28	-2.91	116.32	121.36
2	v	202	JNI	C25-C26-C28	-2.90	116.32	121.36
2	V	202	JNI	C35-N34-C31	-2.90	116.88	121.69
2	t	201	JNI	N3-C2-N7	-2.90	122.17	125.70
2	h	201	JNI	C28-C29-N30	-2.90	119.54	124.32
2	H	202	JNI	C25-C26-C28	-2.89	116.34	121.36
2	C	202	JNI	N3-C2-N7	-2.89	122.18	125.70
2	r	202	JNI	C28-C29-N30	-2.89	119.56	124.32
2	p	202	JNI	C5-C6-N7	-2.89	118.82	123.53
2	f	201	JNI	N3-C2-N7	-2.88	122.19	125.70
2	h	202	JNI	C5-C4-N3	-2.88	120.38	123.96
2	b	202	JNI	N1-C2-N7	2.87	121.72	117.25
2	Z	202	JNI	C28-C29-N30	-2.87	119.59	124.32
2	t	202	JNI	C28-C29-N30	-2.86	119.60	124.32
2	v	201	JNI	C25-C26-C28	-2.86	116.40	121.36
2	p	202	JNI	C23-C22-C21	-2.86	116.28	120.91
2	r	202	JNI	C22-C21-C16	2.86	127.55	123.19
2	p	202	JNI	C20-C21-C22	-2.85	113.05	118.68
2	b	201	JNI	C35-N34-C31	-2.85	116.97	121.69
2	v	201	JNI	C29-C28-C26	-2.84	116.74	121.69
2	j	202	JNI	C28-C29-N30	-2.84	119.64	124.32
2	C	201	JNI	C17-C16-N8	-2.84	114.12	119.23
2	j	202	JNI	C20-C21-C16	-2.83	115.15	117.86
2	X	202	JNI	C19-C20-C21	2.82	125.09	120.33
2	n	202	JNI	C28-C33-N32	-2.81	119.68	124.32
2	J	201	JNI	N32-C31-N34	2.81	119.94	116.90
2	h	202	JNI	C28-C33-N32	-2.81	119.69	124.32
2	n	201	JNI	C27-C22-C21	2.81	125.26	120.61
2	D	201	JNI	C28-C33-N32	-2.81	119.69	124.32
2	Z	201	JNI	C5-C4-N3	-2.79	120.49	123.96
2	l	201	JNI	C39-N34-C31	-2.79	117.06	121.69
2	n	201	JNI	C22-C21-C16	2.79	127.44	123.19
2	X	202	JNI	N1-C2-N7	2.78	121.58	117.25
2	v	202	JNI	C27-C22-C21	2.78	125.22	120.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	X	201	JNI	C10-C9-N8	-2.78	109.49	113.98
2	f	201	JNI	C9-N8-C6	2.77	122.53	118.17
2	H	201	JNI	C28-C33-N32	-2.77	119.75	124.32
2	d	201	JNI	C28-C33-N32	-2.77	119.75	124.32
2	v	202	JNI	C39-N34-C31	-2.76	117.11	121.69
2	p	201	JNI	C28-C29-N30	-2.76	119.77	124.32
2	f	202	JNI	C5-C6-N7	-2.76	119.03	123.53
2	P	202	JNI	C28-C33-N32	-2.76	119.78	124.32
2	J	202	JNI	C25-C26-C28	-2.76	116.58	121.36
2	t	201	JNI	N32-C31-N34	2.75	119.88	116.90
2	H	202	JNI	C35-C36-N37	2.75	118.24	111.12
2	J	202	JNI	C28-C33-N32	-2.75	119.79	124.32
2	Z	202	JNI	C16-N8-C6	2.74	124.26	121.20
2	V	201	JNI	N7-C6-N8	2.74	118.38	115.77
2	j	201	JNI	C9-N8-C16	2.74	122.82	117.78
2	X	201	JNI	C39-N34-C35	2.74	117.57	111.52
2	C	202	JNI	C28-C29-N30	-2.74	119.80	124.32
2	n	202	JNI	C19-C20-C21	2.73	124.95	120.33
2	t	202	JNI	C16-N8-C6	-2.72	118.17	121.20
2	l	201	JNI	N7-C6-N8	2.71	118.35	115.77
2	C	202	JNI	C5-C6-N7	-2.71	119.11	123.53
2	b	201	JNI	C28-C29-N30	-2.70	119.86	124.32
2	f	201	JNI	C28-C33-N32	-2.69	119.88	124.32
2	r	202	JNI	C28-C33-N32	-2.69	119.88	124.32
2	M	201	JNI	C5-C6-N8	2.69	126.40	121.24
2	n	202	JNI	C28-C29-N30	-2.68	119.90	124.32
2	h	201	JNI	N7-C6-N8	2.68	118.32	115.77
2	X	201	JNI	C5-C6-N8	2.67	126.36	121.24
2	v	201	JNI	C28-C29-N30	-2.67	119.92	124.32
2	X	202	JNI	C9-N8-C6	2.67	122.37	118.17
2	b	202	JNI	C23-C22-C27	-2.66	114.40	118.16
2	b	201	JNI	C27-C26-C28	2.66	125.26	120.86
2	R	201	JNI	C28-C33-N32	-2.66	119.94	124.32
2	j	202	JNI	C39-N34-C31	-2.66	117.28	121.69
2	p	202	JNI	C25-C26-C28	-2.65	116.77	121.36
2	d	201	JNI	C27-C22-C21	2.64	124.99	120.61
2	N	201	JNI	N3-C2-N7	-2.64	122.48	125.70
2	l	201	JNI	C10-C9-N8	-2.64	109.71	113.98
2	b	202	JNI	C16-N8-C6	2.64	124.14	121.20
2	U	201	JNI	C5-C4-N3	-2.64	120.68	123.96
2	h	202	JNI	C28-C29-N30	-2.64	119.97	124.32
2	b	202	JNI	C19-C20-C21	2.63	124.77	120.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	h	202	JNI	C22-C21-C16	2.63	127.19	123.19
2	L	201	JNI	C29-C28-C26	2.62	126.27	121.69
2	n	202	JNI	N1-C2-N3	2.62	120.10	117.44
2	b	202	JNI	C24-C23-C22	2.62	123.85	120.56
2	R	201	JNI	C28-C29-N30	-2.61	120.01	124.32
2	A	201	JNI	C5-C6-N7	-2.61	119.27	123.53
2	f	202	JNI	C28-C33-N32	-2.60	120.03	124.32
2	t	201	JNI	C28-C29-N30	-2.60	120.04	124.32
2	U	201	JNI	C5-C6-N8	2.59	126.21	121.24
2	X	202	JNI	C25-C26-C28	-2.59	116.87	121.36
2	J	201	JNI	C28-C29-N30	-2.59	120.05	124.32
2	n	201	JNI	C5-C6-N7	-2.59	119.31	123.53
2	M	201	JNI	C28-C33-N32	-2.58	120.07	124.32
2	F	201	JNI	C39-N34-C31	-2.58	117.41	121.69
2	H	202	JNI	C16-N8-C6	2.58	124.07	121.20
2	f	201	JNI	C28-C29-N30	-2.58	120.07	124.32
2	r	201	JNI	C28-C29-N30	-2.57	120.08	124.32
2	A	202	JNI	C29-C28-C33	2.57	118.67	114.66
2	v	201	JNI	C17-C16-N8	-2.56	114.62	119.23
2	U	201	JNI	C16-N8-C6	2.56	124.05	121.20
2	L	201	JNI	C9-N8-C16	-2.56	113.08	117.78
2	H	201	JNI	C28-C29-N30	-2.55	120.11	124.32
2	Z	202	JNI	C5-C6-N7	-2.55	119.37	123.53
2	N	201	JNI	N30-C31-N34	2.54	119.65	116.90
2	Z	202	JNI	N1-C2-N3	2.53	120.01	117.44
2	d	201	JNI	C23-C22-C21	-2.53	116.81	120.91
2	t	201	JNI	C9-N8-C6	2.53	122.15	118.17
2	V	202	JNI	C28-C29-N30	-2.53	120.15	124.32
2	U	201	JNI	C28-C33-N32	-2.53	120.15	124.32
2	X	201	JNI	C25-C26-C28	-2.52	116.99	121.36
2	l	201	JNI	C9-N8-C6	2.52	122.14	118.17
2	b	202	JNI	C27-C26-C28	2.52	125.03	120.86
2	R	201	JNI	C25-C26-C28	-2.52	117.00	121.36
2	F	202	JNI	N1-C2-N3	2.51	119.99	117.44
2	C	202	JNI	C22-C21-C16	-2.50	119.37	123.19
2	R	201	JNI	C5-C6-N7	-2.50	119.45	123.53
2	t	202	JNI	C28-C33-N32	-2.50	120.20	124.32
2	d	201	JNI	C9-C10-C15	2.50	125.46	120.77
2	F	201	JNI	C28-C29-N30	-2.49	120.21	124.32
2	U	201	JNI	C22-C21-C16	2.49	126.99	123.19
2	L	201	JNI	C5-C4-N3	-2.49	120.86	123.96
2	l	201	JNI	C28-C29-N30	-2.49	120.22	124.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	X	201	JNI	C28-C33-N32	-2.48	120.22	124.32
2	C	202	JNI	C10-C9-N8	-2.48	109.97	113.98
2	t	201	JNI	C25-C26-C28	-2.48	117.06	121.36
2	f	201	JNI	C20-C21-C22	-2.48	113.79	118.68
2	J	202	JNI	C5-C6-N7	-2.48	119.49	123.53
2	Z	202	JNI	C28-C33-N32	-2.47	120.24	124.32
2	L	201	JNI	C23-C22-C27	-2.47	114.67	118.16
2	F	201	JNI	N1-C2-N3	2.47	119.94	117.44
2	b	202	JNI	C28-C29-N30	-2.47	120.25	124.32
2	t	202	JNI	C27-C22-C21	2.47	124.70	120.61
2	h	201	JNI	C27-C22-C21	2.46	124.69	120.61
2	J	201	JNI	C20-C21-C16	2.46	120.21	117.86
2	X	202	JNI	C9-N8-C16	-2.45	113.27	117.78
2	F	202	JNI	C29-C28-C33	2.45	118.48	114.66
2	j	202	JNI	C27-C22-C21	2.45	124.67	120.61
2	b	201	JNI	C22-C21-C16	2.45	126.92	123.19
2	p	202	JNI	C17-C16-N8	-2.44	114.83	119.23
2	v	202	JNI	C10-C9-N8	2.44	117.92	113.98
2	D	201	JNI	N1-C2-N3	2.44	119.91	117.44
2	v	202	JNI	N1-C2-N7	2.43	121.04	117.25
2	o	201	JNI	C28-C33-N32	-2.43	120.31	124.32
2	X	202	JNI	C29-C28-C26	-2.43	117.46	121.69
2	h	201	JNI	C28-C33-N32	-2.43	120.32	124.32
2	r	202	JNI	C18-C17-C16	2.43	123.35	118.26
2	X	202	JNI	C33-C28-C26	2.43	125.92	121.69
2	b	201	JNI	C25-C26-C28	-2.42	117.16	121.36
2	Z	202	JNI	C39-N34-C31	-2.42	117.67	121.69
2	N	201	JNI	C29-C28-C33	2.42	118.43	114.66
2	C	201	JNI	C20-C21-C22	-2.42	113.90	118.68
2	P	201	JNI	C29-C28-C33	2.41	118.43	114.66
2	X	202	JNI	C16-N8-C6	2.41	123.89	121.20
2	Z	202	JNI	C35-N34-C31	-2.41	117.69	121.69
2	V	201	JNI	C28-C29-N30	-2.41	120.34	124.32
2	P	201	JNI	C5-C6-N7	-2.41	119.59	123.53
2	l	201	JNI	C36-C35-N34	2.40	115.69	110.48
2	p	202	JNI	C16-N8-C6	-2.40	118.52	121.20
2	f	201	JNI	N1-C2-N7	-2.40	113.52	117.25
2	Z	202	JNI	C25-C26-C28	-2.40	117.20	121.36
2	U	201	JNI	C28-C29-N30	-2.40	120.37	124.32
2	J	201	JNI	C9-N8-C6	2.39	121.94	118.17
2	X	201	JNI	C23-C22-C21	-2.39	117.03	120.91
2	P	201	JNI	C9-N8-C16	2.39	122.18	117.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	b	202	JNI	C28-C33-N32	-2.39	120.38	124.32
2	v	201	JNI	N30-C31-N34	-2.38	114.31	116.90
2	r	201	JNI	C27-C26-C28	2.38	124.80	120.86
2	h	201	JNI	N1-C2-N3	2.37	119.85	117.44
2	X	202	JNI	C18-C17-C16	2.37	123.22	118.26
2	r	202	JNI	C16-N8-C6	-2.37	118.56	121.20
2	f	202	JNI	N1-C2-N3	2.36	119.83	117.44
2	R	201	JNI	C27-C26-C28	2.36	124.76	120.86
2	Z	202	JNI	N32-C31-N34	2.36	119.45	116.90
2	v	202	JNI	C28-C29-N30	-2.36	120.44	124.32
2	P	202	JNI	C5-C6-N7	-2.35	119.69	123.53
2	F	201	JNI	C23-C22-C21	-2.35	117.10	120.91
2	j	202	JNI	C38-N37-C36	2.35	117.09	110.34
2	d	201	JNI	C35-N34-C31	-2.35	117.80	121.69
2	P	202	JNI	N32-C31-N34	2.34	119.44	116.90
2	A	201	JNI	C9-N8-C6	2.34	121.86	118.17
2	L	201	JNI	C24-C23-C22	2.34	123.50	120.56
2	M	201	JNI	C16-N8-C6	2.34	123.81	121.20
2	Q	201	JNI	N1-C2-N3	2.33	119.81	117.44
2	F	202	JNI	C33-C28-C26	-2.33	117.63	121.69
2	X	202	JNI	C27-C22-C21	2.33	124.46	120.61
2	L	201	JNI	C35-C36-N37	2.32	117.14	111.12
2	r	202	JNI	C39-N34-C31	-2.32	117.84	121.69
2	r	201	JNI	C17-C16-N8	-2.32	115.05	119.23
2	M	201	JNI	C18-C17-C16	2.32	123.12	118.26
2	v	201	JNI	C33-C28-C26	2.32	125.74	121.69
2	r	202	JNI	C19-C20-C21	2.31	124.23	120.33
2	Q	201	JNI	C28-C33-N32	-2.31	120.52	124.32
2	Z	201	JNI	C28-C29-N30	-2.31	120.52	124.32
2	H	202	JNI	N1-C2-N7	2.30	120.83	117.25
2	h	201	JNI	C16-N8-C6	-2.30	118.64	121.20
2	L	201	JNI	C25-C26-C28	-2.30	117.38	121.36
2	L	201	JNI	C19-C20-C21	2.29	124.19	120.33
2	F	201	JNI	C5-C4-N3	-2.28	121.12	123.96
2	n	201	JNI	N1-C2-N3	2.28	119.75	117.44
2	C	201	JNI	C29-C28-C33	2.28	118.21	114.66
2	p	202	JNI	N30-C31-N34	2.28	119.36	116.90
2	V	202	JNI	C39-N34-C31	-2.27	117.92	121.69
2	Z	201	JNI	C38-N37-C36	2.27	116.87	110.34
2	V	202	JNI	C29-C28-C33	2.27	118.20	114.66
2	L	201	JNI	C18-C17-C16	2.26	123.00	118.26
2	L	201	JNI	C28-C29-N30	-2.26	120.60	124.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	b	201	JNI	C5-C6-N8	2.26	125.57	121.24
2	Z	202	JNI	C23-C22-C21	-2.26	117.25	120.91
2	C	202	JNI	C9-N8-C16	2.25	121.92	117.78
2	L	201	JNI	C38-N37-C36	2.25	116.81	110.34
2	H	202	JNI	C20-C21-C22	-2.25	114.24	118.68
2	f	202	JNI	C22-C21-C16	2.25	126.62	123.19
2	M	201	JNI	C25-C26-C28	-2.25	117.47	121.36
2	C	201	JNI	C5-C6-N7	-2.24	119.87	123.53
2	A	202	JNI	C5-C6-N7	-2.24	119.87	123.53
2	v	202	JNI	C22-C21-C16	2.24	126.61	123.19
2	n	202	JNI	C24-C23-C22	2.24	123.37	120.56
2	U	201	JNI	C17-C16-N8	-2.23	115.20	119.23
2	P	202	JNI	C29-C28-C33	2.23	118.14	114.66
2	r	201	JNI	N30-C31-N34	2.23	119.31	116.90
2	U	201	JNI	C20-C21-C22	-2.23	114.28	118.68
2	P	202	JNI	C5-C4-N3	-2.22	121.20	123.96
2	C	202	JNI	C20-C21-C16	2.22	119.99	117.86
2	t	202	JNI	C25-C26-C28	-2.22	117.50	121.36
2	d	201	JNI	C28-C29-N30	-2.22	120.66	124.32
2	l	201	JNI	N1-C2-N3	2.21	119.68	117.44
2	h	201	JNI	C38-C39-N34	2.21	115.26	110.48
2	l	201	JNI	C39-N34-C35	2.20	116.38	111.52
2	p	202	JNI	N1-C2-N7	2.20	120.67	117.25
2	F	201	JNI	N7-C6-N8	2.20	117.86	115.77
2	H	202	JNI	C28-C29-N30	-2.19	120.71	124.32
2	n	202	JNI	C23-C22-C21	-2.19	117.36	120.91
2	j	202	JNI	C36-C35-N34	-2.19	105.75	110.48
2	X	201	JNI	C27-C26-C28	2.18	124.47	120.86
2	v	201	JNI	C35-N34-C31	-2.18	118.07	121.69
2	r	202	JNI	C27-C26-C28	2.18	124.47	120.86
2	n	201	JNI	N30-C31-N34	2.17	119.25	116.90
2	H	202	JNI	C18-C17-C16	2.17	122.81	118.26
2	N	201	JNI	N32-C31-N34	2.17	119.24	116.90
2	X	202	JNI	C24-C23-C22	2.17	123.28	120.56
2	L	201	JNI	C27-C26-C28	2.16	124.44	120.86
2	Z	201	JNI	C39-N34-C35	2.16	116.29	111.52
2	b	202	JNI	C18-C17-C16	2.16	122.79	118.26
2	t	202	JNI	C9-N8-C6	2.16	121.56	118.17
2	Z	202	JNI	C29-C28-C26	2.15	125.45	121.69
2	J	202	JNI	N7-C6-N8	2.15	117.82	115.77
2	j	202	JNI	C19-C20-C21	2.15	123.96	120.33
2	R	201	JNI	C38-N37-C36	2.15	116.51	110.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	o	201	JNI	C20-C21-C22	-2.15	114.44	118.68
2	p	202	JNI	C27-C22-C21	2.15	124.17	120.61
2	j	202	JNI	C29-C28-C33	2.15	118.01	114.66
2	A	201	JNI	C29-C28-C33	2.14	118.00	114.66
2	p	202	JNI	C29-C28-C33	2.14	118.00	114.66
2	t	201	JNI	C27-C26-C28	2.14	124.39	120.86
2	n	201	JNI	C16-N8-C6	-2.13	118.83	121.20
2	J	202	JNI	N30-C31-N34	2.13	119.20	116.90
2	l	201	JNI	C28-C33-N32	-2.13	120.81	124.32
2	o	201	JNI	C22-C21-C16	2.13	126.43	123.19
2	j	201	JNI	C5-C6-N8	2.13	125.32	121.24
2	h	201	JNI	C17-C16-N8	-2.12	115.41	119.23
2	C	201	JNI	N1-C2-N7	2.12	120.55	117.25
2	p	202	JNI	C9-N8-C6	2.12	121.50	118.17
2	d	201	JNI	N1-C2-N3	2.11	119.58	117.44
2	n	202	JNI	C18-C17-C16	2.11	122.69	118.26
2	J	201	JNI	C29-C28-C33	2.11	117.95	114.66
2	r	202	JNI	C23-C22-C27	-2.10	115.19	118.16
2	A	202	JNI	C25-C26-C28	-2.10	117.72	121.36
2	p	201	JNI	N7-C6-N8	2.09	117.76	115.77
2	j	201	JNI	C18-C17-C16	2.09	122.64	118.26
2	X	201	JNI	C38-C39-N34	2.09	115.00	110.48
2	t	202	JNI	C20-C21-C22	-2.09	114.56	118.68
2	F	202	JNI	C20-C21-C16	2.08	119.85	117.86
2	V	201	JNI	C38-N37-C36	2.08	116.32	110.34
2	Z	202	JNI	C33-C28-C26	-2.08	118.08	121.69
2	F	202	JNI	C5-C6-N7	-2.07	120.15	123.53
2	A	202	JNI	N1-C2-N3	2.07	119.54	117.44
2	j	201	JNI	C22-C21-C16	2.07	126.34	123.19
2	n	201	JNI	C36-C35-N34	2.07	114.96	110.48
2	r	202	JNI	C24-C23-C22	2.06	123.15	120.56
2	n	201	JNI	C17-C16-N8	-2.06	115.52	119.23
2	f	202	JNI	C28-C29-N30	-2.06	120.93	124.32
2	F	201	JNI	C38-N37-C36	2.06	116.25	110.34
2	j	201	JNI	C17-C16-N8	-2.06	115.53	119.23
2	r	202	JNI	C10-C9-N8	2.05	117.30	113.98
2	v	201	JNI	C27-C26-C28	2.05	124.25	120.86
2	D	201	JNI	C20-C21-C16	2.05	119.82	117.86
2	C	201	JNI	C27-C26-C28	2.05	124.25	120.86
2	P	201	JNI	C25-C26-C28	-2.05	117.81	121.36
2	X	202	JNI	C28-C29-N30	-2.04	120.95	124.32
2	r	201	JNI	C16-N8-C6	-2.04	118.93	121.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	V	201	JNI	C22-C21-C16	2.04	126.30	123.19
2	t	202	JNI	C22-C21-C16	2.04	126.30	123.19
2	h	202	JNI	C20-C21-C22	-2.03	114.67	118.68
2	o	201	JNI	C17-C16-N8	-2.03	115.58	119.23
2	U	201	JNI	C18-C17-C16	2.03	122.52	118.26
2	P	202	JNI	C10-C9-N8	-2.02	110.71	113.98
2	v	202	JNI	N30-C31-N34	2.02	119.08	116.90
2	V	201	JNI	N30-C31-N34	2.01	119.08	116.90

There are no chirality outliers.

All (330) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	v	201	JNI	N30-C31-N34-C39
2	v	201	JNI	N32-C31-N34-C39
2	Z	201	JNI	N32-C31-N34-C35
2	J	202	JNI	C5-C6-N8-C16
2	J	202	JNI	N7-C6-N8-C16
2	J	202	JNI	N7-C6-N8-C9
2	J	202	JNI	N30-C31-N34-C35
2	J	202	JNI	N32-C31-N34-C35
2	t	201	JNI	N30-C31-N34-C35
2	t	201	JNI	N32-C31-N34-C35
2	r	201	JNI	N30-C31-N34-C39
2	r	201	JNI	N32-C31-N34-C35
2	r	201	JNI	N32-C31-N34-C39
2	F	201	JNI	N30-C31-N34-C39
2	F	201	JNI	N32-C31-N34-C39
2	j	201	JNI	N30-C31-N34-C35
2	j	201	JNI	N32-C31-N34-C35
2	Z	202	JNI	C5-C6-N8-C16
2	C	202	JNI	C5-C6-N8-C16
2	C	202	JNI	N7-C6-N8-C16
2	C	202	JNI	N32-C31-N34-C39
2	P	202	JNI	C16-C21-C22-C23
2	P	202	JNI	C16-C21-C22-C27
2	P	202	JNI	N30-C31-N34-C35
2	P	202	JNI	N30-C31-N34-C39
2	P	202	JNI	N32-C31-N34-C35
2	P	202	JNI	N32-C31-N34-C39
2	t	202	JNI	N30-C31-N34-C35
2	t	202	JNI	N32-C31-N34-C35

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Mol	Chain	Res	Type	Atoms
2	H	202	JNI	N30-C31-N34-C39
2	H	202	JNI	N32-C31-N34-C39
2	n	201	JNI	N30-C31-N34-C35
2	n	201	JNI	N32-C31-N34-C35
2	j	202	JNI	N30-C31-N34-C35
2	j	202	JNI	N32-C31-N34-C35
2	f	201	JNI	N30-C31-N34-C39
2	b	202	JNI	N30-C31-N34-C35
2	b	202	JNI	N32-C31-N34-C35
2	f	202	JNI	C5-C6-N8-C16
2	f	202	JNI	C5-C6-N8-C9
2	f	202	JNI	N7-C6-N8-C16
2	f	202	JNI	N30-C31-N34-C35
2	f	202	JNI	N30-C31-N34-C39
2	f	202	JNI	N32-C31-N34-C35
2	f	202	JNI	N32-C31-N34-C39
2	b	201	JNI	N32-C31-N34-C39
2	p	202	JNI	C5-C6-N8-C16
2	p	202	JNI	N30-C31-N34-C35
2	p	202	JNI	N30-C31-N34-C39
2	p	202	JNI	N32-C31-N34-C35
2	p	202	JNI	N32-C31-N34-C39
2	r	202	JNI	N30-C31-N34-C35
2	r	202	JNI	N32-C31-N34-C35
2	h	202	JNI	N30-C31-N34-C39
2	h	202	JNI	N32-C31-N34-C39
2	Q	201	JNI	N30-C31-N34-C39
2	Q	201	JNI	N32-C31-N34-C39
2	n	202	JNI	N30-C31-N34-C35
2	n	202	JNI	N32-C31-N34-C35
2	n	202	JNI	N32-C31-N34-C39
2	H	201	JNI	C5-C6-N8-C16
2	L	201	JNI	C10-C9-N8-C6
2	M	201	JNI	N30-C31-N34-C39
2	M	201	JNI	N32-C31-N34-C39
2	D	201	JNI	N32-C31-N34-C39
2	V	201	JNI	N30-C31-N34-C35
2	V	201	JNI	N30-C31-N34-C39
2	V	201	JNI	N32-C31-N34-C35
2	V	201	JNI	N32-C31-N34-C39
2	A	202	JNI	C21-C16-N8-C9
2	p	201	JNI	N30-C31-N34-C39

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Mol	Chain	Res	Type	Atoms
2	p	201	JNI	N32-C31-N34-C39
2	h	201	JNI	N30-C31-N34-C39
2	l	201	JNI	N30-C31-N34-C35
2	l	201	JNI	N32-C31-N34-C35
2	o	201	JNI	C5-C6-N8-C16
2	o	201	JNI	N7-C6-N8-C16
2	o	201	JNI	N30-C31-N34-C39
2	o	201	JNI	N32-C31-N34-C39
2	X	202	JNI	N32-C31-N34-C35
2	d	201	JNI	N30-C31-N34-C39
2	d	201	JNI	N32-C31-N34-C39
2	v	201	JNI	C27-C26-C28-C33
2	F	202	JNI	N30-C31-N34-C39
2	D	201	JNI	N30-C31-N34-C39
2	A	202	JNI	N30-C31-N34-C39
2	R	201	JNI	N30-C31-N34-C39
2	h	201	JNI	N32-C31-N34-C39
2	A	201	JNI	N32-C31-N34-C35
2	v	201	JNI	C27-C26-C28-C29
2	v	201	JNI	C25-C26-C28-C33
2	v	201	JNI	C25-C26-C28-C29
2	P	202	JNI	C20-C21-C22-C23
2	P	202	JNI	C20-C21-C22-C27
2	X	202	JNI	C20-C21-C22-C27
2	F	202	JNI	C25-C26-C28-C29
2	p	202	JNI	C27-C26-C28-C33
2	p	202	JNI	C25-C26-C28-C29
2	F	202	JNI	C27-C26-C28-C33
2	V	202	JNI	C27-C26-C28-C29
2	h	202	JNI	C27-C26-C28-C29
2	h	202	JNI	C25-C26-C28-C33
2	Z	201	JNI	N30-C31-N34-C35
2	r	201	JNI	N30-C31-N34-C35
2	C	202	JNI	N30-C31-N34-C39
2	j	202	JNI	N30-C31-N34-C39
2	f	201	JNI	N32-C31-N34-C39
2	b	201	JNI	N30-C31-N34-C39
2	n	202	JNI	N30-C31-N34-C39
2	l	201	JNI	N30-C31-N34-C39
2	X	202	JNI	N30-C31-N34-C35
2	b	202	JNI	C20-C21-C22-C27
2	V	202	JNI	C25-C26-C28-C33

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Mol	Chain	Res	Type	Atoms
2	b	202	JNI	C16-C21-C22-C23
2	b	202	JNI	C16-C21-C22-C27
2	X	202	JNI	C16-C21-C22-C27
2	r	202	JNI	C20-C21-C22-C27
2	X	202	JNI	C20-C21-C22-C23
2	b	202	JNI	C20-C21-C22-C23
2	r	201	JNI	C25-C26-C28-C33
2	F	201	JNI	N32-C31-N34-C35
2	Z	202	JNI	N32-C31-N34-C35
2	h	202	JNI	N32-C31-N34-C35
2	r	202	JNI	C16-C21-C22-C27
2	F	202	JNI	C27-C26-C28-C29
2	r	202	JNI	C20-C21-C22-C23
2	j	202	JNI	C20-C21-C22-C27
2	v	201	JNI	N30-C31-N34-C35
2	F	202	JNI	N32-C31-N34-C39
2	j	202	JNI	N32-C31-N34-C39
2	v	202	JNI	N32-C31-N34-C35
2	H	201	JNI	N32-C31-N34-C39
2	A	202	JNI	N32-C31-N34-C39
2	R	201	JNI	N32-C31-N34-C39
2	A	201	JNI	N30-C31-N34-C35
2	d	201	JNI	N32-C31-N34-C35
2	C	201	JNI	C20-C21-C22-C27
2	n	202	JNI	C20-C21-C22-C27
2	r	202	JNI	C16-C21-C22-C23
2	X	202	JNI	C16-C21-C22-C23
2	r	201	JNI	C27-C26-C28-C29
2	F	202	JNI	C25-C26-C28-C33
2	p	202	JNI	C27-C26-C28-C29
2	p	202	JNI	C25-C26-C28-C33
2	h	202	JNI	C27-C26-C28-C33
2	h	202	JNI	C25-C26-C28-C29
2	F	201	JNI	N30-C31-N34-C35
2	Z	202	JNI	N30-C31-N34-C35
2	l	201	JNI	N32-C31-N34-C39
2	V	202	JNI	C27-C26-C28-C33
2	j	202	JNI	C16-C21-C22-C27
2	v	201	JNI	N32-C31-N34-C35
2	v	202	JNI	N30-C31-N34-C35
2	H	201	JNI	N30-C31-N34-C39
2	C	201	JNI	C20-C21-C22-C23

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Mol	Chain	Res	Type	Atoms
2	h	202	JNI	N30-C31-N34-C35
2	d	201	JNI	N30-C31-N34-C35
2	j	202	JNI	C20-C21-C22-C23
2	C	201	JNI	C16-C21-C22-C27
2	Z	202	JNI	N7-C6-N8-C9
2	C	202	JNI	N7-C6-N8-C9
2	n	201	JNI	N7-C6-N8-C9
2	f	202	JNI	N7-C6-N8-C9
2	p	202	JNI	N7-C6-N8-C9
2	H	201	JNI	N7-C6-N8-C9
2	A	202	JNI	N7-C6-N8-C9
2	U	201	JNI	N7-C6-N8-C9
2	o	201	JNI	N7-C6-N8-C9
2	J	202	JNI	C5-C6-N8-C9
2	Z	202	JNI	C5-C6-N8-C9
2	C	202	JNI	C5-C6-N8-C9
2	t	202	JNI	C5-C6-N8-C9
2	n	201	JNI	C5-C6-N8-C9
2	p	202	JNI	C5-C6-N8-C9
2	H	201	JNI	C5-C6-N8-C9
2	o	201	JNI	C5-C6-N8-C9
2	n	202	JNI	C16-C21-C22-C27
2	F	202	JNI	N7-C6-N8-C16
2	Z	202	JNI	N7-C6-N8-C16
2	p	202	JNI	N7-C6-N8-C16
2	r	202	JNI	N7-C6-N8-C16
2	P	201	JNI	N7-C6-N8-C16
2	H	201	JNI	N7-C6-N8-C16
2	A	202	JNI	N7-C6-N8-C16
2	U	201	JNI	N7-C6-N8-C16
2	t	202	JNI	C5-C6-N8-C16
2	n	201	JNI	C5-C6-N8-C16
2	A	202	JNI	C5-C6-N8-C16
2	U	201	JNI	C5-C6-N8-C16
2	r	201	JNI	C27-C26-C28-C33
2	V	202	JNI	C25-C26-C28-C29
2	n	202	JNI	C20-C21-C22-C23
2	P	202	JNI	C10-C9-N8-C6
2	H	202	JNI	C10-C9-N8-C6
2	b	202	JNI	C10-C9-N8-C6
2	C	201	JNI	C10-C9-N8-C6
2	r	202	JNI	C10-C9-N8-C6

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Mol	Chain	Res	Type	Atoms
2	n	202	JNI	C10-C9-N8-C6
2	V	202	JNI	N32-C31-N34-C35
2	C	201	JNI	N30-C31-N34-C35
2	C	201	JNI	N32-C31-N34-C35
2	C	201	JNI	C16-C21-C22-C23
2	j	202	JNI	C16-C21-C22-C23
2	r	201	JNI	C25-C26-C28-C29
2	V	202	JNI	N30-C31-N34-C35
2	F	202	JNI	N7-C6-N8-C9
2	V	202	JNI	N7-C6-N8-C9
2	P	201	JNI	N7-C6-N8-C9
2	F	202	JNI	C5-C6-N8-C9
2	U	201	JNI	C5-C6-N8-C9
2	j	202	JNI	C25-C26-C28-C29
2	t	202	JNI	N7-C6-N8-C16
2	V	202	JNI	N7-C6-N8-C16
2	n	201	JNI	N7-C6-N8-C16
2	b	201	JNI	N7-C6-N8-C16
2	L	201	JNI	N7-C6-N8-C16
2	J	202	JNI	C27-C26-C28-C33
2	J	202	JNI	C25-C26-C28-C29
2	P	202	JNI	C10-C9-N8-C16
2	H	202	JNI	C10-C9-N8-C16
2	C	201	JNI	C10-C9-N8-C16
2	r	202	JNI	C10-C9-N8-C16
2	L	201	JNI	C10-C9-N8-C16
2	F	202	JNI	C5-C6-N8-C16
2	V	202	JNI	C5-C6-N8-C16
2	J	201	JNI	N30-C31-N34-C39
2	U	201	JNI	N30-C31-N34-C35
2	P	202	JNI	C27-C26-C28-C33
2	n	201	JNI	C27-C26-C28-C33
2	n	202	JNI	C16-C21-C22-C23
2	n	201	JNI	C25-C26-C28-C29
2	P	202	JNI	C25-C26-C28-C29
2	j	202	JNI	C10-C9-N8-C6
2	t	202	JNI	N7-C6-N8-C9
2	r	202	JNI	N7-C6-N8-C9
2	V	202	JNI	C5-C6-N8-C9
2	A	202	JNI	C17-C16-N8-C9
2	J	201	JNI	N32-C31-N34-C39
2	j	201	JNI	N7-C6-N8-C16

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Mol	Chain	Res	Type	Atoms
2	b	202	JNI	N7-C6-N8-C16
2	C	201	JNI	N7-C6-N8-C16
2	Q	201	JNI	N7-C6-N8-C16
2	M	201	JNI	N7-C6-N8-C16
2	X	201	JNI	N7-C6-N8-C16
2	b	202	JNI	C5-C6-N8-C16
2	r	202	JNI	C5-C6-N8-C16
2	P	201	JNI	C5-C6-N8-C16
2	Q	201	JNI	C5-C6-N8-C16
2	L	201	JNI	C5-C6-N8-C16
2	M	201	JNI	C5-C6-N8-C16
2	X	201	JNI	C5-C6-N8-C16
2	v	202	JNI	C20-C21-C22-C27
2	n	202	JNI	C25-C26-C28-C29
2	U	201	JNI	N32-C31-N34-C35
2	J	202	JNI	C27-C26-C28-C29
2	b	202	JNI	N7-C6-N8-C9
2	V	201	JNI	N7-C6-N8-C9
2	A	202	JNI	C5-C6-N8-C9
2	P	202	JNI	C27-C26-C28-C29
2	n	201	JNI	C27-C26-C28-C29
2	F	202	JNI	C10-C9-N8-C6
2	b	202	JNI	C10-C9-N8-C16
2	v	202	JNI	C16-C21-C22-C27
2	V	201	JNI	C5-C6-N8-C9
2	J	202	JNI	C25-C26-C28-C33
2	P	202	JNI	C25-C26-C28-C33
2	j	202	JNI	C27-C26-C28-C33
2	X	201	JNI	N30-C31-N34-C35
2	X	201	JNI	N32-C31-N34-C35
2	n	201	JNI	C25-C26-C28-C33
2	j	202	JNI	C27-C26-C28-C29
2	P	201	JNI	N32-C31-N34-C39
2	j	202	JNI	N7-C6-N8-C9
2	j	202	JNI	C5-C6-N8-C9
2	v	202	JNI	C5-C6-N8-C9
2	o	201	JNI	N32-C31-N34-C35
2	o	201	JNI	N30-C31-N34-C35
2	f	201	JNI	N7-C6-N8-C16
2	v	202	JNI	N7-C6-N8-C16
2	V	201	JNI	N7-C6-N8-C16
2	X	202	JNI	N7-C6-N8-C16

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Mol	Chain	Res	Type	Atoms
2	j	202	JNI	C10-C9-N8-C16
2	n	202	JNI	C10-C9-N8-C16
2	C	201	JNI	C5-C6-N8-C16
2	b	201	JNI	C5-C6-N8-C16
2	v	202	JNI	C5-C6-N8-C16
2	j	202	JNI	C25-C26-C28-C33
2	v	202	JNI	N7-C6-N8-C9
2	n	202	JNI	N7-C6-N8-C9
2	p	201	JNI	N7-C6-N8-C9
2	b	202	JNI	C5-C6-N8-C9
2	r	202	JNI	C5-C6-N8-C9
2	P	201	JNI	C5-C6-N8-C9
2	P	201	JNI	N30-C31-N34-C39
2	v	202	JNI	C20-C21-C22-C23
2	j	202	JNI	N7-C6-N8-C16
2	N	201	JNI	C5-C6-N8-C16
2	n	202	JNI	C5-C6-N8-C16
2	X	202	JNI	C5-C6-N8-C16
2	t	202	JNI	C20-C21-C22-C27
2	f	201	JNI	N7-C6-N8-C9
2	Q	201	JNI	N7-C6-N8-C9
2	X	202	JNI	N7-C6-N8-C9
2	Z	202	JNI	C20-C21-C22-C23
2	Z	202	JNI	C20-C21-C22-C27
2	t	202	JNI	C20-C21-C22-C23
2	f	201	JNI	C5-C6-N8-C9
2	n	202	JNI	C5-C6-N8-C9
2	p	201	JNI	C5-C6-N8-C9
2	C	202	JNI	C20-C21-C22-C27
2	n	202	JNI	C27-C26-C28-C29
2	C	202	JNI	C20-C21-C22-C23
2	f	201	JNI	C5-C6-N8-C16
2	X	201	JNI	N7-C6-N8-C9
2	X	202	JNI	C5-C6-N8-C9
2	J	202	JNI	N30-C31-N34-C39
2	Z	202	JNI	C16-C21-C22-C27
2	t	202	JNI	C16-C21-C22-C27
2	p	202	JNI	C20-C21-C22-C27
2	n	202	JNI	N7-C6-N8-C16
2	p	201	JNI	N7-C6-N8-C16
2	C	201	JNI	N7-C6-N8-C9
2	M	201	JNI	N7-C6-N8-C9

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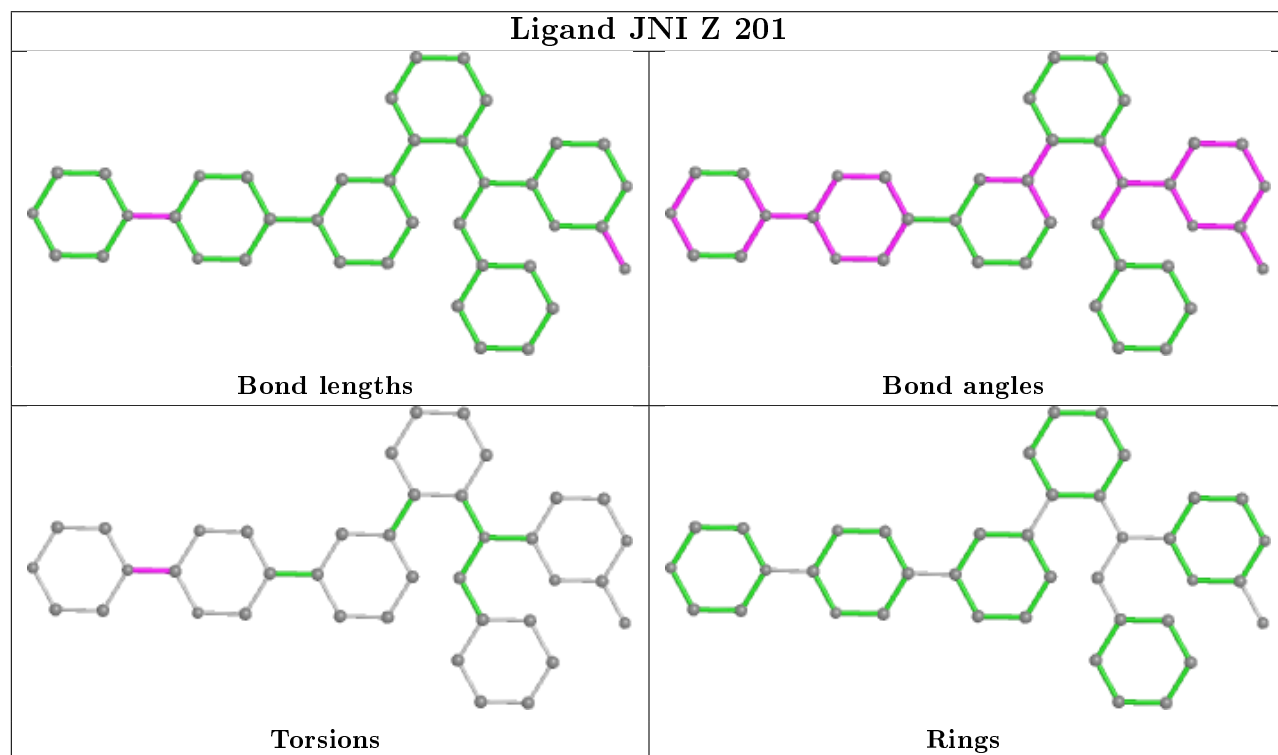
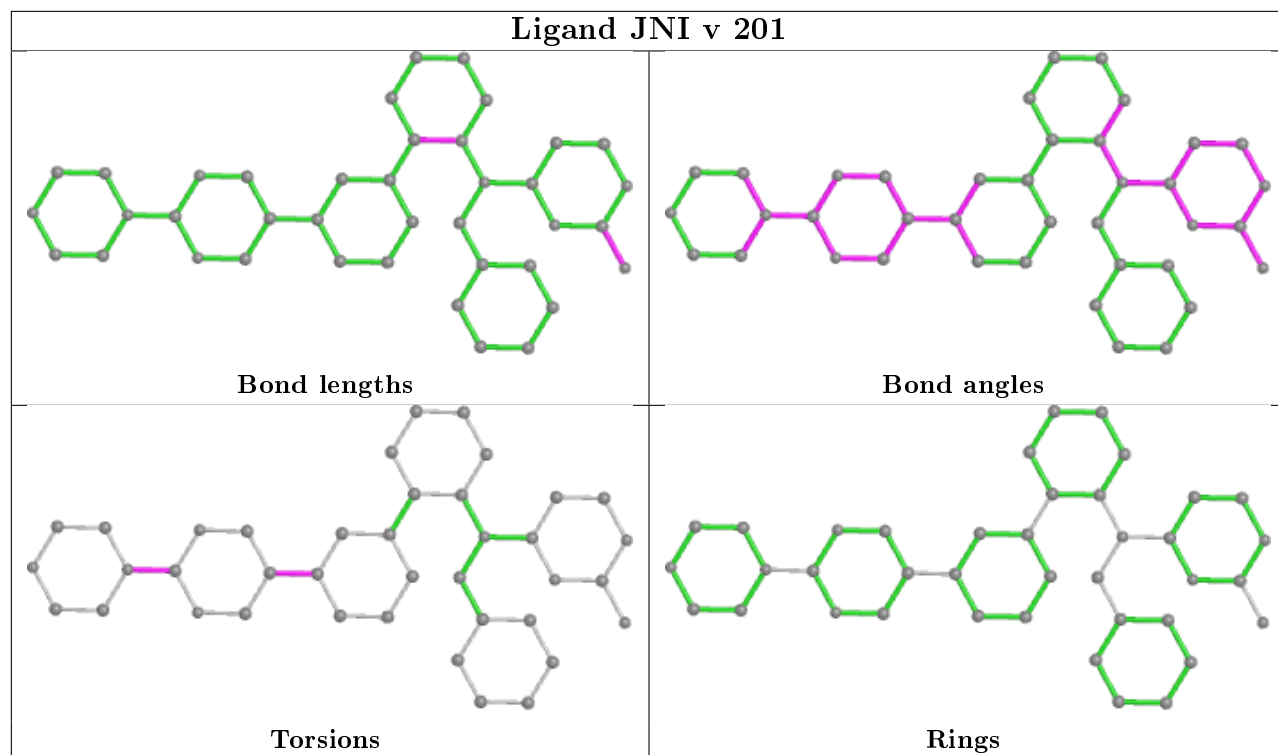
Mol	Chain	Res	Type	Atoms
2	j	202	JNI	C5-C6-N8-C16
2	p	201	JNI	C5-C6-N8-C16
2	C	202	JNI	C16-C21-C22-C27
2	X	202	JNI	C10-C9-N8-C6
2	Z	202	JNI	C16-C21-C22-C23
2	t	202	JNI	C16-C21-C22-C23
2	C	202	JNI	C16-C21-C22-C23

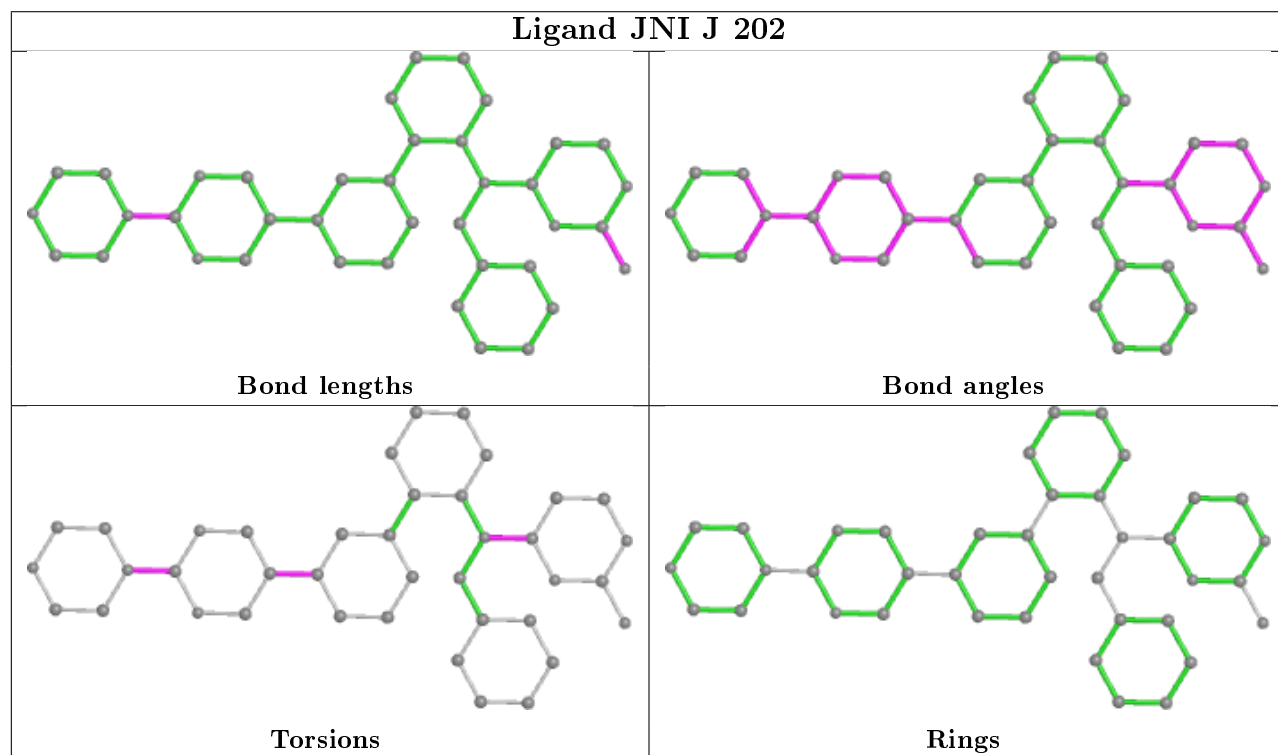
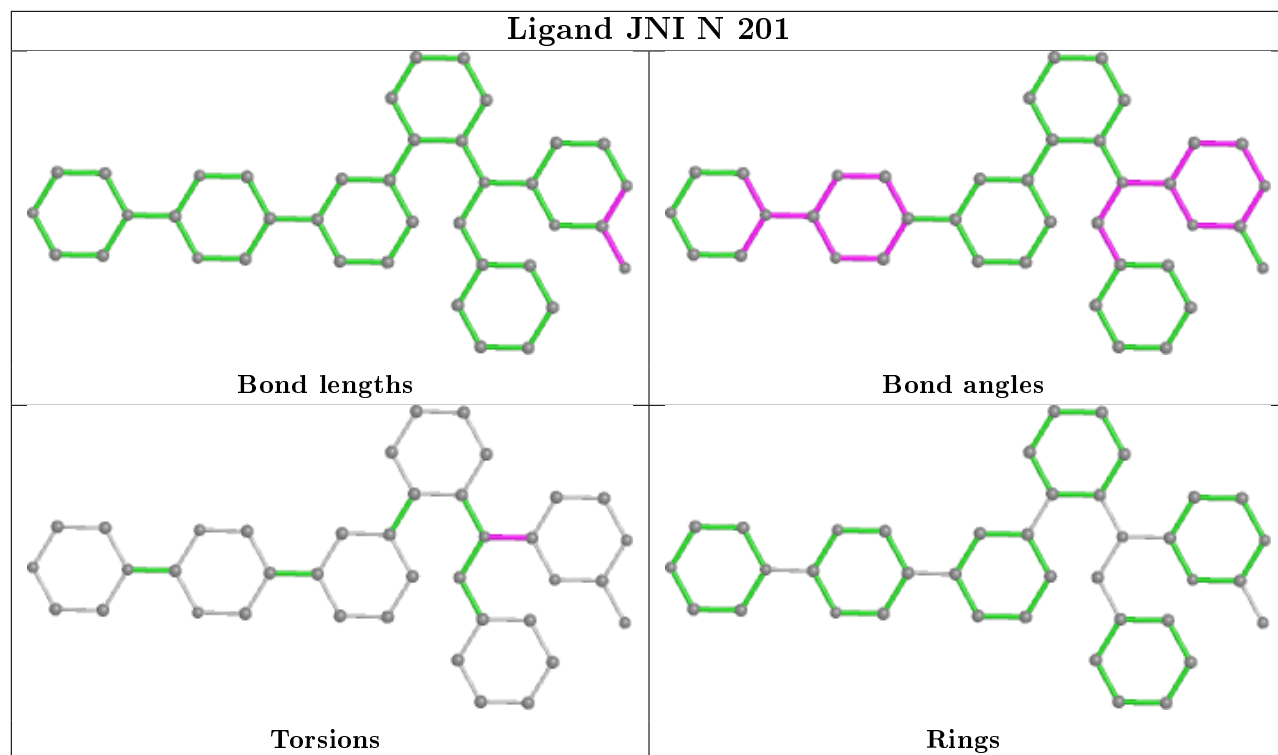
All (1) ring outliers are listed below:

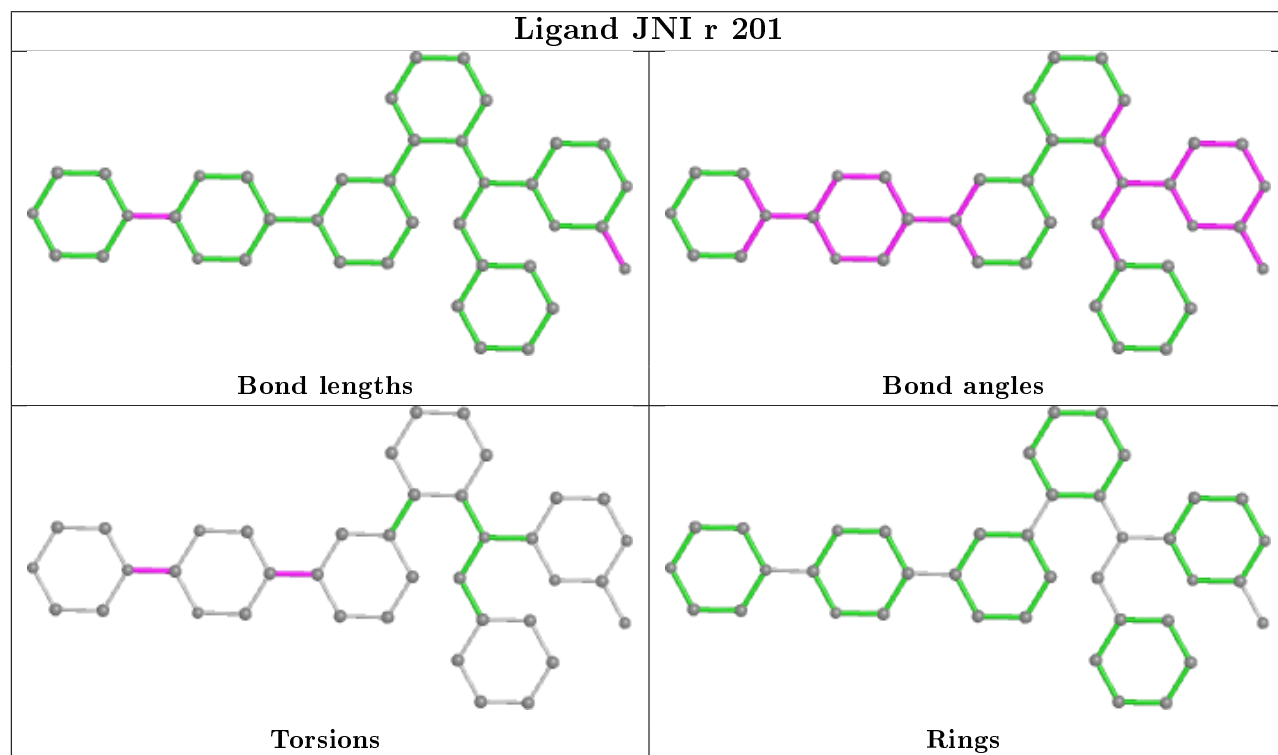
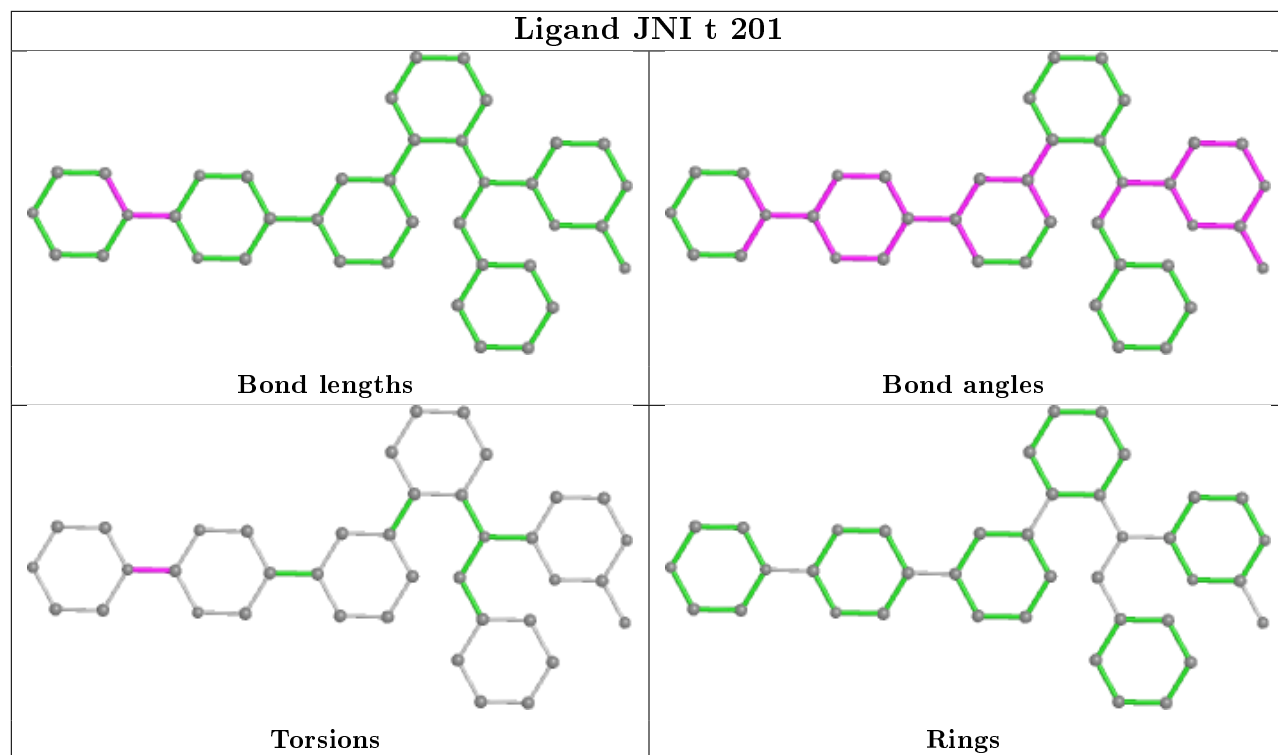
Mol	Chain	Res	Type	Atoms
2	v	202	JNI	C35-C36-C38-C39-N34-N37

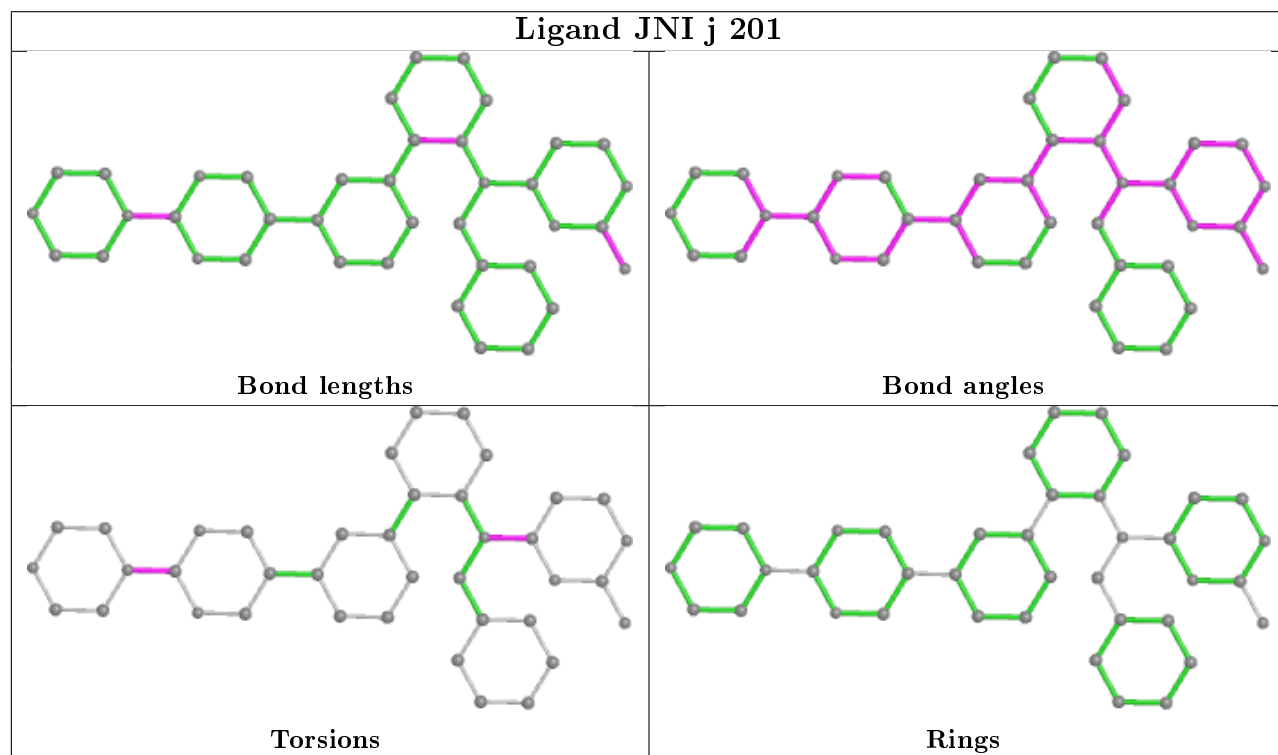
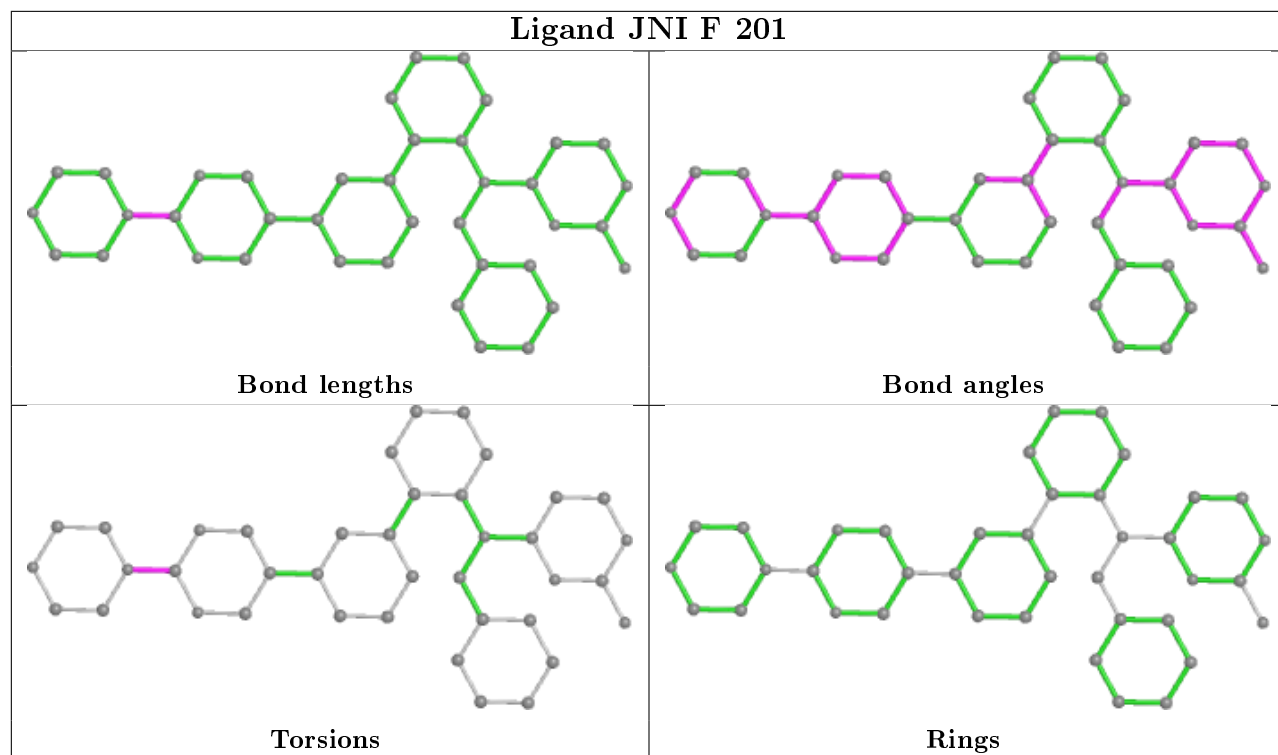
No monomer is involved in short contacts.

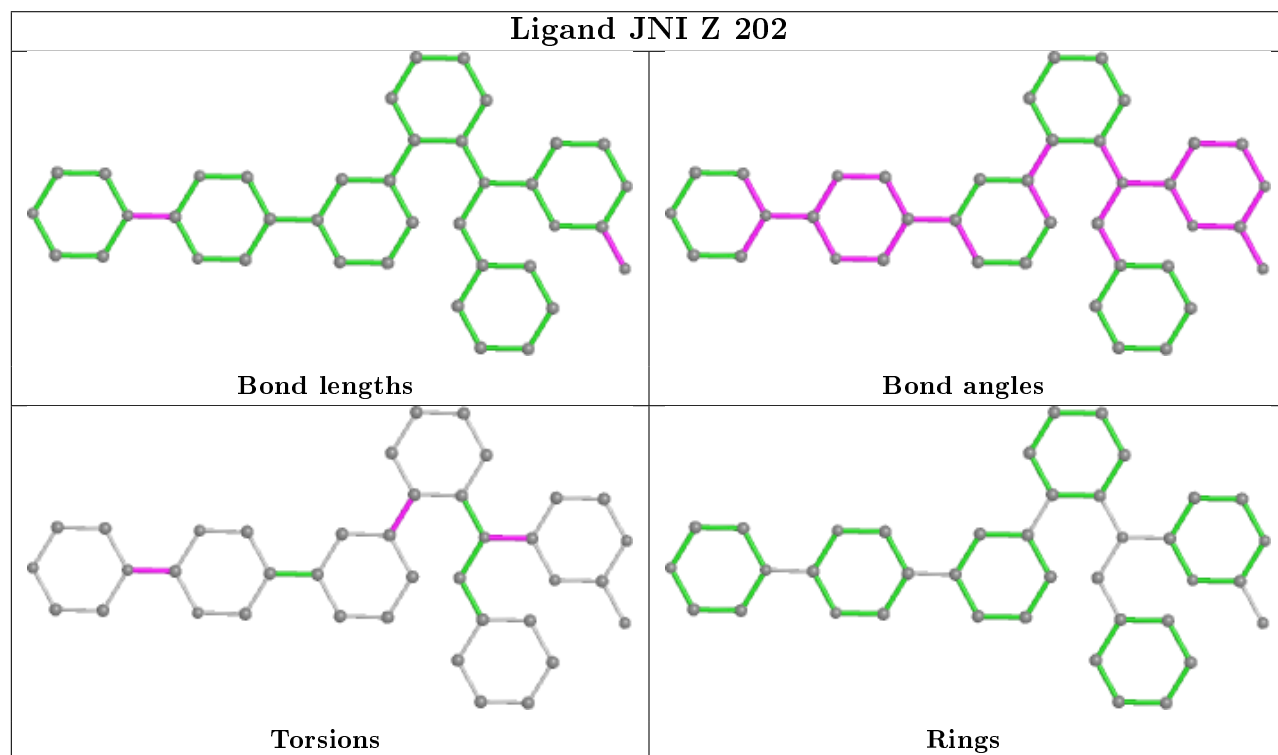
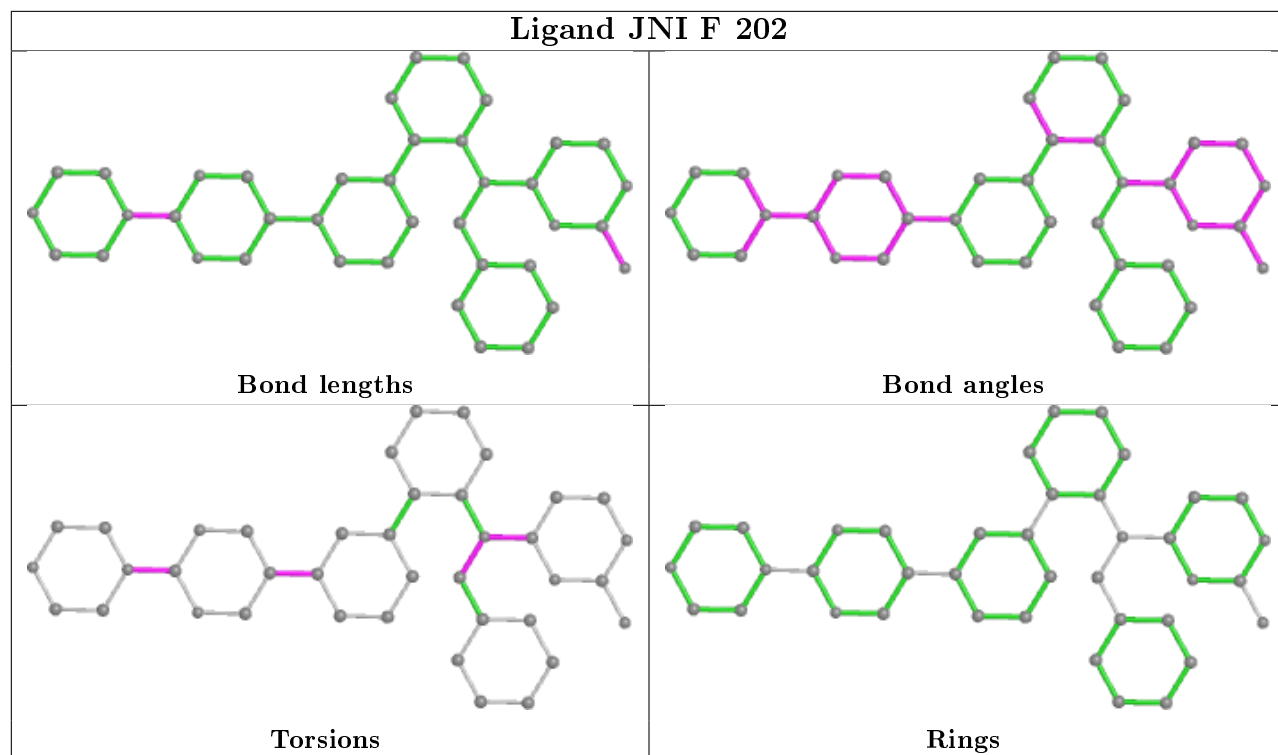
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

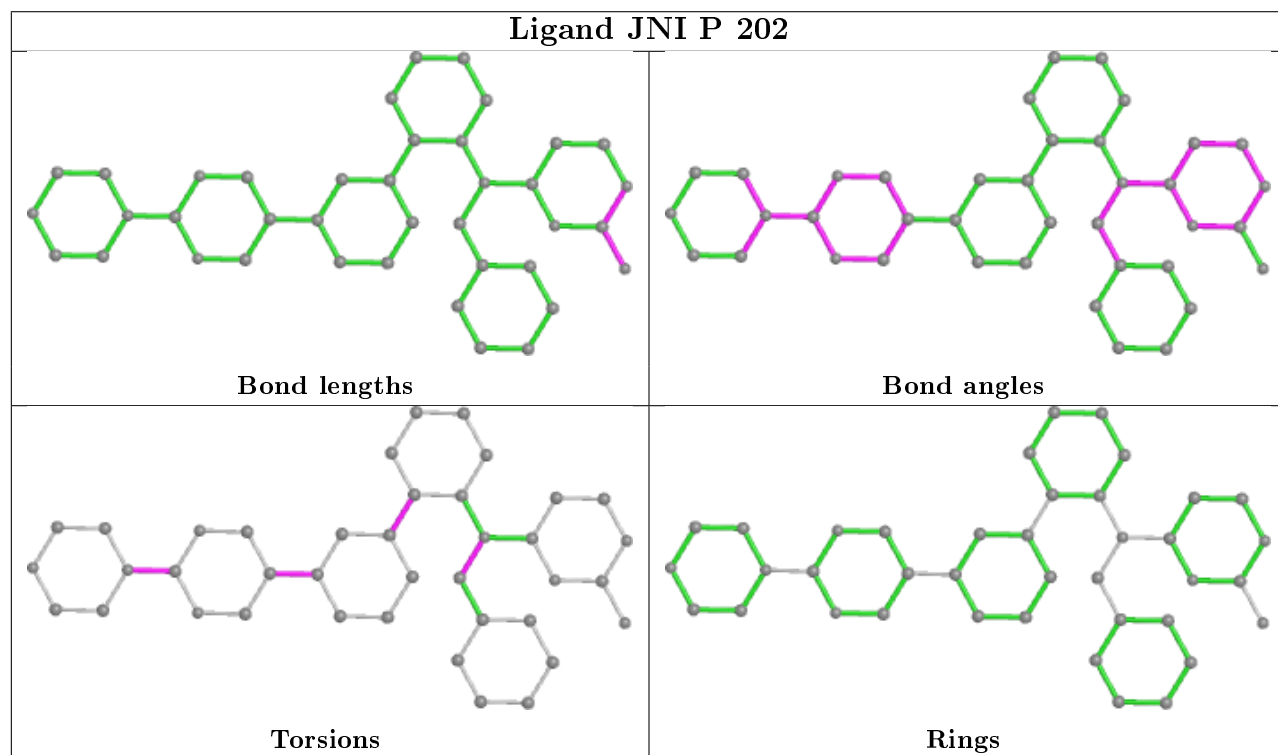
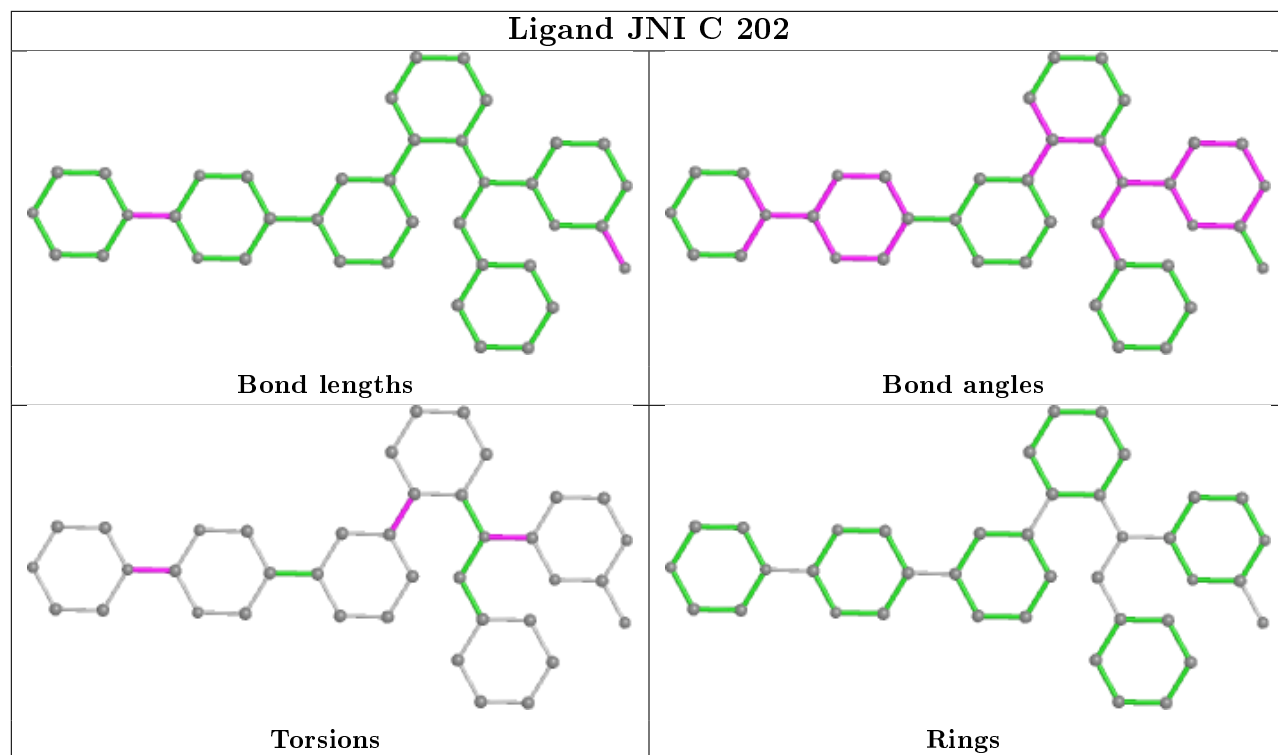


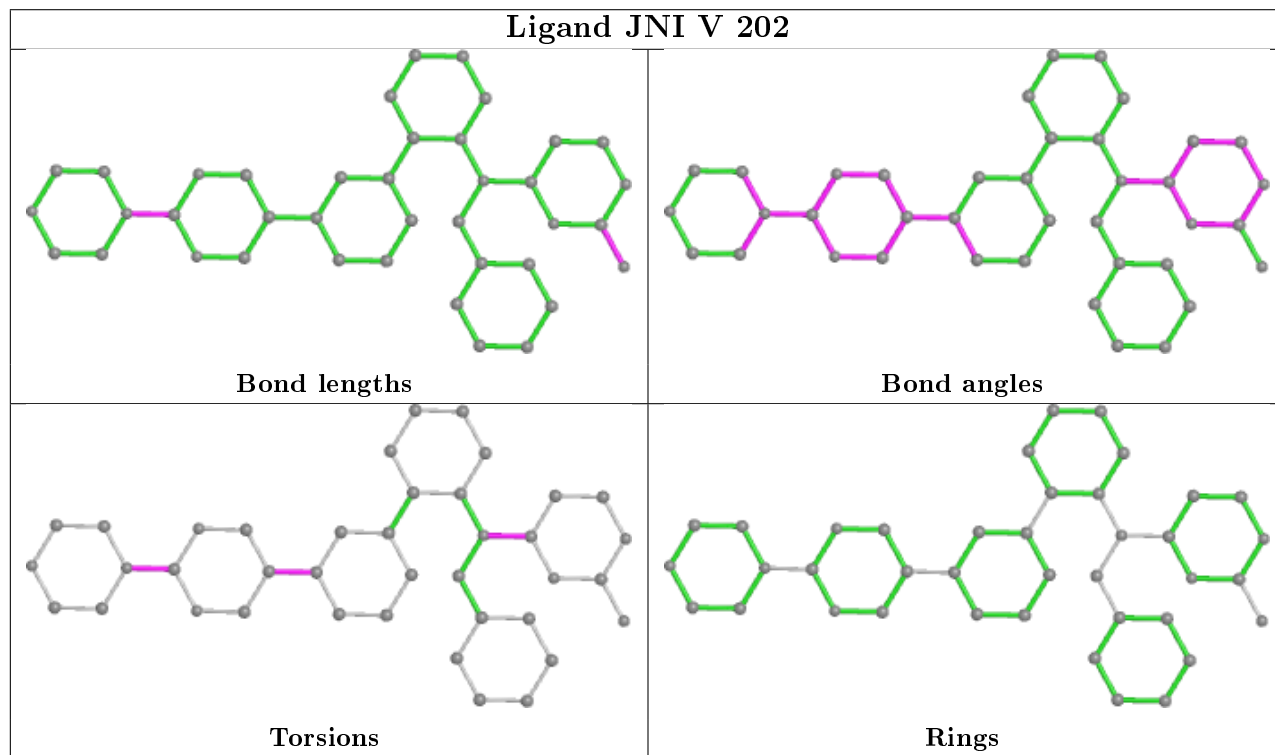
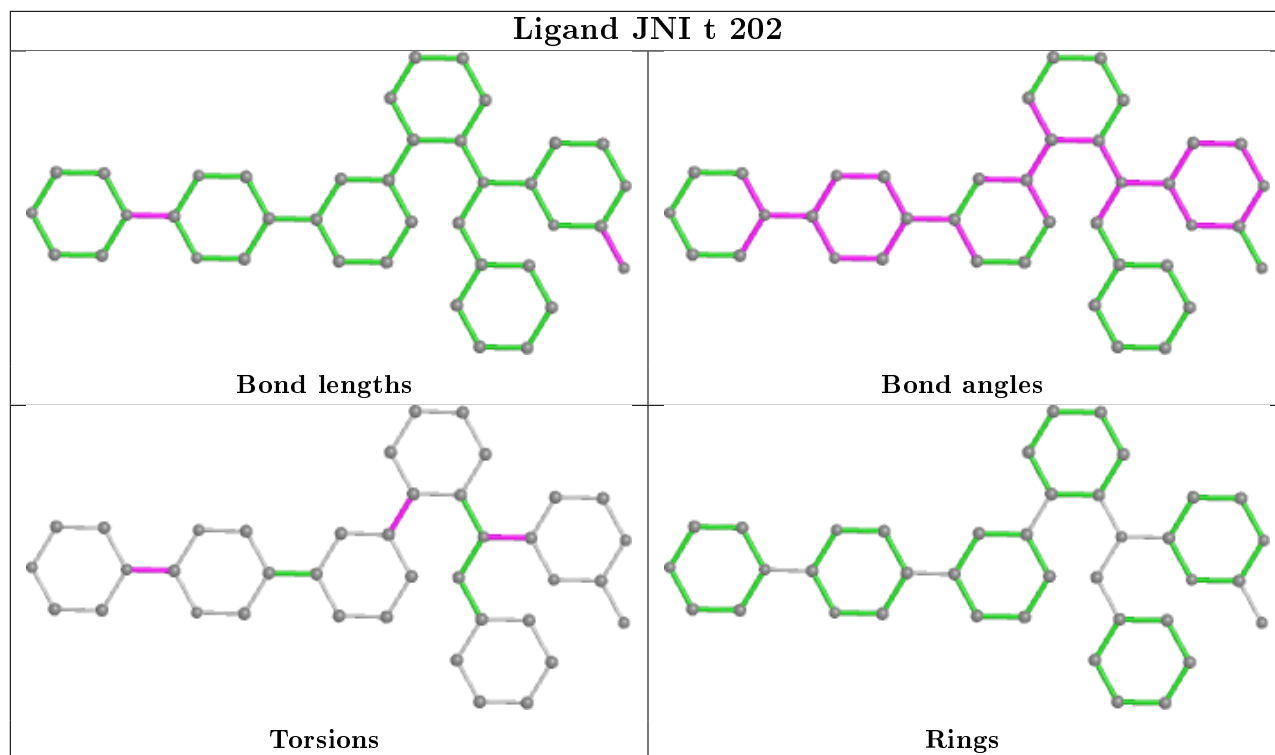


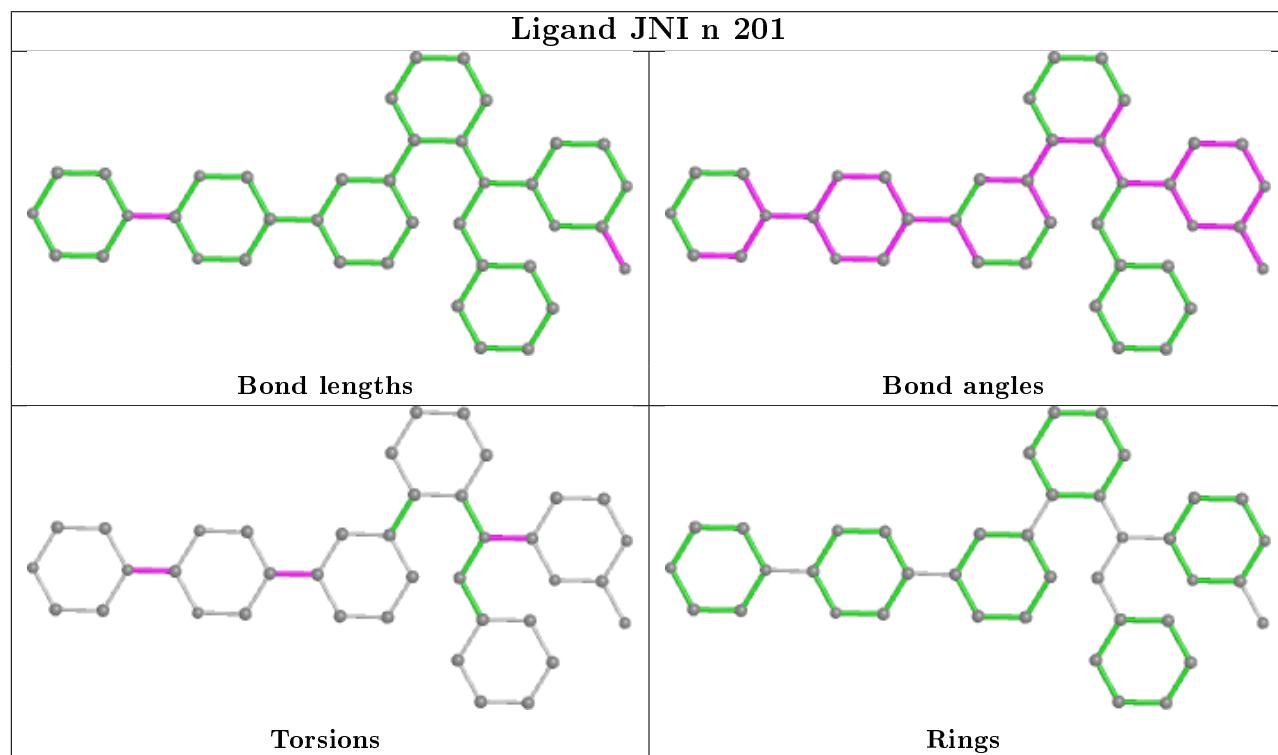
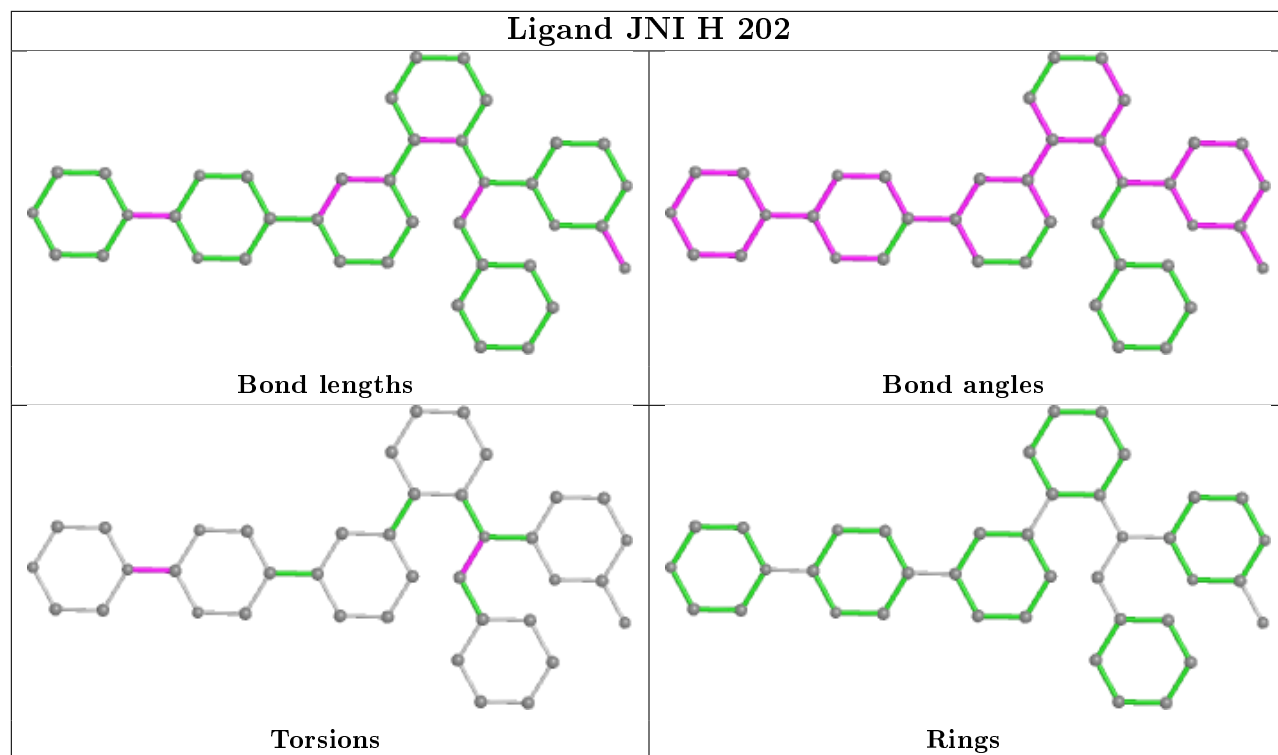


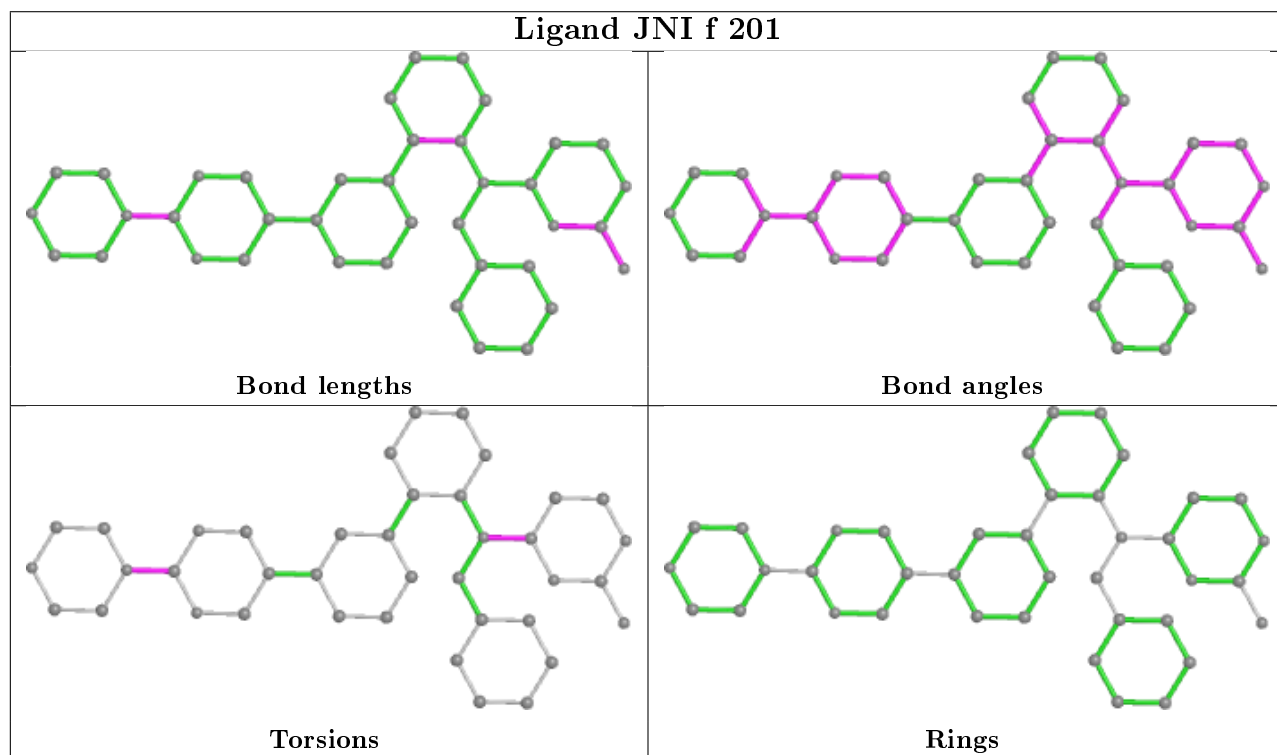
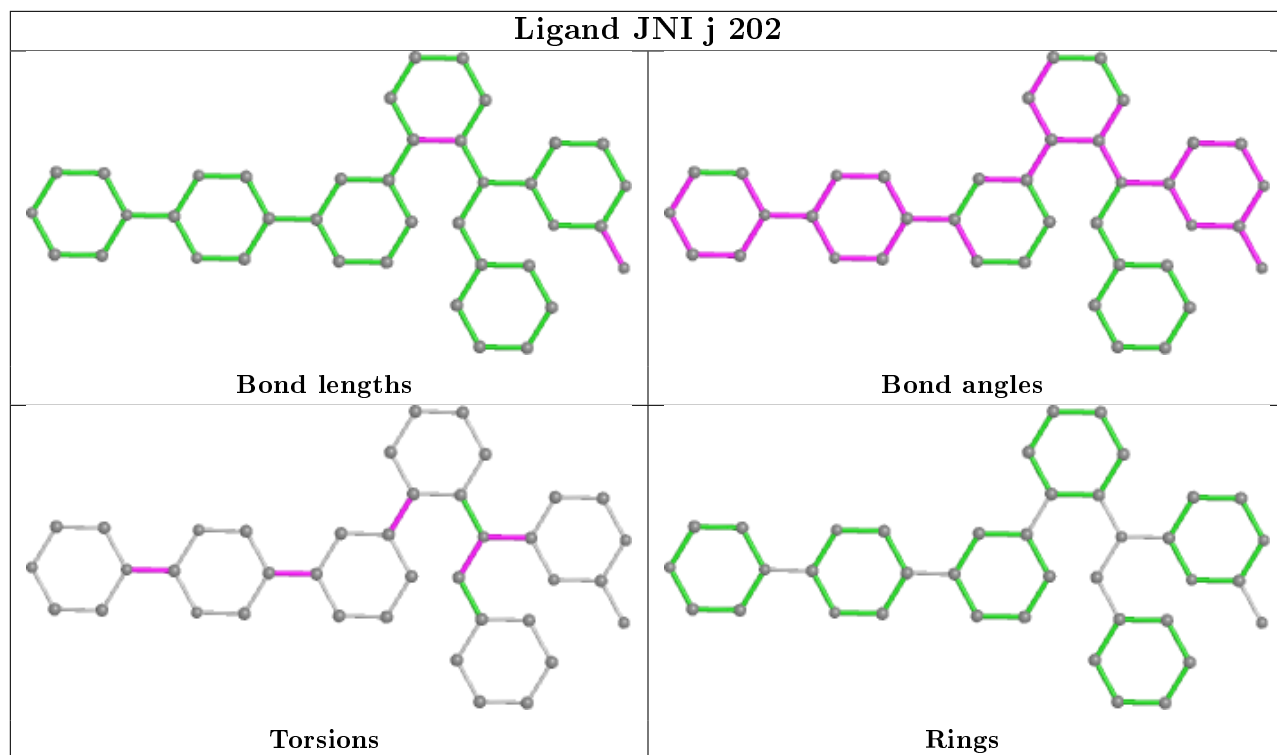


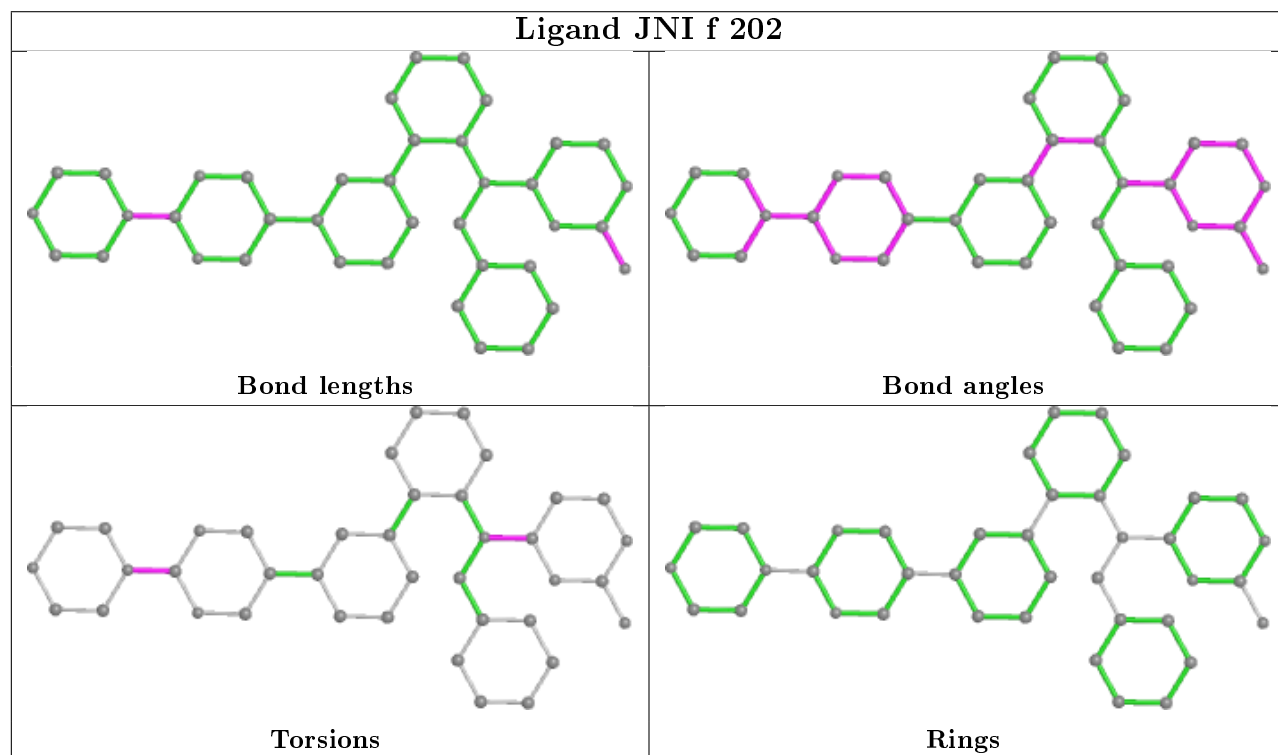
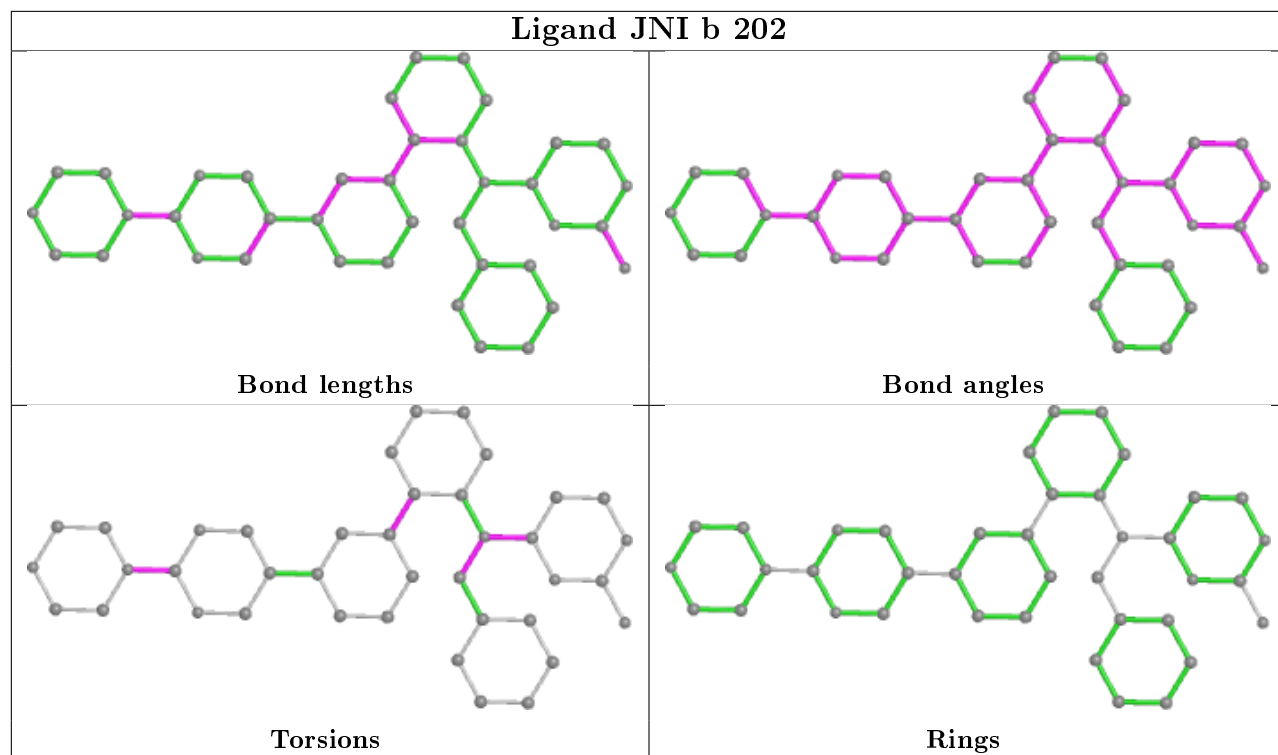


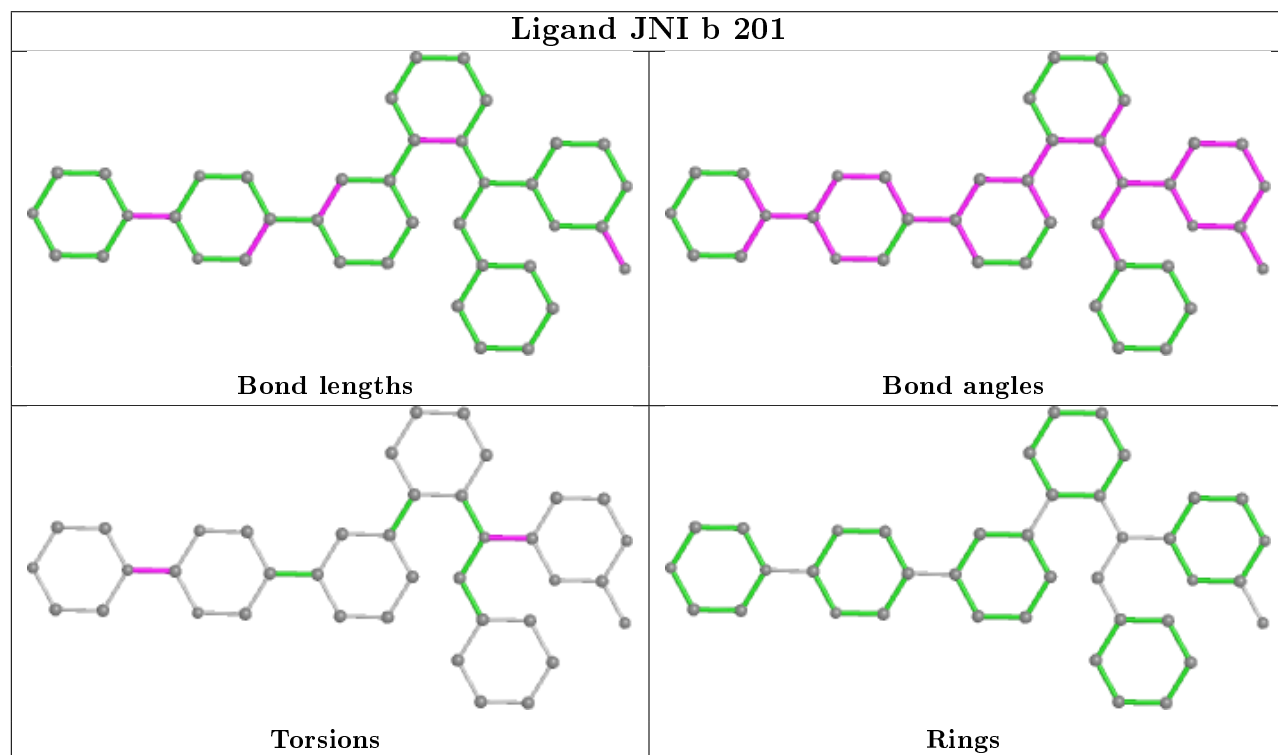
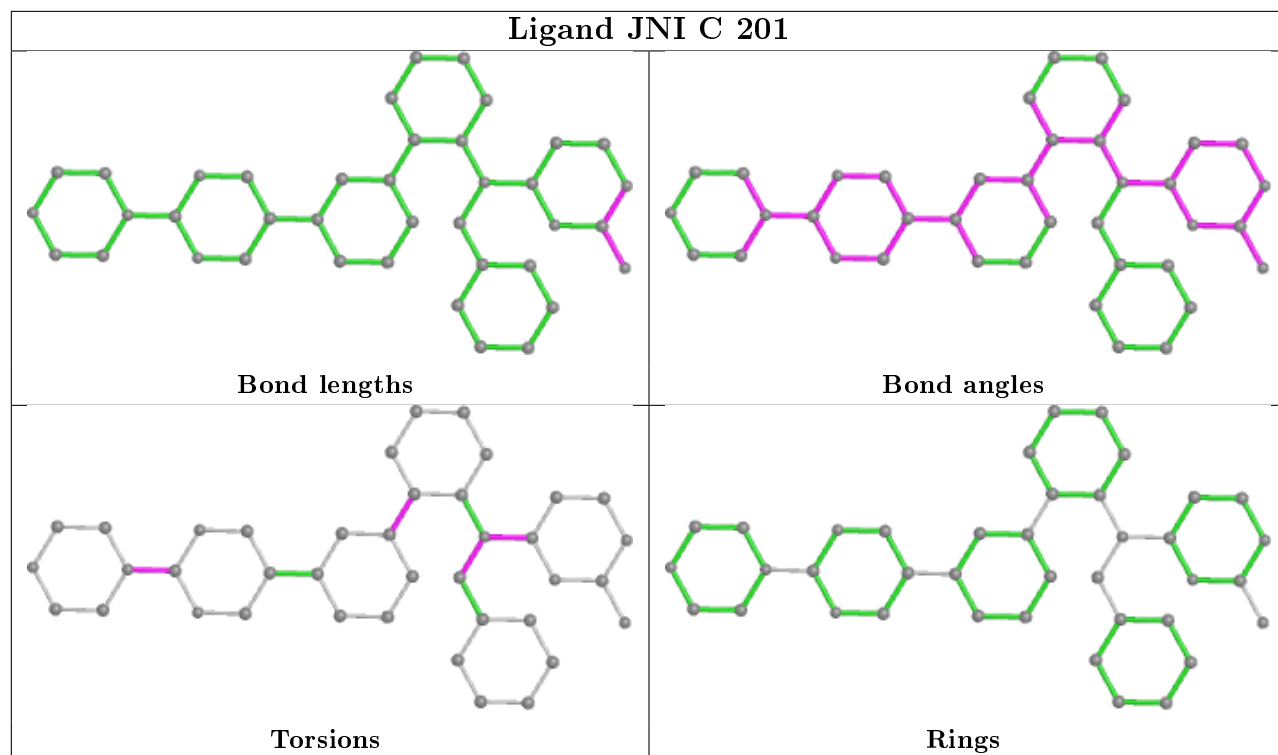


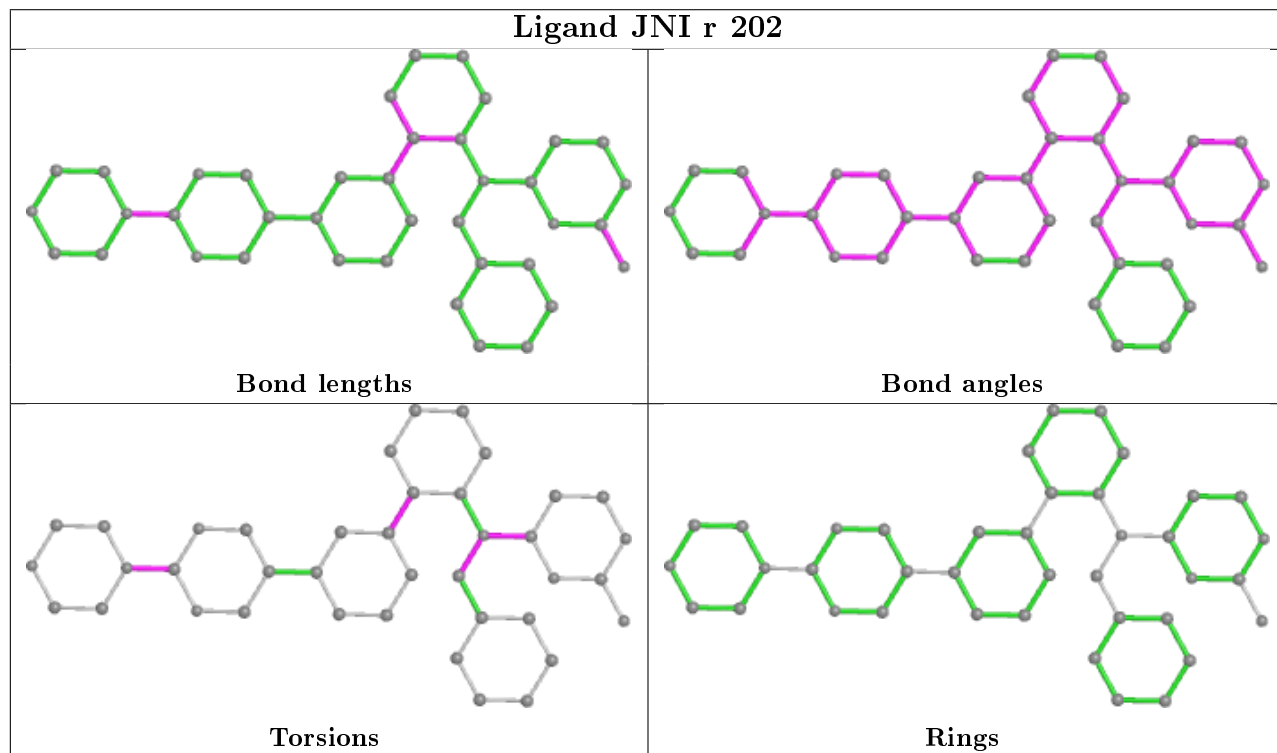
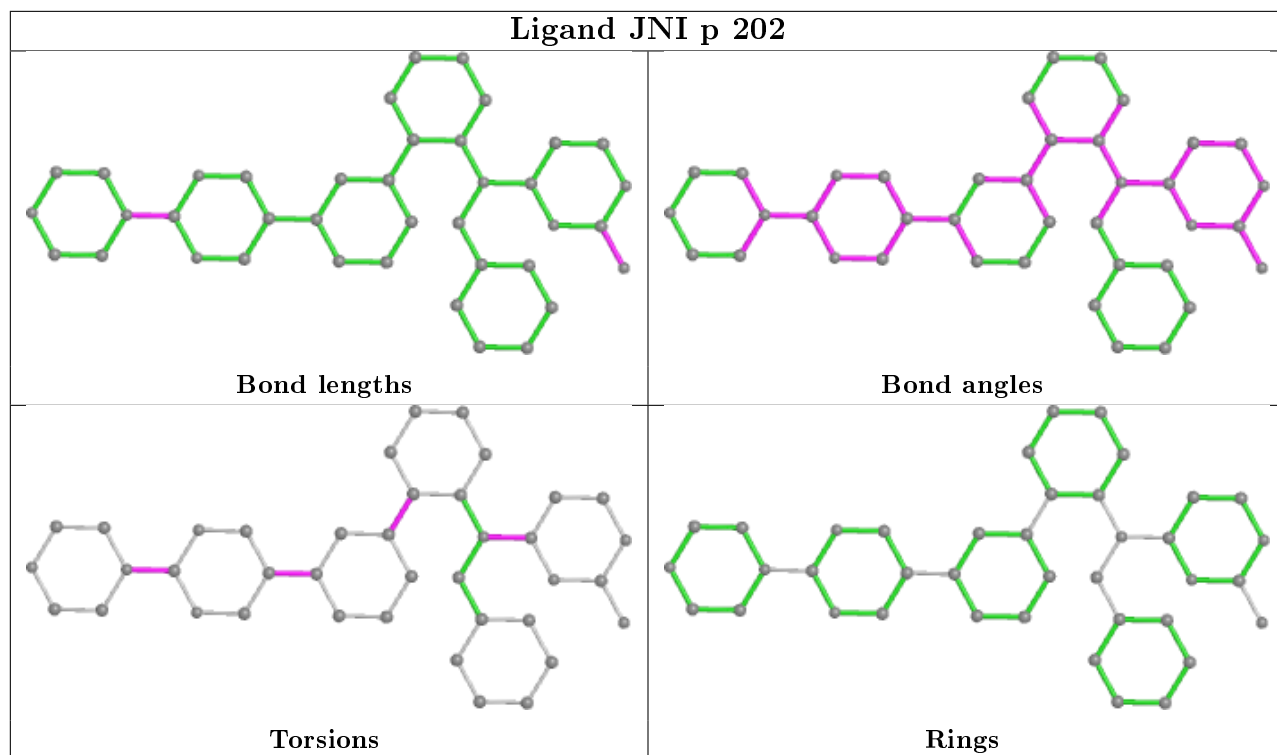


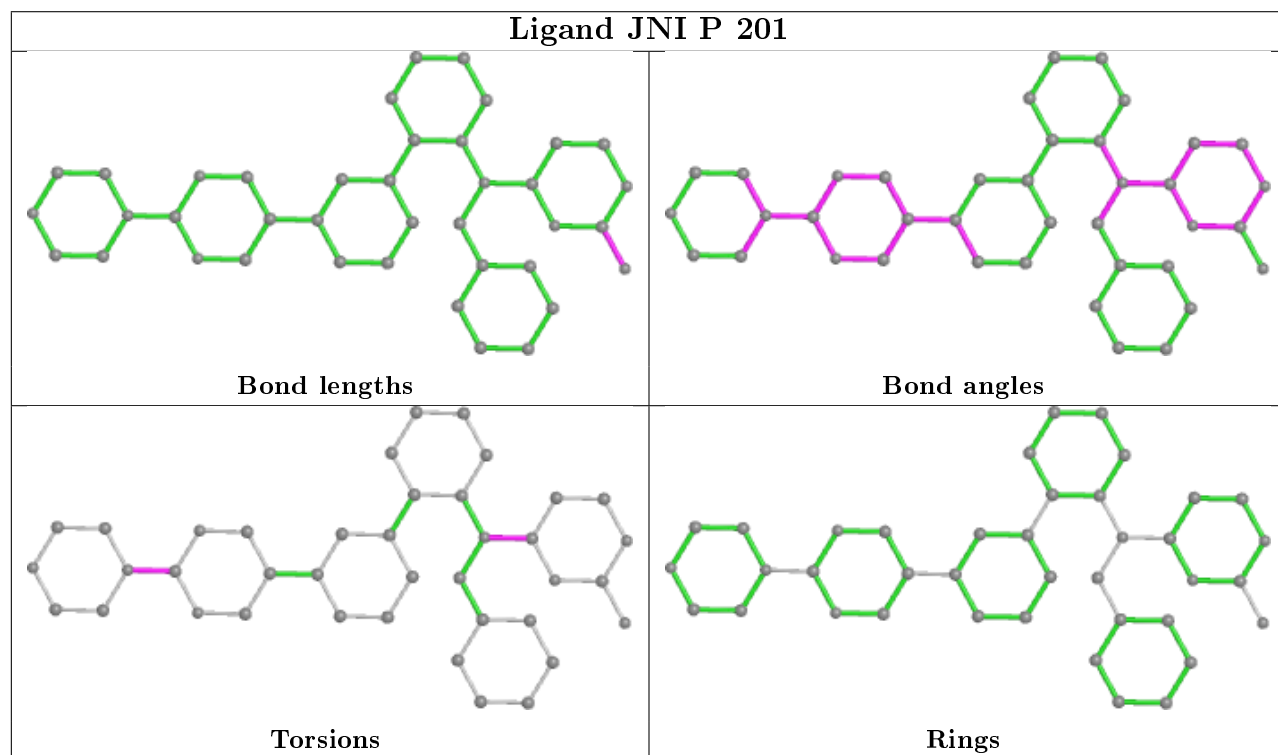
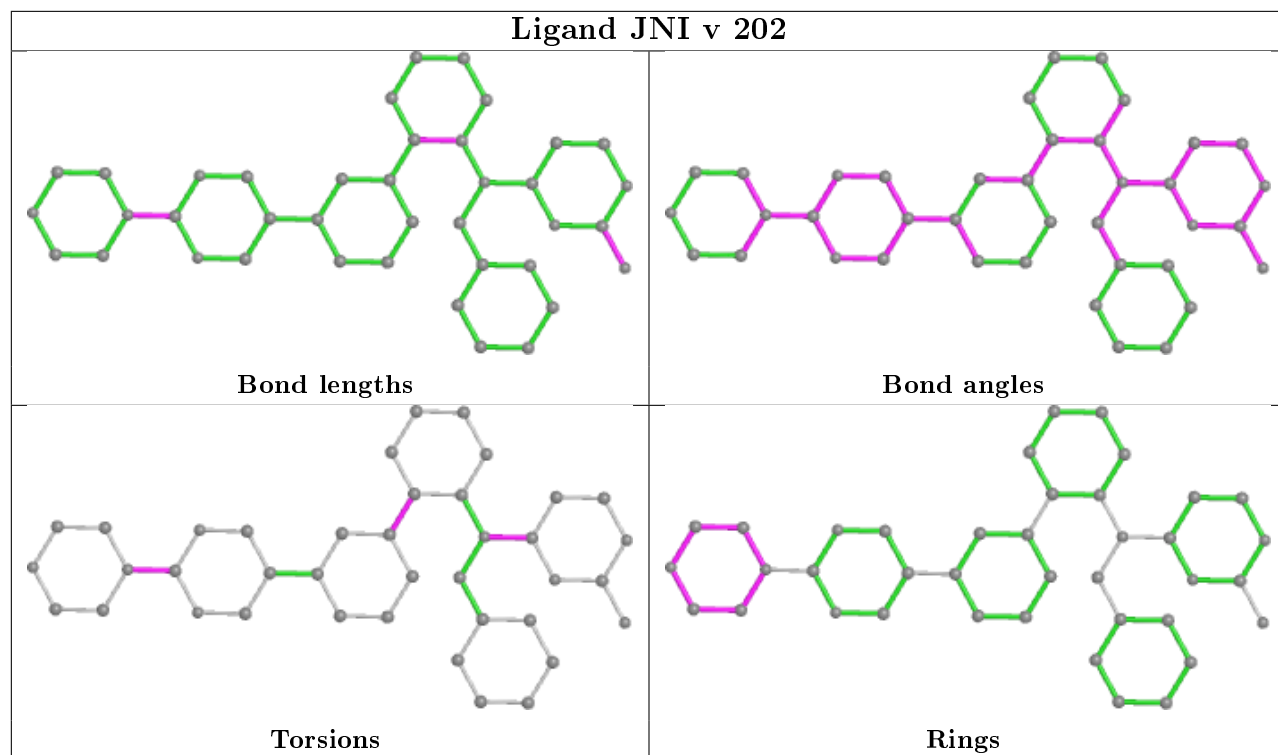


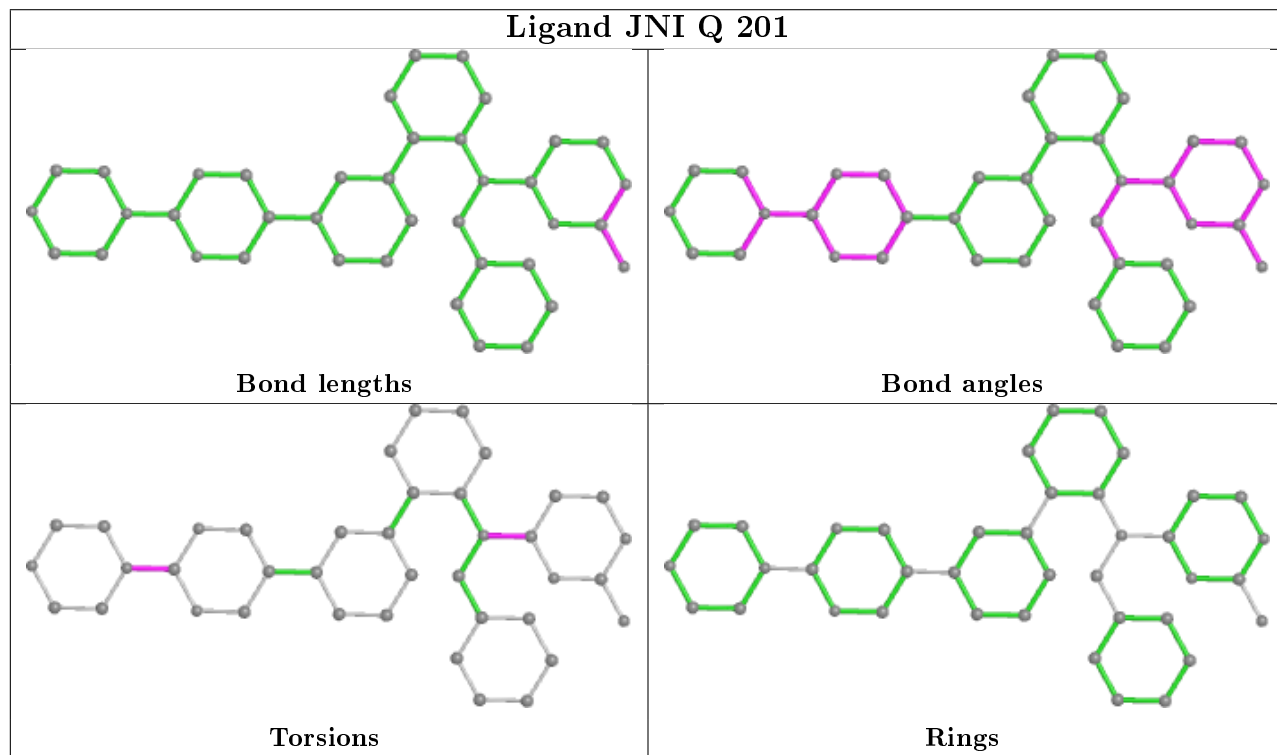
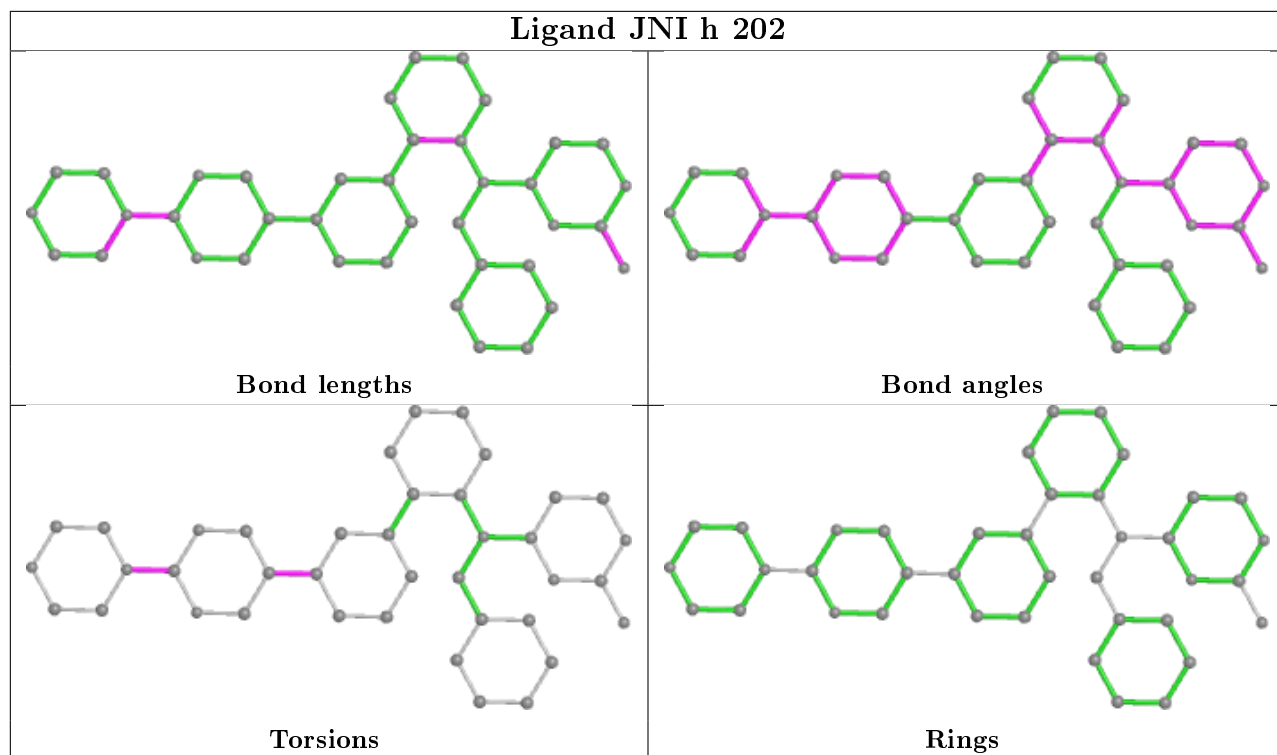


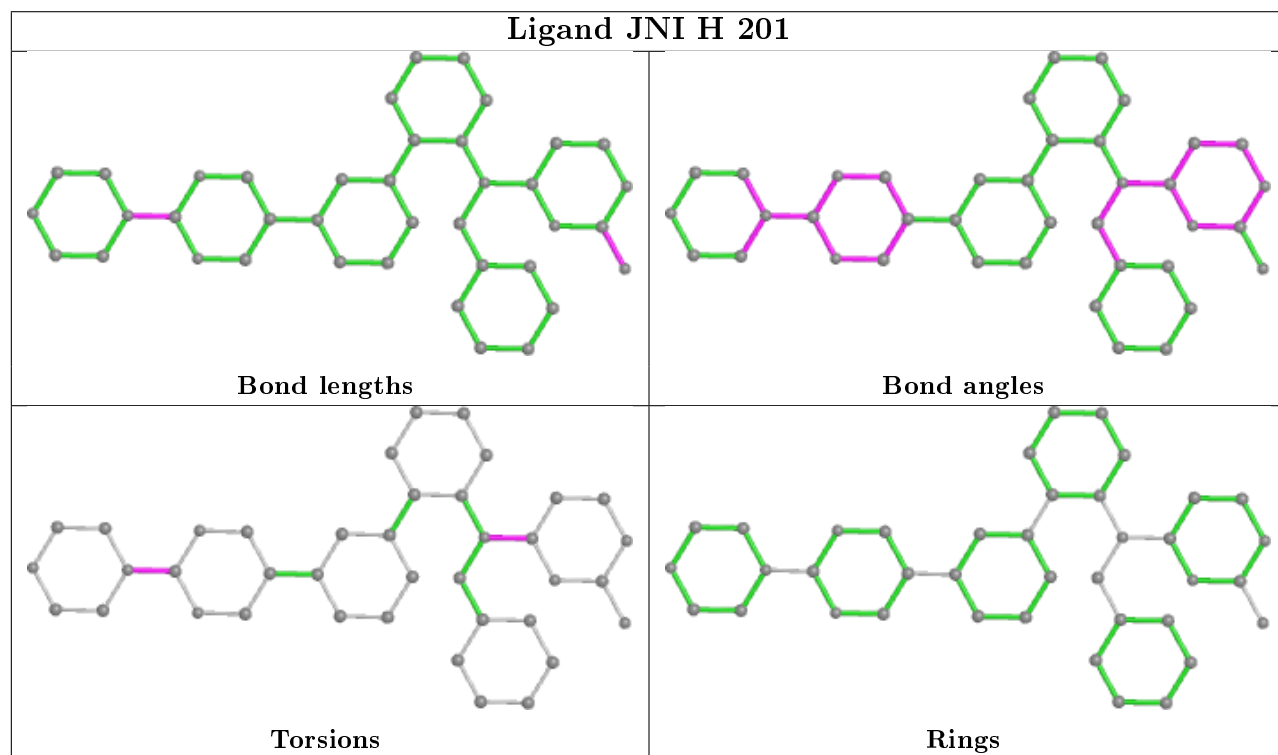
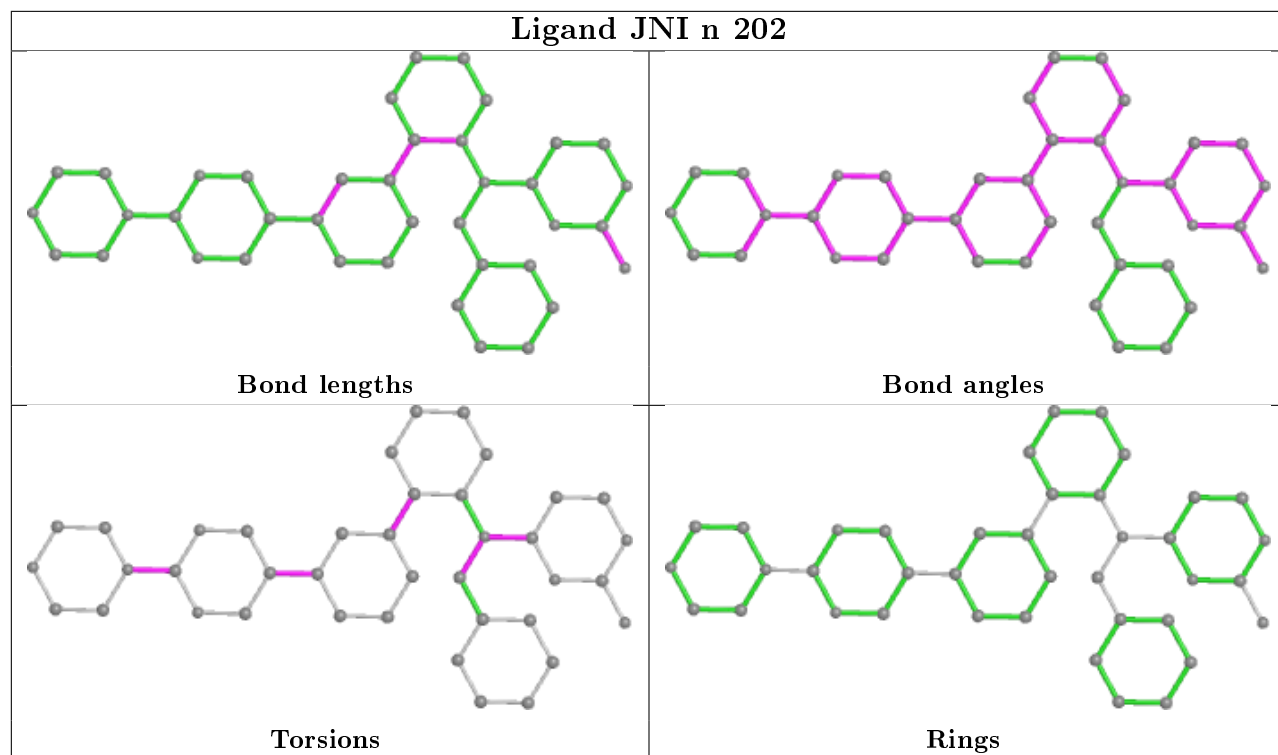


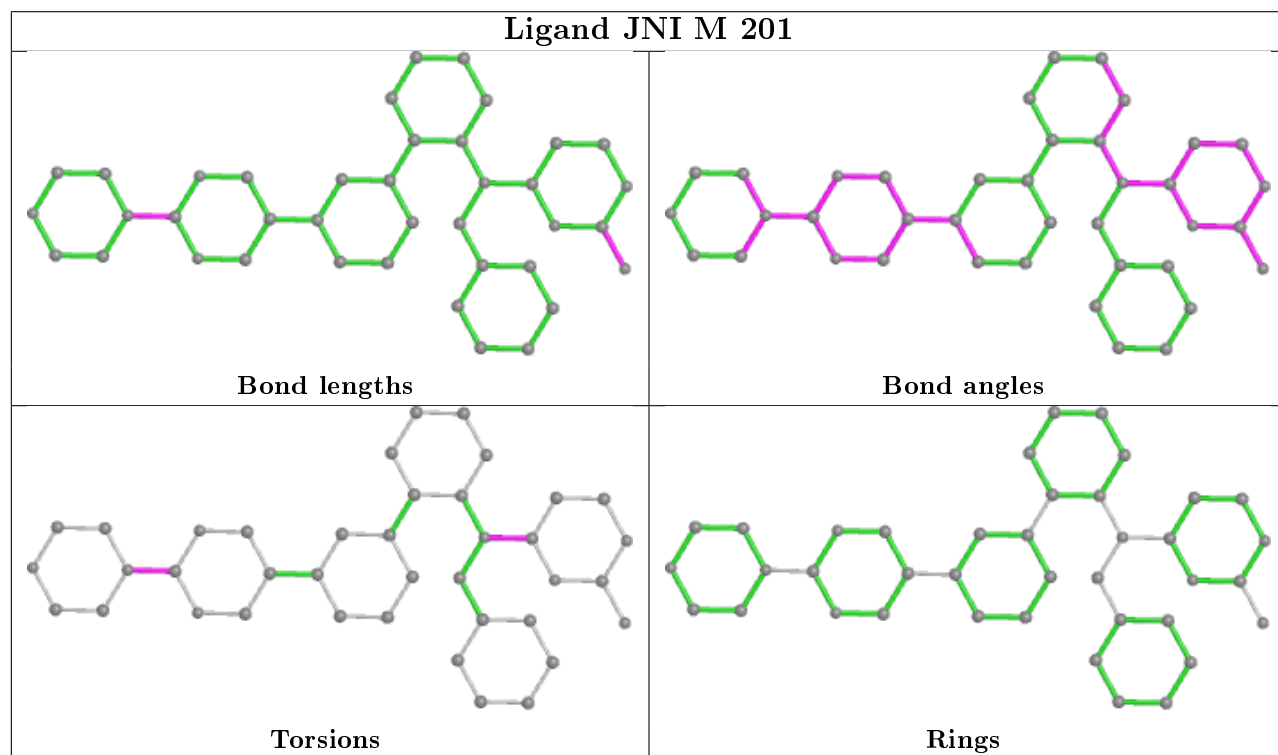
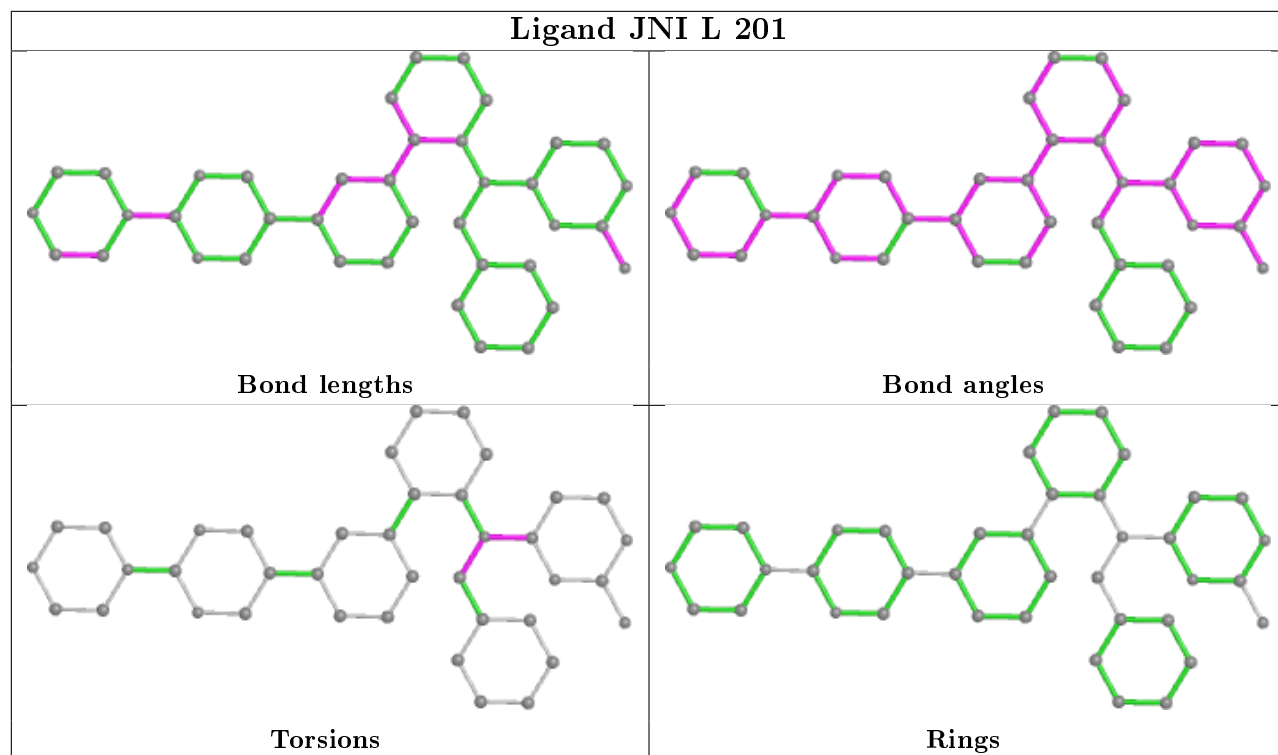


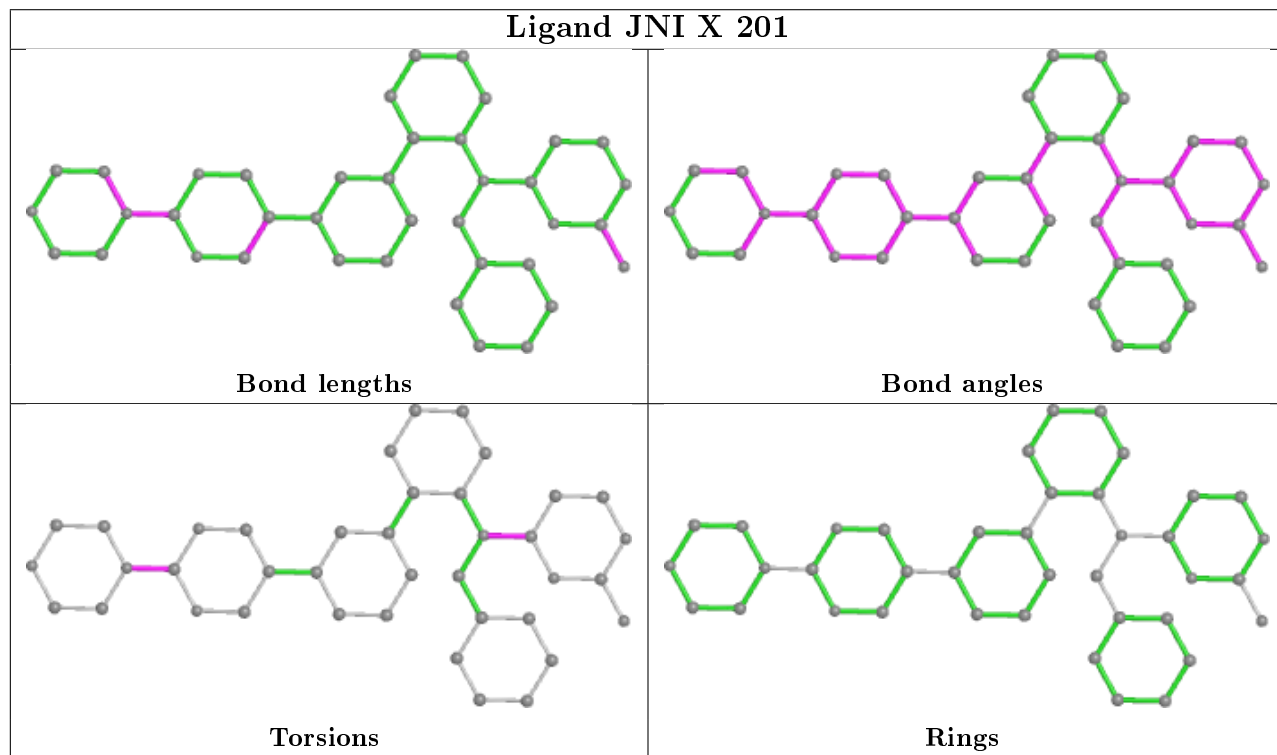
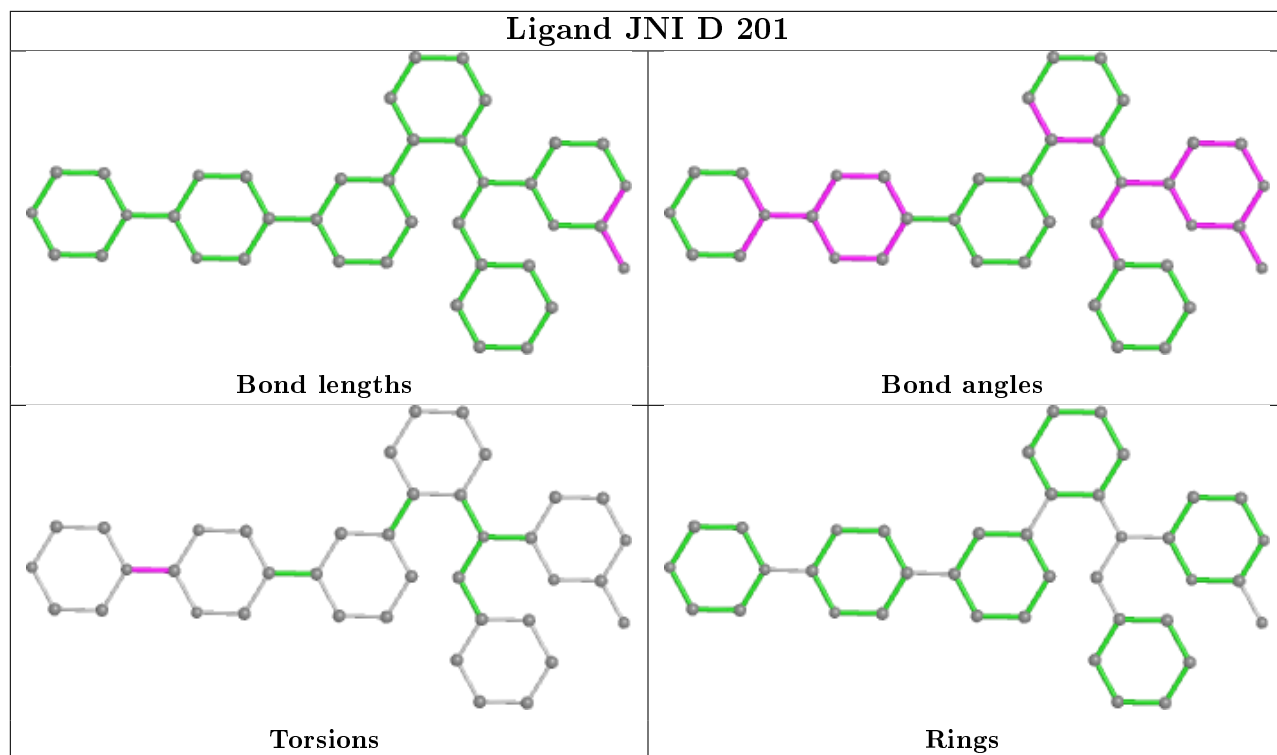


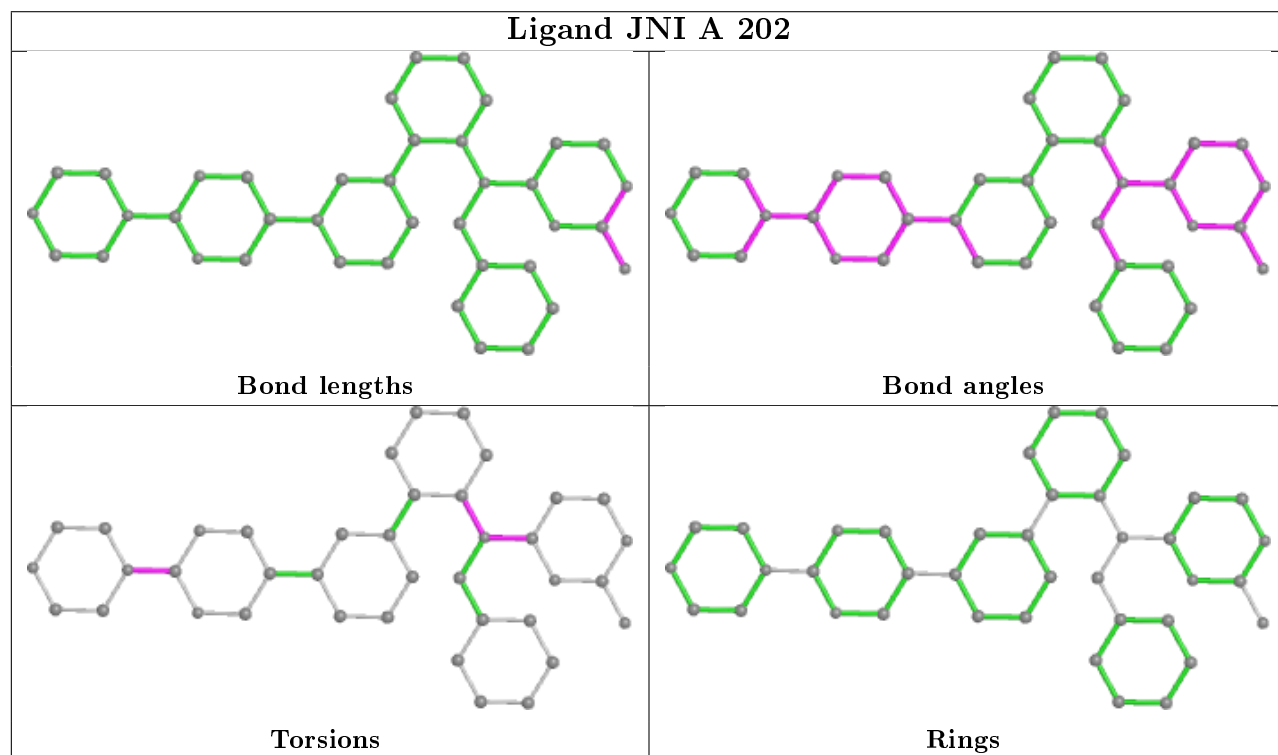
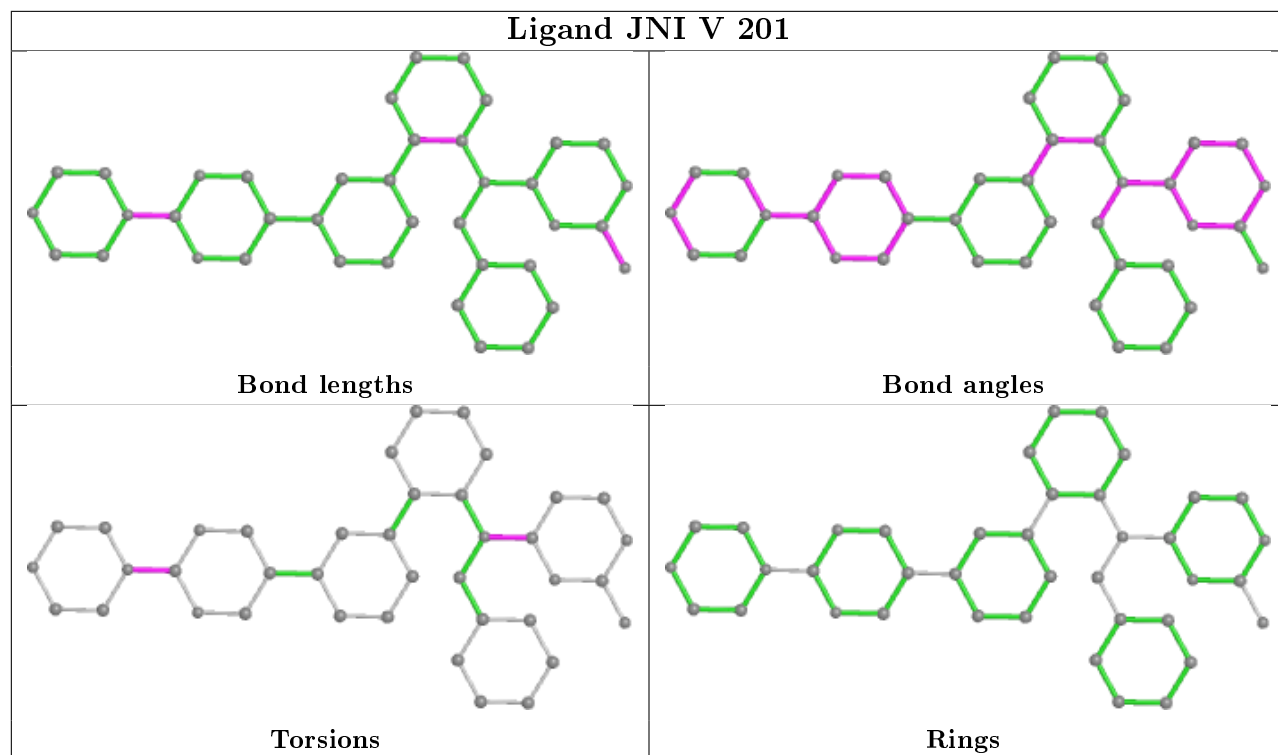


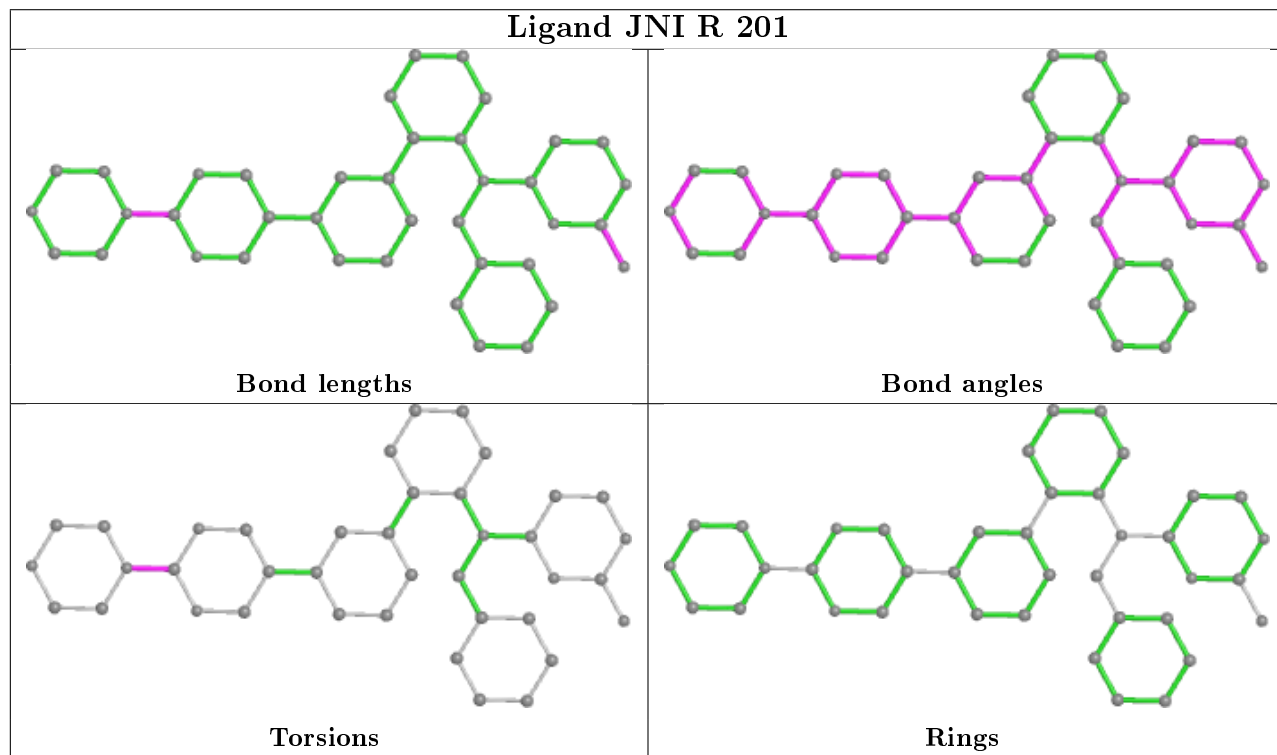
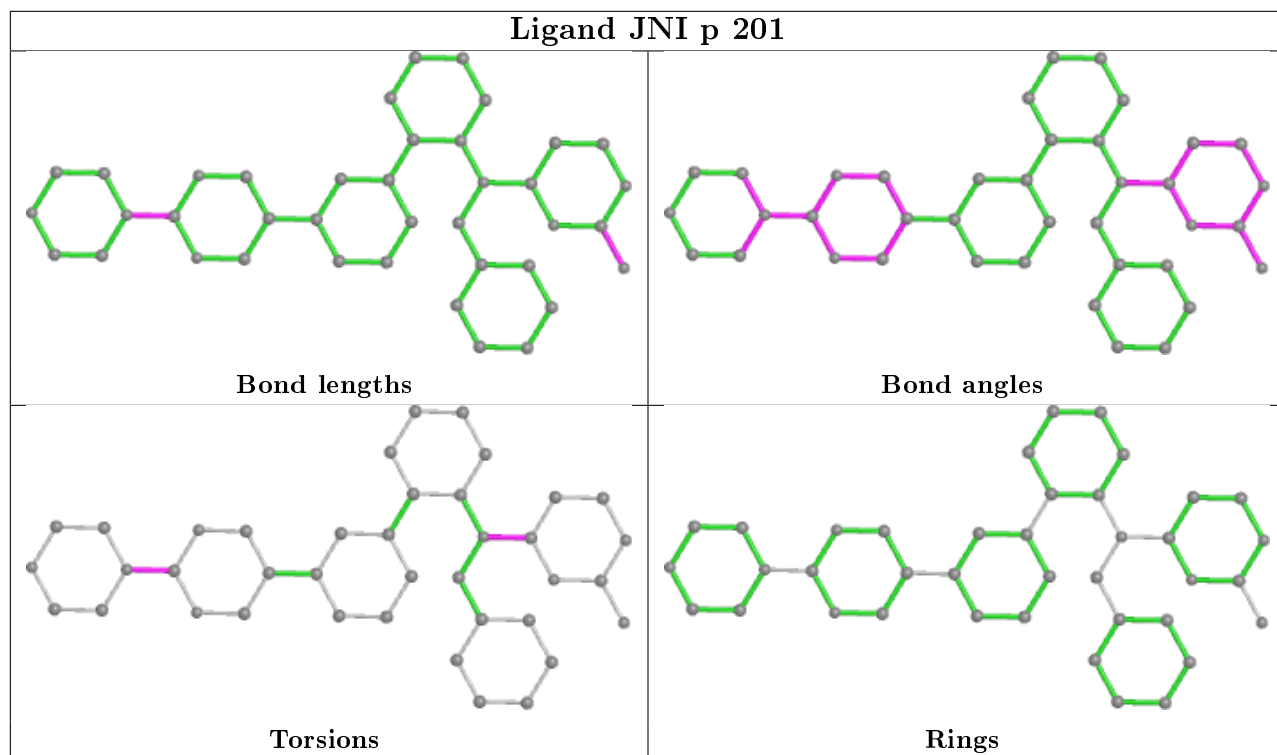


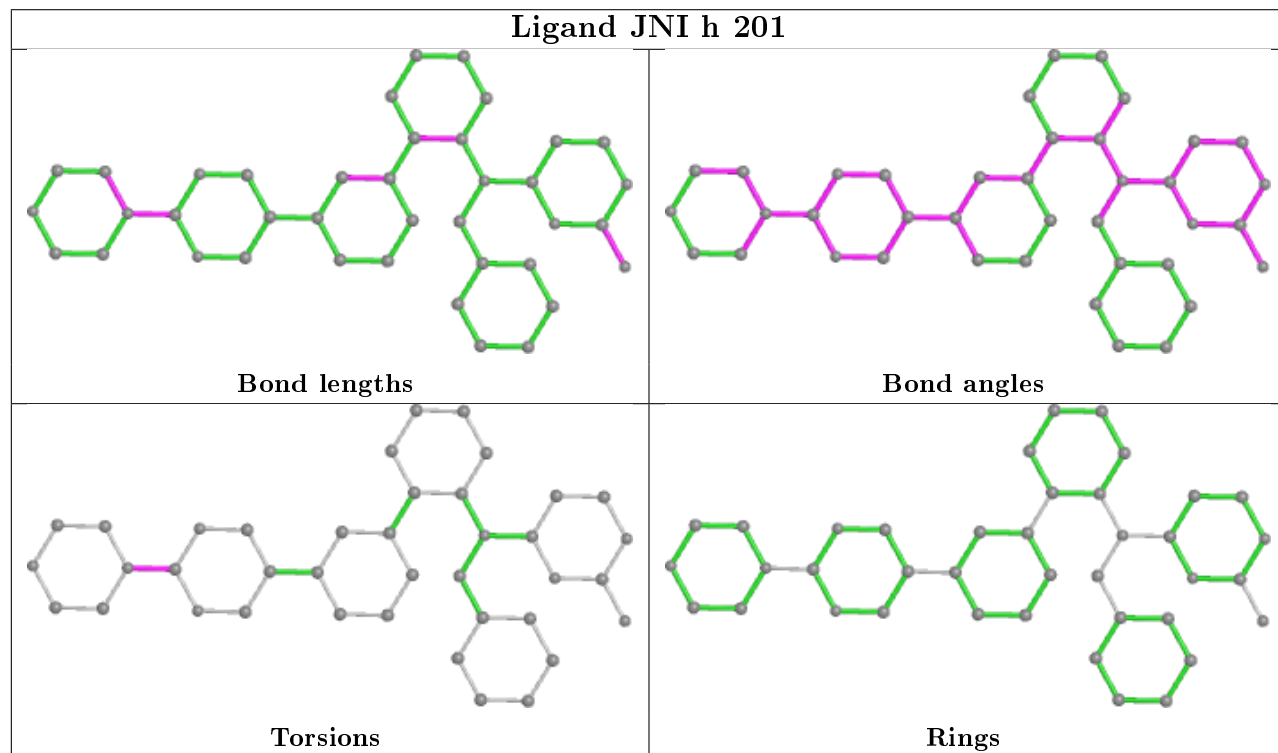
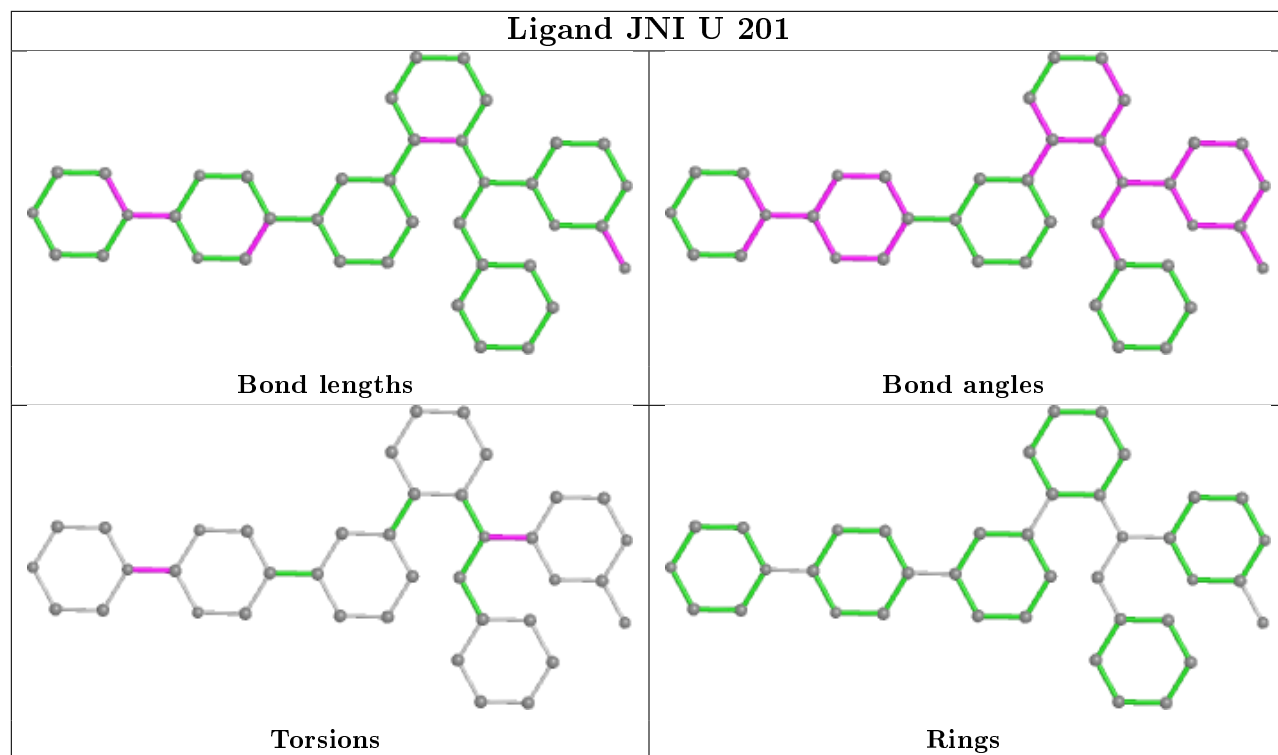


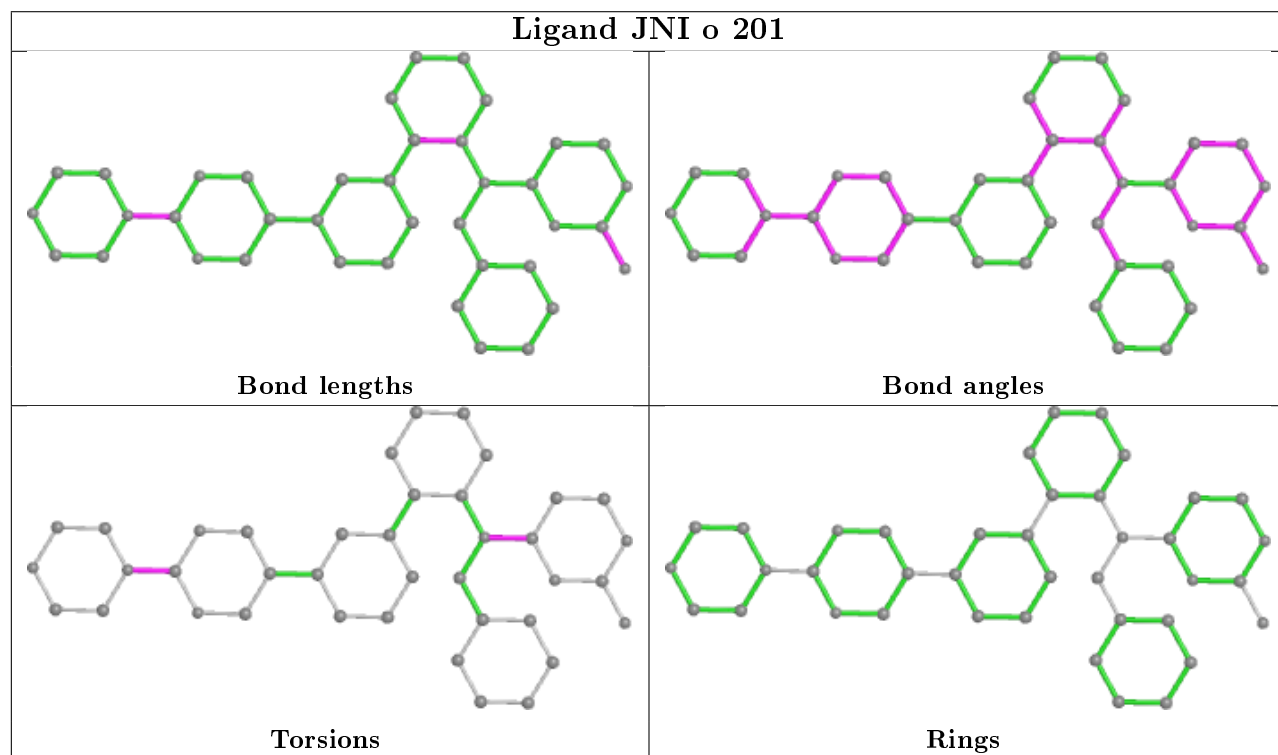
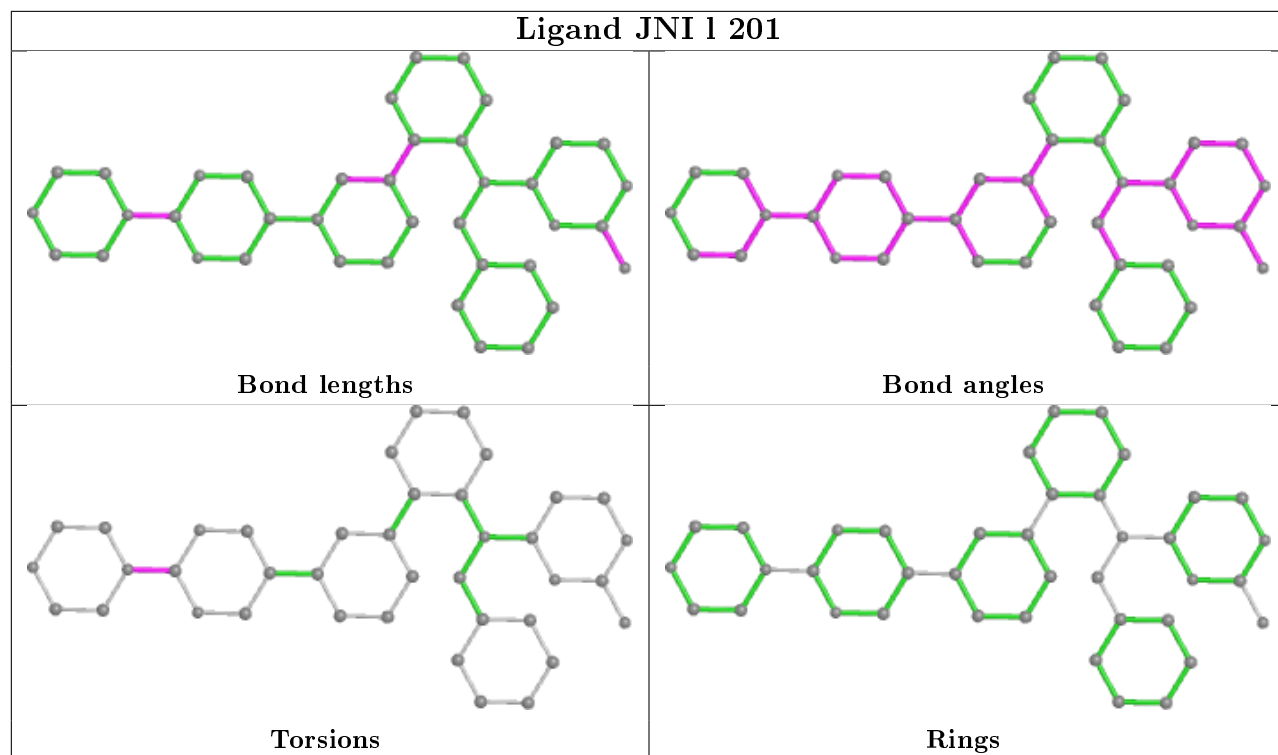


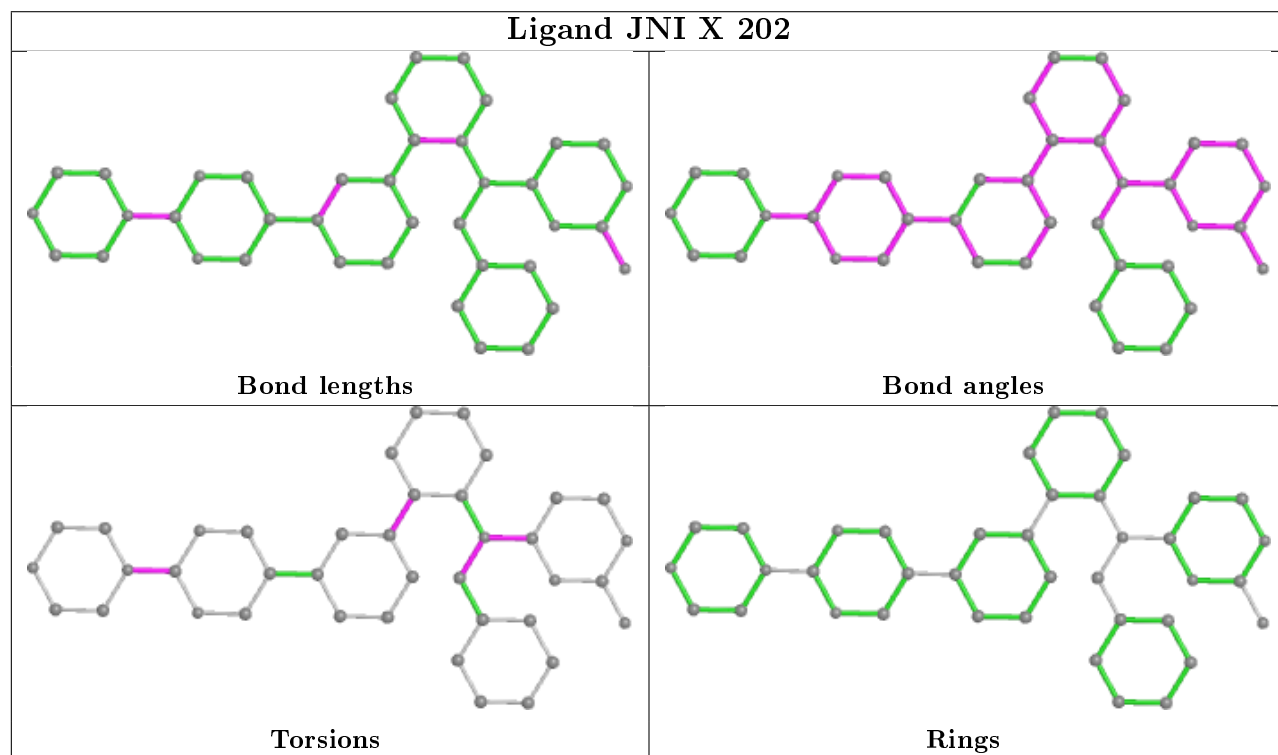
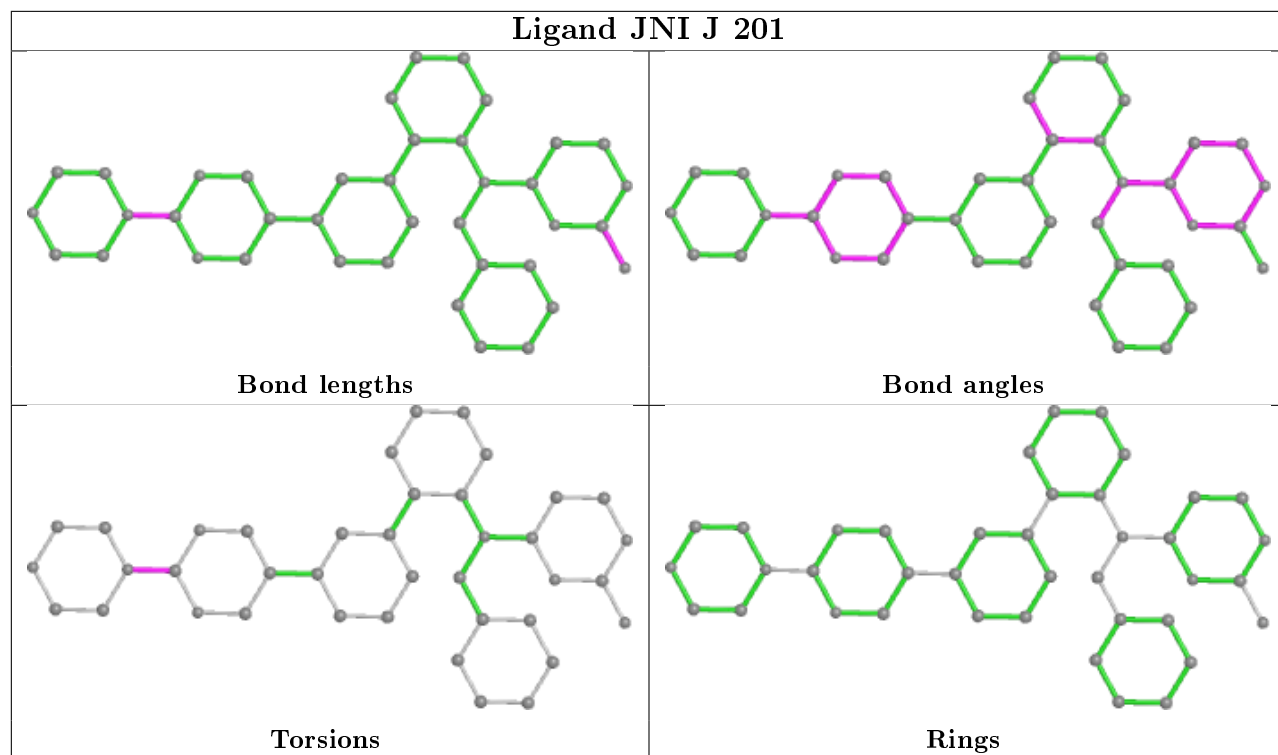


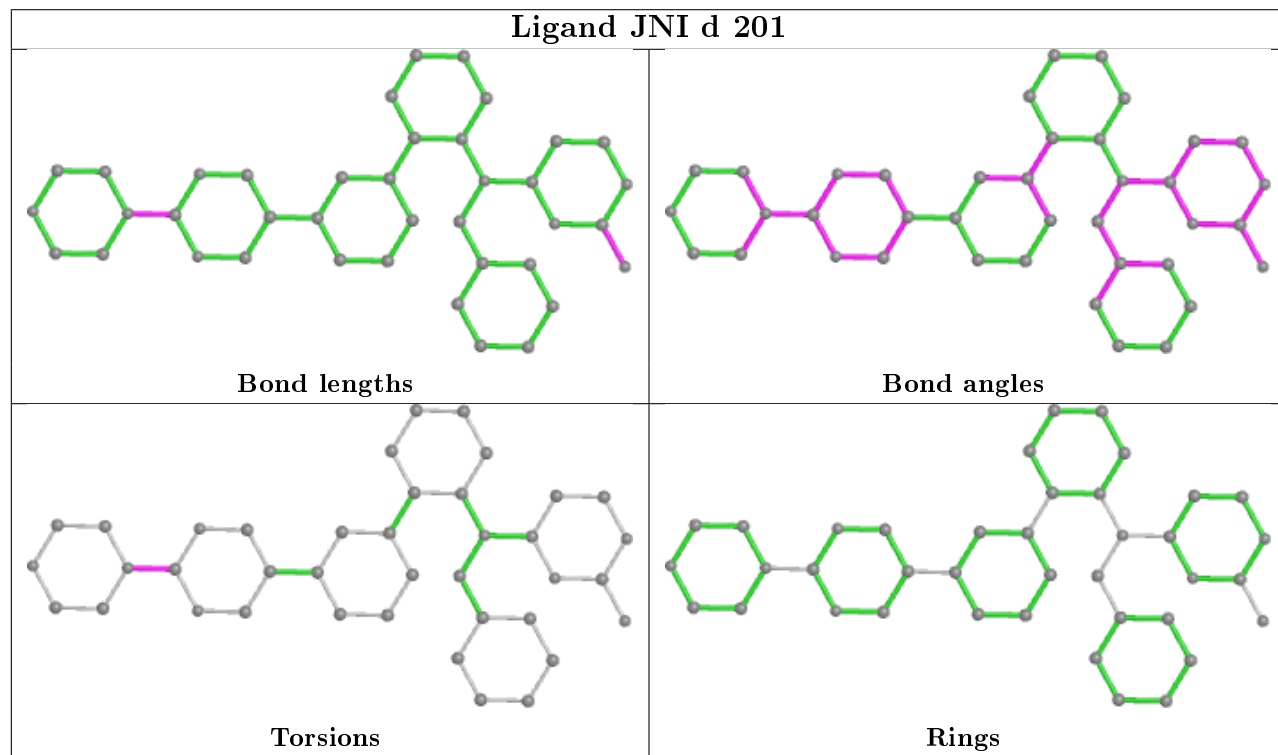
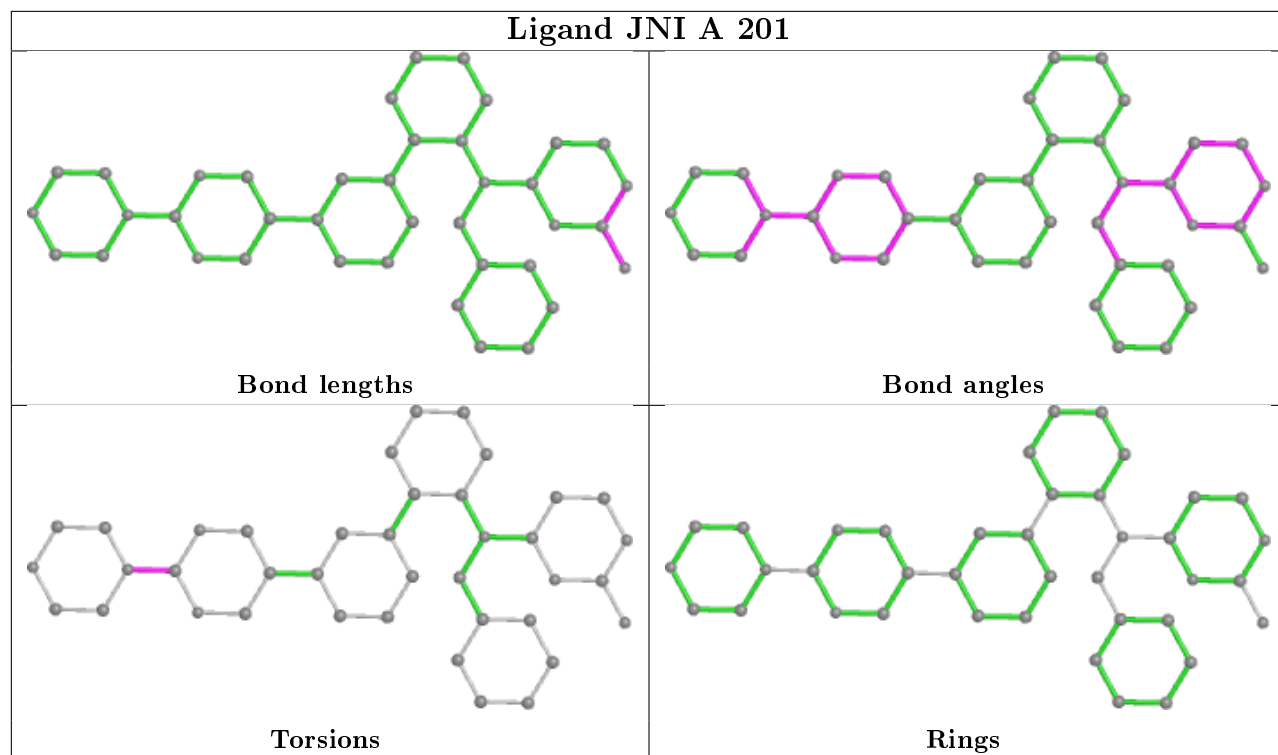












5.7 Other polymers [\(i\)](#)

There are no such residues in this entry.

5.8 Polymer linkage issues

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	141/159 (88%)	-0.46	0 100 100	76, 112, 164, 196	0
1	B	145/159 (91%)	-0.52	3 (2%) 63 34	59, 84, 133, 165	0
1	C	146/159 (91%)	-0.31	3 (2%) 63 34	82, 128, 177, 195	0
1	D	149/159 (93%)	-0.52	0 100 100	66, 83, 151, 180	0
1	F	140/159 (88%)	-0.55	1 (0%) 87 69	64, 95, 175, 222	0
1	G	149/159 (93%)	-0.49	4 (2%) 54 26	56, 84, 154, 189	0
1	H	150/159 (94%)	-0.26	3 (2%) 65 36	84, 127, 182, 217	0
1	I	141/159 (88%)	-0.66	0 100 100	66, 91, 139, 160	0
1	J	138/159 (86%)	-0.09	8 (5%) 23 7	81, 133, 183, 195	0
1	K	149/159 (93%)	-0.45	6 (4%) 38 15	59, 87, 161, 207	0
1	L	142/159 (89%)	0.07	8 (5%) 24 8	95, 142, 198, 234	0
1	M	149/159 (93%)	-0.50	2 (1%) 77 51	64, 89, 157, 194	0
1	N	143/159 (89%)	-0.28	8 (5%) 24 8	74, 100, 167, 211	0
1	O	145/159 (91%)	-0.58	1 (0%) 87 69	66, 90, 136, 161	0
1	P	145/159 (91%)	-0.29	3 (2%) 63 34	86, 131, 178, 217	0
1	Q	149/159 (93%)	-0.57	0 100 100	68, 94, 154, 193	0
1	R	138/159 (86%)	-0.39	2 (1%) 75 49	70, 104, 162, 214	0
1	S	149/159 (93%)	-0.53	4 (2%) 54 26	62, 84, 150, 198	0
1	T	146/159 (91%)	-0.46	1 (0%) 87 69	66, 104, 169, 206	0
1	U	149/159 (93%)	-0.61	0 100 100	61, 95, 162, 207	0
1	V	138/159 (86%)	-0.19	8 (5%) 23 7	79, 123, 187, 207	0
1	W	143/159 (89%)	-0.59	1 (0%) 87 69	61, 82, 133, 160	0
1	X	150/159 (94%)	-0.38	2 (1%) 77 51	68, 99, 183, 212	0
1	Y	149/159 (93%)	-0.62	0 100 100	63, 83, 160, 186	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	Z	143/159 (89%)	-0.21	5 (3%) 44 18	80, 119, 185, 219	0
1	a	149/159 (93%)	-0.44	7 (4%) 31 11	69, 91, 165, 235	0
1	b	144/159 (90%)	-0.31	2 (1%) 75 49	80, 116, 171, 190	0
1	c	145/159 (91%)	-0.57	1 (0%) 87 69	63, 86, 146, 165	0
1	d	138/159 (86%)	-0.41	1 (0%) 87 69	78, 116, 174, 211	0
1	e	149/159 (93%)	-0.66	0 100 100	60, 85, 131, 189	0
1	f	143/159 (89%)	-0.13	3 (2%) 63 34	93, 142, 190, 206	0
1	g	145/159 (91%)	-0.59	0 100 100	70, 98, 148, 170	0
1	h	137/159 (86%)	-0.20	2 (1%) 73 46	84, 120, 185, 204	0
1	i	145/159 (91%)	-0.53	3 (2%) 63 34	66, 89, 158, 186	0
1	j	150/159 (94%)	0.10	12 (8%) 12 4	80, 136, 197, 221	0
1	k	142/159 (89%)	-0.58	1 (0%) 87 69	63, 90, 139, 171	0
1	l	143/159 (89%)	-0.33	3 (2%) 63 34	77, 106, 171, 240	0
1	m	147/159 (92%)	-0.57	0 100 100	72, 94, 145, 186	0
1	n	147/159 (92%)	0.05	7 (4%) 30 11	107, 149, 188, 213	0
1	o	147/159 (92%)	-0.43	2 (1%) 75 49	79, 110, 158, 189	0
1	p	139/159 (87%)	0.06	10 (7%) 15 4	101, 148, 198, 214	0
1	q	149/159 (93%)	-0.56	1 (0%) 87 69	75, 99, 141, 168	0
1	r	144/159 (90%)	-0.05	6 (4%) 36 14	94, 146, 187, 215	0
1	s	149/159 (93%)	-0.52	2 (1%) 77 51	71, 93, 145, 177	0
1	t	143/159 (89%)	-0.08	8 (5%) 24 8	92, 131, 178, 200	0
1	u	145/159 (91%)	-0.53	0 100 100	77, 100, 144, 170	0
1	v	144/159 (90%)	0.27	12 (8%) 11 3	121, 154, 199, 233	0
1	w	145/159 (91%)	-0.53	1 (0%) 87 69	76, 111, 164, 186	0
All	All	6955/7632 (91%)	-0.38	157 (2%) 60 31	56, 106, 177, 240	0

All (157) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	l	109	ALA	8.6
1	a	106	PRO	8.2
1	v	9	SER	7.6
1	l	108	GLY	6.9
1	L	72	THR	6.4

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Mol	Chain	Res	Type	RSRZ
1	j	8	PRO	6.4
1	P	23	GLU	6.1
1	L	71	SER	5.8
1	L	18	ALA	5.8
1	v	34	ASN	5.5
1	R	146	GLU	5.3
1	o	108	GLY	5.1
1	V	106	PRO	4.5
1	j	106	PRO	4.4
1	K	106	PRO	4.4
1	h	71	SER	4.3
1	n	9	SER	4.3
1	l	106	PRO	4.3
1	v	33	ALA	4.2
1	v	24	GLY	4.2
1	v	30	ASN	4.0
1	G	107	GLU	3.9
1	H	109	ALA	3.9
1	Z	109	ALA	3.8
1	L	89	THR	3.7
1	J	67	GLN	3.7
1	j	109	ALA	3.7
1	r	24	GLY	3.5
1	K	108	GLY	3.5
1	r	23	GLU	3.4
1	R	73	HIS	3.4
1	c	9	SER	3.4
1	p	44	ARG	3.4
1	v	8	PRO	3.3
1	L	31	ARG	3.3
1	a	9	SER	3.3
1	a	111	ALA	3.2
1	N	87	TYR	3.2
1	L	73	HIS	3.2
1	a	110	GLU	3.2
1	d	71	SER	3.2
1	G	106	PRO	3.2
1	p	43	LEU	3.1
1	i	9	SER	3.1
1	V	101	CYS	3.1
1	X	33	ALA	3.1
1	M	108	GLY	3.0

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Mol	Chain	Res	Type	RSRZ
1	B	105	THR	3.0
1	j	105	THR	3.0
1	k	9	SER	3.0
1	i	106	PRO	3.0
1	N	73	HIS	3.0
1	J	20	PRO	3.0
1	t	107	GLU	3.0
1	J	24	GLY	3.0
1	J	102	GLN	3.0
1	n	105	THR	3.0
1	r	144	PHE	2.9
1	t	112	LYS	2.9
1	K	111	ALA	2.9
1	H	106	PRO	2.9
1	K	110	GLU	2.9
1	f	33	ALA	2.9
1	o	106	PRO	2.9
1	K	105	THR	2.9
1	j	71	SER	2.9
1	V	105	THR	2.9
1	N	104	GLU	2.8
1	n	8	PRO	2.8
1	s	9	SER	2.8
1	C	24	GLY	2.8
1	J	115	TYR	2.8
1	a	109	ALA	2.7
1	i	111	ALA	2.7
1	t	9	SER	2.7
1	t	106	PRO	2.7
1	a	108	GLY	2.7
1	S	106	PRO	2.7
1	r	30	ASN	2.7
1	q	24	GLY	2.7
1	H	107	GLU	2.7
1	L	23	GLU	2.7
1	O	105	THR	2.6
1	j	73	HIS	2.6
1	v	29	LEU	2.6
1	K	107	GLU	2.6
1	P	73	HIS	2.6
1	P	106	PRO	2.6
1	r	86	SER	2.6

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Mol	Chain	Res	Type	RSRZ
1	p	71	SER	2.6
1	M	110	GLU	2.6
1	T	9	SER	2.5
1	t	71	SER	2.5
1	t	109	ALA	2.5
1	p	20	PRO	2.5
1	j	9	SER	2.5
1	n	40	GLY	2.4
1	S	108	GLY	2.4
1	t	108	GLY	2.4
1	b	21	GLN	2.4
1	f	24	GLY	2.4
1	v	10	ASP	2.4
1	X	110	GLU	2.4
1	h	146	GLU	2.4
1	G	111	ALA	2.4
1	J	103	ARG	2.4
1	v	35	ALA	2.4
1	G	108	GLY	2.4
1	p	72	THR	2.4
1	t	86	SER	2.4
1	n	33	ALA	2.4
1	W	103	ARG	2.4
1	w	106	PRO	2.4
1	p	36	LEU	2.4
1	b	105	THR	2.3
1	Z	108	GLY	2.3
1	S	110	GLU	2.3
1	v	105	THR	2.3
1	S	112	LYS	2.3
1	N	9	SER	2.3
1	n	71	SER	2.3
1	C	23	GLU	2.3
1	p	29	LEU	2.2
1	V	74	VAL	2.2
1	C	106	PRO	2.2
1	v	23	GLU	2.2
1	F	105	THR	2.2
1	L	34	ASN	2.2
1	N	71	SER	2.2
1	N	103	ARG	2.2
1	v	32	ARG	2.2

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Mol	Chain	Res	Type	RSRZ
1	p	27	GLN	2.2
1	n	106	PRO	2.2
1	V	104	GLU	2.2
1	j	40	GLY	2.2
1	B	111	ALA	2.2
1	Z	21	GLN	2.2
1	p	21	GLN	2.2
1	j	107	GLU	2.2
1	Z	111	ALA	2.1
1	j	44	ARG	2.1
1	V	23	GLU	2.1
1	a	107	GLU	2.1
1	j	103	ARG	2.1
1	V	21	GLN	2.1
1	s	110	GLU	2.1
1	j	72	THR	2.1
1	p	10	ASP	2.1
1	Z	112	LYS	2.1
1	J	68	GLY	2.1
1	J	112	LYS	2.1
1	B	71	SER	2.1
1	r	102	GLN	2.1
1	V	103	ARG	2.1
1	N	86	SER	2.1
1	N	106	PRO	2.0
1	f	74	VAL	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [\(i\)](#)

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

6.3 Carbohydrates [\(i\)](#)

There are no monosaccharides in this entry.

6.4 Ligands [\(i\)](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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.

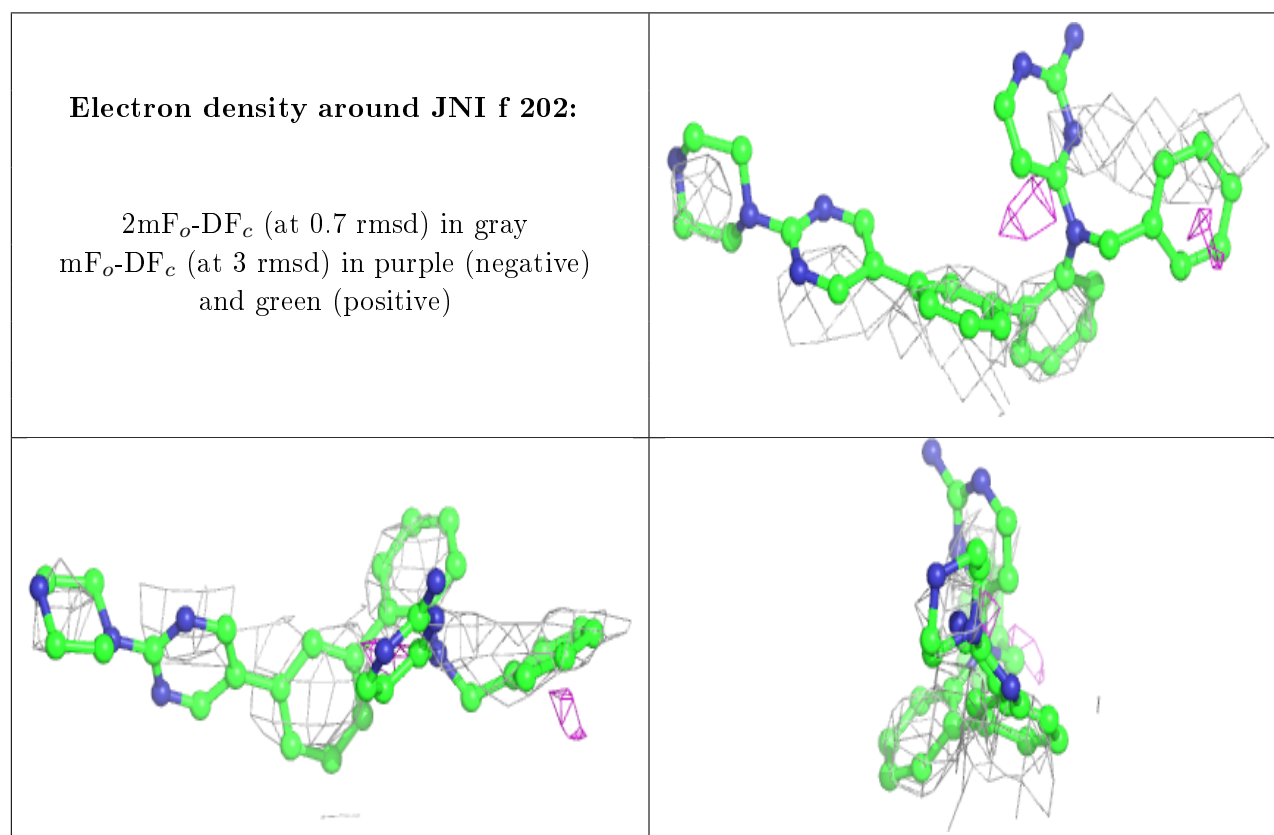
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	JNI	f	202	39/39	0.76	0.44	117,175,241,261	0
2	JNI	j	202	39/39	0.80	0.37	93,148,193,200	0
2	JNI	P	202	39/39	0.80	0.32	80,129,210,215	0
2	JNI	n	202	39/39	0.80	0.33	88,133,183,186	0
2	JNI	r	202	39/39	0.83	0.28	88,144,228,245	0
2	JNI	v	202	39/39	0.85	0.30	97,150,214,219	0
2	JNI	n	201	39/39	0.85	0.30	67,125,200,203	0
2	JNI	J	202	39/39	0.86	0.27	101,150,181,185	0
2	JNI	t	202	39/39	0.86	0.28	87,160,187,203	0
2	JNI	X	202	39/39	0.86	0.30	65,112,179,192	0
2	JNI	U	201	39/39	0.87	0.25	59,93,151,157	0
2	JNI	Z	202	39/39	0.87	0.24	79,130,160,183	0
2	JNI	d	201	39/39	0.87	0.24	91,123,170,180	0
2	JNI	j	201	39/39	0.88	0.28	82,121,168,184	0
2	JNI	L	201	39/39	0.88	0.27	73,119,190,221	0
2	JNI	p	202	39/39	0.88	0.24	103,140,220,241	0
2	JNI	f	201	39/39	0.88	0.23	92,130,170,171	0
2	JNI	b	202	39/39	0.88	0.26	58,126,198,209	0
2	JNI	C	201	39/39	0.89	0.28	59,121,184,199	0
2	JNI	C	202	39/39	0.89	0.23	85,167,208,219	0
2	JNI	r	201	39/39	0.89	0.32	100,172,215,232	0
2	JNI	X	201	39/39	0.90	0.23	67,96,126,165	0
2	JNI	h	202	39/39	0.90	0.26	61,132,171,220	0
2	JNI	o	201	39/39	0.90	0.27	89,119,195,210	0
2	JNI	H	202	39/39	0.90	0.29	59,128,217,244	0
2	JNI	F	202	39/39	0.90	0.22	86,118,162,186	0
2	JNI	h	201	39/39	0.91	0.21	72,111,141,166	0
2	JNI	l	201	39/39	0.91	0.25	69,103,136,147	0
2	JNI	A	202	39/39	0.91	0.19	76,96,124,128	0
2	JNI	R	201	39/39	0.91	0.20	55,91,170,183	0
2	JNI	V	202	39/39	0.91	0.26	85,121,189,247	0
2	JNI	F	201	39/39	0.92	0.27	57,94,163,186	0
2	JNI	J	201	39/39	0.92	0.22	54,115,146,157	0
2	JNI	p	201	39/39	0.92	0.22	64,114,170,175	0
2	JNI	v	201	39/39	0.92	0.26	106,139,183,205	0
2	JNI	b	201	39/39	0.93	0.20	62,94,136,141	0
2	JNI	V	201	39/39	0.93	0.20	63,89,147,155	0
2	JNI	M	201	39/39	0.93	0.20	67,108,136,144	0
2	JNI	H	201	39/39	0.94	0.20	69,91,142,182	0
2	JNI	t	201	39/39	0.94	0.17	75,102,125,129	0
2	JNI	P	201	39/39	0.94	0.18	62,102,142,154	0
2	JNI	D	201	39/39	0.94	0.18	56,71,112,141	0
2	JNI	Q	201	39/39	0.95	0.23	67,88,141,169	0

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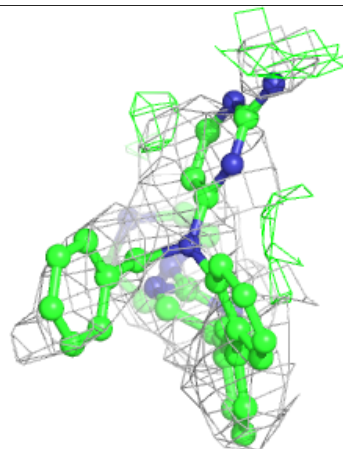
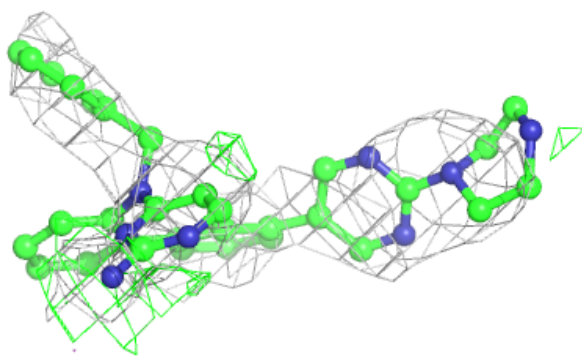
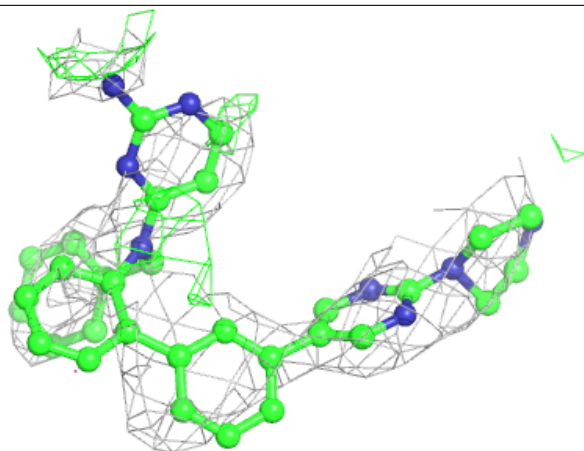
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	JNI	Z	201	39/39	0.95	0.20	68,96,133,138	0
2	JNI	N	201	39/39	0.95	0.18	47,74,95,99	0
2	JNI	A	201	39/39	0.96	0.15	33,84,117,140	0

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.



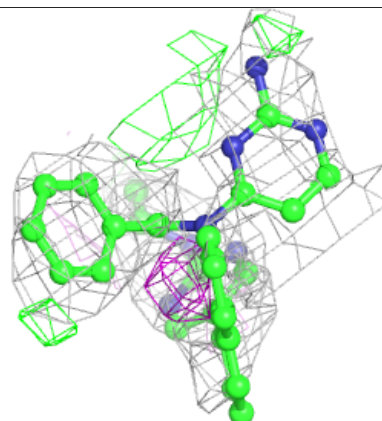
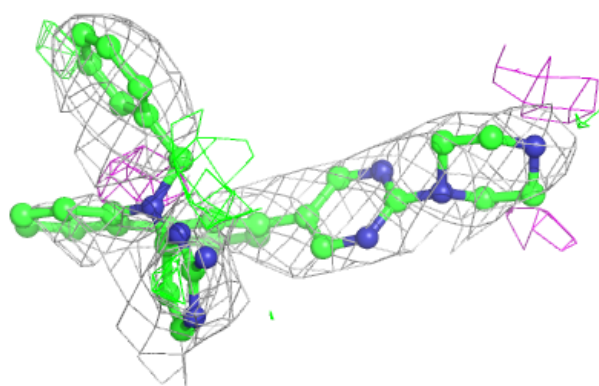
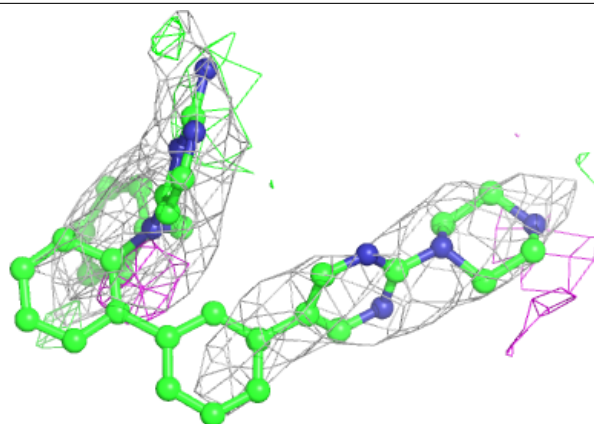
Electron density around JNI j 202:

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

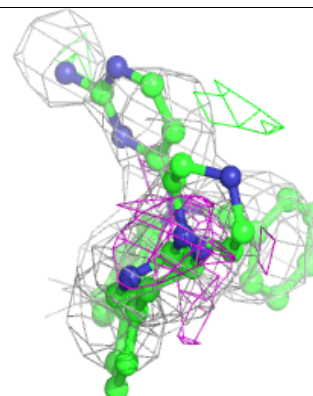
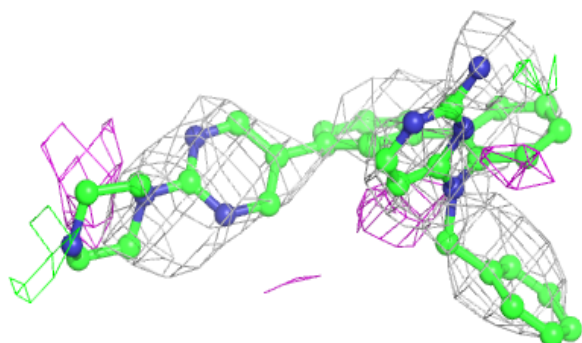
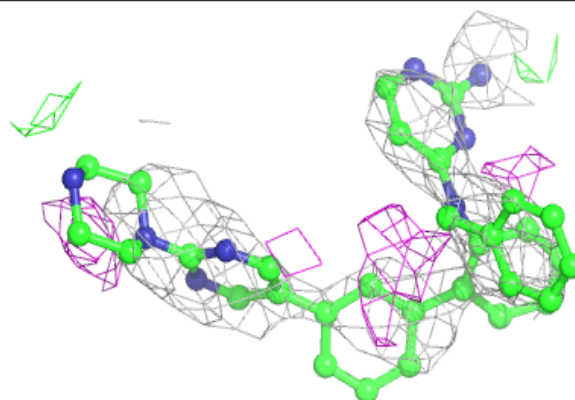


Electron density around JNI P 202:

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

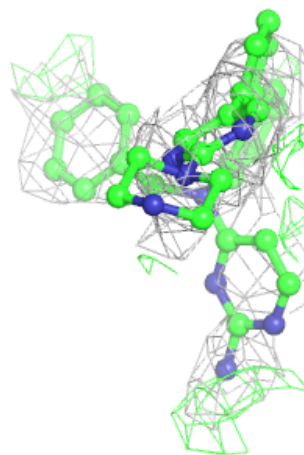
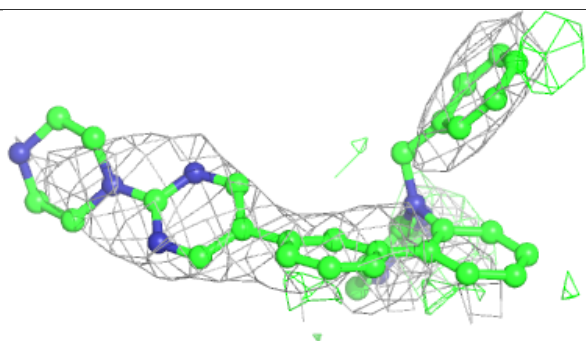
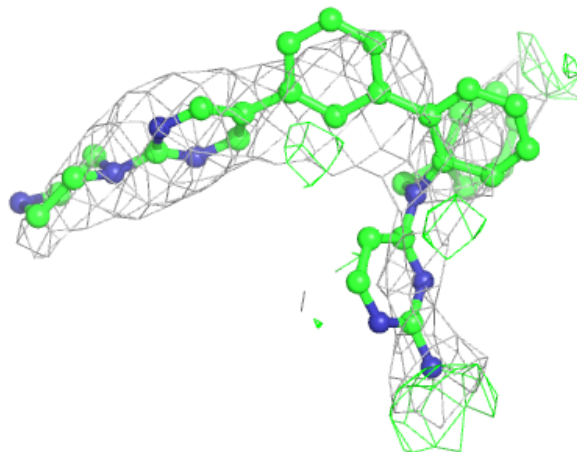
**Electron density around JNI n 202:**

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



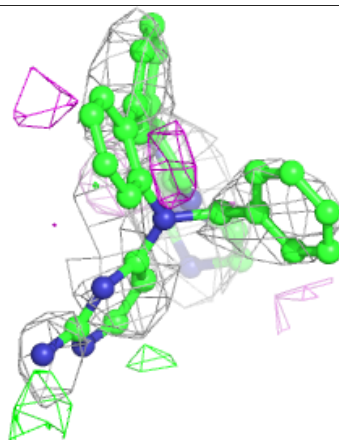
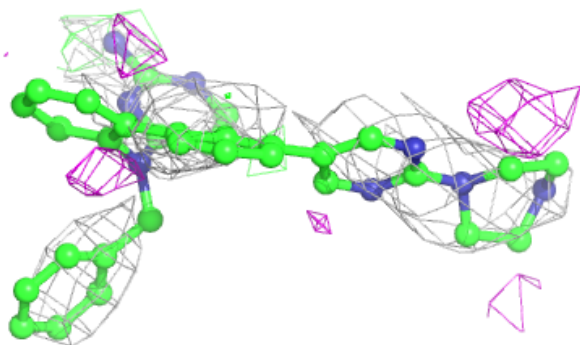
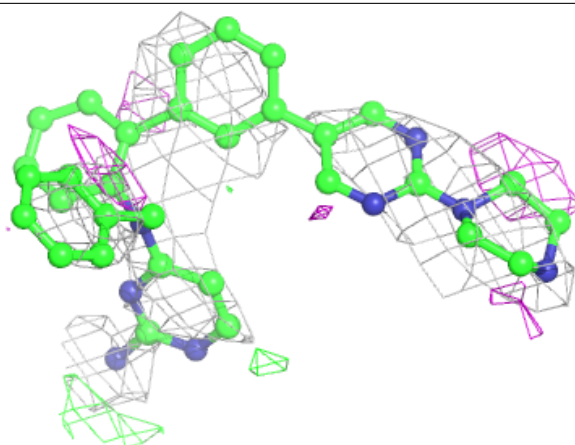
Electron density around JN1 r 202:

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

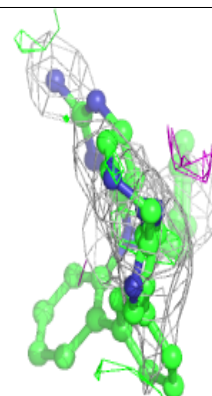
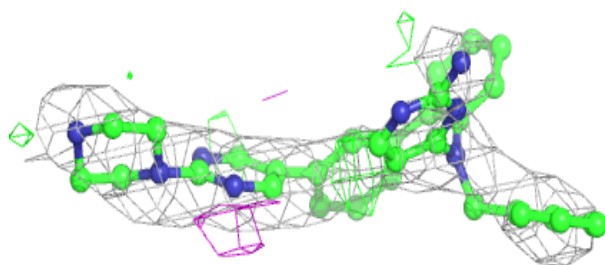
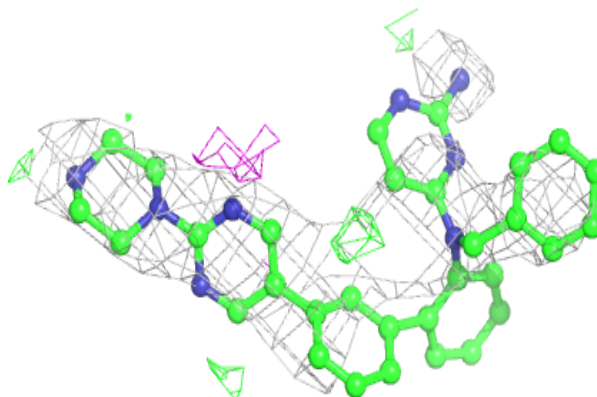


Electron density around JNI v 202:

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

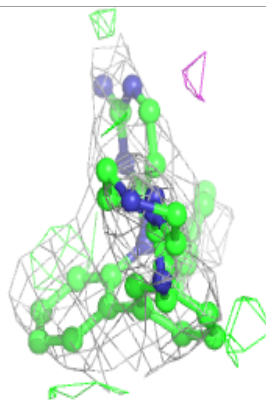
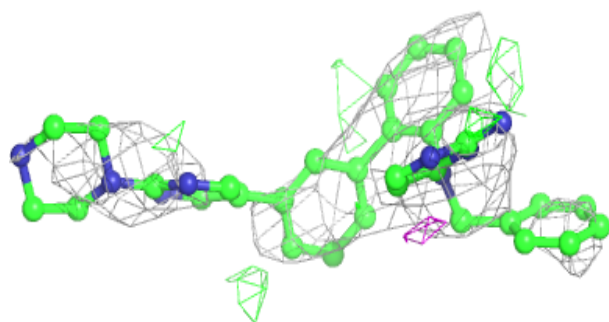
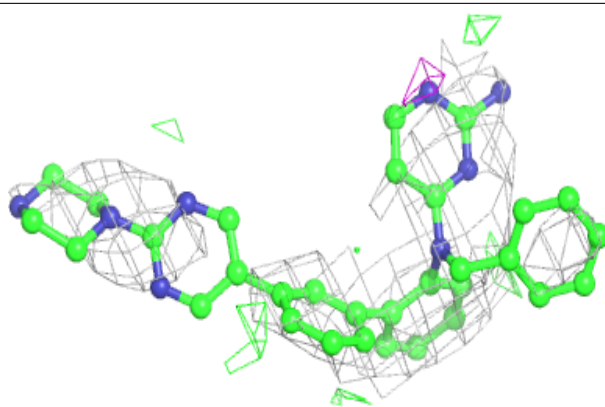
**Electron density around JNI n 201:**

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

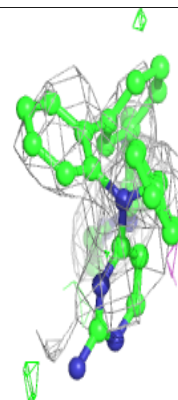
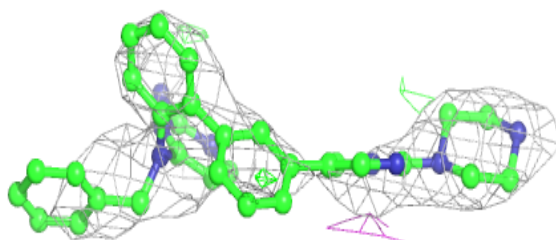
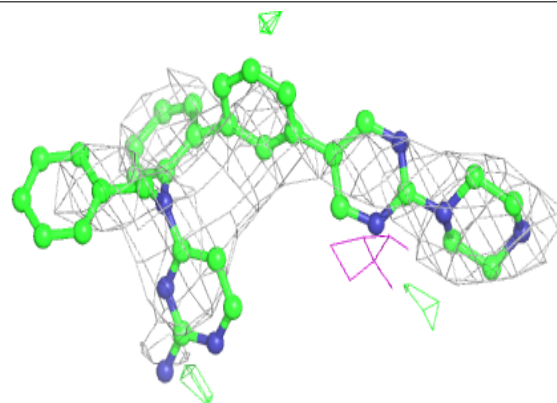


Electron density around JNI J 202:

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

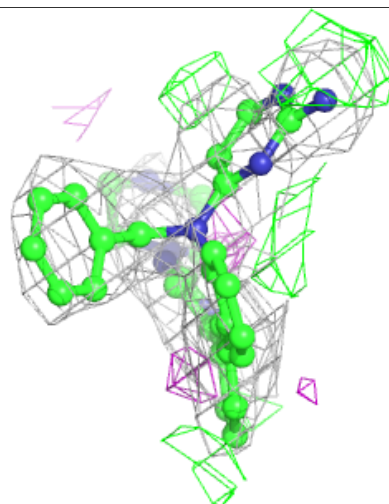
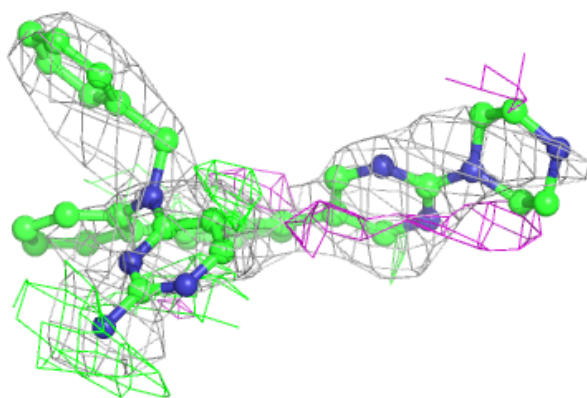
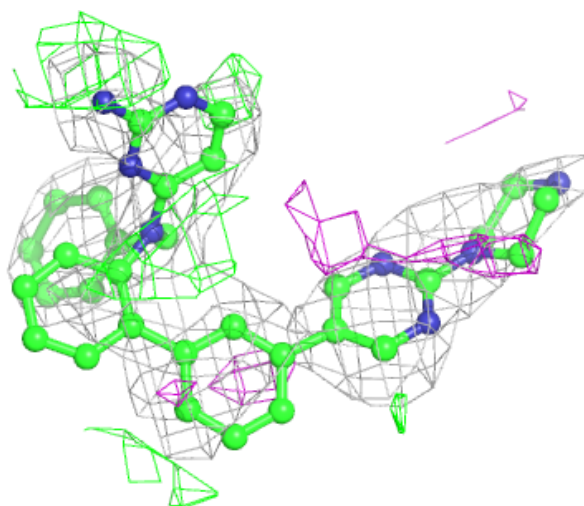
**Electron density around JNI t 202:**

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



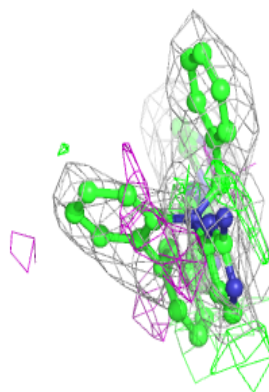
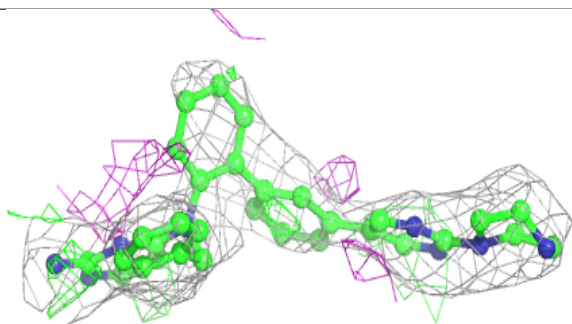
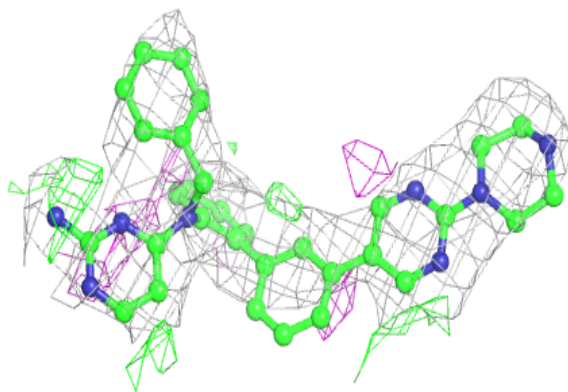
Electron density around JNI X 202:

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

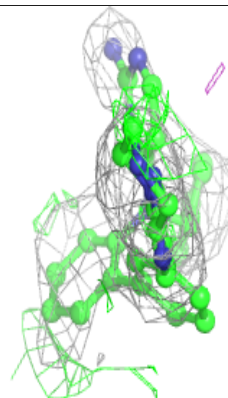
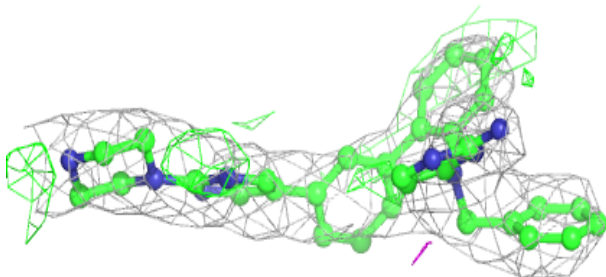
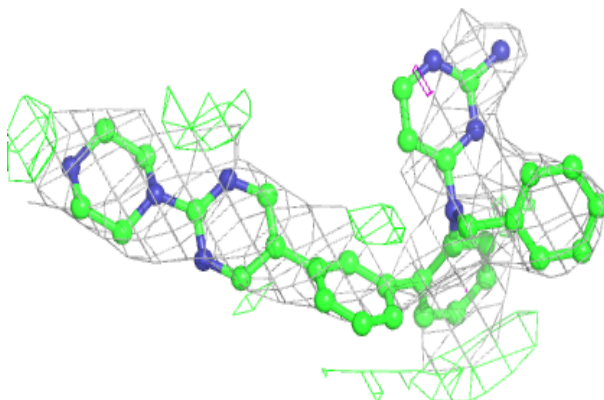


Electron density around JNI U 201:

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

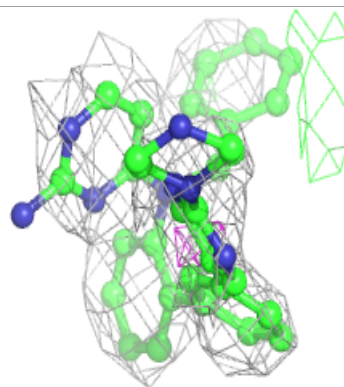
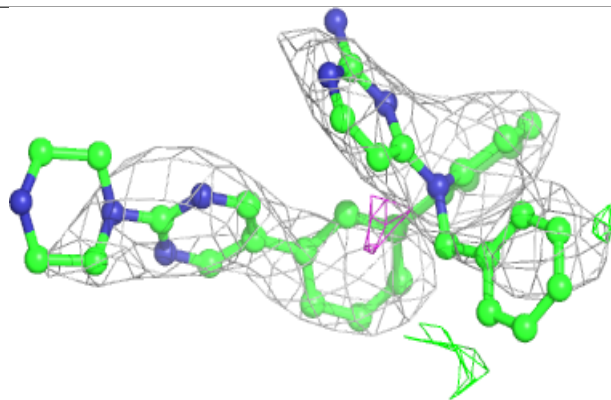
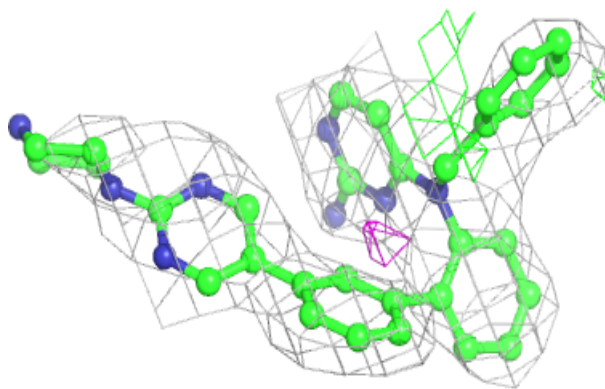
**Electron density around JNI Z 202:**

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

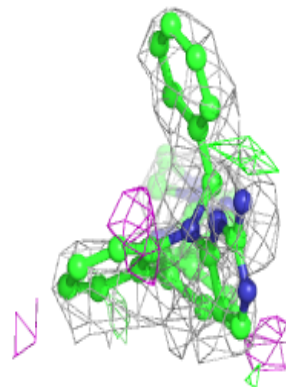
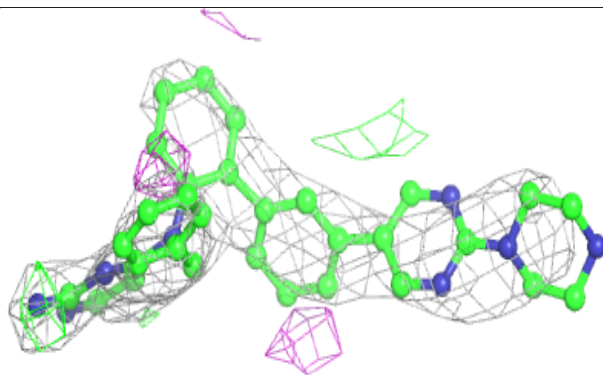
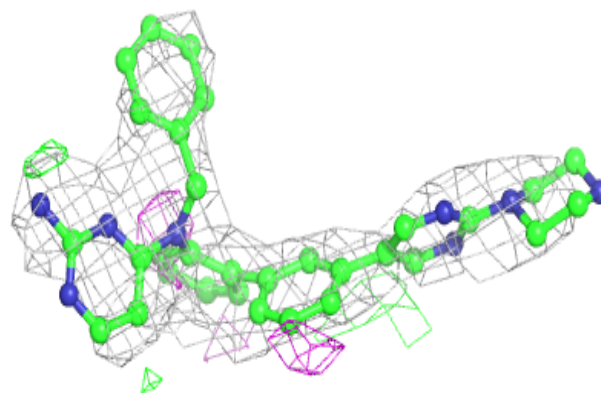


Electron density around JNI d 201:

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

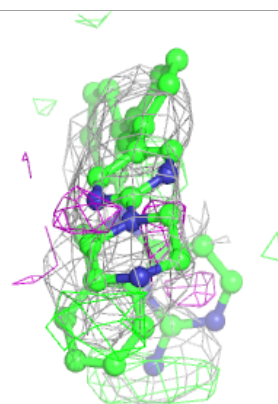
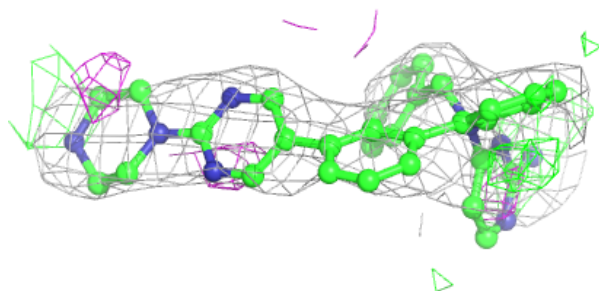
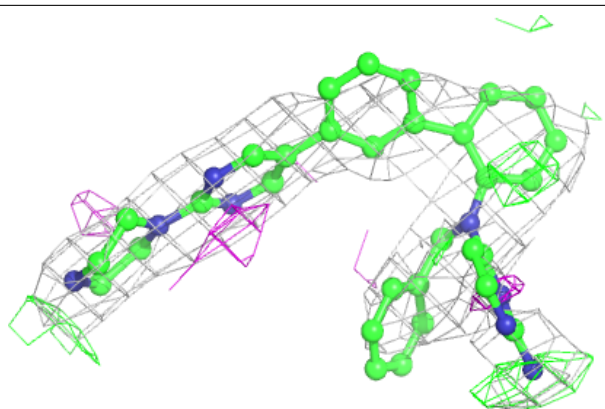
**Electron density around JNI j 201:**

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

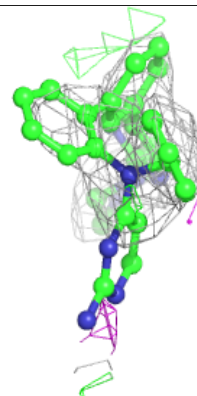
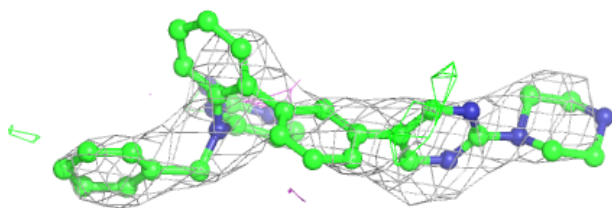
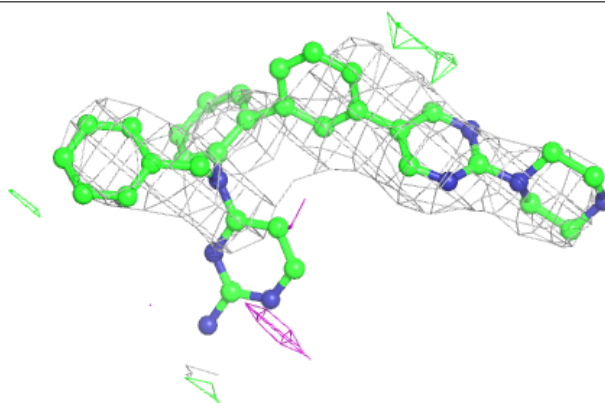


Electron density around JNI L 201:

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

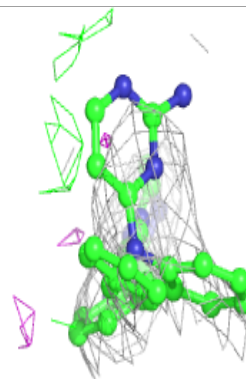
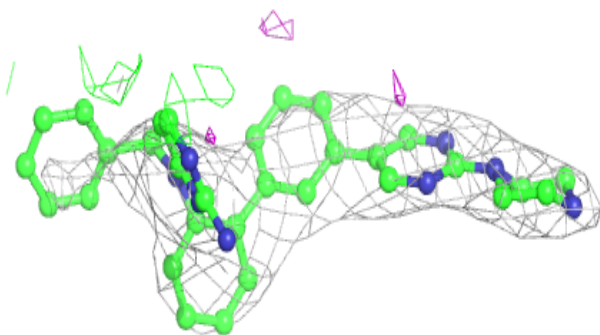
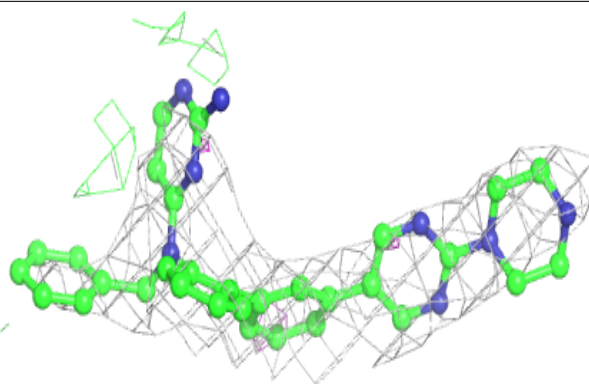
**Electron density around JNI p 202:**

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

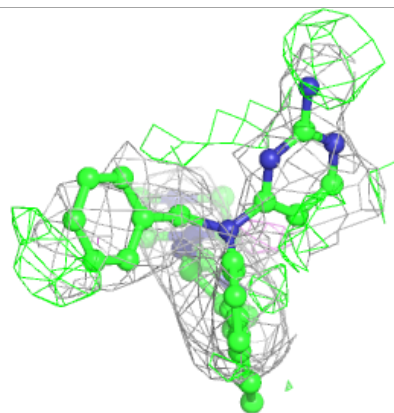
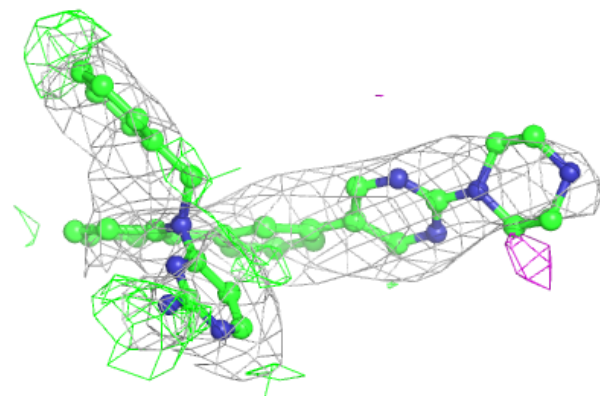
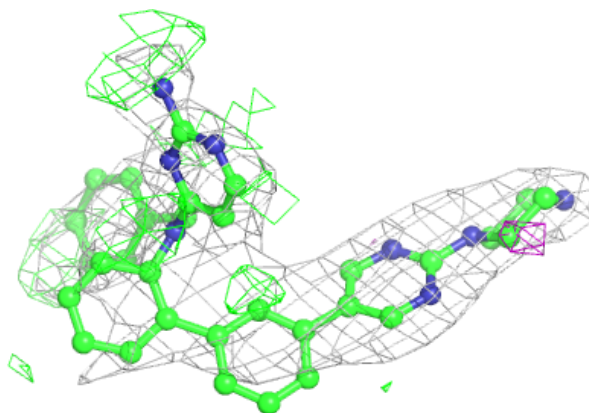


Electron density around JNI f 201:

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

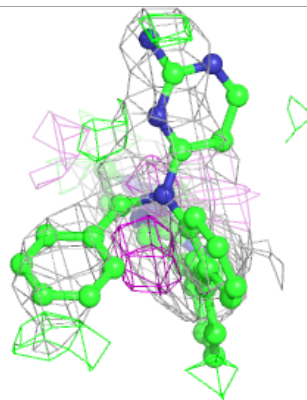
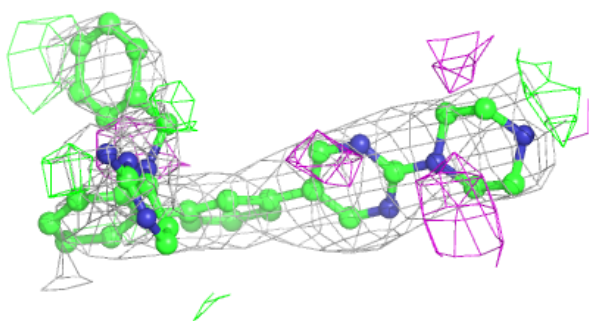
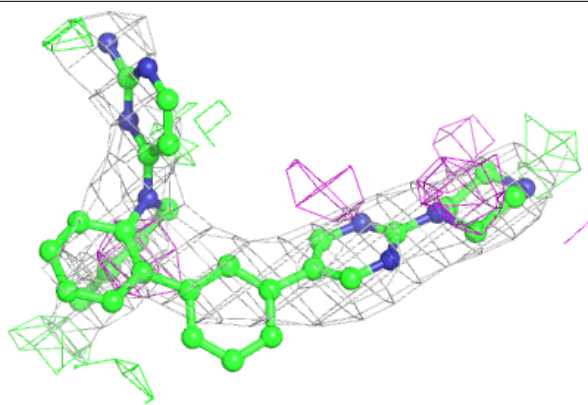
**Electron density around JNI b 202:**

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

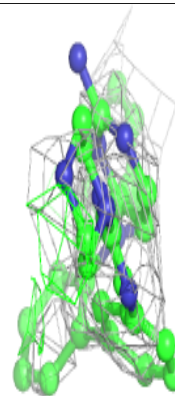
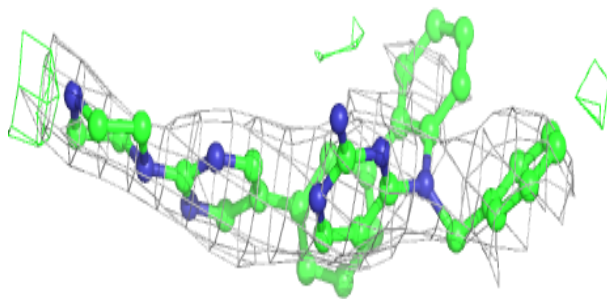
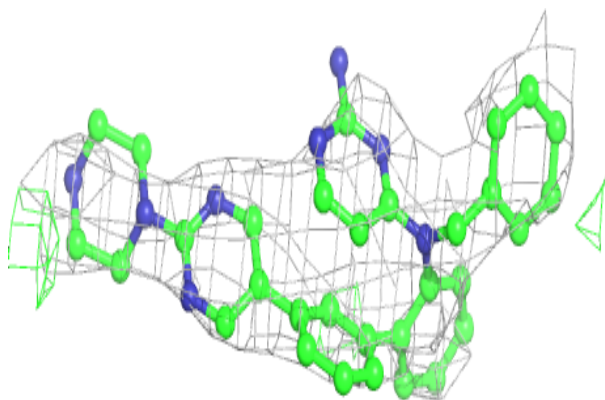


Electron density around JNI C 201:

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

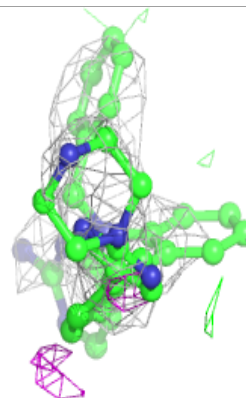
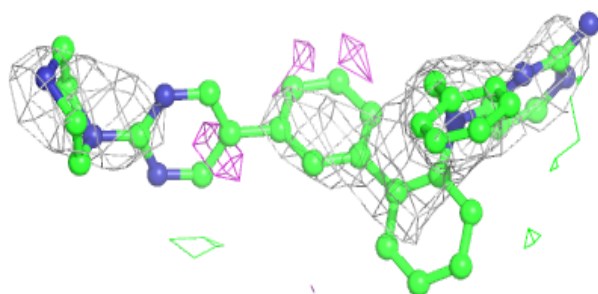
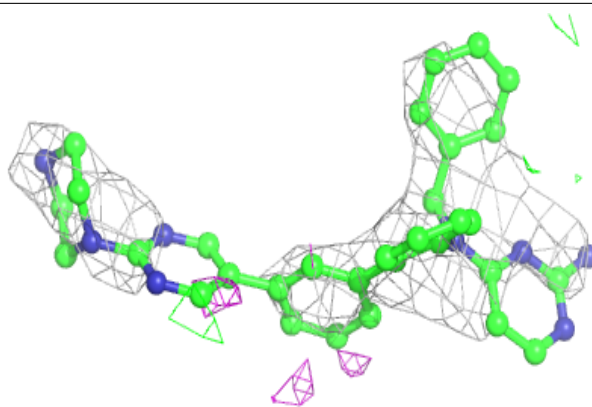
**Electron density around JNI C 202:**

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

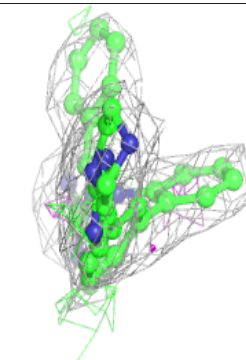
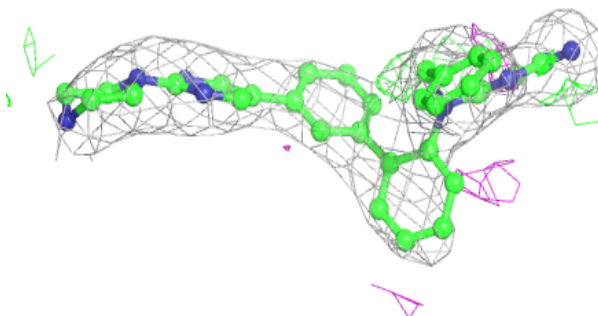
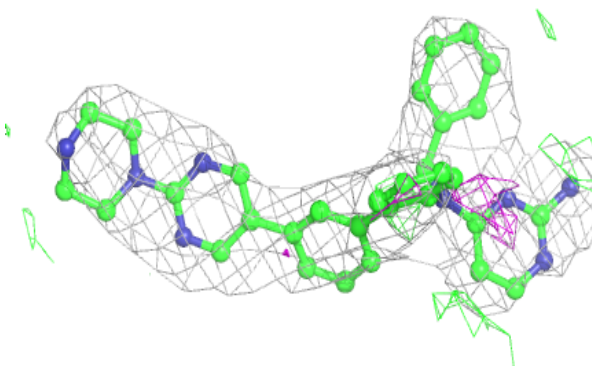


Electron density around JNI r 201:

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

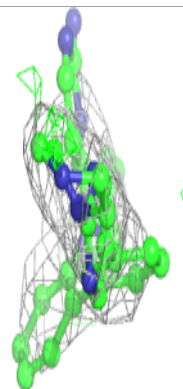
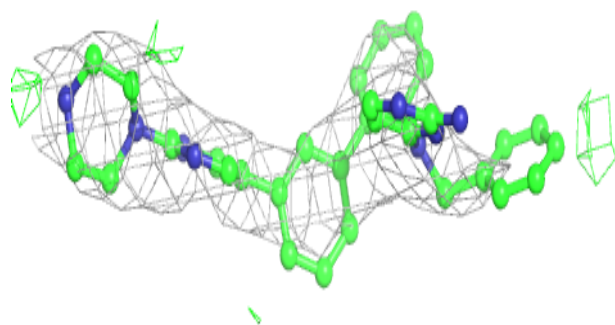
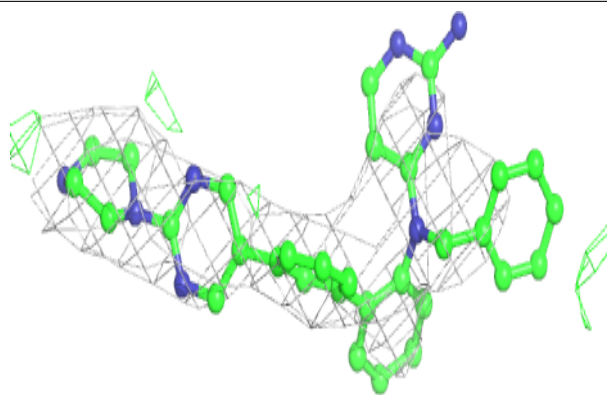
**Electron density around JNI X 201:**

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

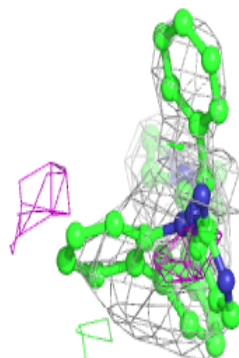
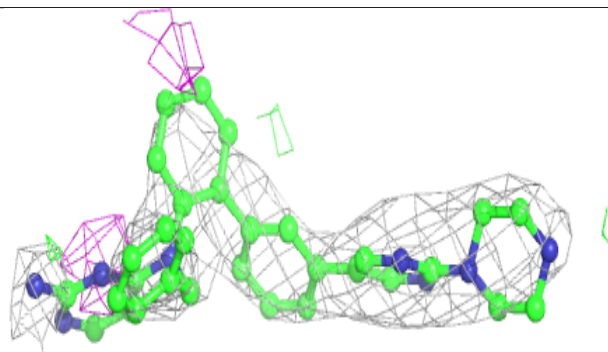
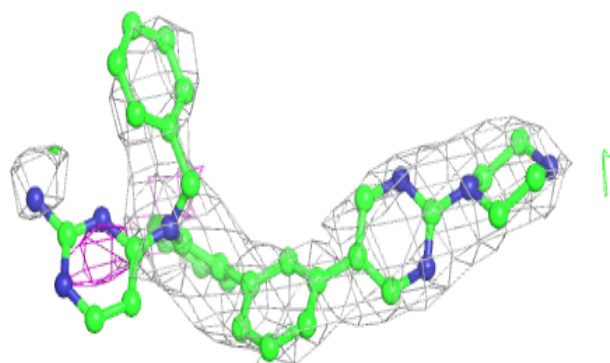


Electron density around JNI h 202:

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

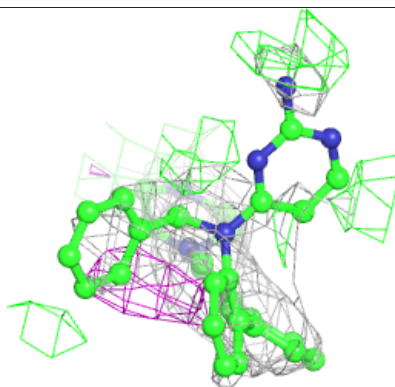
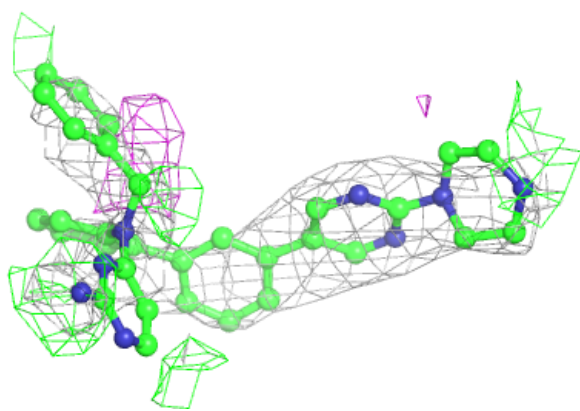
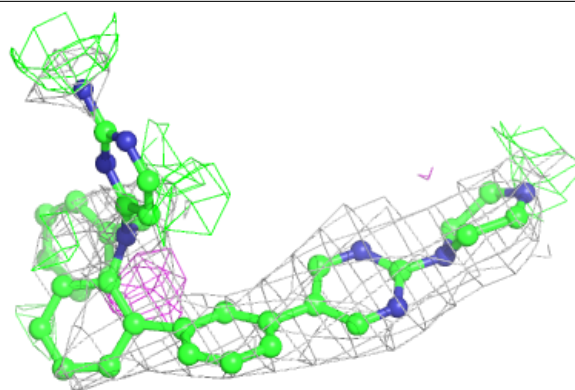
**Electron density around JNI o 201:**

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

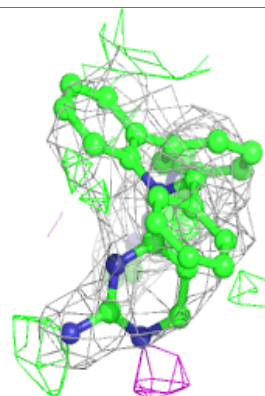
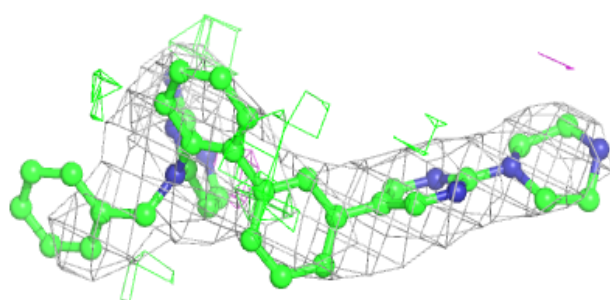
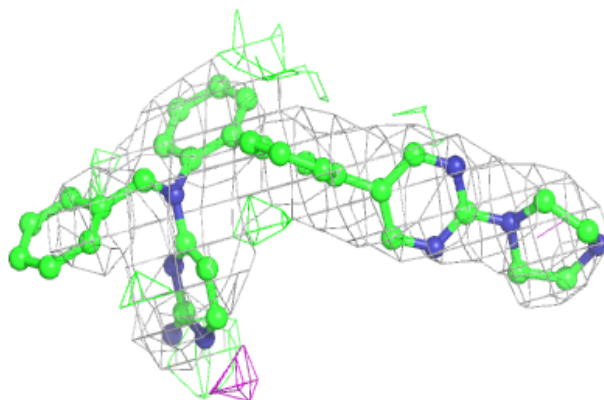


Electron density around JNI H 202:

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

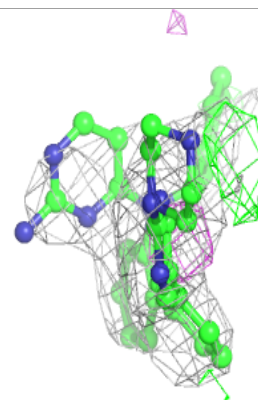
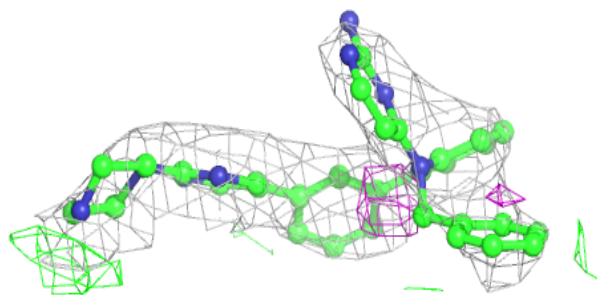
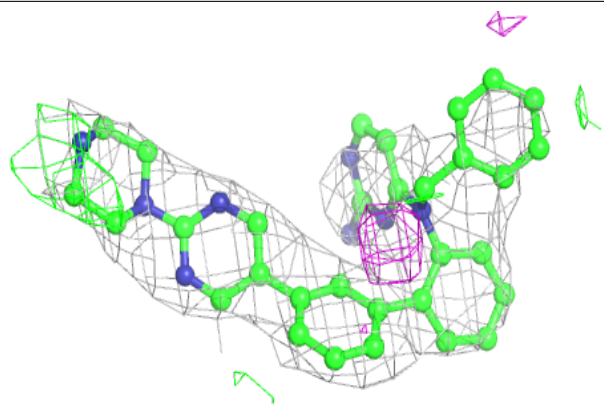
**Electron density around JNI F 202:**

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

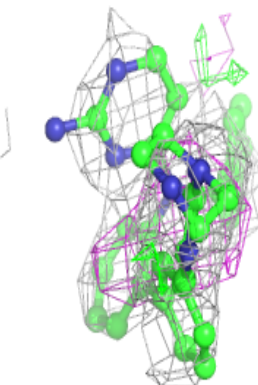
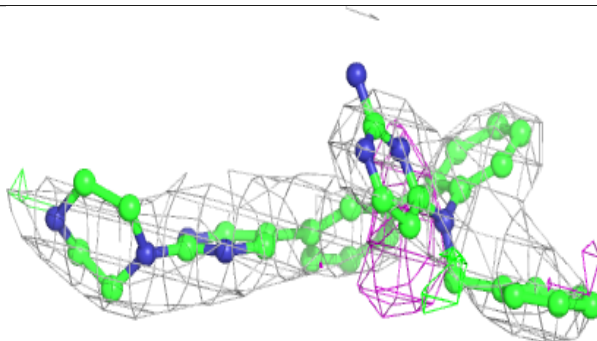
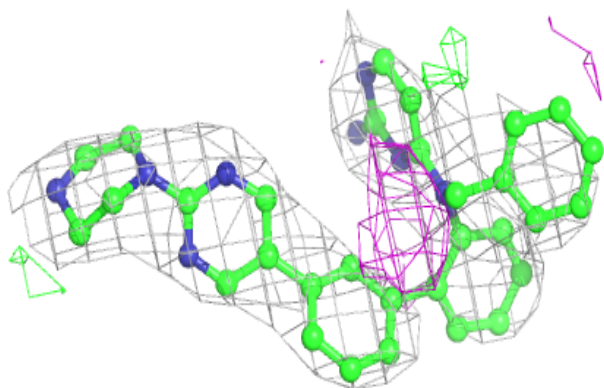


Electron density around JNI h 201:

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

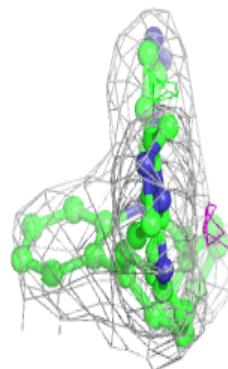
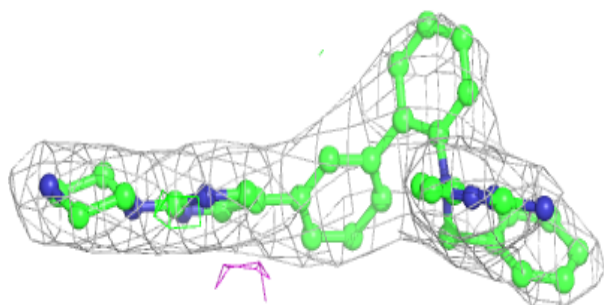
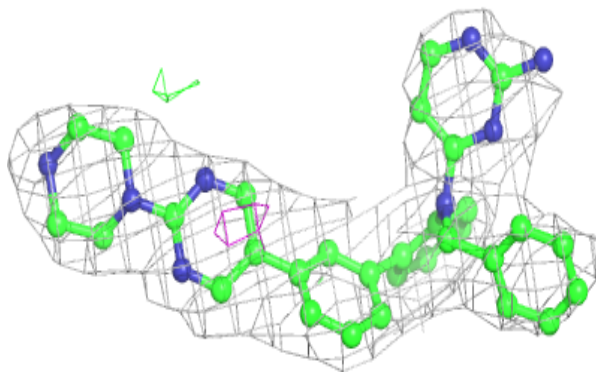
**Electron density around JNI l 201:**

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

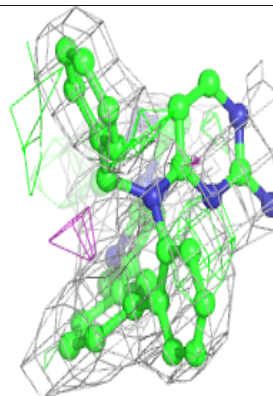
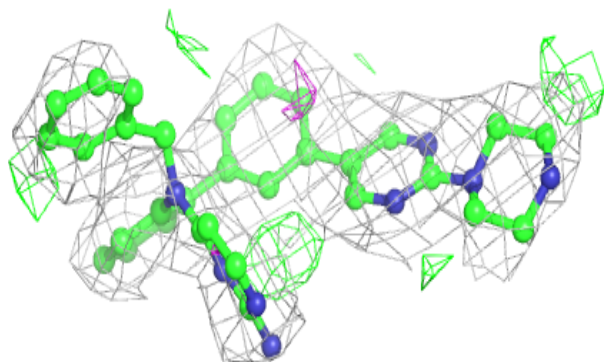
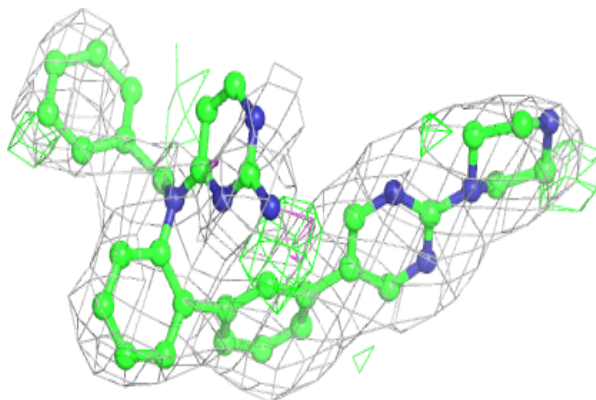


Electron density around JNI A 202:

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

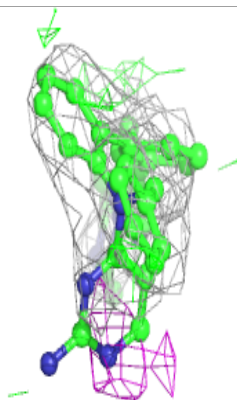
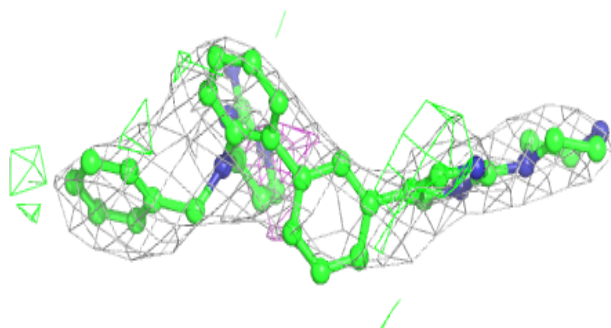
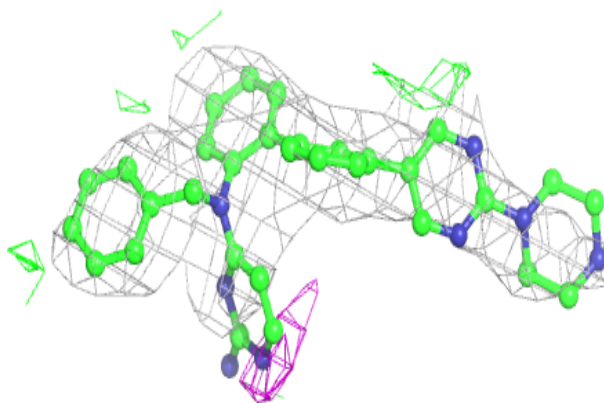
**Electron density around JNI R 201:**

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

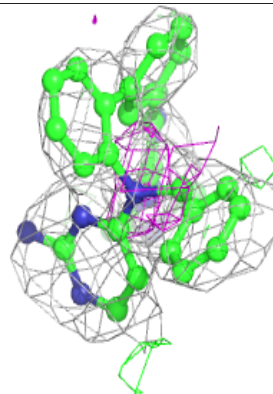
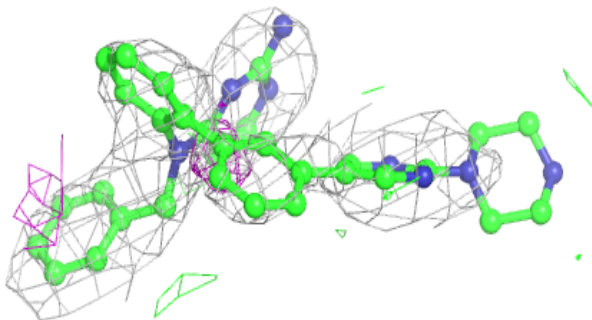
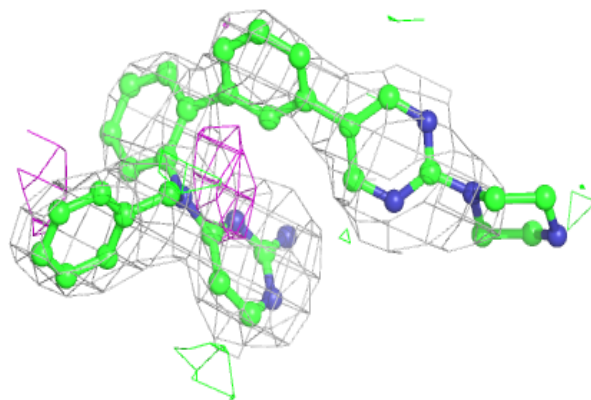


Electron density around JNI V 202:

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

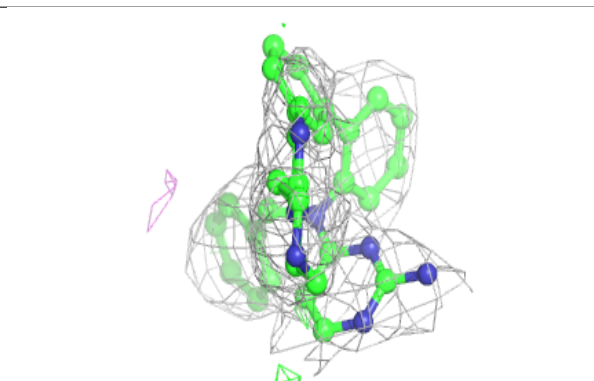
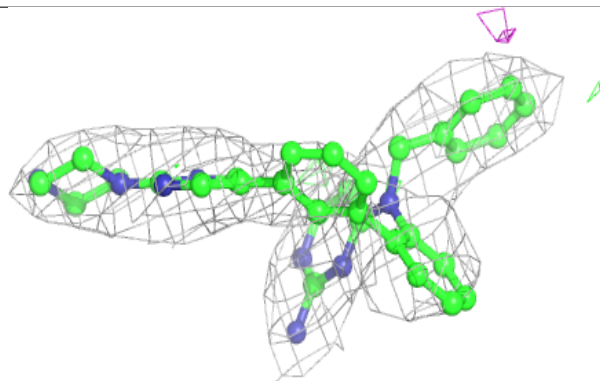
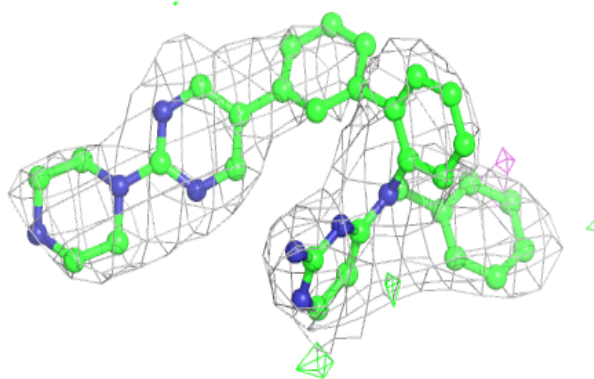
**Electron density around JNI F 201:**

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

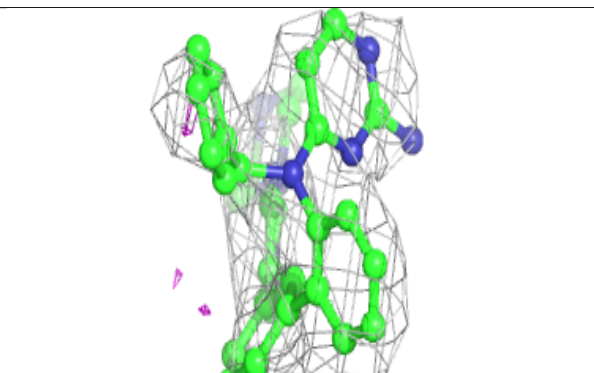
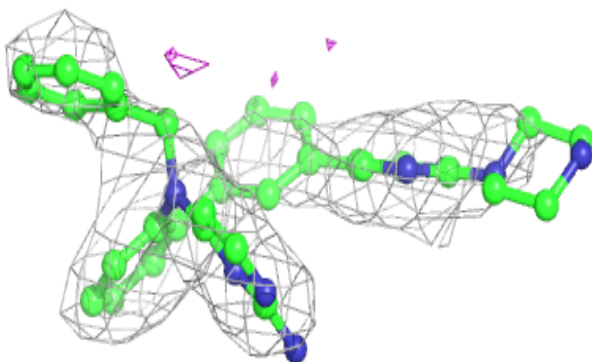
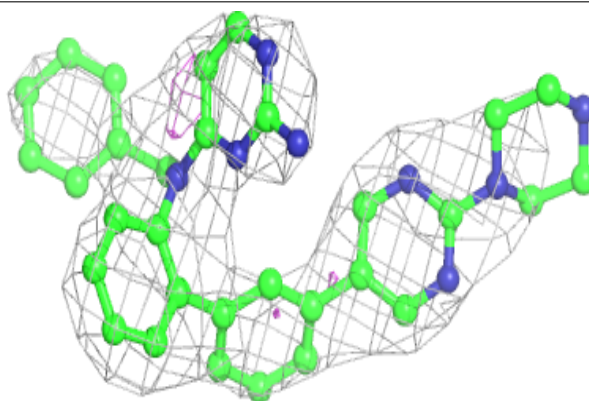


Electron density around JNI J 201:

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

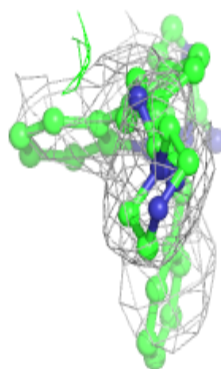
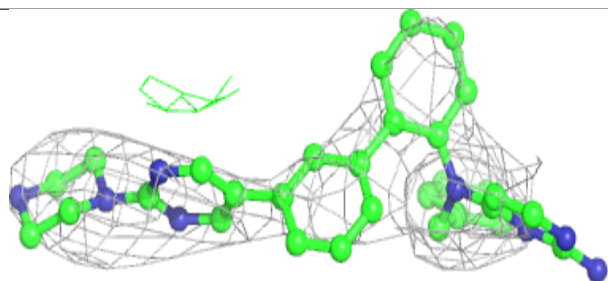
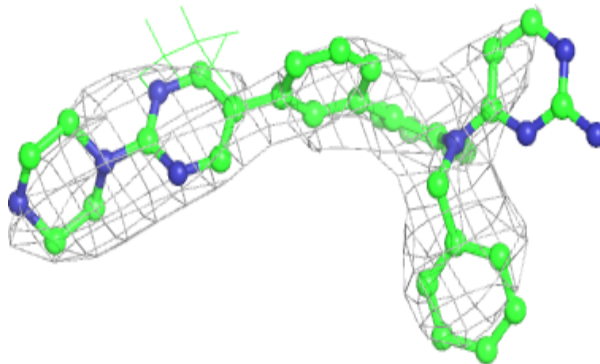
**Electron density around JNI p 201:**

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

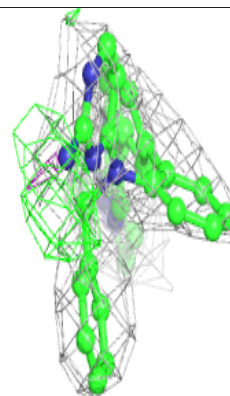
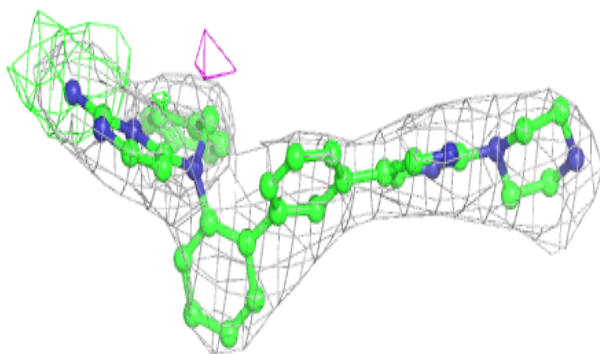
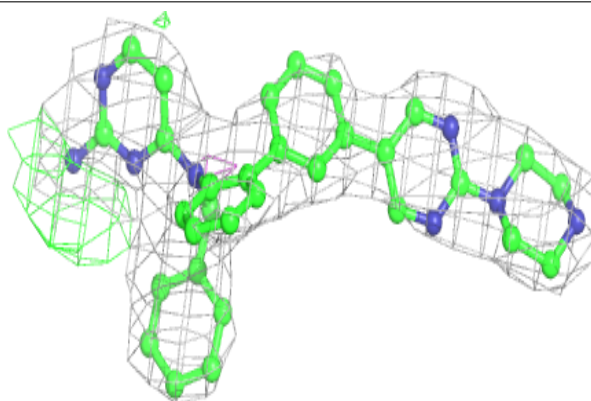


Electron density around JNI v 201:

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

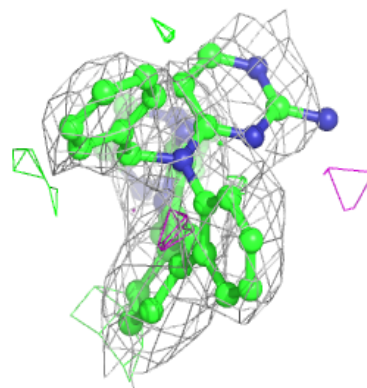
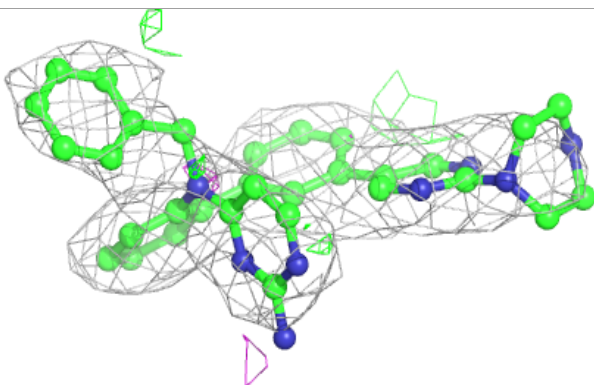
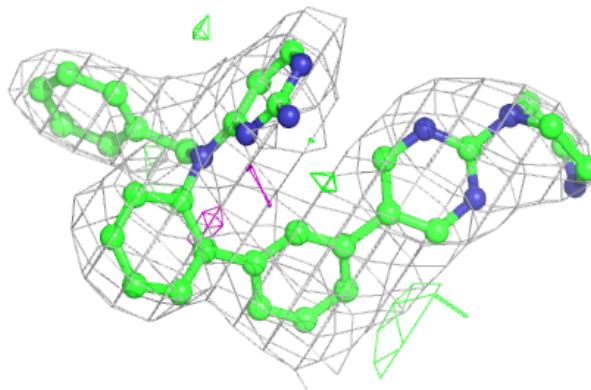
**Electron density around JNI b 201:**

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

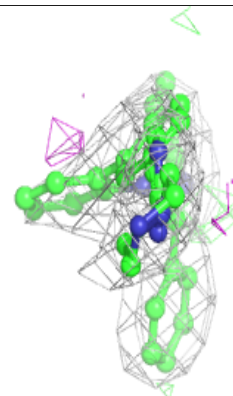
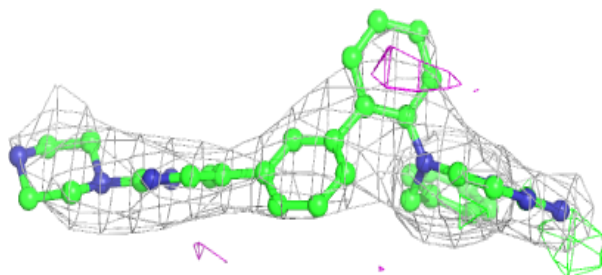
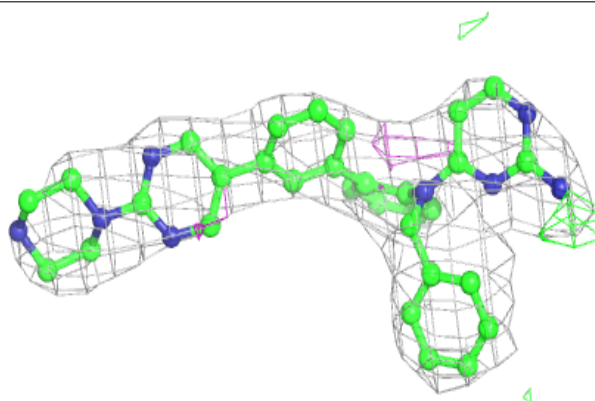


Electron density around JNI V 201:

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

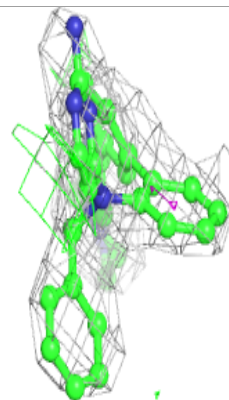
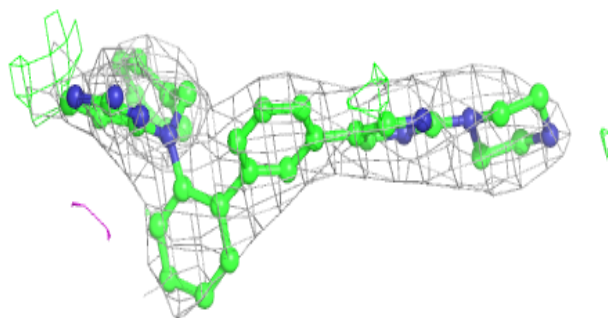
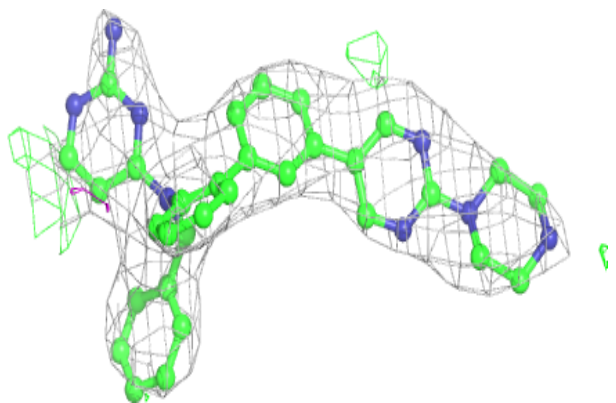
**Electron density around JNI M 201:**

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

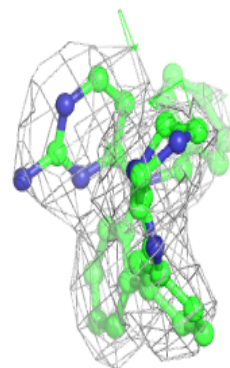
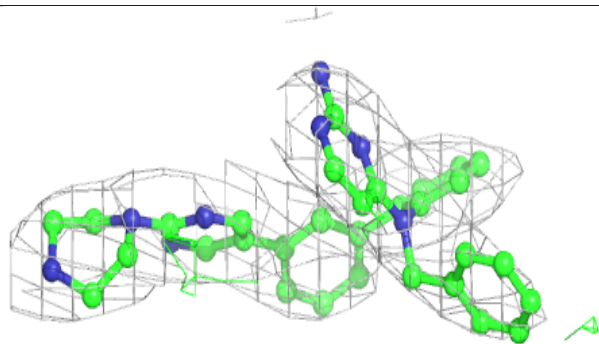
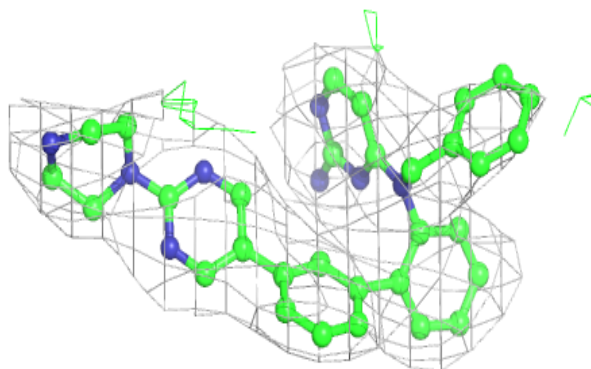


Electron density around JNI H 201:

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

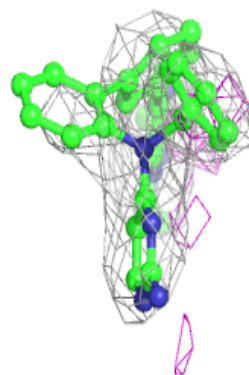
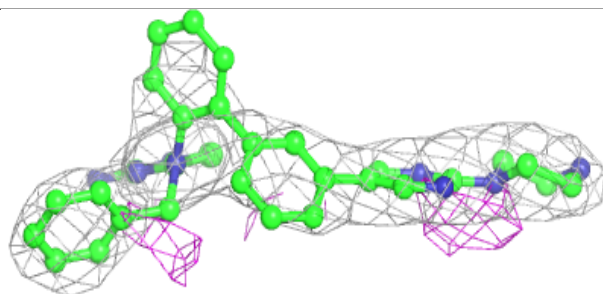
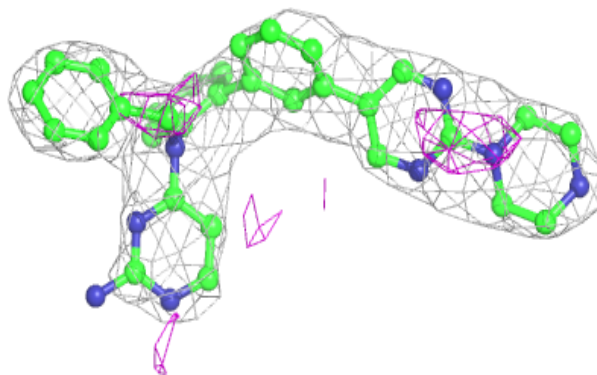
**Electron density around JNI t 201:**

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

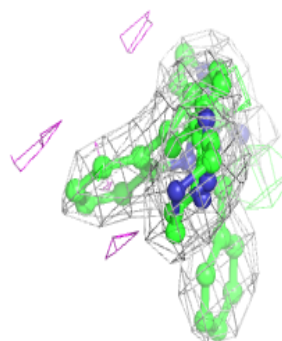
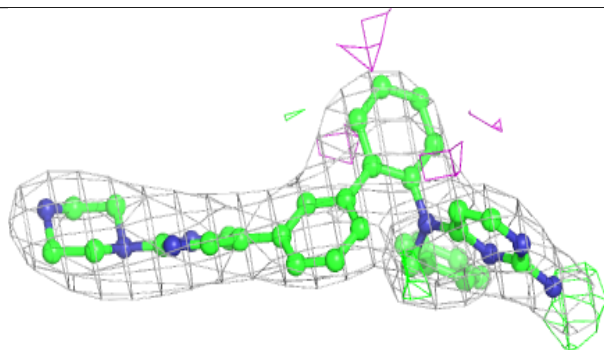
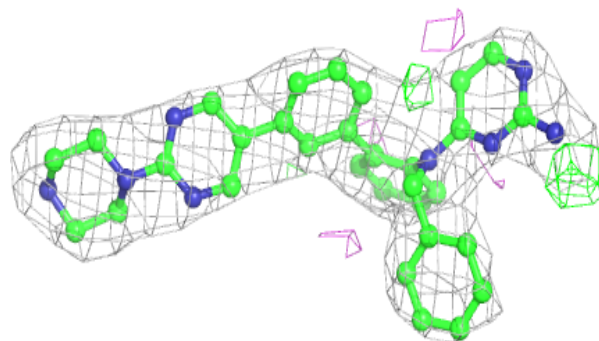


Electron density around JNI P 201:

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

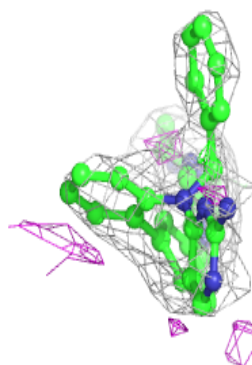
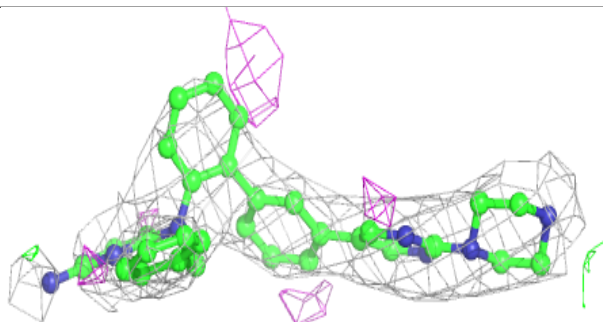
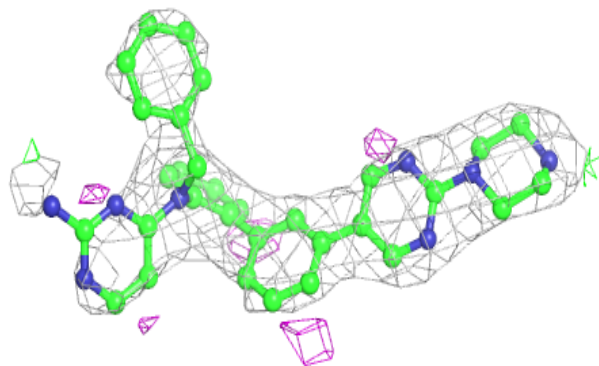
**Electron density around JNI D 201:**

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

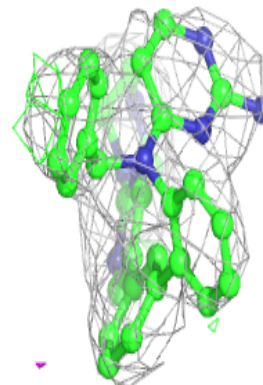
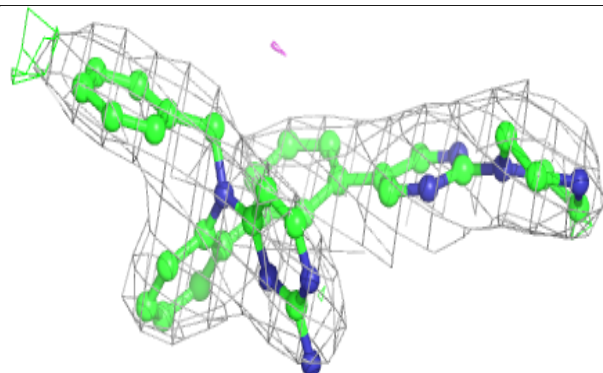
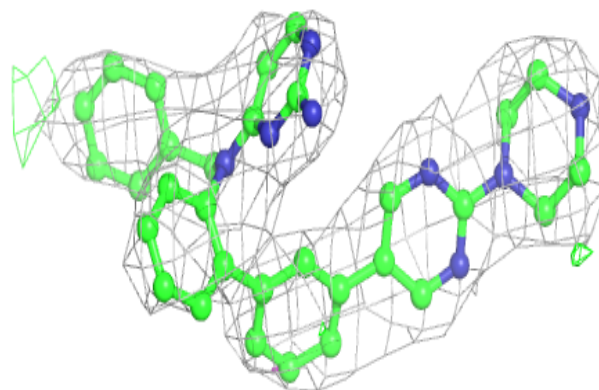


Electron density around JNI Q 201:

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

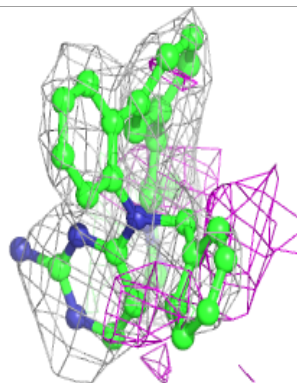
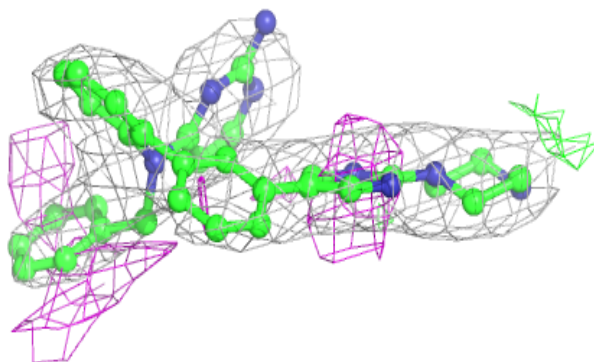
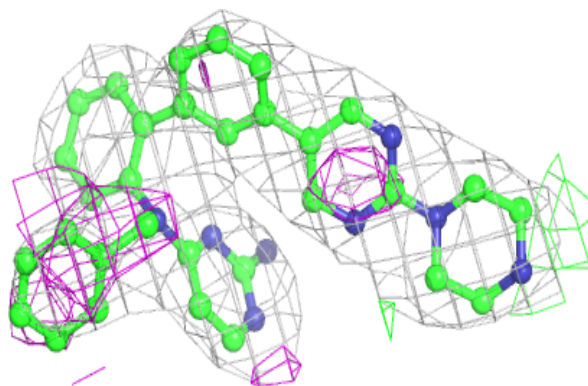
**Electron density around JNI Z 201:**

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

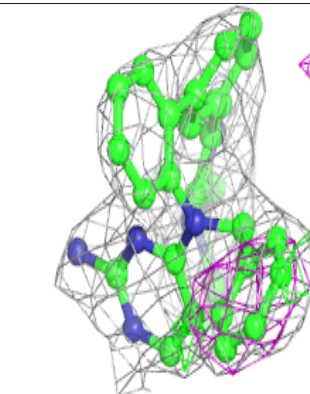
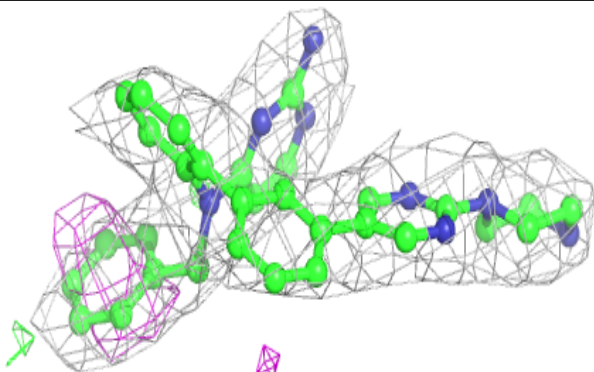
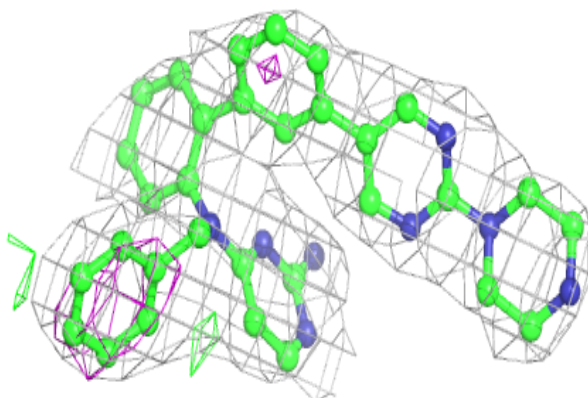


Electron density around JNI N 201:

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

**Electron density around JNI A 201:**

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



6.5 Other polymers

There are no such residues in this entry.