



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 31, 2026 – 12:23 PM UTC

PDB ID : 6SJJ / pdb_00006sjj
Title : A new modulated crystal structure of ANS complex of St John's wort Hyp-1 protein with 36 protein molecules in the asymmetric unit of the supercell
Authors : Smietanska, J.; Sliwiak, J.; Gilski, M.; Dauter, Z.; Strzalka, R.; Wolny, J.; Jaskolski, M.
Deposited on : 2019-08-13
Resolution : 2.30 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 types of validation reports are described at

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

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

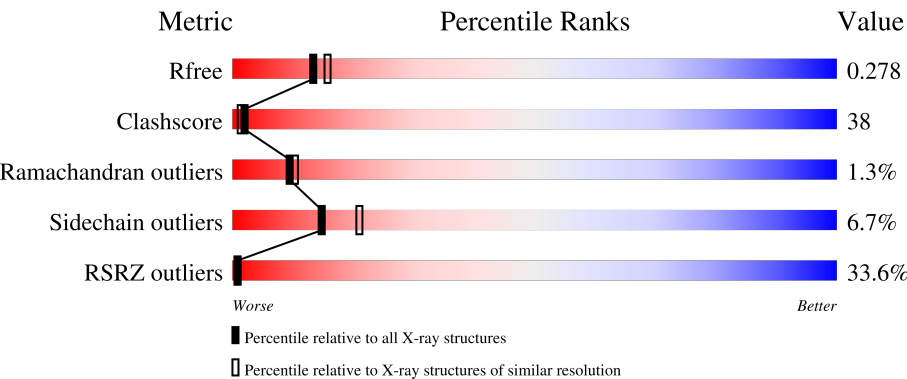
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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}	180053	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (2.30-2.30)

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

Mol	Chain	Length	Quality of chain
1	A	163	44% 39% 54% 6%
1	B	163	25% 52% 42%
1	C	163	48% 48% 48%
1	D	163	39% 44% 47% 7%

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Mol	Chain	Length	Quality of chain
1	E	163	
1	F	163	
1	G	163	
1	H	163	
1	I	163	
1	J	163	
1	K	163	
1	L	163	
1	M	163	
1	N	163	
1	O	163	
1	P	163	
1	Q	163	
1	R	163	
1	S	163	
1	T	163	
1	U	163	
1	V	163	
1	W	163	
1	X	163	
1	Y	163	
1	Z	163	
1	a	163	
1	b	163	
1	c	163	

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Mol	Chain	Length	Quality of chain
1	d	163	
1	e	163	
1	f	163	
1	g	163	
1	h	163	
1	i	163	
1	j	163	

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	2AN	A	202	-	-	X	-
2	2AN	A	204	-	-	-	X
2	2AN	B	201	-	-	X	-
2	2AN	B	202	-	-	X	-
2	2AN	B	203	-	-	X	-
2	2AN	B	204	-	-	X	-
2	2AN	C	202	-	-	X	-
2	2AN	D	201	-	-	X	-
2	2AN	D	203	-	-	X	-
2	2AN	F	201	-	-	X	-
2	2AN	F	202	-	-	X	-
2	2AN	F	203	-	-	X	-
2	2AN	F	204	-	-	X	-
2	2AN	F	206	-	-	X	-
2	2AN	G	203	-	-	X	-
2	2AN	H	204	-	-	X	-
2	2AN	I	203	-	-	X	-
2	2AN	I	204	-	-	X	-
2	2AN	I	205	-	-	X	-
2	2AN	J	202	-	-	X	-
2	2AN	K	202	-	-	X	-
2	2AN	L	201	-	-	X	-
2	2AN	L	204	-	-	X	-
2	2AN	N	201	-	-	X	-
2	2AN	N	203	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	2AN	N	205	-	-	X	-
2	2AN	O	201	-	-	X	-
2	2AN	P	203	-	-	X	-
2	2AN	R	201	-	-	X	-
2	2AN	R	203	-	-	X	-
2	2AN	R	204	-	-	X	-
2	2AN	R	205	-	-	X	-
2	2AN	S	204	-	-	X	X
2	2AN	T	201	-	-	X	-
2	2AN	T	203	-	-	X	-
2	2AN	U	201	-	-	X	-
2	2AN	V	201	-	-	X	-
2	2AN	V	203	-	-	X	-
2	2AN	V	204	-	-	X	-
2	2AN	V	205	-	-	X	-
2	2AN	V	208	-	-	X	-
2	2AN	X	202	-	-	X	-
2	2AN	X	203	-	-	X	-
2	2AN	X	206	-	-	X	-
2	2AN	Y	201	-	-	X	-
2	2AN	Y	204	-	-	X	-
2	2AN	Z	203	-	-	X	-
2	2AN	Z	206	-	-	X	-
2	2AN	a	203	-	-	X	-
2	2AN	a	204	-	-	X	-
2	2AN	b	201	-	-	X	-
2	2AN	b	202	-	-	X	-
2	2AN	b	203	-	-	X	-
2	2AN	b	204	-	-	X	-
2	2AN	b	205	-	-	X	-
2	2AN	c	201	-	-	X	-
2	2AN	c	202	-	-	X	-
2	2AN	c	206	-	-	X	-
2	2AN	d	201	-	-	X	-
2	2AN	d	202	-	-	X	-
2	2AN	d	204	-	-	X	-
2	2AN	f	202	-	-	X	-
2	2AN	f	204	-	-	X	-
2	2AN	f	205	-	-	X	-
2	2AN	f	206	-	-	X	-
2	2AN	g	202	-	-	X	-
2	2AN	h	202	-	-	X	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	2AN	h	204	-	-	X	-
2	2AN	j	201	-	-	X	-
2	2AN	j	203	-	-	X	-
2	2AN	j	204	-	-	X	-
2	2AN	j	205	-	-	X	-
3	SO4	A	205	-	-	X	-
3	SO4	Y	205	-	-	X	-
5	DMS	X	207	-	-	-	X
6	FLC	G	206	-	X	-	-
6	FLC	j	208	-	-	X	-

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 48343 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 PR-10 protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	159	Total	C	N	O	S	0	0	0
			1244	806	202	232	4			
1	A	162	Total	C	N	O	S	0	0	0
			1204	776	195	229	4			
1	R	161	Total	C	N	O	S	0	0	0
			1252	807	205	237	3			
1	Q	162	Total	C	N	O	S	0	0	0
			1266	821	204	237	4			
1	P	159	Total	C	N	O	S	0	0	0
			1249	808	202	236	3			
1	O	161	Total	C	N	O	S	0	0	0
			1215	780	200	231	4			
1	N	163	Total	C	N	O	S	0	0	0
			1265	815	204	243	3			
1	M	162	Total	C	N	O	S	0	0	0
			1271	822	205	240	4			
1	L	160	Total	C	N	O	S	0	0	0
			1256	813	203	236	4			
1	K	162	Total	C	N	O	S	0	0	0
			1266	822	204	237	3			
1	J	163	Total	C	N	O	S	0	0	0
			1257	809	204	241	3			
1	I	161	Total	C	N	O	S	0	0	0
			1253	811	204	234	4			
1	H	160	Total	C	N	O	S	0	0	0
			1232	793	201	234	4			
1	G	162	Total	C	N	O	S	0	0	0
			1232	799	202	227	4			
1	F	159	Total	C	N	O	S	0	0	0
			1188	760	197	227	4			
1	E	161	Total	C	N	O	S	0	0	0
			1250	810	203	235	2			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	D	159	Total	C	N	O	S	0	0	0
			1223	793	199	228	3			
1	C	161	Total	C	N	O	S	0	0	0
			1235	801	203	228	3			
1	f	161	Total	C	N	O	S	0	0	0
			1262	818	201	239	4			
1	e	161	Total	C	N	O	S	0	0	0
			1253	810	203	236	4			
1	d	162	Total	C	N	O	S	0	0	0
			1254	812	206	233	3			
1	c	159	Total	C	N	O	S	0	0	0
			1248	808	202	234	4			
1	b	161	Total	C	N	O	S	0	0	0
			1244	808	197	235	4			
1	a	159	Total	C	N	O	S	0	0	0
			1224	790	198	232	4			
1	Z	159	Total	C	N	O	S	0	0	0
			1218	782	199	233	4			
1	Y	159	Total	C	N	O	S	0	0	0
			1227	791	201	231	4			
1	X	159	Total	C	N	O	S	0	0	0
			1226	792	200	231	3			
1	W	159	Total	C	N	O	S	0	0	0
			1220	789	201	226	4			
1	V	159	Total	C	N	O	S	0	0	0
			1246	806	198	238	4			
1	U	159	Total	C	N	O	S	0	0	0
			1218	787	199	228	4			
1	T	161	Total	C	N	O	S	0	0	0
			1261	817	201	240	3			
1	S	160	Total	C	N	O	S	0	0	0
			1253	813	204	232	4			
1	j	159	Total	C	N	O	S	0	0	0
			1243	805	199	236	3			
1	i	161	Total	C	N	O	S	0	0	0
			1250	808	204	234	4			
1	h	162	Total	C	N	O	S	0	0	0
			1264	817	205	238	4			
1	g	160	Total	C	N	O	S	0	0	0
			1257	815	203	235	4			

There are 144 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-3	ASP	-	expression tag	UNP A0A160HRF0
B	-2	PRO	-	expression tag	UNP A0A160HRF0
B	-1	PHE	-	expression tag	UNP A0A160HRF0
B	0	THR	-	expression tag	UNP A0A160HRF0
A	-3	ASP	-	expression tag	UNP A0A160HRF0
A	-2	PRO	-	expression tag	UNP A0A160HRF0
A	-1	PHE	-	expression tag	UNP A0A160HRF0
A	0	THR	-	expression tag	UNP A0A160HRF0
R	-3	ASP	-	expression tag	UNP A0A160HRF0
R	-2	PRO	-	expression tag	UNP A0A160HRF0
R	-1	PHE	-	expression tag	UNP A0A160HRF0
R	0	THR	-	expression tag	UNP A0A160HRF0
Q	-3	ASP	-	expression tag	UNP A0A160HRF0
Q	-2	PRO	-	expression tag	UNP A0A160HRF0
Q	-1	PHE	-	expression tag	UNP A0A160HRF0
Q	0	THR	-	expression tag	UNP A0A160HRF0
P	-3	ASP	-	expression tag	UNP A0A160HRF0
P	-2	PRO	-	expression tag	UNP A0A160HRF0
P	-1	PHE	-	expression tag	UNP A0A160HRF0
P	0	THR	-	expression tag	UNP A0A160HRF0
O	-3	ASP	-	expression tag	UNP A0A160HRF0
O	-2	PRO	-	expression tag	UNP A0A160HRF0
O	-1	PHE	-	expression tag	UNP A0A160HRF0
O	0	THR	-	expression tag	UNP A0A160HRF0
N	-3	ASP	-	expression tag	UNP A0A160HRF0
N	-2	PRO	-	expression tag	UNP A0A160HRF0
N	-1	PHE	-	expression tag	UNP A0A160HRF0
N	0	THR	-	expression tag	UNP A0A160HRF0
M	-3	ASP	-	expression tag	UNP A0A160HRF0
M	-2	PRO	-	expression tag	UNP A0A160HRF0
M	-1	PHE	-	expression tag	UNP A0A160HRF0
M	0	THR	-	expression tag	UNP A0A160HRF0
L	-3	ASP	-	expression tag	UNP A0A160HRF0
L	-2	PRO	-	expression tag	UNP A0A160HRF0
L	-1	PHE	-	expression tag	UNP A0A160HRF0
L	0	THR	-	expression tag	UNP A0A160HRF0
K	-3	ASP	-	expression tag	UNP A0A160HRF0
K	-2	PRO	-	expression tag	UNP A0A160HRF0
K	-1	PHE	-	expression tag	UNP A0A160HRF0
K	0	THR	-	expression tag	UNP A0A160HRF0
J	-3	ASP	-	expression tag	UNP A0A160HRF0
J	-2	PRO	-	expression tag	UNP A0A160HRF0
J	-1	PHE	-	expression tag	UNP A0A160HRF0

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Chain	Residue	Modelled	Actual	Comment	Reference
J	0	THR	-	expression tag	UNP A0A160HRF0
I	-3	ASP	-	expression tag	UNP A0A160HRF0
I	-2	PRO	-	expression tag	UNP A0A160HRF0
I	-1	PHE	-	expression tag	UNP A0A160HRF0
I	0	THR	-	expression tag	UNP A0A160HRF0
H	-3	ASP	-	expression tag	UNP A0A160HRF0
H	-2	PRO	-	expression tag	UNP A0A160HRF0
H	-1	PHE	-	expression tag	UNP A0A160HRF0
H	0	THR	-	expression tag	UNP A0A160HRF0
G	-3	ASP	-	expression tag	UNP A0A160HRF0
G	-2	PRO	-	expression tag	UNP A0A160HRF0
G	-1	PHE	-	expression tag	UNP A0A160HRF0
G	0	THR	-	expression tag	UNP A0A160HRF0
F	-3	ASP	-	expression tag	UNP A0A160HRF0
F	-2	PRO	-	expression tag	UNP A0A160HRF0
F	-1	PHE	-	expression tag	UNP A0A160HRF0
F	0	THR	-	expression tag	UNP A0A160HRF0
E	-3	ASP	-	expression tag	UNP A0A160HRF0
E	-2	PRO	-	expression tag	UNP A0A160HRF0
E	-1	PHE	-	expression tag	UNP A0A160HRF0
E	0	THR	-	expression tag	UNP A0A160HRF0
D	-3	ASP	-	expression tag	UNP A0A160HRF0
D	-2	PRO	-	expression tag	UNP A0A160HRF0
D	-1	PHE	-	expression tag	UNP A0A160HRF0
D	0	THR	-	expression tag	UNP A0A160HRF0
C	-3	ASP	-	expression tag	UNP A0A160HRF0
C	-2	PRO	-	expression tag	UNP A0A160HRF0
C	-1	PHE	-	expression tag	UNP A0A160HRF0
C	0	THR	-	expression tag	UNP A0A160HRF0
f	-3	ASP	-	expression tag	UNP A0A160HRF0
f	-2	PRO	-	expression tag	UNP A0A160HRF0
f	-1	PHE	-	expression tag	UNP A0A160HRF0
f	0	THR	-	expression tag	UNP A0A160HRF0
e	-3	ASP	-	expression tag	UNP A0A160HRF0
e	-2	PRO	-	expression tag	UNP A0A160HRF0
e	-1	PHE	-	expression tag	UNP A0A160HRF0
e	0	THR	-	expression tag	UNP A0A160HRF0
d	-3	ASP	-	expression tag	UNP A0A160HRF0
d	-2	PRO	-	expression tag	UNP A0A160HRF0
d	-1	PHE	-	expression tag	UNP A0A160HRF0
d	0	THR	-	expression tag	UNP A0A160HRF0
c	-3	ASP	-	expression tag	UNP A0A160HRF0

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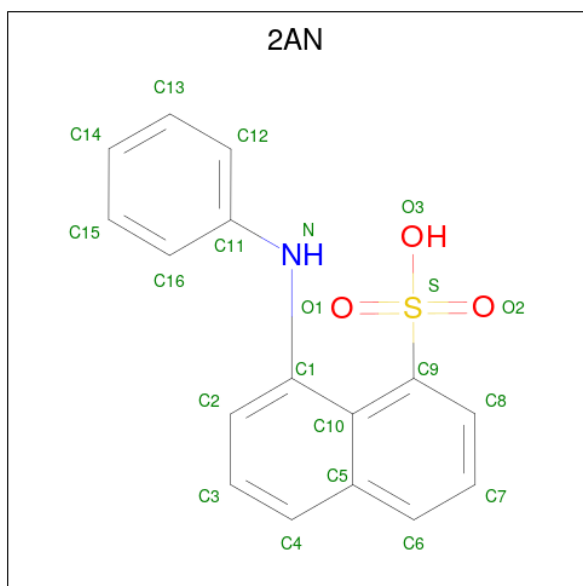
Chain	Residue	Modelled	Actual	Comment	Reference
c	-2	PRO	-	expression tag	UNP A0A160HRF0
c	-1	PHE	-	expression tag	UNP A0A160HRF0
c	0	THR	-	expression tag	UNP A0A160HRF0
b	-3	ASP	-	expression tag	UNP A0A160HRF0
b	-2	PRO	-	expression tag	UNP A0A160HRF0
b	-1	PHE	-	expression tag	UNP A0A160HRF0
b	0	THR	-	expression tag	UNP A0A160HRF0
a	-3	ASP	-	expression tag	UNP A0A160HRF0
a	-2	PRO	-	expression tag	UNP A0A160HRF0
a	-1	PHE	-	expression tag	UNP A0A160HRF0
a	0	THR	-	expression tag	UNP A0A160HRF0
Z	-3	ASP	-	expression tag	UNP A0A160HRF0
Z	-2	PRO	-	expression tag	UNP A0A160HRF0
Z	-1	PHE	-	expression tag	UNP A0A160HRF0
Z	0	THR	-	expression tag	UNP A0A160HRF0
Y	-3	ASP	-	expression tag	UNP A0A160HRF0
Y	-2	PRO	-	expression tag	UNP A0A160HRF0
Y	-1	PHE	-	expression tag	UNP A0A160HRF0
Y	0	THR	-	expression tag	UNP A0A160HRF0
X	-3	ASP	-	expression tag	UNP A0A160HRF0
X	-2	PRO	-	expression tag	UNP A0A160HRF0
X	-1	PHE	-	expression tag	UNP A0A160HRF0
X	0	THR	-	expression tag	UNP A0A160HRF0
W	-3	ASP	-	expression tag	UNP A0A160HRF0
W	-2	PRO	-	expression tag	UNP A0A160HRF0
W	-1	PHE	-	expression tag	UNP A0A160HRF0
W	0	THR	-	expression tag	UNP A0A160HRF0
V	-3	ASP	-	expression tag	UNP A0A160HRF0
V	-2	PRO	-	expression tag	UNP A0A160HRF0
V	-1	PHE	-	expression tag	UNP A0A160HRF0
V	0	THR	-	expression tag	UNP A0A160HRF0
U	-3	ASP	-	expression tag	UNP A0A160HRF0
U	-2	PRO	-	expression tag	UNP A0A160HRF0
U	-1	PHE	-	expression tag	UNP A0A160HRF0
U	0	THR	-	expression tag	UNP A0A160HRF0
T	-3	ASP	-	expression tag	UNP A0A160HRF0
T	-2	PRO	-	expression tag	UNP A0A160HRF0
T	-1	PHE	-	expression tag	UNP A0A160HRF0
T	0	THR	-	expression tag	UNP A0A160HRF0
S	-3	ASP	-	expression tag	UNP A0A160HRF0
S	-2	PRO	-	expression tag	UNP A0A160HRF0
S	-1	PHE	-	expression tag	UNP A0A160HRF0

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Chain	Residue	Modelled	Actual	Comment	Reference
S	0	THR	-	expression tag	UNP A0A160HRF0
j	-3	ASP	-	expression tag	UNP A0A160HRF0
j	-2	PRO	-	expression tag	UNP A0A160HRF0
j	-1	PHE	-	expression tag	UNP A0A160HRF0
j	0	THR	-	expression tag	UNP A0A160HRF0
i	-3	ASP	-	expression tag	UNP A0A160HRF0
i	-2	PRO	-	expression tag	UNP A0A160HRF0
i	-1	PHE	-	expression tag	UNP A0A160HRF0
i	0	THR	-	expression tag	UNP A0A160HRF0
h	-3	ASP	-	expression tag	UNP A0A160HRF0
h	-2	PRO	-	expression tag	UNP A0A160HRF0
h	-1	PHE	-	expression tag	UNP A0A160HRF0
h	0	THR	-	expression tag	UNP A0A160HRF0
g	-3	ASP	-	expression tag	UNP A0A160HRF0
g	-2	PRO	-	expression tag	UNP A0A160HRF0
g	-1	PHE	-	expression tag	UNP A0A160HRF0
g	0	THR	-	expression tag	UNP A0A160HRF0

- Molecule 2 is 8-ANILINO-1-NAPHTHALENE SULFONATE (CCD ID: 2AN) (formula: $C_{16}H_{13}NO_3S$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	B	1	Total	C	N	O	S	0	0
			21	16	1	3	1		
2	B	1	Total	C	N	O	S	0	0
			21	16	1	3	1		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	B	1	Total	C	N	O	S	0	0
			21	16	1	3	1		
2	B	1	Total	C	N	O	S	0	0
			21	16	1	3	1		
2	B	1	Total	C	N	O	S	0	0
			21	16	1	3	1		
2	B	1	Total	C	N	O	S	0	0
			21	16	1	3	1		
2	A	1	Total	C	N	O	S	0	0
			21	16	1	3	1		
2	A	1	Total	C	N	O	S	0	0
			21	16	1	3	1		
2	A	1	Total	C	N	O	S	0	0
			21	16	1	3	1		
2	A	1	Total	C	N	O	S	0	0
			21	16	1	3	1		
2	R	1	Total	C	N	O	S	0	0
			21	16	1	3	1		
2	R	1	Total	C	N	O	S	0	0
			21	16	1	3	1		
2	R	1	Total	C	N	O	S	0	0
			21	16	1	3	1		
2	R	1	Total	C	N	O	S	0	0
			21	16	1	3	1		
2	R	1	Total	C	N	O	S	0	0
			21	16	1	3	1		
2	Q	1	Total	C	N	O	S	0	0
			21	16	1	3	1		
2	Q	1	Total	C	N	O	S	0	0
			21	16	1	3	1		
2	Q	1	Total	C	N	O	S	0	0
			21	16	1	3	1		
2	P	1	Total	C	N	O	S	0	0
			21	16	1	3	1		
2	P	1	Total	C	N	O	S	0	0
			21	16	1	3	1		
2	P	1	Total	C	N	O	S	0	0
			21	16	1	3	1		
2	P	1	Total	C	N	O	S	0	0
			21	16	1	3	1		
2	O	1	Total	C	N	O	S	0	0
			21	16	1	3	1		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	O	1	Total	C	N	O	S	0	0
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2	O	1	Total	C	N	O	S	0	0
			21	16	1	3	1		
2	N	1	Total	C	N	O	S	0	0
			21	16	1	3	1		
2	N	1	Total	C	N	O	S	0	0
			21	16	1	3	1		
2	N	1	Total	C	N	O	S	0	0
			21	16	1	3	1		
2	N	1	Total	C	N	O	S	0	0
			21	16	1	3	1		
2	M	1	Total	C	N	O	S	0	0
			21	16	1	3	1		
2	M	1	Total	C	N	O	S	0	0
			21	16	1	3	1		
2	M	1	Total	C	N	O	S	0	0
			21	16	1	3	1		
2	L	1	Total	C	N	O	S	0	0
			21	16	1	3	1		
2	L	1	Total	C	N	O	S	0	0
			21	16	1	3	1		
2	L	1	Total	C	N	O	S	0	0
			21	16	1	3	1		
2	L	1	Total	C	N	O	S	0	0
			21	16	1	3	1		
2	K	1	Total	C	N	O	S	0	0
			21	16	1	3	1		
2	K	1	Total	C	N	O	S	0	0
			21	16	1	3	1		
2	K	1	Total	C	N	O	S	0	0
			21	16	1	3	1		
2	J	1	Total	C	N	O	S	0	0
			21	16	1	3	1		
2	J	1	Total	C	N	O	S	0	0
			21	16	1	3	1		
2	J	1	Total	C	N	O	S	0	0
			21	16	1	3	1		
2	I	1	Total	C	N	O	S	0	0
			21	16	1	3	1		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	I	1	Total	C	N	O	S	0	0
			21	16	1	3	1		
2	I	1	Total	C	N	O	S	0	0
			21	16	1	3	1		
2	I	1	Total	C	N	O	S	0	0
			21	16	1	3	1		
2	I	1	Total	C	N	O	S	0	0
			21	16	1	3	1		
2	I	1	Total	C	N	O	S	0	0
			21	16	1	3	1		
2	H	1	Total	C	N	O	S	0	0
			21	16	1	3	1		
2	H	1	Total	C	N	O	S	0	0
			21	16	1	3	1		
2	H	1	Total	C	N	O	S	0	0
			21	16	1	3	1		
2	H	1	Total	C	N	O	S	0	0
			21	16	1	3	1		
2	G	1	Total	C	N	O	S	0	0
			21	16	1	3	1		
2	G	1	Total	C	N	O	S	0	0
			21	16	1	3	1		
2	G	1	Total	C	N	O	S	0	0
			21	16	1	3	1		
2	G	1	Total	C	N	O	S	0	0
			21	16	1	3	1		
2	G	1	Total	C	N	O	S	0	0
			21	16	1	3	1		
2	F	1	Total	C	N	O	S	0	0
			21	16	1	3	1		
2	F	1	Total	C	N	O	S	0	0
			21	16	1	3	1		
2	F	1	Total	C	N	O	S	0	0
			21	16	1	3	1		
2	F	1	Total	C	N	O	S	0	0
			21	16	1	3	1		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	F	1	Total	C	N	O	S	0	0
			21	16	1	3	1		
2	E	1	Total	C	N	O	S	0	0
			21	16	1	3	1		
2	E	1	Total	C	N	O	S	0	0
			21	16	1	3	1		
2	E	1	Total	C	N	O	S	0	0
			21	16	1	3	1		
2	E	1	Total	C	N	O	S	0	0
			21	16	1	3	1		
2	D	1	Total	C	N	O	S	0	0
			21	16	1	3	1		
2	D	1	Total	C	N	O	S	0	0
			21	16	1	3	1		
2	D	1	Total	C	N	O	S	0	0
			21	16	1	3	1		
2	D	1	Total	C	N	O	S	0	0
			21	16	1	3	1		
2	C	1	Total	C	N	O	S	0	0
			21	16	1	3	1		
2	C	1	Total	C	N	O	S	0	0
			21	16	1	3	1		
2	C	1	Total	C	N	O	S	0	1
			21	16	1	3	1		
2	f	1	Total	C	N	O	S	0	0
			21	16	1	3	1		
2	f	1	Total	C	N	O	S	0	0
			21	16	1	3	1		
2	f	1	Total	C	N	O	S	0	0
			21	16	1	3	1		
2	f	1	Total	C	N	O	S	0	0
			21	16	1	3	1		
2	f	1	Total	C	N	O	S	0	0
			21	16	1	3	1		
2	e	1	Total	C	N	O	S	0	0
			21	16	1	3	1		
2	d	1	Total	C	N	O	S	0	0
			21	16	1	3	1		
2	d	1	Total	C	N	O	S	0	0
			21	16	1	3	1		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	d	1	Total	C	N	O	S	0	0
			21	16	1	3	1		
2	d	1	Total	C	N	O	S	0	0
			21	16	1	3	1		
2	c	1	Total	C	N	O	S	0	0
			21	16	1	3	1		
2	c	1	Total	C	N	O	S	0	0
			21	16	1	3	1		
2	c	1	Total	C	N	O	S	0	0
			21	16	1	3	1		
2	c	1	Total	C	N	O	S	0	0
			21	16	1	3	1		
2	c	1	Total	C	N	O	S	0	0
			21	16	1	3	1		
2	c	1	Total	C	N	O	S	0	0
			21	16	1	3	1		
2	b	1	Total	C	N	O	S	0	0
			21	16	1	3	1		
2	b	1	Total	C	N	O	S	0	0
			21	16	1	3	1		
2	b	1	Total	C	N	O	S	0	0
			21	16	1	3	1		
2	b	1	Total	C	N	O	S	0	0
			21	16	1	3	1		
2	b	1	Total	C	N	O	S	0	0
			21	16	1	3	1		
2	a	1	Total	C	N	O	S	0	0
			21	16	1	3	1		
2	a	1	Total	C	N	O	S	0	0
			21	16	1	3	1		
2	a	1	Total	C	N	O	S	0	0
			21	16	1	3	1		
2	a	1	Total	C	N	O	S	0	0
			21	16	1	3	1		
2	Z	1	Total	C	N	O	S	0	0
			21	16	1	3	1		
2	Z	1	Total	C	N	O	S	0	0
			21	16	1	3	1		
2	Z	1	Total	C	N	O	S	0	0
			21	16	1	3	1		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	Z	1	Total	C	N	O	S	0	0
			21	16	1	3	1		
2	Z	1	Total	C	N	O	S	0	0
			21	16	1	3	1		
2	Z	1	Total	C	N	O	S	0	0
			21	16	1	3	1		
2	Y	1	Total	C	N	O	S	0	0
			21	16	1	3	1		
2	Y	1	Total	C	N	O	S	0	0
			21	16	1	3	1		
2	Y	1	Total	C	N	O	S	0	0
			21	16	1	3	1		
2	Y	1	Total	C	N	O	S	0	0
			21	16	1	3	1		
2	X	1	Total	C	N	O	S	0	0
			21	16	1	3	1		
2	X	1	Total	C	N	O	S	0	0
			21	16	1	3	1		
2	X	1	Total	C	N	O	S	0	0
			21	16	1	3	1		
2	X	1	Total	C	N	O	S	0	0
			21	16	1	3	1		
2	X	1	Total	C	N	O	S	0	0
			21	16	1	3	1		
2	X	1	Total	C	N	O	S	0	0
			21	16	1	3	1		
2	W	1	Total	C	N	O	S	0	0
			21	16	1	3	1		
2	V	1	Total	C	N	O	S	0	0
			21	16	1	3	1		
2	V	1	Total	C	N	O	S	0	0
			21	16	1	3	1		
2	V	1	Total	C	N	O	S	0	0
			21	16	1	3	1		
2	V	1	Total	C	N	O	S	0	0
			21	16	1	3	1		
2	V	1	Total	C	N	O	S	0	0
			21	16	1	3	1		
2	V	1	Total	C	N	O	S	0	0
			21	16	1	3	1		

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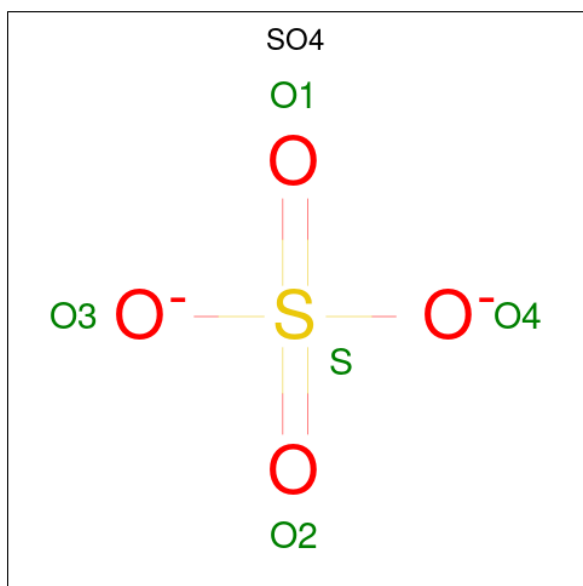
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	V	1	Total	C	N	O	S	0	0
			21	16	1	3	1		
2	U	1	Total	C	N	O	S	0	0
			21	16	1	3	1		
2	U	1	Total	C	N	O	S	0	0
			21	16	1	3	1		
2	T	1	Total	C	N	O	S	0	0
			21	16	1	3	1		
2	T	1	Total	C	N	O	S	0	0
			21	16	1	3	1		
2	T	1	Total	C	N	O	S	0	0
			21	16	1	3	1		
2	T	1	Total	C	N	O	S	0	0
			21	16	1	3	1		
2	S	1	Total	C	N	O	S	0	0
			21	16	1	3	1		
2	S	1	Total	C	N	O	S	0	0
			21	16	1	3	1		
2	S	1	Total	C	N	O	S	0	0
			21	16	1	3	1		
2	S	1	Total	C	N	O	S	0	0
			21	16	1	3	1		
2	j	1	Total	C	N	O	S	0	0
			21	16	1	3	1		
2	j	1	Total	C	N	O	S	0	0
			21	16	1	3	1		
2	j	1	Total	C	N	O	S	0	0
			21	16	1	3	1		
2	j	1	Total	C	N	O	S	0	0
			21	16	1	3	1		
2	j	1	Total	C	N	O	S	0	0
			21	16	1	3	1		
2	j	1	Total	C	N	O	S	0	0
			21	16	1	3	1		
2	i	1	Total	C	N	O	S	0	0
			21	16	1	3	1		
2	h	1	Total	C	N	O	S	0	0
			21	16	1	3	1		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	h	1	Total	C	N	O	S	0	0
			21	16	1	3	1		
2	h	1	Total	C	N	O	S	0	0
			21	16	1	3	1		
2	h	1	Total	C	N	O	S	0	0
			21	16	1	3	1		
2	h	1	Total	C	N	O	S	0	0
			21	16	1	3	1		
2	h	1	Total	C	N	O	S	0	0
			21	16	1	3	1		
2	g	1	Total	C	N	O	S	0	0
			21	16	1	3	1		
2	g	1	Total	C	N	O	S	0	0
			21	16	1	3	1		
2	g	1	Total	C	N	O	S	0	0
			21	16	1	3	1		

- Molecule 3 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



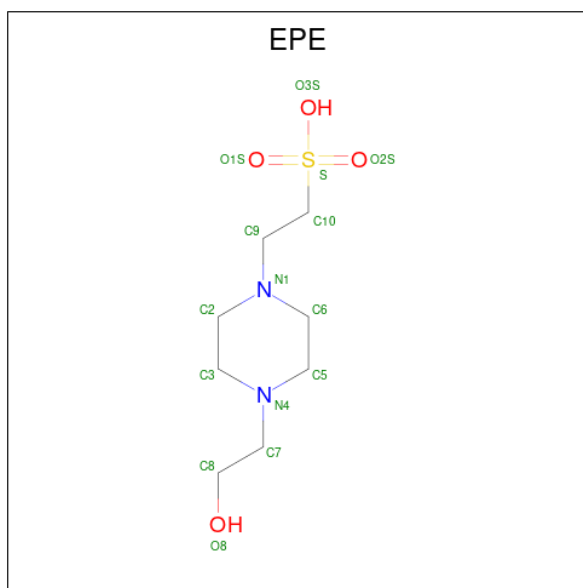
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	S	0	0
			5	4	1		
3	Q	1	Total	O	S	0	0
			5	4	1		
3	I	1	Total	O	S	0	0
			5	4	1		

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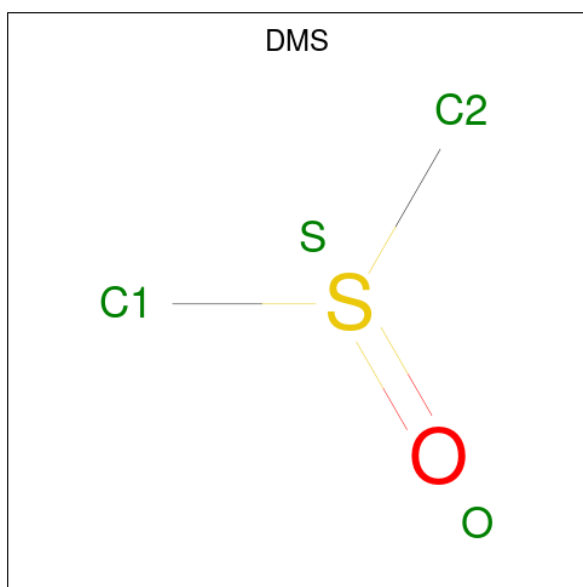
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	G	1	Total	O	S	0	0
			5	4	1		
3	E	1	Total	O	S	0	0
			5	4	1		
3	c	1	Total	O	S	0	0
			5	4	1		
3	c	1	Total	O	S	0	0
			5	4	1		
3	c	1	Total	O	S	0	0
			5	4	1		
3	Y	1	Total	O	S	0	0
			5	4	1		
3	g	1	Total	O	S	0	0
			5	4	1		

- Molecule 4 is 4-(2-HYDROXYETHYL)-1-PIPERAZINE ETHANESULFONIC ACID (CCD ID: EPE) (formula: $C_8H_{18}N_2O_4S$).



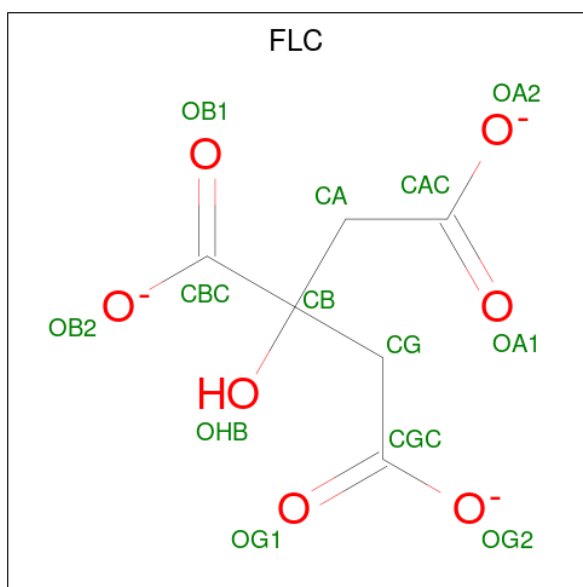
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	P	1	Total	C	N	O	S	0
			15	8	2	4	1	0

- Molecule 5 is DIMETHYL SULFOXIDE (CCD ID: DMS) (formula: C_2H_6OS).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	N	1	Total	C	O	S	0	0
			4	2	1	1		
5	G	1	Total	C	O	S	0	0
			4	2	1	1		
5	X	1	Total	C	O	S	0	0
			4	2	1	1		

- Molecule 6 is CITRATE ANION (CCD ID: FLC) (formula: $C_6H_5O_7$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	G	1	Total	C	O	0	0
			13	6	7		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	e	1	Total C O 13 6 7	0	0
6	a	1	Total C O 13 6 7	0	0
6	a	1	Total C O 13 6 7	0	0
6	j	1	Total C O 13 6 7	0	0
6	i	1	Total C O 13 6 7	0	0
6	i	1	Total C O 13 6 7	0	0

- Molecule 7 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	B	5	Total O 5 5	0	0
7	A	6	Total O 6 6	0	0
7	R	3	Total O 3 3	0	0
7	Q	1	Total O 1 1	0	0
7	P	5	Total O 5 5	0	0
7	O	4	Total O 4 4	0	0
7	N	3	Total O 3 3	0	0
7	M	1	Total O 1 1	0	0
7	L	3	Total O 3 3	0	0
7	K	6	Total O 6 6	0	0
7	J	2	Total O 2 2	0	0
7	I	5	Total O 5 5	0	0
7	H	3	Total O 3 3	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	G	5	Total O 5 5	0	0
7	F	1	Total O 1 1	0	0
7	E	5	Total O 5 5	0	0
7	D	3	Total O 3 3	0	0
7	C	4	Total O 4 4	0	0
7	f	8	Total O 8 8	0	0
7	e	9	Total O 9 9	0	0
7	d	2	Total O 2 2	0	0
7	c	3	Total O 3 3	0	0
7	b	6	Total O 6 6	0	0
7	a	8	Total O 8 8	0	0
7	Z	4	Total O 4 4	0	0
7	Y	4	Total O 4 4	0	0
7	X	3	Total O 3 3	0	0
7	W	2	Total O 2 2	0	0
7	V	9	Total O 9 9	0	0
7	T	5	Total O 5 5	0	0
7	S	1	Total O 1 1	0	0
7	j	5	Total O 5 5	0	0
7	i	6	Total O 6 6	0	0
7	h	8	Total O 8 8	0	0

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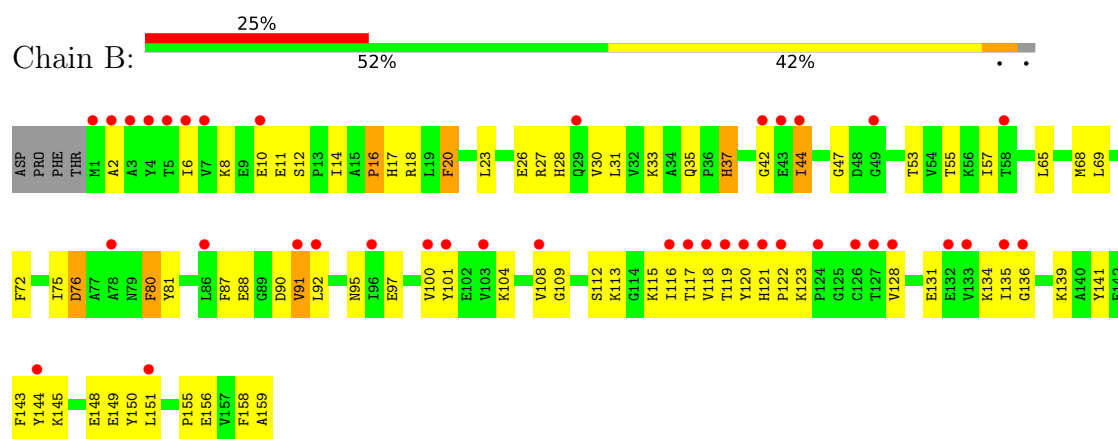
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	g	4	Total	O	0	0
			4	4		

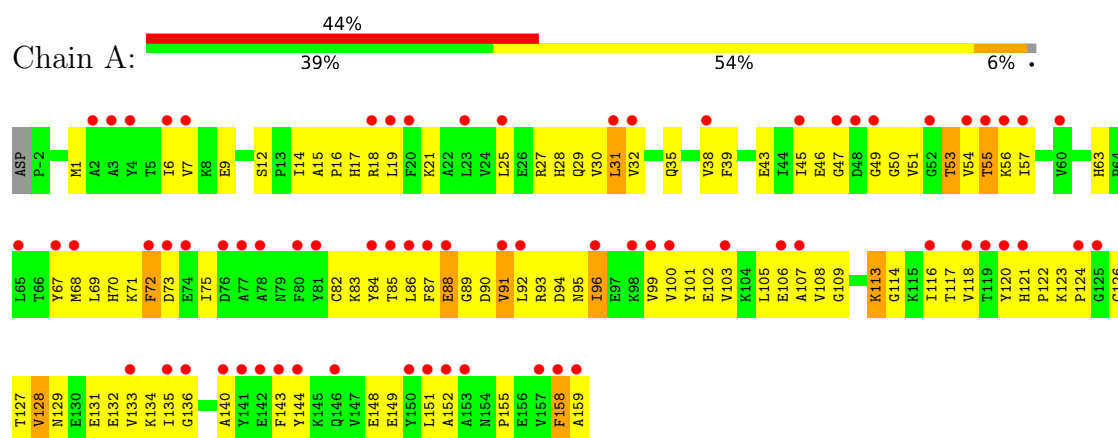
3 Residue-property plots [i](#)

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.

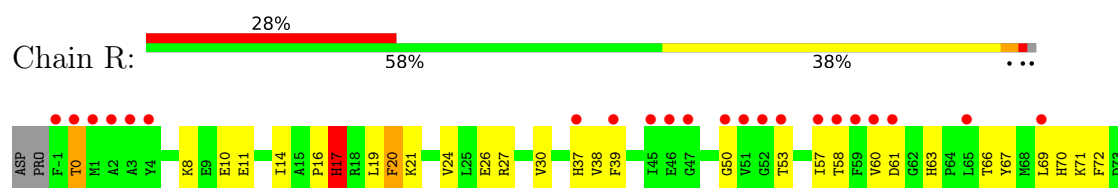
• Molecule 1: PR-10 protein

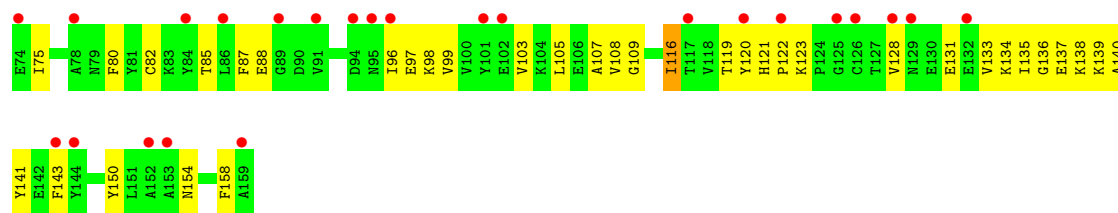


• Molecule 1: PR-10 protein

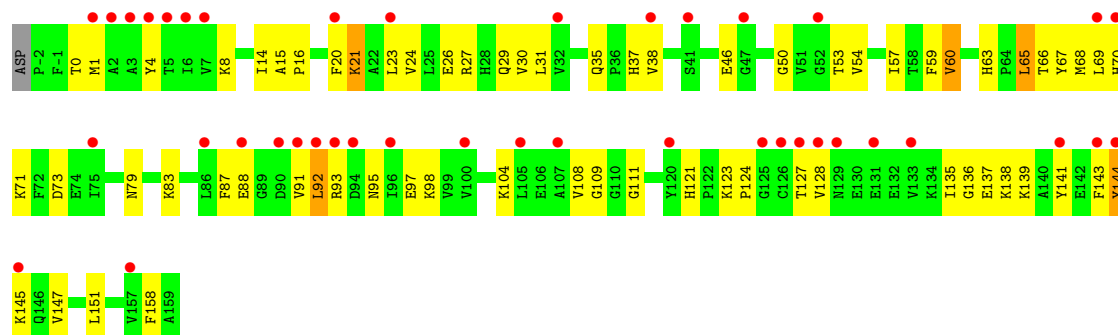


• Molecule 1: PR-10 protein

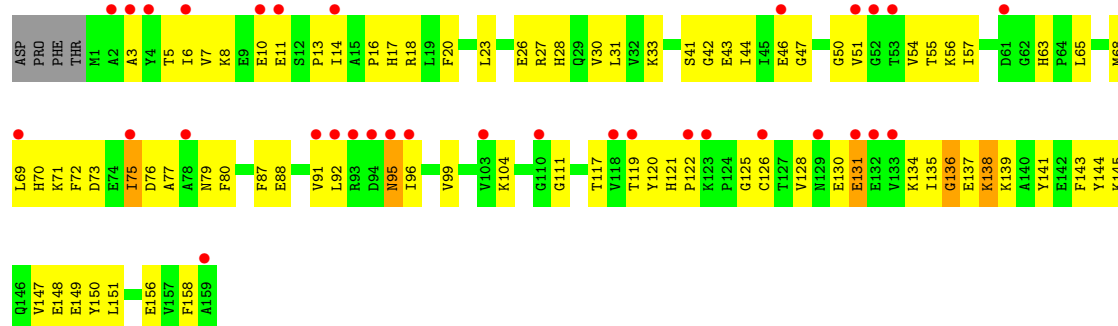




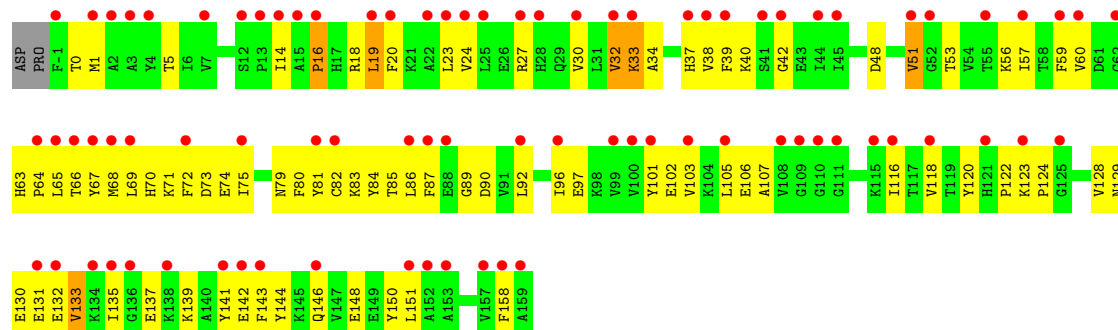
• Molecule 1: PR-10 protein



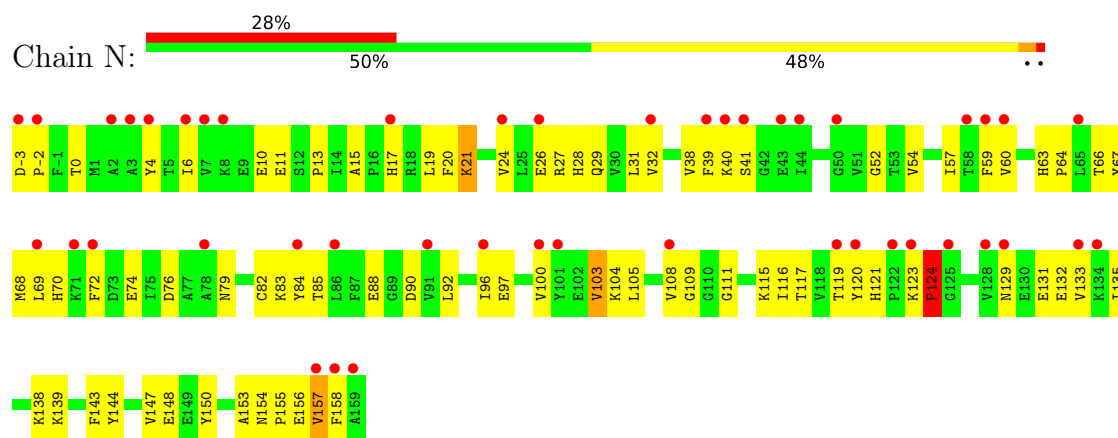
• Molecule 1: PR-10 protein



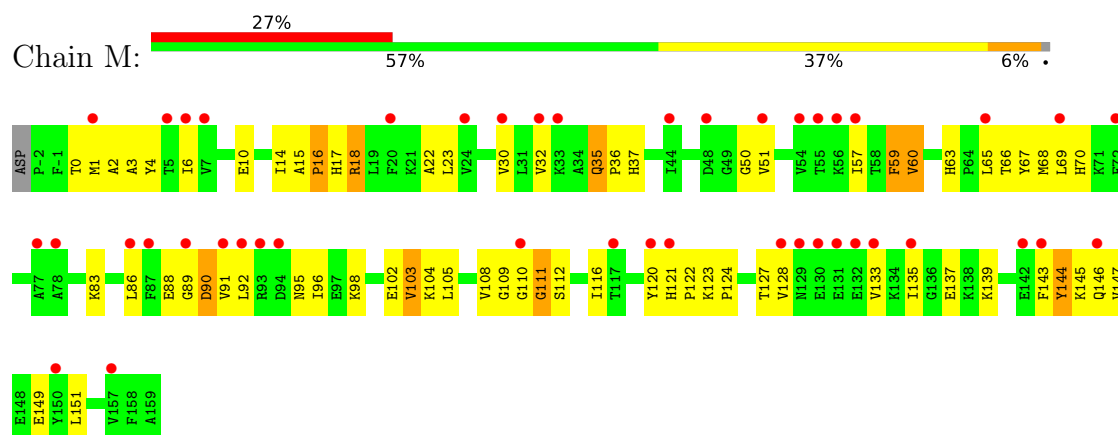
• Molecule 1: PR-10 protein



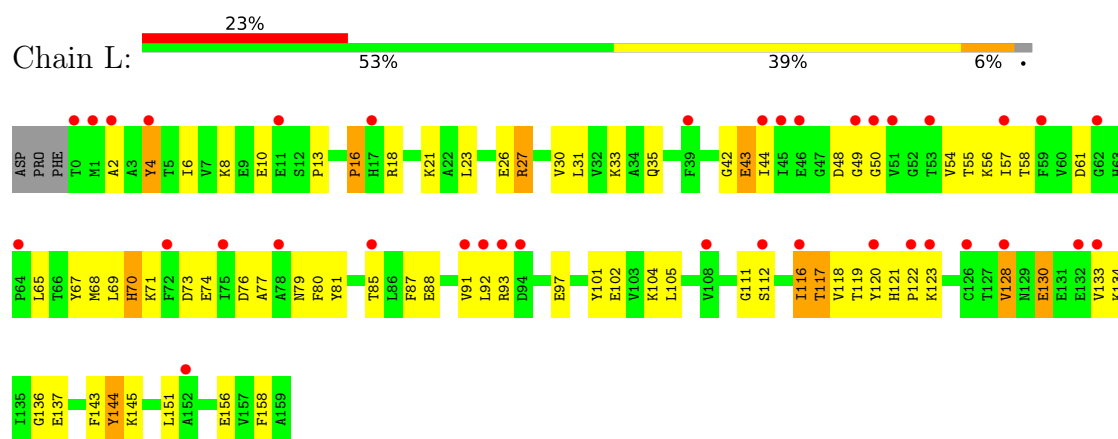
- Molecule 1: PR-10 protein



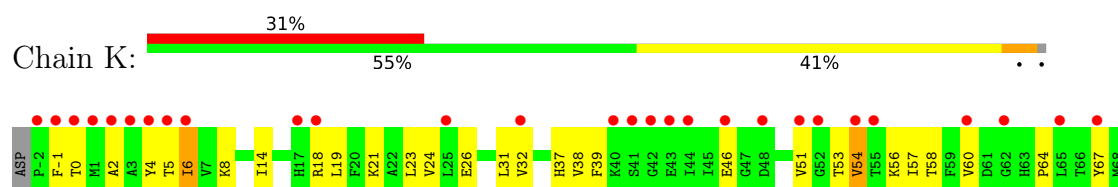
- Molecule 1: PR-10 protein

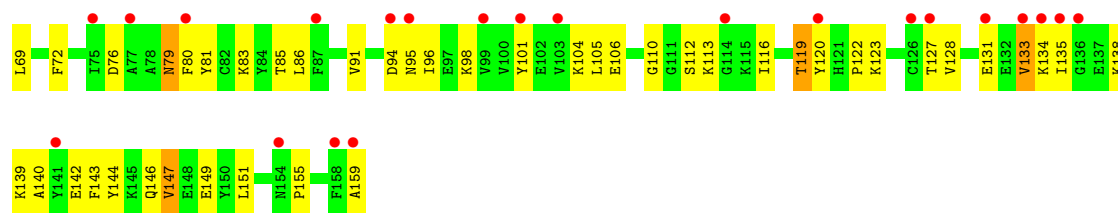


- Molecule 1: PR-10 protein

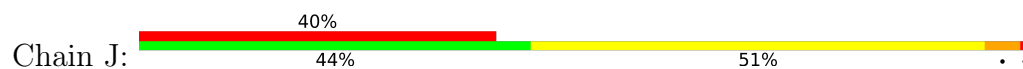


- Molecule 1: PR-10 protein

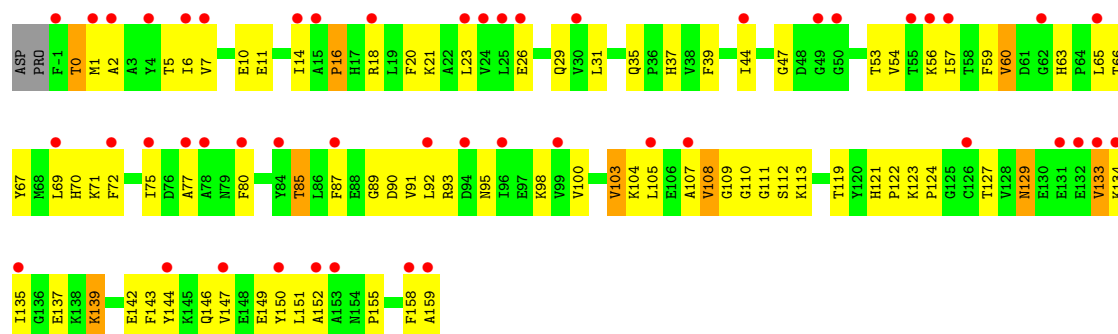




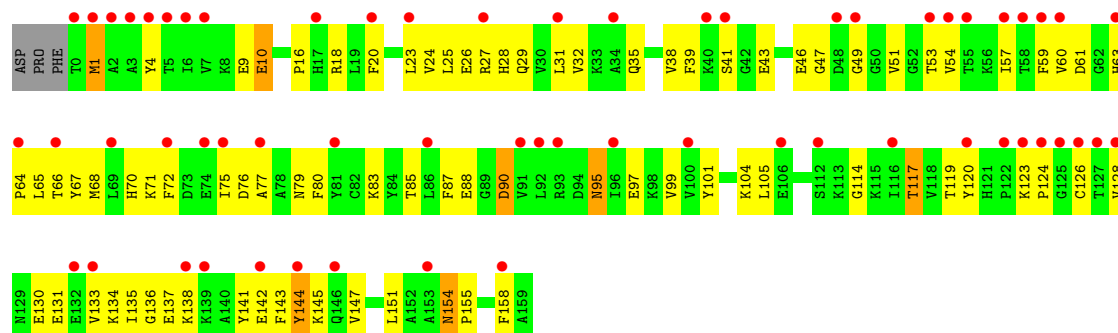
● Molecule 1: PR-10 protein



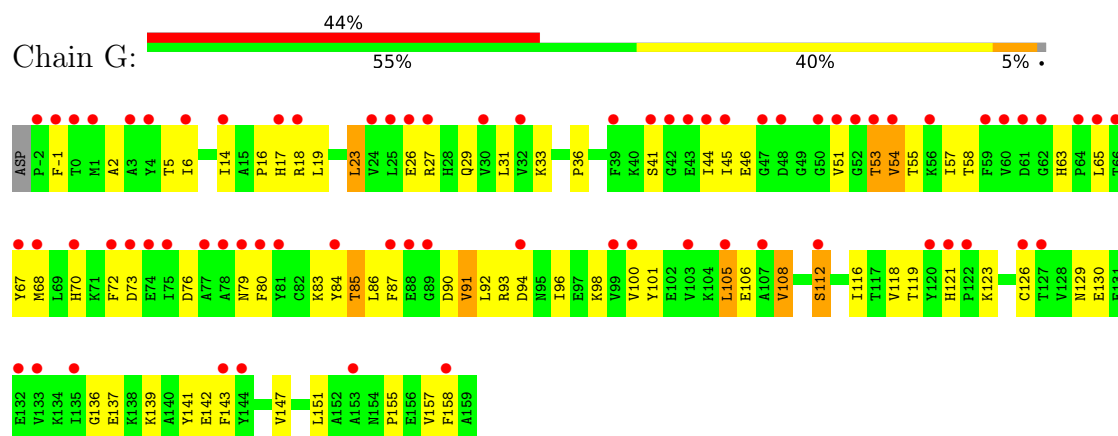
● Molecule 1: PR-10 protein



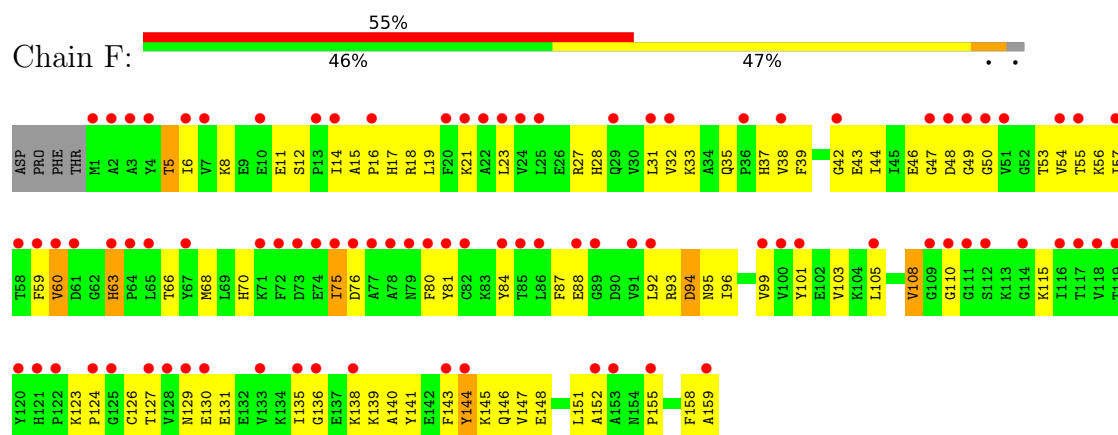
● Molecule 1: PR-10 protein



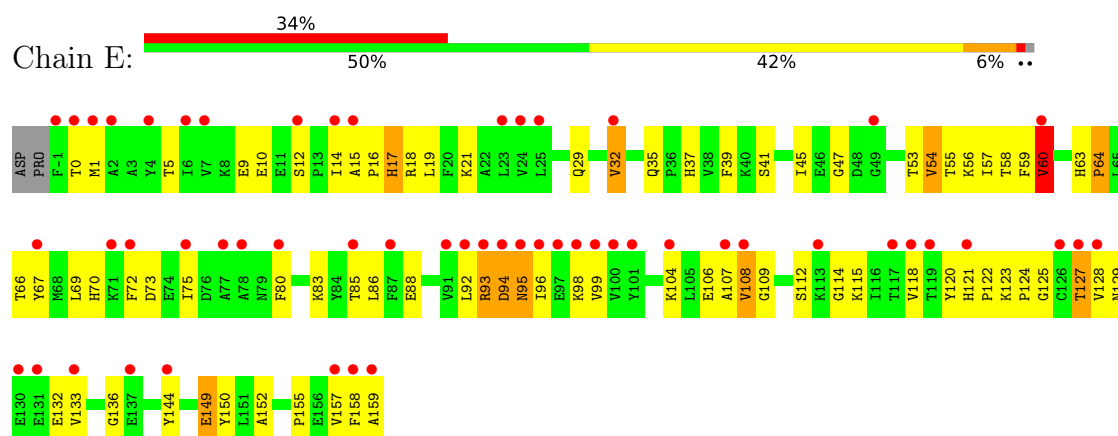
- Molecule 1: PR-10 protein



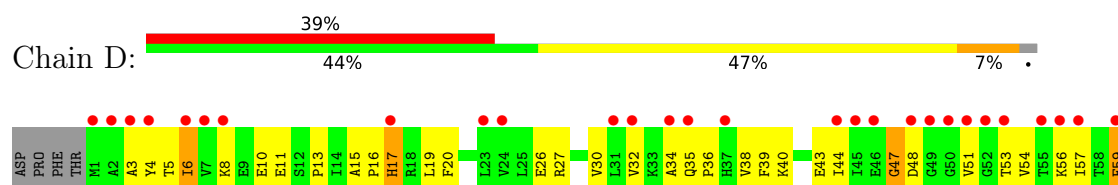
- Molecule 1: PR-10 protein

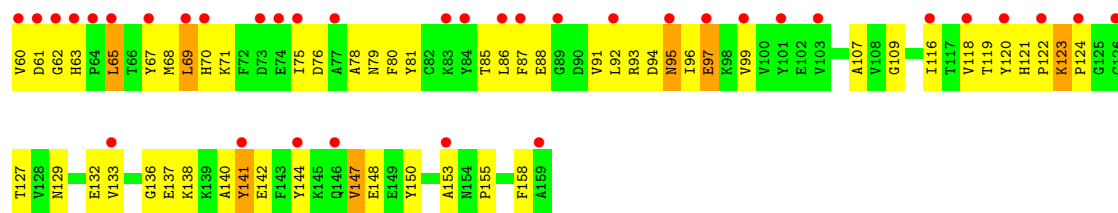


- Molecule 1: PR-10 protein



- Molecule 1: PR-10 protein

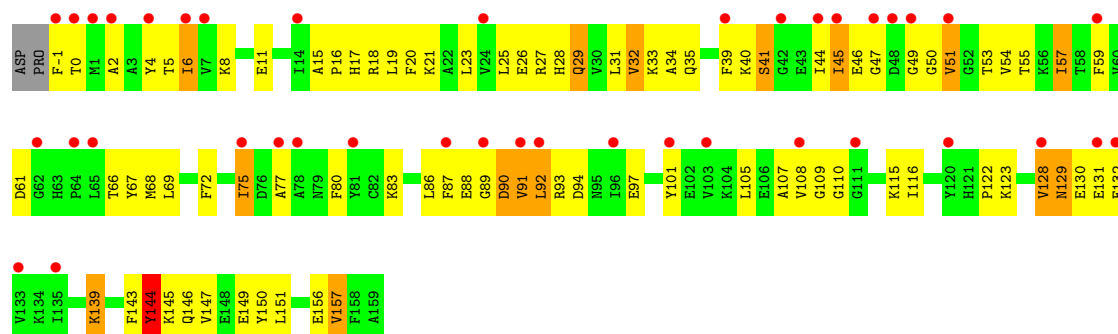
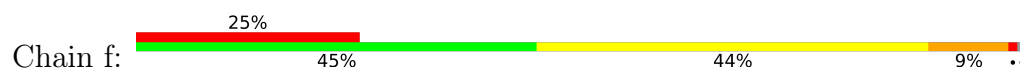




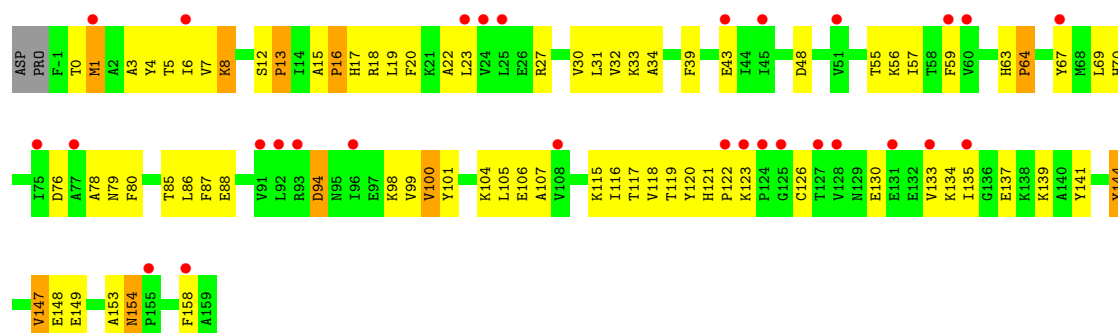
● Molecule 1: PR-10 protein



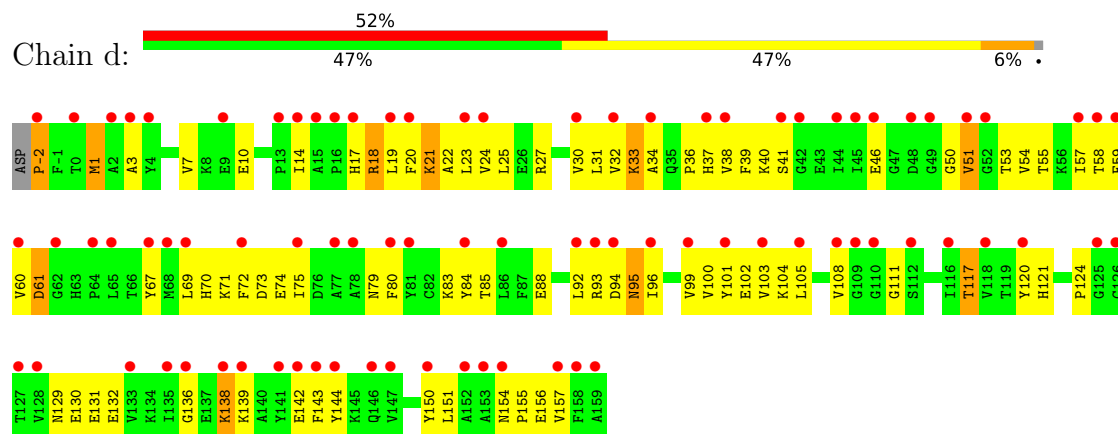
● Molecule 1: PR-10 protein



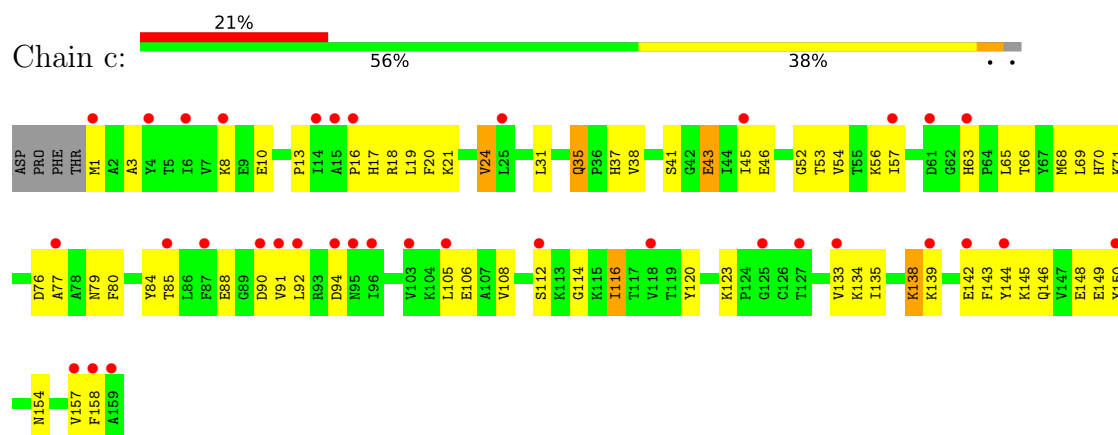
● Molecule 1: PR-10 protein



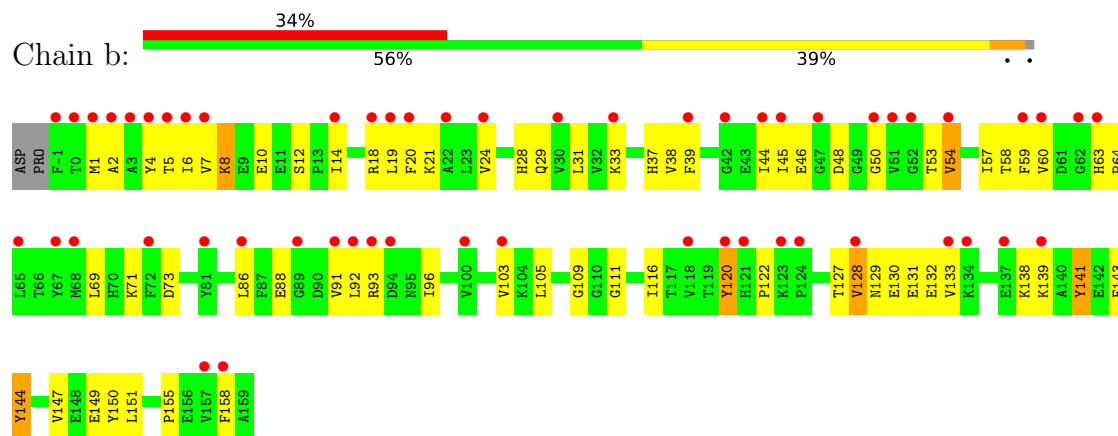
- Molecule 1: PR-10 protein



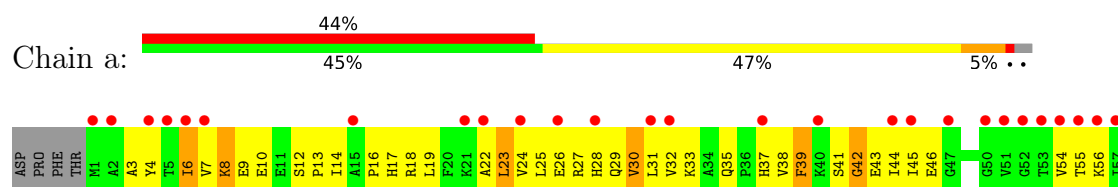
- Molecule 1: PR-10 protein

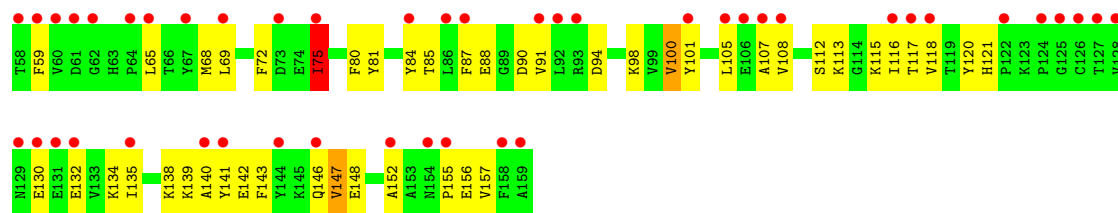


- Molecule 1: PR-10 protein

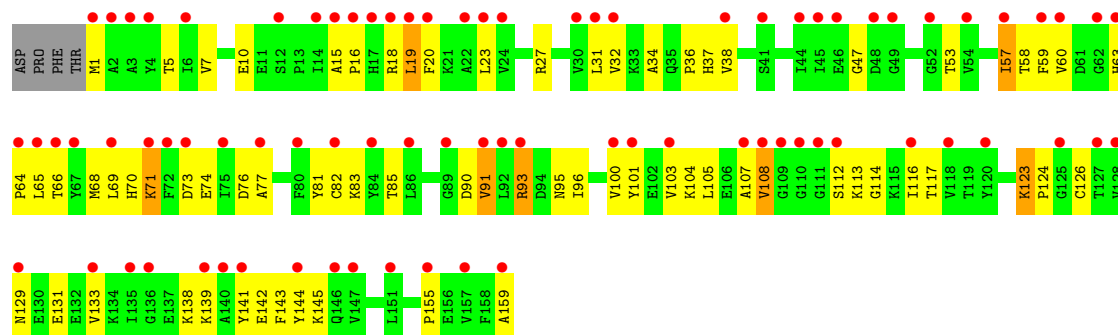


- Molecule 1: PR-10 protein

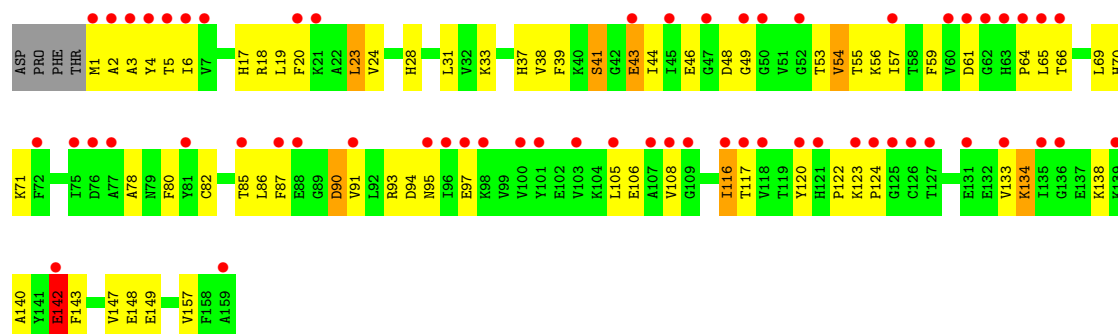




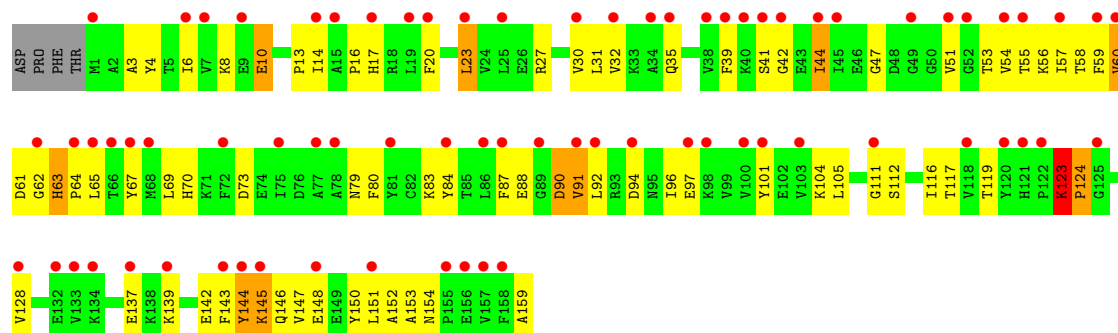
● Molecule 1: PR-10 protein



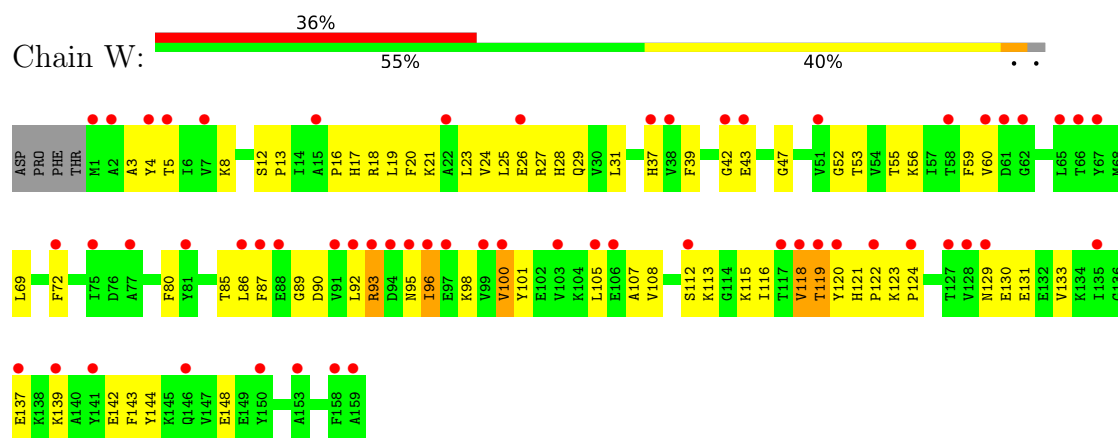
● Molecule 1: PR-10 protein



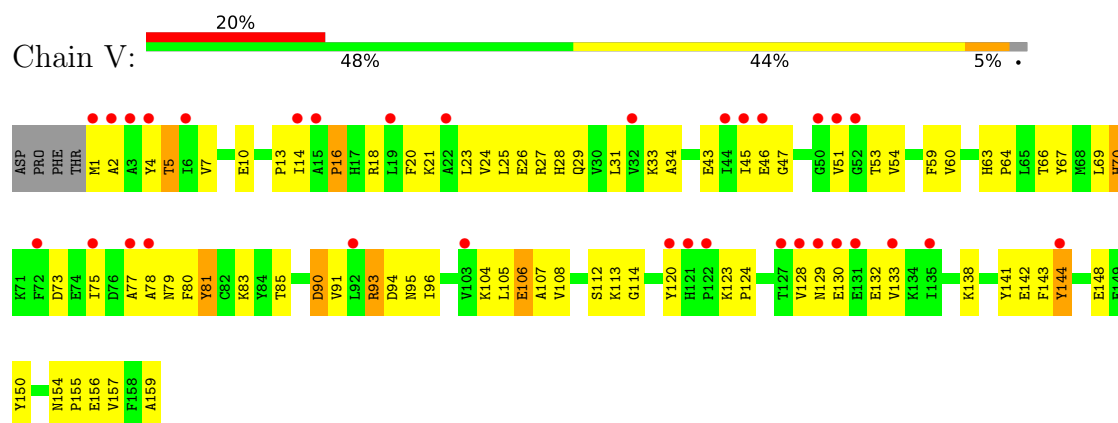
● Molecule 1: PR-10 protein



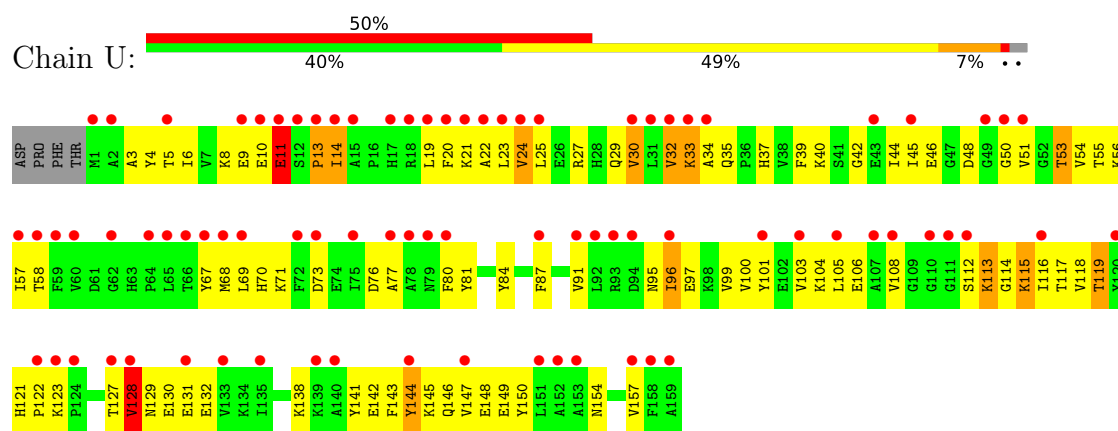
- Molecule 1: PR-10 protein



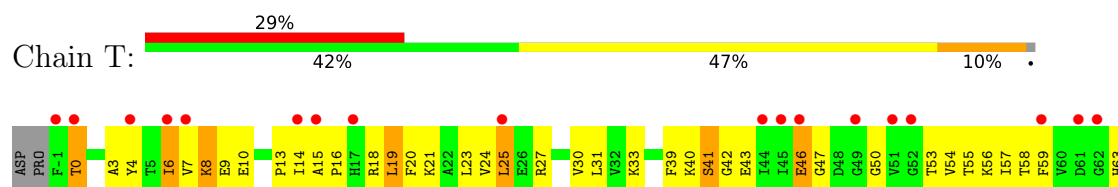
- Molecule 1: PR-10 protein

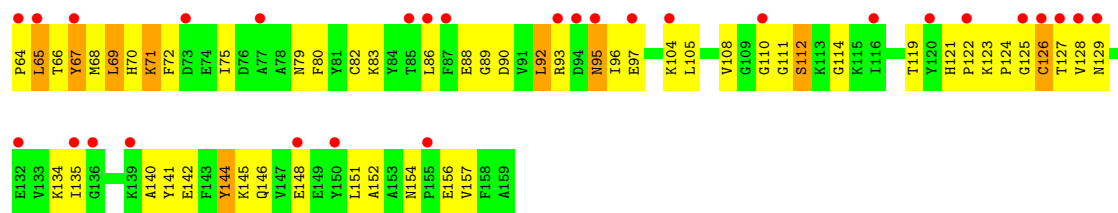


- Molecule 1: PR-10 protein

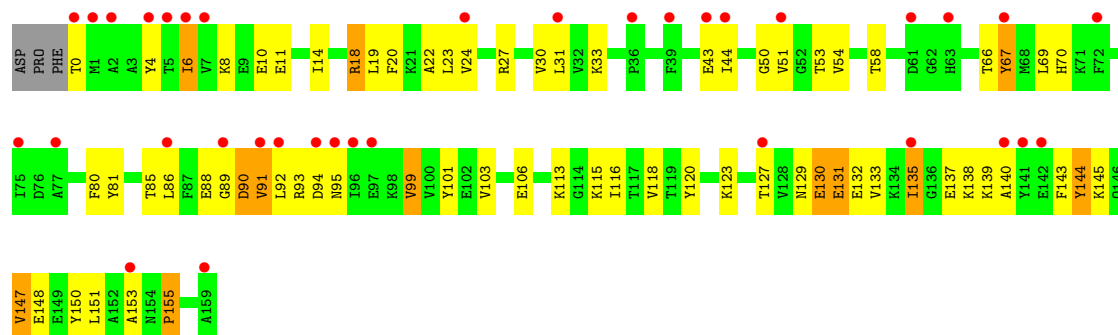


- Molecule 1: PR-10 protein

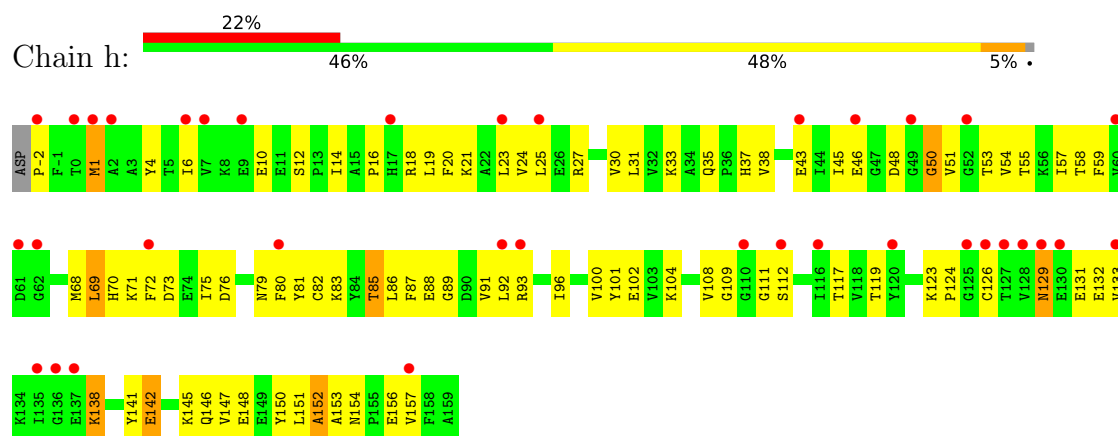




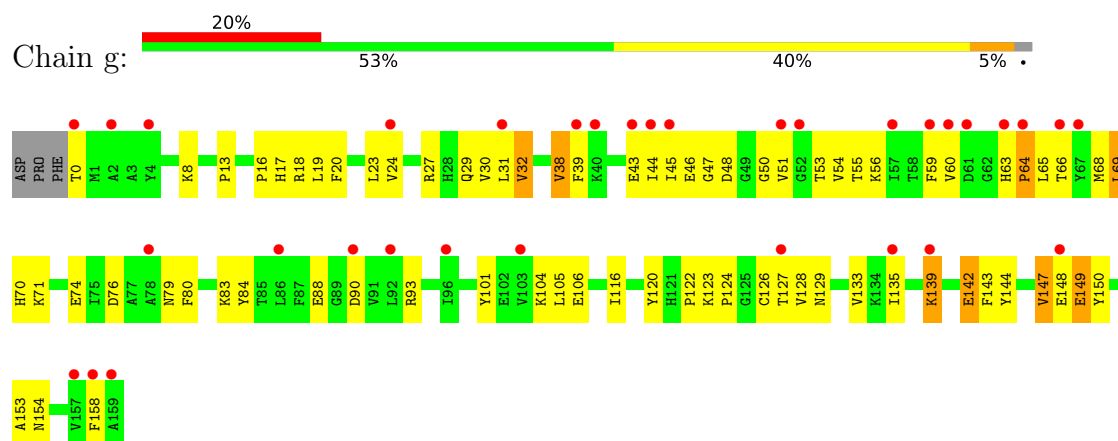
● Molecule 1: PR-10 protein



- Molecule 1: PR-10 protein



- Molecule 1: PR-10 protein



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	145.85Å 145.85Å 385.40Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	31.58 – 2.30 31.58 – 2.30	Depositor EDS
% Data completeness (in resolution range)	99.3 (31.58-2.30) 99.4 (31.58-2.30)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.23 (at 2.29Å)	Xtriage
Refinement program	REFMAC 5.8.0222	Depositor
R, R_{free}	0.226 , 0.255 0.270 , 0.278	Depositor DCC
R_{free} test set	3979 reflections (1.11%)	wwPDB-VP
Wilson B-factor (Å ²)	57.8	Xtriage
Anisotropy	0.131	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 63.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.064 for k,h,-l 0.054 for -k,-h,-l 0.084 for -h,-k,l	Xtriage
Reported twinning fraction	0.241 for H, K, L 0.242 for K, H, -L 0.233 for -K, -H, -L 0.284 for h,-k,-l	Depositor
Outliers	18 of 357481 reflections (0.005%)	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	48343	wwPDB-VP
Average B, all atoms (Å ²)	70.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 74.65 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.4696e-06. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: 2AN, FLC, EPE, DMS, SO4

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	0.83	0/1233	1.26	5/1682 (0.3%)
1	B	0.89	3/1273 (0.2%)	1.27	5/1722 (0.3%)
1	C	0.75	0/1263	1.14	0/1709
1	D	0.80	0/1252	1.29	8/1697 (0.5%)
1	E	0.97	2/1279 (0.2%)	1.29	1/1731 (0.1%)
1	F	0.84	1/1215 (0.1%)	1.23	1/1649 (0.1%)
1	G	0.90	0/1262	1.20	3/1712 (0.2%)
1	H	0.89	1/1261 (0.1%)	1.29	6/1709 (0.4%)
1	I	0.99	5/1282 (0.4%)	1.25	4/1734 (0.2%)
1	J	0.82	0/1287	1.33	7/1746 (0.4%)
1	K	0.95	1/1297 (0.1%)	1.27	5/1755 (0.3%)
1	L	0.90	0/1285	1.25	2/1738 (0.1%)
1	M	0.93	3/1301 (0.2%)	1.23	2/1760 (0.1%)
1	N	0.92	0/1295	1.40	7/1757 (0.4%)
1	O	0.87	0/1242	1.27	6/1684 (0.4%)
1	P	1.03	2/1278 (0.2%)	1.39	8/1729 (0.5%)
1	Q	0.84	0/1296	1.24	3/1753 (0.2%)
1	R	0.93	3/1280 (0.2%)	1.28	1/1732 (0.1%)
1	S	0.93	2/1282 (0.2%)	1.26	2/1733 (0.1%)
1	T	0.91	0/1291	1.34	8/1747 (0.5%)
1	U	0.80	0/1246	1.22	3/1690 (0.2%)
1	V	0.97	3/1275 (0.2%)	1.29	2/1726 (0.1%)
1	W	0.85	0/1249	1.16	0/1689
1	X	0.83	0/1254	1.31	3/1697 (0.2%)
1	Y	0.83	0/1256	1.21	4/1699 (0.2%)
1	Z	0.86	1/1246 (0.1%)	1.20	0/1687
1	a	0.91	0/1253	1.32	3/1695 (0.2%)
1	b	0.79	0/1274	1.24	1/1727 (0.1%)
1	c	0.95	2/1277 (0.2%)	1.30	1/1725 (0.1%)
1	d	0.80	0/1284	1.26	1/1735 (0.1%)
1	e	0.94	3/1282 (0.2%)	1.29	3/1734 (0.2%)
1	f	0.96	2/1292 (0.2%)	1.29	6/1748 (0.3%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	g	0.84	2/1286 (0.2%)	1.27	4/1738 (0.2%)
1	h	0.92	0/1294	1.29	2/1749 (0.1%)
1	i	0.92	2/1279 (0.2%)	1.29	7/1730 (0.4%)
1	j	1.04	1/1272 (0.1%)	1.38	5/1722 (0.3%)
All	All	0.90	39/45773 (0.1%)	1.27	129/61970 (0.2%)

All (39) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	63	HIS	N-CA	7.87	1.54	1.45
1	g	56	LYS	C-O	-7.59	1.15	1.24
1	P	20	PHE	N-CA	-7.01	1.37	1.46
1	S	147	VAL	C-O	-6.67	1.16	1.24
1	E	37	HIS	N-CA	-6.43	1.37	1.46
1	M	32	VAL	C-O	-6.29	1.16	1.24
1	P	41	SER	C-O	-5.99	1.16	1.23
1	I	11	GLU	C-O	-5.94	1.17	1.23
1	V	81	TYR	N-CA	-5.84	1.39	1.46
1	e	147	VAL	C-O	-5.84	1.17	1.24
1	R	20	PHE	N-CA	-5.79	1.39	1.46
1	Z	32	VAL	C-O	-5.76	1.17	1.24
1	M	18	ARG	N-CA	-5.69	1.39	1.46
1	V	70	HIS	CE1-NE2	5.69	1.38	1.32
1	I	44	ILE	N-CA	-5.68	1.39	1.46
1	c	41	SER	C-O	-5.64	1.16	1.23
1	i	16	PRO	C-O	-5.63	1.16	1.24
1	R	14	ILE	N-CA	-5.62	1.39	1.46
1	V	69	LEU	N-CA	-5.60	1.39	1.46
1	e	144	TYR	N-CA	-5.59	1.39	1.46
1	i	36	PRO	C-O	-5.58	1.16	1.24
1	K	147	VAL	N-CA	-5.58	1.39	1.46
1	f	11	GLU	C-O	-5.58	1.17	1.23
1	M	111	GLY	N-CA	5.53	1.49	1.44
1	B	20	PHE	N-CA	-5.53	1.39	1.46
1	B	68	MET	C-O	-5.49	1.17	1.23
1	I	137	GLU	N-CA	-5.44	1.40	1.46
1	c	138	LYS	N-CA	-5.33	1.40	1.46
1	j	13	PRO	C-O	-5.25	1.17	1.24
1	f	144	TYR	C-O	-5.23	1.18	1.24
1	B	37	HIS	CE1-NE2	5.20	1.37	1.32
1	e	13	PRO	C-O	-5.13	1.17	1.24
1	H	155	PRO	C-O	-5.09	1.18	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	S	43	GLU	N-CA	5.08	1.52	1.46
1	I	37	HIS	N-CA	-5.06	1.39	1.46
1	E	60	VAL	N-CA	-5.05	1.40	1.46
1	g	147	VAL	N-CA	-5.04	1.40	1.46
1	R	17	HIS	N-CA	-5.04	1.40	1.46
1	I	16	PRO	C-O	-5.03	1.17	1.24

All (129) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	41	SER	CA-C-N	8.89	127.70	121.65
1	H	41	SER	C-N-CA	8.89	127.70	121.65
1	i	0	THR	CB-CA-C	8.37	123.34	109.53
1	A	90	ASP	CA-CB-CG	6.98	119.58	112.60
1	Q	92	LEU	N-CA-C	-6.81	99.96	110.10
1	O	16	PRO	N-CA-C	6.72	122.29	114.03
1	I	16	PRO	CB-CA-C	-6.68	102.44	113.06
1	T	46	GLU	CB-CG-CD	6.67	123.93	112.60
1	N	157	VAL	CA-C-N	-6.66	113.82	123.00
1	N	157	VAL	C-N-CA	-6.66	113.82	123.00
1	D	97	GLU	N-CA-C	-6.60	104.01	111.14
1	d	95	ASN	N-CA-C	-6.56	105.24	113.18
1	c	35	GLN	CB-CA-C	6.52	119.09	110.81
1	T	112	SER	CA-C-N	6.50	132.74	122.21
1	T	112	SER	C-N-CA	6.50	132.74	122.21
1	L	16	PRO	N-CA-C	6.43	122.27	113.98
1	f	55	THR	CB-CA-C	-6.43	98.64	109.50
1	V	130	GLU	N-CA-C	-6.42	104.28	111.28
1	N	148	GLU	CB-CG-CD	-6.39	101.75	112.60
1	G	53	THR	CA-CB-OG1	-6.34	100.08	109.60
1	R	0	THR	CB-CA-C	6.34	120.69	110.16
1	J	61	ASP	CB-CA-C	6.31	120.08	109.48
1	P	16	PRO	N-CA-C	6.25	121.72	114.03
1	a	30	VAL	N-CA-C	-6.24	105.64	111.45
1	H	16	PRO	CB-CA-C	-6.21	101.31	111.56
1	a	147	VAL	N-CA-C	-6.20	104.70	110.53
1	i	16	PRO	N-CA-C	6.20	122.34	113.47
1	B	149	GLU	CB-CG-CD	6.19	123.13	112.60
1	g	38	VAL	N-CA-C	-6.17	106.94	112.12
1	f	61	ASP	CB-CA-C	-6.10	101.30	110.88
1	X	124	PRO	CB-CA-C	-6.06	102.96	113.20
1	U	32	VAL	N-CA-C	-6.05	105.23	110.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	134	LYS	CA-C-N	6.01	128.22	120.70
1	A	134	LYS	C-N-CA	6.01	128.22	120.70
1	K	147	VAL	N-CA-C	-5.98	104.80	110.42
1	J	90	ASP	CA-CB-CG	5.98	118.58	112.60
1	P	41	SER	CA-C-N	-5.97	117.02	121.61
1	P	41	SER	C-N-CA	-5.97	117.02	121.61
1	X	139	LYS	CA-C-N	5.95	130.65	120.71
1	X	139	LYS	C-N-CA	5.95	130.65	120.71
1	i	15	ALA	CA-C-N	5.86	125.06	118.97
1	i	15	ALA	C-N-CA	5.86	125.06	118.97
1	J	157	VAL	CA-C-N	-5.83	114.77	122.99
1	J	157	VAL	C-N-CA	-5.83	114.77	122.99
1	O	27	ARG	N-CA-C	-5.82	105.44	112.54
1	J	148	GLU	N-CA-C	-5.82	104.16	112.13
1	K	79	ASN	CA-CB-CG	-5.80	106.80	112.60
1	I	137	GLU	N-CA-C	-5.80	104.59	111.03
1	H	61	ASP	CB-CA-C	5.80	118.94	109.90
1	Q	91	VAL	CA-C-N	-5.74	112.73	120.82
1	Q	91	VAL	C-N-CA	-5.74	112.73	120.82
1	e	106	GLU	CA-C-N	5.73	128.90	120.82
1	e	106	GLU	C-N-CA	5.73	128.90	120.82
1	j	16	PRO	N-CA-C	5.72	121.01	113.86
1	D	13	PRO	CB-CA-C	-5.72	102.81	110.88
1	B	136	GLY	CA-C-N	5.70	127.85	120.44
1	B	136	GLY	C-N-CA	5.70	127.85	120.44
1	U	119	THR	CA-CB-OG1	-5.69	101.06	109.60
1	B	16	PRO	N-CA-C	5.67	120.95	113.86
1	P	141	TYR	N-CA-C	-5.61	105.08	111.14
1	O	53	THR	CA-CB-OG1	-5.61	101.18	109.60
1	K	94	ASP	CB-CA-C	5.60	118.13	110.06
1	Y	82	CYS	CA-C-N	5.56	129.11	121.33
1	Y	82	CYS	C-N-CA	5.56	129.11	121.33
1	M	16	PRO	N-CA-C	5.56	120.81	113.86
1	Y	28	HIS	CB-CA-C	5.55	119.70	110.81
1	i	91	VAL	N-CA-C	-5.51	104.17	111.05
1	g	142	GLU	CB-CA-C	5.47	119.47	110.88
1	A	55	THR	CB-CA-C	-5.46	100.78	109.80
1	g	142	GLU	N-CA-C	-5.46	105.23	111.07
1	f	49	GLY	CA-C-N	5.43	126.38	121.82
1	f	49	GLY	C-N-CA	5.43	126.38	121.82
1	e	48	ASP	CA-CB-CG	5.43	118.03	112.60
1	I	133	VAL	N-CA-C	-5.42	105.24	110.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	58	THR	CA-CB-OG1	-5.42	101.47	109.60
1	N	19	LEU	CA-C-N	-5.38	112.13	120.31
1	N	19	LEU	C-N-CA	-5.38	112.13	120.31
1	i	16	PRO	CB-CA-C	-5.38	104.51	113.06
1	a	42	GLY	CA-C-O	-5.37	115.70	120.75
1	S	91	VAL	N-CA-C	-5.37	105.95	112.76
1	N	90	ASP	CA-CB-CG	5.36	117.96	112.60
1	K	64	PRO	CB-CA-C	-5.36	103.32	112.26
1	F	70	HIS	CB-CA-C	5.34	118.46	109.48
1	D	47	GLY	CA-C-N	5.33	127.42	120.28
1	D	47	GLY	C-N-CA	5.33	127.42	120.28
1	j	16	PRO	CB-CA-C	-5.33	103.90	111.68
1	M	17	HIS	N-CA-C	-5.33	105.52	112.23
1	T	47	GLY	CA-C-N	5.32	131.02	122.83
1	T	47	GLY	C-N-CA	5.32	131.02	122.83
1	D	13	PRO	N-CA-C	5.30	120.97	114.35
1	N	13	PRO	CB-CA-C	-5.28	103.07	111.04
1	G	53	THR	CA-C-N	-5.27	116.23	123.14
1	G	53	THR	C-N-CA	-5.27	116.23	123.14
1	P	136	GLY	CA-C-N	5.25	127.63	120.54
1	P	136	GLY	C-N-CA	5.25	127.63	120.54
1	D	141	TYR	CA-C-N	5.23	127.29	120.28
1	D	141	TYR	C-N-CA	5.23	127.29	120.28
1	T	41	SER	CA-C-N	5.21	126.41	121.46
1	T	41	SER	C-N-CA	5.21	126.41	121.46
1	V	16	PRO	N-CA-C	5.20	120.38	113.57
1	f	91	VAL	N-CA-C	-5.19	104.49	111.44
1	O	32	VAL	CA-C-N	-5.18	113.55	120.54
1	O	32	VAL	C-N-CA	-5.18	113.55	120.54
1	J	0	THR	CB-CA-C	5.18	118.29	109.75
1	h	-2	PRO	CA-N-CD	-5.17	104.76	112.00
1	B	134	LYS	CB-CA-C	-5.17	101.07	110.63
1	D	147	VAL	N-CA-C	-5.15	105.58	110.42
1	P	17	HIS	N-CA-C	-5.13	106.87	113.23
1	U	76	ASP	CA-C-O	-5.13	116.47	122.37
1	g	139	LYS	CB-CA-C	-5.12	102.62	110.81
1	j	132	GLU	CA-C-N	5.11	127.00	120.56
1	j	132	GLU	C-N-CA	5.11	127.00	120.56
1	j	73	ASP	N-CA-C	-5.09	106.76	113.12
1	h	142	GLU	N-CA-C	-5.09	105.62	111.07
1	J	62	GLY	N-CA-C	-5.09	107.83	113.79
1	K	149	GLU	CB-CG-CD	5.09	121.25	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	P	138	LYS	CB-CA-C	-5.09	102.35	110.79
1	Y	142	GLU	CB-CG-CD	5.09	121.25	112.60
1	b	141	TYR	N-CA-C	-5.08	105.82	111.36
1	f	11	GLU	CB-CA-C	-5.08	102.82	110.24
1	O	33	LYS	N-CA-C	-5.08	105.02	111.11
1	A	53	THR	CB-CA-C	5.07	118.11	109.80
1	E	29	GLN	CB-CG-CD	-5.06	103.99	112.60
1	i	89	GLY	CA-C-O	-5.03	118.70	122.37
1	H	16	PRO	N-CA-C	5.03	122.83	112.47
1	I	66	THR	CA-CB-OG1	-5.02	102.07	109.60
1	T	93	ARG	N-CA-C	-5.01	103.53	110.35
1	S	18	ARG	N-CA-C	-5.01	105.47	111.03
1	H	10	GLU	CB-CG-CD	5.00	121.11	112.60

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1204	0	1098	133	0
1	B	1244	0	1232	74	0
1	C	1235	0	1201	83	0
1	D	1223	0	1185	116	0
1	E	1250	0	1224	78	0
1	F	1188	0	1101	97	0
1	G	1232	0	1183	93	0
1	H	1232	0	1183	90	0
1	I	1253	0	1234	85	0
1	J	1257	0	1204	92	0
1	K	1266	0	1247	63	0
1	L	1256	0	1245	66	0
1	M	1271	0	1256	72	0
1	N	1265	0	1222	77	0
1	O	1215	0	1153	78	0
1	P	1249	0	1233	80	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	Q	1266	0	1252	65	0
1	R	1252	0	1233	75	0
1	S	1253	0	1250	81	0
1	T	1261	0	1230	91	0
1	U	1218	0	1178	124	0
1	V	1246	0	1222	94	0
1	W	1220	0	1178	68	0
1	X	1226	0	1190	125	0
1	Y	1227	0	1176	78	0
1	Z	1218	0	1159	79	0
1	a	1224	0	1175	94	0
1	b	1244	0	1200	79	0
1	c	1248	0	1233	65	0
1	d	1254	0	1223	112	0
1	e	1253	0	1227	77	0
1	f	1262	0	1238	95	0
1	g	1257	0	1252	59	0
1	h	1264	0	1237	92	0
1	i	1250	0	1225	85	0
1	j	1243	0	1222	83	0
2	A	84	0	48	15	0
2	B	126	0	73	44	0
2	C	63	0	37	18	0
2	D	84	0	49	31	0
2	E	84	0	48	16	0
2	F	126	0	74	66	0
2	G	126	0	74	28	0
2	H	84	0	50	24	0
2	I	147	0	85	46	0
2	J	63	0	37	19	0
2	K	63	0	38	22	0
2	L	84	0	49	27	0
2	M	63	0	37	10	0
2	N	105	0	64	30	0
2	O	63	0	36	22	0
2	P	84	0	51	23	0
2	Q	63	0	36	12	0
2	R	105	0	63	41	0
2	S	84	0	48	27	0
2	T	105	0	62	38	0
2	U	42	0	25	12	0
2	V	168	0	99	77	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	W	21	0	12	6	0
2	X	126	0	72	83	0
2	Y	84	0	49	30	0
2	Z	126	0	74	38	0
2	a	84	0	48	33	0
2	b	126	0	74	51	0
2	c	126	0	74	30	0
2	d	84	0	49	45	0
2	e	21	0	13	4	0
2	f	126	0	73	44	0
2	g	63	0	37	16	0
2	h	126	0	74	39	0
2	i	21	0	13	3	0
2	j	147	0	84	44	0
3	A	5	0	0	6	0
3	E	5	0	0	0	0
3	G	5	0	0	0	0
3	I	5	0	0	0	0
3	Q	5	0	0	0	0
3	Y	5	0	0	2	0
3	c	15	0	0	1	0
3	g	5	0	0	1	0
4	P	15	0	18	6	0
5	G	4	0	6	1	0
5	N	4	0	6	2	0
5	X	4	0	6	0	0
6	G	13	0	5	2	0
6	a	26	0	10	1	0
6	e	13	0	5	1	0
6	i	26	0	10	3	0
6	j	13	0	5	9	0
7	A	6	0	0	8	0
7	B	5	0	0	0	0
7	C	4	0	0	6	0
7	D	3	0	0	0	0
7	E	5	0	0	3	0
7	F	1	0	0	1	0
7	G	5	0	0	3	0
7	H	3	0	0	0	0
7	I	5	0	0	1	0
7	J	2	0	0	2	0
7	K	6	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	L	3	0	0	0	0
7	M	1	0	0	1	0
7	N	3	0	0	0	0
7	O	4	0	0	1	0
7	P	5	0	0	1	0
7	Q	1	0	0	0	0
7	R	3	0	0	1	0
7	S	1	0	0	0	0
7	T	5	0	0	1	0
7	V	9	0	0	2	0
7	W	2	0	0	0	0
7	X	3	0	0	6	0
7	Y	4	0	0	0	0
7	Z	4	0	0	5	0
7	a	8	0	0	1	0
7	b	6	0	0	1	0
7	c	3	0	0	0	0
7	d	2	0	0	1	0
7	e	9	0	0	2	0
7	f	8	0	0	1	0
7	g	4	0	0	0	0
7	h	8	0	0	2	0
7	i	6	0	0	2	0
7	j	5	0	0	0	0
All	All	48343	0	45501	3588	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 38.

All (3588) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:27:ARG:NH1	2:S:204:2AN:H8	1.39	1.34
1:Y:94:ASP:O	1:Y:123:LYS:HD3	1.30	1.28
1:H:138:LYS:HE2	1:G:-1:PHE:CE1	1.69	1.26
1:a:84:TYR:OH	2:a:204:2AN:H6	1.36	1.25
1:X:10:GLU:CG	2:X:206:2AN:H13	1.65	1.24
1:j:137:GLU:OE2	1:i:0:THR:HG23	1.42	1.20
1:S:116:ILE:HG12	2:S:204:2AN:C3	1.73	1.19
1:H:138:LYS:CE	1:G:-1:PHE:CE1	2.26	1.18
1:Y:138:LYS:CE	2:Y:201:2AN:H12	1.73	1.18

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:23:LEU:CD1	2:X:206:2AN:H16	1.73	1.18
1:P:138:LYS:NZ	4:P:205:EPE:H62	1.61	1.16
2:c:204:2AN:H16	2:c:204:2AN:H2	1.27	1.16
2:K:202:2AN:H16	2:K:202:2AN:H2	1.17	1.15
2:Y:202:2AN:H16	2:Y:202:2AN:H2	1.25	1.15
2:J:201:2AN:H16	2:J:201:2AN:H2	1.25	1.14
1:X:10:GLU:CG	2:X:206:2AN:C13	2.25	1.14
2:G:203:2AN:H2	2:G:203:2AN:H16	1.28	1.14
2:F:206:2AN:H2	1:f:77:ALA:HB1	1.28	1.14
2:N:201:2AN:H16	2:N:201:2AN:H2	1.27	1.13
2:B:203:2AN:H16	2:B:203:2AN:H2	1.15	1.13
1:X:62:GLY:O	2:X:203:2AN:H4	1.48	1.13
2:N:204:2AN:H16	2:N:204:2AN:H2	1.30	1.12
2:P:203:2AN:H16	2:P:203:2AN:H2	1.24	1.11
2:I:207:2AN:H16	2:I:207:2AN:H2	1.27	1.11
1:T:33:LYS:HD2	2:T:203:2AN:O3	1.50	1.10
1:W:96:ILE:HG23	1:W:121:HIS:O	1.50	1.10
2:f:205:2AN:H12	2:f:205:2AN:H2	1.17	1.10
1:X:10:GLU:CB	2:X:206:2AN:H13	1.79	1.10
1:V:4:TYR:CD1	1:V:128:VAL:HG11	1.84	1.10
1:Y:93:ARG:HH11	2:Y:204:2AN:C12	1.64	1.10
2:U:201:2AN:H16	2:U:201:2AN:H2	1.34	1.10
2:b:201:2AN:H16	2:b:201:2AN:H2	1.29	1.09
1:I:47:GLY:HA2	2:I:204:2AN:H12	1.26	1.09
2:F:203:2AN:H16	2:F:203:2AN:H2	1.25	1.09
1:X:23:LEU:HB3	2:X:206:2AN:C3	1.83	1.09
1:H:134:LYS:O	1:H:138:LYS:HG3	1.53	1.09
1:E:123:LYS:HG2	1:E:124:PRO:HD2	1.30	1.09
1:D:158:PHE:CZ	2:D:203:2AN:H15	1.89	1.08
1:D:57:ILE:O	1:D:67:TYR:HA	1.53	1.08
2:a:204:2AN:H2	2:a:204:2AN:H12	1.34	1.07
1:g:139:LYS:HE2	2:g:202:2AN:C4	1.84	1.07
2:V:208:2AN:H12	2:V:208:2AN:S	1.95	1.07
1:H:59:PHE:HD1	1:H:66:THR:C	1.62	1.07
2:J:202:2AN:H16	2:J:202:2AN:H2	1.29	1.06
1:X:10:GLU:HG3	2:X:206:2AN:H13	1.24	1.06
2:M:201:2AN:H12	2:M:201:2AN:H2	1.35	1.06
2:I:205:2AN:H2	2:I:205:2AN:H12	1.37	1.05
2:g:201:2AN:H12	2:g:201:2AN:H2	1.10	1.05
1:X:10:GLU:HB3	2:X:206:2AN:H13	1.37	1.05
1:U:9:GLU:HA	1:U:114:GLY:O	1.53	1.05

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:R:201:2AN:H12	2:R:201:2AN:H2	1.36	1.05
2:F:204:2AN:H16	2:F:204:2AN:H2	1.36	1.05
1:P:138:LYS:HZ3	4:P:205:EPE:H62	1.16	1.04
2:j:204:2AN:H16	2:j:204:2AN:H2	1.09	1.04
1:U:106:GLU:HG3	1:U:113:LYS:HD2	1.34	1.04
2:h:204:2AN:H16	2:h:204:2AN:H2	1.39	1.04
1:S:33:LYS:CE	2:S:203:2AN:O1	2.07	1.02
1:S:116:ILE:HG12	2:S:204:2AN:H3	1.41	1.02
2:L:204:2AN:H16	2:L:204:2AN:H2	1.41	1.02
1:X:44:ILE:HD11	1:X:53:THR:HG21	1.39	1.02
1:c:135:ILE:O	1:c:139:LYS:HG2	1.59	1.02
2:R:204:2AN:H12	2:R:204:2AN:H2	1.41	1.02
2:b:203:2AN:O1	2:b:203:2AN:N	1.91	1.02
2:N:201:2AN:H16	2:N:201:2AN:C2	1.81	1.01
2:d:201:2AN:H2	2:d:201:2AN:H12	1.37	1.01
1:V:4:TYR:CD1	1:V:128:VAL:CG1	2.43	1.01
1:Y:138:LYS:HE2	2:Y:201:2AN:H12	1.40	1.01
1:X:23:LEU:HD11	2:X:206:2AN:H16	1.39	1.01
1:H:138:LYS:HE2	1:G:-1:PHE:HE1	0.99	1.01
1:X:10:GLU:HB3	2:X:206:2AN:C13	1.89	1.01
1:J:4:TYR:CE1	1:I:2:ALA:HB2	1.96	1.01
1:J:4:TYR:HE1	1:J:6:ILE:HD11	1.23	1.01
1:Z:10:GLU:HB3	2:Z:203:2AN:H15	1.42	1.01
1:d:101:TYR:OH	2:d:204:2AN:H6	1.59	1.00
2:X:204:2AN:H16	2:X:204:2AN:H2	1.40	0.99
2:j:205:2AN:N	2:j:205:2AN:O3	1.96	0.99
2:f:204:2AN:O3	2:f:204:2AN:N	1.95	0.99
1:Q:69:LEU:HD22	1:Q:88:GLU:OE1	1.62	0.99
2:h:203:2AN:H16	2:h:203:2AN:H2	1.43	0.99
1:X:10:GLU:CB	2:X:206:2AN:C13	2.42	0.98
1:M:135:ILE:O	1:M:139:LYS:HG2	1.62	0.98
2:R:203:2AN:N	2:R:203:2AN:O1	1.97	0.98
2:j:205:2AN:N	2:j:205:2AN:S	2.35	0.97
2:E:201:2AN:H16	2:E:201:2AN:H2	1.44	0.97
2:g:201:2AN:H2	2:g:201:2AN:C12	1.94	0.97
1:U:103:VAL:HG13	1:U:116:ILE:HG22	1.46	0.97
2:L:202:2AN:H2	2:L:202:2AN:H12	1.45	0.97
2:f:205:2AN:H12	2:f:205:2AN:C2	1.89	0.97
1:U:68:MET:HG2	1:U:91:VAL:HG11	1.45	0.97
1:C:65:LEU:HD13	1:C:91:VAL:HG22	1.44	0.97
2:F:201:2AN:H16	2:F:201:2AN:H2	1.44	0.97

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:j:129:ASN:ND2	1:j:132:GLU:HB2	1.78	0.97
2:H:203:2AN:H16	2:H:203:2AN:H2	1.46	0.97
2:R:205:2AN:H2	2:R:205:2AN:H12	1.47	0.96
1:S:129:ASN:HD22	1:S:131:GLU:HG2	1.29	0.96
1:F:139:LYS:C	2:F:202:2AN:C8	2.39	0.96
2:O:201:2AN:H12	2:O:201:2AN:H2	1.45	0.96
2:G:207:2AN:H2	2:G:207:2AN:H12	1.44	0.96
1:B:158:PHE:CZ	2:B:203:2AN:H13	1.99	0.96
1:X:123:LYS:HB3	1:X:124:PRO:CD	1.95	0.96
2:b:204:2AN:H16	2:b:204:2AN:H2	1.45	0.96
1:H:87:PHE:O	1:H:88:GLU:HG3	1.65	0.95
1:X:123:LYS:HB3	1:X:124:PRO:HD2	1.48	0.95
1:R:69:LEU:HD12	1:R:88:GLU:CB	1.96	0.95
2:K:203:2AN:H2	2:K:203:2AN:H12	1.46	0.95
1:U:9:GLU:OE2	1:U:115:LYS:HD3	1.66	0.95
2:j:207:2AN:H16	2:j:207:2AN:H2	1.49	0.95
2:f:205:2AN:H2	2:f:205:2AN:C12	1.94	0.94
1:U:103:VAL:HG13	1:U:116:ILE:CG2	1.98	0.94
2:T:203:2AN:H2	2:T:203:2AN:H12	1.46	0.94
2:c:202:2AN:H16	2:c:202:2AN:H2	1.46	0.94
2:J:202:2AN:H2	2:J:202:2AN:C16	1.94	0.94
1:E:95:ASN:HB2	1:E:127:THR:O	1.67	0.94
1:V:141:TYR:CD2	2:V:208:2AN:C7	2.51	0.94
1:H:138:LYS:CE	1:G:-1:PHE:HE1	1.74	0.94
1:A:107:ALA:HB1	3:A:205:SO4:O2	1.68	0.94
1:E:70:HIS:HD2	7:E:301:HOH:O	1.50	0.94
2:X:202:2AN:H12	2:X:202:2AN:H2	1.46	0.94
2:b:205:2AN:H16	2:b:205:2AN:H2	1.50	0.94
2:B:203:2AN:H2	2:B:203:2AN:C16	1.97	0.93
1:Y:138:LYS:HE2	2:Y:201:2AN:C12	1.98	0.93
1:X:10:GLU:HG3	2:X:206:2AN:C13	1.92	0.93
2:V:206:2AN:H16	2:V:206:2AN:H2	1.48	0.93
1:H:138:LYS:HE3	1:G:-1:PHE:CE1	2.02	0.93
2:I:204:2AN:H15	1:Y:78:ALA:HB2	1.49	0.93
1:U:106:GLU:CG	1:U:113:LYS:HD2	1.98	0.93
2:j:204:2AN:H2	2:j:204:2AN:C16	1.92	0.93
1:G:45:ILE:HD11	1:G:54:VAL:HG22	1.50	0.93
2:I:204:2AN:H4	1:Y:17:HIS:HB2	1.50	0.93
2:T:201:2AN:H2	2:T:201:2AN:H16	1.51	0.93
1:b:2:ALA:HB3	1:a:4:TYR:CE1	2.04	0.93
1:T:10:GLU:HB3	2:T:201:2AN:H13	1.51	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:j:204:2AN:H16	2:j:204:2AN:C2	1.96	0.93
2:a:203:2AN:H16	2:a:203:2AN:H2	1.51	0.92
2:D:201:2AN:H16	2:D:201:2AN:H2	1.49	0.92
2:I:202:2AN:H2	2:I:202:2AN:C16	2.00	0.92
1:b:129:ASN:CB	1:b:132:GLU:HB2	2.00	0.92
2:h:206:2AN:C2	2:h:206:2AN:H12	1.96	0.92
1:F:6:ILE:CB	1:E:1:MET:CB	2.48	0.92
1:g:149:GLU:OE1	1:g:149:GLU:C	2.12	0.92
1:G:70:HIS:CE1	7:G:304:HOH:O	2.22	0.92
1:G:70:HIS:HE1	7:G:304:HOH:O	1.53	0.91
1:Z:23:LEU:O	1:Z:27:ARG:HD2	1.68	0.91
2:T:204:2AN:H2	2:T:204:2AN:H12	1.51	0.91
2:Q:202:2AN:H2	2:Q:202:2AN:H12	1.50	0.91
2:J:202:2AN:H16	2:J:202:2AN:C2	1.90	0.91
1:T:10:GLU:HB3	2:T:201:2AN:C13	1.98	0.91
1:P:46:GLU:HG2	2:V:204:2AN:H12	1.48	0.91
1:U:13:PRO:HD2	1:U:148:GLU:OE2	1.69	0.91
1:V:4:TYR:HD1	1:V:128:VAL:HG11	1.27	0.91
2:V:204:2AN:H16	2:V:204:2AN:H2	1.49	0.91
2:K:203:2AN:O3	2:K:203:2AN:N	2.02	0.91
1:E:70:HIS:HE1	7:E:304:HOH:O	1.52	0.91
1:C:135:ILE:O	1:C:139:LYS:HG2	1.70	0.91
1:F:139:LYS:C	2:F:202:2AN:C7	2.44	0.91
2:b:201:2AN:H2	2:b:201:2AN:C16	2.01	0.91
1:R:96:ILE:O	1:R:123:LYS:HE2	1.71	0.91
1:d:10:GLU:HB3	2:d:201:2AN:H15	1.53	0.91
2:M:201:2AN:H2	2:M:201:2AN:C12	1.98	0.90
1:F:139:LYS:CB	2:F:202:2AN:C8	2.49	0.90
1:Z:10:GLU:CB	2:Z:203:2AN:C15	2.49	0.90
2:I:202:2AN:H2	2:I:202:2AN:H16	1.51	0.90
1:F:140:ALA:HB2	2:F:202:2AN:O3	1.70	0.90
1:C:101:TYR:CE1	7:C:302:HOH:O	2.25	0.90
1:Z:123:LYS:CB	1:Z:124:PRO:HD2	2.02	0.90
2:C:203[A]:2AN:O3	2:C:203[A]:2AN:C11	2.19	0.90
2:N:201:2AN:H2	2:N:201:2AN:C16	1.88	0.90
2:b:201:2AN:H16	2:b:201:2AN:C2	2.00	0.90
1:S:27:ARG:HH12	2:S:204:2AN:H8	1.25	0.90
2:h:203:2AN:H16	2:h:203:2AN:C2	2.00	0.89
2:Y:202:2AN:H2	2:Y:202:2AN:C16	2.01	0.89
1:A:123:LYS:CG	1:A:124:PRO:HD2	2.01	0.89
1:A:123:LYS:HG2	1:A:124:PRO:HD2	1.53	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:203:2AN:H16	2:P:203:2AN:C2	2.02	0.89
1:G:45:ILE:HD11	1:G:54:VAL:CG2	2.03	0.89
1:c:138:LYS:HD3	2:c:202:2AN:C12	2.03	0.89
2:g:201:2AN:H12	2:g:201:2AN:C2	2.02	0.89
1:H:59:PHE:CD1	1:H:66:THR:C	2.51	0.89
1:X:23:LEU:CD1	2:X:206:2AN:C2	2.51	0.89
1:W:92:LEU:HD12	1:W:92:LEU:O	1.73	0.89
2:U:201:2AN:O1	2:U:201:2AN:N	2.06	0.89
1:X:62:GLY:O	2:X:203:2AN:C4	2.21	0.88
1:Z:19:LEU:CD1	1:Z:23:LEU:HD12	2.03	0.88
1:S:116:ILE:CG1	2:S:204:2AN:H3	2.03	0.88
1:Y:94:ASP:O	1:Y:123:LYS:CD	2.21	0.88
1:d:138:LYS:HD2	1:d:142:GLU:OE2	1.73	0.88
1:a:7:VAL:HG23	1:a:117:THR:HG22	1.53	0.88
2:T:205:2AN:H16	2:T:205:2AN:C2	2.02	0.88
2:h:206:2AN:H12	2:h:206:2AN:H2	1.54	0.88
1:d:31:LEU:HA	1:d:143:PHE:CE1	2.09	0.88
2:P:203:2AN:H2	2:P:203:2AN:C16	2.03	0.88
1:C:103:VAL:HG21	2:C:202:2AN:C4	2.03	0.88
1:E:109:GLY:O	1:e:80:PHE:HZ	1.57	0.88
1:R:57:ILE:O	1:R:67:TYR:HA	1.72	0.88
1:F:139:LYS:CB	2:F:202:2AN:C7	2.52	0.88
2:C:202:2AN:H2	2:C:202:2AN:H12	1.53	0.88
1:J:156:GLU:OE1	1:J:156:GLU:N	2.06	0.88
1:E:123:LYS:CG	1:E:124:PRO:HD2	2.03	0.87
1:D:4:TYR:OH	1:C:2:ALA:HB2	1.74	0.87
2:R:201:2AN:H2	2:R:201:2AN:C12	2.04	0.87
2:Y:202:2AN:H16	2:Y:202:2AN:C2	2.04	0.87
1:U:57:ILE:O	1:U:67:TYR:HB2	1.74	0.87
1:R:69:LEU:HD12	1:R:88:GLU:HB3	1.56	0.87
1:X:23:LEU:HD13	2:X:206:2AN:C2	2.02	0.87
1:N:28:HIS:CE1	1:N:29:GLN:HG2	2.09	0.87
1:X:23:LEU:HB3	2:X:206:2AN:H3	1.54	0.87
2:X:205:2AN:H16	2:X:205:2AN:H2	1.54	0.87
2:A:203:2AN:H16	2:A:203:2AN:H2	1.57	0.87
1:I:155:PRO:O	1:I:159:ALA:HB3	1.74	0.87
1:Y:64:PRO:HB2	2:Y:204:2AN:O2	1.75	0.87
2:M:201:2AN:H12	2:M:201:2AN:C2	2.05	0.87
1:T:33:LYS:CD	2:T:203:2AN:O3	2.23	0.87
1:S:116:ILE:HG12	2:S:204:2AN:C4	2.04	0.87
1:i:13:PRO:CD	1:i:148:GLU:OE2	2.23	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:201:2AN:H16	2:A:201:2AN:H2	1.53	0.86
1:d:23:LEU:HD12	2:d:201:2AN:C2	2.05	0.86
1:F:139:LYS:CB	2:F:202:2AN:C9	2.54	0.86
2:b:204:2AN:H16	2:b:204:2AN:C2	2.05	0.86
1:N:139:LYS:HE3	2:N:205:2AN:C8	2.06	0.86
2:C:203[A]:2AN:O3	2:C:203[A]:2AN:N	2.08	0.86
2:c:204:2AN:H2	2:c:204:2AN:C16	2.05	0.86
1:S:33:LYS:NZ	2:S:203:2AN:O1	0.71	0.86
1:H:138:LYS:CE	1:G:-1:PHE:CZ	2.58	0.86
1:E:94:ASP:O	1:E:95:ASN:ND2	2.08	0.86
1:N:138:LYS:CB	2:N:203:2AN:O1	2.24	0.85
2:Z:202:2AN:H16	2:Z:202:2AN:H2	1.55	0.85
1:X:65:LEU:HD13	1:X:91:VAL:HG13	1.58	0.85
2:R:201:2AN:H12	2:R:201:2AN:C2	2.07	0.85
1:i:13:PRO:HD2	1:i:148:GLU:OE2	1.77	0.85
2:W:201:2AN:H16	2:W:201:2AN:H2	1.56	0.85
1:G:65:LEU:HD22	1:G:91:VAL:HG13	1.58	0.85
1:d:31:LEU:HA	1:d:143:PHE:HE1	1.42	0.85
1:U:101:TYR:HD1	1:U:118:VAL:HG22	1.41	0.85
1:h:10:GLU:HB3	2:h:202:2AN:H13	1.58	0.85
1:Q:67:TYR:HE2	1:Q:69:LEU:CD1	1.88	0.85
2:P:203:2AN:N	2:P:203:2AN:O1	2.10	0.85
2:Z:204:2AN:H2	2:Z:204:2AN:H16	1.55	0.85
1:R:158:PHE:CZ	2:R:203:2AN:H13	2.12	0.84
1:F:158:PHE:CE2	2:F:203:2AN:H13	2.13	0.84
2:E:204:2AN:H16	2:E:204:2AN:C2	2.06	0.84
1:e:120:TYR:CE1	1:e:133:VAL:HG13	2.12	0.84
1:T:79:ASN:HB3	1:T:104:LYS:NZ	1.92	0.84
1:h:79:ASN:HB3	1:h:104:LYS:NZ	1.92	0.84
2:Z:205:2AN:S	2:Z:205:2AN:N	2.49	0.84
1:G:65:LEU:CD2	1:G:91:VAL:HG13	2.08	0.84
1:A:6:ILE:HD11	1:A:133:VAL:HG13	1.59	0.84
1:H:70:HIS:HA	1:H:85:THR:O	1.78	0.84
1:i:6:ILE:O	1:i:117:THR:HA	1.77	0.84
1:R:139:LYS:HE3	2:R:205:2AN:C3	2.06	0.84
2:I:202:2AN:H16	2:I:202:2AN:C2	2.07	0.84
2:K:202:2AN:H16	2:K:202:2AN:C2	2.03	0.84
1:F:139:LYS:CB	2:F:202:2AN:C5	2.55	0.83
1:F:139:LYS:CB	2:F:202:2AN:C6	2.56	0.83
1:Z:19:LEU:HD13	1:Z:23:LEU:HD12	1.60	0.83
1:R:71:LYS:HG3	1:R:87:PHE:CE1	2.12	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:d:202:2AN:N	2:d:202:2AN:O1	2.11	0.83
2:c:206:2AN:H16	2:c:206:2AN:C2	2.09	0.83
2:h:205:2AN:H16	2:h:205:2AN:H2	1.61	0.83
1:F:139:LYS:CB	2:F:202:2AN:C10	2.56	0.83
1:i:1:MET:SD	1:i:124:PRO:HA	2.18	0.83
1:d:23:LEU:HB3	2:d:201:2AN:C3	2.09	0.83
1:S:116:ILE:CD1	2:S:204:2AN:H3	2.09	0.83
1:d:101:TYR:OH	2:d:204:2AN:C6	2.27	0.83
1:Z:10:GLU:HB2	2:Z:203:2AN:C15	2.08	0.83
1:D:70:HIS:HA	1:D:85:THR:O	1.79	0.83
1:d:23:LEU:HD12	2:d:201:2AN:H2	1.59	0.83
1:d:23:LEU:CD1	2:d:201:2AN:C2	2.56	0.83
2:X:201:2AN:H2	2:X:201:2AN:H12	1.61	0.83
1:P:158:PHE:CZ	2:P:203:2AN:H15	2.14	0.82
2:K:202:2AN:O3	2:K:202:2AN:N	2.12	0.82
2:j:203:2AN:H16	2:j:203:2AN:C2	2.07	0.82
1:E:109:GLY:O	1:e:80:PHE:CZ	2.33	0.82
2:N:202:2AN:H16	2:N:202:2AN:C2	2.10	0.82
1:X:10:GLU:CB	2:X:206:2AN:C12	2.57	0.82
2:E:201:2AN:H16	2:E:201:2AN:C2	2.09	0.82
1:f:156:GLU:N	1:f:156:GLU:OE1	2.13	0.82
1:Z:10:GLU:HB3	2:Z:203:2AN:C15	2.08	0.82
1:X:23:LEU:HB3	2:X:206:2AN:C4	2.10	0.82
2:M:203:2AN:C2	2:M:203:2AN:H16	2.08	0.82
2:h:206:2AN:C15	7:h:307:HOH:O	2.27	0.82
2:N:204:2AN:O3	2:N:204:2AN:N	2.12	0.82
1:X:23:LEU:HD13	2:X:206:2AN:C3	2.08	0.82
2:J:201:2AN:H16	2:J:201:2AN:C2	2.06	0.82
1:H:77:ALA:O	2:H:204:2AN:H3	1.80	0.82
2:X:202:2AN:O3	2:X:202:2AN:N	2.12	0.82
1:I:123:LYS:HG2	1:I:124:PRO:HD2	1.60	0.82
2:F:205:2AN:O3	2:F:205:2AN:N	2.10	0.82
1:i:28:HIS:CD2	1:i:55:THR:HG21	2.14	0.82
2:V:201:2AN:H16	2:V:201:2AN:H2	1.60	0.82
1:g:143:PHE:O	1:g:147:VAL:HG23	1.80	0.82
2:N:205:2AN:H16	2:N:205:2AN:H2	1.59	0.81
1:F:139:LYS:O	2:F:202:2AN:H7	1.80	0.81
2:P:204:2AN:C2	2:P:204:2AN:H16	2.09	0.81
2:K:202:2AN:H2	2:K:202:2AN:C16	2.01	0.81
1:D:3:ALA:HB3	1:C:5:THR:O	1.80	0.81
1:Y:64:PRO:CB	2:Y:204:2AN:O2	2.27	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:65:LEU:CD1	1:P:91:VAL:HG12	2.11	0.81
1:j:137:GLU:OE2	1:i:0:THR:CG2	2.26	0.81
2:h:203:2AN:H2	2:h:203:2AN:C16	2.02	0.81
2:G:203:2AN:H16	2:G:203:2AN:C2	2.08	0.81
1:X:123:LYS:CB	1:X:124:PRO:CD	2.59	0.81
1:V:129:ASN:HB2	1:V:132:GLU:CB	2.10	0.81
1:P:65:LEU:HD13	1:P:91:VAL:CG1	2.10	0.81
1:N:156:GLU:N	1:N:156:GLU:OE1	2.14	0.81
1:F:43:GLU:O	1:F:55:THR:HA	1.80	0.81
2:X:206:2AN:C7	7:X:302:HOH:O	2.29	0.81
1:j:142:GLU:HG2	6:j:208:FLC:CBC	2.11	0.81
2:h:202:2AN:H16	2:h:202:2AN:H2	1.61	0.81
1:A:73:ASP:HB2	1:A:83:LYS:O	1.80	0.80
2:I:203:2AN:H16	2:I:203:2AN:H2	1.63	0.80
1:f:33:LYS:C	2:f:205:2AN:O3	2.23	0.80
1:Z:138:LYS:NZ	2:Z:206:2AN:H8	1.96	0.80
1:i:156:GLU:N	1:i:156:GLU:OE1	2.14	0.80
1:K:101:TYR:CE2	2:K:202:2AN:C14	2.64	0.80
1:V:94:ASP:O	1:V:123:LYS:HD2	1.81	0.80
1:M:67:TYR:CE2	1:M:89:GLY:HA2	2.16	0.80
2:V:205:2AN:C16	2:V:208:2AN:O2	2.30	0.80
1:I:47:GLY:HA2	2:I:204:2AN:C12	2.09	0.80
1:N:6:ILE:CG2	1:M:0:THR:HB	2.12	0.80
2:J:202:2AN:N	2:J:202:2AN:O1	2.14	0.80
1:H:63:HIS:CE1	1:H:65:LEU:H	1.99	0.80
1:N:92:LEU:HD22	1:N:96:ILE:HB	1.62	0.80
1:d:61:ASP:OD1	1:d:61:ASP:N	2.14	0.80
2:Z:206:2AN:C11	2:Z:206:2AN:O2	2.28	0.80
2:h:206:2AN:H2	2:h:206:2AN:C12	2.09	0.80
1:F:141:TYR:HD1	2:F:201:2AN:O1	1.64	0.80
2:Y:201:2AN:H16	2:Y:201:2AN:H2	1.63	0.80
1:S:27:ARG:NH1	2:S:204:2AN:C8	2.35	0.80
1:H:63:HIS:ND1	1:H:65:LEU:N	2.30	0.80
1:E:149:GLU:C	1:E:149:GLU:OE1	2.23	0.80
1:B:120:TYR:OH	2:B:201:2AN:C15	2.30	0.80
1:J:17:HIS:HB2	7:J:302:HOH:O	1.81	0.80
1:G:45:ILE:CD1	1:G:54:VAL:HG22	2.10	0.80
2:E:201:2AN:H2	2:E:201:2AN:C16	2.07	0.80
1:h:69:LEU:HB2	1:h:88:GLU:HB3	1.61	0.80
1:K:120:TYR:CE2	1:K:133:VAL:HG23	2.16	0.79
1:d:139:LYS:HD3	2:d:204:2AN:H13	1.63	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:123:LYS:HD3	1:X:124:PRO:HD3	1.63	0.79
1:P:138:LYS:HZ1	4:P:205:EPE:H62	1.48	0.79
1:K:6:ILE:HD11	1:K:133:VAL:HG21	1.64	0.79
1:J:4:TYR:CE1	1:J:6:ILE:HD11	2.13	0.79
2:H:201:2AN:H16	2:H:201:2AN:H2	1.62	0.79
2:c:204:2AN:H16	2:c:204:2AN:C2	2.08	0.79
1:S:129:ASN:ND2	1:S:131:GLU:HG2	1.97	0.79
2:c:201:2AN:H16	2:c:201:2AN:C2	2.11	0.79
1:M:23:LEU:CD2	1:M:147:VAL:HG21	2.11	0.79
2:H:204:2AN:H12	2:H:204:2AN:H2	1.63	0.79
1:b:2:ALA:CB	1:a:4:TYR:CE1	2.64	0.79
2:I:205:2AN:H2	2:I:205:2AN:C12	2.09	0.79
1:E:92:LEU:O	1:E:93:ARG:C	2.24	0.79
1:W:5:THR:HA	1:W:118:VAL:O	1.82	0.79
1:j:63:HIS:ND1	1:j:64:PRO:HD2	1.96	0.79
1:j:144:TYR:O	1:j:144:TYR:CD1	2.35	0.79
1:N:4:TYR:CZ	1:M:2:ALA:HB2	2.18	0.79
1:G:45:ILE:CG1	1:G:54:VAL:HG22	2.12	0.79
1:U:9:GLU:HG2	1:U:115:LYS:HB2	1.64	0.79
1:F:47:GLY:HA3	1:F:53:THR:HA	1.64	0.79
2:j:201:2AN:H12	2:j:201:2AN:H2	1.63	0.79
1:f:139:LYS:HE2	2:f:202:2AN:C6	2.13	0.79
1:T:97:GLU:HB3	1:T:121:HIS:O	1.81	0.79
1:R:69:LEU:HD12	1:R:88:GLU:HB2	1.64	0.79
1:c:20:PHE:O	1:c:24:VAL:HG13	1.83	0.79
1:b:131:GLU:HG3	1:b:132:GLU:N	1.97	0.79
1:V:141:TYR:CE2	2:V:208:2AN:H7	2.18	0.79
1:I:149:GLU:OE2	1:I:149:GLU:C	2.26	0.79
2:b:204:2AN:O1	2:b:204:2AN:N	2.16	0.79
1:X:10:GLU:CB	2:X:206:2AN:H12	2.12	0.78
2:L:201:2AN:H2	2:L:201:2AN:H16	1.65	0.78
1:Y:120:TYR:CD2	1:Y:133:VAL:HG22	2.18	0.78
1:g:139:LYS:HE2	2:g:202:2AN:H4	1.60	0.78
2:N:204:2AN:H2	2:N:204:2AN:C16	2.13	0.78
1:d:53:THR:CG2	1:d:72:PHE:CD1	2.66	0.78
2:T:205:2AN:H16	2:T:205:2AN:H2	1.63	0.78
1:B:120:TYR:OH	2:B:201:2AN:H15	1.84	0.78
1:Q:69:LEU:CD2	1:Q:88:GLU:OE1	2.31	0.78
1:d:53:THR:CG2	1:d:72:PHE:CG	2.66	0.78
1:Z:138:LYS:NZ	2:Z:206:2AN:C8	2.47	0.78
1:Y:93:ARG:HH11	2:Y:204:2AN:H12	1.46	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:T:30:VAL:HG13	2:T:203:2AN:C4	2.13	0.78
1:V:95:ASN:HD21	1:V:129:ASN:ND2	1.81	0.78
1:A:72:PHE:CG	1:A:75:ILE:HD11	2.19	0.78
1:X:23:LEU:CD1	2:X:206:2AN:C3	2.61	0.78
2:V:208:2AN:H12	2:V:208:2AN:O3	1.82	0.78
2:G:203:2AN:S	2:G:203:2AN:N	2.45	0.77
1:Y:138:LYS:HE2	2:Y:201:2AN:C13	2.14	0.77
1:X:27:ARG:NH1	2:X:206:2AN:H6	1.99	0.77
1:V:129:ASN:HB2	1:V:132:GLU:HB2	1.65	0.77
1:V:144:TYR:CE2	2:V:203:2AN:H12	2.19	0.77
2:S:202:2AN:H16	2:S:202:2AN:C2	2.13	0.77
2:j:205:2AN:H16	2:j:205:2AN:C2	2.13	0.77
1:A:54:VAL:HA	1:A:71:LYS:HA	1.66	0.77
1:J:21:LYS:HD3	1:J:158:PHE:CD1	2.19	0.77
2:a:201:2AN:H16	2:a:201:2AN:C2	2.14	0.77
1:Y:93:ARG:NH1	2:Y:204:2AN:C12	2.46	0.77
1:P:138:LYS:NZ	4:P:205:EPE:C6	2.47	0.77
1:G:87:PHE:HA	1:G:98:LYS:HB3	1.65	0.77
2:H:204:2AN:O3	2:H:204:2AN:N	2.16	0.77
1:X:10:GLU:HB3	2:X:206:2AN:C12	2.15	0.77
1:A:109:GLY:O	1:i:80:PHE:CZ	2.37	0.77
2:V:205:2AN:S	2:V:205:2AN:N	2.57	0.77
1:T:95:ASN:HD22	1:T:95:ASN:H	1.32	0.77
1:F:60:VAL:HG23	1:F:63:HIS:HB2	1.67	0.77
2:I:205:2AN:H12	2:I:205:2AN:C2	2.15	0.77
1:X:80:PHE:HB3	1:X:105:LEU:HB2	1.66	0.77
1:K:106:GLU:OE2	1:K:113:LYS:HE3	1.85	0.77
1:E:96:ILE:HD11	1:E:132:GLU:OE1	1.84	0.77
1:S:89:GLY:O	1:S:92:LEU:HG	1.85	0.76
1:j:66:THR:HG22	1:j:67:TYR:HD2	1.50	0.76
1:j:96:ILE:CD1	1:j:128:VAL:HG12	2.14	0.76
1:j:137:GLU:CD	1:i:0:THR:HG23	2.08	0.76
2:X:205:2AN:H16	2:X:205:2AN:C2	2.13	0.76
1:J:4:TYR:CE1	1:I:2:ALA:CB	2.68	0.76
1:d:53:THR:HG22	1:d:72:PHE:CG	2.21	0.76
1:T:123:LYS:CB	1:T:124:PRO:HD2	2.15	0.76
1:U:11:GLU:HB2	1:U:113:LYS:HA	1.65	0.76
1:Q:67:TYR:CE2	1:Q:69:LEU:CD1	2.69	0.76
1:H:54:VAL:HG22	1:H:71:LYS:HG3	1.67	0.76
2:a:204:2AN:H12	2:a:204:2AN:C2	2.13	0.76
1:W:96:ILE:H	1:W:123:LYS:N	1.83	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:119:THR:HG22	1:R:121:HIS:NE2	2.01	0.76
1:P:65:LEU:HD13	1:P:91:VAL:HG12	1.68	0.76
1:N:32:VAL:HG13	1:N:39:PHE:O	1.86	0.76
1:L:70:HIS:HA	1:L:85:THR:O	1.85	0.76
1:G:46:GLU:HB2	1:G:54:VAL:HG13	1.67	0.76
2:c:206:2AN:H16	2:c:206:2AN:H2	1.67	0.76
1:h:10:GLU:HB3	2:h:202:2AN:C13	2.14	0.76
2:h:202:2AN:H16	2:h:202:2AN:C2	2.15	0.76
1:N:32:VAL:HG21	1:N:41:SER:HA	1.66	0.76
1:I:155:PRO:O	1:I:159:ALA:CB	2.32	0.76
2:G:203:2AN:H2	2:G:203:2AN:C16	2.09	0.76
2:G:203:2AN:N	2:G:203:2AN:O1	2.19	0.76
2:G:204:2AN:H16	2:G:204:2AN:H2	1.65	0.76
1:D:40:LYS:CB	1:D:59:PHE:O	2.34	0.76
2:B:206:2AN:H2	2:B:206:2AN:H12	1.66	0.76
1:A:55:THR:OG1	1:A:70:HIS:HB2	1.84	0.76
1:c:138:LYS:CD	2:c:202:2AN:H12	2.16	0.76
2:T:201:2AN:H16	2:T:201:2AN:C2	2.16	0.76
2:j:206:2AN:H16	2:j:206:2AN:H2	1.67	0.76
2:L:201:2AN:H2	2:L:201:2AN:C16	2.14	0.76
2:I:207:2AN:H2	2:I:207:2AN:C16	2.04	0.76
1:D:99:VAL:HG13	1:D:119:THR:O	1.84	0.76
2:f:204:2AN:N	2:f:204:2AN:S	2.54	0.76
2:f:206:2AN:C2	2:f:206:2AN:H12	2.16	0.76
1:W:89:GLY:O	1:W:92:LEU:HG	1.86	0.76
1:g:135:ILE:O	1:g:139:LYS:HG2	1.85	0.76
1:R:158:PHE:CE1	2:R:203:2AN:H13	2.20	0.76
1:Y:19:LEU:HD22	1:Y:23:LEU:HD22	1.67	0.76
1:V:47:GLY:HA2	2:V:201:2AN:C13	2.16	0.76
1:E:98:LYS:HE3	1:E:121:HIS:CE1	2.21	0.75
1:E:120:TYR:OH	1:E:136:GLY:HA3	1.85	0.75
1:f:33:LYS:HB3	2:f:205:2AN:O3	1.86	0.75
1:N:92:LEU:HD22	1:N:96:ILE:CG2	2.16	0.75
2:O:202:2AN:H12	2:O:202:2AN:H2	1.66	0.75
1:a:135:ILE:O	1:a:139:LYS:HG2	1.87	0.75
1:B:12:SER:HB3	1:B:144:TYR:OH	1.86	0.75
1:O:139:LYS:O	1:O:142:GLU:HG2	1.86	0.75
1:a:43:GLU:O	1:a:56:LYS:N	2.20	0.75
1:d:40:LYS:HD3	1:d:58:THR:HG21	1.67	0.75
2:X:206:2AN:C6	7:X:302:HOH:O	2.34	0.75
1:Z:10:GLU:CB	2:Z:203:2AN:H15	2.12	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:j:203:2AN:H2	2:j:203:2AN:C16	2.15	0.75
1:P:95:ASN:HA	1:P:126:CYS:HB2	1.68	0.74
2:L:201:2AN:H16	2:L:201:2AN:C2	2.17	0.74
1:T:95:ASN:H	1:T:95:ASN:ND2	1.83	0.74
1:F:84:TYR:OH	2:F:201:2AN:H4	1.86	0.74
2:I:207:2AN:H16	2:I:207:2AN:C2	2.10	0.74
1:H:1:MET:HA	1:H:1:MET:HE3	1.68	0.74
1:h:1:MET:O	1:h:1:MET:SD	2.44	0.74
2:c:206:2AN:H2	2:c:206:2AN:C16	2.16	0.74
1:E:95:ASN:O	1:E:96:ILE:HD13	1.87	0.74
1:S:94:ASP:O	1:S:123:LYS:HD2	1.86	0.74
1:O:32:VAL:O	1:O:33:LYS:C	2.30	0.74
1:G:23:LEU:N	1:G:23:LEU:HD23	2.02	0.74
1:V:142:GLU:OE2	2:V:208:2AN:C11	2.36	0.74
1:U:101:TYR:HD1	1:U:118:VAL:CG2	2.01	0.74
1:j:142:GLU:HG2	6:j:208:FLC:OB2	1.87	0.74
1:b:8:LYS:HE2	1:b:10:GLU:OE2	1.88	0.74
1:G:18:ARG:NH1	1:G:157:VAL:O	2.21	0.74
2:b:204:2AN:H2	2:b:204:2AN:C16	2.16	0.74
1:Z:138:LYS:HZ1	2:Z:206:2AN:C7	2.01	0.74
1:Q:67:TYR:HE2	1:Q:69:LEU:HD13	1.53	0.73
2:d:202:2AN:H16	2:d:202:2AN:H2	1.69	0.73
1:b:10:GLU:HB3	2:b:201:2AN:H13	1.70	0.73
1:G:70:HIS:CE1	1:G:86:LEU:HB2	2.23	0.73
1:U:57:ILE:O	1:U:67:TYR:CB	2.36	0.73
1:N:6:ILE:HG23	1:M:0:THR:HB	1.70	0.73
1:D:99:VAL:HA	1:D:119:THR:O	1.88	0.73
1:d:93:ARG:NH2	1:d:132:GLU:HB2	2.03	0.73
1:S:103:VAL:HG21	2:S:204:2AN:H6	1.70	0.73
1:K:139:LYS:O	1:K:142:GLU:HG2	1.88	0.73
2:H:201:2AN:H16	2:H:201:2AN:C2	2.18	0.73
1:U:9:GLU:CA	1:U:114:GLY:O	2.36	0.73
1:i:52:GLY:HA2	1:i:71:LYS:HE2	1.71	0.73
1:R:70:HIS:HA	1:R:85:THR:O	1.88	0.73
2:h:204:2AN:H2	2:h:204:2AN:C16	2.18	0.73
1:d:39:PHE:CE1	1:d:59:PHE:CE1	2.76	0.73
1:j:10:GLU:HB3	2:j:203:2AN:C13	2.19	0.73
2:j:206:2AN:N	2:j:206:2AN:O1	2.21	0.73
2:a:204:2AN:H2	2:a:204:2AN:C12	2.15	0.73
1:e:86:LEU:N	1:e:99:VAL:O	2.20	0.73
2:R:203:2AN:H12	2:R:203:2AN:H2	1.69	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:53:THR:HG22	1:J:72:PHE:HB2	1.69	0.73
1:X:123:LYS:HD3	1:X:124:PRO:CD	2.19	0.73
2:R:204:2AN:H12	2:R:204:2AN:C2	2.17	0.73
2:H:201:2AN:H2	2:H:201:2AN:C16	2.19	0.73
2:X:204:2AN:N	2:X:204:2AN:O2	2.22	0.73
2:V:205:2AN:C12	2:V:205:2AN:O3	2.37	0.73
1:C:92:LEU:HG	1:C:96:ILE:HG22	1.69	0.72
1:U:103:VAL:HG22	1:U:116:ILE:CG2	2.19	0.72
1:a:84:TYR:OH	2:a:204:2AN:C6	2.28	0.72
2:V:205:2AN:H16	2:V:208:2AN:O2	1.88	0.72
1:O:141:TYR:O	1:O:144:TYR:N	2.22	0.72
1:d:53:THR:HG22	1:d:72:PHE:HB2	1.70	0.72
1:X:23:LEU:HD12	2:X:206:2AN:C2	2.19	0.72
2:S:202:2AN:H16	2:S:202:2AN:H2	1.72	0.72
1:V:47:GLY:HA2	2:V:201:2AN:C12	2.18	0.72
1:V:141:TYR:HD2	2:V:208:2AN:C7	2.01	0.72
1:A:136:GLY:HA2	2:A:202:2AN:C14	2.20	0.72
1:U:23:LEU:O	1:U:27:ARG:HD2	1.89	0.72
2:F:204:2AN:H16	2:F:204:2AN:C2	2.17	0.72
2:C:202:2AN:H12	2:C:202:2AN:C2	2.19	0.72
1:e:6:ILE:HG22	1:e:118:VAL:HB	1.70	0.72
1:b:28:HIS:ND1	7:b:301:HOH:O	2.23	0.72
1:A:92:LEU:HD22	1:A:96:ILE:CD1	2.20	0.72
2:f:204:2AN:H16	2:f:204:2AN:C2	2.18	0.72
1:d:60:VAL:HG21	2:d:202:2AN:C14	2.20	0.72
1:X:14:ILE:HD11	1:X:152:ALA:HB2	1.70	0.72
1:U:103:VAL:CG1	1:U:116:ILE:HG22	2.18	0.72
1:A:109:GLY:O	1:i:80:PHE:HZ	1.71	0.72
2:J:201:2AN:H2	2:J:201:2AN:C16	2.04	0.72
1:a:84:TYR:CZ	2:a:204:2AN:H6	2.25	0.72
2:V:201:2AN:O2	2:V:201:2AN:N	2.20	0.72
1:B:120:TYR:OH	2:B:201:2AN:C14	2.38	0.72
1:J:17:HIS:CB	7:J:302:HOH:O	2.37	0.72
1:c:76:ASP:OD2	1:c:79:ASN:ND2	2.23	0.72
1:R:138:LYS:HE2	2:R:204:2AN:O2	1.90	0.72
2:G:203:2AN:N	2:G:203:2AN:O3	2.23	0.72
1:J:54:VAL:HA	1:J:70:HIS:O	1.88	0.71
1:f:35:GLN:NE2	1:f:146:GLN:HE22	1.88	0.71
1:X:23:LEU:HD11	2:X:206:2AN:C16	2.17	0.71
1:X:23:LEU:CD1	2:X:206:2AN:C16	2.63	0.71
1:X:91:VAL:HG23	1:X:92:LEU:HD12	1.72	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:W:96:ILE:CG2	1:W:121:HIS:O	2.33	0.71
1:R:96:ILE:HG23	1:R:121:HIS:O	1.90	0.71
1:B:44:ILE:N	1:B:44:ILE:HD12	2.05	0.71
1:M:23:LEU:HD23	1:M:147:VAL:HG21	1.72	0.71
1:W:85:THR:OG1	1:W:100:VAL:HG22	1.90	0.71
1:W:95:ASN:HA	1:W:123:LYS:CB	2.20	0.71
1:T:14:ILE:HD11	1:T:152:ALA:HB2	1.72	0.71
1:O:123:LYS:HG2	1:O:124:PRO:HD2	1.72	0.71
1:N:54:VAL:HA	1:N:70:HIS:O	1.91	0.71
2:L:204:2AN:H13	1:Z:47:GLY:HA2	1.71	0.71
1:G:80:PHE:HB2	1:G:105:LEU:O	1.90	0.71
1:a:26:GLU:O	1:a:30:VAL:HG13	1.91	0.71
1:X:20:PHE:HB2	1:X:105:LEU:HD12	1.70	0.71
2:T:201:2AN:S	2:T:201:2AN:N	2.62	0.71
1:S:6:ILE:HD12	1:S:118:VAL:O	1.90	0.71
2:B:202:2AN:O3	2:B:202:2AN:N	2.24	0.71
1:A:18:ARG:NH2	1:A:151:LEU:O	2.24	0.71
2:P:201:2AN:H16	2:P:201:2AN:C2	2.21	0.71
1:C:26:GLU:OE1	1:C:29:GLN:NE2	2.22	0.71
1:X:10:GLU:HG2	2:X:206:2AN:C13	2.18	0.71
2:j:201:2AN:H2	2:j:201:2AN:C12	2.18	0.71
1:d:75:ILE:HD12	1:d:75:ILE:O	1.91	0.71
2:K:202:2AN:N	2:K:202:2AN:O1	2.23	0.71
2:j:203:2AN:H16	2:j:203:2AN:H2	1.71	0.71
2:g:202:2AN:H16	2:g:202:2AN:C2	2.20	0.71
2:P:204:2AN:C2	2:P:204:2AN:C16	2.63	0.71
1:U:154:ASN:HB3	1:U:157:VAL:HG23	1.71	0.71
1:A:92:LEU:HD22	1:A:96:ILE:HD12	1.73	0.71
2:I:206:2AN:H16	2:I:206:2AN:C2	2.21	0.71
1:F:158:PHE:CZ	2:F:203:2AN:H13	2.25	0.71
2:D:202:2AN:H16	2:D:202:2AN:C2	2.21	0.71
1:b:10:GLU:CB	2:b:201:2AN:C13	2.69	0.71
2:V:205:2AN:N	2:V:205:2AN:O3	2.23	0.71
1:F:139:LYS:O	2:F:202:2AN:C7	2.38	0.70
1:X:10:GLU:HB2	2:X:206:2AN:H12	1.72	0.70
1:N:92:LEU:HD22	1:N:96:ILE:CB	2.21	0.70
2:F:206:2AN:H4	1:f:17:HIS:HB2	1.74	0.70
1:D:57:ILE:O	1:D:67:TYR:CA	2.37	0.70
1:Q:57:ILE:O	1:Q:67:TYR:HA	1.90	0.70
1:H:59:PHE:HD1	1:H:66:THR:O	1.73	0.70
1:F:140:ALA:CB	2:F:202:2AN:O3	2.39	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:V:23:LEU:O	1:V:27:ARG:HD2	1.90	0.70
1:j:47:GLY:HA2	2:j:201:2AN:C16	2.19	0.70
1:j:129:ASN:CG	1:j:132:GLU:HB2	2.16	0.70
2:R:202:2AN:C2	2:R:202:2AN:H12	2.22	0.70
1:P:51:VAL:HG13	1:P:73:ASP:O	1.91	0.70
1:H:138:LYS:HE2	1:G:-1:PHE:CZ	2.24	0.70
1:U:105:LEU:CD2	1:U:114:GLY:HA2	2.22	0.70
2:S:202:2AN:H2	2:S:202:2AN:C16	2.22	0.70
2:j:206:2AN:N	2:j:206:2AN:S	2.55	0.70
2:h:206:2AN:C16	7:h:307:HOH:O	2.38	0.70
2:B:203:2AN:H16	2:B:203:2AN:C2	2.03	0.70
1:c:21:LYS:HG2	1:c:158:PHE:CD1	2.26	0.70
2:T:201:2AN:H2	2:T:201:2AN:C16	2.20	0.70
2:B:206:2AN:S	2:B:206:2AN:N	2.64	0.70
1:A:16:PRO:HD2	3:A:205:SO4:O4	1.92	0.70
1:N:60:VAL:HG22	1:N:63:HIS:HB2	1.74	0.70
1:L:27:ARG:O	1:L:30:VAL:N	2.24	0.70
1:D:142:GLU:HA	2:D:204:2AN:H2	1.74	0.70
1:d:27:ARG:NE	2:d:204:2AN:O1	2.25	0.70
1:d:40:LYS:HB3	1:d:58:THR:HG22	1.72	0.70
1:Y:71:LYS:N	1:Y:85:THR:O	2.24	0.70
1:j:116:ILE:N	1:j:116:ILE:HD12	2.06	0.70
1:A:93:ARG:O	1:A:94:ASP:HB2	1.92	0.70
2:F:204:2AN:O3	2:F:204:2AN:N	2.25	0.70
1:U:141:TYR:O	1:U:144:TYR:N	2.24	0.70
2:g:203:2AN:H16	2:g:203:2AN:C2	2.19	0.70
1:P:6:ILE:HG23	1:O:1:MET:CB	2.21	0.70
2:Z:205:2AN:H16	2:Z:205:2AN:H2	1.72	0.70
1:U:105:LEU:HD22	1:U:113:LYS:O	1.92	0.70
2:i:201:2AN:H2	2:i:201:2AN:H12	1.74	0.70
1:d:46:GLU:O	1:d:53:THR:HA	1.91	0.70
1:c:66:THR:HB	1:c:90:ASP:OD2	1.92	0.70
1:Z:129:ASN:CB	1:Z:131:GLU:OE1	2.40	0.70
1:j:33:LYS:C	2:j:204:2AN:O3	2.35	0.70
1:j:122:PRO:HB3	1:j:128:VAL:HG13	1.73	0.70
1:h:141:TYR:O	1:h:145:LYS:HG2	1.91	0.70
2:Q:202:2AN:H2	2:Q:202:2AN:C12	2.22	0.69
1:K:57:ILE:O	1:K:67:TYR:HA	1.91	0.69
1:D:158:PHE:CZ	2:D:203:2AN:C15	2.73	0.69
1:a:84:TYR:HH	2:a:204:2AN:H6	1.57	0.69
2:Z:203:2AN:H12	2:Z:203:2AN:H2	1.73	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:129:ASN:HD22	1:S:131:GLU:CG	2.03	0.69
2:P:204:2AN:C16	2:P:204:2AN:H2	2.22	0.69
1:N:150:TYR:CE1	1:N:154:ASN:OD1	2.45	0.69
1:L:87:PHE:O	1:L:88:GLU:HG3	1.92	0.69
1:j:141:TYR:HD2	6:j:208:FLC:CA	2.06	0.69
1:D:69:LEU:O	1:D:86:LEU:HA	1.93	0.69
1:C:51:VAL:CG1	1:C:75:ILE:HG13	2.22	0.69
1:Z:19:LEU:HD13	1:Z:23:LEU:CD1	2.23	0.69
2:R:201:2AN:O3	2:R:201:2AN:N	2.26	0.69
1:G:18:ARG:NH2	1:G:151:LEU:O	2.26	0.69
1:b:46:GLU:HB2	1:b:54:VAL:HB	1.72	0.69
1:U:68:MET:HG2	1:U:91:VAL:CG1	2.21	0.69
1:E:9:GLU:HG2	1:E:115:LYS:HG2	1.72	0.69
2:Y:203:2AN:H2	2:Y:203:2AN:H12	1.73	0.69
1:V:43:GLU:OE2	1:V:45:ILE:HG22	1.92	0.69
2:d:201:2AN:H12	2:d:201:2AN:C2	2.18	0.69
1:X:123:LYS:CG	1:X:124:PRO:HD3	2.23	0.69
1:B:18:ARG:NH1	1:B:151:LEU:O	2.25	0.69
1:J:76:ASP:OD1	1:J:78:ALA:HB3	1.92	0.69
1:c:45:ILE:HD12	1:c:46:GLU:HB2	1.73	0.69
2:a:202:2AN:H2	2:a:202:2AN:H12	1.75	0.69
2:B:206:2AN:H12	2:B:206:2AN:C2	2.22	0.69
1:R:150:TYR:CE1	1:R:154:ASN:ND2	2.61	0.69
2:Q:202:2AN:H12	2:Q:202:2AN:C2	2.22	0.69
1:P:131:GLU:O	1:P:135:ILE:HG13	1.93	0.69
1:H:49:GLY:N	1:H:53:THR:OG1	2.25	0.69
1:D:6:ILE:HD11	1:C:0:THR:HG21	1.75	0.69
2:b:206:2AN:C11	2:b:206:2AN:O3	2.41	0.69
1:V:142:GLU:HG2	2:V:208:2AN:C12	2.23	0.69
1:h:129:ASN:OD1	1:h:129:ASN:N	2.19	0.69
1:N:108:VAL:O	1:N:109:GLY:C	2.33	0.69
2:b:205:2AN:H16	2:b:205:2AN:C2	2.22	0.69
1:V:144:TYR:CD1	1:V:144:TYR:O	2.46	0.69
2:j:203:2AN:C2	2:j:203:2AN:C16	2.64	0.69
1:B:155:PRO:O	1:B:159:ALA:HB2	1.92	0.69
1:H:95:ASN:OD1	1:H:95:ASN:N	2.18	0.69
1:C:51:VAL:HG12	1:C:75:ILE:HG13	1.74	0.69
1:Y:93:ARG:CZ	2:Y:204:2AN:H2	2.23	0.69
2:V:204:2AN:H2	2:V:204:2AN:C16	2.23	0.69
2:B:205:2AN:C2	2:B:205:2AN:H12	2.23	0.68
1:A:123:LYS:HG2	1:A:124:PRO:CD	2.22	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:21:LYS:HE2	1:R:158:PHE:CD1	2.28	0.68
1:O:129:ASN:O	1:O:132:GLU:HG2	1.93	0.68
1:K:18:ARG:NH1	1:K:151:LEU:O	2.26	0.68
1:J:4:TYR:CZ	1:I:2:ALA:HB2	2.27	0.68
2:X:204:2AN:H2	2:X:204:2AN:C16	2.21	0.68
1:V:141:TYR:CD2	2:V:208:2AN:H7	2.28	0.68
1:L:102:GLU:HB3	1:L:117:THR:HB	1.75	0.68
2:D:201:2AN:H16	2:D:201:2AN:C2	2.20	0.68
2:D:201:2AN:H2	2:D:201:2AN:C16	2.19	0.68
1:Y:138:LYS:CE	2:Y:201:2AN:C12	2.59	0.68
1:X:65:LEU:HA	1:X:90:ASP:OD2	1.93	0.68
1:L:65:LEU:HD13	1:L:91:VAL:HB	1.74	0.68
1:K:142:GLU:HG3	1:K:143:PHE:N	2.07	0.68
1:I:16:PRO:HD3	1:I:111:GLY:O	1.92	0.68
1:H:134:LYS:O	1:H:138:LYS:CG	2.36	0.68
1:f:143:PHE:HA	1:f:146:GLN:HE21	1.59	0.68
2:c:203:2AN:H16	2:c:203:2AN:H2	1.74	0.68
2:N:203:2AN:O3	2:N:203:2AN:N	2.27	0.68
2:I:204:2AN:H16	2:I:204:2AN:H2	1.75	0.68
1:D:119:THR:HG22	1:D:121:HIS:CD2	2.28	0.68
2:D:204:2AN:C10	2:D:204:2AN:H16	2.23	0.68
2:d:202:2AN:H16	2:d:202:2AN:C2	2.21	0.68
1:U:8:LYS:O	1:U:115:LYS:HA	1.94	0.68
2:T:205:2AN:H2	2:T:205:2AN:C16	2.22	0.68
1:j:141:TYR:CD2	6:j:208:FLC:HA1	2.27	0.68
1:X:10:GLU:OE1	1:X:10:GLU:HA	1.94	0.68
2:X:205:2AN:H2	2:X:205:2AN:C16	2.20	0.68
1:J:86:LEU:HD21	1:J:91:VAL:HG11	1.76	0.68
1:b:10:GLU:HB3	2:b:201:2AN:C13	2.24	0.68
2:B:204:2AN:H16	2:B:204:2AN:H2	1.75	0.68
1:E:69:LEU:O	1:E:86:LEU:HD12	1.92	0.68
1:f:89:GLY:O	1:f:92:LEU:HB2	1.93	0.68
1:Y:1:MET:CE	1:Y:4:TYR:HA	2.24	0.68
1:S:27:ARG:HH12	2:S:204:2AN:C8	2.02	0.68
1:N:57:ILE:O	1:N:68:MET:N	2.27	0.68
1:L:77:ALA:HB3	2:L:204:2AN:C16	2.24	0.68
1:H:77:ALA:O	2:H:204:2AN:C3	2.41	0.68
1:U:9:GLU:HG2	1:U:115:LYS:CB	2.24	0.68
1:S:129:ASN:OD1	1:S:129:ASN:N	2.22	0.68
2:j:201:2AN:H12	2:j:201:2AN:C2	2.23	0.68
1:A:105:LEU:HD23	1:A:114:GLY:HA2	1.76	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:129:ASN:N	1:O:132:GLU:OE2	2.27	0.68
1:b:91:VAL:HG21	2:b:202:2AN:C13	2.24	0.68
2:V:201:2AN:H2	2:V:201:2AN:C16	2.24	0.68
2:V:205:2AN:H16	2:V:205:2AN:C2	2.24	0.68
2:j:205:2AN:O3	2:j:205:2AN:C11	2.42	0.68
1:A:21:LYS:HE2	1:A:158:PHE:CE1	2.29	0.67
1:M:23:LEU:HD21	1:M:147:VAL:HG21	1.75	0.67
1:G:17:HIS:HA	1:G:80:PHE:HE1	1.59	0.67
2:b:203:2AN:H12	2:b:203:2AN:H2	1.75	0.67
2:h:204:2AN:N	2:h:204:2AN:O2	2.27	0.67
2:Q:203:2AN:H16	2:Q:203:2AN:C2	2.24	0.67
1:E:98:LYS:HE2	1:E:121:HIS:CD2	2.28	0.67
2:f:201:2AN:C16	2:f:201:2AN:C2	2.70	0.67
2:f:204:2AN:O3	2:f:204:2AN:C11	2.41	0.67
2:i:201:2AN:H12	2:i:201:2AN:C2	2.23	0.67
1:A:155:PRO:O	1:A:159:ALA:HB3	1.94	0.67
2:A:202:2AN:C2	2:A:202:2AN:H12	2.24	0.67
1:O:101:TYR:HE1	2:O:201:2AN:H14	1.60	0.67
2:f:206:2AN:H12	2:f:206:2AN:H2	1.75	0.67
1:c:148:GLU:O	1:c:149:GLU:C	2.36	0.67
1:Z:138:LYS:HE3	1:Z:142:GLU:OE2	1.93	0.67
1:Y:38:VAL:O	1:Y:59:PHE:CD2	2.47	0.67
1:g:13:PRO:HD2	1:g:148:GLU:OE2	1.93	0.67
1:M:95:ASN:ND2	1:M:128:VAL:HA	2.10	0.67
1:L:134:LYS:HE3	1:K:-1:PHE:CE2	2.30	0.67
1:H:131:GLU:O	1:H:135:ILE:HG13	1.94	0.67
1:F:5:THR:HG21	1:E:5:THR:HB	1.76	0.67
2:f:202:2AN:H12	2:f:202:2AN:C2	2.24	0.67
1:X:116:ILE:HD13	2:X:206:2AN:O2	1.95	0.67
1:W:96:ILE:HA	1:W:121:HIS:O	1.95	0.67
1:A:14:ILE:HG22	1:A:18:ARG:HB2	1.74	0.67
1:O:70:HIS:HB2	7:O:302:HOH:O	1.94	0.67
1:V:144:TYR:CD1	1:V:144:TYR:C	2.72	0.67
1:S:131:GLU:HG3	1:S:132:GLU:N	2.08	0.67
1:j:129:ASN:HB2	1:j:131:GLU:HG2	1.77	0.67
2:R:203:2AN:O1	2:R:203:2AN:H16	1.95	0.67
2:N:202:2AN:C2	2:N:202:2AN:C16	2.68	0.67
1:M:59:PHE:CZ	1:M:68:MET:HE2	2.29	0.67
1:M:95:ASN:HD22	1:M:128:VAL:HA	1.59	0.67
1:K:83:LYS:HA	1:K:101:TYR:O	1.94	0.67
1:K:101:TYR:CE2	2:K:202:2AN:H14	2.30	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:16:PRO:HG2	1:a:107:ALA:HB2	1.77	0.67
1:Z:66:THR:N	1:Z:90:ASP:OD2	2.28	0.67
1:A:47:GLY:HA3	1:A:53:THR:HG22	1.77	0.67
1:M:96:ILE:HD13	1:M:128:VAL:HG22	1.77	0.67
1:I:135:ILE:O	1:I:139:LYS:HG2	1.94	0.67
2:I:203:2AN:H16	2:I:203:2AN:C2	2.24	0.67
1:b:18:ARG:HG2	1:b:158:PHE:O	1.94	0.67
1:a:30:VAL:HG23	1:a:143:PHE:CZ	2.29	0.67
1:A:51:VAL:HG13	1:A:73:ASP:O	1.95	0.67
2:c:201:2AN:C2	2:c:201:2AN:C16	2.65	0.67
1:a:141:TYR:HD1	2:a:204:2AN:C14	2.07	0.67
2:V:203:2AN:H16	2:V:203:2AN:C2	2.25	0.67
1:A:68:MET:HE3	1:A:91:VAL:HG21	1.76	0.67
1:I:149:GLU:OE2	1:I:149:GLU:O	2.13	0.67
1:d:10:GLU:HB3	2:d:201:2AN:C15	2.25	0.67
2:A:201:2AN:H2	2:A:201:2AN:C16	2.26	0.66
2:F:205:2AN:N	2:F:205:2AN:S	2.65	0.66
1:j:8:LYS:NZ	2:j:203:2AN:O2	2.28	0.66
1:c:138:LYS:CD	2:c:202:2AN:C12	2.72	0.66
1:Y:120:TYR:CE2	1:Y:133:VAL:HG22	2.29	0.66
1:W:96:ILE:H	1:W:123:LYS:CB	2.08	0.66
1:W:98:LYS:HG3	1:W:98:LYS:O	1.95	0.66
2:V:205:2AN:O3	2:V:205:2AN:C11	2.43	0.66
2:V:206:2AN:N	2:V:206:2AN:O1	2.26	0.66
1:U:54:VAL:HA	1:U:70:HIS:O	1.94	0.66
1:A:85:THR:CB	1:A:100:VAL:HA	2.26	0.66
2:F:206:2AN:H12	1:D:109:GLY:CA	2.25	0.66
1:K:101:TYR:HE2	2:K:202:2AN:C14	2.09	0.66
1:F:44:ILE:HA	1:F:54:VAL:O	1.95	0.66
1:E:16:PRO:O	1:E:18:ARG:N	2.28	0.66
1:X:35:GLN:NE2	1:X:146:GLN:OE1	2.29	0.66
1:j:40:LYS:HD2	1:j:60:VAL:HA	1.77	0.66
1:A:70:HIS:NE2	7:A:302:HOH:O	2.22	0.66
1:L:97:GLU:HB2	1:L:123:LYS:HG3	1.77	0.66
1:I:16:PRO:HG3	1:I:112:SER:HB3	1.78	0.66
1:H:35:GLN:NE2	1:H:39:PHE:HE2	1.93	0.66
2:h:202:2AN:H2	2:h:202:2AN:C16	2.25	0.66
1:A:122:PRO:HG2	7:A:306:HOH:O	1.96	0.66
1:O:123:LYS:HG2	1:O:124:PRO:CD	2.26	0.66
2:F:203:2AN:S	2:F:203:2AN:N	2.65	0.66
1:D:27:ARG:O	1:D:30:VAL:N	2.28	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:b:91:VAL:HG21	2:b:202:2AN:C12	2.26	0.66
1:U:10:GLU:N	1:U:114:GLY:O	2.29	0.66
1:S:90:ASP:OD1	1:S:90:ASP:N	2.20	0.66
1:P:6:ILE:HG23	1:O:1:MET:HB2	1.76	0.66
1:T:30:VAL:O	1:T:31:LEU:C	2.39	0.66
1:N:97:GLU:N	1:N:121:HIS:O	2.27	0.66
1:J:153:ALA:O	1:J:155:PRO:HD3	1.96	0.66
1:I:63:HIS:CE1	2:I:205:2AN:H15	2.30	0.66
1:G:158:PHE:CZ	2:G:204:2AN:H15	2.31	0.66
2:D:203:2AN:O2	2:D:203:2AN:N	2.23	0.66
2:e:201:2AN:C2	2:e:201:2AN:H16	2.26	0.66
2:d:201:2AN:H2	2:d:201:2AN:C12	2.20	0.66
1:V:107:ALA:HB1	7:V:302:HOH:O	1.96	0.66
1:T:4:TYR:CE1	1:T:128:VAL:CB	2.79	0.66
1:I:63:HIS:CE1	2:I:205:2AN:C15	2.79	0.66
2:f:204:2AN:H16	2:f:204:2AN:H2	1.77	0.66
1:X:123:LYS:CD	1:X:124:PRO:HD3	2.25	0.66
2:U:201:2AN:H16	2:U:201:2AN:C2	2.19	0.66
1:i:27:ARG:O	1:i:31:LEU:HG	1.96	0.66
1:A:92:LEU:HA	1:A:96:ILE:HD11	1.78	0.66
1:K:116:ILE:HD13	2:K:202:2AN:C9	2.26	0.66
2:J:201:2AN:N	2:J:201:2AN:O1	2.28	0.66
1:X:63:HIS:ND1	1:X:64:PRO:HD2	2.11	0.66
1:P:54:VAL:HG22	1:P:71:LYS:HB2	1.78	0.65
1:K:46:GLU:HB3	1:K:54:VAL:HG23	1.78	0.65
1:G:106:GLU:N	1:G:106:GLU:OE2	2.29	0.65
2:f:201:2AN:C16	2:f:201:2AN:H2	2.24	0.65
2:T:203:2AN:S	2:T:203:2AN:N	2.66	0.65
1:g:23:LEU:O	1:g:27:ARG:NH1	2.28	0.65
1:M:98:LYS:HE2	1:M:121:HIS:CG	2.32	0.65
2:F:205:2AN:H16	2:F:205:2AN:H2	1.79	0.65
1:D:57:ILE:HD13	1:D:68:MET:HB2	1.79	0.65
1:e:87:PHE:O	1:e:87:PHE:CD1	2.49	0.65
1:e:87:PHE:O	1:e:87:PHE:HD1	1.78	0.65
2:a:202:2AN:H12	2:a:202:2AN:C2	2.25	0.65
2:Z:205:2AN:N	2:Z:205:2AN:O1	2.28	0.65
1:X:3:ALA:O	1:W:4:TYR:HA	1.95	0.65
1:P:138:LYS:HZ3	4:P:205:EPE:C6	2.02	0.65
2:K:201:2AN:O3	2:K:201:2AN:N	2.20	0.65
1:C:36:PRO:HD2	7:C:303:HOH:O	1.96	0.65
2:N:201:2AN:O3	2:N:201:2AN:N	2.30	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:202:2AN:N	2:J:202:2AN:S	2.54	0.65
1:d:54:VAL:HA	1:d:70:HIS:O	1.96	0.65
1:c:70:HIS:HA	1:c:85:THR:O	1.96	0.65
1:Q:69:LEU:HB2	1:Q:88:GLU:HB3	1.79	0.65
1:J:69:LEU:CB	1:J:88:GLU:HB3	2.26	0.65
1:Y:38:VAL:O	1:Y:59:PHE:HD2	1.79	0.65
1:S:66:THR:N	1:S:90:ASP:OD2	2.30	0.65
1:S:116:ILE:CG1	2:S:204:2AN:C3	2.62	0.65
1:B:131:GLU:O	1:B:135:ILE:HG13	1.96	0.65
1:L:120:TYR:CD2	1:L:133:VAL:HG22	2.32	0.65
1:D:10:GLU:HG3	2:D:201:2AN:H13	1.79	0.65
1:f:69:LEU:HD12	1:f:88:GLU:HB3	1.78	0.65
1:e:27:ARG:O	1:e:31:LEU:HG	1.97	0.65
1:d:14:ILE:O	1:d:111:GLY:HA2	1.97	0.65
1:Z:65:LEU:HA	1:Z:90:ASP:OD2	1.96	0.65
1:e:85:THR:HG23	1:e:100:VAL:HG23	1.79	0.65
2:A:203:2AN:H16	2:A:203:2AN:C2	2.26	0.65
1:P:63:HIS:CE1	1:P:65:LEU:HB2	2.31	0.65
1:H:4:TYR:CE1	1:G:2:ALA:CB	2.80	0.65
2:H:203:2AN:N	2:H:203:2AN:O2	2.25	0.65
1:X:54:VAL:HA	1:X:70:HIS:O	1.97	0.65
1:F:138:LYS:HE2	2:F:204:2AN:O1	1.96	0.65
2:E:204:2AN:C2	2:E:204:2AN:C16	2.65	0.65
1:D:4:TYR:OH	1:C:2:ALA:CB	2.45	0.65
1:Z:123:LYS:CB	1:Z:124:PRO:CD	2.74	0.65
1:W:3:ALA:HB1	1:W:120:TYR:O	1.97	0.65
1:i:79:ASN:O	1:i:104:LYS:NZ	2.24	0.65
1:M:57:ILE:HB	1:M:68:MET:HB2	1.78	0.65
1:I:158:PHE:CZ	2:I:207:2AN:H7	2.32	0.65
2:G:202:2AN:C2	2:G:202:2AN:H12	2.26	0.65
2:j:207:2AN:H16	2:j:207:2AN:C2	2.26	0.65
1:A:107:ALA:HB2	1:i:107:ALA:CB	2.27	0.64
2:N:201:2AN:N	2:N:201:2AN:S	2.61	0.64
1:d:51:VAL:H	1:d:75:ILE:HG12	1.62	0.64
1:X:44:ILE:HD11	1:X:53:THR:CG2	2.22	0.64
2:j:206:2AN:N	2:j:206:2AN:O2	2.30	0.64
1:G:139:LYS:HE2	1:G:139:LYS:HA	1.78	0.64
1:F:140:ALA:N	2:F:202:2AN:H8	2.12	0.64
2:f:201:2AN:C2	2:f:201:2AN:H16	2.25	0.64
2:c:206:2AN:C2	2:c:206:2AN:C16	2.67	0.64
1:a:46:GLU:HB2	1:a:54:VAL:HB	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Z:68:MET:O	1:Z:69:LEU:HD23	1.97	0.64
1:X:23:LEU:CB	2:X:206:2AN:C3	2.70	0.64
1:h:50:GLY:C	1:h:75:ILE:HD12	2.22	0.64
1:B:75:ILE:HG22	1:B:76:ASP:H	1.61	0.64
1:J:-3:ASP:O	1:I:134:LYS:HE2	1.97	0.64
1:F:139:LYS:CA	2:F:202:2AN:C7	2.75	0.64
1:b:10:GLU:HB2	2:b:201:2AN:C13	2.27	0.64
1:N:6:ILE:HG21	1:M:0:THR:HB	1.80	0.64
1:G:63:HIS:HE1	1:G:65:LEU:HD12	1.62	0.64
1:Y:140:ALA:O	1:Y:143:PHE:HB3	1.97	0.64
2:j:205:2AN:C2	2:j:205:2AN:C16	2.74	0.64
1:i:45:ILE:HG21	1:i:56:LYS:HD3	1.79	0.64
1:A:85:THR:CB	1:A:99:VAL:O	2.45	0.64
1:P:125:GLY:O	1:P:126:CYS:SG	2.55	0.64
1:J:-3:ASP:N	1:J:-2:PRO:CD	2.60	0.64
1:c:18:ARG:NE	1:c:157:VAL:O	2.28	0.64
1:S:8:LYS:HG3	2:S:204:2AN:H14	1.79	0.64
1:Q:4:TYR:CE1	1:Q:128:VAL:HB	2.32	0.64
1:I:2:ALA:O	1:I:122:PRO:HG3	1.97	0.64
1:e:6:ILE:O	1:e:117:THR:HA	1.98	0.64
1:B:31:LEU:HD23	1:B:143:PHE:CE1	2.32	0.64
1:N:105:LEU:HD22	2:N:201:2AN:H15	1.79	0.64
2:F:203:2AN:H16	2:F:203:2AN:C2	2.11	0.64
1:D:53:THR:HG22	1:D:54:VAL:O	1.98	0.64
1:C:57:ILE:O	1:C:67:TYR:HA	1.98	0.64
1:c:8:LYS:NZ	3:c:207:SO4:O1	2.30	0.64
1:h:43:GLU:HG3	1:h:45:ILE:HG23	1.80	0.64
1:I:143:PHE:O	1:I:146:GLN:HB2	1.98	0.64
2:H:202:2AN:H16	2:H:202:2AN:C2	2.27	0.64
1:W:96:ILE:N	1:W:123:LYS:CB	2.60	0.64
1:S:129:ASN:ND2	1:S:131:GLU:CG	2.60	0.64
1:R:141:TYR:CD2	2:R:204:2AN:H4	2.32	0.64
1:O:75:ILE:HG12	1:O:82:CYS:SG	2.38	0.64
1:O:101:TYR:CE1	2:O:201:2AN:H14	2.33	0.64
2:K:203:2AN:H12	2:K:203:2AN:C2	2.26	0.64
1:Y:91:VAL:HG21	2:Y:203:2AN:C13	2.27	0.64
1:g:150:TYR:O	1:g:154:ASN:ND2	2.30	0.64
1:X:23:LEU:HD13	2:X:206:2AN:H16	1.76	0.64
1:K:122:PRO:HG3	1:K:128:VAL:HG23	1.79	0.63
1:G:57:ILE:O	1:G:67:TYR:HA	1.97	0.63
1:F:140:ALA:N	2:F:202:2AN:C8	2.61	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:b:91:VAL:CG2	2:b:202:2AN:C13	2.76	0.63
1:Z:19:LEU:CD1	1:Z:23:LEU:CD1	2.74	0.63
1:T:57:ILE:HD12	1:T:68:MET:HE3	1.79	0.63
1:S:93:ARG:HG2	2:S:201:2AN:H4	1.80	0.63
1:h:18:ARG:NE	1:h:157:VAL:O	2.25	0.63
1:R:60:VAL:HG22	1:R:63:HIS:HB2	1.80	0.63
1:R:139:LYS:HE3	2:R:205:2AN:H3	1.77	0.63
1:D:97:GLU:HA	1:D:123:LYS:HE2	1.80	0.63
2:Z:205:2AN:N	2:Z:205:2AN:O3	2.29	0.63
1:Y:93:ARG:NH1	2:Y:204:2AN:H12	2.12	0.63
1:V:129:ASN:HB2	1:V:132:GLU:HB3	1.78	0.63
1:T:46:GLU:HG3	1:T:54:VAL:HB	1.80	0.63
1:h:33:LYS:NZ	2:h:204:2AN:C12	2.61	0.63
1:N:131:GLU:O	1:N:135:ILE:HG13	1.98	0.63
1:J:105:LEU:CD2	2:J:202:2AN:H15	2.27	0.63
2:F:204:2AN:H2	2:F:204:2AN:C16	2.14	0.63
1:Z:141:TYR:OH	2:Z:206:2AN:H15	1.99	0.63
1:X:80:PHE:CB	1:X:105:LEU:HB2	2.27	0.63
1:F:81:TYR:CD1	1:F:81:TYR:C	2.76	0.63
2:E:203:2AN:H16	2:E:203:2AN:H2	1.80	0.63
1:U:108:VAL:CG2	1:U:113:LYS:HE2	2.29	0.63
1:S:120:TYR:CE1	1:S:133:VAL:HG22	2.34	0.63
1:K:31:LEU:HD12	1:K:57:ILE:HD13	1.80	0.63
2:I:203:2AN:H12	1:Y:46:GLU:HG2	1.80	0.63
1:d:1:MET:SD	1:d:1:MET:N	2.67	0.63
2:b:202:2AN:H12	2:b:202:2AN:H2	1.80	0.63
1:V:10:GLU:CD	1:V:141:TYR:HE1	2.06	0.63
2:V:203:2AN:H16	2:V:203:2AN:H2	1.80	0.63
1:U:101:TYR:CD1	1:U:118:VAL:HG22	2.28	0.63
1:j:129:ASN:HD21	1:j:132:GLU:HB2	1.61	0.63
1:F:87:PHE:O	1:F:92:LEU:HD11	1.98	0.63
1:a:35:GLN:HB2	1:a:39:PHE:HE1	1.63	0.63
1:X:96:ILE:HD11	1:X:128:VAL:CB	2.29	0.63
1:W:13:PRO:HD2	1:W:148:GLU:OE2	1.98	0.63
2:V:203:2AN:H2	2:V:203:2AN:C16	2.26	0.63
1:U:100:VAL:O	1:U:118:VAL:HA	1.97	0.63
1:i:57:ILE:O	1:i:67:TYR:HB2	1.99	0.63
1:Q:59:PHE:CZ	1:Q:68:MET:HE2	2.33	0.63
1:O:80:PHE:CB	1:O:105:LEU:HD12	2.29	0.63
1:F:87:PHE:C	1:F:92:LEU:HD11	2.24	0.63
2:F:201:2AN:H2	2:F:201:2AN:C16	2.24	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:141:TYR:O	1:U:144:TYR:HB3	1.99	0.63
1:U:145:LYS:O	1:U:146:GLN:C	2.42	0.63
2:S:202:2AN:C2	2:S:202:2AN:C16	2.73	0.63
1:O:142:GLU:HG3	1:O:143:PHE:N	2.13	0.63
2:O:203:2AN:H16	2:O:203:2AN:C2	2.28	0.63
2:M:203:2AN:C2	2:M:203:2AN:C16	2.68	0.63
1:H:68:MET:HB3	1:H:70:HIS:HE1	1.63	0.63
1:G:18:ARG:HH21	1:G:151:LEU:CA	2.11	0.63
1:h:33:LYS:CE	2:h:204:2AN:O3	2.47	0.63
2:F:206:2AN:H12	1:D:109:GLY:HA3	1.80	0.63
1:D:140:ALA:HB1	2:D:201:2AN:C8	2.29	0.63
1:Z:138:LYS:HZ1	2:Z:206:2AN:H7	1.63	0.63
1:X:27:ARG:NH1	2:X:206:2AN:C6	2.62	0.63
1:S:27:ARG:CZ	2:S:204:2AN:H8	2.22	0.63
1:P:31:LEU:CD1	1:P:57:ILE:HD13	2.29	0.62
1:D:92:LEU:HA	1:D:96:ILE:HB	1.81	0.62
1:b:33:LYS:HB3	2:b:204:2AN:O3	1.98	0.62
1:Z:138:LYS:HZ3	2:Z:206:2AN:C8	2.10	0.62
1:X:8:LYS:HE3	2:X:206:2AN:O3	1.99	0.62
1:V:13:PRO:HD2	1:V:148:GLU:OE2	1.99	0.62
2:g:203:2AN:C2	2:g:203:2AN:C16	2.72	0.62
2:M:202:2AN:C2	2:M:202:2AN:H16	2.29	0.62
1:K:104:LYS:O	1:K:105:LEU:HD23	1.98	0.62
1:K:139:LYS:O	1:K:142:GLU:CG	2.47	0.62
1:H:32:VAL:HG22	1:H:39:PHE:CB	2.27	0.62
1:D:4:TYR:CZ	1:C:2:ALA:CB	2.83	0.62
1:d:23:LEU:CB	2:d:201:2AN:C3	2.77	0.62
1:d:70:HIS:NE2	2:d:204:2AN:H7	2.14	0.62
2:V:205:2AN:C7	2:V:208:2AN:C6	2.77	0.62
1:Z:57:ILE:N	1:Z:57:ILE:HD12	2.14	0.62
2:Y:203:2AN:H12	2:Y:203:2AN:C2	2.29	0.62
1:j:94:ASP:O	1:j:123:LYS:HD2	1.99	0.62
1:J:87:PHE:CE2	1:J:88:GLU:HB2	2.34	0.62
1:G:23:LEU:HD22	1:G:147:VAL:HG21	1.80	0.62
1:d:21:LYS:HA	1:d:25:LEU:HB2	1.81	0.62
1:d:138:LYS:O	1:d:142:GLU:HG3	2.00	0.62
2:V:204:2AN:H16	2:V:204:2AN:C2	2.26	0.62
1:N:17:HIS:CB	5:N:206:DMS:H22	2.28	0.62
1:M:10:GLU:HG2	2:M:201:2AN:C16	2.29	0.62
1:F:48:ASP:N	1:F:53:THR:OG1	2.32	0.62
1:C:103:VAL:HG21	2:C:202:2AN:H4	1.82	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:d:23:LEU:HD13	2:d:201:2AN:C2	2.27	0.62
1:Z:138:LYS:HZ3	2:Z:206:2AN:H8	1.62	0.62
1:V:21:LYS:O	1:V:26:GLU:HB2	1.99	0.62
1:U:127:THR:O	1:U:128:VAL:HG12	1.99	0.62
1:Q:54:VAL:HG22	1:Q:71:LYS:HG3	1.81	0.62
1:F:139:LYS:C	2:F:202:2AN:H8	2.23	0.62
1:Z:141:TYR:CD1	7:Z:304:HOH:O	2.51	0.62
1:P:10:GLU:C	1:P:11:GLU:HG3	2.24	0.62
1:P:26:GLU:O	1:P:27:ARG:C	2.43	0.62
1:O:80:PHE:CB	1:O:105:LEU:CD1	2.78	0.62
1:K:6:ILE:HD11	1:K:133:VAL:CG2	2.29	0.62
1:J:96:ILE:HA	1:J:122:PRO:HA	1.82	0.62
1:F:47:GLY:CA	1:F:53:THR:HA	2.30	0.62
2:C:201:2AN:H12	2:C:201:2AN:C2	2.27	0.62
1:h:18:ARG:NH2	1:h:154:ASN:O	2.31	0.62
1:A:82:CYS:N	1:A:103:VAL:O	2.30	0.62
1:A:123:LYS:HG3	1:A:124:PRO:HD2	1.82	0.62
1:O:1:MET:N	1:O:1:MET:SD	2.73	0.62
1:H:120:TYR:HE2	1:H:133:VAL:HG13	1.65	0.62
1:X:32:VAL:O	1:X:32:VAL:HG12	1.99	0.62
1:V:150:TYR:O	1:V:154:ASN:ND2	2.21	0.62
1:M:10:GLU:HG2	2:M:201:2AN:H16	1.81	0.62
1:H:138:LYS:HE3	1:G:-1:PHE:CZ	2.30	0.62
1:j:96:ILE:HD11	1:j:128:VAL:HG12	1.81	0.62
1:j:144:TYR:CD1	1:j:144:TYR:C	2.78	0.62
1:i:20:PHE:HB2	1:i:105:LEU:HD12	1.81	0.62
1:B:139:LYS:HE2	2:B:201:2AN:C4	2.30	0.62
2:B:204:2AN:H16	1:j:77:ALA:HB3	1.80	0.62
1:M:57:ILE:O	1:M:67:TYR:HA	1.99	0.62
1:I:123:LYS:HG2	1:I:124:PRO:CD	2.30	0.62
2:D:202:2AN:H16	2:D:202:2AN:H2	1.82	0.62
2:D:203:2AN:H16	2:D:203:2AN:C2	2.29	0.62
1:C:46:GLU:O	1:C:53:THR:HG23	2.00	0.62
2:a:203:2AN:S	2:a:203:2AN:N	2.70	0.62
1:T:19:LEU:HD13	1:T:23:LEU:HD12	1.80	0.62
1:J:105:LEU:HD22	2:J:202:2AN:H15	1.82	0.61
1:F:15:ALA:HB3	1:F:18:ARG:CD	2.30	0.61
1:C:92:LEU:HG	1:C:96:ILE:CG2	2.30	0.61
1:Y:138:LYS:HE2	2:Y:201:2AN:H13	1.79	0.61
2:Y:201:2AN:H16	2:Y:201:2AN:C2	2.29	0.61
2:T:204:2AN:H2	2:T:204:2AN:C12	2.25	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:76:ASP:OD2	1:G:79:ASN:ND2	2.33	0.61
1:D:99:VAL:CG1	1:D:119:THR:O	2.47	0.61
1:H:32:VAL:HG22	1:H:39:PHE:HB3	1.82	0.61
1:H:66:THR:N	1:H:90:ASP:OD1	2.29	0.61
1:a:141:TYR:HB2	2:a:204:2AN:C13	2.29	0.61
1:V:33:LYS:HD3	2:V:207:2AN:O3	2.00	0.61
1:j:2:ALA:HB2	1:i:4:TYR:OH	2.00	0.61
1:i:57:ILE:HD12	1:i:68:MET:HE3	1.82	0.61
2:h:205:2AN:N	2:h:205:2AN:O2	2.32	0.61
1:J:24:VAL:HG12	1:J:25:LEU:HD23	1.82	0.61
1:E:21:LYS:HE2	1:E:158:PHE:CD1	2.34	0.61
1:E:123:LYS:CG	1:E:124:PRO:CD	2.78	0.61
1:C:23:LEU:HD23	2:C:202:2AN:C2	2.30	0.61
1:e:153:ALA:C	1:e:154:ASN:OD1	2.42	0.61
1:d:53:THR:HG22	1:d:72:PHE:CB	2.30	0.61
1:Z:138:LYS:HZ1	2:Z:206:2AN:C8	2.10	0.61
1:X:123:LYS:CB	1:X:124:PRO:HD3	2.30	0.61
2:W:201:2AN:H2	2:W:201:2AN:C16	2.26	0.61
1:j:141:TYR:HD2	6:j:208:FLC:HA1	1.62	0.61
1:i:18:ARG:HG2	1:i:158:PHE:O	2.00	0.61
1:B:28:HIS:O	1:B:42:GLY:HA3	2.00	0.61
1:A:7:VAL:HA	1:A:116:ILE:O	2.00	0.61
1:A:93:ARG:O	1:A:94:ASP:CB	2.48	0.61
1:P:95:ASN:HA	1:P:126:CYS:CB	2.31	0.61
1:d:93:ARG:HH21	1:d:132:GLU:HB2	1.64	0.61
1:Z:16:PRO:N	1:Z:112:SER:OG	2.34	0.61
1:Q:57:ILE:HB	1:Q:68:MET:HB2	1.81	0.61
1:O:69:LEU:O	1:O:86:LEU:HD12	2.00	0.61
1:O:128:VAL:HA	1:O:132:GLU:OE2	1.99	0.61
1:M:1:MET:HE1	1:M:124:PRO:HA	1.82	0.61
2:L:202:2AN:N	2:L:202:2AN:O3	2.33	0.61
1:F:48:ASP:C	1:F:50:GLY:H	2.08	0.61
1:e:32:VAL:HG22	1:e:39:PHE:HB3	1.83	0.61
1:a:7:VAL:HG23	1:a:117:THR:CG2	2.29	0.61
2:Y:201:2AN:H2	2:Y:201:2AN:C16	2.26	0.61
1:h:85:THR:HG23	1:h:100:VAL:HG22	1.81	0.61
1:f:35:GLN:HE21	1:f:146:GLN:HE22	1.47	0.61
1:c:46:GLU:HG2	2:c:205:2AN:H12	1.83	0.61
1:T:80:PHE:CB	1:T:105:LEU:HB2	2.31	0.61
1:S:116:ILE:HD12	1:S:116:ILE:N	2.16	0.61
1:A:69:LEU:O	1:A:86:LEU:HA	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:65:LEU:HD13	1:P:91:VAL:HG13	1.80	0.61
2:P:201:2AN:H2	2:P:201:2AN:C16	2.31	0.61
1:J:31:LEU:CD1	1:J:57:ILE:HD13	2.30	0.61
1:e:20:PHE:HB2	1:e:105:LEU:HD12	1.83	0.61
1:W:52:GLY:N	1:W:72:PHE:O	2.33	0.61
1:A:46:GLU:O	1:A:53:THR:HA	2.01	0.61
1:R:120:TYR:OH	1:R:136:GLY:HA3	2.01	0.61
1:L:130:GLU:O	1:L:134:LYS:HG3	2.01	0.61
1:f:143:PHE:HA	1:f:146:GLN:NE2	2.15	0.61
1:d:156:GLU:OE1	1:d:156:GLU:N	2.33	0.61
1:h:123:LYS:O	1:h:126:CYS:SG	2.59	0.61
1:A:86:LEU:HD12	1:A:86:LEU:O	2.01	0.61
1:A:86:LEU:HD23	7:A:302:HOH:O	2.00	0.61
1:A:122:PRO:CG	7:A:306:HOH:O	2.49	0.61
1:b:8:LYS:CE	1:b:10:GLU:OE2	2.49	0.61
1:O:143:PHE:O	1:O:146:GLN:HB2	2.00	0.60
1:L:4:TYR:O	1:L:119:THR:HA	2.00	0.60
1:E:16:PRO:O	1:E:17:HIS:C	2.43	0.60
1:D:118:VAL:HG12	1:D:119:THR:H	1.66	0.60
1:h:33:LYS:HD3	2:h:204:2AN:O3	2.01	0.60
1:A:43:GLU:OE2	1:A:56:LYS:HD3	2.01	0.60
1:e:43:GLU:O	1:e:56:LYS:N	2.33	0.60
1:d:53:THR:HG23	1:d:72:PHE:CD1	2.35	0.60
2:B:205:2AN:C2	2:B:205:2AN:C12	2.78	0.60
1:A:92:LEU:CD2	1:A:96:ILE:HD11	2.31	0.60
1:K:21:LYS:O	1:K:26:GLU:HB2	2.00	0.60
1:J:92:LEU:HD22	1:J:96:ILE:HB	1.83	0.60
1:f:18:ARG:NH2	1:f:157:VAL:O	2.30	0.60
1:d:101:TYR:HH	2:d:204:2AN:H6	1.66	0.60
2:d:203:2AN:S	2:d:203:2AN:N	2.74	0.60
2:b:203:2AN:C4	2:b:205:2AN:O1	2.50	0.60
2:W:201:2AN:H16	2:W:201:2AN:C2	2.30	0.60
1:g:47:GLY:HA3	1:g:53:THR:HG23	1.84	0.60
1:J:60:VAL:HG22	1:J:63:HIS:HB2	1.83	0.60
1:J:92:LEU:HB3	1:J:96:ILE:HB	1.82	0.60
1:f:20:PHE:HB2	1:f:105:LEU:HD12	1.82	0.60
1:W:129:ASN:C	1:W:131:GLU:H	2.09	0.60
2:T:202:2AN:H16	2:T:202:2AN:C2	2.30	0.60
1:B:30:VAL:HA	1:B:33:LYS:HG3	1.84	0.60
2:Q:203:2AN:C2	2:Q:203:2AN:C16	2.78	0.60
1:K:106:GLU:OE2	1:K:113:LYS:CE	2.49	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:77:ALA:O	2:H:204:2AN:H2	2.02	0.60
1:d:138:LYS:CD	1:d:142:GLU:OE2	2.48	0.60
1:X:55:THR:O	1:X:69:LEU:HA	2.01	0.60
1:h:150:TYR:O	1:h:153:ALA:HB3	2.02	0.60
1:J:97:GLU:N	1:J:121:HIS:O	2.31	0.60
1:V:138:LYS:HA	2:V:208:2AN:C3	2.31	0.60
2:g:202:2AN:C2	2:g:202:2AN:C16	2.78	0.60
1:A:32:VAL:HA	1:A:39:PHE:HB2	1.84	0.60
1:N:32:VAL:HG21	1:N:41:SER:CA	2.32	0.60
2:N:204:2AN:N	2:N:204:2AN:S	2.64	0.60
2:E:203:2AN:H16	2:E:203:2AN:C2	2.32	0.60
1:X:23:LEU:CB	2:X:206:2AN:H3	2.28	0.60
1:U:144:TYR:CD2	1:U:145:LYS:HD2	2.37	0.60
1:h:33:LYS:HD3	2:h:204:2AN:N	2.16	0.60
2:K:203:2AN:N	2:K:203:2AN:S	2.59	0.60
1:G:46:GLU:HB2	1:G:54:VAL:CG1	2.31	0.60
2:f:202:2AN:C2	2:f:202:2AN:C12	2.75	0.60
1:e:56:LYS:HG3	1:e:69:LEU:HD21	1.83	0.60
1:d:139:LYS:HD3	2:d:204:2AN:C13	2.31	0.60
1:Z:23:LEU:HD12	2:Z:203:2AN:C2	2.32	0.60
1:Z:155:PRO:O	1:Z:159:ALA:HB2	2.01	0.60
2:X:206:2AN:N	2:X:206:2AN:S	2.74	0.60
1:V:31:LEU:HA	1:V:143:PHE:CE1	2.37	0.60
2:T:203:2AN:H2	2:T:203:2AN:C12	2.27	0.60
1:R:21:LYS:HD2	1:R:158:PHE:HB3	1.83	0.60
2:K:203:2AN:H2	2:K:203:2AN:C12	2.27	0.60
2:I:203:2AN:H2	2:I:203:2AN:C16	2.31	0.60
1:X:41:SER:OG	1:X:58:THR:HB	2.02	0.60
1:X:116:ILE:CD1	2:X:206:2AN:O2	2.50	0.60
2:X:203:2AN:S	2:X:203:2AN:N	2.73	0.60
1:j:4:TYR:CD1	1:j:128:VAL:CG2	2.85	0.60
1:g:120:TYR:CE1	1:g:133:VAL:HG13	2.37	0.60
1:L:43:GLU:O	1:L:56:LYS:N	2.26	0.60
2:G:207:2AN:H2	2:G:207:2AN:C12	2.24	0.60
1:c:138:LYS:HD2	2:c:202:2AN:H12	1.82	0.60
1:V:10:GLU:HB2	2:V:203:2AN:C13	2.32	0.60
1:i:101:TYR:CD2	1:i:118:VAL:HG22	2.36	0.60
2:O:201:2AN:C16	2:O:201:2AN:O2	2.49	0.59
1:M:116:ILE:HD13	2:M:201:2AN:O2	2.01	0.59
1:J:-3:ASP:O	1:I:134:LYS:CE	2.49	0.59
1:F:46:GLU:HG3	2:F:206:2AN:O1	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:f:203:2AN:S	2:f:203:2AN:N	2.74	0.59
1:e:1:MET:SD	1:e:1:MET:N	2.71	0.59
1:S:23:LEU:O	2:S:204:2AN:H7	2.02	0.59
1:B:2:ALA:HB3	1:B:122:PRO:HG3	1.84	0.59
1:Q:57:ILE:N	1:Q:68:MET:O	2.36	0.59
1:H:4:TYR:CE1	1:G:2:ALA:HB2	2.37	0.59
2:f:205:2AN:S	2:f:205:2AN:N	2.74	0.59
1:Z:31:LEU:HA	1:Z:143:PHE:CE1	2.37	0.59
1:j:70:HIS:HA	1:j:85:THR:O	2.02	0.59
1:B:44:ILE:HA	1:B:55:THR:HA	1.84	0.59
2:D:203:2AN:H16	2:D:203:2AN:H2	1.82	0.59
1:e:154:ASN:OD1	1:e:154:ASN:N	2.35	0.59
2:V:208:2AN:H12	2:V:208:2AN:O1	2.02	0.59
1:h:57:ILE:HD12	1:h:68:MET:HE3	1.83	0.59
1:P:130:GLU:O	1:P:134:LYS:HG3	2.03	0.59
1:E:53:THR:HB	1:E:72:PHE:HD2	1.66	0.59
1:Y:97:GLU:HG3	1:Y:123:LYS:HA	1.84	0.59
1:U:14:ILE:HD12	1:U:14:ILE:N	2.17	0.59
2:T:201:2AN:N	2:T:201:2AN:O1	2.33	0.59
1:i:30:VAL:O	1:i:34:ALA:N	2.33	0.59
1:g:31:LEU:HD23	1:g:143:PHE:CE1	2.37	0.59
1:P:63:HIS:ND1	1:P:65:LEU:HB2	2.17	0.59
1:P:68:MET:HG2	1:P:91:VAL:CG2	2.33	0.59
1:O:67:TYR:O	1:O:90:ASP:OD1	2.20	0.59
1:D:96:ILE:HD12	1:D:120:TYR:HD2	1.68	0.59
1:c:135:ILE:O	1:c:139:LYS:CG	2.44	0.59
1:b:144:TYR:O	1:b:144:TYR:CD1	2.55	0.59
1:S:20:PHE:O	1:S:24:VAL:HB	2.03	0.59
1:j:8:LYS:NZ	1:j:10:GLU:OE1	2.34	0.59
1:B:150:TYR:CD2	2:B:203:2AN:O3	2.55	0.59
1:F:152:ALA:HB3	7:F:301:HOH:O	2.02	0.59
1:C:133:VAL:O	1:C:137:GLU:N	2.34	0.59
1:d:74:GLU:HG2	1:d:83:LYS:HB2	1.84	0.59
2:X:206:2AN:C8	7:X:302:HOH:O	2.47	0.59
1:U:8:LYS:O	1:U:116:ILE:N	2.31	0.59
1:S:67:TYR:CE1	1:S:89:GLY:HA2	2.38	0.59
1:B:120:TYR:OH	2:B:201:2AN:H14	2.02	0.59
1:H:154:ASN:HD22	1:H:154:ASN:N	2.00	0.59
1:Y:1:MET:HE3	1:Y:4:TYR:HA	1.84	0.59
1:Y:91:VAL:HG21	2:Y:203:2AN:C12	2.32	0.59
1:B:87:PHE:CD2	1:B:88:GLU:HG2	2.37	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:201:2AN:O3	2:P:201:2AN:N	2.36	0.59
1:N:59:PHE:N	1:N:66:THR:O	2.35	0.59
1:d:83:LYS:HA	1:d:101:TYR:O	2.02	0.59
1:i:94:ASP:O	1:i:123:LYS:HD2	2.03	0.59
1:i:104:LYS:NZ	1:i:105:LEU:O	2.32	0.59
1:B:65:LEU:HD13	1:B:91:VAL:HB	1.84	0.59
2:H:203:2AN:H2	2:H:203:2AN:C16	2.26	0.59
1:E:16:PRO:O	1:E:19:LEU:N	2.35	0.59
2:C:201:2AN:C2	2:C:201:2AN:C12	2.74	0.59
1:e:17:HIS:HA	1:e:80:PHE:CE1	2.38	0.59
1:X:144:TYR:CD1	1:X:144:TYR:C	2.79	0.59
1:g:63:HIS:CD2	1:g:64:PRO:HD2	2.38	0.59
1:A:45:ILE:HD12	1:A:46:GLU:N	2.18	0.59
1:R:57:ILE:O	1:R:67:TYR:CA	2.48	0.59
2:N:202:2AN:C16	2:N:202:2AN:H2	2.32	0.59
1:E:72:PHE:CD1	1:E:75:ILE:HD11	2.38	0.59
1:D:4:TYR:CE1	1:C:2:ALA:HB1	2.37	0.59
1:c:91:VAL:HG23	2:c:203:2AN:C7	2.32	0.59
1:W:108:VAL:HG21	1:W:113:LYS:HG3	1.85	0.59
1:S:31:LEU:HD23	1:S:143:PHE:CE1	2.38	0.59
1:Q:69:LEU:HD22	1:Q:88:GLU:HB3	1.84	0.58
1:O:103:VAL:HG22	1:O:116:ILE:CG1	2.33	0.58
1:C:20:PHE:O	1:C:24:VAL:HB	2.03	0.58
1:d:20:PHE:HB2	1:d:105:LEU:HD12	1.85	0.58
1:a:16:PRO:O	1:a:17:HIS:C	2.45	0.58
1:T:80:PHE:HB3	1:T:105:LEU:HB2	1.83	0.58
2:i:201:2AN:H2	2:i:201:2AN:C12	2.32	0.58
1:A:51:VAL:CG1	1:A:73:ASP:O	2.51	0.58
2:Q:201:2AN:C16	2:Q:201:2AN:C2	2.79	0.58
2:Q:201:2AN:C2	2:Q:201:2AN:H16	2.33	0.58
1:I:18:ARG:NH2	1:I:151:LEU:O	2.36	0.58
1:D:20:PHE:CE1	1:D:80:PHE:C	2.82	0.58
1:D:20:PHE:HZ	1:D:81:TYR:O	1.86	0.58
1:V:70:HIS:HA	1:V:85:THR:O	2.02	0.58
1:U:32:VAL:O	1:U:33:LYS:C	2.45	0.58
1:i:76:ASP:HB3	1:i:81:TYR:HB3	1.83	0.58
1:B:156:GLU:OE1	1:B:156:GLU:N	2.34	0.58
1:P:148:GLU:O	1:P:149:GLU:C	2.45	0.58
2:P:201:2AN:H16	2:P:201:2AN:H2	1.84	0.58
2:G:202:2AN:C2	2:G:202:2AN:C12	2.74	0.58
1:E:107:ALA:HB2	1:e:107:ALA:HB2	1.84	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:80:PHE:O	1:B:104:LYS:HA	2.03	0.58
1:R:140:ALA:HB1	2:R:201:2AN:H8	1.85	0.58
1:J:6:ILE:CG2	1:I:0:THR:HG22	2.34	0.58
1:G:70:HIS:HA	1:G:85:THR:O	2.02	0.58
1:G:76:ASP:OD2	1:G:79:ASN:HB2	2.03	0.58
1:f:57:ILE:O	1:f:67:TYR:HA	2.03	0.58
1:e:19:LEU:O	1:e:22:ALA:N	2.37	0.58
1:Z:73:ASP:HB2	1:Z:83:LYS:O	2.03	0.58
1:U:103:VAL:HA	1:U:116:ILE:HG22	1.85	0.58
2:I:204:2AN:H2	2:I:204:2AN:C16	2.34	0.58
2:H:203:2AN:H16	2:H:203:2AN:C2	2.27	0.58
1:D:69:LEU:HB3	1:D:88:GLU:H	1.68	0.58
1:C:53:THR:O	1:C:71:LYS:HA	2.03	0.58
1:d:93:ARG:HH21	1:d:129:ASN:ND2	2.01	0.58
1:c:71:LYS:O	1:c:84:TYR:HA	2.04	0.58
1:Z:108:VAL:HG12	1:Z:108:VAL:O	2.02	0.58
1:h:73:ASP:OD2	1:h:85:THR:OG1	2.22	0.58
1:B:20:PHE:CD1	1:B:80:PHE:HA	2.38	0.58
3:A:205:SO4:O1	1:i:17:HIS:ND1	2.37	0.58
1:N:40:LYS:HE2	1:N:60:VAL:HA	1.85	0.58
1:E:45:ILE:HG12	1:E:54:VAL:HG12	1.86	0.58
1:D:10:GLU:C	1:D:11:GLU:HG3	2.28	0.58
1:D:53:THR:HG22	1:D:54:VAL:N	2.17	0.58
1:d:37:HIS:CD2	1:d:38:VAL:HG23	2.39	0.58
2:M:202:2AN:C2	2:M:202:2AN:C16	2.78	0.58
1:f:19:LEU:O	1:f:23:LEU:HB2	2.03	0.58
1:d:14:ILE:HG21	1:d:151:LEU:CD1	2.33	0.58
1:Z:68:MET:HG2	1:Z:91:VAL:HG11	1.85	0.58
1:g:55:THR:O	1:g:69:LEU:HA	2.04	0.58
1:H:77:ALA:O	2:H:204:2AN:C2	2.51	0.58
1:H:123:LYS:CB	1:H:124:PRO:HD2	2.33	0.58
2:C:202:2AN:H2	2:C:202:2AN:C12	2.28	0.58
2:V:207:2AN:O1	2:V:207:2AN:N	2.33	0.58
1:h:151:LEU:O	1:h:153:ALA:N	2.36	0.58
1:R:27:ARG:NH2	2:R:202:2AN:O3	2.33	0.58
1:M:109:GLY:O	1:W:80:PHE:CZ	2.57	0.58
1:G:136:GLY:O	1:G:139:LYS:N	2.36	0.58
1:f:28:HIS:O	1:f:32:VAL:HG23	2.03	0.58
2:g:202:2AN:C16	2:g:202:2AN:H2	2.34	0.58
1:A:92:LEU:CD2	1:A:96:ILE:CD1	2.82	0.58
1:N:57:ILE:O	1:N:67:TYR:HA	2.04	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:69:LEU:N	1:M:88:GLU:O	2.31	0.58
1:M:103:VAL:HG22	1:M:116:ILE:CG1	2.34	0.58
1:G:46:GLU:O	1:G:53:THR:HG23	2.04	0.58
1:e:56:LYS:HA	1:e:69:LEU:HD23	1.86	0.58
1:b:129:ASN:O	1:b:132:GLU:CB	2.52	0.58
1:V:108:VAL:HG21	1:V:113:LYS:HD3	1.86	0.58
1:g:8:LYS:NZ	3:g:204:SO4:O4	2.33	0.58
2:B:201:2AN:C2	2:B:201:2AN:H12	2.34	0.57
1:e:87:PHE:CD1	1:e:87:PHE:C	2.82	0.57
1:a:29:GLN:O	1:a:33:LYS:HG3	2.03	0.57
1:a:30:VAL:HG23	1:a:143:PHE:HZ	1.68	0.57
1:X:80:PHE:HB2	1:X:105:LEU:O	2.03	0.57
1:J:105:LEU:HA	1:J:113:LYS:O	2.04	0.57
1:H:4:TYR:CE1	1:G:2:ALA:HB1	2.37	0.57
2:e:201:2AN:H16	2:e:201:2AN:H2	1.85	0.57
1:Y:142:GLU:HG3	3:Y:205:SO4:O1	2.04	0.57
2:Y:203:2AN:H2	2:Y:203:2AN:C12	2.34	0.57
2:V:202:2AN:H16	2:V:202:2AN:C2	2.34	0.57
1:g:59:PHE:CZ	1:g:68:MET:HE2	2.38	0.57
2:B:203:2AN:N	2:B:203:2AN:S	2.75	0.57
1:A:57:ILE:O	1:A:67:TYR:HA	2.03	0.57
1:A:120:TYR:O	1:A:122:PRO:HD3	2.03	0.57
1:J:30:VAL:HG11	1:J:147:VAL:HG11	1.85	0.57
1:H:57:ILE:HB	1:H:68:MET:HB2	1.86	0.57
1:a:141:TYR:CD1	2:a:204:2AN:C14	2.87	0.57
1:Z:77:ALA:HB1	2:Z:202:2AN:H2	1.86	0.57
1:X:44:ILE:CD1	1:X:53:THR:HG21	2.26	0.57
1:W:28:HIS:O	1:W:42:GLY:HA3	2.04	0.57
1:V:142:GLU:OE2	2:V:208:2AN:N	2.36	0.57
1:j:2:ALA:HB2	1:i:4:TYR:CZ	2.38	0.57
1:h:30:VAL:O	1:h:31:LEU:C	2.47	0.57
1:g:68:MET:HA	1:g:88:GLU:O	2.04	0.57
1:J:103:VAL:HG22	1:J:116:ILE:HG23	1.86	0.57
1:H:68:MET:HB3	1:H:70:HIS:CE1	2.39	0.57
1:C:80:PHE:HB2	1:C:105:LEU:O	2.04	0.57
1:Z:70:HIS:HA	1:Z:85:THR:O	2.04	0.57
1:T:50:GLY:C	1:T:75:ILE:HD12	2.29	0.57
1:M:35:GLN:HB3	1:M:37:HIS:CE1	2.39	0.57
2:f:205:2AN:N	2:f:205:2AN:O1	2.37	0.57
1:d:60:VAL:HG21	2:d:202:2AN:H14	1.85	0.57
1:c:31:LEU:HD23	1:c:143:PHE:CE1	2.39	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:b:63:HIS:ND1	1:b:64:PRO:HD2	2.19	0.57
1:a:28:HIS:O	1:a:42:GLY:HA3	2.03	0.57
1:X:14:ILE:CD1	1:X:152:ALA:HB2	2.32	0.57
1:T:57:ILE:HD12	1:T:68:MET:CE	2.34	0.57
1:G:14:ILE:O	1:G:112:SER:OG	2.22	0.57
1:E:17:HIS:NE2	1:E:159:ALA:HB3	2.20	0.57
2:f:204:2AN:H2	2:f:204:2AN:C16	2.35	0.57
6:e:202:FLC:OG2	6:e:202:FLC:OHB	2.18	0.57
1:b:8:LYS:NZ	2:b:201:2AN:O3	2.36	0.57
1:a:13:PRO:HD2	1:a:148:GLU:OE2	2.05	0.57
1:Z:141:TYR:CE1	7:Z:304:HOH:O	2.58	0.57
1:Y:70:HIS:HA	1:Y:85:THR:O	2.05	0.57
1:X:10:GLU:CG	2:X:206:2AN:C12	2.80	0.57
1:X:79:ASN:O	1:X:104:LYS:NZ	2.33	0.57
1:U:21:LYS:HA	1:U:25:LEU:HB3	1.87	0.57
1:T:31:LEU:CD1	1:T:57:ILE:HD13	2.35	0.57
1:g:45:ILE:HD12	1:g:46:GLU:HB2	1.85	0.57
1:B:47:GLY:HA3	1:B:53:THR:HA	1.86	0.57
1:A:16:PRO:O	1:A:18:ARG:N	2.38	0.57
1:K:122:PRO:CG	1:K:128:VAL:HG23	2.34	0.57
1:E:41:SER:OG	1:E:58:THR:HB	2.04	0.57
1:Y:59:PHE:CZ	1:Y:65:LEU:HD13	2.39	0.57
1:T:13:PRO:HD2	1:T:148:GLU:OE2	2.05	0.57
1:Q:73:ASP:HB2	1:Q:83:LYS:O	2.04	0.57
1:K:76:ASP:OD2	1:K:79:ASN:ND2	2.37	0.57
1:f:128:VAL:O	1:f:128:VAL:HG12	2.04	0.57
2:b:202:2AN:N	2:b:202:2AN:S	2.75	0.57
1:Z:31:LEU:HA	1:Z:143:PHE:CZ	2.39	0.57
2:j:207:2AN:H2	2:j:207:2AN:C16	2.26	0.57
1:i:53:THR:O	1:i:71:LYS:HA	2.04	0.57
1:Y:20:PHE:HB2	1:Y:105:LEU:HD12	1.87	0.57
1:T:4:TYR:O	1:T:119:THR:HA	2.04	0.57
1:S:8:LYS:HG3	2:S:204:2AN:C14	2.34	0.57
1:A:107:ALA:CB	3:A:205:SO4:O2	2.49	0.57
2:R:205:2AN:H2	2:R:205:2AN:C12	2.27	0.57
2:O:203:2AN:O3	2:O:203:2AN:N	2.31	0.57
1:J:129:ASN:O	1:J:133:VAL:HG23	2.04	0.57
1:F:155:PRO:O	1:F:159:ALA:HB2	2.04	0.57
2:E:202:2AN:H12	2:E:202:2AN:C2	2.35	0.57
1:e:70:HIS:HA	1:e:85:THR:O	2.05	0.57
1:d:102:GLU:HB3	1:d:117:THR:HB	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:b:46:GLU:O	1:b:53:THR:HA	2.05	0.57
1:V:129:ASN:CB	1:V:132:GLU:HB2	2.34	0.57
1:j:63:HIS:CE1	1:j:64:PRO:HD2	2.38	0.57
1:B:100:VAL:O	1:B:119:THR:N	2.38	0.56
1:Q:50:GLY:O	1:Q:53:THR:OG1	2.20	0.56
1:M:16:PRO:HD3	1:M:111:GLY:O	2.05	0.56
1:L:76:ASP:OD1	1:L:79:ASN:ND2	2.38	0.56
1:G:17:HIS:CA	1:G:80:PHE:HE1	2.17	0.56
2:b:205:2AN:H2	2:b:205:2AN:C16	2.28	0.56
1:a:87:PHE:CD1	1:a:87:PHE:C	2.83	0.56
1:g:32:VAL:HG13	1:g:39:PHE:O	2.04	0.56
2:A:203:2AN:O3	2:A:203:2AN:N	2.37	0.56
1:M:104:LYS:O	1:M:105:LEU:HD23	2.05	0.56
1:L:105:LEU:HD21	2:L:201:2AN:H15	1.87	0.56
1:J:-3:ASP:H2	1:J:-2:PRO:HD2	1.69	0.56
1:I:103:VAL:HG21	2:I:202:2AN:C4	2.35	0.56
6:G:206:FLC:OG1	2:G:207:2AN:C7	2.53	0.56
1:E:0:THR:O	1:E:0:THR:HG22	2.04	0.56
1:E:98:LYS:HE2	1:E:121:HIS:CG	2.40	0.56
1:Z:16:PRO:CA	1:Z:112:SER:OG	2.54	0.56
2:Z:201:2AN:C2	2:Z:201:2AN:H12	2.36	0.56
1:j:129:ASN:N	1:j:129:ASN:OD1	2.38	0.56
1:g:44:ILE:HG23	1:g:54:VAL:O	2.05	0.56
2:B:205:2AN:N	2:B:205:2AN:O2	2.36	0.56
2:N:201:2AN:C2	2:N:201:2AN:C16	2.47	0.56
2:N:205:2AN:N	2:N:205:2AN:O1	2.38	0.56
2:N:205:2AN:N	2:N:205:2AN:S	2.72	0.56
2:L:204:2AN:H2	2:L:204:2AN:C16	2.23	0.56
1:H:23:LEU:O	1:H:27:ARG:HD2	2.05	0.56
2:F:206:2AN:H6	1:f:17:HIS:HB2	1.87	0.56
1:C:139:LYS:HA	1:C:139:LYS:HE2	1.87	0.56
1:f:91:VAL:HG21	2:f:202:2AN:C13	2.36	0.56
1:f:122:PRO:HG3	1:f:128:VAL:HG23	1.87	0.56
1:e:63:HIS:ND1	1:e:64:PRO:HD2	2.20	0.56
1:e:101:TYR:CD1	1:e:118:VAL:HG22	2.40	0.56
1:Z:63:HIS:ND1	1:Z:64:PRO:HD2	2.18	0.56
1:Z:83:LYS:HA	1:Z:101:TYR:O	2.05	0.56
1:U:97:GLU:HA	1:U:123:LYS:HG3	1.86	0.56
1:B:44:ILE:HD12	1:B:44:ILE:H	1.69	0.56
1:G:31:LEU:HD23	1:G:143:PHE:CE1	2.40	0.56
1:D:70:HIS:NE2	1:D:86:LEU:HD13	2.21	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:74:GLU:OE1	1:C:83:LYS:HE2	2.06	0.56
1:b:4:TYR:HA	1:a:3:ALA:O	2.05	0.56
2:b:204:2AN:N	2:b:204:2AN:S	2.73	0.56
1:X:92:LEU:HD23	1:X:97:GLU:C	2.30	0.56
2:X:206:2AN:C5	7:X:302:HOH:O	2.53	0.56
1:V:142:GLU:OE2	2:V:208:2AN:C16	2.54	0.56
1:T:95:ASN:HA	1:T:126:CYS:HB3	1.86	0.56
1:A:16:PRO:O	1:A:17:HIS:C	2.48	0.56
1:Q:59:PHE:CD2	1:Q:63:HIS:CE1	2.94	0.56
1:Q:79:ASN:O	1:Q:104:LYS:NZ	2.35	0.56
1:D:137:GLU:OE1	1:C:0:THR:HG22	2.05	0.56
1:f:4:TYR:HA	1:e:3:ALA:O	2.06	0.56
1:h:83:LYS:HA	1:h:101:TYR:O	2.05	0.56
1:M:90:ASP:OD1	1:M:90:ASP:N	2.36	0.56
1:C:10:GLU:HB3	2:C:202:2AN:C15	2.35	0.56
1:a:6:ILE:N	1:a:6:ILE:HD12	2.20	0.56
1:V:77:ALA:HB3	2:V:204:2AN:H16	1.87	0.56
1:S:143:PHE:O	1:S:147:VAL:HG23	2.05	0.56
2:R:202:2AN:H12	2:R:202:2AN:H2	1.87	0.56
1:N:103:VAL:HG21	2:N:201:2AN:C4	2.36	0.56
2:D:203:2AN:O2	2:D:203:2AN:H12	2.05	0.56
1:C:0:THR:O	1:C:0:THR:HG23	2.03	0.56
1:b:39:PHE:CE1	1:b:59:PHE:CE1	2.94	0.56
1:T:19:LEU:CD1	1:T:23:LEU:HD12	2.36	0.56
1:T:43:GLU:HG2	1:T:56:LYS:O	2.06	0.56
1:g:122:PRO:HB3	1:g:128:VAL:HG23	1.87	0.56
1:B:158:PHE:CE2	2:B:203:2AN:H13	2.39	0.56
2:B:203:2AN:C16	2:B:203:2AN:C2	2.68	0.56
1:A:53:THR:O	1:A:72:PHE:N	2.32	0.56
1:P:31:LEU:HD23	1:P:143:PHE:CE1	2.40	0.56
2:N:202:2AN:H16	2:N:202:2AN:H2	1.87	0.56
2:I:204:2AN:H16	2:I:204:2AN:C2	2.36	0.56
1:G:16:PRO:HB2	1:G:80:PHE:CE1	2.40	0.56
1:C:63:HIS:HE1	1:C:65:LEU:HD12	1.70	0.56
2:d:202:2AN:H2	2:d:202:2AN:C16	2.34	0.56
2:b:202:2AN:H12	2:b:202:2AN:C2	2.34	0.56
1:a:6:ILE:O	1:a:117:THR:HA	2.06	0.56
1:Y:65:LEU:HD22	1:Y:91:VAL:HB	1.87	0.56
1:Y:66:THR:HB	1:Y:90:ASP:OD2	2.06	0.56
1:W:31:LEU:HD23	1:W:143:PHE:CD1	2.41	0.56
2:V:204:2AN:N	2:V:204:2AN:O1	2.37	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:103:VAL:CB	1:U:116:ILE:HG22	2.35	0.56
1:h:51:VAL:N	1:h:75:ILE:HD12	2.20	0.56
1:N:21:LYS:HE2	1:N:158:PHE:CD1	2.41	0.56
1:I:95:ASN:HB2	1:I:127:THR:O	2.05	0.56
1:F:93:ARG:O	1:F:94:ASP:C	2.49	0.56
1:e:135:ILE:O	1:e:139:LYS:HG2	2.06	0.56
1:d:50:GLY:HA2	1:d:75:ILE:HG21	1.88	0.56
1:c:13:PRO:HD2	1:c:148:GLU:OE2	2.05	0.56
1:b:129:ASN:O	1:b:132:GLU:N	2.39	0.56
1:V:28:HIS:CD2	1:V:29:GLN:HG2	2.41	0.56
1:U:24:VAL:HG22	1:U:25:LEU:N	2.20	0.56
2:K:201:2AN:N	2:K:201:2AN:S	2.79	0.56
2:f:203:2AN:H16	2:f:203:2AN:C2	2.35	0.56
1:e:16:PRO:HB2	1:e:80:PHE:CE2	2.41	0.56
2:b:203:2AN:H12	2:b:203:2AN:C2	2.35	0.56
1:X:144:TYR:CD1	2:X:206:2AN:H15	2.41	0.56
1:V:141:TYR:CD2	2:V:208:2AN:C6	2.89	0.56
2:V:201:2AN:H16	2:V:201:2AN:C2	2.32	0.56
1:T:20:PHE:O	1:T:24:VAL:N	2.39	0.56
1:g:139:LYS:CE	2:g:202:2AN:C4	2.72	0.56
1:A:108:VAL:HG21	1:A:113:LYS:HB2	1.88	0.55
1:O:40:LYS:HB3	1:O:60:VAL:HA	1.87	0.55
1:H:76:ASP:OD1	1:H:79:ASN:ND2	2.38	0.55
1:F:43:GLU:CG	1:F:56:LYS:HB3	2.36	0.55
1:d:73:ASP:OD2	1:d:85:THR:OG1	2.21	0.55
1:b:20:PHE:HB2	1:b:105:LEU:CD1	2.35	0.55
2:X:202:2AN:H12	2:X:202:2AN:C2	2.26	0.55
1:U:45:ILE:CG2	1:U:56:LYS:HB2	2.35	0.55
1:j:139:LYS:HE2	2:j:202:2AN:C6	2.37	0.55
1:i:69:LEU:HD12	1:i:88:GLU:OE1	2.06	0.55
1:B:135:ILE:O	1:B:139:LYS:HG2	2.06	0.55
1:A:30:VAL:O	1:A:31:LEU:C	2.46	0.55
2:L:202:2AN:H12	2:L:202:2AN:C2	2.30	0.55
1:K:134:LYS:O	1:K:138:LYS:HB2	2.05	0.55
1:H:20:PHE:O	1:H:24:VAL:HB	2.07	0.55
1:D:35:GLN:OE1	1:D:39:PHE:HE2	1.89	0.55
1:f:46:GLU:HB3	1:f:54:VAL:HB	1.88	0.55
1:X:144:TYR:CD1	2:X:206:2AN:C15	2.89	0.55
1:V:10:GLU:CB	2:V:203:2AN:C13	2.84	0.55
1:T:4:TYR:CE1	1:S:4:TYR:HE1	2.24	0.55
1:T:144:TYR:CD1	1:T:144:TYR:C	2.85	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:h:55:THR:HG23	1:h:72:PHE:HE1	1.71	0.55
1:A:55:THR:HG1	1:A:70:HIS:HB2	1.68	0.55
1:H:47:GLY:HA3	1:H:53:THR:HA	1.87	0.55
1:H:120:TYR:CE2	1:H:133:VAL:HG13	2.42	0.55
1:D:15:ALA:HB1	1:D:17:HIS:NE2	2.21	0.55
1:e:148:GLU:O	1:e:149:GLU:C	2.49	0.55
1:c:120:TYR:CE1	1:c:133:VAL:HG13	2.41	0.55
2:b:202:2AN:N	2:b:202:2AN:O1	2.40	0.55
1:Y:148:GLU:O	1:Y:149:GLU:C	2.48	0.55
2:h:202:2AN:S	2:h:202:2AN:N	2.80	0.55
1:Q:16:PRO:HD3	1:Q:111:GLY:O	2.06	0.55
1:K:31:LEU:CD1	1:K:57:ILE:HD13	2.36	0.55
1:I:110:GLY:HA2	1:a:17:HIS:CB	2.36	0.55
1:F:84:TYR:HE1	1:F:103:VAL:CG2	2.19	0.55
2:b:206:2AN:H12	2:b:206:2AN:C10	2.37	0.55
1:Q:8:LYS:NZ	2:Q:202:2AN:O3	2.39	0.55
1:O:103:VAL:HG22	1:O:116:ILE:HG12	1.87	0.55
1:F:47:GLY:HA3	1:F:53:THR:HG23	1.89	0.55
1:a:37:HIS:CD2	1:a:38:VAL:HG23	2.41	0.55
1:X:65:LEU:HD13	1:X:91:VAL:CG1	2.34	0.55
1:U:48:ASP:C	1:U:50:GLY:N	2.61	0.55
1:h:20:PHE:O	1:h:24:VAL:N	2.39	0.55
2:B:202:2AN:C2	2:B:202:2AN:H12	2.36	0.55
1:A:45:ILE:HD12	1:A:46:GLU:CB	2.37	0.55
1:A:47:GLY:CA	1:A:53:THR:HG22	2.36	0.55
1:J:84:TYR:OH	2:J:202:2AN:H4	2.05	0.55
1:H:99:VAL:HG22	1:H:120:TYR:CD1	2.42	0.55
1:Y:91:VAL:CG2	2:Y:203:2AN:C13	2.85	0.55
1:U:68:MET:CG	1:U:91:VAL:HG11	2.26	0.55
1:U:154:ASN:CB	1:U:157:VAL:HG23	2.36	0.55
6:i:203:FLC:CG	6:i:203:FLC:OA1	2.53	0.55
2:B:206:2AN:N	2:B:206:2AN:O1	2.39	0.55
1:O:59:PHE:CD1	1:O:65:LEU:O	2.60	0.55
1:f:39:PHE:CE1	1:f:59:PHE:CE1	2.95	0.55
1:c:43:GLU:OE2	1:c:56:LYS:O	2.25	0.55
2:Z:202:2AN:N	2:Z:202:2AN:O1	2.40	0.55
1:Y:2:ALA:O	1:Y:122:PRO:HG3	2.07	0.55
1:U:11:GLU:HB2	1:U:112:SER:O	2.07	0.55
1:U:20:PHE:CE1	1:U:80:PHE:HA	2.41	0.55
1:U:81:TYR:HB2	1:U:104:LYS:HD3	1.89	0.55
1:U:105:LEU:HD21	1:U:114:GLY:HA2	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:113:LYS:HB3	1:U:113:LYS:HZ3	1.72	0.55
1:j:31:LEU:HA	1:j:143:PHE:CZ	2.42	0.55
1:i:138:LYS:HE3	1:i:139:LYS:HE2	1.87	0.55
1:A:70:HIS:C	1:A:87:PHE:HE1	2.15	0.55
1:R:139:LYS:CE	2:R:205:2AN:C3	2.81	0.55
1:Q:37:HIS:CD2	1:Q:38:VAL:HG23	2.42	0.55
2:N:205:2AN:H2	2:N:205:2AN:C16	2.34	0.55
1:K:104:LYS:C	1:K:105:LEU:HD23	2.32	0.55
1:J:100:VAL:N	1:J:119:THR:O	2.32	0.55
1:H:27:ARG:NH1	1:H:143:PHE:HE2	2.04	0.55
1:e:98:LYS:HG3	1:e:121:HIS:ND1	2.22	0.55
1:d:67:TYR:HB2	7:d:302:HOH:O	2.06	0.55
1:Y:2:ALA:O	1:Y:122:PRO:CG	2.55	0.55
2:g:202:2AN:H16	2:g:202:2AN:H2	1.89	0.55
1:K:51:VAL:O	1:K:72:PHE:O	2.25	0.55
2:F:203:2AN:H2	2:F:203:2AN:C16	2.10	0.55
1:D:158:PHE:HZ	2:D:203:2AN:H15	1.63	0.55
1:C:5:THR:OG1	1:C:119:THR:HG23	2.07	0.55
2:f:205:2AN:C2	2:f:205:2AN:C12	2.59	0.55
1:j:129:ASN:C	1:j:131:GLU:N	2.65	0.55
2:j:204:2AN:O1	2:j:204:2AN:N	2.33	0.55
1:i:52:GLY:HA2	1:i:71:LYS:CE	2.37	0.55
2:R:205:2AN:O1	2:R:205:2AN:N	2.37	0.55
1:J:31:LEU:HD12	1:J:57:ILE:HD13	1.89	0.55
1:J:139:LYS:HB3	2:J:203:2AN:C6	2.37	0.55
2:I:203:2AN:O3	2:I:203:2AN:N	2.40	0.55
1:V:18:ARG:NH2	1:V:157:VAL:O	2.39	0.55
1:T:42:GLY:HA2	1:T:57:ILE:HA	1.89	0.55
1:j:4:TYR:HA	1:i:3:ALA:O	2.07	0.55
1:g:71:LYS:O	1:g:84:TYR:HA	2.07	0.55
1:R:69:LEU:CD1	1:R:88:GLU:HB2	2.37	0.54
1:R:131:GLU:O	1:R:135:ILE:HG13	2.06	0.54
2:P:203:2AN:C2	2:P:203:2AN:C16	2.69	0.54
2:L:204:2AN:O2	2:L:204:2AN:N	2.31	0.54
1:G:18:ARG:HH21	1:G:151:LEU:HA	1.70	0.54
1:C:37:HIS:CE1	1:C:38:VAL:HG23	2.43	0.54
1:X:151:LEU:O	1:X:152:ALA:C	2.49	0.54
2:P:201:2AN:C2	2:P:201:2AN:C16	2.79	0.54
1:M:18:ARG:NH2	1:M:151:LEU:O	2.39	0.54
2:G:201:2AN:C2	2:G:201:2AN:H12	2.37	0.54
1:f:50:GLY:N	1:f:53:THR:OG1	2.40	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:d:93:ARG:NH2	1:d:129:ASN:ND2	2.55	0.54
1:X:116:ILE:HG12	2:X:206:2AN:O2	2.07	0.54
1:U:57:ILE:CG2	1:U:58:THR:N	2.71	0.54
1:P:33:LYS:HB3	2:P:203:2AN:O2	2.07	0.54
1:P:68:MET:HG2	1:P:91:VAL:HG21	1.88	0.54
1:P:77:ALA:HB3	2:V:201:2AN:H16	1.88	0.54
2:F:206:2AN:C12	1:D:109:GLY:HA3	2.37	0.54
1:D:39:PHE:HA	1:D:59:PHE:HA	1.88	0.54
1:d:129:ASN:C	1:d:131:GLU:H	2.14	0.54
1:c:54:VAL:HG13	1:c:70:HIS:O	2.08	0.54
1:b:144:TYR:CD1	1:b:144:TYR:C	2.84	0.54
1:Y:18:ARG:NE	1:Y:157:VAL:O	2.40	0.54
1:T:10:GLU:CB	2:T:201:2AN:C13	2.78	0.54
2:R:204:2AN:H2	2:R:204:2AN:C12	2.17	0.54
1:O:133:VAL:O	1:O:137:GLU:CB	2.55	0.54
1:F:50:GLY:HA2	1:F:75:ILE:HD12	1.89	0.54
1:E:155:PRO:O	1:E:159:ALA:O	2.25	0.54
1:d:17:HIS:O	1:d:21:LYS:HB2	2.07	0.54
2:a:202:2AN:H2	2:a:202:2AN:C12	2.35	0.54
1:P:18:ARG:NH2	1:P:151:LEU:O	2.41	0.54
1:O:84:TYR:CE1	1:O:101:TYR:CD2	2.95	0.54
1:N:74:GLU:HB2	1:N:83:LYS:HB2	1.89	0.54
1:J:12:SER:HB3	1:J:112:SER:OG	2.07	0.54
1:f:97:GLU:HB2	1:f:123:LYS:HG2	1.88	0.54
1:e:12:SER:OG	1:e:13:PRO:HD2	2.08	0.54
1:c:66:THR:CB	1:c:90:ASP:OD2	2.54	0.54
1:b:1:MET:HE1	1:b:122:PRO:O	2.07	0.54
1:W:31:LEU:HD23	1:W:143:PHE:CE1	2.43	0.54
1:B:6:ILE:HG23	1:A:1:MET:HB3	1.89	0.54
1:B:16:PRO:HB2	1:B:80:PHE:CD2	2.42	0.54
1:B:87:PHE:HD2	1:B:88:GLU:HG2	1.72	0.54
2:B:202:2AN:H12	2:B:202:2AN:H2	1.89	0.54
2:A:201:2AN:H16	2:A:201:2AN:C2	2.27	0.54
2:R:203:2AN:O1	2:R:203:2AN:C16	2.54	0.54
1:L:105:LEU:CD2	2:L:201:2AN:H15	2.38	0.54
1:K:133:VAL:CG1	1:K:134:LYS:N	2.70	0.54
1:I:57:ILE:O	1:I:67:TYR:HA	2.07	0.54
1:E:80:PHE:O	1:E:104:LYS:HA	2.06	0.54
1:D:6:ILE:HD11	1:C:0:THR:CG2	2.38	0.54
2:c:201:2AN:S	2:c:201:2AN:N	2.80	0.54
2:Z:206:2AN:O2	2:Z:206:2AN:N	2.40	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:V:4:TYR:CE1	1:V:128:VAL:CG1	2.90	0.54
1:i:44:ILE:HG23	1:i:53:THR:HG23	1.89	0.54
2:g:202:2AN:C15	2:g:203:2AN:H7	2.38	0.54
1:B:108:VAL:O	1:B:109:GLY:C	2.47	0.54
1:R:99:VAL:HG22	1:R:120:TYR:CD2	2.43	0.54
2:N:204:2AN:H16	2:N:204:2AN:C2	2.15	0.54
1:L:77:ALA:HB3	2:L:204:2AN:H16	1.90	0.54
1:f:57:ILE:HG21	1:f:68:MET:HE2	1.89	0.54
2:e:201:2AN:H2	2:e:201:2AN:C16	2.37	0.54
1:d:154:ASN:HB3	1:d:157:VAL:CG2	2.38	0.54
1:b:116:ILE:N	1:b:116:ILE:HD12	2.23	0.54
1:a:65:LEU:HD22	1:a:90:ASP:OD1	2.07	0.54
1:V:90:ASP:N	1:V:90:ASP:OD1	2.40	0.54
1:j:66:THR:HG22	1:j:67:TYR:CD2	2.38	0.54
1:g:79:ASN:O	1:g:104:LYS:NZ	2.40	0.54
1:B:10:GLU:C	1:B:11:GLU:HG3	2.32	0.54
1:B:87:PHE:O	1:B:92:LEU:CD2	2.55	0.54
1:A:72:PHE:CD2	1:A:75:ILE:HD11	2.42	0.54
1:Q:57:ILE:O	1:Q:67:TYR:CA	2.56	0.54
1:N:6:ILE:HG23	1:M:0:THR:CB	2.36	0.54
1:I:89:GLY:C	1:I:91:VAL:H	2.16	0.54
2:F:201:2AN:O2	2:F:201:2AN:N	2.31	0.54
1:D:69:LEU:HD13	1:D:69:LEU:C	2.33	0.54
2:b:203:2AN:H4	2:b:205:2AN:O1	2.08	0.54
2:X:203:2AN:C2	2:X:203:2AN:H16	2.38	0.54
1:W:85:THR:OG1	1:W:100:VAL:CG2	2.56	0.54
1:U:97:GLU:CA	1:U:123:LYS:HG3	2.38	0.54
1:S:81:TYR:HA	1:S:103:VAL:O	2.08	0.54
1:j:31:LEU:HA	1:j:143:PHE:CE1	2.43	0.54
1:i:25:LEU:HD23	1:i:25:LEU:H	1.72	0.54
1:A:92:LEU:HD23	1:A:96:ILE:HD11	1.90	0.54
1:N:84:TYR:OH	2:N:201:2AN:H6	2.07	0.54
1:E:57:ILE:O	1:E:67:TYR:HA	2.08	0.54
1:C:57:ILE:O	1:C:67:TYR:CA	2.56	0.54
2:a:203:2AN:H2	2:a:203:2AN:C16	2.34	0.54
1:Y:33:LYS:HD3	2:Y:202:2AN:C1	2.38	0.54
1:V:95:ASN:HD21	1:V:129:ASN:CG	2.15	0.54
1:h:138:LYS:O	1:h:142:GLU:HG3	2.06	0.54
2:A:203:2AN:H2	2:A:203:2AN:C16	2.33	0.54
1:K:56:LYS:HE3	1:K:67:TYR:CD2	2.43	0.54
1:G:16:PRO:O	1:G:17:HIS:C	2.50	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:e:85:THR:HG23	1:e:100:VAL:CG2	2.37	0.54
2:e:201:2AN:C2	2:e:201:2AN:C16	2.85	0.54
1:d:70:HIS:NE2	2:d:204:2AN:C7	2.70	0.54
1:Z:7:VAL:HA	1:Z:116:ILE:O	2.08	0.54
1:X:144:TYR:CE1	2:X:206:2AN:C15	2.91	0.54
1:I:108:VAL:HG22	1:I:108:VAL:O	2.08	0.53
1:E:59:PHE:O	1:E:60:VAL:C	2.49	0.53
1:f:69:LEU:N	1:f:88:GLU:O	2.39	0.53
1:c:91:VAL:HG23	2:c:203:2AN:H7	1.89	0.53
2:Z:203:2AN:H2	2:Z:203:2AN:C12	2.36	0.53
1:V:25:LEU:CD2	1:V:75:ILE:HD11	2.38	0.53
1:U:32:VAL:O	1:U:34:ALA:N	2.40	0.53
1:T:4:TYR:CE2	1:S:4:TYR:OH	2.52	0.53
1:j:142:GLU:CG	6:j:208:FLC:CBC	2.84	0.53
1:L:48:ASP:C	1:L:50:GLY:H	2.16	0.53
1:C:30:VAL:O	1:C:31:LEU:C	2.50	0.53
1:c:120:TYR:CD1	1:c:133:VAL:HG22	2.42	0.53
1:a:139:LYS:NZ	2:a:201:2AN:O1	2.38	0.53
1:Z:57:ILE:HD12	1:Z:57:ILE:H	1.72	0.53
1:W:142:GLU:O	1:W:143:PHE:C	2.51	0.53
1:U:51:VAL:CG1	1:U:73:ASP:O	2.56	0.53
1:i:135:ILE:O	1:i:139:LYS:HG2	2.08	0.53
1:B:6:ILE:HG23	1:A:1:MET:CB	2.38	0.53
1:E:9:GLU:HA	1:E:114:GLY:O	2.09	0.53
1:U:101:TYR:CD1	1:U:118:VAL:CG2	2.88	0.53
1:T:141:TYR:O	1:T:145:LYS:HG2	2.08	0.53
2:j:206:2AN:C13	6:j:208:FLC:OB1	2.56	0.53
1:M:96:ILE:HD11	1:M:128:VAL:HG13	1.89	0.53
1:F:84:TYR:CE1	1:F:103:VAL:CG2	2.92	0.53
1:D:97:GLU:HA	1:D:123:LYS:HG2	1.90	0.53
1:C:38:VAL:O	1:C:59:PHE:HA	2.08	0.53
1:a:107:ALA:O	1:a:108:VAL:HG13	2.08	0.53
1:Z:19:LEU:HD11	1:Z:23:LEU:HD12	1.87	0.53
1:X:116:ILE:CG1	2:X:206:2AN:O2	2.57	0.53
1:U:13:PRO:CD	1:U:148:GLU:OE2	2.52	0.53
1:U:40:LYS:HB3	1:U:58:THR:O	2.09	0.53
1:T:95:ASN:HB2	1:T:127:THR:O	2.08	0.53
1:T:156:GLU:O	1:T:157:VAL:C	2.51	0.53
1:i:73:ASP:C	1:i:74:GLU:HG3	2.34	0.53
1:i:120:TYR:CE1	1:i:133:VAL:HG13	2.43	0.53
1:A:53:THR:O	1:A:72:PHE:HB2	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:98:LYS:HE3	1:Q:121:HIS:CD2	2.43	0.53
1:N:52:GLY:N	1:N:72:PHE:O	2.42	0.53
2:L:204:2AN:H16	2:L:204:2AN:C2	2.27	0.53
1:e:18:ARG:NH1	7:e:301:HOH:O	2.27	0.53
1:a:24:VAL:HG22	2:a:204:2AN:H7	1.90	0.53
1:Z:23:LEU:CD1	2:Z:203:2AN:C2	2.86	0.53
1:U:141:TYR:O	1:U:142:GLU:C	2.50	0.53
1:R:58:THR:HA	1:R:66:THR:O	2.09	0.53
1:O:101:TYR:CE1	2:O:201:2AN:C14	2.91	0.53
2:O:201:2AN:H12	2:O:201:2AN:C2	2.26	0.53
1:J:28:HIS:NE2	1:J:44:ILE:HD11	2.24	0.53
1:X:63:HIS:HD2	2:X:203:2AN:C6	2.22	0.53
1:U:48:ASP:C	1:U:50:GLY:H	2.15	0.53
1:T:20:PHE:HB2	1:T:105:LEU:HD12	1.90	0.53
1:T:55:THR:HG23	1:T:72:PHE:HE1	1.73	0.53
1:Q:71:LYS:HB2	1:Q:87:PHE:CE2	2.44	0.53
1:M:109:GLY:O	1:W:80:PHE:HZ	1.92	0.53
1:K:81:TYR:CD1	1:K:81:TYR:C	2.85	0.53
1:G:87:PHE:HA	1:G:98:LYS:CB	2.36	0.53
1:f:4:TYR:HD1	1:f:128:VAL:HG21	1.74	0.53
2:f:206:2AN:N	2:f:206:2AN:O2	2.41	0.53
1:X:147:VAL:HG13	2:X:202:2AN:H14	1.89	0.53
1:V:144:TYR:CD2	2:V:203:2AN:H12	2.44	0.53
1:S:140:ALA:HB1	2:S:204:2AN:O3	2.09	0.53
1:j:46:GLU:O	1:j:53:THR:HA	2.08	0.53
1:A:107:ALA:HB2	1:i:107:ALA:HB2	1.91	0.53
1:J:138:LYS:C	1:J:138:LYS:HD3	2.33	0.53
2:G:202:2AN:N	2:G:202:2AN:O1	2.42	0.53
1:D:54:VAL:HG22	1:D:71:LYS:HG2	1.91	0.53
1:C:91:VAL:HG11	2:C:201:2AN:H2	1.91	0.53
1:c:105:LEU:HD23	1:c:114:GLY:HA3	1.91	0.53
1:Y:46:GLU:O	1:Y:53:THR:HA	2.09	0.53
1:V:47:GLY:N	2:V:201:2AN:H12	2.24	0.53
1:U:69:LEU:HB3	1:U:87:PHE:CE1	2.42	0.53
1:S:144:TYR:CD1	1:S:144:TYR:C	2.87	0.53
1:A:21:LYS:HA	1:A:25:LEU:HB2	1.89	0.53
1:Q:144:TYR:O	1:Q:145:LYS:C	2.52	0.53
1:M:103:VAL:HG22	1:M:116:ILE:HG13	1.91	0.53
1:H:1:MET:HA	1:H:1:MET:CE	2.37	0.53
1:H:27:ARG:NH1	1:H:143:PHE:CE2	2.77	0.53
1:H:120:TYR:CD2	1:H:133:VAL:HG22	2.44	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:118:VAL:HG12	1:D:119:THR:N	2.23	0.53
1:D:120:TYR:OH	1:D:136:GLY:HA3	2.09	0.53
1:f:147:VAL:O	1:f:151:LEU:HG	2.09	0.53
2:X:201:2AN:H12	2:X:201:2AN:C2	2.37	0.53
1:T:30:VAL:CG1	2:T:203:2AN:C4	2.85	0.53
1:h:16:PRO:HB3	1:h:112:SER:HB3	1.90	0.53
1:h:33:LYS:CD	2:h:204:2AN:O3	2.56	0.53
1:A:129:ASN:CB	1:A:132:GLU:CB	2.87	0.53
1:J:6:ILE:HD13	1:I:2:ALA:HA	1.91	0.53
1:I:10:GLU:HG2	2:I:202:2AN:C12	2.39	0.53
1:I:158:PHE:CE2	2:I:207:2AN:H7	2.44	0.53
1:a:85:THR:HG23	1:a:100:VAL:HG23	1.91	0.53
1:Y:1:MET:HE2	1:Y:4:TYR:HA	1.89	0.53
2:V:204:2AN:N	2:V:204:2AN:S	2.69	0.53
1:S:27:ARG:O	1:S:31:LEU:HG	2.08	0.53
1:i:86:LEU:N	1:i:99:VAL:O	2.36	0.53
1:R:134:LYS:HG3	2:R:204:2AN:C14	2.39	0.52
1:N:6:ILE:HG23	1:M:0:THR:CG2	2.39	0.52
1:L:16:PRO:HB2	1:L:80:PHE:CE2	2.45	0.52
1:K:46:GLU:O	1:K:53:THR:HA	2.09	0.52
1:J:31:LEU:HD12	1:J:57:ILE:CD1	2.39	0.52
2:F:205:2AN:H16	2:F:205:2AN:C2	2.39	0.52
1:D:44:ILE:HD12	1:D:44:ILE:N	2.24	0.52
1:C:35:GLN:NE2	1:C:146:GLN:OE1	2.42	0.52
1:d:79:ASN:O	1:d:104:LYS:HE3	2.09	0.52
1:c:80:PHE:HB3	1:c:105:LEU:HB2	1.90	0.52
1:c:116:ILE:HD12	1:c:116:ILE:N	2.25	0.52
2:S:201:2AN:H16	2:S:201:2AN:C2	2.39	0.52
1:i:70:HIS:HA	1:i:85:THR:O	2.09	0.52
1:h:81:TYR:HB2	1:h:104:LYS:HD3	1.90	0.52
1:R:141:TYR:HB3	2:R:204:2AN:H4	1.90	0.52
1:K:18:ARG:HH12	1:K:155:PRO:HA	1.74	0.52
1:I:139:LYS:NZ	2:I:205:2AN:C13	2.72	0.52
1:e:69:LEU:HD12	1:e:88:GLU:OE1	2.10	0.52
1:a:6:ILE:HD12	1:a:118:VAL:O	2.09	0.52
2:a:203:2AN:N	2:a:203:2AN:O3	2.42	0.52
1:S:115:LYS:C	1:S:116:ILE:HD12	2.34	0.52
1:g:153:ALA:C	1:g:154:ASN:ND2	2.67	0.52
1:L:21:LYS:HG2	1:L:158:PHE:HB3	1.92	0.52
1:L:88:GLU:HA	1:L:92:LEU:CD2	2.40	0.52
1:I:23:LEU:HD21	1:I:147:VAL:HG21	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:65:LEU:HD21	1:G:91:VAL:HG13	1.86	0.52
1:d:51:VAL:HG23	1:d:75:ILE:HG12	1.92	0.52
2:Z:203:2AN:H12	2:Z:203:2AN:C2	2.38	0.52
1:X:4:TYR:O	1:X:119:THR:HA	2.09	0.52
1:g:127:THR:OG1	1:g:128:VAL:N	2.42	0.52
1:B:144:TYR:CZ	2:B:202:2AN:H15	2.44	0.52
1:Q:144:TYR:O	1:Q:147:VAL:N	2.43	0.52
1:J:139:LYS:HB3	2:J:203:2AN:C7	2.40	0.52
1:G:158:PHE:CE1	2:G:204:2AN:H15	2.45	0.52
1:b:149:GLU:O	1:b:150:TYR:C	2.53	0.52
1:Q:59:PHE:CD2	1:Q:63:HIS:ND1	2.76	0.52
1:P:77:ALA:HB3	2:V:201:2AN:H15	1.92	0.52
1:P:80:PHE:O	1:P:104:LYS:HA	2.10	0.52
1:P:120:TYR:OH	2:P:202:2AN:H14	2.10	0.52
1:L:97:GLU:OE1	1:L:123:LYS:HG2	2.10	0.52
1:K:80:PHE:HB2	1:K:105:LEU:O	2.09	0.52
1:I:63:HIS:HE2	2:I:205:2AN:C14	2.23	0.52
1:e:16:PRO:O	1:e:17:HIS:C	2.52	0.52
1:d:27:ARG:NH2	2:d:204:2AN:O1	2.42	0.52
1:S:69:LEU:HG	1:S:88:GLU:HB3	1.90	0.52
1:j:47:GLY:CA	2:j:201:2AN:C16	2.88	0.52
1:i:100:VAL:O	1:i:118:VAL:HA	2.09	0.52
1:R:16:PRO:HG3	1:R:107:ALA:HB2	1.92	0.52
1:R:60:VAL:HG23	1:R:63:HIS:H	1.75	0.52
1:N:17:HIS:HB2	5:N:206:DMS:H22	1.91	0.52
1:N:154:ASN:O	1:N:157:VAL:HG23	2.09	0.52
2:I:201:2AN:H16	2:I:201:2AN:C2	2.40	0.52
1:H:59:PHE:CZ	1:H:68:MET:HE2	2.44	0.52
1:H:154:ASN:N	1:H:154:ASN:ND2	2.58	0.52
1:c:20:PHE:CD1	1:c:24:VAL:HG11	2.44	0.52
1:a:30:VAL:O	1:a:31:LEU:C	2.52	0.52
1:W:96:ILE:H	1:W:123:LYS:H	1.53	0.52
1:i:13:PRO:HD3	1:i:148:GLU:OE2	2.06	0.52
1:B:44:ILE:HG13	1:B:55:THR:HG22	1.91	0.52
1:A:82:CYS:O	1:A:102:GLU:HA	2.09	0.52
1:N:15:ALA:HB1	1:N:17:HIS:CE1	2.44	0.52
1:J:0:THR:HG21	1:I:7:VAL:O	2.10	0.52
1:H:38:VAL:C	1:H:60:VAL:HG13	2.35	0.52
1:F:43:GLU:HG3	1:F:56:LYS:HB3	1.91	0.52
1:D:65:LEU:HD21	1:D:91:VAL:CA	2.40	0.52
1:D:153:ALA:O	1:D:155:PRO:HD3	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:d:55:THR:O	1:d:69:LEU:HA	2.09	0.52
1:c:3:ALA:HB1	1:c:120:TYR:O	2.10	0.52
1:Z:20:PHE:HB2	1:Z:105:LEU:HD12	1.91	0.52
1:X:23:LEU:O	2:X:206:2AN:H4	2.10	0.52
1:U:145:LYS:O	1:U:148:GLU:N	2.43	0.52
2:j:205:2AN:O3	2:j:205:2AN:C12	2.58	0.52
2:j:205:2AN:C16	2:j:205:2AN:H2	2.39	0.52
1:A:86:LEU:HD12	1:A:86:LEU:C	2.34	0.52
1:Q:63:HIS:CE1	1:Q:65:LEU:HB2	2.44	0.52
1:O:18:ARG:HG2	1:O:158:PHE:O	2.09	0.52
1:F:49:GLY:N	1:F:53:THR:OG1	2.43	0.52
2:E:202:2AN:C2	2:E:202:2AN:C12	2.84	0.52
1:C:85:THR:HG23	1:C:99:VAL:O	2.09	0.52
1:d:51:VAL:HG23	1:d:75:ILE:CG1	2.40	0.52
2:c:202:2AN:H2	2:c:202:2AN:C16	2.24	0.52
1:W:12:SER:HB3	1:W:19:LEU:HD11	1.91	0.52
1:W:120:TYR:CE2	1:W:133:VAL:HG22	2.44	0.52
1:V:129:ASN:HB3	1:V:132:GLU:H	1.75	0.52
1:R:108:VAL:O	1:R:109:GLY:C	2.53	0.52
1:R:135:ILE:HG21	2:R:205:2AN:H4	1.92	0.52
1:F:35:GLN:C	1:F:37:HIS:H	2.18	0.52
1:C:128:VAL:HG12	1:C:130:GLU:H	1.75	0.52
1:g:18:ARG:HG2	1:g:158:PHE:O	2.10	0.52
1:A:108:VAL:O	1:A:108:VAL:HG12	2.09	0.52
1:K:95:ASN:HB2	1:K:127:THR:O	2.09	0.52
1:G:41:SER:CB	1:G:58:THR:OG1	2.58	0.52
1:G:46:GLU:CB	1:G:54:VAL:HG13	2.38	0.52
1:F:140:ALA:HB3	2:F:201:2AN:C7	2.40	0.52
1:D:59:PHE:CZ	1:D:68:MET:HE2	2.45	0.52
2:d:203:2AN:H16	2:d:203:2AN:C2	2.39	0.52
1:U:11:GLU:CB	1:U:113:LYS:HA	2.38	0.52
1:T:89:GLY:O	1:T:92:LEU:HB2	2.09	0.52
1:h:33:LYS:NZ	2:h:204:2AN:C11	2.73	0.52
1:P:44:ILE:HA	1:P:55:THR:HA	1.90	0.51
1:M:143:PHE:O	1:M:146:GLN:HB2	2.10	0.51
1:K:8:LYS:HE3	7:K:303:HOH:O	2.11	0.51
1:J:10:GLU:C	1:J:11:GLU:HG3	2.35	0.51
1:f:21:LYS:HG2	1:f:25:LEU:HD12	1.92	0.51
1:Z:142:GLU:HG2	2:Z:206:2AN:H7	1.92	0.51
1:W:96:ILE:HG12	1:W:122:PRO:HA	1.92	0.51
1:U:27:ARG:HE	2:U:202:2AN:C13	2.23	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:T:19:LEU:O	1:T:23:LEU:HB2	2.11	0.51
1:T:23:LEU:HB3	2:T:201:2AN:C3	2.40	0.51
1:T:63:HIS:CD2	1:T:65:LEU:HB2	2.45	0.51
2:h:201:2AN:H16	2:h:201:2AN:C2	2.40	0.51
1:A:105:LEU:HD23	1:A:114:GLY:CA	2.40	0.51
1:M:96:ILE:CD1	1:M:128:VAL:HG13	2.40	0.51
1:H:28:HIS:CD2	1:H:29:GLN:HG2	2.46	0.51
1:G:72:PHE:CD1	1:G:84:TYR:HB3	2.46	0.51
1:f:108:VAL:HG13	1:f:108:VAL:O	2.10	0.51
1:f:149:GLU:O	1:f:150:TYR:C	2.53	0.51
1:d:99:VAL:HG22	1:d:120:TYR:CD1	2.45	0.51
1:Z:15:ALA:HB3	1:Z:18:ARG:HD3	1.92	0.51
1:V:142:GLU:CD	2:V:208:2AN:C11	2.83	0.51
1:U:129:ASN:HB2	1:U:131:GLU:HG2	1.92	0.51
1:g:116:ILE:N	1:g:116:ILE:HD12	2.25	0.51
1:O:51:VAL:O	1:O:72:PHE:O	2.27	0.51
1:G:68:MET:CE	1:G:91:VAL:HG21	2.40	0.51
1:b:20:PHE:HB2	1:b:105:LEU:HD12	1.91	0.51
1:b:131:GLU:HG3	1:b:132:GLU:H	1.73	0.51
1:X:27:ARG:CZ	2:X:206:2AN:H6	2.39	0.51
1:W:116:ILE:N	1:W:116:ILE:HD12	2.26	0.51
1:i:18:ARG:NH1	7:i:302:HOH:O	2.26	0.51
1:i:26:GLU:O	1:i:30:VAL:HB	2.10	0.51
1:B:44:ILE:N	1:B:44:ILE:CD1	2.73	0.51
1:J:104:LYS:C	1:J:105:LEU:HD23	2.35	0.51
1:E:10:GLU:HG3	2:E:201:2AN:H13	1.91	0.51
1:D:147:VAL:O	1:D:150:TYR:N	2.43	0.51
2:b:206:2AN:O3	2:b:206:2AN:N	2.43	0.51
1:Z:58:THR:HG22	1:Z:59:PHE:O	2.10	0.51
1:Y:2:ALA:O	1:Y:122:PRO:CD	2.58	0.51
1:X:17:HIS:NE2	1:X:159:ALA:OXT	2.43	0.51
1:h:151:LEU:O	1:h:152:ALA:C	2.53	0.51
1:Q:54:VAL:HA	1:Q:70:HIS:O	2.10	0.51
1:Q:109:GLY:O	1:S:80:PHE:CZ	2.64	0.51
1:N:26:GLU:O	1:N:27:ARG:C	2.52	0.51
1:I:65:LEU:CD1	2:I:205:2AN:H16	2.41	0.51
1:D:51:VAL:HG22	1:D:75:ILE:HB	1.93	0.51
1:a:140:ALA:HB1	2:a:204:2AN:C2	2.41	0.51
2:V:208:2AN:C12	2:V:208:2AN:O1	2.59	0.51
1:A:15:ALA:HA	3:A:205:SO4:O4	2.11	0.51
1:Q:46:GLU:O	1:Q:53:THR:HG23	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:16:PRO:CG	1:O:107:ALA:HB2	2.41	0.51
1:O:66:THR:HG22	1:O:67:TYR:HD1	1.75	0.51
1:O:68:MET:HE1	2:O:203:2AN:O3	2.11	0.51
1:M:67:TYR:CZ	1:M:89:GLY:HA2	2.44	0.51
1:F:130:GLU:CD	1:F:130:GLU:C	2.79	0.51
1:E:107:ALA:HB2	1:e:107:ALA:CB	2.40	0.51
1:D:4:TYR:CZ	1:C:2:ALA:HB1	2.45	0.51
1:D:69:LEU:HD11	1:D:87:PHE:CZ	2.45	0.51
1:C:3:ALA:HB1	1:C:120:TYR:O	2.10	0.51
1:f:19:LEU:HG	1:f:23:LEU:HD12	1.93	0.51
1:f:130:GLU:OE1	1:f:130:GLU:HA	2.10	0.51
2:f:203:2AN:C2	2:f:203:2AN:C16	2.87	0.51
1:d:3:ALA:HB1	1:d:120:TYR:O	2.11	0.51
1:X:144:TYR:CD1	1:X:144:TYR:O	2.64	0.51
2:V:205:2AN:C8	2:V:208:2AN:C7	2.89	0.51
1:A:135:ILE:N	1:A:135:ILE:HD12	2.26	0.51
1:P:120:TYR:OH	2:P:202:2AN:C14	2.59	0.51
1:I:53:THR:HB	1:I:72:PHE:CD2	2.46	0.51
1:D:129:ASN:CB	1:D:132:GLU:CD	2.84	0.51
2:C:202:2AN:S	2:C:202:2AN:N	2.81	0.51
1:a:141:TYR:CD1	2:a:204:2AN:H14	2.46	0.51
2:X:201:2AN:H2	2:X:201:2AN:C12	2.36	0.51
1:V:81:TYR:C	1:V:81:TYR:CD2	2.89	0.51
1:T:40:LYS:N	1:T:58:THR:O	2.40	0.51
1:j:18:ARG:NE	1:j:157:VAL:O	2.43	0.51
1:j:85:THR:HG23	1:j:100:VAL:HG22	1.92	0.51
1:h:46:GLU:HB2	1:h:54:VAL:HB	1.92	0.51
1:R:8:LYS:HB2	1:R:116:ILE:HD13	1.92	0.51
1:R:96:ILE:C	1:R:123:LYS:HG3	2.35	0.51
1:P:135:ILE:O	1:P:136:GLY:C	2.52	0.51
2:O:201:2AN:O2	2:O:201:2AN:H16	2.10	0.51
1:M:104:LYS:C	1:M:105:LEU:HD23	2.35	0.51
1:I:5:THR:HA	1:I:119:THR:HA	1.92	0.51
1:C:101:TYR:CZ	7:C:302:HOH:O	2.51	0.51
1:C:142:GLU:O	1:C:146:GLN:HG3	2.10	0.51
2:B:206:2AN:H2	2:B:206:2AN:C12	2.40	0.51
1:H:83:LYS:HA	1:H:101:TYR:O	2.11	0.51
2:G:204:2AN:O3	2:G:204:2AN:N	2.39	0.51
2:D:203:2AN:H2	2:D:203:2AN:C16	2.40	0.51
1:f:69:LEU:O	1:f:86:LEU:HD12	2.11	0.51
1:c:8:LYS:HE2	1:c:10:GLU:OE2	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Y:39:PHE:HA	1:Y:59:PHE:HA	1.93	0.51
1:X:4:TYR:CZ	1:W:4:TYR:CE2	2.98	0.51
1:B:44:ILE:HG23	1:B:53:THR:HG22	1.93	0.51
1:R:69:LEU:CD1	1:R:88:GLU:OE1	2.58	0.51
1:I:95:ASN:OD1	1:I:95:ASN:N	2.43	0.51
1:f:129:ASN:ND2	1:f:132:GLU:CB	2.74	0.51
1:b:92:LEU:O	1:b:93:ARG:CB	2.58	0.51
1:Y:5:THR:CG2	1:Y:117:THR:HG22	2.41	0.51
1:N:129:ASN:ND2	1:N:132:GLU:CB	2.74	0.50
1:e:120:TYR:O	1:e:122:PRO:HD3	2.11	0.50
1:b:69:LEU:HB2	1:b:88:GLU:HB3	1.93	0.50
1:X:10:GLU:HG2	2:X:206:2AN:C12	2.40	0.50
1:T:79:ASN:HB3	1:T:104:LYS:HZ2	1.75	0.50
1:A:53:THR:OG1	1:A:72:PHE:HD2	1.94	0.50
2:A:202:2AN:C2	2:A:202:2AN:C12	2.80	0.50
1:R:10:GLU:HB3	2:R:201:2AN:C15	2.42	0.50
1:L:68:MET:HB3	1:L:70:HIS:CE1	2.46	0.50
1:L:92:LEU:N	1:L:92:LEU:CD1	2.73	0.50
1:F:84:TYR:HH	2:F:201:2AN:H4	1.76	0.50
2:D:203:2AN:C2	2:D:203:2AN:C16	2.89	0.50
2:Y:202:2AN:O2	2:Y:202:2AN:N	2.30	0.50
1:W:43:GLU:O	1:W:55:THR:HA	2.11	0.50
1:U:13:PRO:C	1:U:14:ILE:HD12	2.36	0.50
1:h:68:MET:HA	1:h:88:GLU:O	2.11	0.50
1:g:149:GLU:OE1	1:g:149:GLU:O	2.29	0.50
1:A:68:MET:CE	1:A:91:VAL:HG21	2.40	0.50
1:G:16:PRO:HB3	1:G:105:LEU:HD12	1.93	0.50
1:D:120:TYR:CE1	1:D:133:VAL:HG13	2.46	0.50
1:C:71:LYS:HB2	1:C:87:PHE:CE1	2.47	0.50
1:b:2:ALA:CB	1:a:4:TYR:HE1	2.24	0.50
1:X:4:TYR:CE2	1:W:4:TYR:OH	2.65	0.50
1:X:6:ILE:O	1:X:117:THR:HA	2.10	0.50
2:V:207:2AN:N	2:V:207:2AN:S	2.74	0.50
2:T:202:2AN:H16	2:T:202:2AN:H2	1.92	0.50
2:R:203:2AN:H12	2:R:203:2AN:C2	2.40	0.50
1:P:30:VAL:HA	1:P:33:LYS:HG3	1.94	0.50
1:O:144:TYR:OH	1:O:148:GLU:OE1	2.23	0.50
1:I:23:LEU:CD2	1:I:147:VAL:HG21	2.41	0.50
2:I:206:2AN:C2	2:I:206:2AN:C16	2.80	0.50
1:E:63:HIS:O	1:E:64:PRO:C	2.55	0.50
2:E:204:2AN:N	2:E:204:2AN:O1	2.44	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:69:LEU:C	1:D:69:LEU:CD1	2.84	0.50
1:f:2:ALA:HB2	1:e:4:TYR:OH	2.12	0.50
1:d:14:ILE:HG21	1:d:151:LEU:HD12	1.92	0.50
2:b:203:2AN:H2	2:b:203:2AN:C12	2.41	0.50
1:Y:41:SER:HB2	1:Y:43:GLU:OE1	2.11	0.50
1:X:60:VAL:HG12	1:X:61:ASP:H	1.77	0.50
1:U:84:TYR:O	1:U:101:TYR:N	2.34	0.50
1:U:143:PHE:O	1:U:147:VAL:HG23	2.11	0.50
2:T:204:2AN:H12	2:T:204:2AN:C2	2.34	0.50
2:S:201:2AN:C2	2:S:201:2AN:C16	2.83	0.50
1:j:63:HIS:ND1	1:j:64:PRO:CD	2.72	0.50
1:j:90:ASP:OD1	1:j:90:ASP:N	2.39	0.50
1:i:44:ILE:HG12	1:i:55:THR:HG22	1.94	0.50
2:B:203:2AN:N	2:B:203:2AN:O1	2.44	0.50
1:A:122:PRO:HB3	1:A:126:CYS:SG	2.52	0.50
1:d:144:TYR:CD2	2:d:201:2AN:O1	2.65	0.50
1:b:18:ARG:NH2	1:b:155:PRO:HA	2.27	0.50
1:X:144:TYR:CE1	2:X:206:2AN:H15	2.46	0.50
1:X:147:VAL:HG22	2:X:202:2AN:H14	1.93	0.50
1:V:77:ALA:HB1	2:V:204:2AN:H2	1.94	0.50
1:U:11:GLU:O	1:U:11:GLU:HG3	2.11	0.50
1:U:138:LYS:HA	2:U:201:2AN:C3	2.41	0.50
1:T:53:THR:HB	1:T:72:PHE:CD1	2.47	0.50
1:i:28:HIS:NE2	1:i:55:THR:HG21	2.26	0.50
1:B:144:TYR:O	1:B:145:LYS:C	2.51	0.50
2:L:202:2AN:H2	2:L:202:2AN:C12	2.25	0.50
1:C:155:PRO:O	1:C:159:ALA:HB2	2.12	0.50
1:f:47:GLY:CA	2:f:203:2AN:H2	2.41	0.50
1:d:129:ASN:C	1:d:131:GLU:N	2.68	0.50
1:c:105:LEU:HD23	1:c:114:GLY:CA	2.41	0.50
1:T:33:LYS:HD2	2:T:203:2AN:N	2.26	0.50
1:j:130:GLU:O	1:j:133:VAL:HB	2.11	0.50
1:h:91:VAL:O	1:h:132:GLU:OE2	2.30	0.50
1:g:48:ASP:C	1:g:48:ASP:OD1	2.55	0.50
1:g:69:LEU:HD12	1:g:88:GLU:HB3	1.92	0.50
2:B:202:2AN:H2	2:B:202:2AN:C12	2.42	0.50
1:N:139:LYS:HE3	2:N:205:2AN:C9	2.42	0.50
1:K:21:LYS:O	1:K:26:GLU:CB	2.59	0.50
1:H:32:VAL:HG22	1:H:39:PHE:HB2	1.93	0.50
1:F:140:ALA:N	2:F:202:2AN:O3	2.45	0.50
1:E:73:ASP:HB2	1:E:83:LYS:HG2	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:137:GLU:OE1	1:C:0:THR:CG2	2.59	0.50
1:f:34:ALA:HB3	1:f:143:PHE:HE1	1.77	0.50
1:c:108:VAL:O	1:c:108:VAL:HG12	2.12	0.50
1:Z:105:LEU:HD23	1:Z:114:GLY:HA3	1.93	0.50
1:Y:18:ARG:NH1	1:Y:157:VAL:O	2.40	0.50
1:W:139:LYS:HD3	2:W:201:2AN:C4	2.41	0.50
1:U:39:PHE:HE2	2:U:202:2AN:C4	2.25	0.50
2:j:202:2AN:C2	2:j:202:2AN:H12	2.42	0.50
1:h:129:ASN:C	1:h:131:GLU:N	2.69	0.50
1:h:151:LEU:C	1:h:153:ALA:N	2.69	0.50
2:h:204:2AN:H16	2:h:204:2AN:C2	2.24	0.50
1:P:43:GLU:OE2	7:P:301:HOH:O	2.20	0.50
1:P:95:ASN:OD1	1:P:95:ASN:N	2.45	0.50
1:I:110:GLY:HA2	1:a:17:HIS:CG	2.47	0.50
1:C:132:GLU:H	1:C:132:GLU:CD	2.16	0.50
1:e:18:ARG:O	1:e:19:LEU:C	2.53	0.50
1:Z:76:ASP:HB3	1:Z:81:TYR:HB3	1.94	0.50
1:W:47:GLY:HA3	1:W:53:THR:HG23	1.94	0.50
1:P:23:LEU:HD22	1:P:143:PHE:CE2	2.46	0.50
1:O:101:TYR:CE1	2:O:201:2AN:H13	2.47	0.50
1:N:69:LEU:CB	1:N:88:GLU:HB3	2.41	0.50
1:G:136:GLY:O	1:G:137:GLU:C	2.55	0.50
1:D:62:GLY:O	1:D:63:HIS:C	2.55	0.50
1:f:129:ASN:O	1:f:130:GLU:C	2.53	0.50
2:f:204:2AN:O3	2:f:204:2AN:C12	2.60	0.50
2:f:206:2AN:H2	2:f:206:2AN:C12	2.40	0.50
2:c:206:2AN:S	2:c:206:2AN:N	2.85	0.50
2:b:201:2AN:O1	2:b:201:2AN:N	2.36	0.50
1:S:86:LEU:N	1:S:99:VAL:O	2.42	0.50
1:j:33:LYS:HB3	2:j:204:2AN:O3	2.12	0.50
1:h:92:LEU:HD23	1:h:96:ILE:HG22	1.93	0.50
1:g:84:TYR:CE1	1:g:101:TYR:CD2	3.00	0.50
1:N:70:HIS:HA	1:N:85:THR:O	2.12	0.49
1:K:143:PHE:O	1:K:146:GLN:HB2	2.12	0.49
1:J:12:SER:CB	1:J:19:LEU:HD11	2.42	0.49
1:G:18:ARG:NH1	1:G:155:PRO:O	2.45	0.49
1:c:149:GLU:C	1:c:149:GLU:OE1	2.55	0.49
1:Y:44:ILE:HG12	1:Y:55:THR:HG22	1.92	0.49
1:Y:59:PHE:CZ	1:Y:65:LEU:CD1	2.96	0.49
1:W:23:LEU:O	1:W:27:ARG:NH1	2.41	0.49
1:V:14:ILE:O	1:V:112:SER:OG	2.25	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:V:90:ASP:O	1:V:91:VAL:C	2.55	0.49
1:T:55:THR:HG23	1:T:72:PHE:CE1	2.47	0.49
1:S:106:GLU:CD	1:S:113:LYS:HB2	2.38	0.49
1:h:33:LYS:HZ3	2:h:204:2AN:C12	2.24	0.49
1:B:81:TYR:CD1	1:B:81:TYR:C	2.89	0.49
1:A:1:MET:SD	1:A:1:MET:N	2.85	0.49
1:Q:141:TYR:O	1:Q:145:LYS:HG2	2.12	0.49
1:L:26:GLU:O	1:L:27:ARG:C	2.54	0.49
1:H:99:VAL:HA	1:H:119:THR:O	2.12	0.49
1:D:97:GLU:CA	1:D:123:LYS:HG2	2.42	0.49
1:d:18:ARG:NH2	1:d:154:ASN:O	2.45	0.49
1:b:5:THR:HG22	1:b:7:VAL:HG23	1.94	0.49
1:Z:85:THR:OG1	1:Z:100:VAL:HG22	2.11	0.49
1:W:120:TYR:CE2	1:W:133:VAL:HG13	2.47	0.49
1:V:105:LEU:C	1:V:106:GLU:HG2	2.37	0.49
1:U:35:GLN:C	1:U:37:HIS:H	2.19	0.49
1:U:103:VAL:HG22	1:U:116:ILE:HB	1.93	0.49
2:T:201:2AN:C2	2:T:201:2AN:C16	2.80	0.49
1:i:141:TYR:O	1:i:144:TYR:N	2.45	0.49
1:Q:59:PHE:HD1	1:Q:66:THR:C	2.21	0.49
1:P:138:LYS:HZ1	4:P:205:EPE:C6	2.17	0.49
1:M:23:LEU:HD21	1:M:147:VAL:CG2	2.42	0.49
1:K:5:THR:OG1	1:K:119:THR:HG23	2.12	0.49
1:I:31:LEU:CD1	1:I:57:ILE:HD13	2.41	0.49
1:I:77:ALA:HB3	2:I:203:2AN:H16	1.92	0.49
2:I:201:2AN:C2	2:I:201:2AN:C16	2.88	0.49
1:e:13:PRO:HD2	1:e:148:GLU:OE1	2.13	0.49
1:e:15:ALA:HB1	1:e:16:PRO:HD2	1.94	0.49
1:d:55:THR:OG1	1:d:70:HIS:HB2	2.13	0.49
1:d:92:LEU:C	1:d:94:ASP:H	2.20	0.49
1:X:4:TYR:CE2	1:W:4:TYR:CZ	3.00	0.49
1:W:96:ILE:HA	1:W:122:PRO:C	2.37	0.49
1:W:129:ASN:O	1:W:131:GLU:N	2.45	0.49
1:V:47:GLY:CA	2:V:201:2AN:C12	2.87	0.49
1:U:69:LEU:HB3	1:U:87:PHE:CZ	2.47	0.49
1:i:34:ALA:CB	1:i:143:PHE:HE1	2.25	0.49
1:h:33:LYS:HD3	2:h:204:2AN:C1	2.42	0.49
1:g:38:VAL:C	1:g:60:VAL:HG13	2.37	0.49
1:O:56:LYS:O	1:O:57:ILE:HD13	2.12	0.49
1:N:6:ILE:CG2	1:M:0:THR:CB	2.88	0.49
1:M:3:ALA:HB1	1:M:120:TYR:O	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:76:ASP:OD1	1:D:78:ALA:HB3	2.12	0.49
1:C:18:ARG:HH22	1:C:155:PRO:HA	1.76	0.49
1:C:122:PRO:HB3	1:C:128:VAL:HG23	1.93	0.49
1:f:45:ILE:HD12	1:f:46:GLU:HB2	1.94	0.49
1:e:57:ILE:O	1:e:67:TYR:HB2	2.11	0.49
1:U:105:LEU:CD2	1:U:113:LYS:O	2.59	0.49
2:T:203:2AN:H12	2:T:203:2AN:C2	2.29	0.49
1:L:81:TYR:HB2	1:L:104:LYS:HD3	1.94	0.49
2:G:203:2AN:C2	2:G:203:2AN:C16	2.74	0.49
1:F:138:LYS:HG2	2:F:204:2AN:C1	2.42	0.49
1:E:32:VAL:HA	1:E:39:PHE:HB2	1.93	0.49
1:C:39:PHE:C	1:C:60:VAL:HG13	2.38	0.49
1:C:57:ILE:HB	1:C:68:MET:HG2	1.94	0.49
1:a:44:ILE:HA	1:a:55:THR:HA	1.95	0.49
2:X:203:2AN:C2	2:X:203:2AN:C16	2.90	0.49
1:V:46:GLU:O	1:V:54:VAL:N	2.36	0.49
1:S:145:LYS:HD2	1:S:148:GLU:OE1	2.13	0.49
1:i:68:MET:HG2	1:i:91:VAL:HG11	1.93	0.49
1:h:102:GLU:HB3	1:h:117:THR:HB	1.95	0.49
1:A:106:GLU:O	1:A:108:VAL:HG23	2.13	0.49
1:A:148:GLU:O	1:A:152:ALA:N	2.35	0.49
1:P:117:THR:O	1:P:117:THR:HG22	2.13	0.49
1:N:6:ILE:HD11	1:N:133:VAL:CG1	2.42	0.49
1:M:83:LYS:HG3	1:M:102:GLU:HG3	1.94	0.49
1:L:16:PRO:HD3	1:L:112:SER:HB3	1.94	0.49
2:L:204:2AN:C13	1:Z:47:GLY:HA2	2.40	0.49
1:J:87:PHE:CD2	1:J:88:GLU:HB2	2.48	0.49
1:F:57:ILE:HB	1:F:68:MET:HG3	1.94	0.49
1:f:83:LYS:HA	1:f:101:TYR:O	2.11	0.49
1:b:69:LEU:HD12	1:b:88:GLU:HB3	1.94	0.49
1:X:13:PRO:O	1:X:111:GLY:HA3	2.12	0.49
1:U:45:ILE:HG12	1:U:54:VAL:O	2.13	0.49
1:T:56:LYS:HA	1:T:68:MET:O	2.11	0.49
1:h:131:GLU:HG2	1:h:132:GLU:N	2.26	0.49
1:B:17:HIS:HB3	1:h:109:GLY:O	2.13	0.49
1:B:47:GLY:HA3	1:B:53:THR:HG23	1.94	0.49
1:A:116:ILE:HG22	1:A:118:VAL:HG23	1.95	0.49
1:J:37:HIS:O	1:J:60:VAL:HG11	2.13	0.49
1:H:18:ARG:NH2	1:H:151:LEU:O	2.42	0.49
1:F:141:TYR:CD1	2:F:201:2AN:O1	2.54	0.49
1:C:135:ILE:O	1:C:139:LYS:CG	2.54	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:d:51:VAL:N	1:d:75:ILE:HG21	2.27	0.49
1:a:25:LEU:C	1:a:26:GLU:OE1	2.55	0.49
2:j:205:2AN:H16	2:j:205:2AN:H2	1.90	0.49
1:Q:71:LYS:HB2	1:Q:87:PHE:HE2	1.78	0.49
1:L:54:VAL:HG22	1:L:71:LYS:HB3	1.94	0.49
1:H:72:PHE:CD2	1:H:75:ILE:HD11	2.47	0.49
1:F:95:ASN:HD21	1:F:129:ASN:HB2	1.77	0.49
1:F:140:ALA:CA	2:F:202:2AN:H8	2.43	0.49
1:U:39:PHE:CE2	2:U:202:2AN:C4	2.95	0.49
1:j:2:ALA:CB	1:i:4:TYR:CZ	2.95	0.49
2:P:201:2AN:N	2:P:201:2AN:S	2.86	0.49
1:N:100:VAL:HB	1:N:119:THR:HB	1.95	0.49
1:M:59:PHE:O	1:M:60:VAL:C	2.56	0.49
1:F:108:VAL:HG22	1:F:108:VAL:O	2.12	0.49
1:F:131:GLU:O	1:F:135:ILE:CB	2.61	0.49
1:D:47:GLY:HA3	1:D:53:THR:HG23	1.94	0.49
1:C:132:GLU:O	1:C:136:GLY:N	2.44	0.49
1:V:51:VAL:HG23	1:V:75:ILE:HG22	1.95	0.49
1:T:30:VAL:HG13	2:T:203:2AN:C3	2.43	0.49
1:S:31:LEU:HD23	1:S:143:PHE:CD1	2.48	0.49
1:S:95:ASN:OD1	1:S:95:ASN:N	2.33	0.49
1:S:129:ASN:O	1:S:130:GLU:C	2.56	0.49
1:i:73:ASP:O	1:i:74:GLU:HG3	2.13	0.49
1:g:31:LEU:HD23	1:g:143:PHE:CD1	2.48	0.49
1:P:87:PHE:O	1:P:88:GLU:HG3	2.13	0.49
1:P:88:GLU:HA	1:P:92:LEU:HD12	1.94	0.49
1:P:99:VAL:HA	1:P:119:THR:O	2.12	0.49
1:N:69:LEU:N	1:N:88:GLU:O	2.46	0.49
1:N:92:LEU:HD22	1:N:96:ILE:HG22	1.95	0.49
1:G:108:VAL:O	1:G:108:VAL:CG2	2.60	0.49
1:e:69:LEU:HD12	1:e:88:GLU:HB3	1.95	0.49
1:a:65:LEU:HD11	1:a:91:VAL:HG23	1.94	0.49
1:Z:77:ALA:HB1	2:Z:202:2AN:C2	2.43	0.49
1:g:51:VAL:HG22	1:g:74:GLU:HA	1.95	0.49
2:B:204:2AN:C2	1:j:77:ALA:HB1	2.43	0.48
2:R:204:2AN:O1	2:R:204:2AN:N	2.36	0.48
1:L:101:TYR:HD1	1:L:118:VAL:HG22	1.77	0.48
1:F:14:ILE:HG21	1:F:151:LEU:HD13	1.94	0.48
2:f:206:2AN:N	2:f:206:2AN:S	2.85	0.48
1:d:32:VAL:C	1:d:33:LYS:HE3	2.37	0.48
1:c:142:GLU:O	1:c:146:GLN:HG3	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:56:LYS:HA	1:U:69:LEU:HD23	1.94	0.48
1:P:137:GLU:OE2	1:O:1:MET:SD	2.71	0.48
1:N:4:TYR:OH	1:M:2:ALA:HB2	2.13	0.48
1:M:14:ILE:HG22	1:M:15:ALA:O	2.14	0.48
1:L:158:PHE:CE1	2:L:202:2AN:H13	2.48	0.48
1:G:23:LEU:N	1:G:23:LEU:CD2	2.74	0.48
2:G:204:2AN:N	2:G:204:2AN:O1	2.46	0.48
1:C:0:THR:O	1:C:0:THR:CG2	2.60	0.48
1:f:80:PHE:HB3	1:f:105:LEU:HB2	1.95	0.48
1:e:43:GLU:O	1:e:55:THR:HA	2.14	0.48
1:c:21:LYS:CG	1:c:158:PHE:CD1	2.96	0.48
2:b:205:2AN:C2	2:b:205:2AN:C16	2.88	0.48
1:a:142:GLU:O	1:a:146:GLN:HG3	2.13	0.48
1:X:32:VAL:O	1:X:32:VAL:CG1	2.60	0.48
1:W:139:LYS:CD	2:W:201:2AN:C4	2.91	0.48
1:T:3:ALA:O	1:S:4:TYR:HA	2.13	0.48
1:B:20:PHE:CE1	1:B:80:PHE:HA	2.48	0.48
2:B:205:2AN:C12	2:B:205:2AN:H2	2.43	0.48
1:J:96:ILE:HG22	1:J:121:HIS:O	2.13	0.48
1:F:140:ALA:CB	2:F:201:2AN:C7	2.92	0.48
1:E:14:ILE:O	1:E:15:ALA:C	2.54	0.48
1:f:129:ASN:C	1:f:131:GLU:N	2.69	0.48
1:c:63:HIS:HE1	1:c:65:LEU:HD12	1.78	0.48
1:b:138:LYS:CB	2:b:205:2AN:O3	2.61	0.48
1:T:6:ILE:HD12	1:T:6:ILE:N	2.28	0.48
1:S:92:LEU:O	1:S:93:ARG:HB2	2.13	0.48
1:S:120:TYR:CZ	1:S:133:VAL:HG22	2.49	0.48
1:h:35:GLN:HE21	1:h:146:GLN:NE2	2.10	0.48
1:h:154:ASN:N	1:h:154:ASN:ND2	2.61	0.48
1:g:63:HIS:CE1	1:g:65:LEU:HG	2.49	0.48
1:A:136:GLY:HA2	2:A:202:2AN:C13	2.44	0.48
1:O:74:GLU:HB2	1:O:83:LYS:HB3	1.94	0.48
1:N:39:PHE:CE1	1:N:59:PHE:CE1	3.01	0.48
2:N:203:2AN:C16	2:N:203:2AN:C2	2.84	0.48
1:M:86:LEU:HD21	1:M:91:VAL:HG11	1.94	0.48
1:G:139:LYS:O	1:G:142:GLU:HB3	2.13	0.48
1:F:15:ALA:HB1	1:F:17:HIS:CD2	2.49	0.48
1:D:158:PHE:CE1	2:D:203:2AN:H15	2.44	0.48
1:f:-1:PHE:HE2	1:e:134:LYS:O	1.96	0.48
1:d:-2:PRO:HB3	1:c:134:LYS:HB3	1.96	0.48
2:a:201:2AN:C2	2:a:201:2AN:C16	2.75	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Y:108:VAL:O	1:Y:108:VAL:HG12	2.11	0.48
1:X:152:ALA:O	1:X:153:ALA:C	2.56	0.48
1:V:144:TYR:O	1:V:144:TYR:HD1	1.96	0.48
1:h:37:HIS:CD2	1:h:38:VAL:HG23	2.48	0.48
1:h:53:THR:HB	1:h:72:PHE:CD1	2.49	0.48
1:h:123:LYS:C	1:h:126:CYS:HG	2.22	0.48
1:L:116:ILE:N	1:L:116:ILE:HD12	2.28	0.48
1:K:32:VAL:HG22	1:K:39:PHE:HB3	1.95	0.48
2:J:203:2AN:C2	2:J:203:2AN:H12	2.44	0.48
1:D:92:LEU:CA	1:D:96:ILE:HB	2.43	0.48
1:C:18:ARG:NH1	1:C:157:VAL:O	2.46	0.48
1:C:80:PHE:HB3	1:C:105:LEU:HB2	1.94	0.48
1:d:18:ARG:O	1:d:22:ALA:N	2.47	0.48
1:d:31:LEU:HD23	1:d:143:PHE:CE1	2.47	0.48
1:d:70:HIS:CE1	2:d:204:2AN:C8	2.95	0.48
1:d:93:ARG:NH1	1:d:131:GLU:OE1	2.47	0.48
1:b:96:ILE:HD13	1:b:122:PRO:HB3	1.95	0.48
1:a:115:LYS:C	1:a:116:ILE:HD12	2.38	0.48
2:X:204:2AN:H16	2:X:204:2AN:C2	2.26	0.48
1:W:92:LEU:O	1:W:93:ARG:O	2.31	0.48
1:V:46:GLU:O	1:V:53:THR:HA	2.14	0.48
1:U:103:VAL:CG1	1:U:116:ILE:CG2	2.80	0.48
1:N:20:PHE:O	1:N:24:VAL:HB	2.13	0.48
1:N:153:ALA:O	1:N:155:PRO:HD3	2.14	0.48
1:I:10:GLU:HG2	2:I:202:2AN:H12	1.95	0.48
1:I:71:LYS:HB2	1:I:87:PHE:CE2	2.49	0.48
2:H:202:2AN:C2	2:H:202:2AN:C16	2.85	0.48
1:G:23:LEU:HD12	2:G:203:2AN:C16	2.44	0.48
1:f:8:LYS:O	1:f:115:LYS:HA	2.13	0.48
1:e:8:LYS:O	1:e:115:LYS:HA	2.11	0.48
1:d:131:GLU:O	1:d:132:GLU:C	2.56	0.48
1:a:12:SER:OG	1:a:13:PRO:HD2	2.14	0.48
1:Y:93:ARG:HE	2:Y:204:2AN:C11	2.27	0.48
1:j:31:LEU:CD1	1:j:57:ILE:HD13	2.44	0.48
1:g:50:GLY:H	1:g:53:THR:HG1	1.59	0.48
1:K:85:THR:HG21	1:K:98:LYS:HD2	1.94	0.48
1:H:136:GLY:O	1:H:137:GLU:C	2.57	0.48
1:C:30:VAL:O	1:C:32:VAL:N	2.47	0.48
1:e:18:ARG:HG2	1:e:158:PHE:O	2.14	0.48
1:V:31:LEU:HA	1:V:143:PHE:CZ	2.47	0.48
1:V:156:GLU:OE1	1:V:156:GLU:N	2.27	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:V:205:2AN:O3	2:V:205:2AN:H12	2.14	0.48
1:j:57:ILE:O	1:j:67:TYR:HA	2.14	0.48
1:i:57:ILE:O	1:i:67:TYR:HA	2.14	0.48
1:h:82:CYS:SG	1:h:83:LYS:N	2.86	0.48
1:h:151:LEU:O	1:h:154:ASN:N	2.47	0.48
1:A:6:ILE:HD11	1:A:133:VAL:CG1	2.36	0.48
1:I:26:GLU:OE1	1:I:29:GLN:NE2	2.47	0.48
2:I:205:2AN:C12	2:I:205:2AN:C2	2.79	0.48
2:G:207:2AN:H12	2:G:207:2AN:C2	2.29	0.48
1:D:93:ARG:O	1:D:94:ASP:HB2	2.13	0.48
1:f:67:TYR:OH	1:f:88:GLU:OE2	2.23	0.48
1:d:20:PHE:CE2	1:d:80:PHE:HA	2.48	0.48
1:Z:101:TYR:OH	7:Z:301:HOH:O	2.20	0.48
1:W:39:PHE:CE1	1:W:59:PHE:CE1	3.01	0.48
1:U:6:ILE:O	1:U:117:THR:HA	2.14	0.48
1:i:25:LEU:HD12	1:i:26:GLU:OE2	2.13	0.48
1:B:44:ILE:H	1:B:44:ILE:CD1	2.26	0.48
1:B:47:GLY:HA2	2:B:204:2AN:C13	2.44	0.48
1:O:83:LYS:HA	1:O:101:TYR:O	2.12	0.48
1:O:128:VAL:CA	1:O:132:GLU:OE2	2.61	0.48
2:O:201:2AN:H2	2:O:201:2AN:C12	2.29	0.48
1:M:66:THR:HB	1:M:90:ASP:OD2	2.14	0.48
1:K:95:ASN:OD1	1:K:96:ILE:HG13	2.12	0.48
1:H:77:ALA:HB1	2:H:204:2AN:C2	2.44	0.48
1:F:27:ARG:O	1:F:31:LEU:N	2.47	0.48
1:E:69:LEU:O	1:E:86:LEU:CD1	2.61	0.48
1:C:32:VAL:O	1:C:33:LYS:C	2.57	0.48
1:a:30:VAL:HG23	1:a:143:PHE:CE1	2.48	0.48
1:a:138:LYS:HA	2:a:203:2AN:C14	2.43	0.48
1:Z:19:LEU:HD11	1:Z:23:LEU:CD1	2.44	0.48
1:T:140:ALA:O	7:T:301:HOH:O	2.20	0.48
1:S:27:ARG:NH2	2:S:204:2AN:O3	2.31	0.48
2:B:204:2AN:H2	2:B:204:2AN:C16	2.44	0.48
2:B:204:2AN:O1	2:B:204:2AN:N	2.44	0.48
1:A:19:LEU:HD13	2:A:201:2AN:C15	2.43	0.48
1:R:96:ILE:HG22	1:R:98:LYS:N	2.29	0.48
2:O:202:2AN:O3	2:O:202:2AN:N	2.39	0.48
1:M:92:LEU:HD22	1:M:96:ILE:CG2	2.43	0.48
1:K:140:ALA:CB	2:K:202:2AN:C13	2.91	0.48
1:H:26:GLU:HA	1:H:26:GLU:OE2	2.14	0.48
1:H:144:TYR:CD1	1:H:144:TYR:C	2.90	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:51:VAL:O	1:G:51:VAL:HG23	2.14	0.48
1:F:88:GLU:HA	1:F:92:LEU:CD1	2.44	0.48
1:E:16:PRO:HD3	1:E:112:SER:HB3	1.95	0.48
1:d:40:LYS:HD3	1:d:58:THR:CG2	2.39	0.48
1:d:40:LYS:HB3	1:d:58:THR:CG2	2.43	0.48
1:b:8:LYS:NZ	1:b:10:GLU:OE2	2.47	0.48
1:B:35:GLN:C	1:B:37:HIS:H	2.20	0.47
2:B:204:2AN:H16	1:j:77:ALA:CB	2.44	0.47
1:A:47:GLY:HA3	1:A:53:THR:CG2	2.43	0.47
1:Q:95:ASN:ND2	1:Q:127:THR:O	2.42	0.47
1:P:77:ALA:HB3	2:V:201:2AN:C16	2.43	0.47
2:O:202:2AN:N	2:O:202:2AN:S	2.71	0.47
1:N:63:HIS:O	1:N:64:PRO:C	2.55	0.47
1:J:3:ALA:HB1	1:J:120:TYR:O	2.14	0.47
1:J:6:ILE:HD12	1:I:0:THR:O	2.14	0.47
2:F:206:2AN:C12	1:D:109:GLY:CA	2.93	0.47
1:E:124:PRO:O	1:E:125:GLY:C	2.57	0.47
1:f:28:HIS:HA	1:f:31:LEU:HD12	1.95	0.47
2:d:201:2AN:S	2:d:201:2AN:N	2.83	0.47
1:b:92:LEU:HD22	1:b:96:ILE:O	2.14	0.47
1:a:18:ARG:NE	1:a:157:VAL:O	2.47	0.47
1:Y:48:ASP:OD1	1:Y:49:GLY:N	2.47	0.47
1:W:107:ALA:O	1:W:108:VAL:CG2	2.62	0.47
1:T:69:LEU:HB2	1:T:88:GLU:HB3	1.96	0.47
1:S:120:TYR:CD1	1:S:133:VAL:HG22	2.49	0.47
2:B:202:2AN:C2	2:B:202:2AN:C12	2.92	0.47
1:F:8:LYS:O	1:F:115:LYS:HA	2.14	0.47
1:E:85:THR:HG23	1:E:99:VAL:C	2.38	0.47
1:d:18:ARG:NE	1:d:157:VAL:O	2.47	0.47
2:c:203:2AN:H16	2:c:203:2AN:C2	2.43	0.47
1:i:17:HIS:ND1	1:i:17:HIS:N	2.61	0.47
1:i:131:GLU:O	1:i:132:GLU:C	2.57	0.47
1:g:66:THR:HB	1:g:90:ASP:OD2	2.14	0.47
1:B:26:GLU:O	1:B:27:ARG:C	2.56	0.47
1:N:103:VAL:HA	1:N:115:LYS:O	2.14	0.47
1:a:141:TYR:HD1	2:a:204:2AN:C15	2.26	0.47
1:Z:95:ASN:O	1:Z:96:ILE:HD13	2.14	0.47
1:U:99:VAL:HG12	1:U:118:VAL:CG1	2.43	0.47
1:S:138:LYS:O	1:S:139:LYS:C	2.55	0.47
1:g:149:GLU:OE1	1:g:150:TYR:N	2.47	0.47
1:B:100:VAL:O	1:B:118:VAL:HA	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:53:THR:HG1	1:A:72:PHE:HD2	1.61	0.47
1:P:3:ALA:HB1	1:P:120:TYR:O	2.15	0.47
1:P:28:HIS:ND1	1:P:55:THR:HG21	2.30	0.47
1:M:36:PRO:HD2	7:M:301:HOH:O	2.14	0.47
1:L:8:LYS:HG2	1:K:0:THR:HG21	1.96	0.47
1:J:53:THR:O	1:J:71:LYS:HA	2.14	0.47
1:J:107:ALA:O	1:J:108:VAL:CG2	2.62	0.47
1:I:92:LEU:O	1:I:93:ARG:C	2.57	0.47
1:H:105:LEU:CD2	2:H:201:2AN:H15	2.44	0.47
1:E:59:PHE:C	1:E:60:VAL:O	2.58	0.47
1:D:150:TYR:CE2	2:D:203:2AN:C1	2.97	0.47
2:b:202:2AN:C12	2:b:202:2AN:H2	2.43	0.47
2:b:205:2AN:O1	2:b:205:2AN:N	2.47	0.47
1:a:134:LYS:NZ	6:a:205:FLC:OB1	2.41	0.47
1:Z:107:ALA:O	1:Z:108:VAL:HG23	2.14	0.47
1:X:42:GLY:HA2	1:X:56:LYS:O	2.15	0.47
1:T:41:SER:O	1:T:58:THR:N	2.24	0.47
1:B:119:THR:HG22	1:B:121:HIS:CE1	2.49	0.47
1:O:18:ARG:C	1:O:20:PHE:H	2.23	0.47
1:H:25:LEU:O	1:H:26:GLU:OE2	2.32	0.47
6:G:206:FLC:OG1	2:G:207:2AN:H7	2.14	0.47
2:D:202:2AN:C2	2:D:202:2AN:C16	2.84	0.47
1:d:14:ILE:HG21	1:d:151:LEU:HD13	1.96	0.47
1:b:63:HIS:CG	1:b:64:PRO:HD2	2.49	0.47
1:a:8:LYS:O	1:a:115:LYS:HA	2.14	0.47
1:T:92:LEU:HD12	1:T:96:ILE:HG22	1.96	0.47
1:h:71:LYS:HB2	1:h:87:PHE:HE1	1.80	0.47
2:h:201:2AN:H16	2:h:201:2AN:H2	1.97	0.47
1:B:115:LYS:C	1:B:116:ILE:HD12	2.39	0.47
1:A:102:GLU:HB2	1:A:117:THR:HB	1.96	0.47
1:P:55:THR:O	1:P:69:LEU:HA	2.14	0.47
1:N:31:LEU:HD12	1:N:57:ILE:HD13	1.97	0.47
1:M:3:ALA:HA	1:M:122:PRO:HD3	1.96	0.47
2:K:201:2AN:H16	2:K:201:2AN:C2	2.45	0.47
1:J:53:THR:CG2	1:J:72:PHE:CD1	2.97	0.47
1:f:47:GLY:HA2	2:f:203:2AN:H2	1.97	0.47
1:f:129:ASN:OD1	1:f:129:ASN:N	2.47	0.47
1:c:63:HIS:ND1	1:c:65:LEU:HB2	2.29	0.47
1:Z:37:HIS:CD2	1:Z:38:VAL:HG23	2.50	0.47
1:Y:143:PHE:O	1:Y:147:VAL:HG23	2.15	0.47
2:X:202:2AN:H2	2:X:202:2AN:C12	2.30	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:32:VAL:O	1:U:35:GLN:N	2.47	0.47
1:j:2:ALA:CB	1:i:4:TYR:CE1	2.98	0.47
1:i:28:HIS:CE1	1:i:29:GLN:HG2	2.48	0.47
1:i:57:ILE:O	1:i:67:TYR:CB	2.62	0.47
2:B:202:2AN:N	2:B:202:2AN:S	2.87	0.47
1:R:96:ILE:O	1:R:123:LYS:HG3	2.15	0.47
1:Q:109:GLY:O	1:S:80:PHE:HZ	1.98	0.47
1:Q:123:LYS:HB3	1:Q:124:PRO:HD2	1.97	0.47
1:O:37:HIS:CE1	1:O:38:VAL:HG13	2.50	0.47
1:O:37:HIS:ND1	1:O:38:VAL:HG13	2.30	0.47
1:O:101:TYR:CE1	2:O:201:2AN:C13	2.98	0.47
1:O:101:TYR:CD1	2:O:201:2AN:H13	2.50	0.47
1:N:144:TYR:HB2	2:N:201:2AN:O1	2.14	0.47
1:M:149:GLU:O	1:M:149:GLU:CD	2.57	0.47
1:L:18:ARG:NH2	1:L:151:LEU:O	2.47	0.47
1:G:68:MET:HE3	1:G:91:VAL:HG21	1.96	0.47
1:G:141:TYR:O	1:G:142:GLU:C	2.58	0.47
1:F:136:GLY:HA2	2:F:202:2AN:C13	2.45	0.47
1:E:16:PRO:C	1:E:18:ARG:N	2.71	0.47
1:E:54:VAL:HG22	1:E:70:HIS:O	2.15	0.47
1:E:98:LYS:CE	1:E:121:HIS:CD2	2.97	0.47
1:f:2:ALA:HB2	1:e:4:TYR:CZ	2.50	0.47
1:f:72:PHE:CD2	1:f:75:ILE:HD11	2.50	0.47
1:e:32:VAL:O	1:e:33:LYS:C	2.57	0.47
1:c:139:LYS:HE2	2:c:206:2AN:C4	2.44	0.47
1:b:129:ASN:O	1:b:132:GLU:HB3	2.15	0.47
1:U:101:TYR:OH	2:U:202:2AN:H16	2.14	0.47
1:T:8:LYS:NZ	2:T:201:2AN:O2	2.28	0.47
1:T:123:LYS:CB	1:T:124:PRO:CD	2.89	0.47
2:T:205:2AN:C2	2:T:205:2AN:C16	2.68	0.47
1:S:144:TYR:CD1	1:S:144:TYR:O	2.68	0.47
1:i:98:LYS:HG3	1:i:121:HIS:CD2	2.49	0.47
1:g:139:LYS:CE	2:g:202:2AN:H4	2.39	0.47
1:B:75:ILE:HG22	1:B:76:ASP:N	2.29	0.47
1:A:9:GLU:HA	1:A:114:GLY:O	2.14	0.47
1:N:10:GLU:C	1:N:11:GLU:HG3	2.38	0.47
1:H:63:HIS:CE1	1:H:65:LEU:CB	2.97	0.47
1:F:38:VAL:O	1:F:38:VAL:HG12	2.15	0.47
1:E:56:LYS:HG3	1:E:69:LEU:HD23	1.96	0.47
1:D:20:PHE:CD1	1:D:80:PHE:HB3	2.49	0.47
1:f:139:LYS:HE2	2:f:202:2AN:H6	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:e:23:LEU:HD11	1:e:147:VAL:HG11	1.97	0.47
2:c:204:2AN:O2	2:c:204:2AN:N	2.40	0.47
1:b:48:ASP:CB	2:b:206:2AN:O1	2.63	0.47
1:Y:3:ALA:HB1	1:Y:120:TYR:O	2.14	0.47
2:V:202:2AN:C2	2:V:202:2AN:C16	2.90	0.47
1:U:9:GLU:OE2	1:U:115:LYS:CD	2.53	0.47
1:U:113:LYS:HB3	1:U:113:LYS:NZ	2.29	0.47
1:h:33:LYS:HZ2	2:h:204:2AN:C11	2.27	0.47
1:Q:135:ILE:O	1:Q:139:LYS:HG2	2.15	0.47
1:O:68:MET:HB2	1:O:86:LEU:HD11	1.97	0.47
2:L:201:2AN:C16	2:L:201:2AN:C2	2.72	0.47
1:F:15:ALA:HB3	1:F:18:ARG:HD3	1.95	0.47
1:f:31:LEU:HA	1:f:143:PHE:CE1	2.50	0.47
2:f:202:2AN:C12	2:f:202:2AN:H2	2.44	0.47
1:b:14:ILE:C	1:b:111:GLY:HA2	2.40	0.47
1:U:103:VAL:CA	1:U:116:ILE:HG22	2.45	0.47
2:T:203:2AN:O3	2:T:203:2AN:N	2.34	0.47
1:h:35:GLN:HE21	1:h:146:GLN:HE22	1.63	0.47
2:B:206:2AN:C2	2:B:206:2AN:C12	2.88	0.47
1:A:15:ALA:O	1:A:16:PRO:C	2.58	0.47
2:R:203:2AN:H2	2:R:203:2AN:C12	2.43	0.47
1:P:144:TYR:O	1:P:145:LYS:C	2.56	0.47
1:N:28:HIS:ND1	1:N:29:GLN:HG2	2.28	0.47
1:L:23:LEU:HD22	1:L:143:PHE:CE2	2.50	0.47
1:J:76:ASP:O	1:J:77:ALA:C	2.57	0.47
1:E:129:ASN:CB	1:E:132:GLU:HG3	2.45	0.47
1:D:140:ALA:CB	2:D:201:2AN:H8	2.45	0.47
1:d:30:VAL:HG13	2:d:203:2AN:C7	2.45	0.47
1:d:150:TYR:CE1	1:d:154:ASN:ND2	2.82	0.47
1:Z:16:PRO:HG3	1:Z:107:ALA:HB2	1.97	0.47
1:W:20:PHE:HB2	1:W:105:LEU:HD12	1.97	0.47
1:V:77:ALA:HB1	2:V:204:2AN:C2	2.45	0.47
1:S:10:GLU:O	1:S:113:LYS:HA	2.14	0.47
1:S:101:TYR:HD1	1:S:118:VAL:HG22	1.80	0.47
2:j:205:2AN:C4	6:j:208:FLC:OHB	2.63	0.47
1:g:44:ILE:CG2	1:g:54:VAL:O	2.63	0.47
1:R:26:GLU:O	1:R:30:VAL:HG23	2.16	0.46
1:Q:69:LEU:HD22	1:Q:88:GLU:CD	2.36	0.46
1:P:147:VAL:O	1:P:148:GLU:C	2.56	0.46
2:O:202:2AN:N	2:O:202:2AN:O1	2.48	0.46
1:K:69:LEU:O	1:K:86:LEU:HD12	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:12:SER:HB3	1:F:144:TYR:OH	2.15	0.46
1:F:87:PHE:O	1:F:92:LEU:CD1	2.61	0.46
1:E:55:THR:O	1:E:69:LEU:HA	2.15	0.46
2:C:202:2AN:C2	2:C:202:2AN:C12	2.86	0.46
1:f:0:THR:HB	1:e:6:ILE:HD11	1.96	0.46
1:e:76:ASP:C	1:e:78:ALA:H	2.23	0.46
1:d:27:ARG:CZ	2:d:204:2AN:O1	2.63	0.46
1:c:17:HIS:HB3	1:c:80:PHE:CE1	2.50	0.46
2:c:201:2AN:N	2:c:201:2AN:O3	2.47	0.46
1:a:39:PHE:HA	1:a:59:PHE:HA	1.97	0.46
1:a:85:THR:HG23	1:a:100:VAL:CG2	2.44	0.46
1:W:5:THR:CB	1:W:119:THR:HG23	2.45	0.46
1:T:9:GLU:HA	1:T:114:GLY:O	2.15	0.46
1:S:66:THR:CB	1:S:90:ASP:OD2	2.63	0.46
1:i:27:ARG:HH22	1:i:140:ALA:HB1	1.79	0.46
1:i:59:PHE:HD2	1:i:63:HIS:CD2	2.33	0.46
1:h:54:VAL:HA	1:h:70:HIS:O	2.15	0.46
1:h:147:VAL:O	1:h:148:GLU:C	2.58	0.46
1:A:55:THR:OG1	7:A:301:HOH:O	2.20	0.46
1:A:136:GLY:CA	2:A:202:2AN:C14	2.93	0.46
1:N:59:PHE:CD1	1:N:63:HIS:CE1	3.03	0.46
1:J:129:ASN:N	1:J:129:ASN:OD1	2.49	0.46
2:E:203:2AN:H2	2:E:203:2AN:C16	2.44	0.46
1:D:118:VAL:O	1:D:119:THR:OG1	2.24	0.46
1:C:27:ARG:NH2	7:C:301:HOH:O	2.26	0.46
1:C:86:LEU:HB2	7:C:302:HOH:O	2.14	0.46
1:e:23:LEU:O	1:e:27:ARG:HD2	2.15	0.46
1:W:69:LEU:O	1:W:86:LEU:HD12	2.15	0.46
1:V:77:ALA:CB	2:V:204:2AN:H16	2.45	0.46
1:V:79:ASN:OD1	1:V:79:ASN:N	2.47	0.46
1:S:135:ILE:O	1:S:139:LYS:HG2	2.15	0.46
1:h:14:ILE:HD11	1:h:152:ALA:HB2	1.97	0.46
1:R:119:THR:HG22	1:R:121:HIS:CD2	2.51	0.46
1:R:137:GLU:CD	1:Q:0:THR:HG1	2.23	0.46
1:J:146:GLN:C	1:J:148:GLU:H	2.22	0.46
1:G:85:THR:HG23	1:G:100:VAL:HG13	1.97	0.46
1:f:129:ASN:O	1:f:131:GLU:N	2.49	0.46
2:f:202:2AN:S	2:f:202:2AN:N	2.88	0.46
1:e:79:ASN:O	1:e:104:LYS:CE	2.64	0.46
1:d:70:HIS:CE1	2:d:204:2AN:H8	2.50	0.46
1:a:4:TYR:HB3	1:a:120:TYR:HB2	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Z:205:2AN:HN	2:Z:205:2AN:HO3	1.59	0.46
1:Y:6:ILE:HD11	1:Y:133:VAL:CG1	2.46	0.46
2:X:202:2AN:O3	2:X:202:2AN:H16	2.15	0.46
1:A:131:GLU:OE1	1:A:131:GLU:N	2.49	0.46
1:O:14:ILE:HD12	1:O:14:ILE:N	2.31	0.46
1:N:-3:ASP:O	1:N:-2:PRO:C	2.58	0.46
1:J:60:VAL:CG2	1:J:63:HIS:HB2	2.44	0.46
1:H:31:LEU:HD23	1:H:143:PHE:CE1	2.49	0.46
1:H:54:VAL:HG22	1:H:71:LYS:CG	2.43	0.46
2:F:201:2AN:H16	2:F:201:2AN:C2	2.29	0.46
1:E:132:GLU:O	1:E:133:VAL:C	2.58	0.46
1:D:138:LYS:HG3	2:D:204:2AN:O1	2.16	0.46
1:c:91:VAL:O	1:c:91:VAL:HG22	2.15	0.46
1:b:2:ALA:CB	1:a:4:TYR:CD1	2.99	0.46
1:b:141:TYR:CZ	2:b:203:2AN:O3	2.61	0.46
1:X:23:LEU:HD13	2:X:206:2AN:C1	2.43	0.46
1:U:32:VAL:C	1:U:34:ALA:N	2.72	0.46
1:U:45:ILE:HG13	1:U:46:GLU:N	2.31	0.46
1:T:53:THR:O	1:T:71:LYS:HA	2.15	0.46
2:T:202:2AN:C2	2:T:202:2AN:C16	2.91	0.46
1:h:92:LEU:CD2	1:h:96:ILE:HG22	2.45	0.46
1:g:93:ARG:NH2	1:g:129:ASN:HD21	2.13	0.46
1:A:127:THR:O	1:A:128:VAL:C	2.57	0.46
1:R:99:VAL:CG2	1:R:120:TYR:CD2	2.99	0.46
1:K:6:ILE:H	1:K:6:ILE:HD12	1.80	0.46
1:H:158:PHE:CE1	2:H:203:2AN:H15	2.51	0.46
2:F:206:2AN:C13	1:D:109:GLY:HA3	2.46	0.46
1:a:43:GLU:O	1:a:56:LYS:O	2.34	0.46
2:Z:206:2AN:O2	2:Z:206:2AN:C16	2.62	0.46
1:j:141:TYR:CD2	6:j:208:FLC:HG2	2.50	0.46
1:i:16:PRO:HG2	1:i:107:ALA:CA	2.46	0.46
1:h:156:GLU:O	1:h:157:VAL:C	2.58	0.46
1:P:28:HIS:O	1:P:42:GLY:HA3	2.15	0.46
1:P:77:ALA:HB3	2:V:201:2AN:C15	2.45	0.46
2:P:202:2AN:H12	2:P:202:2AN:C2	2.45	0.46
2:N:205:2AN:H16	2:N:205:2AN:C2	2.37	0.46
1:M:98:LYS:CG	1:M:121:HIS:HB2	2.45	0.46
1:L:18:ARG:NH1	1:L:151:LEU:O	2.48	0.46
1:I:105:LEU:HA	1:I:113:LYS:O	2.16	0.46
1:H:4:TYR:HE1	1:G:2:ALA:HB2	1.80	0.46
1:H:147:VAL:O	1:H:151:LEU:HG	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:f:44:ILE:HG23	1:f:53:THR:HG23	1.98	0.46
1:f:144:TYR:CD1	1:f:144:TYR:O	2.69	0.46
1:f:145:LYS:HE2	2:f:204:2AN:C13	2.45	0.46
2:c:203:2AN:H7	2:c:206:2AN:H15	1.98	0.46
2:b:203:2AN:O1	2:b:203:2AN:H16	2.16	0.46
1:a:141:TYR:HB2	2:a:204:2AN:C14	2.45	0.46
1:Z:138:LYS:HD2	1:Z:138:LYS:HA	1.71	0.46
2:T:205:2AN:O2	2:T:205:2AN:N	2.48	0.46
1:S:90:ASP:C	1:S:92:LEU:N	2.73	0.46
1:i:59:PHE:CD2	1:i:63:HIS:CD2	3.04	0.46
1:P:77:ALA:CB	2:V:201:2AN:H16	2.46	0.46
1:M:22:ALA:HA	1:M:30:VAL:HG21	1.97	0.46
1:J:96:ILE:CG2	1:J:121:HIS:O	2.64	0.46
1:H:59:PHE:HD1	1:H:67:TYR:N	2.10	0.46
1:G:116:ILE:HD13	2:G:203:2AN:O1	2.15	0.46
1:F:18:ARG:NH1	1:F:151:LEU:O	2.49	0.46
1:C:95:ASN:ND2	1:C:128:VAL:HA	2.30	0.46
1:d:10:GLU:CB	2:d:201:2AN:H15	2.33	0.46
1:c:150:TYR:O	1:c:154:ASN:ND2	2.41	0.46
1:b:12:SER:OG	1:b:14:ILE:HG12	2.16	0.46
1:X:69:LEU:HD12	1:X:88:GLU:CG	2.45	0.46
1:S:106:GLU:OE2	1:S:113:LYS:HB2	2.16	0.46
1:j:18:ARG:NH2	1:j:157:VAL:O	2.49	0.46
1:j:129:ASN:O	1:j:132:GLU:N	2.48	0.46
1:A:83:LYS:HA	1:A:101:TYR:O	2.15	0.46
1:Q:30:VAL:HG12	1:Q:143:PHE:CE1	2.51	0.46
1:O:96:ILE:HD11	1:O:132:GLU:CD	2.40	0.46
1:K:139:LYS:HA	1:K:139:LYS:HE2	1.97	0.46
1:H:59:PHE:CD1	1:H:66:THR:O	2.60	0.46
2:H:204:2AN:H2	2:H:204:2AN:C12	2.41	0.46
2:G:201:2AN:C2	2:G:201:2AN:C12	2.89	0.46
1:F:145:LYS:O	1:F:146:GLN:C	2.59	0.46
2:d:203:2AN:C2	2:d:203:2AN:C16	2.91	0.46
1:b:44:ILE:HG23	1:b:53:THR:CG2	2.46	0.46
1:b:131:GLU:O	1:b:132:GLU:C	2.58	0.46
1:Y:6:ILE:O	1:Y:117:THR:HA	2.15	0.46
1:U:29:GLN:OE1	1:U:42:GLY:O	2.33	0.46
1:U:95:ASN:HD21	1:U:129:ASN:H	1.63	0.46
1:T:67:TYR:N	1:T:67:TYR:CD1	2.84	0.46
1:S:85:THR:HA	1:S:99:VAL:O	2.16	0.46
2:j:204:2AN:C16	2:j:204:2AN:C2	2.64	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:122:PRO:HB3	1:B:128:VAL:HG23	1.96	0.46
1:O:79:ASN:O	1:O:80:PHE:CB	2.63	0.46
1:L:91:VAL:HG22	1:L:91:VAL:O	2.16	0.46
1:H:87:PHE:C	1:H:88:GLU:HG3	2.38	0.46
1:G:65:LEU:HD21	1:G:91:VAL:CG1	2.46	0.46
1:F:110:GLY:HA2	1:d:17:HIS:CB	2.46	0.46
1:F:144:TYR:O	1:F:148:GLU:N	2.43	0.46
1:D:147:VAL:O	1:D:148:GLU:C	2.59	0.46
1:d:92:LEU:HD22	1:d:96:ILE:HG22	1.97	0.46
1:c:63:HIS:CE1	1:c:65:LEU:HD12	2.51	0.46
1:Y:54:VAL:HA	1:Y:70:HIS:O	2.16	0.46
1:X:16:PRO:CD	1:X:112:SER:OG	2.64	0.46
1:S:30:VAL:O	1:S:33:LYS:N	2.49	0.46
1:O:5:THR:CB	1:O:118:VAL:O	2.64	0.46
1:L:4:TYR:HE1	1:K:2:ALA:CB	2.29	0.46
2:K:202:2AN:N	2:K:202:2AN:S	2.54	0.46
1:I:21:LYS:O	1:I:26:GLU:HB2	2.15	0.46
1:C:8:LYS:NZ	2:C:202:2AN:O3	2.46	0.46
1:C:51:VAL:HG13	1:C:75:ILE:HG13	1.96	0.46
1:f:26:GLU:O	1:f:29:GLN:HB2	2.16	0.46
1:f:27:ARG:NH1	7:f:302:HOH:O	2.36	0.46
1:e:8:LYS:N	1:e:116:ILE:O	2.40	0.46
1:d:33:LYS:HG3	2:d:203:2AN:O3	2.15	0.46
2:d:202:2AN:N	2:d:202:2AN:S	2.89	0.46
1:V:90:ASP:O	1:V:93:ARG:N	2.45	0.46
1:A:45:ILE:HD12	1:A:46:GLU:HB2	1.97	0.45
2:R:203:2AN:O1	2:R:203:2AN:C11	2.64	0.45
1:P:8:LYS:HD3	1:O:1:MET:HE2	1.98	0.45
1:P:31:LEU:HD12	1:P:57:ILE:HD13	1.96	0.45
1:M:92:LEU:HD22	1:M:96:ILE:HG22	1.97	0.45
1:J:20:PHE:O	1:J:24:VAL:HB	2.16	0.45
1:F:32:VAL:HG22	1:F:39:PHE:HB3	1.98	0.45
1:F:105:LEU:HD21	2:F:201:2AN:H15	1.98	0.45
1:D:26:GLU:O	1:D:27:ARG:C	2.59	0.45
1:C:81:TYR:CD1	1:C:81:TYR:C	2.94	0.45
1:d:41:SER:OG	1:d:58:THR:HB	2.16	0.45
1:d:99:VAL:HG22	1:d:120:TYR:HD1	1.80	0.45
1:c:20:PHE:CE2	1:c:77:ALA:HA	2.51	0.45
1:X:69:LEU:HD12	1:X:88:GLU:HB3	1.98	0.45
2:X:206:2AN:H16	2:X:206:2AN:C2	2.45	0.45
1:W:96:ILE:H	1:W:123:LYS:CA	2.29	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:W:129:ASN:C	1:W:131:GLU:N	2.74	0.45
1:U:44:ILE:HG22	1:U:55:THR:HG22	1.98	0.45
1:T:30:VAL:O	1:T:33:LYS:N	2.44	0.45
1:h:12:SER:OG	1:h:14:ILE:HG12	2.17	0.45
1:L:119:THR:CG2	1:L:121:HIS:CE1	2.99	0.45
1:J:39:PHE:CE1	1:J:57:ILE:CG2	2.99	0.45
1:H:70:HIS:CA	1:H:85:THR:O	2.58	0.45
1:F:16:PRO:HB2	1:F:80:PHE:CD2	2.51	0.45
2:D:202:2AN:H2	2:D:202:2AN:C16	2.44	0.45
1:c:1:MET:HB2	1:c:1:MET:HE3	1.75	0.45
2:c:201:2AN:C16	2:c:201:2AN:H2	2.43	0.45
2:b:201:2AN:N	2:b:201:2AN:S	2.75	0.45
1:a:101:TYR:CD1	1:a:118:VAL:HG22	2.51	0.45
1:W:16:PRO:HD3	1:W:112:SER:HB3	1.98	0.45
1:U:57:ILE:HG22	1:U:58:THR:N	2.30	0.45
1:j:91:VAL:HG21	2:j:202:2AN:C13	2.47	0.45
1:j:129:ASN:O	1:j:131:GLU:N	2.49	0.45
1:B:44:ILE:HG21	1:B:53:THR:CG2	2.46	0.45
1:A:89:GLY:O	1:A:91:VAL:N	2.50	0.45
1:R:20:PHE:O	1:R:24:VAL:HB	2.15	0.45
1:P:43:GLU:O	1:P:56:LYS:N	2.39	0.45
2:L:203:2AN:H16	2:L:203:2AN:C2	2.46	0.45
1:G:65:LEU:HD23	1:G:90:ASP:HB2	1.97	0.45
2:G:207:2AN:O3	5:G:208:DMS:H12	2.16	0.45
1:F:138:LYS:CE	2:F:204:2AN:O1	2.63	0.45
2:F:206:2AN:H13	1:D:109:GLY:HA3	1.98	0.45
1:f:89:GLY:O	1:f:92:LEU:CB	2.63	0.45
1:c:157:VAL:HG12	1:c:158:PHE:CD2	2.52	0.45
1:X:80:PHE:O	1:X:104:LYS:HA	2.16	0.45
2:X:206:2AN:C2	2:X:206:2AN:C16	2.94	0.45
1:V:95:ASN:ND2	1:V:129:ASN:CG	2.75	0.45
2:B:201:2AN:C2	2:B:201:2AN:C12	2.87	0.45
1:A:50:GLY:C	1:A:75:ILE:HD12	2.41	0.45
1:A:87:PHE:N	1:A:87:PHE:CD1	2.84	0.45
1:A:103:VAL:HG22	1:A:116:ILE:HG23	1.98	0.45
1:O:18:ARG:O	1:O:20:PHE:N	2.50	0.45
1:L:35:GLN:HE22	2:L:203:2AN:H7	1.79	0.45
1:K:155:PRO:O	1:K:159:ALA:HB2	2.16	0.45
1:W:98:LYS:HE3	1:W:121:HIS:ND1	2.32	0.45
2:V:207:2AN:C2	2:V:207:2AN:C12	2.93	0.45
1:S:19:LEU:O	1:S:22:ALA:N	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:54:VAL:HA	1:S:70:HIS:O	2.16	0.45
2:j:202:2AN:C2	2:j:202:2AN:C12	2.93	0.45
1:B:90:ASP:O	1:B:92:LEU:N	2.49	0.45
1:P:13:PRO:O	1:P:111:GLY:HA2	2.17	0.45
1:P:96:ILE:HA	1:P:122:PRO:HA	1.99	0.45
1:P:158:PHE:CE1	2:P:203:2AN:H15	2.51	0.45
1:J:53:THR:HG22	1:J:72:PHE:CB	2.42	0.45
1:J:132:GLU:O	1:J:136:GLY:N	2.44	0.45
1:G:96:ILE:HA	1:G:121:HIS:O	2.17	0.45
1:G:123:LYS:HB3	1:G:126:CYS:HB2	1.99	0.45
1:F:38:VAL:O	1:F:59:PHE:HD2	1.99	0.45
2:F:206:2AN:H2	1:f:77:ALA:CB	2.20	0.45
1:e:76:ASP:C	1:e:78:ALA:N	2.74	0.45
1:d:23:LEU:CB	2:d:201:2AN:H3	2.47	0.45
2:b:202:2AN:C12	2:b:202:2AN:C2	2.94	0.45
1:a:108:VAL:HG21	1:a:113:LYS:HD2	1.99	0.45
1:Y:142:GLU:CG	3:Y:205:SO4:O1	2.64	0.45
1:V:23:LEU:HD13	2:V:203:2AN:C2	2.47	0.45
1:U:99:VAL:HA	1:U:119:THR:O	2.17	0.45
1:U:115:LYS:HZ2	1:U:115:LYS:HB3	1.81	0.45
1:j:14:ILE:O	1:j:112:SER:OG	2.33	0.45
1:j:30:VAL:O	1:j:31:LEU:C	2.59	0.45
1:g:20:PHE:O	1:g:24:VAL:HB	2.17	0.45
1:B:12:SER:HB2	1:B:148:GLU:OE2	2.17	0.45
1:O:19:LEU:O	1:O:23:LEU:HB2	2.16	0.45
1:N:21:LYS:CD	1:N:158:PHE:CD1	3.00	0.45
1:J:27:ARG:NH2	2:J:203:2AN:O3	2.49	0.45
1:J:90:ASP:OD2	1:J:90:ASP:N	2.50	0.45
1:I:147:VAL:O	1:I:150:TYR:HB3	2.16	0.45
1:H:35:GLN:HE22	2:H:202:2AN:H6	1.81	0.45
1:F:123:LYS:HB3	1:F:124:PRO:HD2	1.98	0.45
1:E:144:TYR:CE1	2:E:201:2AN:C12	3.00	0.45
1:C:14:ILE:HD11	1:C:152:ALA:HB2	1.97	0.45
1:f:139:LYS:HE2	2:f:202:2AN:C5	2.47	0.45
1:b:69:LEU:O	1:b:86:LEU:HD12	2.16	0.45
1:Y:116:ILE:HD12	1:Y:116:ILE:N	2.32	0.45
1:U:14:ILE:HD13	1:U:148:GLU:HG3	1.98	0.45
1:T:124:PRO:C	1:T:126:CYS:H	2.25	0.45
1:T:151:LEU:O	1:T:152:ALA:C	2.59	0.45
1:i:16:PRO:HG2	1:i:107:ALA:HA	1.97	0.45
1:h:4:TYR:O	1:h:119:THR:HA	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:h:21:LYS:HA	1:h:25:LEU:HB2	1.98	0.45
1:h:79:ASN:HB3	1:h:104:LYS:HZ3	1.74	0.45
1:g:16:PRO:O	1:g:17:HIS:C	2.58	0.45
1:A:95:ASN:HD22	1:A:129:ASN:H	1.63	0.45
1:A:123:LYS:N	1:A:126:CYS:SG	2.84	0.45
1:R:63:HIS:HE2	2:R:205:2AN:H13	1.82	0.45
1:N:156:GLU:H	1:N:156:GLU:CD	2.16	0.45
1:M:123:LYS:HG2	1:M:124:PRO:HD2	1.99	0.45
1:I:72:PHE:CD2	1:I:75:ILE:HD11	2.52	0.45
1:G:45:ILE:HG13	1:G:54:VAL:HG22	1.92	0.45
1:D:4:TYR:CE1	1:C:2:ALA:CB	3.00	0.45
1:D:36:PRO:C	1:D:38:VAL:H	2.25	0.45
1:C:73:ASP:C	1:C:74:GLU:HG3	2.42	0.45
1:C:136:GLY:O	1:C:137:GLU:C	2.58	0.45
1:c:16:PRO:HD3	1:c:112:SER:HB3	1.98	0.45
1:X:147:VAL:O	1:X:148:GLU:C	2.60	0.45
1:W:8:LYS:HE2	1:W:137:GLU:OE2	2.16	0.45
1:U:129:ASN:OD1	1:U:129:ASN:N	2.48	0.45
1:j:2:ALA:HA	1:i:4:TYR:CE1	2.52	0.45
1:i:16:PRO:CG	1:i:107:ALA:HA	2.47	0.45
1:h:1:MET:SD	1:h:1:MET:N	2.90	0.45
1:g:120:TYR:CD1	1:g:133:VAL:HG22	2.52	0.45
1:P:56:LYS:HG3	1:P:69:LEU:HD23	1.98	0.45
1:N:76:ASP:CG	1:N:79:ASN:HD22	2.25	0.45
1:M:98:LYS:HG2	1:M:121:HIS:HB2	1.99	0.45
1:K:95:ASN:O	1:K:123:LYS:N	2.34	0.45
1:H:141:TYR:OH	1:H:145:LYS:HE2	2.16	0.45
1:F:5:THR:HG21	1:E:5:THR:CB	2.43	0.45
1:E:35:GLN:OE1	2:E:202:2AN:H7	2.17	0.45
1:f:40:LYS:C	1:f:41:SER:OG	2.58	0.45
1:d:20:PHE:CD2	1:d:80:PHE:HA	2.52	0.45
1:d:23:LEU:HD13	2:d:201:2AN:C1	2.47	0.45
1:Z:116:ILE:N	1:Z:116:ILE:HD12	2.32	0.45
1:X:13:PRO:O	1:X:111:GLY:CA	2.64	0.45
1:h:71:LYS:HB2	1:h:87:PHE:CE1	2.51	0.45
1:g:59:PHE:HZ	1:g:68:MET:HE2	1.80	0.45
1:O:89:GLY:CA	1:O:92:LEU:HD23	2.46	0.45
1:L:33:LYS:HD3	2:L:202:2AN:N	2.32	0.45
1:J:26:GLU:O	1:J:29:GLN:N	2.47	0.45
1:J:86:LEU:HD21	1:J:91:VAL:CG1	2.43	0.45
1:J:147:VAL:O	1:J:147:VAL:HG12	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:80:PHE:O	1:I:104:LYS:HA	2.17	0.45
1:D:99:VAL:CA	1:D:119:THR:O	2.62	0.45
1:C:54:VAL:HA	1:C:70:HIS:O	2.16	0.45
1:f:-1:PHE:HE1	2:f:206:2AN:H8	1.82	0.45
1:f:45:ILE:HD12	1:f:45:ILE:C	2.41	0.45
1:f:151:LEU:HD22	1:f:157:VAL:CG2	2.47	0.45
1:a:30:VAL:CG2	1:a:143:PHE:HZ	2.29	0.45
1:Z:34:ALA:C	1:Z:36:PRO:HD3	2.42	0.45
1:T:16:PRO:HB3	1:T:112:SER:OG	2.17	0.45
1:T:144:TYR:CD1	1:T:144:TYR:O	2.70	0.45
1:i:50:GLY:O	1:i:53:THR:OG1	2.26	0.45
1:h:20:PHE:CE1	1:h:80:PHE:HA	2.51	0.45
1:h:23:LEU:HB3	2:h:202:2AN:C3	2.46	0.45
1:g:20:PHE:CD1	1:g:24:VAL:HG21	2.51	0.45
1:B:141:TYR:CD2	2:B:205:2AN:H3	2.52	0.45
1:A:89:GLY:C	1:A:91:VAL:H	2.24	0.45
1:A:107:ALA:CB	1:i:107:ALA:HB2	2.46	0.45
1:R:116:ILE:N	1:R:116:ILE:HD12	2.32	0.45
1:O:42:GLY:HA2	1:O:57:ILE:HA	1.97	0.45
1:L:13:PRO:O	1:L:111:GLY:HA2	2.18	0.45
1:L:42:GLY:C	1:L:43:GLU:HG3	2.42	0.45
1:I:14:ILE:HD11	1:I:152:ALA:HB2	1.98	0.45
1:I:110:GLY:HA2	1:a:17:HIS:HB3	1.99	0.45
1:H:80:PHE:O	1:H:104:LYS:HA	2.17	0.45
1:D:4:TYR:CD1	1:D:4:TYR:C	2.95	0.45
1:b:37:HIS:CD2	1:b:38:VAL:HG23	2.52	0.45
1:a:143:PHE:HA	1:a:146:GLN:OE1	2.16	0.45
1:U:39:PHE:HE2	2:U:202:2AN:H4	1.82	0.45
1:U:103:VAL:HG22	1:U:116:ILE:HG22	1.98	0.45
1:j:76:ASP:C	1:j:78:ALA:N	2.74	0.45
1:i:141:TYR:HD1	7:i:306:HOH:O	1.99	0.45
2:g:201:2AN:O1	2:g:201:2AN:N	2.50	0.45
1:A:7:VAL:HG12	1:A:117:THR:HA	1.98	0.44
1:A:148:GLU:O	1:A:149:GLU:C	2.60	0.44
1:R:17:HIS:ND1	7:R:301:HOH:O	2.35	0.44
1:R:66:THR:HG22	1:R:67:TYR:HD2	1.82	0.44
1:R:141:TYR:CB	2:R:204:2AN:H4	2.47	0.44
1:Q:69:LEU:HD22	1:Q:88:GLU:CB	2.47	0.44
1:O:39:PHE:HA	1:O:59:PHE:HA	1.98	0.44
1:D:35:GLN:O	1:D:39:PHE:HD2	2.00	0.44
1:D:80:PHE:HZ	1:f:109:GLY:O	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:c:138:LYS:NZ	2:c:201:2AN:O3	2.38	0.44
1:a:35:GLN:NE2	1:a:143:PHE:HB2	2.32	0.44
1:U:53:THR:O	1:U:71:LYS:HA	2.17	0.44
2:U:201:2AN:H2	2:U:201:2AN:C16	2.15	0.44
1:T:15:ALA:HA	1:T:111:GLY:HA2	1.99	0.44
1:T:18:ARG:NE	1:T:157:VAL:O	2.35	0.44
1:T:70:HIS:NE2	1:T:86:LEU:HB2	2.32	0.44
1:T:92:LEU:HD13	1:T:92:LEU:HA	1.82	0.44
1:i:106:GLU:HG3	1:i:113:LYS:HB2	1.98	0.44
1:h:33:LYS:HE2	2:h:204:2AN:O3	2.16	0.44
2:B:205:2AN:H12	2:B:205:2AN:H2	1.99	0.44
1:A:21:LYS:HG2	1:A:158:PHE:CD1	2.53	0.44
1:A:28:HIS:CD2	1:A:29:GLN:HG3	2.51	0.44
1:R:140:ALA:O	1:R:143:PHE:HB3	2.18	0.44
1:Q:57:ILE:O	1:Q:68:MET:N	2.50	0.44
1:P:47:GLY:HA2	2:V:204:2AN:C12	2.48	0.44
1:N:108:VAL:O	1:N:111:GLY:N	2.40	0.44
1:M:123:LYS:CG	1:M:124:PRO:HD2	2.47	0.44
1:L:2:ALA:HB2	1:K:4:TYR:CZ	2.52	0.44
1:L:88:GLU:HA	1:L:92:LEU:HD22	1.97	0.44
1:I:16:PRO:HB2	1:I:80:PHE:CE2	2.52	0.44
1:I:54:VAL:HA	1:I:70:HIS:O	2.17	0.44
1:G:45:ILE:HG12	1:G:54:VAL:O	2.17	0.44
2:F:206:2AN:H12	1:D:109:GLY:HA2	1.98	0.44
1:E:122:PRO:HB3	1:E:128:VAL:CG2	2.48	0.44
1:D:92:LEU:HB3	1:D:96:ILE:HB	1.99	0.44
1:D:116:ILE:N	1:D:116:ILE:HD12	2.32	0.44
1:C:46:GLU:HB3	1:C:54:VAL:HB	1.98	0.44
2:f:206:2AN:C2	2:f:206:2AN:C12	2.81	0.44
1:Z:90:ASP:O	1:Z:93:ARG:HG2	2.17	0.44
1:Z:104:LYS:O	1:Z:104:LYS:HG3	2.14	0.44
1:X:116:ILE:CD1	2:X:206:2AN:HN	2.30	0.44
1:W:115:LYS:C	1:W:116:ILE:HD12	2.42	0.44
1:V:104:LYS:O	1:V:114:GLY:HA2	2.16	0.44
2:V:206:2AN:O3	2:V:208:2AN:C2	2.65	0.44
1:S:153:ALA:C	1:S:155:PRO:HD3	2.43	0.44
1:g:122:PRO:HB3	1:g:128:VAL:CG2	2.46	0.44
1:A:85:THR:CA	1:A:99:VAL:O	2.66	0.44
1:Q:26:GLU:OE1	1:Q:29:GLN:OE1	2.35	0.44
1:J:6:ILE:CG2	1:I:0:THR:CG2	2.95	0.44
1:I:142:GLU:HB2	2:I:206:2AN:H8	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:59:PHE:CD1	1:H:67:TYR:N	2.85	0.44
1:G:83:LYS:HA	1:G:101:TYR:O	2.17	0.44
1:G:92:LEU:O	1:G:94:ASP:N	2.42	0.44
1:G:129:ASN:O	1:G:130:GLU:C	2.60	0.44
1:E:12:SER:OG	1:E:14:ILE:HG12	2.16	0.44
1:C:143:PHE:O	1:C:144:TYR:C	2.59	0.44
2:C:201:2AN:C12	2:C:201:2AN:H2	2.47	0.44
1:b:8:LYS:NZ	2:b:201:2AN:S	2.91	0.44
1:a:18:ARG:NH2	1:a:155:PRO:HA	2.32	0.44
1:Z:142:GLU:CG	2:Z:206:2AN:H7	2.47	0.44
1:W:43:GLU:O	1:W:56:LYS:N	2.41	0.44
1:V:47:GLY:H	2:V:201:2AN:H12	1.81	0.44
2:V:207:2AN:C12	2:V:207:2AN:H2	2.46	0.44
1:T:15:ALA:HB2	1:T:110:GLY:O	2.16	0.44
1:T:54:VAL:HA	1:T:70:HIS:O	2.17	0.44
1:h:6:ILE:HD11	1:h:133:VAL:CG1	2.47	0.44
1:g:19:LEU:HD12	1:g:19:LEU:HA	1.88	0.44
2:g:202:2AN:H15	2:g:203:2AN:H7	1.99	0.44
1:N:104:LYS:C	1:N:105:LEU:HD23	2.42	0.44
1:I:108:VAL:HG13	1:I:112:SER:HA	2.00	0.44
2:H:201:2AN:S	2:H:201:2AN:N	2.83	0.44
1:E:21:LYS:CE	1:E:158:PHE:CD1	3.00	0.44
1:D:43:GLU:C	1:D:44:ILE:HD12	2.42	0.44
1:a:10:GLU:HG3	2:a:204:2AN:H15	1.99	0.44
1:a:87:PHE:CD1	1:a:88:GLU:HB2	2.52	0.44
1:Y:1:MET:HE2	1:Y:4:TYR:CD1	2.53	0.44
1:Y:59:PHE:CE1	1:Y:65:LEU:HB3	2.52	0.44
1:S:150:TYR:C	1:S:150:TYR:CD1	2.96	0.44
1:B:8:LYS:HB2	1:B:116:ILE:HB	1.99	0.44
1:B:95:ASN:OD1	1:B:95:ASN:N	2.50	0.44
1:P:68:MET:HG2	1:P:91:VAL:HG22	1.99	0.44
1:N:40:LYS:HG3	1:N:60:VAL:HA	2.00	0.44
1:F:15:ALA:HB3	1:F:18:ARG:HD2	1.99	0.44
1:F:140:ALA:HA	2:F:202:2AN:H8	2.00	0.44
1:D:53:THR:CG2	1:D:54:VAL:N	2.80	0.44
1:f:151:LEU:CD2	1:f:157:VAL:CG2	2.94	0.44
1:e:144:TYR:O	1:e:147:VAL:N	2.49	0.44
1:Z:74:GLU:O	1:Z:82:CYS:HA	2.17	0.44
1:Y:31:LEU:HD22	1:Y:39:PHE:CE2	2.52	0.44
1:U:51:VAL:HG13	1:U:73:ASP:O	2.16	0.44
1:A:35:GLN:HB2	1:A:39:PHE:CE2	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:55:THR:N	1:A:70:HIS:O	2.49	0.44
1:R:140:ALA:O	1:R:141:TYR:C	2.61	0.44
1:Q:4:TYR:CD1	1:Q:4:TYR:N	2.85	0.44
1:Q:20:PHE:O	1:Q:24:VAL:HB	2.16	0.44
1:Q:98:LYS:HE3	1:Q:121:HIS:CG	2.52	0.44
1:K:14:ILE:O	1:K:112:SER:OG	2.28	0.44
1:F:47:GLY:HA3	1:F:53:THR:CA	2.39	0.44
1:f:2:ALA:CB	1:e:4:TYR:CZ	3.01	0.44
1:b:69:LEU:HD12	1:b:88:GLU:CG	2.47	0.44
1:a:101:TYR:HD1	1:a:118:VAL:HG22	1.82	0.44
1:X:44:ILE:O	1:X:44:ILE:CG2	2.65	0.44
1:X:150:TYR:O	1:X:153:ALA:HB3	2.17	0.44
1:V:120:TYR:N	1:V:120:TYR:CD1	2.86	0.44
1:U:115:LYS:HB3	1:U:115:LYS:NZ	2.33	0.44
1:T:21:LYS:HA	1:T:25:LEU:HB2	2.00	0.44
1:S:30:VAL:O	1:S:31:LEU:C	2.60	0.44
1:g:76:ASP:OD2	1:g:79:ASN:ND2	2.43	0.44
1:P:65:LEU:CD1	1:P:91:VAL:CG1	2.81	0.44
2:P:203:2AN:O1	2:P:203:2AN:H12	2.17	0.44
1:M:95:ASN:OD1	1:M:95:ASN:N	2.50	0.44
1:L:92:LEU:O	1:L:93:ARG:HB2	2.18	0.44
1:J:53:THR:HG23	1:J:72:PHE:CD1	2.53	0.44
2:G:202:2AN:N	2:G:202:2AN:S	2.90	0.44
1:d:71:LYS:O	1:d:84:TYR:HB2	2.18	0.44
1:b:96:ILE:HA	1:b:122:PRO:HA	2.00	0.44
1:a:68:MET:SD	1:a:91:VAL:HG11	2.58	0.44
1:T:23:LEU:CB	2:T:201:2AN:C3	2.96	0.44
1:S:14:ILE:HD13	1:S:14:ILE:N	2.32	0.44
1:A:85:THR:HA	1:A:99:VAL:O	2.18	0.44
1:A:127:THR:O	1:A:127:THR:HG23	2.18	0.44
1:Q:138:LYS:HG2	2:Q:203:2AN:H7	1.99	0.44
1:N:74:GLU:O	1:N:82:CYS:HA	2.18	0.44
2:N:205:2AN:O1	2:N:205:2AN:H12	2.18	0.44
1:L:81:TYR:C	1:L:81:TYR:CD1	2.96	0.44
1:L:144:TYR:C	1:L:144:TYR:CD1	2.93	0.44
1:L:144:TYR:CE2	1:L:145:LYS:HD3	2.53	0.44
1:E:123:LYS:O	1:E:124:PRO:C	2.60	0.44
1:C:150:TYR:O	1:C:154:ASN:N	2.45	0.44
1:c:21:LYS:HG2	1:c:158:PHE:HD1	1.78	0.44
1:c:120:TYR:CG	1:c:133:VAL:HG22	2.53	0.44
1:b:127:THR:OG1	1:b:128:VAL:N	2.49	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Y:93:ARG:HH11	2:Y:204:2AN:C13	2.24	0.44
1:X:151:LEU:O	1:X:154:ASN:N	2.50	0.44
1:W:26:GLU:OE1	1:W:29:GLN:NE2	2.51	0.44
1:V:10:GLU:HB3	2:V:203:2AN:C13	2.48	0.44
1:V:144:TYR:CE1	1:V:148:GLU:OE1	2.71	0.44
1:T:33:LYS:HD2	2:T:203:2AN:HN	1.82	0.44
1:h:53:THR:O	1:h:71:LYS:HA	2.17	0.44
1:h:150:TYR:CD1	1:h:150:TYR:C	2.96	0.44
1:B:144:TYR:CD2	2:B:202:2AN:H16	2.53	0.44
2:P:204:2AN:H16	2:P:204:2AN:H2	1.86	0.44
1:M:57:ILE:HD12	1:M:70:HIS:CE1	2.53	0.44
1:K:37:HIS:CD2	1:K:38:VAL:HG23	2.53	0.44
1:D:6:ILE:HG23	1:D:6:ILE:O	2.18	0.44
2:a:203:2AN:H16	2:a:203:2AN:C2	2.31	0.44
1:X:27:ARG:HH12	2:X:206:2AN:C6	2.31	0.44
1:X:47:GLY:HA3	1:X:53:THR:HA	1.99	0.44
1:T:55:THR:O	1:T:69:LEU:HA	2.17	0.44
2:T:202:2AN:H2	2:T:202:2AN:C16	2.47	0.44
1:j:129:ASN:C	1:j:131:GLU:H	2.25	0.44
2:j:203:2AN:S	2:j:203:2AN:N	2.90	0.44
1:h:19:LEU:O	1:h:23:LEU:HB2	2.17	0.44
1:h:33:LYS:HZ2	2:h:204:2AN:C12	2.30	0.44
1:P:27:ARG:O	1:P:30:VAL:N	2.49	0.43
1:K:91:VAL:HG21	2:K:201:2AN:C16	2.48	0.43
1:J:29:GLN:O	1:J:31:LEU:N	2.51	0.43
1:I:65:LEU:HD11	2:I:205:2AN:H16	2.00	0.43
1:H:136:GLY:HA2	2:H:202:2AN:C15	2.48	0.43
1:F:35:GLN:C	1:F:37:HIS:N	2.75	0.43
1:D:56:LYS:HA	1:D:68:MET:O	2.17	0.43
1:f:50:GLY:O	1:f:53:THR:OG1	2.27	0.43
1:d:10:GLU:CB	2:d:201:2AN:C15	2.95	0.43
1:W:101:TYR:CD1	1:W:118:VAL:HG13	2.53	0.43
1:U:14:ILE:N	1:U:14:ILE:CD1	2.80	0.43
1:T:63:HIS:HD2	1:T:65:LEU:HB2	1.83	0.43
1:S:66:THR:HB	1:S:90:ASP:OD2	2.17	0.43
1:i:31:LEU:HD23	1:i:143:PHE:CE1	2.53	0.43
1:g:44:ILE:HA	1:g:55:THR:HA	2.00	0.43
1:B:75:ILE:O	1:B:76:ASP:HB2	2.18	0.43
1:Q:23:LEU:CD2	1:Q:147:VAL:HG11	2.48	0.43
1:Q:143:PHE:O	1:Q:144:TYR:C	2.60	0.43
1:O:105:LEU:HD12	1:O:105:LEU:C	2.43	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:21:LYS:HE2	1:N:158:PHE:CE1	2.52	0.43
1:L:70:HIS:CA	1:L:85:THR:O	2.61	0.43
1:J:53:THR:HG22	1:J:72:PHE:CG	2.53	0.43
1:E:70:HIS:CD2	7:E:301:HOH:O	2.40	0.43
1:D:4:TYR:C	1:D:4:TYR:HD1	2.26	0.43
1:D:119:THR:HG22	1:D:121:HIS:HD2	1.80	0.43
1:f:87:PHE:CD1	1:f:87:PHE:C	2.95	0.43
1:b:18:ARG:HH22	1:b:155:PRO:HA	1.84	0.43
1:b:20:PHE:O	1:b:24:VAL:HB	2.18	0.43
1:a:8:LYS:HB3	1:a:8:LYS:NZ	2.32	0.43
1:a:14:ILE:HD11	1:a:152:ALA:HB2	2.00	0.43
1:a:30:VAL:O	1:a:33:LYS:N	2.51	0.43
1:T:97:GLU:OE1	1:T:122:PRO:O	2.36	0.43
1:j:51:VAL:CG1	1:j:75:ILE:H	2.31	0.43
1:i:26:GLU:O	1:i:30:VAL:HG23	2.18	0.43
2:h:206:2AN:C2	2:h:206:2AN:C12	2.59	0.43
1:R:50:GLY:C	1:R:75:ILE:HD12	2.43	0.43
2:P:202:2AN:C2	2:P:202:2AN:C12	2.93	0.43
2:O:203:2AN:H16	2:O:203:2AN:H2	1.99	0.43
1:L:68:MET:HB3	1:L:70:HIS:HE1	1.82	0.43
1:K:23:LEU:HD21	1:K:147:VAL:HB	1.99	0.43
1:J:10:GLU:O	1:J:114:GLY:N	2.50	0.43
1:I:95:ASN:CB	1:I:127:THR:O	2.65	0.43
1:I:109:GLY:O	1:a:80:PHE:HZ	2.01	0.43
1:I:139:LYS:HZ3	2:I:205:2AN:C13	2.31	0.43
1:f:105:LEU:HD22	2:f:201:2AN:H15	1.99	0.43
1:d:18:ARG:HH12	1:d:155:PRO:HA	1.83	0.43
1:a:16:PRO:HD3	1:a:112:SER:HB3	1.99	0.43
1:a:27:ARG:O	1:a:31:LEU:HG	2.18	0.43
1:a:81:TYR:CD1	1:a:81:TYR:C	2.96	0.43
1:a:100:VAL:HG12	7:a:308:HOH:O	2.18	0.43
1:Z:47:GLY:HA3	1:Z:53:THR:HA	1.99	0.43
1:A:12:SER:OG	1:A:14:ILE:HG12	2.18	0.43
2:Q:201:2AN:C16	2:Q:201:2AN:H2	2.47	0.43
1:P:138:LYS:HE3	1:P:139:LYS:HD2	1.99	0.43
1:L:144:TYR:CE2	1:L:145:LYS:CD	3.01	0.43
1:e:63:HIS:O	1:e:64:PRO:C	2.60	0.43
1:d:136:GLY:HA2	2:d:204:2AN:H3	1.99	0.43
1:c:8:LYS:CE	1:c:10:GLU:OE2	2.67	0.43
1:X:57:ILE:O	1:X:67:TYR:HA	2.18	0.43
2:V:203:2AN:S	2:V:203:2AN:N	2.87	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:j:131:GLU:O	1:j:132:GLU:C	2.61	0.43
1:j:150:TYR:HE1	1:j:157:VAL:HG21	1.83	0.43
1:i:131:GLU:O	1:i:134:LYS:N	2.51	0.43
1:h:55:THR:O	1:h:69:LEU:HA	2.18	0.43
1:g:29:GLN:O	1:g:32:VAL:HG23	2.18	0.43
1:g:123:LYS:O	1:g:124:PRO:C	2.60	0.43
1:R:53:THR:O	1:R:72:PHE:N	2.52	0.43
1:R:71:LYS:HG3	1:R:87:PHE:CZ	2.52	0.43
1:N:154:ASN:HB3	1:N:157:VAL:CG2	2.49	0.43
1:I:20:PHE:CD2	1:I:20:PHE:O	2.71	0.43
2:H:204:2AN:C3	1:b:109:GLY:HA2	2.48	0.43
1:E:150:TYR:CE2	2:E:203:2AN:C10	3.02	0.43
1:b:147:VAL:O	1:b:151:LEU:HG	2.18	0.43
1:Z:139:LYS:HD3	1:Z:139:LYS:HA	1.94	0.43
2:X:203:2AN:N	2:X:203:2AN:O3	2.51	0.43
1:W:20:PHE:O	1:W:24:VAL:HB	2.18	0.43
1:V:5:THR:CG2	1:V:7:VAL:HG23	2.48	0.43
1:h:153:ALA:C	1:h:154:ASN:ND2	2.77	0.43
1:A:16:PRO:O	1:A:19:LEU:N	2.52	0.43
1:R:0:THR:HG23	1:Q:137:GLU:OE2	2.19	0.43
1:Q:23:LEU:HD13	2:Q:202:2AN:C2	2.49	0.43
1:K:39:PHE:O	1:K:60:VAL:HG13	2.18	0.43
1:J:6:ILE:HG22	1:I:0:THR:HG22	2.00	0.43
1:E:150:TYR:CD2	2:E:203:2AN:C5	3.02	0.43
1:f:131:GLU:O	1:f:132:GLU:C	2.62	0.43
1:e:16:PRO:C	1:e:18:ARG:N	2.75	0.43
1:b:21:LYS:HE3	1:b:158:PHE:CE1	2.53	0.43
1:Y:93:ARG:NH1	2:Y:204:2AN:H2	2.33	0.43
1:W:107:ALA:C	1:W:108:VAL:HG23	2.44	0.43
1:T:66:THR:OG1	1:T:90:ASP:OD2	2.24	0.43
1:T:129:ASN:OD1	1:T:129:ASN:N	2.51	0.43
1:i:133:VAL:O	1:i:137:GLU:N	2.48	0.43
1:R:19:LEU:C	1:R:21:LYS:N	2.72	0.43
1:Q:67:TYR:CE2	1:Q:69:LEU:HD13	2.40	0.43
1:I:31:LEU:HD13	1:I:57:ILE:HD13	2.01	0.43
1:I:98:LYS:HE3	1:I:121:HIS:CD2	2.54	0.43
1:H:77:ALA:C	2:H:204:2AN:H2	2.42	0.43
1:G:5:THR:HA	1:G:118:VAL:O	2.18	0.43
1:G:18:ARG:CZ	1:G:157:VAL:O	2.67	0.43
1:F:130:GLU:OE1	1:F:131:GLU:N	2.51	0.43
1:D:4:TYR:CZ	1:C:2:ALA:HB2	2.46	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:140:ALA:O	1:D:141:TYR:C	2.58	0.43
1:c:94:ASP:O	1:c:123:LYS:CD	2.66	0.43
1:X:147:VAL:HG13	2:X:202:2AN:C14	2.49	0.43
1:V:16:PRO:HG3	1:V:107:ALA:HB2	2.00	0.43
1:g:50:GLY:O	1:g:51:VAL:C	2.60	0.43
1:g:83:LYS:HA	1:g:101:TYR:O	2.19	0.43
1:R:37:HIS:CD2	1:R:38:VAL:HG23	2.54	0.43
1:K:19:LEU:O	1:K:23:LEU:N	2.41	0.43
1:J:107:ALA:O	1:J:108:VAL:HG22	2.18	0.43
1:J:147:VAL:O	1:J:151:LEU:HG	2.19	0.43
1:G:44:ILE:HA	1:G:55:THR:HG22	2.00	0.43
1:e:59:PHE:HD2	1:e:63:HIS:CD2	2.36	0.43
1:e:79:ASN:O	1:e:104:LYS:HE2	2.19	0.43
1:b:50:GLY:N	1:b:53:THR:OG1	2.51	0.43
1:a:16:PRO:HG2	1:a:107:ALA:CB	2.47	0.43
1:Z:66:THR:H	1:Z:90:ASP:CG	2.26	0.43
1:W:120:TYR:CD2	1:W:133:VAL:HG22	2.54	0.43
1:T:97:GLU:HB2	1:T:122:PRO:C	2.44	0.43
1:j:83:LYS:HA	1:j:101:TYR:O	2.19	0.43
1:i:29:GLN:NE2	1:i:42:GLY:O	2.52	0.43
1:i:99:VAL:HA	1:i:119:THR:O	2.18	0.43
1:h:50:GLY:C	1:h:75:ILE:CD1	2.90	0.43
1:A:31:LEU:HA	1:A:143:PHE:CE1	2.53	0.43
1:R:103:VAL:HG21	2:R:201:2AN:C4	2.49	0.43
2:R:202:2AN:H2	2:R:202:2AN:C12	2.47	0.43
1:P:76:ASP:CG	1:P:79:ASN:HD22	2.27	0.43
1:P:122:PRO:HB3	1:P:128:VAL:CG2	2.49	0.43
1:M:59:PHE:N	1:M:59:PHE:CD1	2.87	0.43
1:L:44:ILE:HA	1:L:55:THR:HA	2.01	0.43
2:F:204:2AN:C2	2:F:204:2AN:C16	2.83	0.43
1:C:55:THR:O	1:C:69:LEU:HA	2.18	0.43
1:C:57:ILE:HB	1:C:68:MET:CG	2.49	0.43
1:f:90:ASP:OD1	1:f:90:ASP:N	2.49	0.43
1:e:30:VAL:O	1:e:34:ALA:N	2.48	0.43
1:d:-2:PRO:HG3	2:c:202:2AN:C16	2.49	0.43
2:c:201:2AN:N	2:c:201:2AN:O1	2.52	0.43
1:a:19:LEU:O	1:a:22:ALA:N	2.52	0.43
1:Y:80:PHE:HB3	1:Y:105:LEU:HB2	2.00	0.43
2:V:205:2AN:C16	2:V:205:2AN:C2	2.88	0.43
1:T:0:THR:CG2	1:S:137:GLU:OE2	2.66	0.43
1:T:134:LYS:O	1:T:135:ILE:C	2.61	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:j:20:PHE:HB2	1:j:105:LEU:HD12	2.01	0.43
1:j:47:GLY:N	2:j:201:2AN:H16	2.33	0.43
1:A:151:LEU:HD23	1:A:151:LEU:HA	1.69	0.43
1:P:147:VAL:O	1:P:150:TYR:N	2.52	0.43
1:N:26:GLU:OE1	1:N:26:GLU:HA	2.19	0.43
1:M:4:TYR:CD1	1:M:4:TYR:N	2.87	0.43
1:M:59:PHE:O	1:M:60:VAL:O	2.37	0.43
1:J:59:PHE:CD2	1:J:65:LEU:HB2	2.52	0.43
1:G:36:PRO:HD2	7:G:305:HOH:O	2.18	0.43
1:f:15:ALA:HA	1:f:16:PRO:HD3	1.90	0.43
1:d:-2:PRO:CB	1:c:134:LYS:HB3	2.48	0.43
1:c:19:LEU:HA	1:c:19:LEU:HD23	1.72	0.43
1:a:16:PRO:C	1:a:18:ARG:N	2.73	0.43
1:T:63:HIS:CG	1:T:64:PRO:HD2	2.53	0.43
1:S:91:VAL:HG23	2:S:201:2AN:C7	2.49	0.43
1:h:35:GLN:HE21	1:h:146:GLN:CD	2.27	0.43
1:g:30:VAL:O	1:g:31:LEU:C	2.61	0.43
1:g:80:PHE:HB3	1:g:105:LEU:HB2	2.00	0.43
1:B:31:LEU:HD12	1:B:57:ILE:HD13	2.01	0.42
1:A:123:LYS:O	1:A:126:CYS:SG	2.75	0.42
1:R:0:THR:CG2	1:Q:137:GLU:OE2	2.67	0.42
1:Q:92:LEU:CD1	1:Q:97:GLU:O	2.67	0.42
1:O:129:ASN:O	1:O:130:GLU:C	2.61	0.42
1:L:73:ASP:HB3	1:L:74:GLU:OE1	2.18	0.42
1:I:63:HIS:NE2	2:I:205:2AN:C15	2.82	0.42
1:H:49:GLY:HA2	1:H:53:THR:HG21	2.00	0.42
1:F:48:ASP:C	1:F:50:GLY:N	2.77	0.42
1:D:57:ILE:HD12	1:D:57:ILE:N	2.34	0.42
1:D:97:GLU:HA	1:D:123:LYS:CE	2.48	0.42
1:a:35:GLN:HB2	1:a:39:PHE:CE1	2.49	0.42
1:X:6:ILE:HG21	1:X:137:GLU:OE2	2.18	0.42
1:V:10:GLU:OE2	1:V:141:TYR:HE1	2.02	0.42
1:V:63:HIS:ND1	1:V:64:PRO:HD2	2.34	0.42
1:V:66:THR:N	1:V:90:ASP:OD2	2.52	0.42
1:T:80:PHE:O	1:T:104:LYS:HA	2.19	0.42
1:j:51:VAL:CG1	1:j:74:GLU:HA	2.48	0.42
1:A:31:LEU:HD21	2:A:202:2AN:C8	2.49	0.42
1:P:5:THR:HG22	1:P:7:VAL:HG23	2.01	0.42
1:P:42:GLY:O	1:P:43:GLU:HB3	2.19	0.42
1:O:30:VAL:O	1:O:34:ALA:HB3	2.18	0.42
1:N:0:THR:HG22	1:M:6:ILE:HG23	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:48:ASP:C	1:L:50:GLY:N	2.77	0.42
1:L:67:TYR:HE2	1:L:69:LEU:HD11	1.84	0.42
1:I:35:GLN:OE1	2:I:201:2AN:H7	2.19	0.42
1:I:98:LYS:HE2	1:I:121:HIS:CG	2.53	0.42
1:H:70:HIS:ND1	1:H:70:HIS:N	2.67	0.42
1:G:108:VAL:O	1:G:108:VAL:HG23	2.18	0.42
1:D:34:ALA:C	1:D:36:PRO:HD3	2.43	0.42
1:C:55:THR:N	1:C:70:HIS:O	2.39	0.42
2:C:202:2AN:C10	7:C:301:HOH:O	2.67	0.42
1:e:16:PRO:O	1:e:18:ARG:N	2.52	0.42
1:V:59:PHE:C	1:V:60:VAL:O	2.61	0.42
1:U:144:TYR:CD2	1:U:145:LYS:CD	3.02	0.42
1:T:142:GLU:O	1:T:146:GLN:HG3	2.19	0.42
1:j:4:TYR:CD1	1:j:128:VAL:HG21	2.52	0.42
1:h:48:ASP:OD1	1:h:48:ASP:N	2.52	0.42
1:A:70:HIS:CE1	7:A:302:HOH:O	2.70	0.42
1:O:101:TYR:CD1	2:O:201:2AN:C13	3.02	0.42
2:O:202:2AN:H2	2:O:202:2AN:C12	2.45	0.42
1:K:133:VAL:HG12	1:K:134:LYS:N	2.34	0.42
1:H:97:GLU:HG2	1:H:123:LYS:HA	2.01	0.42
1:F:46:GLU:CG	2:F:206:2AN:O1	2.68	0.42
1:D:140:ALA:HB1	2:D:201:2AN:H8	1.99	0.42
1:c:69:LEU:HD12	1:c:88:GLU:CB	2.49	0.42
1:b:6:ILE:HD11	1:b:133:VAL:CG1	2.49	0.42
1:a:55:THR:HG23	1:a:72:PHE:HE2	1.85	0.42
1:X:73:ASP:HB2	1:X:83:LYS:O	2.19	0.42
1:U:149:GLU:O	1:U:150:TYR:C	2.62	0.42
1:L:31:LEU:CD1	1:L:57:ILE:HD13	2.49	0.42
1:K:110:GLY:HA2	1:Y:17:HIS:CD2	2.54	0.42
1:I:2:ALA:O	1:I:122:PRO:CG	2.67	0.42
1:F:14:ILE:HG21	1:F:151:LEU:CD1	2.48	0.42
1:F:19:LEU:O	1:F:23:LEU:HB2	2.19	0.42
1:E:108:VAL:O	1:E:108:VAL:HG12	2.18	0.42
1:D:69:LEU:HG	1:D:88:GLU:HB2	2.01	0.42
1:D:141:TYR:HB3	2:D:204:2AN:H12	2.00	0.42
1:c:144:TYR:CE2	1:c:145:LYS:HD2	2.55	0.42
2:b:203:2AN:O1	2:b:203:2AN:C16	2.67	0.42
1:W:87:PHE:CD1	1:W:87:PHE:C	2.98	0.42
1:V:155:PRO:O	1:V:159:ALA:HB2	2.19	0.42
1:j:76:ASP:C	1:j:78:ALA:H	2.28	0.42
2:j:201:2AN:H16	2:j:201:2AN:O2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:i:16:PRO:HG2	1:i:107:ALA:HB2	2.01	0.42
1:h:19:LEU:O	1:h:19:LEU:HD13	2.20	0.42
1:B:44:ILE:CG2	1:B:53:THR:CG2	2.97	0.42
2:A:202:2AN:C12	2:A:202:2AN:H2	2.50	0.42
1:R:103:VAL:HG21	2:R:201:2AN:H4	2.02	0.42
1:Q:27:ARG:O	1:Q:31:LEU:HG	2.19	0.42
1:Q:59:PHE:O	1:Q:60:VAL:C	2.63	0.42
1:O:0:THR:O	1:O:0:THR:HG22	2.19	0.42
1:O:73:ASP:N	1:O:83:LYS:O	2.53	0.42
1:N:6:ILE:O	1:N:117:THR:HA	2.19	0.42
1:F:130:GLU:C	1:F:130:GLU:OE1	2.62	0.42
1:E:59:PHE:O	1:E:60:VAL:O	2.37	0.42
1:D:16:PRO:HG3	1:D:107:ALA:N	2.35	0.42
1:f:116:ILE:HD12	1:f:116:ILE:N	2.34	0.42
1:e:94:ASP:O	1:e:123:LYS:HD2	2.19	0.42
1:e:100:VAL:HG12	7:e:307:HOH:O	2.19	0.42
1:d:154:ASN:HB3	1:d:157:VAL:HG23	2.00	0.42
1:b:128:VAL:O	1:b:128:VAL:HG12	2.19	0.42
1:a:138:LYS:HA	2:a:203:2AN:C15	2.50	0.42
1:Z:1:MET:HE1	1:Y:134:LYS:CE	2.50	0.42
1:Z:53:THR:O	1:Z:71:LYS:HA	2.20	0.42
1:V:10:GLU:HB3	2:V:203:2AN:H13	2.01	0.42
1:j:69:LEU:HD12	1:j:88:GLU:HB3	2.02	0.42
1:i:30:VAL:O	1:i:34:ALA:CB	2.67	0.42
1:h:153:ALA:C	1:h:154:ASN:HD22	2.27	0.42
1:R:120:TYR:CE1	1:R:133:VAL:HG13	2.55	0.42
1:R:137:GLU:OE2	1:Q:0:THR:OG1	2.32	0.42
1:Q:57:ILE:HG21	1:Q:68:MET:HE3	2.02	0.42
1:L:122:PRO:HB3	1:L:128:VAL:HG22	2.01	0.42
1:J:14:ILE:HD12	1:J:151:LEU:HB2	2.01	0.42
1:I:16:PRO:CG	1:I:107:ALA:HA	2.49	0.42
1:F:143:PHE:O	1:F:147:VAL:HG23	2.20	0.42
1:D:92:LEU:HA	1:D:96:ILE:HG13	2.01	0.42
2:a:204:2AN:O1	2:a:204:2AN:N	2.52	0.42
1:X:16:PRO:HD3	1:X:112:SER:OG	2.19	0.42
1:U:30:VAL:HA	1:U:33:LYS:HD2	2.01	0.42
2:T:201:2AN:N	2:T:201:2AN:O2	2.53	0.42
1:h:70:HIS:NE2	1:h:86:LEU:HB2	2.35	0.42
1:h:150:TYR:CE2	2:h:204:2AN:C8	3.03	0.42
1:B:23:LEU:HD22	1:B:143:PHE:CE2	2.54	0.42
1:A:38:VAL:HG13	1:A:63:HIS:CD2	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:21:LYS:HD3	1:R:158:PHE:CD2	2.54	0.42
1:R:96:ILE:CG2	1:R:97:GLU:N	2.82	0.42
1:P:119:THR:HG22	1:P:121:HIS:CD2	2.55	0.42
1:O:16:PRO:HG3	1:O:107:ALA:N	2.35	0.42
1:N:120:TYR:CE1	1:N:133:VAL:HG13	2.55	0.42
1:N:143:PHE:CE1	1:N:147:VAL:HG21	2.54	0.42
1:L:2:ALA:CB	1:K:4:TYR:CE2	3.02	0.42
1:E:47:GLY:HA3	1:E:53:THR:HA	2.01	0.42
1:E:107:ALA:CB	1:e:107:ALA:HB2	2.48	0.42
1:D:123:LYS:O	1:D:124:PRO:C	2.60	0.42
1:e:6:ILE:CG2	1:e:118:VAL:HB	2.46	0.42
1:a:116:ILE:HG12	2:a:204:2AN:O3	2.20	0.42
1:Z:27:ARG:NH1	7:Z:302:HOH:O	2.36	0.42
1:Y:31:LEU:HD12	1:Y:57:ILE:HD13	2.00	0.42
1:V:4:TYR:HA	1:U:3:ALA:O	2.19	0.42
1:U:149:GLU:CD	1:U:149:GLU:C	2.87	0.42
1:i:26:GLU:O	1:i:30:VAL:CG2	2.67	0.42
1:h:89:GLY:O	1:h:92:LEU:HB2	2.20	0.42
1:A:72:PHE:CD1	1:A:75:ILE:HD11	2.54	0.42
1:Q:108:VAL:O	1:Q:108:VAL:HG12	2.19	0.42
1:P:14:ILE:HD13	1:P:148:GLU:HG3	2.01	0.42
1:O:18:ARG:C	1:O:20:PHE:N	2.78	0.42
1:O:120:TYR:O	1:O:122:PRO:HD3	2.20	0.42
1:L:119:THR:HG22	1:L:121:HIS:CE1	2.55	0.42
1:J:129:ASN:C	1:J:131:GLU:H	2.27	0.42
1:J:158:PHE:CE2	2:J:201:2AN:H13	2.55	0.42
2:I:206:2AN:H12	7:I:303:HOH:O	2.19	0.42
1:D:65:LEU:HD21	1:D:91:VAL:HA	2.00	0.42
1:f:2:ALA:HA	1:e:4:TYR:CE1	2.54	0.42
2:d:203:2AN:N	2:d:203:2AN:O1	2.53	0.42
1:b:39:PHE:CE1	1:b:59:PHE:CZ	3.08	0.42
1:a:43:GLU:N	1:a:56:LYS:O	2.48	0.42
1:U:9:GLU:HA	1:U:115:LYS:HA	2.02	0.42
1:h:43:GLU:HG3	1:h:45:ILE:CG2	2.47	0.42
1:M:110:GLY:HA2	1:W:17:HIS:CG	2.55	0.42
1:F:38:VAL:O	1:F:59:PHE:CD2	2.73	0.42
1:E:152:ALA:O	1:E:155:PRO:HD3	2.20	0.42
1:D:70:HIS:CD2	1:D:86:LEU:HD13	2.55	0.42
2:D:202:2AN:S	2:D:202:2AN:N	2.93	0.42
1:C:14:ILE:C	1:C:111:GLY:HA2	2.45	0.42
1:f:-1:PHE:CE1	2:f:206:2AN:C8	3.03	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:b:28:HIS:ND1	1:b:28:HIS:N	2.62	0.42
1:b:120:TYR:N	1:b:120:TYR:CD1	2.88	0.42
1:a:8:LYS:HG3	1:a:116:ILE:O	2.20	0.42
2:Z:204:2AN:H16	2:Z:204:2AN:C2	2.37	0.42
1:X:20:PHE:CE1	1:X:80:PHE:HA	2.55	0.42
2:X:206:2AN:C9	7:X:302:HOH:O	2.66	0.42
1:T:27:ARG:NH2	2:T:202:2AN:O2	2.48	0.42
1:R:87:PHE:CD1	1:R:87:PHE:N	2.88	0.42
1:Q:14:ILE:HG22	1:Q:15:ALA:O	2.20	0.42
1:M:96:ILE:CD1	1:M:128:VAL:HG22	2.46	0.42
1:L:91:VAL:HG13	1:L:92:LEU:CD1	2.50	0.42
1:H:57:ILE:HD12	1:H:70:HIS:CE1	2.55	0.42
1:H:57:ILE:N	1:H:68:MET:O	2.29	0.42
2:F:203:2AN:N	2:F:203:2AN:O3	2.36	0.42
2:F:206:2AN:H4	1:f:17:HIS:CB	2.47	0.42
1:D:19:LEU:HD23	1:D:19:LEU:HA	1.94	0.42
1:C:59:PHE:HD1	1:C:66:THR:C	2.27	0.42
1:f:6:ILE:HG13	1:e:0:THR:HB	2.01	0.42
1:f:16:PRO:HG3	1:f:107:ALA:HA	2.01	0.42
1:f:34:ALA:N	2:f:205:2AN:O3	2.53	0.42
1:f:144:TYR:CD1	1:f:144:TYR:C	2.98	0.42
1:d:19:LEU:HD21	2:d:201:2AN:C12	2.49	0.42
1:d:57:ILE:HD12	1:d:57:ILE:N	2.34	0.42
1:c:17:HIS:H	1:c:17:HIS:CD2	2.37	0.42
1:c:37:HIS:CD2	1:c:38:VAL:HG23	2.55	0.42
1:T:82:CYS:SG	1:T:83:LYS:N	2.93	0.42
1:h:93:ARG:HG2	1:h:132:GLU:OE1	2.20	0.42
1:N:123:LYS:O	1:N:124:PRO:C	2.63	0.41
1:L:80:PHE:O	1:L:104:LYS:HA	2.20	0.41
2:L:203:2AN:C2	2:L:203:2AN:C16	2.95	0.41
1:G:17:HIS:N	1:G:80:PHE:CE1	2.87	0.41
2:G:204:2AN:N	2:G:204:2AN:S	2.70	0.41
1:F:110:GLY:HA2	1:d:17:HIS:HB2	2.02	0.41
1:D:17:HIS:HB3	1:f:110:GLY:HA2	2.02	0.41
1:C:109:GLY:O	1:g:80:PHE:HZ	2.03	0.41
2:C:203[A]:2AN:N	2:C:203[A]:2AN:S	2.92	0.41
1:d:34:ALA:C	1:d:36:PRO:HD3	2.45	0.41
1:c:18:ARG:NH2	1:c:154:ASN:O	2.52	0.41
1:b:158:PHE:CZ	2:b:204:2AN:H6	2.54	0.41
2:a:204:2AN:N	2:a:204:2AN:O3	2.44	0.41
1:W:96:ILE:CA	1:W:121:HIS:O	2.65	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:W:101:TYR:OH	2:W:201:2AN:H12	2.19	0.41
1:V:142:GLU:HG2	2:V:208:2AN:H12	1.98	0.41
1:U:103:VAL:CG2	1:U:116:ILE:CG2	2.95	0.41
1:S:50:GLY:O	1:S:51:VAL:C	2.62	0.41
1:i:141:TYR:O	1:i:142:GLU:C	2.63	0.41
1:R:96:ILE:HG22	1:R:97:GLU:N	2.35	0.41
1:O:74:GLU:O	1:O:83:LYS:N	2.39	0.41
1:M:16:PRO:HD3	1:M:112:SER:HB3	2.01	0.41
1:L:54:VAL:HG22	1:L:71:LYS:CB	2.49	0.41
1:I:20:PHE:CE2	1:I:77:ALA:HA	2.54	0.41
2:I:203:2AN:N	2:I:203:2AN:S	2.90	0.41
1:G:26:GLU:O	1:G:29:GLN:N	2.47	0.41
1:G:85:THR:HG22	1:G:100:VAL:HG22	2.01	0.41
1:E:67:TYR:OH	1:E:88:GLU:OE2	2.37	0.41
1:D:5:THR:HG1	1:C:5:THR:CB	2.29	0.41
1:D:79:ASN:O	1:D:80:PHE:C	2.63	0.41
1:C:82:CYS:SG	1:C:83:LYS:N	2.93	0.41
1:e:100:VAL:O	1:e:118:VAL:HA	2.20	0.41
1:d:100:VAL:HG23	1:d:121:HIS:CD2	2.55	0.41
1:b:12:SER:C	1:b:14:ILE:H	2.28	0.41
1:W:17:HIS:O	1:W:21:LYS:HB2	2.20	0.41
2:V:206:2AN:H2	2:V:206:2AN:C16	2.30	0.41
1:T:53:THR:O	1:T:72:PHE:HD1	2.03	0.41
1:j:136:GLY:O	1:j:137:GLU:C	2.60	0.41
1:A:27:ARG:NH2	7:A:303:HOH:O	2.24	0.41
1:A:82:CYS:O	1:A:103:VAL:N	2.44	0.41
1:N:129:ASN:OD1	1:N:129:ASN:N	2.53	0.41
1:J:5:THR:HA	1:J:118:VAL:O	2.20	0.41
1:D:32:VAL:O	1:D:36:PRO:HB3	2.20	0.41
2:D:203:2AN:O2	2:D:203:2AN:C12	2.69	0.41
1:e:141:TYR:O	1:e:144:TYR:HB3	2.19	0.41
1:d:24:VAL:HG21	1:d:103:VAL:HG11	2.02	0.41
1:Y:71:LYS:O	1:Y:85:THR:N	2.42	0.41
1:X:143:PHE:O	1:X:147:VAL:HG23	2.19	0.41
1:V:20:PHE:CD1	1:V:24:VAL:HG21	2.55	0.41
1:j:6:ILE:HD13	1:j:137:GLU:OE2	2.20	0.41
1:i:63:HIS:O	1:i:64:PRO:C	2.62	0.41
1:h:129:ASN:C	1:h:131:GLU:H	2.27	0.41
1:B:11:GLU:HA	1:B:113:LYS:HA	2.01	0.41
1:B:72:PHE:CD2	1:B:75:ILE:HD11	2.55	0.41
1:N:92:LEU:HD13	1:N:96:ILE:O	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:136:GLY:O	1:L:137:GLU:C	2.61	0.41
1:K:86:LEU:HD21	1:K:91:VAL:CG1	2.50	0.41
1:J:105:LEU:HD23	1:J:105:LEU:N	2.35	0.41
1:I:63:HIS:HE1	2:I:205:2AN:C15	2.29	0.41
1:G:27:ARG:NH2	2:G:201:2AN:O2	2.46	0.41
1:D:8:LYS:HG2	1:D:116:ILE:HB	2.02	0.41
1:c:68:MET:HA	1:c:88:GLU:O	2.20	0.41
2:b:206:2AN:S	2:b:206:2AN:C12	3.09	0.41
1:Z:141:TYR:HD1	7:Z:304:HOH:O	1.93	0.41
1:X:54:VAL:HG13	1:X:87:PHE:CE1	2.56	0.41
1:W:37:HIS:O	1:W:60:VAL:HG11	2.19	0.41
1:V:10:GLU:CD	1:V:141:TYR:CE1	2.93	0.41
2:V:202:2AN:O1	7:V:301:HOH:O	2.22	0.41
1:U:5:THR:HG23	1:U:119:THR:OG1	2.20	0.41
1:U:95:ASN:HD21	1:U:129:ASN:N	2.18	0.41
1:O:0:THR:HB	1:O:1:MET:CE	2.50	0.41
1:O:81:TYR:HA	1:O:103:VAL:O	2.20	0.41
1:O:97:GLU:HB2	1:O:123:LYS:HA	2.01	0.41
1:G:29:GLN:O	1:G:33:LYS:HG3	2.20	0.41
2:F:203:2AN:N	2:F:203:2AN:O1	2.54	0.41
1:D:40:LYS:N	1:D:59:PHE:O	2.54	0.41
1:f:4:TYR:CG	1:f:128:VAL:HG11	2.56	0.41
1:d:19:LEU:HD21	2:d:201:2AN:H12	2.02	0.41
2:a:203:2AN:O3	2:a:203:2AN:H12	2.20	0.41
1:X:16:PRO:CG	1:X:112:SER:OG	2.69	0.41
1:X:20:PHE:CB	1:X:105:LEU:HD12	2.47	0.41
1:U:57:ILE:O	1:U:67:TYR:HB3	2.18	0.41
1:U:131:GLU:CG	1:U:132:GLU:N	2.83	0.41
1:h:1:MET:O	1:h:1:MET:CG	2.68	0.41
1:h:14:ILE:C	1:h:111:GLY:HA2	2.46	0.41
1:B:55:THR:O	1:B:69:LEU:HA	2.21	0.41
1:R:24:VAL:CG1	1:R:82:CYS:SG	3.08	0.41
1:R:38:VAL:HB	1:R:39:PHE:CD2	2.56	0.41
1:O:73:ASP:OD2	1:O:85:THR:OG1	2.33	0.41
1:N:38:VAL:HG13	1:N:63:HIS:NE2	2.35	0.41
2:I:204:2AN:C4	1:Y:17:HIS:HB2	2.36	0.41
1:G:16:PRO:HB2	1:G:80:PHE:CZ	2.56	0.41
1:F:33:LYS:HD3	2:F:203:2AN:C11	2.50	0.41
1:E:15:ALA:O	1:E:16:PRO:C	2.63	0.41
1:E:149:GLU:O	1:E:150:TYR:C	2.62	0.41
1:f:-1:PHE:HE1	2:f:206:2AN:C8	2.33	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:b:158:PHE:CE2	2:b:204:2AN:H6	2.54	0.41
1:a:32:VAL:HG22	1:a:39:PHE:HB2	2.01	0.41
1:W:90:ASP:OD1	1:W:90:ASP:N	2.53	0.41
1:B:14:ILE:O	1:B:112:SER:OG	2.22	0.41
1:B:101:TYR:CD2	1:B:118:VAL:HG13	2.56	0.41
1:B:117:THR:O	1:B:117:THR:HG22	2.20	0.41
1:R:135:ILE:CG2	2:R:205:2AN:H4	2.51	0.41
1:P:54:VAL:HG22	1:P:71:LYS:CB	2.49	0.41
1:P:72:PHE:CD2	1:P:75:ILE:HD11	2.55	0.41
2:J:201:2AN:N	2:J:201:2AN:S	2.76	0.41
1:G:29:GLN:HB3	1:G:33:LYS:HE3	2.02	0.41
1:G:31:LEU:HD23	1:G:143:PHE:CZ	2.55	0.41
1:G:57:ILE:O	1:G:67:TYR:CA	2.66	0.41
1:G:76:ASP:OD2	1:G:79:ASN:CG	2.64	0.41
1:F:57:ILE:HB	1:F:68:MET:CG	2.51	0.41
1:f:150:TYR:CE2	2:f:205:2AN:O1	2.74	0.41
1:e:147:VAL:O	1:e:148:GLU:C	2.64	0.41
1:Z:1:MET:HE2	1:Z:1:MET:HB3	1.90	0.41
2:Z:201:2AN:C2	2:Z:201:2AN:C12	2.94	0.41
2:Z:204:2AN:O3	2:Z:204:2AN:N	2.53	0.41
1:Y:23:LEU:HD11	1:Y:147:VAL:HG21	2.03	0.41
1:V:78:ALA:C	1:V:79:ASN:OD1	2.64	0.41
1:U:20:PHE:CZ	1:U:77:ALA:HA	2.55	0.41
1:U:96:ILE:HG12	1:U:128:VAL:HG23	2.02	0.41
1:U:142:GLU:CB	2:U:201:2AN:H15	2.51	0.41
2:U:201:2AN:C2	2:U:201:2AN:C16	2.84	0.41
1:j:153:ALA:C	1:j:155:PRO:HD3	2.45	0.41
1:A:16:PRO:HD2	3:A:205:SO4:S	2.61	0.41
1:R:69:LEU:HD12	1:R:88:GLU:OE1	2.19	0.41
1:O:96:ILE:HD11	1:O:132:GLU:OE1	2.20	0.41
1:K:101:TYR:CE2	2:K:202:2AN:C15	3.03	0.41
1:J:50:GLY:O	1:J:51:VAL:C	2.63	0.41
2:J:203:2AN:C2	2:J:203:2AN:C12	2.94	0.41
1:H:46:GLU:OE1	1:H:47:GLY:N	2.49	0.41
1:E:122:PRO:HB3	1:E:128:VAL:HG23	2.03	0.41
1:C:97:GLU:HB3	1:C:121:HIS:O	2.21	0.41
1:e:69:LEU:HB2	1:e:88:GLU:HB3	2.02	0.41
1:c:52:GLY:O	1:c:53:THR:C	2.63	0.41
1:Z:7:VAL:HG13	1:Z:117:THR:OG1	2.20	0.41
1:X:84:TYR:CE1	1:X:101:TYR:HB2	2.55	0.41
1:V:108:VAL:O	1:V:108:VAL:HG12	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:108:VAL:HG21	1:U:113:LYS:HE2	2.01	0.41
1:U:113:LYS:NZ	1:U:113:LYS:CB	2.84	0.41
1:A:49:GLY:N	1:A:53:THR:HG21	2.36	0.41
1:A:51:VAL:HG22	1:A:75:ILE:HG13	2.01	0.41
1:A:84:TYR:CZ	1:A:101:TYR:CB	3.04	0.41
2:O:203:2AN:N	2:O:203:2AN:S	2.94	0.41
1:M:95:ASN:CB	1:M:127:THR:O	2.68	0.41
1:M:133:VAL:O	1:M:137:GLU:N	2.47	0.41
1:K:120:TYR:CD2	1:K:133:VAL:HG23	2.54	0.41
1:J:56:LYS:HE3	1:J:67:TYR:CB	2.51	0.41
1:I:98:LYS:HE2	1:I:121:HIS:ND1	2.36	0.41
1:I:108:VAL:HG11	1:I:113:LYS:HG3	2.03	0.41
1:G:19:LEU:O	1:G:23:LEU:N	2.44	0.41
1:F:28:HIS:O	1:F:42:GLY:HA3	2.19	0.41
1:f:20:PHE:HE2	1:f:77:ALA:HA	1.84	0.41
1:f:50:GLY:O	1:f:51:VAL:C	2.63	0.41
1:e:23:LEU:CD1	1:e:147:VAL:HG11	2.50	0.41
1:e:57:ILE:O	1:e:67:TYR:HA	2.20	0.41
1:e:99:VAL:HA	1:e:119:THR:O	2.21	0.41
1:d:69:LEU:HD12	1:d:88:GLU:CG	2.51	0.41
1:d:74:GLU:CG	1:d:83:LYS:HB2	2.48	0.41
1:b:31:LEU:HD21	1:b:143:PHE:CD2	2.56	0.41
1:b:91:VAL:HG22	2:b:202:2AN:C13	2.50	0.41
1:b:139:LYS:HE2	2:b:202:2AN:C4	2.51	0.41
1:Z:81:TYR:CD1	1:Z:81:TYR:C	2.99	0.41
1:Y:37:HIS:CD2	1:Y:38:VAL:HG23	2.56	0.41
1:X:30:VAL:HG13	2:X:202:2AN:C13	2.50	0.41
1:X:31:LEU:HA	1:X:143:PHE:CZ	2.56	0.41
1:W:107:ALA:O	1:W:108:VAL:HG22	2.21	0.41
1:V:34:ALA:HB3	1:V:143:PHE:HE1	1.85	0.41
1:V:46:GLU:HB3	1:V:54:VAL:HB	2.02	0.41
1:V:47:GLY:N	2:V:201:2AN:C12	2.84	0.41
1:V:73:ASP:HB2	1:V:83:LYS:O	2.21	0.41
1:U:8:LYS:O	1:U:115:LYS:CA	2.68	0.41
1:j:28:HIS:CD2	1:j:29:GLN:HG2	2.54	0.41
1:j:34:ALA:HB3	1:j:143:PHE:HE1	1.85	0.41
1:j:129:ASN:O	1:j:130:GLU:C	2.63	0.41
1:i:14:ILE:HG23	1:i:18:ARG:NH1	2.36	0.41
6:i:203:FLC:OG2	6:i:203:FLC:OHB	2.30	0.41
1:h:27:ARG:NH2	2:h:201:2AN:O2	2.47	0.41
1:A:87:PHE:O	1:A:88:GLU:HB2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:16:PRO:CB	1:O:105:LEU:HD13	2.51	0.41
1:O:69:LEU:HB3	1:O:87:PHE:CE1	2.56	0.41
1:M:57:ILE:HG21	1:M:68:MET:HE3	2.02	0.41
2:K:203:2AN:C2	2:K:203:2AN:C12	2.93	0.41
1:J:4:TYR:CZ	1:I:2:ALA:CB	3.01	0.41
1:J:119:THR:HG22	1:J:121:HIS:NE2	2.36	0.41
1:H:95:ASN:CB	1:H:126:CYS:HB3	2.50	0.41
1:G:16:PRO:HG3	1:G:112:SER:HB3	2.03	0.41
1:E:73:ASP:HB2	1:E:83:LYS:O	2.21	0.41
1:D:56:LYS:C	1:D:57:ILE:HD12	2.46	0.41
1:X:142:GLU:O	1:X:146:GLN:HG3	2.21	0.41
1:U:121:HIS:HA	1:U:122:PRO:HD3	1.93	0.41
1:T:18:ARG:NH2	1:T:154:ASN:O	2.54	0.41
1:S:44:ILE:HG21	1:S:53:THR:HG23	2.02	0.41
1:S:66:THR:HB	1:S:90:ASP:CG	2.46	0.41
1:S:130:GLU:O	1:S:133:VAL:N	2.45	0.41
1:B:44:ILE:HG21	1:B:53:THR:HG23	2.03	0.40
1:B:97:GLU:OE1	1:B:123:LYS:HE3	2.21	0.40
1:A:16:PRO:C	1:A:18:ARG:N	2.76	0.40
1:A:140:ALA:HB1	7:A:303:HOH:O	2.19	0.40
1:R:150:TYR:CE2	2:R:203:2AN:C10	3.04	0.40
2:R:204:2AN:C2	2:R:204:2AN:C12	2.83	0.40
1:Q:1:MET:SD	1:Q:124:PRO:HA	2.61	0.40
1:Q:92:LEU:HD13	1:Q:97:GLU:C	2.47	0.40
1:Q:136:GLY:O	1:Q:137:GLU:C	2.64	0.40
1:P:54:VAL:HA	1:P:70:HIS:O	2.21	0.40
1:O:71:LYS:O	1:O:84:TYR:HB2	2.20	0.40
1:L:136:GLY:HA2	2:L:203:2AN:C15	2.51	0.40
1:I:85:THR:HG23	1:I:100:VAL:HG22	2.03	0.40
2:D:204:2AN:C10	2:D:204:2AN:C16	2.91	0.40
1:f:4:TYR:CD1	1:f:128:VAL:HG11	2.57	0.40
1:c:148:GLU:O	1:c:150:TYR:N	2.54	0.40
1:b:33:LYS:C	2:b:204:2AN:O3	2.63	0.40
1:a:56:LYS:HG3	1:a:69:LEU:CD2	2.51	0.40
1:Y:70:HIS:CE1	1:Y:86:LEU:HB2	2.56	0.40
1:Y:71:LYS:HB2	1:Y:87:PHE:CE1	2.56	0.40
1:X:39:PHE:CE1	1:X:59:PHE:CE1	3.08	0.40
1:V:96:ILE:O	1:V:123:LYS:HE2	2.21	0.40
1:U:103:VAL:HG22	1:U:116:ILE:CB	2.50	0.40
1:S:18:ARG:NH2	1:S:151:LEU:O	2.53	0.40
1:j:43:GLU:O	1:j:55:THR:HA	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:i:31:LEU:HD23	1:i:31:LEU:HA	1.93	0.40
6:i:203:FLC:OA1	6:i:203:FLC:HG1	2.22	0.40
1:h:76:ASP:OD1	1:h:76:ASP:C	2.64	0.40
1:Q:14:ILE:HD12	1:Q:151:LEU:HB3	2.03	0.40
2:Q:202:2AN:O2	2:Q:202:2AN:N	2.53	0.40
1:P:92:LEU:HD22	1:P:96:ILE:HG22	2.02	0.40
1:O:74:GLU:OE1	1:O:81:TYR:OH	2.25	0.40
1:M:144:TYR:O	1:M:145:LYS:C	2.60	0.40
1:L:4:TYR:CE1	1:K:2:ALA:CB	3.04	0.40
1:I:59:PHE:O	1:I:60:VAL:C	2.64	0.40
1:H:9:GLU:HA	1:H:114:GLY:O	2.20	0.40
1:G:26:GLU:O	1:G:27:ARG:C	2.64	0.40
1:E:92:LEU:O	1:E:94:ASP:N	2.52	0.40
1:f:20:PHE:HB2	1:f:105:LEU:CD1	2.50	0.40
1:b:19:LEU:HD12	1:b:19:LEU:HA	1.94	0.40
1:b:28:HIS:HE2	1:b:44:ILE:HD11	1.86	0.40
1:a:23:LEU:CD1	1:a:147:VAL:HG11	2.52	0.40
1:a:80:PHE:HB2	1:a:105:LEU:HB2	2.03	0.40
1:Z:145:LYS:HE3	2:Z:206:2AN:H16	2.02	0.40
1:Y:56:LYS:HA	1:Y:69:LEU:HD23	2.03	0.40
1:Y:95:ASN:O	1:Y:95:ASN:OD1	2.39	0.40
1:X:144:TYR:CZ	2:X:206:2AN:C14	3.04	0.40
1:X:145:LYS:HG3	2:X:205:2AN:H15	2.02	0.40
1:W:18:ARG:O	1:W:19:LEU:C	2.64	0.40
1:V:2:ALA:HB1	1:U:4:TYR:CE1	2.57	0.40
1:V:25:LEU:HD23	1:V:75:ILE:HD11	2.03	0.40
1:T:66:THR:CB	1:T:90:ASP:OD2	2.69	0.40
1:i:101:TYR:CD2	1:i:118:VAL:CG2	3.04	0.40
1:h:58:THR:HG22	1:h:59:PHE:O	2.22	0.40
1:h:69:LEU:HG	1:h:88:GLU:HG2	2.02	0.40
1:g:16:PRO:O	1:g:19:LEU:N	2.54	0.40
1:A:96:ILE:HA	1:A:121:HIS:O	2.21	0.40
1:A:149:GLU:OE1	1:A:149:GLU:HA	2.20	0.40
1:R:122:PRO:HB3	1:R:128:VAL:CG2	2.51	0.40
1:M:30:VAL:HG12	1:M:143:PHE:CZ	2.56	0.40
1:J:21:LYS:HD3	1:J:158:PHE:CE1	2.56	0.40
1:I:35:GLN:HB2	1:I:39:PHE:HD2	1.87	0.40
1:I:56:LYS:HG3	1:I:69:LEU:HD23	2.04	0.40
1:H:63:HIS:O	1:H:64:PRO:C	2.64	0.40
1:F:47:GLY:HA3	1:F:53:THR:CB	2.51	0.40
1:F:84:TYR:CE1	1:F:103:VAL:HG23	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:93:ARG:O	1:D:95:ASN:OD1	2.39	0.40
1:c:31:LEU:HD12	1:c:57:ILE:HD13	2.03	0.40
1:b:103:VAL:HG13	1:b:116:ILE:HG13	2.03	0.40
1:U:19:LEU:O	1:U:22:ALA:N	2.48	0.40
2:j:207:2AN:C2	2:j:207:2AN:C16	2.91	0.40
2:h:205:2AN:H16	2:h:205:2AN:C2	2.43	0.40
1:A:70:HIS:CD2	1:A:86:LEU:HB3	2.56	0.40
1:A:84:TYR:CE2	1:A:101:TYR:HB2	2.57	0.40
1:A:89:GLY:C	1:A:91:VAL:N	2.79	0.40
1:N:32:VAL:HG21	1:N:41:SER:C	2.46	0.40
1:M:50:GLY:O	1:M:51:VAL:C	2.64	0.40
1:M:63:HIS:CE1	1:M:65:LEU:HB2	2.57	0.40
1:J:39:PHE:CE1	1:J:59:PHE:CE1	3.10	0.40
1:J:103:VAL:HG12	1:J:105:LEU:HD21	2.02	0.40
1:E:5:THR:HA	1:E:118:VAL:O	2.22	0.40
1:D:96:ILE:CD1	1:D:120:TYR:HD2	2.33	0.40
1:D:138:LYS:HA	2:D:204:2AN:H12	2.02	0.40
1:a:17:HIS:HA	1:a:80:PHE:CE1	2.56	0.40
1:a:18:ARG:O	1:a:19:LEU:C	2.61	0.40
1:a:98:LYS:O	1:a:121:HIS:HB2	2.22	0.40
1:V:67:TYR:CD2	1:V:67:TYR:C	2.99	0.40
2:V:205:2AN:H16	2:V:205:2AN:H2	2.01	0.40
1:j:47:GLY:N	2:j:201:2AN:C16	2.84	0.40
2:h:204:2AN:N	2:h:204:2AN:S	2.68	0.40
1:g:54:VAL:HA	1:g:70:HIS:O	2.21	0.40
1:B:47:GLY:HA2	2:B:204:2AN:C12	2.51	0.40
1:B:90:ASP:C	1:B:92:LEU:N	2.80	0.40
1:A:84:TYR:O	1:A:101:TYR:N	2.38	0.40
1:R:16:PRO:HB2	1:R:80:PHE:CE2	2.56	0.40
1:R:19:LEU:O	1:R:20:PHE:C	2.58	0.40
1:Q:21:LYS:HG2	1:Q:158:PHE:CD1	2.57	0.40
1:O:63:HIS:ND1	1:O:64:PRO:HD2	2.35	0.40
1:O:81:TYR:CE1	1:O:102:GLU:HG3	2.57	0.40
1:O:150:TYR:CD1	1:O:151:LEU:HD23	2.57	0.40
1:L:77:ALA:CB	2:L:204:2AN:H16	2.51	0.40
1:L:77:ALA:O	2:L:204:2AN:H3	2.20	0.40
2:L:201:2AN:S	2:L:201:2AN:N	2.89	0.40
1:J:-3:ASP:H3	1:J:-2:PRO:CD	2.33	0.40
1:I:59:PHE:C	1:I:60:VAL:O	2.63	0.40
1:I:95:ASN:HD21	1:I:129:ASN:CG	2.29	0.40
1:H:117:THR:O	1:H:117:THR:HG22	2.20	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:127:THR:OG1	1:E:128:VAL:N	2.54	0.40
1:D:116:ILE:HD11	2:D:201:2AN:C16	2.52	0.40
1:f:57:ILE:O	1:f:57:ILE:HG22	2.22	0.40
1:b:31:LEU:CD2	1:b:143:PHE:CE2	3.05	0.40
1:a:75:ILE:O	1:a:75:ILE:HG22	2.20	0.40
1:X:16:PRO:CB	1:X:112:SER:OG	2.69	0.40
2:X:206:2AN:C10	7:X:302:HOH:O	2.69	0.40
1:V:80:PHE:HB3	1:V:105:LEU:HB2	2.03	0.40
1:U:144:TYR:CE2	1:U:145:LYS:HD2	2.56	0.40
1:T:39:PHE:CE1	1:T:59:PHE:CE1	3.10	0.40
1:S:101:TYR:CD1	1:S:118:VAL:HG22	2.55	0.40
1:h:80:PHE:O	1:h:104:LYS:HA	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	160/163 (98%)	137 (86%)	20 (12%)	3 (2%)	6	5
1	B	157/163 (96%)	134 (85%)	21 (13%)	2 (1%)	9	10
1	C	159/163 (98%)	141 (89%)	16 (10%)	2 (1%)	9	10
1	D	157/163 (96%)	122 (78%)	30 (19%)	5 (3%)	3	2
1	E	159/163 (98%)	134 (84%)	21 (13%)	4 (2%)	4	3
1	F	157/163 (96%)	142 (90%)	12 (8%)	3 (2%)	6	5
1	G	160/163 (98%)	137 (86%)	22 (14%)	1 (1%)	21	27
1	H	158/163 (97%)	145 (92%)	13 (8%)	0	100	100
1	I	159/163 (98%)	143 (90%)	13 (8%)	3 (2%)	6	5
1	J	161/163 (99%)	138 (86%)	22 (14%)	1 (1%)	21	27

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	K	160/163 (98%)	148 (92%)	10 (6%)	2 (1%)	9	10
1	L	158/163 (97%)	142 (90%)	13 (8%)	3 (2%)	6	5
1	M	160/163 (98%)	145 (91%)	13 (8%)	2 (1%)	9	10
1	N	161/163 (99%)	144 (89%)	16 (10%)	1 (1%)	21	27
1	O	159/163 (98%)	140 (88%)	15 (9%)	4 (2%)	4	3
1	P	157/163 (96%)	137 (87%)	19 (12%)	1 (1%)	21	27
1	Q	160/163 (98%)	148 (92%)	11 (7%)	1 (1%)	21	27
1	R	159/163 (98%)	146 (92%)	13 (8%)	0	100	100
1	S	158/163 (97%)	146 (92%)	11 (7%)	1 (1%)	21	27
1	T	159/163 (98%)	141 (89%)	16 (10%)	2 (1%)	9	10
1	U	157/163 (96%)	136 (87%)	17 (11%)	4 (2%)	4	3
1	V	157/163 (96%)	146 (93%)	9 (6%)	2 (1%)	9	10
1	W	157/163 (96%)	134 (85%)	19 (12%)	4 (2%)	4	3
1	X	157/163 (96%)	139 (88%)	16 (10%)	2 (1%)	9	10
1	Y	157/163 (96%)	143 (91%)	12 (8%)	2 (1%)	9	10
1	Z	157/163 (96%)	134 (85%)	20 (13%)	3 (2%)	6	5
1	a	157/163 (96%)	140 (89%)	16 (10%)	1 (1%)	21	27
1	b	159/163 (98%)	142 (89%)	16 (10%)	1 (1%)	21	27
1	c	157/163 (96%)	145 (92%)	12 (8%)	0	100	100
1	d	160/163 (98%)	139 (87%)	17 (11%)	4 (2%)	4	3
1	e	159/163 (98%)	137 (86%)	20 (13%)	2 (1%)	9	10
1	f	159/163 (98%)	141 (89%)	15 (9%)	3 (2%)	6	5
1	g	158/163 (97%)	140 (89%)	18 (11%)	0	100	100
1	h	160/163 (98%)	144 (90%)	13 (8%)	3 (2%)	6	5
1	i	159/163 (98%)	145 (91%)	12 (8%)	2 (1%)	9	10
1	j	157/163 (96%)	144 (92%)	12 (8%)	1 (1%)	21	27
All	All	5705/5868 (97%)	5059 (89%)	571 (10%)	75 (1%)	9	10

All (75) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	76	ASP
1	O	51	VAL

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Mol	Chain	Res	Type
1	F	94	ASP
1	X	123	LYS
1	O	24	VAL
1	M	60	VAL
1	K	24	VAL
1	J	51	VAL
1	F	76	ASP
1	f	93	ARG
1	f	129	ASN
1	d	108	VAL
1	Z	108	VAL
1	W	130	GLU
1	U	128	VAL
1	i	24	VAL
1	B	91	VAL
1	A	158	PHE
1	Q	60	VAL
1	P	50	GLY
1	O	19	LEU
1	I	90	ASP
1	G	93	ARG
1	D	59	PHE
1	Y	24	VAL
1	W	93	ARG
1	U	11	GLU
1	h	50	GLY
1	h	152	ALA
1	A	128	VAL
1	L	49	GLY
1	L	61	ASP
1	I	1	MET
1	E	32	VAL
1	D	65	LEU
1	C	24	VAL
1	C	93	ARG
1	f	139	LYS
1	d	51	VAL
1	a	75	ILE
1	X	94	ASP
1	W	96	ILE
1	U	13	PRO
1	U	33	LYS

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Mol	Chain	Res	Type
1	T	126	CYS
1	j	129	ASN
1	A	88	GLU
1	L	27	ARG
1	F	126	CYS
1	E	17	HIS
1	D	122	PRO
1	e	64	PRO
1	d	124	PRO
1	Z	93	ARG
1	V	93	ARG
1	O	135	ILE
1	E	60	VAL
1	D	6	ILE
1	d	130	GLU
1	Y	124	PRO
1	K	135	ILE
1	h	124	PRO
1	N	124	PRO
1	I	60	VAL
1	T	125	GLY
1	i	51	VAL
1	E	108	VAL
1	e	16	PRO
1	b	60	VAL
1	S	155	PRO
1	M	108	VAL
1	D	60	VAL
1	Z	123	LYS
1	W	124	PRO
1	V	124	PRO

5.3.2 Protein sidechains ⓘ

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

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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	114/138 (83%)	108 (95%)	6 (5%)	20	30
1	B	130/138 (94%)	128 (98%)	2 (2%)	57	75
1	C	124/138 (90%)	121 (98%)	3 (2%)	43	62
1	D	123/138 (89%)	115 (94%)	8 (6%)	15	22
1	E	128/138 (93%)	118 (92%)	10 (8%)	11	16
1	F	114/138 (83%)	102 (90%)	12 (10%)	6	8
1	G	122/138 (88%)	112 (92%)	10 (8%)	10	14
1	H	125/138 (91%)	113 (90%)	12 (10%)	8	10
1	I	130/138 (94%)	121 (93%)	9 (7%)	14	20
1	J	128/138 (93%)	117 (91%)	11 (9%)	10	13
1	K	132/138 (96%)	125 (95%)	7 (5%)	20	30
1	L	132/138 (96%)	121 (92%)	11 (8%)	10	14
1	M	134/138 (97%)	129 (96%)	5 (4%)	30	45
1	N	131/138 (95%)	127 (97%)	4 (3%)	35	52
1	O	120/138 (87%)	116 (97%)	4 (3%)	33	50
1	P	131/138 (95%)	127 (97%)	4 (3%)	35	52
1	Q	132/138 (96%)	127 (96%)	5 (4%)	29	44
1	R	130/138 (94%)	125 (96%)	5 (4%)	29	44
1	S	131/138 (95%)	119 (91%)	12 (9%)	8	11
1	T	131/138 (95%)	117 (89%)	14 (11%)	6	8
1	U	123/138 (89%)	112 (91%)	11 (9%)	9	12
1	V	131/138 (95%)	125 (95%)	6 (5%)	24	36
1	W	121/138 (88%)	116 (96%)	5 (4%)	27	41
1	X	124/138 (90%)	113 (91%)	11 (9%)	9	12
1	Y	123/138 (89%)	113 (92%)	10 (8%)	11	14
1	Z	122/138 (88%)	111 (91%)	11 (9%)	9	12
1	a	123/138 (89%)	110 (89%)	13 (11%)	6	8
1	b	127/138 (92%)	115 (91%)	12 (9%)	8	11
1	c	130/138 (94%)	124 (95%)	6 (5%)	24	36
1	d	127/138 (92%)	117 (92%)	10 (8%)	11	15

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	e	129/138 (94%)	119 (92%)	10 (8%)	11	16
1	f	132/138 (96%)	116 (88%)	16 (12%)	5	5
1	g	132/138 (96%)	122 (92%)	10 (8%)	12	16
1	h	131/138 (95%)	125 (95%)	6 (5%)	24	36
1	i	129/138 (94%)	122 (95%)	7 (5%)	20	29
1	j	130/138 (94%)	120 (92%)	10 (8%)	12	16
All	All	4576/4968 (92%)	4268 (93%)	308 (7%)	15	21

All (308) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	44	ILE
1	B	80	PHE
1	A	31	LEU
1	A	72	PHE
1	A	91	VAL
1	A	96	ILE
1	A	113	LYS
1	A	144	TYR
1	R	11	GLU
1	R	17	HIS
1	R	61	ASP
1	R	105	LEU
1	R	116	ILE
1	Q	21	LYS
1	Q	35	GLN
1	Q	65	LEU
1	Q	93	ARG
1	Q	144	TYR
1	P	75	ILE
1	P	95	ASN
1	P	131	GLU
1	P	156	GLU
1	O	48	ASP
1	O	106	GLU
1	O	131	GLU
1	O	133	VAL
1	N	21	LYS
1	N	103	VAL
1	N	116	ILE

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Mol	Chain	Res	Type
1	N	124	PRO
1	M	35	GLN
1	M	59	PHE
1	M	90	ASP
1	M	103	VAL
1	M	144	TYR
1	L	4	TYR
1	L	6	ILE
1	L	10	GLU
1	L	43	GLU
1	L	70	HIS
1	L	116	ILE
1	L	117	THR
1	L	128	VAL
1	L	130	GLU
1	L	144	TYR
1	L	156	GLU
1	K	6	ILE
1	K	54	VAL
1	K	58	THR
1	K	119	THR
1	K	131	GLU
1	K	133	VAL
1	K	144	TYR
1	J	51	VAL
1	J	57	ILE
1	J	58	THR
1	J	66	THR
1	J	75	ILE
1	J	85	THR
1	J	90	ASP
1	J	117	THR
1	J	118	VAL
1	J	119	THR
1	J	158	PHE
1	I	0	THR
1	I	6	ILE
1	I	85	THR
1	I	103	VAL
1	I	108	VAL
1	I	129	ASN
1	I	133	VAL

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Mol	Chain	Res	Type
1	I	139	LYS
1	I	144	TYR
1	H	1	MET
1	H	10	GLU
1	H	43	GLU
1	H	51	VAL
1	H	90	ASP
1	H	95	ASN
1	H	117	THR
1	H	128	VAL
1	H	130	GLU
1	H	142	GLU
1	H	144	TYR
1	H	154	ASN
1	G	6	ILE
1	G	23	LEU
1	G	54	VAL
1	G	73	ASP
1	G	85	THR
1	G	91	VAL
1	G	105	LEU
1	G	108	VAL
1	G	112	SER
1	G	119	THR
1	F	5	THR
1	F	11	GLU
1	F	21	LYS
1	F	60	VAL
1	F	66	THR
1	F	75	ILE
1	F	96	ILE
1	F	99	VAL
1	F	101	TYR
1	F	108	VAL
1	F	127	THR
1	F	144	TYR
1	E	54	VAL
1	E	64	PRO
1	E	66	THR
1	E	93	ARG
1	E	94	ASP
1	E	95	ASN

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Mol	Chain	Res	Type
1	E	106	GLU
1	E	127	THR
1	E	149	GLU
1	E	157	VAL
1	D	17	HIS
1	D	48	ASP
1	D	61	ASP
1	D	69	LEU
1	D	95	ASN
1	D	123	LYS
1	D	127	THR
1	D	144	TYR
1	C	93	ARG
1	C	96	ILE
1	C	132	GLU
1	f	5	THR
1	f	6	ILE
1	f	29	GLN
1	f	32	VAL
1	f	41	SER
1	f	45	ILE
1	f	51	VAL
1	f	57	ILE
1	f	66	THR
1	f	75	ILE
1	f	90	ASP
1	f	92	LEU
1	f	94	ASP
1	f	128	VAL
1	f	144	TYR
1	f	157	VAL
1	e	1	MET
1	e	5	THR
1	e	7	VAL
1	e	8	LYS
1	e	94	ASP
1	e	100	VAL
1	e	126	CYS
1	e	130	GLU
1	e	137	GLU
1	e	154	ASN
1	d	-2	PRO

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Mol	Chain	Res	Type
1	d	1	MET
1	d	7	VAL
1	d	18	ARG
1	d	21	LYS
1	d	33	LYS
1	d	61	ASP
1	d	95	ASN
1	d	117	THR
1	d	138	LYS
1	c	24	VAL
1	c	35	GLN
1	c	43	GLU
1	c	92	LEU
1	c	106	GLU
1	c	116	ILE
1	b	8	LYS
1	b	29	GLN
1	b	45	ILE
1	b	54	VAL
1	b	57	ILE
1	b	58	THR
1	b	71	LYS
1	b	73	ASP
1	b	120	TYR
1	b	128	VAL
1	b	130	GLU
1	b	144	TYR
1	a	6	ILE
1	a	8	LYS
1	a	9	GLU
1	a	23	LEU
1	a	39	PHE
1	a	41	SER
1	a	45	ILE
1	a	75	ILE
1	a	94	ASP
1	a	100	VAL
1	a	130	GLU
1	a	132	GLU
1	a	156	GLU
1	Z	5	THR
1	Z	19	LEU

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Mol	Chain	Res	Type
1	Z	57	ILE
1	Z	60	VAL
1	Z	71	LYS
1	Z	91	VAL
1	Z	103	VAL
1	Z	113	LYS
1	Z	126	CYS
1	Z	133	VAL
1	Z	144	TYR
1	Y	23	LEU
1	Y	41	SER
1	Y	43	GLU
1	Y	54	VAL
1	Y	61	ASP
1	Y	90	ASP
1	Y	106	GLU
1	Y	116	ILE
1	Y	134	LYS
1	Y	142	GLU
1	X	10	GLU
1	X	23	LEU
1	X	44	ILE
1	X	51	VAL
1	X	60	VAL
1	X	63	HIS
1	X	90	ASP
1	X	91	VAL
1	X	123	LYS
1	X	144	TYR
1	X	145	LYS
1	W	25	LEU
1	W	100	VAL
1	W	118	VAL
1	W	119	THR
1	W	144	TYR
1	V	1	MET
1	V	5	THR
1	V	90	ASP
1	V	106	GLU
1	V	133	VAL
1	V	144	TYR
1	U	11	GLU

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Mol	Chain	Res	Type
1	U	14	ILE
1	U	24	VAL
1	U	30	VAL
1	U	53	THR
1	U	96	ILE
1	U	113	LYS
1	U	115	LYS
1	U	128	VAL
1	U	130	GLU
1	U	144	TYR
1	T	0	THR
1	T	6	ILE
1	T	7	VAL
1	T	8	LYS
1	T	19	LEU
1	T	25	LEU
1	T	65	LEU
1	T	67	TYR
1	T	69	LEU
1	T	71	LYS
1	T	92	LEU
1	T	95	ASN
1	T	108	VAL
1	T	144	TYR
1	S	0	THR
1	S	6	ILE
1	S	11	GLU
1	S	58	THR
1	S	67	TYR
1	S	90	ASP
1	S	99	VAL
1	S	127	THR
1	S	130	GLU
1	S	131	GLU
1	S	135	ILE
1	S	144	TYR
1	j	5	THR
1	j	6	ILE
1	j	10	GLU
1	j	33	LYS
1	j	90	ASP
1	j	112	SER

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Mol	Chain	Res	Type
1	j	116	ILE
1	j	124	PRO
1	j	129	ASN
1	j	144	TYR
1	i	0	THR
1	i	8	LYS
1	i	25	LEU
1	i	91	VAL
1	i	94	ASP
1	i	95	ASN
1	i	144	TYR
1	h	1	MET
1	h	69	LEU
1	h	85	THR
1	h	108	VAL
1	h	129	ASN
1	h	138	LYS
1	g	0	THR
1	g	32	VAL
1	g	43	GLU
1	g	64	PRO
1	g	69	LEU
1	g	106	GLU
1	g	126	CYS
1	g	142	GLU
1	g	144	TYR
1	g	149	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (66) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	95	ASN
1	R	95	ASN
1	R	154	ASN
1	Q	37	HIS
1	P	79	ASN
1	P	146	GLN
1	O	121	HIS
1	N	17	HIS
1	N	28	HIS
1	M	35	GLN
1	M	146	GLN

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Mol	Chain	Res	Type
1	L	17	HIS
1	L	29	GLN
1	L	35	GLN
1	L	79	ASN
1	K	17	HIS
1	K	35	GLN
1	K	121	HIS
1	J	79	ASN
1	J	146	GLN
1	I	28	HIS
1	I	79	ASN
1	H	35	GLN
1	H	70	HIS
1	H	154	ASN
1	G	35	GLN
1	G	63	HIS
1	G	70	HIS
1	G	154	ASN
1	F	79	ASN
1	E	95	ASN
1	C	17	HIS
1	f	35	GLN
1	f	79	ASN
1	f	146	GLN
1	d	37	HIS
1	d	95	ASN
1	d	121	HIS
1	d	146	GLN
1	d	154	ASN
1	c	17	HIS
1	c	35	GLN
1	c	146	GLN
1	a	79	ASN
1	Z	17	HIS
1	X	29	GLN
1	X	35	GLN
1	W	70	HIS
1	V	95	ASN
1	U	79	ASN
1	T	35	GLN
1	T	63	HIS
1	T	95	ASN

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Mol	Chain	Res	Type
1	T	121	HIS
1	T	146	GLN
1	j	35	GLN
1	j	121	HIS
1	i	79	ASN
1	i	129	ASN
1	i	146	GLN
1	h	29	GLN
1	h	35	GLN
1	h	154	ASN
1	g	28	HIS
1	g	35	GLN
1	g	121	HIS

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

178 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	2AN	e	201	-	22,23,23	2.01	6 (27%)	29,33,33	1.59	6 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	2AN	T	202	-	22,23,23	2.00	4 (18%)	29,33,33	1.58	3 (10%)
2	2AN	a	202	-	22,23,23	1.96	4 (18%)	29,33,33	1.54	6 (20%)
3	SO4	A	205	-	4,4,4	0.41	0	6,6,6	0.78	0
2	2AN	J	203	-	22,23,23	1.76	4 (18%)	29,33,33	1.63	6 (20%)
2	2AN	T	205	-	22,23,23	2.27	6 (27%)	29,33,33	2.23	10 (34%)
2	2AN	Z	204	-	22,23,23	1.78	4 (18%)	29,33,33	1.42	3 (10%)
2	2AN	a	204	-	22,23,23	1.90	5 (22%)	29,33,33	1.21	2 (6%)
4	EPE	P	205	-	15,15,15	2.10	1 (6%)	19,20,20	1.74	7 (36%)
2	2AN	E	203	-	22,23,23	1.91	4 (18%)	29,33,33	1.87	8 (27%)
2	2AN	Q	201	-	22,23,23	1.94	5 (22%)	29,33,33	1.73	6 (20%)
2	2AN	V	208	-	22,23,23	2.11	6 (27%)	29,33,33	3.43	10 (34%)
2	2AN	d	201	-	22,23,23	1.58	3 (13%)	29,33,33	1.59	5 (17%)
2	2AN	a	203	-	22,23,23	2.19	7 (31%)	29,33,33	1.51	3 (10%)
2	2AN	d	202	-	22,23,23	1.96	5 (22%)	29,33,33	1.41	2 (6%)
3	SO4	c	208	-	4,4,4	0.45	0	6,6,6	0.38	0
2	2AN	j	201	-	22,23,23	1.66	4 (18%)	29,33,33	1.60	5 (17%)
2	2AN	d	204	-	22,23,23	1.64	4 (18%)	29,33,33	2.01	5 (17%)
5	DMS	N	206	-	3,3,3	0.50	0	3,3,3	0.85	0
2	2AN	f	204	-	22,23,23	1.67	7 (31%)	29,33,33	1.35	2 (6%)
2	2AN	W	201	-	22,23,23	2.06	5 (22%)	29,33,33	1.63	5 (17%)
2	2AN	h	206	-	22,23,23	2.03	4 (18%)	29,33,33	1.63	6 (20%)
2	2AN	N	205	-	22,23,23	2.42	7 (31%)	29,33,33	1.65	5 (17%)
2	2AN	F	203	-	22,23,23	1.45	4 (18%)	29,33,33	1.36	4 (13%)
3	SO4	c	209	-	4,4,4	0.49	0	6,6,6	0.62	0
2	2AN	I	202	-	22,23,23	1.78	5 (22%)	29,33,33	1.36	4 (13%)
2	2AN	I	207	-	22,23,23	2.37	4 (18%)	29,33,33	1.69	10 (34%)
3	SO4	E	205	-	4,4,4	0.19	0	6,6,6	0.13	0
2	2AN	E	202	-	22,23,23	1.44	3 (13%)	29,33,33	1.68	7 (24%)
2	2AN	f	205	-	22,23,23	1.68	4 (18%)	29,33,33	1.29	5 (17%)
2	2AN	M	202	-	22,23,23	1.58	5 (22%)	29,33,33	2.09	9 (31%)
2	2AN	c	205	-	22,23,23	1.66	5 (22%)	29,33,33	1.09	2 (6%)
2	2AN	c	206	-	22,23,23	1.35	3 (13%)	29,33,33	1.25	3 (10%)
2	2AN	Y	203	-	22,23,23	1.71	5 (22%)	29,33,33	1.54	6 (20%)
2	2AN	D	203	-	22,23,23	1.87	6 (27%)	29,33,33	1.62	5 (17%)
2	2AN	j	203	-	22,23,23	1.71	6 (27%)	29,33,33	1.73	8 (27%)
2	2AN	A	202	-	22,23,23	2.07	7 (31%)	29,33,33	1.79	8 (27%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	2AN	h	204	-	22,23,23	1.51	4 (18%)	29,33,33	1.58	2 (6%)
6	FLC	G	206	-	12,12,12	1.04	0	17,17,17	1.93	5 (29%)
2	2AN	F	202	-	22,23,23	2.04	4 (18%)	29,33,33	2.07	13 (44%)
2	2AN	Z	206	-	22,23,23	2.02	5 (22%)	29,33,33	1.73	6 (20%)
2	2AN	I	201	-	22,23,23	1.32	3 (13%)	29,33,33	1.89	7 (24%)
2	2AN	X	206	-	22,23,23	1.81	5 (22%)	29,33,33	0.90	2 (6%)
2	2AN	D	201	-	22,23,23	1.77	6 (27%)	29,33,33	1.56	5 (17%)
2	2AN	V	201	-	22,23,23	1.83	5 (22%)	29,33,33	1.58	6 (20%)
2	2AN	P	201	-	22,23,23	1.68	3 (13%)	29,33,33	1.16	3 (10%)
2	2AN	K	201	-	22,23,23	1.70	5 (22%)	29,33,33	1.79	7 (24%)
2	2AN	J	201	-	22,23,23	1.48	3 (13%)	29,33,33	1.01	1 (3%)
2	2AN	F	206	-	22,23,23	1.88	5 (22%)	29,33,33	1.61	7 (24%)
2	2AN	X	205	-	22,23,23	2.06	5 (22%)	29,33,33	1.30	3 (10%)
2	2AN	f	203	-	22,23,23	1.81	5 (22%)	29,33,33	0.91	2 (6%)
2	2AN	c	202	-	22,23,23	2.14	5 (22%)	29,33,33	1.80	10 (34%)
2	2AN	R	201	-	22,23,23	1.84	5 (22%)	29,33,33	1.00	1 (3%)
2	2AN	A	204	-	22,23,23	1.81	5 (22%)	29,33,33	0.88	2 (6%)
2	2AN	c	203	-	22,23,23	1.69	3 (13%)	29,33,33	1.19	2 (6%)
2	2AN	Y	204	-	22,23,23	1.68	4 (18%)	29,33,33	0.90	2 (6%)
2	2AN	f	202	-	22,23,23	1.36	2 (9%)	29,33,33	1.52	4 (13%)
2	2AN	F	204	-	22,23,23	1.77	4 (18%)	29,33,33	1.29	4 (13%)
2	2AN	Z	201	-	22,23,23	2.32	6 (27%)	29,33,33	1.60	8 (27%)
2	2AN	A	203	-	22,23,23	2.11	4 (18%)	29,33,33	1.39	4 (13%)
2	2AN	C	202	-	22,23,23	1.75	5 (22%)	29,33,33	1.02	1 (3%)
2	2AN	h	202	-	22,23,23	1.63	5 (22%)	29,33,33	1.68	6 (20%)
2	2AN	O	203	-	22,23,23	2.08	4 (18%)	29,33,33	1.52	3 (10%)
2	2AN	T	204	-	22,23,23	2.27	5 (22%)	29,33,33	1.64	9 (31%)
2	2AN	b	201	-	22,23,23	1.78	4 (18%)	29,33,33	1.01	1 (3%)
2	2AN	I	204	-	22,23,23	2.03	5 (22%)	29,33,33	1.43	4 (13%)
2	2AN	S	202	-	22,23,23	1.85	4 (18%)	29,33,33	1.85	9 (31%)
2	2AN	P	204	-	22,23,23	1.81	5 (22%)	29,33,33	1.51	3 (10%)
2	2AN	O	201	-	22,23,23	1.44	2 (9%)	29,33,33	1.42	3 (10%)
2	2AN	g	201	-	22,23,23	1.96	6 (27%)	29,33,33	1.75	8 (27%)
2	2AN	P	203	-	22,23,23	1.65	6 (27%)	29,33,33	1.57	4 (13%)
3	SO4	g	204	-	4,4,4	0.60	0	6,6,6	0.47	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	2AN	E	204	-	22,23,23	2.09	6 (27%)	29,33,33	1.89	5 (17%)
2	2AN	M	201	-	22,23,23	2.11	4 (18%)	29,33,33	2.09	9 (31%)
6	FLC	j	208	-	12,12,12	2.27	1 (8%)	17,17,17	2.39	6 (35%)
2	2AN	h	205	-	22,23,23	2.11	5 (22%)	29,33,33	1.30	2 (6%)
2	2AN	G	202	-	22,23,23	1.51	4 (18%)	29,33,33	1.62	5 (17%)
2	2AN	B	201	-	22,23,23	1.80	5 (22%)	29,33,33	2.02	12 (41%)
2	2AN	R	203	-	22,23,23	1.84	6 (27%)	29,33,33	1.36	3 (10%)
2	2AN	X	202	-	22,23,23	1.82	6 (27%)	29,33,33	1.33	2 (6%)
2	2AN	Y	202	-	22,23,23	1.85	6 (27%)	29,33,33	1.42	6 (20%)
6	FLC	a	206	-	12,12,12	1.15	0	17,17,17	1.43	3 (17%)
2	2AN	L	202	-	22,23,23	1.76	4 (18%)	29,33,33	1.29	3 (10%)
2	2AN	D	202	-	22,23,23	1.81	6 (27%)	29,33,33	1.21	2 (6%)
2	2AN	V	202	-	22,23,23	1.48	5 (22%)	29,33,33	1.71	7 (24%)
2	2AN	j	205	-	22,23,23	1.80	4 (18%)	29,33,33	1.87	10 (34%)
2	2AN	b	206	-	22,23,23	2.33	5 (22%)	29,33,33	1.60	4 (13%)
6	FLC	i	202	-	12,12,12	1.34	2 (16%)	17,17,17	1.21	1 (5%)
2	2AN	K	203	-	22,23,23	1.74	4 (18%)	29,33,33	1.26	1 (3%)
2	2AN	G	205	-	22,23,23	1.88	4 (18%)	29,33,33	1.19	3 (10%)
2	2AN	Q	202	-	22,23,23	1.80	4 (18%)	29,33,33	1.24	2 (6%)
2	2AN	B	204	-	22,23,23	1.60	4 (18%)	29,33,33	1.49	4 (13%)
2	2AN	S	203	-	22,23,23	1.72	4 (18%)	29,33,33	1.08	2 (6%)
2	2AN	R	204	-	22,23,23	2.16	4 (18%)	29,33,33	1.56	6 (20%)
2	2AN	H	203	-	22,23,23	1.69	5 (22%)	29,33,33	1.29	2 (6%)
2	2AN	K	202	-	22,23,23	1.63	4 (18%)	29,33,33	1.10	4 (13%)
2	2AN	J	202	-	22,23,23	1.49	4 (18%)	29,33,33	0.99	2 (6%)
2	2AN	f	206	-	22,23,23	1.87	4 (18%)	29,33,33	1.28	2 (6%)
2	2AN	E	201	-	22,23,23	1.71	4 (18%)	29,33,33	1.14	2 (6%)
2	2AN	a	201	-	22,23,23	1.98	5 (22%)	29,33,33	2.21	8 (27%)
2	2AN	M	203	-	22,23,23	1.87	7 (31%)	29,33,33	1.84	6 (20%)
2	2AN	G	207	-	22,23,23	2.04	5 (22%)	29,33,33	1.05	1 (3%)
2	2AN	R	202	-	22,23,23	2.09	8 (36%)	29,33,33	1.30	5 (17%)
2	2AN	j	207	-	22,23,23	2.30	5 (22%)	29,33,33	1.13	2 (6%)
3	SO4	c	207	-	4,4,4	0.43	0	6,6,6	0.45	0
2	2AN	g	203	-	22,23,23	1.79	6 (27%)	29,33,33	1.55	4 (13%)
2	2AN	V	205	-	22,23,23	1.58	7 (31%)	29,33,33	1.65	6 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	DMS	X	207	-	3,3,3	0.56	0	3,3,3	0.62	0
2	2AN	b	205	-	22,23,23	2.00	5 (22%)	29,33,33	1.57	5 (17%)
2	2AN	N	201	-	22,23,23	1.39	4 (18%)	29,33,33	1.22	2 (6%)
2	2AN	B	202	-	22,23,23	1.65	3 (13%)	29,33,33	0.95	1 (3%)
2	2AN	H	201	-	22,23,23	1.60	5 (22%)	29,33,33	1.38	3 (10%)
2	2AN	g	202	-	22,23,23	1.63	4 (18%)	29,33,33	1.86	7 (24%)
3	SO4	G	209	-	4,4,4	0.52	0	6,6,6	0.20	0
2	2AN	U	201	-	22,23,23	1.94	5 (22%)	29,33,33	1.26	1 (3%)
2	2AN	S	204	-	22,23,23	1.69	6 (27%)	29,33,33	2.56	4 (13%)
5	DMS	G	208	-	3,3,3	0.52	0	3,3,3	1.10	0
2	2AN	c	204	-	22,23,23	1.44	4 (18%)	29,33,33	1.52	4 (13%)
2	2AN	f	201	-	22,23,23	2.07	6 (27%)	29,33,33	1.92	9 (31%)
2	2AN	Q	203	-	22,23,23	2.14	5 (22%)	29,33,33	1.75	5 (17%)
2	2AN	T	201	-	22,23,23	1.77	7 (31%)	29,33,33	1.31	2 (6%)
2	2AN	h	201	-	22,23,23	2.23	4 (18%)	29,33,33	1.35	6 (20%)
6	FLC	i	203	-	12,12,12	1.39	1 (8%)	17,17,17	2.32	5 (29%)
2	2AN	B	206	-	22,23,23	1.81	4 (18%)	29,33,33	0.96	1 (3%)
2	2AN	Y	201	-	22,23,23	2.49	6 (27%)	29,33,33	2.18	12 (41%)
2	2AN	j	202	-	22,23,23	1.39	3 (13%)	29,33,33	1.99	8 (27%)
2	2AN	b	202	-	22,23,23	1.86	5 (22%)	29,33,33	1.24	3 (10%)
2	2AN	Z	205	-	22,23,23	1.63	4 (18%)	29,33,33	1.61	5 (17%)
2	2AN	X	203	-	22,23,23	1.79	5 (22%)	29,33,33	0.90	1 (3%)
2	2AN	V	204	-	22,23,23	1.74	5 (22%)	29,33,33	1.37	3 (10%)
6	FLC	e	202	-	12,12,12	1.54	1 (8%)	17,17,17	1.85	3 (17%)
2	2AN	I	203	-	22,23,23	1.92	5 (22%)	29,33,33	1.26	3 (10%)
2	2AN	V	207	-	22,23,23	1.74	5 (22%)	29,33,33	0.90	1 (3%)
2	2AN	A	201	-	22,23,23	1.67	6 (27%)	29,33,33	1.40	6 (20%)
2	2AN	D	204	-	22,23,23	2.40	5 (22%)	29,33,33	2.15	10 (34%)
2	2AN	V	203	-	22,23,23	1.97	6 (27%)	29,33,33	1.59	6 (20%)
2	2AN	h	203	-	22,23,23	2.21	6 (27%)	29,33,33	1.84	8 (27%)
2	2AN	O	202	-	22,23,23	2.12	4 (18%)	29,33,33	1.29	4 (13%)
2	2AN	G	203	-	22,23,23	1.39	4 (18%)	29,33,33	1.23	3 (10%)
2	2AN	Z	202	-	22,23,23	2.01	5 (22%)	29,33,33	1.55	5 (17%)
2	2AN	c	201	-	22,23,23	1.69	6 (27%)	29,33,33	1.52	4 (13%)
2	2AN	N	202	-	22,23,23	1.73	6 (27%)	29,33,33	1.59	6 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	2AN	H	202	-	22,23,23	1.82	4 (18%)	29,33,33	1.55	5 (17%)
2	2AN	G	201	-	22,23,23	1.71	4 (18%)	29,33,33	1.38	5 (17%)
2	2AN	j	206	-	22,23,23	1.94	6 (27%)	29,33,33	1.36	3 (10%)
2	2AN	P	202	-	22,23,23	1.84	7 (31%)	29,33,33	1.96	10 (34%)
2	2AN	C	201	-	22,23,23	1.64	5 (22%)	29,33,33	1.39	4 (13%)
2	2AN	B	205	-	22,23,23	1.71	4 (18%)	29,33,33	1.31	4 (13%)
2	2AN	X	201	-	22,23,23	2.00	5 (22%)	29,33,33	1.63	4 (13%)
2	2AN	N	204	-	22,23,23	1.56	5 (22%)	29,33,33	1.90	5 (17%)
2	2AN	I	205	-	22,23,23	2.69	5 (22%)	29,33,33	1.61	7 (24%)
2	2AN	L	204	-	22,23,23	1.98	5 (22%)	29,33,33	1.55	6 (20%)
2	2AN	b	204	-	22,23,23	1.73	3 (13%)	29,33,33	1.11	2 (6%)
6	FLC	a	205	-	12,12,12	1.33	1 (8%)	17,17,17	1.47	5 (29%)
2	2AN	d	203	-	22,23,23	1.74	5 (22%)	29,33,33	0.92	1 (3%)
2	2AN	F	201	-	22,23,23	1.55	4 (18%)	29,33,33	1.45	6 (20%)
2	2AN	Z	203	-	22,23,23	1.90	5 (22%)	29,33,33	1.64	7 (24%)
3	SO4	Q	204	-	4,4,4	0.53	0	6,6,6	0.58	0
2	2AN	G	204	-	22,23,23	2.05	5 (22%)	29,33,33	1.39	5 (17%)
2	2AN	j	204	-	22,23,23	1.68	5 (22%)	29,33,33	1.50	4 (13%)
2	2AN	N	203	-	22,23,23	1.97	5 (22%)	29,33,33	2.66	9 (31%)
2	2AN	X	204	-	22,23,23	1.91	4 (18%)	29,33,33	1.41	5 (17%)
2	2AN	R	205	-	22,23,23	1.83	5 (22%)	29,33,33	1.36	2 (6%)
2	2AN	S	201	-	22,23,23	2.06	4 (18%)	29,33,33	1.84	4 (13%)
2	2AN	U	202	-	22,23,23	1.79	5 (22%)	29,33,33	1.30	2 (6%)
3	SO4	I	208	-	4,4,4	0.32	0	6,6,6	0.90	0
2	2AN	C	203[A]	-	22,23,23	0.61	0	29,33,33	1.44	5 (17%)
2	2AN	H	204	-	22,23,23	2.01	5 (22%)	29,33,33	1.41	2 (6%)
2	2AN	L	203	-	22,23,23	1.60	4 (18%)	29,33,33	1.92	8 (27%)
2	2AN	b	203	-	22,23,23	1.75	5 (22%)	29,33,33	1.06	2 (6%)
2	2AN	F	205	-	22,23,23	1.71	4 (18%)	29,33,33	1.27	3 (10%)
2	2AN	T	203	-	22,23,23	1.60	5 (22%)	29,33,33	1.92	7 (24%)
3	SO4	Y	205	-	4,4,4	0.31	0	6,6,6	0.63	0
2	2AN	B	203	-	22,23,23	1.71	5 (22%)	29,33,33	1.53	4 (13%)
2	2AN	L	201	-	22,23,23	1.62	5 (22%)	29,33,33	1.25	2 (6%)
2	2AN	I	206	-	22,23,23	2.36	6 (27%)	29,33,33	1.81	7 (24%)
2	2AN	V	206	-	22,23,23	1.71	4 (18%)	29,33,33	1.87	8 (27%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	2AN	i	201	-	22,23,23	1.75	4 (18%)	29,33,33	1.72	6 (20%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	2AN	e	201	-	-	4/10/10/10	0/3/3/3
2	2AN	T	202	-	-	1/10/10/10	0/3/3/3
2	2AN	a	202	-	-	0/10/10/10	0/3/3/3
2	2AN	J	203	-	-	2/10/10/10	0/3/3/3
2	2AN	T	205	-	-	5/10/10/10	0/3/3/3
2	2AN	Z	204	-	-	0/10/10/10	0/3/3/3
2	2AN	a	204	-	-	0/10/10/10	0/3/3/3
4	EPE	P	205	-	-	2/9/19/19	0/1/1/1
2	2AN	E	203	-	-	3/10/10/10	0/3/3/3
2	2AN	Q	201	-	-	1/10/10/10	0/3/3/3
2	2AN	V	208	-	-	4/10/10/10	0/3/3/3
2	2AN	d	201	-	-	0/10/10/10	0/3/3/3
2	2AN	a	203	-	-	0/10/10/10	0/3/3/3
2	2AN	d	202	-	-	6/10/10/10	0/3/3/3
2	2AN	j	201	-	-	6/10/10/10	0/3/3/3
2	2AN	d	204	-	-	0/10/10/10	0/3/3/3
2	2AN	f	204	-	-	0/10/10/10	0/3/3/3
2	2AN	W	201	-	-	6/10/10/10	0/3/3/3
2	2AN	h	206	-	-	0/10/10/10	0/3/3/3
2	2AN	N	205	-	-	0/10/10/10	0/3/3/3
2	2AN	F	203	-	-	0/10/10/10	0/3/3/3
2	2AN	I	202	-	-	0/10/10/10	0/3/3/3
2	2AN	I	207	-	-	5/10/10/10	0/3/3/3
2	2AN	E	202	-	-	1/10/10/10	0/3/3/3
2	2AN	f	205	-	-	0/10/10/10	0/3/3/3
2	2AN	M	202	-	-	3/10/10/10	0/3/3/3
2	2AN	c	205	-	-	0/10/10/10	0/3/3/3
2	2AN	c	206	-	-	0/10/10/10	0/3/3/3
2	2AN	Y	203	-	-	0/10/10/10	0/3/3/3
2	2AN	D	203	-	-	6/10/10/10	0/3/3/3
2	2AN	j	203	-	-	0/10/10/10	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	2AN	A	202	-	-	2/10/10/10	0/3/3/3
2	2AN	h	204	-	-	0/10/10/10	0/3/3/3
6	FLC	G	206	-	-	14/16/16/16	-
2	2AN	F	202	-	-	8/10/10/10	0/3/3/3
2	2AN	Z	206	-	-	6/10/10/10	0/3/3/3
2	2AN	I	201	-	-	2/10/10/10	0/3/3/3
2	2AN	X	206	-	-	2/10/10/10	0/3/3/3
2	2AN	D	201	-	-	0/10/10/10	0/3/3/3
2	2AN	V	201	-	-	2/10/10/10	0/3/3/3
2	2AN	P	201	-	-	0/10/10/10	0/3/3/3
2	2AN	K	201	-	-	4/10/10/10	0/3/3/3
2	2AN	J	201	-	-	0/10/10/10	0/3/3/3
2	2AN	F	206	-	-	2/10/10/10	0/3/3/3
2	2AN	X	205	-	-	0/10/10/10	0/3/3/3
2	2AN	f	203	-	-	2/10/10/10	0/3/3/3
2	2AN	c	202	-	-	0/10/10/10	0/3/3/3
2	2AN	R	201	-	-	0/10/10/10	0/3/3/3
2	2AN	A	204	-	-	4/10/10/10	0/3/3/3
2	2AN	c	203	-	-	3/10/10/10	0/3/3/3
2	2AN	Y	204	-	-	7/10/10/10	0/3/3/3
2	2AN	f	202	-	-	1/10/10/10	0/3/3/3
2	2AN	F	204	-	-	2/10/10/10	0/3/3/3
2	2AN	Z	201	-	-	2/10/10/10	0/3/3/3
2	2AN	A	203	-	-	6/10/10/10	0/3/3/3
2	2AN	C	202	-	-	0/10/10/10	0/3/3/3
2	2AN	h	202	-	-	0/10/10/10	0/3/3/3
2	2AN	O	203	-	-	6/10/10/10	0/3/3/3
2	2AN	T	204	-	-	6/10/10/10	0/3/3/3
2	2AN	b	201	-	-	0/10/10/10	0/3/3/3
2	2AN	I	204	-	-	0/10/10/10	0/3/3/3
2	2AN	S	202	-	-	6/10/10/10	0/3/3/3
2	2AN	P	204	-	-	1/10/10/10	0/3/3/3
2	2AN	O	201	-	-	5/10/10/10	0/3/3/3
2	2AN	g	201	-	-	0/10/10/10	0/3/3/3
2	2AN	P	203	-	-	6/10/10/10	0/3/3/3
6	FLC	j	208	-	-	7/16/16/16	-
2	2AN	E	204	-	-	8/10/10/10	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	2AN	M	201	-	-	0/10/10/10	0/3/3/3
2	2AN	h	205	-	-	0/10/10/10	0/3/3/3
2	2AN	G	202	-	-	2/10/10/10	0/3/3/3
2	2AN	B	201	-	-	2/10/10/10	0/3/3/3
2	2AN	R	203	-	-	6/10/10/10	0/3/3/3
2	2AN	X	202	-	-	0/10/10/10	0/3/3/3
2	2AN	Y	202	-	-	6/10/10/10	0/3/3/3
6	FLC	a	206	-	-	7/16/16/16	-
2	2AN	L	202	-	-	0/10/10/10	0/3/3/3
2	2AN	D	202	-	-	1/10/10/10	0/3/3/3
2	2AN	V	202	-	-	1/10/10/10	0/3/3/3
2	2AN	j	205	-	-	1/10/10/10	0/3/3/3
2	2AN	b	206	-	-	7/10/10/10	0/3/3/3
6	FLC	i	202	-	-	8/16/16/16	-
2	2AN	K	203	-	-	0/10/10/10	0/3/3/3
2	2AN	G	205	-	-	6/10/10/10	0/3/3/3
2	2AN	Q	202	-	-	0/10/10/10	0/3/3/3
2	2AN	B	204	-	-	0/10/10/10	0/3/3/3
2	2AN	S	203	-	-	0/10/10/10	0/3/3/3
2	2AN	R	204	-	-	6/10/10/10	0/3/3/3
2	2AN	H	203	-	-	6/10/10/10	0/3/3/3
2	2AN	K	202	-	-	0/10/10/10	0/3/3/3
2	2AN	J	202	-	-	0/10/10/10	0/3/3/3
2	2AN	f	206	-	-	1/10/10/10	0/3/3/3
2	2AN	E	201	-	-	0/10/10/10	0/3/3/3
2	2AN	a	201	-	-	2/10/10/10	0/3/3/3
2	2AN	M	203	-	-	8/10/10/10	0/3/3/3
2	2AN	G	207	-	-	0/10/10/10	0/3/3/3
2	2AN	R	202	-	-	2/10/10/10	0/3/3/3
2	2AN	j	207	-	-	0/10/10/10	0/3/3/3
2	2AN	g	203	-	-	2/10/10/10	0/3/3/3
2	2AN	V	205	-	-	2/10/10/10	0/3/3/3
2	2AN	b	205	-	-	0/10/10/10	0/3/3/3
2	2AN	N	201	-	-	0/10/10/10	0/3/3/3
2	2AN	B	202	-	-	0/10/10/10	0/3/3/3
2	2AN	H	201	-	-	0/10/10/10	0/3/3/3
2	2AN	g	202	-	-	4/10/10/10	0/3/3/3
2	2AN	U	201	-	-	6/10/10/10	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	2AN	S	204	-	-	8/10/10/10	0/3/3/3
2	2AN	c	204	-	-	2/10/10/10	0/3/3/3
2	2AN	f	201	-	-	0/10/10/10	0/3/3/3
2	2AN	Q	203	-	-	5/10/10/10	0/3/3/3
2	2AN	T	201	-	-	0/10/10/10	0/3/3/3
2	2AN	h	201	-	-	0/10/10/10	0/3/3/3
6	FLC	i	203	-	-	9/16/16/16	-
2	2AN	B	206	-	-	1/10/10/10	0/3/3/3
2	2AN	Y	201	-	-	0/10/10/10	0/3/3/3
2	2AN	j	202	-	-	1/10/10/10	0/3/3/3
2	2AN	b	202	-	-	0/10/10/10	0/3/3/3
2	2AN	Z	205	-	-	0/10/10/10	0/3/3/3
2	2AN	X	203	-	-	2/10/10/10	0/3/3/3
2	2AN	V	204	-	-	0/10/10/10	0/3/3/3
6	FLC	e	202	-	-	11/16/16/16	-
2	2AN	I	203	-	-	0/10/10/10	0/3/3/3
2	2AN	V	207	-	-	0/10/10/10	0/3/3/3
2	2AN	A	201	-	-	0/10/10/10	0/3/3/3
2	2AN	D	204	-	-	8/10/10/10	0/3/3/3
2	2AN	V	203	-	-	1/10/10/10	0/3/3/3
2	2AN	h	203	-	-	3/10/10/10	0/3/3/3
2	2AN	O	202	-	-	0/10/10/10	0/3/3/3
2	2AN	G	203	-	-	0/10/10/10	0/3/3/3
2	2AN	Z	202	-	-	0/10/10/10	0/3/3/3
2	2AN	c	201	-	-	2/10/10/10	0/3/3/3
2	2AN	N	202	-	-	1/10/10/10	0/3/3/3
2	2AN	H	202	-	-	2/10/10/10	0/3/3/3
2	2AN	G	201	-	-	1/10/10/10	0/3/3/3
2	2AN	j	206	-	-	0/10/10/10	0/3/3/3
2	2AN	P	202	-	-	2/10/10/10	0/3/3/3
2	2AN	C	201	-	-	1/10/10/10	0/3/3/3
2	2AN	B	205	-	-	7/10/10/10	0/3/3/3
2	2AN	X	201	-	-	0/10/10/10	0/3/3/3
2	2AN	N	204	-	-	0/10/10/10	0/3/3/3
2	2AN	I	205	-	-	6/10/10/10	0/3/3/3
2	2AN	L	204	-	-	5/10/10/10	0/3/3/3
2	2AN	b	204	-	-	0/10/10/10	0/3/3/3
6	FLC	a	205	-	-	9/16/16/16	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	2AN	d	203	-	-	2/10/10/10	0/3/3/3
2	2AN	F	201	-	-	6/10/10/10	0/3/3/3
2	2AN	Z	203	-	-	0/10/10/10	0/3/3/3
2	2AN	G	204	-	-	0/10/10/10	0/3/3/3
2	2AN	j	204	-	-	5/10/10/10	0/3/3/3
2	2AN	N	203	-	-	8/10/10/10	0/3/3/3
2	2AN	X	204	-	-	3/10/10/10	0/3/3/3
2	2AN	R	205	-	-	0/10/10/10	0/3/3/3
2	2AN	S	201	-	-	8/10/10/10	0/3/3/3
2	2AN	U	202	-	-	5/10/10/10	0/3/3/3
2	2AN	C	203[A]	-	-	7/10/10/10	0/3/3/3
2	2AN	H	204	-	-	2/10/10/10	0/3/3/3
2	2AN	L	203	-	-	2/10/10/10	0/3/3/3
2	2AN	b	203	-	-	6/10/10/10	0/3/3/3
2	2AN	F	205	-	-	3/10/10/10	0/3/3/3
2	2AN	T	203	-	-	0/10/10/10	0/3/3/3
2	2AN	B	203	-	-	0/10/10/10	0/3/3/3
2	2AN	L	201	-	-	0/10/10/10	0/3/3/3
2	2AN	I	206	-	-	2/10/10/10	0/3/3/3
2	2AN	V	206	-	-	0/10/10/10	0/3/3/3
2	2AN	i	201	-	-	3/10/10/10	0/3/3/3

All (754) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	I	205	2AN	C1-C10	8.45	1.54	1.43
2	M	201	2AN	C1-C10	7.97	1.53	1.43
2	Y	201	2AN	C1-C10	7.65	1.53	1.43
2	j	207	2AN	C1-C10	7.55	1.52	1.43
4	P	205	EPE	C10-S	-7.51	1.67	1.77
2	I	207	2AN	C1-C10	7.45	1.52	1.43
6	j	208	FLC	CB-CBC	-7.01	1.46	1.53
2	b	206	2AN	C1-C10	6.81	1.51	1.43
2	h	206	2AN	C1-C10	6.80	1.51	1.43
2	T	204	2AN	C1-C10	6.73	1.51	1.43
2	I	206	2AN	C1-C10	6.72	1.51	1.43
2	D	204	2AN	C1-C10	6.72	1.51	1.43
2	h	201	2AN	C1-C10	6.69	1.51	1.43
2	R	204	2AN	C1-C10	6.69	1.51	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	Z	201	2AN	C1-C10	6.65	1.51	1.43
2	T	202	2AN	C1-C10	6.51	1.51	1.43
2	I	204	2AN	C1-C10	6.51	1.51	1.43
2	a	202	2AN	C1-C10	6.43	1.51	1.43
2	a	201	2AN	C1-C10	6.42	1.51	1.43
2	N	205	2AN	C1-C10	6.39	1.51	1.43
2	X	205	2AN	C1-C10	6.37	1.51	1.43
2	Z	206	2AN	C1-C10	6.27	1.51	1.43
2	f	201	2AN	C1-C10	6.27	1.51	1.43
2	O	202	2AN	C1-C10	6.26	1.51	1.43
2	b	205	2AN	C1-C10	6.24	1.51	1.43
2	h	205	2AN	C1-C10	6.22	1.51	1.43
2	Z	202	2AN	C1-C10	6.20	1.51	1.43
2	G	204	2AN	C1-C10	6.11	1.51	1.43
2	A	203	2AN	C1-C10	6.07	1.50	1.43
2	S	201	2AN	C1-C10	6.05	1.50	1.43
2	X	201	2AN	C1-C10	6.04	1.50	1.43
2	H	204	2AN	C1-C10	5.99	1.50	1.43
2	c	202	2AN	C1-C10	5.97	1.50	1.43
2	e	201	2AN	C1-C10	5.95	1.50	1.43
2	V	203	2AN	C1-C10	5.93	1.50	1.43
2	Q	203	2AN	C1-C10	5.92	1.50	1.43
2	U	201	2AN	C1-C10	5.86	1.50	1.43
2	F	202	2AN	C1-C10	5.84	1.50	1.43
2	T	205	2AN	C1-C10	5.83	1.50	1.43
2	Q	201	2AN	C1-C10	5.81	1.50	1.43
2	G	207	2AN	C1-C10	5.80	1.50	1.43
2	S	202	2AN	C1-C10	5.75	1.50	1.43
2	I	202	2AN	C1-C10	5.75	1.50	1.43
2	a	203	2AN	C1-C10	5.74	1.50	1.43
2	g	201	2AN	C1-C10	5.70	1.50	1.43
2	O	203	2AN	C1-C10	5.61	1.50	1.43
2	X	204	2AN	C1-C10	5.60	1.50	1.43
2	L	204	2AN	C1-C10	5.57	1.50	1.43
2	d	202	2AN	C1-C10	5.56	1.50	1.43
2	i	201	2AN	C1-C10	5.48	1.50	1.43
2	A	202	2AN	C1-C10	5.45	1.50	1.43
2	F	206	2AN	C1-C10	5.45	1.50	1.43
2	R	201	2AN	C1-C10	5.45	1.50	1.43
2	W	201	2AN	C1-C10	5.43	1.50	1.43
2	R	205	2AN	C1-C10	5.40	1.50	1.43
2	I	205	2AN	C10-C5	5.34	1.53	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	204	2AN	C1-C10	5.34	1.50	1.43
2	B	202	2AN	C1-C10	5.27	1.49	1.43
2	G	205	2AN	C1-C10	5.27	1.49	1.43
2	H	202	2AN	C1-C10	5.26	1.49	1.43
2	j	206	2AN	C1-C10	5.23	1.49	1.43
2	f	206	2AN	C1-C10	5.17	1.49	1.43
2	Q	202	2AN	C1-C10	5.16	1.49	1.43
2	E	201	2AN	C1-C10	5.16	1.49	1.43
2	c	203	2AN	C1-C10	5.16	1.49	1.43
2	P	201	2AN	C1-C10	5.16	1.49	1.43
2	V	208	2AN	C1-C10	5.15	1.49	1.43
2	F	204	2AN	C1-C10	5.14	1.49	1.43
2	b	201	2AN	C1-C10	5.12	1.49	1.43
2	K	203	2AN	C1-C10	5.12	1.49	1.43
2	b	203	2AN	C1-C10	5.06	1.49	1.43
2	N	203	2AN	C1-N	-5.05	1.23	1.38
2	h	203	2AN	C1-C10	5.02	1.49	1.43
2	B	206	2AN	C1-C10	4.99	1.49	1.43
2	D	204	2AN	C9-C10	4.93	1.54	1.44
2	D	201	2AN	C1-C10	4.90	1.49	1.43
2	I	203	2AN	C1-C10	4.88	1.49	1.43
2	c	202	2AN	C9-C10	4.87	1.53	1.44
2	F	205	2AN	C1-C10	4.85	1.49	1.43
2	Y	203	2AN	C1-C10	4.78	1.49	1.43
2	O	203	2AN	O1-S	4.77	1.66	1.43
2	I	205	2AN	C9-C10	4.76	1.53	1.44
2	Y	202	2AN	C1-C10	4.75	1.49	1.43
2	b	206	2AN	C9-C10	4.75	1.53	1.44
2	E	204	2AN	O2-S	4.74	1.66	1.43
2	B	201	2AN	C1-C10	4.74	1.49	1.43
2	Z	204	2AN	C1-C10	4.70	1.49	1.43
2	E	203	2AN	C1-C10	4.69	1.49	1.43
2	Y	201	2AN	C9-C10	4.68	1.53	1.44
2	C	202	2AN	C1-C10	4.67	1.49	1.43
2	L	202	2AN	C1-C10	4.67	1.49	1.43
2	R	203	2AN	C1-C10	4.67	1.49	1.43
2	A	204	2AN	C1-C10	4.63	1.49	1.43
2	A	202	2AN	O1-S	4.57	1.65	1.43
2	f	203	2AN	C1-C10	4.57	1.49	1.43
2	X	206	2AN	C1-C10	4.56	1.49	1.43
2	V	207	2AN	C1-C10	4.55	1.49	1.43
2	W	201	2AN	O2-S	4.55	1.65	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	j	203	2AN	C1-C10	4.54	1.48	1.43
2	d	203	2AN	C1-C10	4.53	1.48	1.43
2	I	206	2AN	C9-C10	4.52	1.53	1.44
2	I	207	2AN	O2-S	4.52	1.65	1.43
2	L	202	2AN	O2-S	4.48	1.65	1.43
2	g	201	2AN	O1-S	4.47	1.65	1.43
2	Z	201	2AN	O1-S	4.46	1.65	1.43
2	Z	203	2AN	C1-C10	4.44	1.48	1.43
2	X	203	2AN	C1-C10	4.44	1.48	1.43
2	G	207	2AN	O2-S	4.42	1.65	1.43
2	E	203	2AN	O1-S	4.42	1.65	1.43
2	M	202	2AN	C1-C10	4.42	1.48	1.43
2	R	202	2AN	C11-N	-4.41	1.31	1.40
2	g	203	2AN	C1-C10	4.40	1.48	1.43
2	I	205	2AN	O1-S	4.40	1.64	1.43
2	b	204	2AN	C1-C10	4.39	1.48	1.43
2	V	204	2AN	O1-S	4.39	1.64	1.43
2	S	203	2AN	O1-S	4.38	1.64	1.43
2	c	205	2AN	O1-S	4.37	1.64	1.43
2	X	205	2AN	O1-S	4.37	1.64	1.43
2	D	202	2AN	O2-S	4.35	1.64	1.43
2	I	207	2AN	C9-C10	4.34	1.52	1.44
2	J	203	2AN	C1-C10	4.33	1.48	1.43
2	C	201	2AN	O1-S	4.32	1.64	1.43
2	N	205	2AN	C10-C5	4.32	1.51	1.42
2	Q	203	2AN	O2-S	4.32	1.64	1.43
2	R	202	2AN	C1-C10	4.32	1.48	1.43
2	T	204	2AN	C10-C5	4.31	1.51	1.42
2	F	206	2AN	O1-S	4.31	1.64	1.43
2	S	204	2AN	O2-S	4.30	1.64	1.43
2	V	201	2AN	O1-S	4.30	1.64	1.43
2	I	203	2AN	O1-S	4.29	1.64	1.43
2	K	201	2AN	O1-S	4.29	1.64	1.43
2	b	202	2AN	C1-C10	4.29	1.48	1.43
2	h	201	2AN	C9-C10	4.29	1.52	1.44
2	a	204	2AN	O1-S	4.28	1.64	1.43
2	V	201	2AN	C1-C10	4.28	1.48	1.43
2	g	202	2AN	C1-C10	4.28	1.48	1.43
2	G	204	2AN	O1-S	4.27	1.64	1.43
2	G	201	2AN	O1-S	4.27	1.64	1.43
2	b	206	2AN	O1-S	4.26	1.64	1.43
2	U	202	2AN	O2-S	4.26	1.64	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	201	2AN	C1-C10	4.24	1.48	1.43
2	L	204	2AN	O2-S	4.24	1.64	1.43
2	N	205	2AN	C9-C10	4.24	1.52	1.44
2	d	201	2AN	O1-S	4.24	1.64	1.43
2	X	201	2AN	O2-S	4.23	1.64	1.43
2	g	203	2AN	O2-S	4.23	1.64	1.43
2	a	204	2AN	C1-C10	4.23	1.48	1.43
2	Y	201	2AN	O2-S	4.21	1.64	1.43
2	O	202	2AN	O1-S	4.21	1.64	1.43
2	f	203	2AN	O2-S	4.20	1.64	1.43
2	Z	201	2AN	C9-C10	4.20	1.52	1.44
2	b	202	2AN	O1-S	4.20	1.64	1.43
2	a	203	2AN	O1-S	4.20	1.64	1.43
2	A	204	2AN	O2-S	4.20	1.63	1.43
2	T	205	2AN	O2-S	4.19	1.63	1.43
2	h	201	2AN	O1-S	4.19	1.63	1.43
2	h	205	2AN	O1-S	4.19	1.63	1.43
2	E	202	2AN	O1-S	4.19	1.63	1.43
2	X	203	2AN	O1-S	4.18	1.63	1.43
2	D	204	2AN	C10-C5	4.18	1.51	1.42
2	X	206	2AN	O2-S	4.18	1.63	1.43
2	j	207	2AN	O1-S	4.18	1.63	1.43
2	S	201	2AN	O1-S	4.18	1.63	1.43
2	d	204	2AN	O2-S	4.17	1.63	1.43
2	B	203	2AN	O1-S	4.17	1.63	1.43
2	S	203	2AN	C1-C10	4.17	1.48	1.43
2	K	202	2AN	C11-N	-4.16	1.31	1.40
2	K	201	2AN	C1-C10	4.16	1.48	1.43
2	e	201	2AN	C9-C10	4.16	1.52	1.44
2	j	205	2AN	C12-C11	-4.16	1.32	1.39
2	d	201	2AN	C1-C10	4.15	1.48	1.43
2	a	202	2AN	C9-C10	4.15	1.52	1.44
2	A	203	2AN	O1-S	4.14	1.63	1.43
2	D	202	2AN	C1-C10	4.14	1.48	1.43
2	H	202	2AN	O2-S	4.14	1.63	1.43
2	N	203	2AN	C11-N	-4.13	1.31	1.40
2	Z	206	2AN	O1-S	4.13	1.63	1.43
2	a	201	2AN	O2-S	4.13	1.63	1.43
6	e	202	FLC	CB-CBC	-4.12	1.49	1.53
2	B	205	2AN	C1-C10	4.11	1.48	1.43
2	Z	202	2AN	O1-S	4.11	1.63	1.43
2	Y	201	2AN	C10-C5	4.11	1.51	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	X	202	2AN	O1-S	4.10	1.63	1.43
2	X	204	2AN	O2-S	4.08	1.63	1.43
2	U	202	2AN	C1-C10	4.08	1.48	1.43
2	H	203	2AN	O2-S	4.07	1.63	1.43
2	B	204	2AN	O1-S	4.07	1.63	1.43
2	D	204	2AN	O1-S	4.07	1.63	1.43
2	Y	204	2AN	C1-C10	4.06	1.48	1.43
2	H	203	2AN	C1-C10	4.06	1.48	1.43
2	j	206	2AN	O2-S	4.06	1.63	1.43
2	T	202	2AN	O1-S	4.06	1.63	1.43
2	B	205	2AN	O1-S	4.04	1.63	1.43
2	R	204	2AN	O2-S	4.03	1.63	1.43
2	D	203	2AN	O2-S	4.02	1.63	1.43
2	b	204	2AN	O1-S	4.02	1.63	1.43
2	f	205	2AN	O1-S	4.02	1.63	1.43
2	T	205	2AN	C9-C10	4.02	1.52	1.44
2	Q	203	2AN	C9-C10	4.01	1.52	1.44
2	H	201	2AN	C1-C10	4.01	1.48	1.43
2	B	206	2AN	O2-S	3.99	1.63	1.43
2	Y	204	2AN	O2-S	3.99	1.63	1.43
2	P	203	2AN	C1-C10	3.99	1.48	1.43
2	T	205	2AN	C10-C5	3.99	1.50	1.42
2	d	204	2AN	C1-C10	3.98	1.48	1.43
2	R	204	2AN	C9-C10	3.97	1.52	1.44
2	M	203	2AN	O2-S	3.96	1.62	1.43
2	J	201	2AN	O1-S	3.95	1.62	1.43
2	j	204	2AN	O1-S	3.95	1.62	1.43
2	T	201	2AN	O2-S	3.95	1.62	1.43
2	I	206	2AN	O2-S	3.94	1.62	1.43
2	h	203	2AN	C11-N	-3.92	1.32	1.40
2	A	203	2AN	C9-C10	3.92	1.52	1.44
2	X	202	2AN	C1-C10	3.91	1.48	1.43
2	Q	201	2AN	O1-S	3.90	1.62	1.43
2	h	202	2AN	C1-C10	3.90	1.48	1.43
2	L	201	2AN	C1-C10	3.88	1.48	1.43
2	V	206	2AN	C1-C10	3.87	1.48	1.43
2	G	205	2AN	C11-N	-3.87	1.32	1.40
2	d	202	2AN	O1-S	3.87	1.62	1.43
2	c	205	2AN	C1-C10	3.84	1.48	1.43
2	P	202	2AN	C11-N	-3.84	1.32	1.40
2	T	201	2AN	C1-C10	3.83	1.48	1.43
2	a	203	2AN	C10-C5	3.82	1.50	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	201	2AN	O2-S	3.80	1.62	1.43
2	I	207	2AN	C10-C5	3.80	1.50	1.42
2	a	203	2AN	C9-C10	3.80	1.51	1.44
2	b	206	2AN	C10-C5	3.79	1.50	1.42
2	Z	203	2AN	O2-S	3.79	1.62	1.43
2	I	206	2AN	C10-C5	3.79	1.50	1.42
2	Y	202	2AN	O2-S	3.78	1.62	1.43
2	c	203	2AN	O3-S	3.77	1.65	1.45
2	f	206	2AN	O2-S	3.77	1.61	1.43
2	f	205	2AN	C11-N	-3.76	1.32	1.40
2	V	204	2AN	C1-C10	3.75	1.47	1.43
2	F	205	2AN	O1-S	3.74	1.61	1.43
2	c	202	2AN	C10-C5	3.74	1.50	1.42
2	G	201	2AN	C1-C10	3.74	1.47	1.43
2	F	203	2AN	O1-S	3.73	1.61	1.43
2	S	204	2AN	C1-C10	3.73	1.47	1.43
2	V	208	2AN	C9-C10	3.73	1.51	1.44
2	D	203	2AN	C11-N	-3.71	1.32	1.40
2	V	208	2AN	O3-S	3.70	1.64	1.45
2	c	202	2AN	O2-S	3.70	1.61	1.43
2	Q	202	2AN	O2-S	3.69	1.61	1.43
2	D	203	2AN	C1-C10	3.68	1.47	1.43
2	F	202	2AN	C9-C10	3.68	1.51	1.44
2	O	201	2AN	O2-S	3.68	1.61	1.43
2	P	204	2AN	C4-C5	-3.67	1.34	1.42
2	J	203	2AN	O2-S	3.67	1.61	1.43
2	V	208	2AN	C11-N	-3.67	1.32	1.40
2	Z	205	2AN	O3-S	3.66	1.64	1.45
2	T	204	2AN	O2-S	3.66	1.61	1.43
2	U	201	2AN	O3-S	3.66	1.64	1.45
2	V	206	2AN	C10-C5	3.66	1.50	1.42
2	f	202	2AN	O1-S	3.65	1.61	1.43
2	Z	204	2AN	O3-S	3.65	1.64	1.45
2	Q	203	2AN	C10-C5	3.64	1.50	1.42
2	I	204	2AN	O3-S	3.64	1.64	1.45
2	V	203	2AN	O2-S	3.64	1.61	1.43
2	a	204	2AN	C11-N	-3.63	1.32	1.40
2	B	201	2AN	O1-S	3.63	1.61	1.43
2	W	201	2AN	C9-C10	3.62	1.51	1.44
2	E	203	2AN	C10-C5	3.62	1.49	1.42
2	A	202	2AN	C9-C10	3.62	1.51	1.44
2	Z	203	2AN	C10-C5	3.62	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	201	2AN	O2-S	3.61	1.61	1.43
2	S	201	2AN	C9-C10	3.61	1.51	1.44
2	H	204	2AN	O3-S	3.61	1.64	1.45
2	R	203	2AN	O3-S	3.60	1.64	1.45
2	F	202	2AN	C10-C5	3.59	1.49	1.42
2	h	201	2AN	C10-C5	3.59	1.49	1.42
2	f	204	2AN	C1-C10	3.59	1.47	1.43
2	V	205	2AN	C1-C10	3.58	1.47	1.43
2	T	203	2AN	O3-S	3.58	1.64	1.45
2	F	201	2AN	O2-S	3.58	1.61	1.43
2	N	205	2AN	O3-S	3.57	1.64	1.45
2	j	207	2AN	C9-C10	3.56	1.51	1.44
2	C	202	2AN	O3-S	3.55	1.64	1.45
2	P	202	2AN	O2-S	3.55	1.60	1.43
2	G	205	2AN	O3-S	3.55	1.63	1.45
2	d	203	2AN	O3-S	3.55	1.63	1.45
2	A	203	2AN	C10-C5	3.55	1.49	1.42
2	P	204	2AN	O3-S	3.55	1.63	1.45
2	M	203	2AN	C9-C10	3.55	1.51	1.44
2	c	201	2AN	C4-C5	-3.54	1.34	1.42
2	V	207	2AN	O3-S	3.54	1.63	1.45
2	G	202	2AN	C1-C10	3.54	1.47	1.43
2	M	203	2AN	C1-C10	3.54	1.47	1.43
2	L	203	2AN	C1-C10	3.53	1.47	1.43
2	h	202	2AN	O2-S	3.53	1.60	1.43
2	c	204	2AN	O2-S	3.52	1.60	1.43
2	R	205	2AN	O3-S	3.52	1.63	1.45
2	e	201	2AN	C10-C5	3.52	1.49	1.42
2	J	201	2AN	C1-C10	3.50	1.47	1.43
2	J	202	2AN	O3-S	3.50	1.63	1.45
2	Z	203	2AN	C9-C10	3.50	1.51	1.44
2	M	202	2AN	O3-S	3.49	1.63	1.45
2	V	202	2AN	O1-S	3.49	1.60	1.43
2	i	201	2AN	C10-C5	3.49	1.49	1.42
2	h	203	2AN	O1-S	3.48	1.60	1.43
2	N	202	2AN	C1-C10	3.48	1.47	1.43
2	G	202	2AN	O3-S	3.48	1.63	1.45
2	L	203	2AN	O2-S	3.47	1.60	1.43
2	H	204	2AN	C10-C5	3.47	1.49	1.42
2	R	204	2AN	C10-C5	3.47	1.49	1.42
2	K	203	2AN	O3-S	3.46	1.63	1.45
2	S	202	2AN	C9-C10	3.45	1.51	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	P	204	2AN	C1-C10	3.45	1.47	1.43
2	j	204	2AN	C1-C10	3.45	1.47	1.43
2	N	202	2AN	O2-S	3.45	1.60	1.43
2	I	201	2AN	O1-S	3.45	1.60	1.43
2	O	203	2AN	C9-C10	3.44	1.51	1.44
2	P	203	2AN	C11-N	-3.44	1.33	1.40
2	T	203	2AN	C4-C5	-3.43	1.34	1.42
2	j	201	2AN	C4-C5	-3.43	1.34	1.42
2	j	201	2AN	C1-C10	3.43	1.47	1.43
2	K	202	2AN	C1-C10	3.42	1.47	1.43
2	B	203	2AN	C11-N	-3.42	1.33	1.40
2	Y	203	2AN	O3-S	3.42	1.63	1.45
2	b	205	2AN	O3-S	3.41	1.63	1.45
2	T	204	2AN	C8-C9	3.41	1.41	1.37
2	G	207	2AN	C9-C10	3.41	1.50	1.44
2	Z	201	2AN	C10-C5	3.40	1.49	1.42
2	j	202	2AN	O1-S	3.40	1.60	1.43
2	F	201	2AN	C1-C10	3.39	1.47	1.43
2	j	205	2AN	O1-S	3.39	1.60	1.43
2	h	205	2AN	C10-C5	3.38	1.49	1.42
2	j	201	2AN	O2-S	3.38	1.60	1.43
2	B	204	2AN	C1-C10	3.37	1.47	1.43
2	R	203	2AN	C11-N	-3.37	1.33	1.40
2	I	203	2AN	C10-C5	3.37	1.49	1.42
2	X	202	2AN	C11-N	-3.37	1.33	1.40
2	N	204	2AN	C4-C5	-3.37	1.34	1.42
2	U	202	2AN	C11-N	-3.36	1.33	1.40
2	L	201	2AN	C4-C5	-3.35	1.34	1.42
2	L	203	2AN	C10-C5	3.35	1.49	1.42
2	V	202	2AN	C1-C10	3.34	1.47	1.43
2	S	202	2AN	C10-C5	3.33	1.49	1.42
2	N	205	2AN	C8-C9	3.33	1.41	1.37
2	h	206	2AN	O3-S	3.33	1.62	1.45
2	c	201	2AN	O1-S	3.33	1.59	1.43
2	h	205	2AN	C9-C10	3.33	1.50	1.44
2	Q	201	2AN	C9-C10	3.32	1.50	1.44
2	O	202	2AN	C10-C5	3.32	1.49	1.42
2	T	204	2AN	C9-C10	3.30	1.50	1.44
2	G	201	2AN	C9-C10	3.30	1.50	1.44
2	b	202	2AN	C11-N	-3.29	1.33	1.40
2	D	201	2AN	C10-C5	3.28	1.49	1.42
2	L	204	2AN	C10-C5	3.28	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	204	2AN	O3-S	3.28	1.62	1.45
2	F	202	2AN	O3-S	3.27	1.62	1.45
2	h	203	2AN	C9-C10	3.26	1.50	1.44
2	Z	202	2AN	C10-C5	3.26	1.49	1.42
2	Z	205	2AN	C1-C10	3.26	1.47	1.43
2	h	204	2AN	C1-C10	3.23	1.47	1.43
2	j	207	2AN	C10-C5	3.23	1.49	1.42
2	D	203	2AN	C9-C10	3.23	1.50	1.44
2	Z	206	2AN	C10-C5	3.23	1.49	1.42
2	M	201	2AN	O2-S	3.21	1.59	1.43
2	h	203	2AN	C10-C5	3.21	1.49	1.42
2	j	206	2AN	C11-N	-3.20	1.33	1.40
2	P	201	2AN	O3-S	3.20	1.62	1.45
2	b	205	2AN	C10-C5	3.20	1.49	1.42
2	N	204	2AN	O3-S	3.19	1.62	1.45
2	h	206	2AN	C9-C10	3.19	1.50	1.44
2	c	204	2AN	C1-C10	3.19	1.47	1.43
2	I	204	2AN	C10-C5	3.19	1.49	1.42
2	E	204	2AN	C9-C10	3.17	1.50	1.44
2	h	204	2AN	C6-C5	-3.17	1.35	1.42
2	L	204	2AN	C9-C10	3.17	1.50	1.44
2	Y	202	2AN	C10-C5	3.17	1.49	1.42
2	i	201	2AN	O3-S	3.16	1.61	1.45
2	P	203	2AN	O3-S	3.16	1.61	1.45
2	d	202	2AN	C10-C5	3.16	1.49	1.42
2	T	202	2AN	C9-C10	3.15	1.50	1.44
2	W	201	2AN	C10-C5	3.14	1.48	1.42
2	j	206	2AN	C10-C5	3.14	1.48	1.42
2	U	201	2AN	C10-C5	3.14	1.48	1.42
2	R	205	2AN	C4-C5	-3.14	1.35	1.42
2	S	202	2AN	O3-S	3.14	1.61	1.45
2	X	201	2AN	C9-C10	3.13	1.50	1.44
2	b	205	2AN	C9-C10	3.13	1.50	1.44
2	b	203	2AN	O3-S	3.13	1.61	1.45
2	F	204	2AN	C9-C10	3.12	1.50	1.44
2	K	201	2AN	C9-C10	3.12	1.50	1.44
2	b	202	2AN	C10-C5	3.11	1.48	1.42
2	X	205	2AN	C9-C10	3.11	1.50	1.44
2	N	202	2AN	C9-C10	3.11	1.50	1.44
2	E	204	2AN	C10-C5	3.10	1.48	1.42
2	E	204	2AN	C11-N	-3.10	1.34	1.40
2	c	201	2AN	C6-C5	-3.10	1.35	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	R	202	2AN	C4-C5	-3.10	1.35	1.42
2	A	202	2AN	C10-C5	3.09	1.48	1.42
2	f	201	2AN	C4-C5	-3.09	1.35	1.42
2	B	202	2AN	O3-S	3.09	1.61	1.45
2	I	202	2AN	O2-S	3.09	1.58	1.43
2	X	204	2AN	C10-C5	3.09	1.48	1.42
2	Y	203	2AN	C10-C5	3.08	1.48	1.42
2	G	207	2AN	C10-C5	3.08	1.48	1.42
2	O	202	2AN	C9-C10	3.07	1.50	1.44
2	Z	206	2AN	C9-C10	3.07	1.50	1.44
2	V	201	2AN	C4-C5	-3.05	1.35	1.42
2	J	203	2AN	C9-C10	3.05	1.50	1.44
2	M	203	2AN	C10-C5	3.04	1.48	1.42
2	C	201	2AN	C1-C10	3.04	1.47	1.43
2	a	204	2AN	C9-C10	3.04	1.50	1.44
2	f	206	2AN	C10-C5	3.04	1.48	1.42
2	J	202	2AN	C4-C5	-3.04	1.35	1.42
2	Z	201	2AN	C8-C9	3.03	1.41	1.37
2	b	201	2AN	O2-S	3.03	1.58	1.43
2	V	204	2AN	C10-C5	3.02	1.48	1.42
2	J	202	2AN	C11-N	-3.01	1.34	1.40
2	N	202	2AN	C11-N	-3.00	1.34	1.40
2	c	206	2AN	O3-S	3.00	1.61	1.45
2	X	205	2AN	C10-C5	3.00	1.48	1.42
2	V	208	2AN	C10-C5	3.00	1.48	1.42
2	O	203	2AN	C10-C5	2.99	1.48	1.42
2	X	204	2AN	C9-C10	2.99	1.50	1.44
2	X	202	2AN	C9-C10	2.99	1.50	1.44
2	d	202	2AN	C9-C10	2.98	1.50	1.44
2	b	203	2AN	C9-C10	2.98	1.50	1.44
2	f	206	2AN	C9-C10	2.97	1.50	1.44
2	Y	201	2AN	C8-C9	2.96	1.41	1.37
2	D	202	2AN	C9-C10	2.96	1.50	1.44
2	E	203	2AN	C9-C10	2.96	1.50	1.44
2	d	202	2AN	C11-N	-2.95	1.34	1.40
2	R	201	2AN	O3-S	2.95	1.60	1.45
2	N	203	2AN	O3-S	2.95	1.60	1.45
2	C	202	2AN	C9-C10	2.95	1.50	1.44
2	g	202	2AN	C10-C5	2.94	1.48	1.42
2	j	202	2AN	C1-C10	2.94	1.46	1.43
2	c	205	2AN	C10-C5	2.93	1.48	1.42
2	B	204	2AN	C10-C5	2.93	1.48	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	201	2AN	O3-S	2.93	1.60	1.45
2	h	204	2AN	O3-S	2.93	1.60	1.45
2	Z	204	2AN	C9-C10	2.92	1.49	1.44
2	N	205	2AN	C11-N	-2.92	1.34	1.40
2	N	201	2AN	C6-C5	-2.92	1.35	1.42
2	Z	205	2AN	C10-C5	2.91	1.48	1.42
2	Z	204	2AN	C10-C5	2.90	1.48	1.42
2	h	206	2AN	C10-C5	2.88	1.48	1.42
2	b	202	2AN	C9-C10	2.88	1.49	1.44
2	H	204	2AN	C9-C10	2.87	1.49	1.44
2	T	203	2AN	C1-C10	2.86	1.46	1.43
2	P	202	2AN	C10-C5	2.86	1.48	1.42
2	R	202	2AN	C6-C5	-2.86	1.35	1.42
2	C	201	2AN	C9-C10	2.86	1.49	1.44
2	Y	203	2AN	C9-C10	2.86	1.49	1.44
2	X	206	2AN	C10-C5	2.86	1.48	1.42
2	f	203	2AN	C10-C5	2.85	1.48	1.42
2	V	207	2AN	C10-C5	2.85	1.48	1.42
2	C	202	2AN	C10-C5	2.85	1.48	1.42
2	D	202	2AN	C11-N	-2.84	1.34	1.40
2	j	207	2AN	C8-C9	2.84	1.41	1.37
2	A	204	2AN	C10-C5	2.84	1.48	1.42
2	e	201	2AN	C8-C9	2.84	1.41	1.37
2	Y	204	2AN	C11-N	-2.84	1.34	1.40
2	I	201	2AN	C1-C10	2.83	1.46	1.43
2	b	201	2AN	C11-N	-2.83	1.34	1.40
2	G	203	2AN	C11-N	-2.83	1.34	1.40
2	K	202	2AN	O3-S	2.83	1.60	1.45
2	B	206	2AN	C10-C5	2.83	1.48	1.42
2	H	202	2AN	C10-C5	2.83	1.48	1.42
2	U	201	2AN	C9-C10	2.83	1.49	1.44
2	I	203	2AN	C9-C10	2.83	1.49	1.44
2	V	205	2AN	O3-S	2.82	1.60	1.45
2	X	203	2AN	C10-C5	2.82	1.48	1.42
2	d	203	2AN	C10-C5	2.82	1.48	1.42
2	N	203	2AN	C9-C10	2.82	1.49	1.44
2	S	203	2AN	C10-C5	2.81	1.48	1.42
2	D	203	2AN	C10-C5	2.81	1.48	1.42
2	V	206	2AN	O3-S	2.81	1.60	1.45
2	a	202	2AN	O2-S	2.80	1.57	1.43
2	K	203	2AN	C10-C5	2.80	1.48	1.42
2	Y	202	2AN	C9-C10	2.80	1.49	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	j	203	2AN	C10-C5	2.80	1.48	1.42
2	F	203	2AN	C11-N	-2.80	1.34	1.40
2	A	201	2AN	C9-C10	2.80	1.49	1.44
2	S	201	2AN	C10-C5	2.80	1.48	1.42
2	N	204	2AN	C6-C5	-2.79	1.35	1.42
2	j	205	2AN	C11-N	-2.79	1.34	1.40
2	I	204	2AN	C9-C10	2.78	1.49	1.44
2	N	201	2AN	O3-S	2.78	1.59	1.45
2	g	202	2AN	O3-S	2.78	1.59	1.45
2	F	206	2AN	C11-N	-2.78	1.34	1.40
2	P	204	2AN	C9-C10	2.77	1.49	1.44
2	T	201	2AN	C8-C9	2.76	1.41	1.37
2	G	204	2AN	C10-C5	2.76	1.48	1.42
2	R	203	2AN	C9-C10	2.76	1.49	1.44
2	D	204	2AN	C8-C9	2.75	1.41	1.37
2	V	203	2AN	C9-C10	2.75	1.49	1.44
2	H	201	2AN	O3-S	2.75	1.59	1.45
2	I	206	2AN	C8-C9	2.74	1.41	1.37
2	B	201	2AN	C10-C5	2.74	1.48	1.42
2	H	201	2AN	C10-C5	2.74	1.48	1.42
2	P	203	2AN	C6-C5	-2.73	1.36	1.42
2	a	203	2AN	C11-N	-2.73	1.34	1.40
2	G	205	2AN	C9-C10	2.72	1.49	1.44
2	G	203	2AN	O1-S	2.71	1.56	1.43
2	G	203	2AN	C4-C5	-2.70	1.36	1.42
2	V	204	2AN	C11-N	-2.70	1.34	1.40
2	f	204	2AN	O3-S	2.70	1.59	1.45
2	I	206	2AN	C11-N	-2.70	1.34	1.40
2	L	201	2AN	O3-S	2.70	1.59	1.45
2	J	203	2AN	C10-C5	2.70	1.48	1.42
2	f	202	2AN	C9-C10	2.69	1.49	1.44
2	Z	202	2AN	C9-C10	2.68	1.49	1.44
2	f	204	2AN	C12-C11	-2.68	1.34	1.39
2	T	201	2AN	C11-N	-2.68	1.35	1.40
2	F	204	2AN	C10-C5	2.68	1.48	1.42
2	B	203	2AN	C1-C10	2.68	1.46	1.43
2	h	205	2AN	C8-C9	2.67	1.40	1.37
2	M	203	2AN	C11-N	-2.67	1.35	1.40
2	F	205	2AN	C10-C5	2.66	1.47	1.42
2	V	203	2AN	C10-C5	2.66	1.47	1.42
2	T	203	2AN	C10-C5	2.66	1.47	1.42
2	N	201	2AN	C11-N	-2.66	1.35	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	j	203	2AN	O2-S	2.66	1.56	1.43
2	V	206	2AN	C9-C10	2.66	1.49	1.44
2	G	207	2AN	C8-C9	2.65	1.40	1.37
2	h	204	2AN	C4-C5	-2.65	1.36	1.42
2	I	201	2AN	C4-C5	-2.64	1.36	1.42
2	b	203	2AN	C11-N	-2.64	1.35	1.40
2	Q	202	2AN	C10-C5	2.64	1.47	1.42
2	f	204	2AN	C11-N	-2.64	1.35	1.40
2	a	204	2AN	C10-C5	2.64	1.47	1.42
2	L	204	2AN	C8-C9	2.63	1.40	1.37
2	f	201	2AN	O2-S	2.63	1.56	1.43
2	B	203	2AN	C4-C5	-2.63	1.36	1.42
2	Q	202	2AN	C11-N	-2.61	1.35	1.40
2	G	204	2AN	C9-C10	2.61	1.49	1.44
2	T	205	2AN	C8-C9	2.60	1.40	1.37
2	I	202	2AN	C10-C5	2.60	1.47	1.42
2	R	201	2AN	C9-C10	2.60	1.49	1.44
2	F	206	2AN	C10-C5	2.60	1.47	1.42
2	T	201	2AN	C4-C5	-2.59	1.36	1.42
2	V	202	2AN	C10-C5	2.59	1.47	1.42
2	N	201	2AN	C4-C5	-2.59	1.36	1.42
2	f	201	2AN	C9-C10	2.59	1.49	1.44
2	E	202	2AN	C6-C5	-2.58	1.36	1.42
2	F	201	2AN	C10-C5	2.58	1.47	1.42
2	M	201	2AN	C9-C10	2.58	1.49	1.44
2	g	202	2AN	C6-C5	-2.57	1.36	1.42
2	E	201	2AN	C9-C10	2.57	1.49	1.44
2	I	203	2AN	C8-C9	2.57	1.40	1.37
2	a	201	2AN	C10-C5	2.56	1.47	1.42
2	V	205	2AN	C10-C5	2.56	1.47	1.42
2	B	205	2AN	C10-C5	2.56	1.47	1.42
2	D	201	2AN	C9-C10	2.55	1.49	1.44
2	d	204	2AN	C10-C5	2.55	1.47	1.42
2	R	205	2AN	C8-C9	2.54	1.40	1.37
6	a	205	FLC	CB-CBC	-2.54	1.50	1.53
2	I	202	2AN	C9-C10	2.54	1.49	1.44
2	R	202	2AN	O2-S	2.53	1.56	1.43
2	B	201	2AN	C11-N	-2.53	1.35	1.40
2	g	201	2AN	C10-C5	2.53	1.47	1.42
2	F	201	2AN	C9-C10	2.51	1.49	1.44
2	R	201	2AN	C10-C5	2.51	1.47	1.42
2	B	204	2AN	C9-C10	2.51	1.49	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	203	2AN	C10-C5	2.51	1.47	1.42
2	j	201	2AN	C11-N	-2.51	1.35	1.40
2	Z	206	2AN	C11-N	-2.50	1.35	1.40
2	i	201	2AN	C9-C10	2.49	1.49	1.44
2	f	201	2AN	C10-C5	2.49	1.47	1.42
2	M	202	2AN	C10-C5	2.48	1.47	1.42
2	S	203	2AN	C9-C10	2.48	1.49	1.44
2	f	203	2AN	C11-N	-2.47	1.35	1.40
2	Q	201	2AN	C10-C5	2.47	1.47	1.42
2	Y	204	2AN	C10-C5	2.47	1.47	1.42
2	d	203	2AN	C11-N	-2.47	1.35	1.40
2	X	203	2AN	C11-N	-2.46	1.35	1.40
2	b	204	2AN	C11-N	-2.46	1.35	1.40
2	D	201	2AN	C4-C5	-2.46	1.36	1.42
2	X	206	2AN	C11-N	-2.45	1.35	1.40
2	b	206	2AN	C8-C9	2.45	1.40	1.37
2	X	203	2AN	C9-C10	2.45	1.49	1.44
2	f	201	2AN	C7-C8	2.45	1.43	1.38
2	X	206	2AN	C9-C10	2.45	1.49	1.44
2	g	201	2AN	C8-C9	2.45	1.40	1.37
2	V	207	2AN	C11-N	-2.45	1.35	1.40
2	O	201	2AN	C11-N	-2.44	1.35	1.40
2	j	204	2AN	C11-N	-2.44	1.35	1.40
2	A	204	2AN	C11-N	-2.44	1.35	1.40
2	d	203	2AN	C9-C10	2.43	1.49	1.44
2	P	202	2AN	C8-C9	-2.43	1.34	1.37
2	R	201	2AN	C4-C5	-2.43	1.36	1.42
2	f	203	2AN	C9-C10	2.42	1.48	1.44
2	R	203	2AN	C10-C5	2.42	1.47	1.42
2	f	205	2AN	C1-C10	2.42	1.46	1.43
2	V	207	2AN	C9-C10	2.42	1.48	1.44
2	c	204	2AN	C6-C5	-2.41	1.36	1.42
2	E	202	2AN	C1-C10	2.41	1.46	1.43
2	G	204	2AN	C8-C9	2.40	1.40	1.37
2	H	203	2AN	C4-C5	-2.40	1.36	1.42
2	P	204	2AN	C8-C9	-2.40	1.34	1.37
2	B	203	2AN	C6-C5	-2.39	1.36	1.42
2	X	201	2AN	C4-C5	-2.39	1.36	1.42
2	D	203	2AN	C6-C5	-2.39	1.36	1.42
2	b	205	2AN	C8-C9	2.39	1.40	1.37
2	L	201	2AN	C9-C10	2.39	1.48	1.44
2	c	202	2AN	C8-C9	2.38	1.40	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	L	203	2AN	C9-C10	2.38	1.48	1.44
2	H	201	2AN	C11-N	-2.38	1.35	1.40
2	D	202	2AN	C10-C5	2.38	1.47	1.42
2	L	202	2AN	C8-C9	2.37	1.40	1.37
2	A	204	2AN	C9-C10	2.37	1.48	1.44
2	N	204	2AN	C10-C5	2.36	1.47	1.42
2	j	203	2AN	C6-C5	-2.36	1.36	1.42
2	a	202	2AN	C10-C5	2.36	1.47	1.42
2	d	204	2AN	C11-N	-2.36	1.35	1.40
2	F	203	2AN	C1-C10	2.34	1.46	1.43
2	T	205	2AN	C11-N	-2.34	1.35	1.40
2	h	202	2AN	C10-C5	2.34	1.47	1.42
2	W	201	2AN	C8-C9	2.34	1.40	1.37
2	N	202	2AN	C6-C5	-2.33	1.36	1.42
2	c	201	2AN	C1-N	-2.33	1.31	1.38
2	X	202	2AN	C10-C5	2.33	1.47	1.42
2	c	201	2AN	C1-C10	2.33	1.46	1.43
2	b	201	2AN	C10-C5	2.33	1.47	1.42
2	G	201	2AN	C6-C5	-2.32	1.36	1.42
2	c	204	2AN	C10-C5	2.32	1.47	1.42
2	H	204	2AN	C8-C9	2.32	1.40	1.37
2	V	205	2AN	C4-C5	-2.32	1.36	1.42
2	j	202	2AN	C9-C10	2.32	1.48	1.44
2	j	206	2AN	C9-C10	2.32	1.48	1.44
2	R	203	2AN	C6-C5	-2.32	1.36	1.42
2	S	204	2AN	C1-N	-2.31	1.31	1.38
6	i	203	FLC	OB1-CBC	2.31	1.29	1.22
2	A	201	2AN	C6-C5	-2.31	1.37	1.42
2	H	203	2AN	C11-N	-2.31	1.35	1.40
2	M	203	2AN	C8-C9	2.30	1.40	1.37
2	A	201	2AN	C10-C5	2.30	1.47	1.42
2	P	201	2AN	C9-C10	2.30	1.48	1.44
2	I	202	2AN	C6-C5	-2.30	1.37	1.42
2	N	202	2AN	C4-C5	-2.30	1.37	1.42
2	j	204	2AN	C1-N	-2.30	1.31	1.38
2	I	205	2AN	C8-C9	2.30	1.40	1.37
2	I	204	2AN	C8-C9	2.29	1.40	1.37
2	L	202	2AN	C10-C5	2.29	1.47	1.42
2	d	201	2AN	C4-C5	-2.29	1.37	1.42
2	e	201	2AN	C11-N	-2.29	1.35	1.40
2	V	205	2AN	C8-C9	2.28	1.40	1.37
2	Q	203	2AN	C8-C9	2.28	1.40	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	206	2AN	C3-C4	2.27	1.41	1.36
2	Z	201	2AN	C11-N	-2.27	1.35	1.40
2	g	203	2AN	C11-N	-2.27	1.35	1.40
2	g	201	2AN	C4-C5	-2.26	1.37	1.42
2	U	202	2AN	C10-C5	2.26	1.47	1.42
2	c	203	2AN	C9-C10	2.26	1.48	1.44
2	M	202	2AN	C6-C5	-2.26	1.37	1.42
2	Y	202	2AN	C11-N	-2.25	1.35	1.40
2	f	204	2AN	C8-C9	2.25	1.40	1.37
2	M	202	2AN	C4-C5	-2.24	1.37	1.42
2	H	202	2AN	C9-C10	2.24	1.48	1.44
2	F	205	2AN	C9-C10	2.24	1.48	1.44
2	a	201	2AN	C9-C10	2.24	1.48	1.44
2	h	203	2AN	C4-C5	-2.23	1.37	1.42
2	h	202	2AN	C4-C5	-2.23	1.37	1.42
2	B	205	2AN	C9-C10	2.23	1.48	1.44
2	j	205	2AN	C4-C5	-2.22	1.37	1.42
2	X	201	2AN	C8-C9	2.22	1.40	1.37
2	N	204	2AN	C11-N	-2.22	1.36	1.40
2	K	201	2AN	C6-C5	-2.22	1.37	1.42
2	G	203	2AN	C6-C5	-2.21	1.37	1.42
2	V	203	2AN	C4-C5	-2.21	1.37	1.42
2	j	203	2AN	C4-C5	-2.21	1.37	1.42
2	f	204	2AN	C4-C5	-2.21	1.37	1.42
2	X	205	2AN	C8-C9	2.21	1.40	1.37
2	J	201	2AN	C4-C5	-2.20	1.37	1.42
2	c	201	2AN	C11-N	-2.20	1.36	1.40
2	S	204	2AN	C11-N	-2.20	1.36	1.40
2	h	202	2AN	C11-N	-2.19	1.36	1.40
6	i	202	FLC	CB-CBC	-2.19	1.51	1.53
2	Z	202	2AN	C8-C9	2.19	1.40	1.37
2	B	201	2AN	C4-C5	-2.18	1.37	1.42
2	D	202	2AN	C6-C5	-2.18	1.37	1.42
2	B	202	2AN	C4-C5	-2.17	1.37	1.42
2	P	202	2AN	C6-C5	-2.17	1.37	1.42
2	A	202	2AN	C11-N	-2.17	1.36	1.40
2	C	201	2AN	C8-C9	2.17	1.40	1.37
2	P	202	2AN	C12-C11	-2.17	1.35	1.39
2	f	204	2AN	C15-C14	-2.17	1.33	1.38
2	A	202	2AN	C4-C5	-2.17	1.37	1.42
2	N	205	2AN	C7-C6	2.16	1.41	1.36
2	Z	203	2AN	C8-C9	2.16	1.40	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	c	206	2AN	C8-C9	-2.16	1.34	1.37
2	T	201	2AN	C9-C10	2.16	1.48	1.44
2	N	203	2AN	C16-C11	-2.15	1.35	1.39
2	V	205	2AN	C6-C5	-2.15	1.37	1.42
2	a	203	2AN	C8-C9	2.14	1.40	1.37
6	i	202	FLC	OG2-CGC	-2.14	1.23	1.30
2	M	203	2AN	C1-N	-2.14	1.32	1.38
2	J	202	2AN	C1-N	-2.14	1.32	1.38
2	R	202	2AN	C9-C10	2.13	1.48	1.44
2	V	205	2AN	C11-N	-2.13	1.36	1.40
2	Y	202	2AN	C4-C5	-2.13	1.37	1.42
2	V	208	2AN	C3-C2	-2.13	1.35	1.38
2	g	203	2AN	C4-C5	-2.12	1.37	1.42
2	R	205	2AN	C9-C10	2.12	1.48	1.44
2	g	203	2AN	C9-C10	2.12	1.48	1.44
2	C	201	2AN	C10-C5	2.11	1.46	1.42
2	g	201	2AN	C9-C10	2.11	1.48	1.44
2	g	203	2AN	C1-N	-2.11	1.32	1.38
2	a	201	2AN	C4-C5	-2.11	1.37	1.42
2	V	201	2AN	C11-N	-2.11	1.36	1.40
2	V	201	2AN	C8-C9	2.11	1.40	1.37
2	V	204	2AN	C9-C10	2.11	1.48	1.44
2	b	203	2AN	C4-C5	-2.10	1.37	1.42
2	U	202	2AN	C9-C10	2.10	1.48	1.44
2	F	206	2AN	C9-C10	2.10	1.48	1.44
2	T	202	2AN	C10-C5	2.09	1.46	1.42
2	c	205	2AN	C11-N	-2.09	1.36	1.40
2	f	205	2AN	C10-C5	2.09	1.46	1.42
2	A	201	2AN	C11-N	-2.09	1.36	1.40
2	C	202	2AN	C11-N	-2.08	1.36	1.40
2	G	202	2AN	C4-C5	-2.08	1.37	1.42
2	T	203	2AN	C11-N	-2.07	1.36	1.40
2	H	201	2AN	C9-C10	2.07	1.48	1.44
2	j	203	2AN	C9-C10	2.06	1.48	1.44
2	F	203	2AN	C10-C5	2.06	1.46	1.42
2	c	206	2AN	C6-C5	-2.06	1.37	1.42
2	V	203	2AN	C7-C6	2.05	1.41	1.36
2	K	202	2AN	C4-C5	-2.05	1.37	1.42
2	P	202	2AN	C1-C10	2.05	1.45	1.43
2	V	202	2AN	C4-C5	-2.05	1.37	1.42
2	Q	201	2AN	C11-N	-2.05	1.36	1.40
2	D	201	2AN	C11-N	-2.04	1.36	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	K	201	2AN	C11-N	-2.04	1.36	1.40
2	Y	201	2AN	C4-C5	-2.04	1.37	1.42
2	K	203	2AN	C9-C10	2.04	1.48	1.44
2	E	201	2AN	C11-N	-2.04	1.36	1.40
2	c	205	2AN	C9-C10	2.04	1.48	1.44
2	L	201	2AN	C11-N	-2.04	1.36	1.40
2	e	201	2AN	O3-S	2.04	1.56	1.45
2	S	204	2AN	C4-C5	-2.03	1.37	1.42
2	V	202	2AN	C11-N	-2.03	1.36	1.40
2	Z	205	2AN	C11-N	-2.03	1.36	1.40
2	A	202	2AN	C8-C9	2.03	1.40	1.37
2	T	201	2AN	C10-C5	2.03	1.46	1.42
2	M	201	2AN	C4-C5	-2.03	1.37	1.42
2	j	206	2AN	C8-C9	2.03	1.40	1.37
2	Y	203	2AN	C11-N	-2.02	1.36	1.40
2	X	202	2AN	C7-C6	2.02	1.41	1.36
2	P	203	2AN	C9-C10	2.02	1.48	1.44
2	P	203	2AN	C4-C5	-2.02	1.37	1.42
2	R	202	2AN	C7-C8	-2.02	1.35	1.38
2	G	202	2AN	C10-C5	2.02	1.46	1.42
2	S	204	2AN	C6-C5	-2.02	1.37	1.42
2	a	203	2AN	C4-C5	-2.02	1.37	1.42
2	E	204	2AN	C1-N	-2.01	1.32	1.38
2	U	201	2AN	C4-C5	-2.01	1.37	1.42
2	j	204	2AN	C10-C5	2.01	1.46	1.42
2	R	202	2AN	C1-N	-2.01	1.32	1.38

All (780) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	V	208	2AN	C10-C1-N	11.92	137.79	120.39
2	S	204	2AN	C11-N-C1	-10.66	103.10	126.36
2	V	208	2AN	C2-C1-N	-7.89	103.51	123.47
2	E	204	2AN	C11-N-C1	-7.89	109.16	126.36
2	N	203	2AN	C2-C1-C10	7.18	126.86	120.21
2	N	204	2AN	C2-C1-C10	-6.93	113.79	120.21
2	S	201	2AN	C11-N-C1	-6.83	111.45	126.36
2	D	204	2AN	C11-N-C1	-6.79	111.56	126.36
2	T	203	2AN	C2-C1-C10	-6.54	114.15	120.21
2	T	205	2AN	C2-C1-C10	-6.37	114.32	120.21
2	M	203	2AN	C11-N-C1	-6.36	112.49	126.36
2	Q	203	2AN	C11-N-C1	-6.33	112.56	126.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	j	208	FLC	OHB-CB-CBC	-6.30	100.03	108.96
2	d	204	2AN	C10-C1-N	6.23	129.48	120.39
2	a	201	2AN	C11-N-C1	-6.20	112.85	126.36
2	V	208	2AN	C11-N-C1	6.19	139.86	126.36
2	N	203	2AN	C1-C10-C5	-6.16	110.68	118.91
2	N	203	2AN	C11-N-C1	-6.09	113.08	126.36
6	i	203	FLC	OHB-CB-CBC	5.79	117.16	108.96
2	g	203	2AN	C11-N-C1	-5.64	114.06	126.36
2	d	204	2AN	C11-N-C1	-5.59	114.16	126.36
2	d	202	2AN	C2-C1-C10	-5.48	115.14	120.21
2	h	204	2AN	C2-C1-C10	-5.48	115.14	120.21
2	Z	205	2AN	C2-C1-C10	-5.47	115.15	120.21
2	I	206	2AN	C11-N-C1	-5.46	114.44	126.36
2	g	201	2AN	C2-C1-C10	-5.46	115.16	120.21
6	e	202	FLC	OHB-CB-CBC	-5.45	101.23	108.96
2	Z	202	2AN	C2-C1-C10	-5.40	115.21	120.21
2	V	206	2AN	C2-C1-C10	-5.31	115.30	120.21
2	G	202	2AN	C11-N-C1	-5.28	114.84	126.36
2	V	208	2AN	C1-C10-C5	-5.26	111.88	118.91
2	T	202	2AN	C2-C1-C10	-5.22	115.38	120.21
2	O	201	2AN	C10-C1-N	-5.14	112.89	120.39
2	U	202	2AN	C11-N-C1	-5.13	115.17	126.36
2	M	202	2AN	C2-C1-C10	-5.13	115.46	120.21
2	W	201	2AN	O2-S-C9	5.12	121.22	106.37
2	M	202	2AN	C11-N-C1	-5.04	115.37	126.36
2	K	203	2AN	C2-C1-C10	-5.03	115.55	120.21
2	X	202	2AN	C10-C1-N	-5.03	113.05	120.39
2	H	204	2AN	C2-C1-C10	-4.99	115.59	120.21
2	j	202	2AN	C2-C1-C10	-4.97	115.61	120.21
2	h	202	2AN	O2-S-C9	4.90	120.56	106.37
2	c	201	2AN	C11-N-C1	-4.87	115.74	126.36
2	K	201	2AN	O2-S-C9	4.83	120.36	106.37
2	D	201	2AN	C2-C1-C10	-4.83	115.74	120.21
2	S	204	2AN	C2-C1-N	-4.83	111.26	123.47
2	V	202	2AN	C2-C1-C10	-4.81	115.76	120.21
2	J	203	2AN	C11-N-C1	-4.78	115.93	126.36
2	I	201	2AN	C2-C1-C10	-4.78	115.79	120.21
2	Y	201	2AN	C13-C12-C11	4.77	125.23	119.73
2	D	203	2AN	O2-S-C9	4.75	120.13	106.37
2	X	201	2AN	C2-C1-C10	-4.66	115.90	120.21
2	Z	206	2AN	C11-N-C1	-4.62	116.28	126.36
2	P	202	2AN	C2-C1-C10	-4.62	115.94	120.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	h	203	2AN	O3-S-O2	-4.60	90.19	111.55
2	E	203	2AN	C2-C1-C10	-4.58	115.97	120.21
2	d	204	2AN	C2-C1-N	-4.57	111.90	123.47
2	d	201	2AN	O1-S-C9	4.55	119.56	106.37
2	L	203	2AN	C2-C1-C10	-4.54	116.01	120.21
2	Y	203	2AN	C2-C1-C10	-4.53	116.02	120.21
2	j	205	2AN	C2-C1-C10	-4.51	116.03	120.21
2	a	203	2AN	C2-C1-C10	-4.49	116.06	120.21
2	S	204	2AN	C10-C1-N	4.48	126.94	120.39
2	b	205	2AN	C2-C1-C10	-4.42	116.12	120.21
2	j	204	2AN	O1-S-C9	4.37	119.04	106.37
2	X	204	2AN	C2-C1-C10	-4.34	116.19	120.21
2	a	201	2AN	C2-C1-C10	-4.33	116.21	120.21
2	f	201	2AN	C10-C1-N	4.31	126.69	120.39
2	j	201	2AN	O1-S-C9	-4.27	94.01	106.37
2	i	201	2AN	C2-C1-C10	-4.24	116.29	120.21
2	j	202	2AN	O2-S-O1	-4.22	91.65	112.88
2	V	201	2AN	O1-S-C9	-4.21	94.18	106.37
2	L	204	2AN	C2-C1-C10	-4.20	116.32	120.21
2	V	205	2AN	C2-C1-C10	-4.19	116.33	120.21
2	j	202	2AN	C3-C2-C1	4.19	126.66	120.05
2	E	203	2AN	C7-C8-C9	4.17	125.01	120.37
2	g	202	2AN	C2-C1-C10	-4.16	116.36	120.21
2	M	201	2AN	C10-C1-N	4.15	126.44	120.39
2	M	201	2AN	C15-C16-C11	4.14	124.51	119.73
2	T	204	2AN	C2-C1-C10	-4.14	116.38	120.21
2	B	201	2AN	C7-C8-C9	4.13	124.97	120.37
2	c	204	2AN	C2-C1-C10	-4.13	116.39	120.21
2	N	201	2AN	C11-N-C1	-4.13	117.36	126.36
2	B	201	2AN	C2-C1-C10	-4.11	116.40	120.21
2	O	202	2AN	C2-C1-C10	-4.08	116.43	120.21
2	S	201	2AN	C2-C1-N	-4.08	113.15	123.47
2	f	204	2AN	C2-C1-C10	-4.07	116.45	120.21
2	a	201	2AN	C10-C1-N	4.04	126.29	120.39
2	Q	201	2AN	C10-C1-N	4.03	126.28	120.39
2	B	203	2AN	C2-C1-C10	-4.00	116.50	120.21
2	B	204	2AN	C2-C1-C10	-4.00	116.50	120.21
2	f	201	2AN	C13-C12-C11	4.00	124.34	119.73
2	Y	201	2AN	C10-C1-N	4.00	126.23	120.39
2	N	202	2AN	O1-S-C9	3.99	117.93	106.37
2	M	201	2AN	C16-C11-C12	-3.98	113.76	119.04
2	h	205	2AN	C2-C1-C10	-3.96	116.55	120.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	i	203	FLC	OB2-CBC-CB	3.95	120.73	113.14
2	R	205	2AN	C2-C1-C10	-3.92	116.58	120.21
2	j	203	2AN	C13-C12-C11	3.92	124.25	119.73
2	Z	204	2AN	C2-C1-C10	-3.92	116.58	120.21
2	F	206	2AN	C10-C1-N	3.90	126.08	120.39
2	T	201	2AN	O2-S-C9	3.89	117.63	106.37
2	D	204	2AN	C1-C10-C5	-3.88	113.72	118.91
2	H	203	2AN	C2-C1-C10	-3.88	116.62	120.21
2	j	206	2AN	C2-C1-C10	-3.88	116.62	120.21
2	g	202	2AN	C7-C8-C9	3.87	124.67	120.37
2	j	205	2AN	C11-N-C1	-3.86	117.94	126.36
2	U	201	2AN	C2-C1-C10	-3.85	116.64	120.21
2	P	203	2AN	O1-S-C9	3.84	117.50	106.37
2	G	204	2AN	C2-C1-C10	-3.84	116.66	120.21
2	f	201	2AN	C2-C1-N	-3.84	113.76	123.47
2	T	205	2AN	C11-N-C1	-3.80	118.07	126.36
2	Q	201	2AN	C2-C1-N	-3.77	113.92	123.47
2	F	205	2AN	O1-S-C9	3.76	117.26	106.37
2	e	201	2AN	O1-S-C9	3.74	117.22	106.37
2	b	206	2AN	C11-N-C1	-3.74	118.20	126.36
2	h	203	2AN	C8-C9-C10	-3.74	114.50	120.18
2	F	202	2AN	C2-C1-N	-3.72	114.06	123.47
2	Z	203	2AN	O2-S-C9	3.72	117.14	106.37
2	B	201	2AN	C10-C1-N	3.71	125.80	120.39
2	G	205	2AN	C10-C1-N	-3.70	114.98	120.39
2	D	204	2AN	C2-C1-N	-3.70	114.10	123.47
2	S	202	2AN	C10-C1-N	3.70	125.79	120.39
2	T	205	2AN	C3-C2-C1	3.65	125.81	120.05
2	M	201	2AN	C15-C14-C13	-3.64	114.88	119.87
6	G	206	FLC	OHB-CB-CBC	3.63	114.11	108.96
2	V	208	2AN	C6-C5-C4	-3.62	114.75	123.01
2	C	203[A]	2AN	C11-N-C1	3.62	134.26	126.36
2	f	202	2AN	C2-C1-C10	-3.61	116.87	120.21
2	P	203	2AN	C10-C1-N	-3.60	115.13	120.39
2	H	202	2AN	C2-C1-C10	-3.60	116.88	120.21
2	P	202	2AN	O1-S-C9	3.60	116.79	106.37
2	K	201	2AN	C8-C9-C10	-3.59	114.72	120.18
2	X	201	2AN	C15-C16-C11	3.59	123.86	119.73
2	f	205	2AN	O1-S-C9	3.58	116.75	106.37
2	M	202	2AN	C13-C12-C11	3.56	123.83	119.73
2	i	201	2AN	C7-C8-C9	3.55	124.32	120.37
6	i	203	FLC	OB1-CBC-CB	-3.55	115.22	122.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	M	201	2AN	C2-C1-C10	-3.54	116.93	120.21
2	V	204	2AN	C2-C1-C10	-3.54	116.94	120.21
2	S	202	2AN	C2-C1-C10	-3.53	116.94	120.21
2	j	201	2AN	O2-S-C9	3.51	116.55	106.37
2	Y	201	2AN	C16-C11-C12	-3.50	114.39	119.04
2	I	206	2AN	O2-S-C9	3.50	116.51	106.37
2	N	205	2AN	O2-S-C9	3.50	116.50	106.37
2	A	202	2AN	C2-C1-C10	-3.49	116.98	120.21
2	A	202	2AN	C10-C1-N	3.49	125.48	120.39
2	F	202	2AN	C10-C1-N	3.48	125.47	120.39
2	L	203	2AN	C11-N-C1	-3.48	118.77	126.36
2	I	203	2AN	C2-C1-C10	-3.48	116.99	120.21
2	h	206	2AN	C15-C16-C11	3.45	123.71	119.73
2	R	203	2AN	C10-C1-N	-3.45	115.36	120.39
2	F	206	2AN	C2-C1-C10	-3.45	117.02	120.21
2	P	202	2AN	C7-C8-C9	3.44	124.20	120.37
2	X	205	2AN	C2-C1-C10	-3.44	117.03	120.21
2	N	205	2AN	C10-C1-N	-3.43	115.38	120.39
2	E	201	2AN	O1-S-C9	3.42	116.29	106.37
6	j	208	FLC	CB-CA-CAC	-3.42	104.56	113.92
2	j	204	2AN	O2-S-C9	-3.42	96.45	106.37
2	c	204	2AN	O2-S-C9	3.42	116.27	106.37
2	V	208	2AN	C3-C2-C1	3.42	125.45	120.05
2	f	202	2AN	C11-N-C1	-3.42	118.91	126.36
2	B	205	2AN	O2-S-C9	3.41	116.25	106.37
2	h	203	2AN	C7-C8-C9	3.41	124.17	120.37
2	Z	201	2AN	C1-C10-C5	-3.41	114.35	118.91
2	C	203[A]	2AN	C10-C1-N	3.41	125.36	120.39
2	N	203	2AN	C7-C6-C5	3.39	125.20	120.48
2	c	203	2AN	C2-C1-C10	-3.39	117.08	120.21
2	Z	206	2AN	C2-C1-N	-3.36	114.96	123.47
2	F	202	2AN	C11-N-C1	-3.36	119.03	126.36
2	F	202	2AN	O1-S-C9	3.36	116.10	106.37
2	P	204	2AN	C1-C10-C5	-3.36	114.42	118.91
2	a	201	2AN	C2-C1-N	-3.35	114.98	123.47
2	F	202	2AN	C7-C8-C9	3.35	124.10	120.37
2	L	201	2AN	C13-C12-C11	3.32	123.56	119.73
2	O	203	2AN	O2-S-C9	3.32	115.99	106.37
2	N	205	2AN	C2-C1-C10	-3.31	117.15	120.21
2	P	204	2AN	C2-C1-N	-3.30	115.11	123.47
6	G	206	FLC	OHB-CB-CG	-3.30	101.84	109.38
2	C	201	2AN	C2-C1-N	-3.29	115.14	123.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	206	2AN	C2-C1-N	-3.29	115.15	123.47
2	G	203	2AN	C10-C1-N	-3.28	115.60	120.39
6	j	208	FLC	CG-CB-CA	3.28	117.72	109.31
2	N	203	2AN	C2-C1-N	-3.28	115.18	123.47
2	Z	203	2AN	C2-C1-C10	-3.27	117.18	120.21
2	g	203	2AN	C2-C1-N	-3.27	115.19	123.47
2	C	203[A]	2AN	C2-C1-C10	-3.27	117.19	120.21
2	Y	201	2AN	C6-C5-C4	-3.26	115.56	123.01
4	P	205	EPE	C5-N4-C3	3.26	115.87	108.84
2	I	204	2AN	C13-C12-C11	3.26	123.49	119.73
2	b	206	2AN	C2-C1-N	-3.26	115.22	123.47
2	F	204	2AN	C2-C1-C10	-3.25	117.20	120.21
2	c	202	2AN	C1-C10-C5	-3.24	114.58	118.91
6	G	206	FLC	OB2-CBC-CB	3.24	119.36	113.14
2	V	205	2AN	C8-C9-C10	-3.24	115.25	120.18
2	E	202	2AN	C11-N-C1	-3.24	119.30	126.36
2	h	202	2AN	O1-S-C9	3.22	115.71	106.37
2	I	201	2AN	C6-C5-C4	-3.22	115.66	123.01
2	S	202	2AN	C7-C8-C9	3.22	123.95	120.37
2	T	205	2AN	C10-C1-N	3.21	125.08	120.39
2	c	206	2AN	C7-C8-C9	3.21	123.94	120.37
2	L	203	2AN	O3-S-O2	-3.21	96.68	111.55
2	c	202	2AN	C2-C1-C10	-3.20	117.25	120.21
2	Q	201	2AN	C13-C12-C11	3.19	123.40	119.73
2	a	202	2AN	C2-C1-C10	-3.18	117.26	120.21
2	j	201	2AN	C2-C1-C10	-3.18	117.27	120.21
2	V	203	2AN	C8-C9-C10	-3.17	115.36	120.18
2	T	201	2AN	C2-C1-C10	-3.14	117.30	120.21
2	j	203	2AN	C11-N-C1	-3.14	119.50	126.36
2	Z	205	2AN	C10-C1-N	-3.14	115.80	120.39
2	I	205	2AN	C2-C1-C10	-3.14	117.30	120.21
2	T	205	2AN	C15-C16-C11	3.13	123.34	119.73
2	I	206	2AN	C2-C1-N	-3.13	115.55	123.47
2	j	203	2AN	C8-C9-C10	-3.13	115.42	120.18
2	a	204	2AN	C10-C1-N	-3.13	115.82	120.39
2	Y	201	2AN	C2-C1-C10	-3.13	117.32	120.21
2	Y	201	2AN	C1-C10-C5	-3.12	114.73	118.91
2	b	204	2AN	C2-C1-C10	-3.12	117.32	120.21
2	V	202	2AN	C3-C2-C1	3.12	124.97	120.05
2	L	203	2AN	C7-C8-C9	3.11	123.83	120.37
2	C	201	2AN	C11-N-C1	-3.11	119.58	126.36
2	e	201	2AN	C2-C1-C10	-3.11	117.33	120.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	a	201	2AN	C16-C11-C12	-3.10	114.92	119.04
2	F	201	2AN	C13-C12-C11	3.10	123.30	119.73
2	a	202	2AN	O1-S-C9	3.09	115.33	106.37
2	J	203	2AN	O1-S-C9	3.09	115.32	106.37
2	h	206	2AN	C11-N-C1	-3.07	119.67	126.36
2	N	205	2AN	C8-C9-C10	-3.07	115.52	120.18
2	j	207	2AN	C2-C1-C10	-3.06	117.38	120.21
2	N	202	2AN	C11-N-C1	-3.06	119.69	126.36
2	A	203	2AN	C2-C1-C10	-3.06	117.38	120.21
2	N	204	2AN	C3-C2-C1	3.05	124.87	120.05
2	V	206	2AN	O2-S-C9	3.05	115.21	106.37
2	Q	203	2AN	C2-C1-N	-3.05	115.75	123.47
2	A	202	2AN	C11-N-C1	-3.04	119.72	126.36
2	f	206	2AN	C2-C1-C10	-3.04	117.40	120.21
2	g	201	2AN	C13-C12-C11	3.04	123.23	119.73
2	N	203	2AN	C4-C3-C2	-3.03	116.33	121.00
2	D	204	2AN	C10-C1-N	3.03	124.82	120.39
2	d	201	2AN	C2-C1-C10	-3.03	117.41	120.21
2	F	202	2AN	O3-S-O1	-3.03	97.51	111.55
2	F	203	2AN	C10-C1-N	-3.02	115.98	120.39
2	G	202	2AN	C2-C1-N	-3.02	115.82	123.47
2	I	201	2AN	C11-N-C1	-3.02	119.78	126.36
2	a	203	2AN	C10-C1-N	-3.02	115.99	120.39
2	V	202	2AN	C10-C1-N	3.02	124.79	120.39
2	V	205	2AN	C11-N-C1	-3.02	119.78	126.36
2	Z	206	2AN	C10-C1-N	3.02	124.79	120.39
2	P	202	2AN	C3-C2-C1	3.01	124.81	120.05
2	I	204	2AN	C2-C1-C10	-3.01	117.42	120.21
2	d	204	2AN	C2-C1-C10	-3.00	117.43	120.21
2	R	204	2AN	C1-C10-C5	-3.00	114.90	118.91
2	j	205	2AN	C8-C9-C10	-2.99	115.63	120.18
2	d	203	2AN	C11-N-C1	-2.99	119.84	126.36
2	V	203	2AN	C2-C1-C10	-2.99	117.45	120.21
2	i	201	2AN	C8-C9-C10	-2.98	115.64	120.18
2	f	206	2AN	C11-N-C1	-2.97	119.89	126.36
2	M	201	2AN	C13-C12-C11	2.96	123.14	119.73
2	S	201	2AN	C1-C10-C5	-2.95	114.96	118.91
2	c	202	2AN	C3-C2-C1	2.95	124.71	120.05
6	j	208	FLC	OA1-CAC-CA	-2.95	114.60	122.95
2	D	202	2AN	O2-S-C9	2.95	114.91	106.37
6	i	203	FLC	OG1-CGC-CG	-2.94	114.61	122.95
2	M	203	2AN	O2-S-C9	2.94	114.88	106.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	j	202	2AN	C7-C8-C9	2.94	123.64	120.37
2	I	207	2AN	C1-C10-C5	-2.93	114.99	118.91
2	f	203	2AN	C11-N-C1	-2.93	119.97	126.36
2	b	206	2AN	C10-C1-N	2.93	124.66	120.39
2	X	203	2AN	C11-N-C1	-2.92	119.99	126.36
2	X	206	2AN	C11-N-C1	-2.91	120.02	126.36
2	E	203	2AN	C8-C9-C10	-2.91	115.76	120.18
2	h	202	2AN	C2-C1-C10	-2.90	117.53	120.21
2	Y	201	2AN	C2-C1-N	-2.90	116.14	123.47
2	V	207	2AN	C11-N-C1	-2.89	120.05	126.36
2	V	208	2AN	C4-C5-C10	2.89	123.99	118.27
2	A	201	2AN	O1-S-C9	2.89	114.73	106.37
2	Y	202	2AN	O1-S-C9	2.89	114.73	106.37
2	D	203	2AN	C10-C1-N	-2.88	116.18	120.39
2	j	201	2AN	C7-C8-C9	2.88	123.58	120.37
2	Y	203	2AN	C7-C8-C9	2.87	123.57	120.37
2	M	202	2AN	C10-C1-N	2.87	124.58	120.39
2	E	204	2AN	C2-C1-N	-2.87	116.20	123.47
2	Q	202	2AN	C2-C1-C10	-2.87	117.56	120.21
2	c	201	2AN	C2-C1-C10	-2.86	117.56	120.21
2	A	202	2AN	C2-C1-N	-2.86	116.23	123.47
2	h	203	2AN	C1-C10-C5	-2.86	115.08	118.91
2	G	201	2AN	C8-C9-C10	-2.86	115.83	120.18
2	V	206	2AN	C8-C9-C10	-2.86	115.83	120.18
2	D	201	2AN	C7-C8-C9	2.86	123.55	120.37
2	h	206	2AN	C10-C1-N	2.85	124.56	120.39
2	f	201	2AN	C15-C14-C13	-2.85	115.97	119.87
2	F	201	2AN	C2-C1-C10	-2.85	117.57	120.21
2	H	203	2AN	O2-S-C9	2.85	114.61	106.37
2	S	204	2AN	C7-C8-C9	2.84	123.53	120.37
2	h	201	2AN	C2-C1-C10	-2.84	117.58	120.21
2	e	201	2AN	C3-C2-C1	2.84	124.53	120.05
2	P	204	2AN	C11-N-C1	-2.84	120.17	126.36
2	I	205	2AN	C16-C11-C12	-2.83	115.28	119.04
2	j	206	2AN	C10-C1-N	-2.83	116.25	120.39
2	H	202	2AN	C11-N-C1	-2.83	120.19	126.36
2	I	201	2AN	C10-C1-N	2.83	124.52	120.39
2	E	203	2AN	O1-S-C9	2.83	114.56	106.37
2	O	203	2AN	C13-C12-C11	2.82	122.98	119.73
2	L	202	2AN	C2-C1-C10	-2.82	117.60	120.21
2	d	201	2AN	O2-S-C9	2.82	114.53	106.37
2	V	201	2AN	O2-S-C9	2.82	114.53	106.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	K	201	2AN	C6-C7-C8	2.82	125.32	121.00
2	N	203	2AN	C13-C12-C11	2.82	122.97	119.73
2	I	207	2AN	C6-C5-C4	-2.81	116.60	123.01
2	Z	206	2AN	C2-C1-C10	-2.81	117.61	120.21
2	H	201	2AN	C8-C9-C10	-2.81	115.91	120.18
2	G	203	2AN	C7-C8-C9	-2.80	117.24	120.37
2	j	202	2AN	C8-C9-C10	-2.80	115.92	120.18
2	Q	202	2AN	O1-S-C9	2.80	114.49	106.37
2	T	203	2AN	O3-S-O2	-2.80	98.57	111.55
2	F	205	2AN	C2-C1-C10	-2.80	117.62	120.21
2	I	207	2AN	C2-C1-C10	-2.80	117.62	120.21
2	B	203	2AN	C3-C2-C1	2.79	124.46	120.05
2	c	202	2AN	C13-C12-C11	2.79	122.95	119.73
2	P	202	2AN	O3-S-O2	-2.79	98.60	111.55
2	F	205	2AN	C10-C1-N	-2.79	116.32	120.39
2	W	201	2AN	C2-C1-C10	-2.78	117.64	120.21
2	M	202	2AN	C3-C2-C1	2.78	124.44	120.05
2	G	205	2AN	C16-C11-N	-2.77	111.22	120.61
2	I	205	2AN	C13-C12-C11	2.76	122.92	119.73
2	B	201	2AN	C2-C1-N	-2.76	116.47	123.47
2	b	206	2AN	C1-C10-C5	-2.76	115.22	118.91
2	S	203	2AN	C2-C1-C10	-2.76	117.66	120.21
2	M	201	2AN	C2-C1-N	-2.75	116.50	123.47
2	T	202	2AN	C3-C2-C1	2.75	124.40	120.05
2	T	202	2AN	C13-C12-C11	2.75	122.90	119.73
2	e	201	2AN	C1-C10-C5	-2.74	115.25	118.91
2	V	206	2AN	C7-C8-C9	2.73	123.41	120.37
2	V	208	2AN	C16-C11-N	-2.73	111.36	120.61
2	c	203	2AN	C10-C1-N	-2.73	116.41	120.39
2	f	201	2AN	C7-C8-C9	2.73	123.41	120.37
2	b	205	2AN	C15-C16-C11	2.73	122.88	119.73
2	L	204	2AN	C15-C16-C11	2.72	122.87	119.73
2	c	204	2AN	O1-S-C9	2.72	114.25	106.37
2	S	202	2AN	C2-C1-N	-2.72	116.59	123.47
2	T	203	2AN	C8-C9-C10	-2.71	116.05	120.18
4	P	205	EPE	C5-C6-N1	-2.71	105.19	110.65
2	A	204	2AN	C11-N-C1	-2.70	120.47	126.36
2	Z	206	2AN	O1-S-C9	2.69	114.18	106.37
2	j	203	2AN	C7-C8-C9	2.69	123.37	120.37
2	A	202	2AN	C6-C5-C4	-2.69	116.87	123.01
2	S	202	2AN	C3-C2-C1	2.69	124.29	120.05
2	G	202	2AN	C10-C1-N	2.68	124.30	120.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	V	208	2AN	O3-S-O2	-2.68	99.12	111.55
2	E	202	2AN	C6-C5-C4	-2.68	116.90	123.01
2	H	201	2AN	C13-C12-C11	2.67	122.81	119.73
2	a	203	2AN	C8-C9-C10	-2.67	116.11	120.18
2	Y	202	2AN	C2-C1-C10	-2.67	117.74	120.21
2	K	201	2AN	C1-C10-C5	-2.67	115.34	118.91
2	Z	203	2AN	C8-C9-C10	-2.66	116.13	120.18
2	V	205	2AN	C7-C8-C9	2.66	123.33	120.37
2	F	206	2AN	C16-C11-N	-2.66	111.62	120.61
2	e	201	2AN	C8-C9-C10	-2.66	116.14	120.18
2	V	201	2AN	C2-C1-C10	-2.65	117.76	120.21
2	g	202	2AN	C6-C5-C4	-2.65	116.96	123.01
2	B	201	2AN	C15-C16-C11	2.65	122.78	119.73
2	B	201	2AN	C6-C5-C4	-2.65	116.97	123.01
2	j	205	2AN	O2-S-C9	2.64	114.03	106.37
2	Z	204	2AN	O2-S-C9	2.64	114.03	106.37
2	E	202	2AN	C7-C8-C9	2.64	123.31	120.37
2	E	203	2AN	C6-C5-C4	-2.64	116.99	123.01
2	T	203	2AN	C7-C8-C9	2.64	123.30	120.37
2	d	202	2AN	C3-C2-C1	2.64	124.22	120.05
2	F	202	2AN	C6-C5-C4	-2.64	117.00	123.01
2	h	206	2AN	C2-C1-N	-2.63	116.80	123.47
2	h	202	2AN	O2-S-O1	-2.63	99.63	112.88
2	E	204	2AN	O2-S-C9	2.63	113.99	106.37
2	C	201	2AN	C10-C1-N	2.63	124.23	120.39
2	c	202	2AN	C16-C11-C12	-2.63	115.56	119.04
2	Y	201	2AN	C7-C8-C9	2.62	123.29	120.37
2	A	201	2AN	C2-C1-C10	-2.62	117.78	120.21
2	Z	201	2AN	O2-S-O1	-2.62	99.70	112.88
2	V	203	2AN	C7-C6-C5	-2.62	116.84	120.48
2	C	202	2AN	C2-C1-C10	-2.62	117.79	120.21
2	V	206	2AN	C15-C16-C11	2.61	122.74	119.73
2	R	204	2AN	C3-C2-C1	2.61	124.18	120.05
2	b	202	2AN	C2-C1-C10	-2.61	117.80	120.21
2	Z	201	2AN	O2-S-C9	2.61	113.92	106.37
2	c	202	2AN	O1-S-C9	2.59	113.89	106.37
2	V	206	2AN	C3-C2-C1	2.59	124.15	120.05
2	g	201	2AN	C10-C1-N	2.59	124.17	120.39
2	G	207	2AN	C2-C1-C10	-2.59	117.81	120.21
4	P	205	EPE	O3S-S-C10	2.59	111.07	106.00
2	b	205	2AN	O1-S-C9	2.59	113.87	106.37
2	O	203	2AN	C8-C9-C10	-2.59	116.25	120.18

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	c	205	2AN	C11-N-C1	-2.58	120.73	126.36
2	C	201	2AN	O1-S-C9	2.58	113.85	106.37
2	O	201	2AN	C8-C9-C10	-2.58	116.25	120.18
2	I	203	2AN	C7-C8-C9	2.58	123.24	120.37
6	e	202	FLC	OHB-CB-CA	2.58	115.26	109.38
2	K	202	2AN	O2-S-C9	2.58	113.84	106.37
6	a	205	FLC	CG-CB-CBC	2.58	115.73	110.03
2	B	201	2AN	O1-S-C9	2.57	113.83	106.37
2	j	206	2AN	C11-N-C1	2.57	131.97	126.36
2	D	204	2AN	C8-C9-C10	-2.57	116.27	120.18
2	R	202	2AN	C10-C1-N	2.57	124.14	120.39
2	I	205	2AN	O1-S-C9	2.57	113.80	106.37
2	g	202	2AN	C3-C2-C1	2.56	124.10	120.05
2	Y	202	2AN	C7-C8-C9	2.56	123.21	120.37
2	V	205	2AN	O1-S-C9	2.55	113.77	106.37
2	L	204	2AN	C7-C8-C9	2.55	123.21	120.37
2	b	205	2AN	C16-C11-C12	-2.55	115.66	119.04
2	a	201	2AN	C15-C16-C11	2.55	122.67	119.73
2	K	201	2AN	C10-C1-N	-2.55	116.67	120.39
2	I	201	2AN	C3-C2-C1	2.55	124.07	120.05
2	Y	202	2AN	C8-C9-C10	-2.55	116.31	120.18
2	f	201	2AN	O2-S-C9	-2.54	99.00	106.37
2	Q	201	2AN	C11-N-C1	-2.54	120.82	126.36
2	c	202	2AN	C6-C5-C4	-2.54	117.22	123.01
2	D	204	2AN	C3-C2-C1	2.54	124.06	120.05
4	P	205	EPE	O3S-S-O1S	-2.54	105.05	111.40
2	N	204	2AN	C8-C9-C10	-2.54	116.32	120.18
2	E	202	2AN	O1-S-C9	2.54	113.72	106.37
2	R	204	2AN	C6-C5-C4	-2.54	117.23	123.01
2	i	201	2AN	C3-C2-C1	2.53	124.05	120.05
2	f	205	2AN	O2-S-C9	-2.53	99.03	106.37
2	a	202	2AN	C4-C5-C10	2.53	123.29	118.27
2	Q	203	2AN	C1-C10-C5	-2.53	115.53	118.91
2	L	203	2AN	C8-C9-C10	-2.53	116.33	120.18
2	B	204	2AN	C11-N-C1	2.52	131.86	126.36
2	V	202	2AN	C6-C5-C4	-2.52	117.27	123.01
2	T	204	2AN	C6-C5-C4	-2.52	117.27	123.01
2	V	201	2AN	C13-C12-C11	2.51	122.63	119.73
4	P	205	EPE	C2-C3-N4	2.51	115.71	110.65
2	P	201	2AN	C2-C1-C10	-2.50	117.89	120.21
2	B	201	2AN	C11-N-C1	-2.50	120.90	126.36
2	Y	204	2AN	C2-C1-C10	-2.50	117.89	120.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	203	2AN	C7-C8-C9	2.50	123.15	120.37
2	F	202	2AN	C8-C9-C10	-2.50	116.38	120.18
2	V	203	2AN	O1-S-C9	2.49	113.60	106.37
2	g	201	2AN	C16-C11-C12	-2.49	115.73	119.04
2	I	207	2AN	C10-C1-N	2.49	124.03	120.39
2	K	201	2AN	C9-C10-C5	2.49	121.33	115.98
2	P	202	2AN	C4-C5-C10	2.49	123.21	118.27
2	g	202	2AN	C10-C1-N	2.49	124.03	120.39
2	G	204	2AN	C13-C12-C11	2.49	122.60	119.73
2	G	202	2AN	C15-C16-C11	2.49	122.60	119.73
2	b	204	2AN	O1-S-C9	2.49	113.57	106.37
2	b	202	2AN	O2-S-C9	2.49	113.57	106.37
2	S	202	2AN	C6-C5-C4	-2.48	117.34	123.01
2	Z	206	2AN	C7-C8-C9	2.48	123.13	120.37
2	f	204	2AN	C15-C16-C11	2.48	122.59	119.73
2	P	202	2AN	C16-C11-N	-2.48	112.22	120.61
2	Y	201	2AN	C3-C2-C1	2.48	123.96	120.05
2	X	204	2AN	C13-C12-C11	2.48	122.58	119.73
2	R	204	2AN	C2-C1-C10	-2.47	117.92	120.21
2	T	205	2AN	C6-C5-C4	-2.47	117.38	123.01
2	M	203	2AN	C2-C1-N	-2.47	117.23	123.47
2	V	203	2AN	C7-C8-C9	2.46	123.11	120.37
2	A	201	2AN	C1-C10-C5	-2.46	115.62	118.91
2	Q	201	2AN	O2-S-C9	2.46	113.49	106.37
2	M	202	2AN	C7-C8-C9	2.46	123.10	120.37
2	A	202	2AN	C3-C2-C1	2.46	123.93	120.05
2	M	202	2AN	C6-C5-C4	-2.46	117.41	123.01
2	I	206	2AN	C1-C10-C5	-2.45	115.63	118.91
6	a	206	FLC	OB2-CBC-CB	2.45	117.84	113.14
2	Z	202	2AN	C15-C16-C11	2.45	122.55	119.73
2	Y	201	2AN	C16-C11-N	2.45	128.90	120.61
2	b	201	2AN	C14-C15-C16	2.44	123.25	120.24
2	a	202	2AN	C1-C10-C5	-2.44	115.64	118.91
6	a	205	FLC	CA-CB-CBC	-2.44	104.64	110.03
2	f	202	2AN	C3-C2-C1	2.44	123.90	120.05
2	B	205	2AN	C11-N-C1	-2.44	121.05	126.36
2	J	201	2AN	C2-C1-C10	-2.44	117.95	120.21
2	W	201	2AN	C13-C12-C11	2.43	122.53	119.73
2	D	204	2AN	C6-C5-C4	-2.43	117.47	123.01
2	L	204	2AN	O2-S-C9	2.43	113.40	106.37
6	a	206	FLC	OHB-CB-CBC	-2.43	105.52	108.96
2	A	201	2AN	C3-C2-C1	2.43	123.88	120.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	N	205	2AN	C7-C8-C9	2.43	123.07	120.37
2	L	203	2AN	C3-C2-C1	2.43	123.88	120.05
2	I	202	2AN	C13-C12-C11	2.42	122.52	119.73
2	E	202	2AN	C8-C9-C10	-2.42	116.50	120.18
2	j	203	2AN	C15-C14-C13	-2.42	116.56	119.87
2	h	206	2AN	O2-S-C9	2.41	113.36	106.37
2	F	206	2AN	C3-C2-C1	2.41	123.86	120.05
2	B	204	2AN	C3-C2-C1	2.41	123.85	120.05
2	j	205	2AN	C6-C7-C8	2.41	124.69	121.00
2	J	202	2AN	C11-N-C1	-2.40	121.12	126.36
2	P	203	2AN	O2-S-O1	-2.40	100.78	112.88
2	h	202	2AN	C7-C8-C9	2.40	123.04	120.37
2	f	205	2AN	C2-C1-C10	-2.40	117.99	120.21
2	V	202	2AN	C7-C8-C9	2.40	123.04	120.37
2	a	201	2AN	C6-C5-C4	-2.40	117.54	123.01
2	W	201	2AN	C7-C8-C9	2.40	123.04	120.37
2	I	207	2AN	C3-C2-C1	2.40	123.84	120.05
2	M	202	2AN	C8-C9-C10	-2.39	116.54	120.18
2	g	203	2AN	O2-S-C9	2.39	113.30	106.37
2	M	201	2AN	C6-C5-C10	2.39	123.00	118.27
2	d	201	2AN	O2-S-O1	-2.39	100.85	112.88
2	N	202	2AN	C2-C1-C10	-2.39	118.00	120.21
2	N	202	2AN	C4-C5-C10	2.39	123.00	118.27
2	F	202	2AN	C2-C1-C10	-2.39	118.00	120.21
2	j	204	2AN	C2-C1-C10	-2.39	118.00	120.21
2	W	201	2AN	O3-S-O2	-2.39	100.48	111.55
2	C	203[A]	2AN	C2-C1-N	-2.38	117.44	123.47
2	I	205	2AN	C10-C1-N	2.38	123.87	120.39
2	Y	201	2AN	O3-S-O1	-2.38	100.50	111.55
2	h	203	2AN	O2-S-C9	2.38	113.27	106.37
2	P	203	2AN	C8-C9-C10	-2.38	116.56	120.18
2	c	204	2AN	C3-C2-C1	2.38	123.81	120.05
2	I	201	2AN	O1-S-C9	2.38	113.25	106.37
2	R	202	2AN	C2-C1-N	-2.37	117.46	123.47
2	c	201	2AN	C2-C1-N	-2.37	117.47	123.47
2	a	202	2AN	C6-C5-C4	-2.36	117.62	123.01
2	h	206	2AN	C2-C1-C10	-2.36	118.02	120.21
2	S	202	2AN	C13-C12-C11	2.36	122.45	119.73
2	Z	201	2AN	C8-C9-C10	-2.36	116.59	120.18
2	H	202	2AN	C13-C12-C11	2.36	122.45	119.73
2	S	201	2AN	C10-C1-N	2.36	123.83	120.39
2	b	203	2AN	C2-C1-C10	-2.36	118.03	120.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	S	202	2AN	C1-C10-C5	-2.36	115.76	118.91
2	I	206	2AN	C10-C1-N	2.35	123.83	120.39
2	f	201	2AN	C6-C5-C10	2.35	122.93	118.27
2	L	204	2AN	C16-C11-C12	-2.35	115.92	119.04
6	G	206	FLC	CB-CG-CGC	-2.35	107.49	113.92
2	X	204	2AN	C3-C2-C1	2.35	123.76	120.05
2	j	205	2AN	C7-C6-C5	-2.35	117.22	120.48
2	D	202	2AN	C2-C1-C10	-2.35	118.04	120.21
2	T	204	2AN	O3-S-O2	-2.35	100.67	111.55
2	F	206	2AN	C11-N-C1	-2.34	121.25	126.36
2	f	205	2AN	C10-C1-N	-2.34	116.97	120.39
2	A	203	2AN	C6-C5-C4	-2.34	117.67	123.01
2	a	201	2AN	C13-C12-C11	2.34	122.42	119.73
2	F	202	2AN	C15-C16-C11	2.34	122.42	119.73
2	B	202	2AN	C15-C16-C11	2.33	122.42	119.73
4	P	205	EPE	C6-N1-C2	-2.33	103.82	108.84
2	G	202	2AN	C2-C1-C10	-2.33	118.05	120.21
2	I	207	2AN	C16-C11-C12	-2.33	115.96	119.04
2	j	205	2AN	C1-C10-C5	2.32	122.01	118.91
2	E	203	2AN	C3-C2-C1	2.32	123.72	120.05
2	P	202	2AN	C11-N-C1	-2.32	121.30	126.36
2	F	201	2AN	C6-C5-C4	-2.32	117.71	123.01
2	J	203	2AN	C2-C1-N	-2.32	117.59	123.47
2	D	201	2AN	C15-C16-C11	2.31	122.40	119.73
2	I	204	2AN	C16-C11-N	2.31	128.44	120.61
2	c	206	2AN	C8-C9-C10	-2.31	116.67	120.18
2	B	204	2AN	C7-C8-C9	2.31	122.94	120.37
2	B	201	2AN	C8-C9-C10	-2.31	116.67	120.18
2	c	201	2AN	O2-S-C9	-2.31	99.69	106.37
2	R	205	2AN	C6-C5-C10	2.31	122.84	118.27
2	B	206	2AN	C2-C1-C10	-2.30	118.08	120.21
2	e	201	2AN	C7-C8-C9	2.30	122.93	120.37
6	i	203	FLC	CA-CB-CBC	-2.30	104.94	110.03
2	h	205	2AN	C11-N-C1	2.30	131.38	126.36
2	H	201	2AN	C7-C8-C9	2.30	122.93	120.37
2	H	204	2AN	C11-N-C1	2.30	131.37	126.36
2	D	204	2AN	C7-C8-C9	2.30	122.92	120.37
2	V	208	2AN	C12-C11-N	2.29	128.38	120.61
2	g	202	2AN	C15-C16-C11	2.29	122.37	119.73
2	G	204	2AN	C11-N-C1	2.29	131.35	126.36
2	U	202	2AN	C2-C1-N	-2.29	117.68	123.47
2	h	201	2AN	C8-C9-C10	-2.29	116.70	120.18

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	R	202	2AN	C7-C8-C9	2.29	122.91	120.37
2	M	203	2AN	C7-C8-C9	2.28	122.91	120.37
2	b	203	2AN	O1-S-C9	2.28	112.98	106.37
2	F	201	2AN	C3-C2-C1	2.28	123.64	120.05
2	R	203	2AN	O1-S-C9	2.27	112.96	106.37
2	I	207	2AN	O1-S-C9	2.27	112.96	106.37
2	Y	203	2AN	C3-C2-C1	2.27	123.64	120.05
2	T	203	2AN	C3-C4-C5	-2.27	117.33	120.48
2	f	202	2AN	C8-C9-C10	-2.27	116.73	120.18
2	j	205	2AN	O3-S-O2	-2.27	101.04	111.55
2	B	205	2AN	C2-C1-N	-2.27	117.74	123.47
2	F	202	2AN	C1-C10-C5	-2.26	115.88	118.91
2	E	203	2AN	O2-S-O1	-2.26	101.50	112.88
2	Z	203	2AN	O2-S-O1	-2.26	101.50	112.88
2	b	202	2AN	O2-S-O1	-2.25	101.53	112.88
2	J	203	2AN	C2-C1-C10	-2.25	118.13	120.21
2	j	203	2AN	C2-C1-C10	-2.25	118.13	120.21
2	g	201	2AN	C6-C5-C4	-2.25	117.88	123.01
2	R	202	2AN	O1-S-C9	2.25	112.88	106.37
2	O	202	2AN	C11-N-C1	2.25	131.26	126.36
2	A	202	2AN	C1-C10-C5	-2.24	115.91	118.91
2	P	202	2AN	C8-C9-C10	-2.24	116.77	120.18
2	F	206	2AN	C12-C11-N	2.23	128.18	120.61
2	R	204	2AN	O2-S-C9	2.23	112.84	106.37
2	h	202	2AN	C8-C9-C10	-2.23	116.78	120.18
2	i	201	2AN	O2-S-O1	-2.23	101.65	112.88
2	J	203	2AN	C8-C9-C10	-2.22	116.80	120.18
2	R	203	2AN	C2-C1-C10	-2.22	118.15	120.21
2	N	204	2AN	C6-C5-C4	-2.22	117.94	123.01
2	F	204	2AN	O1-S-C9	2.22	112.79	106.37
2	a	204	2AN	C2-C1-C10	-2.21	118.16	120.21
2	T	205	2AN	C8-C9-C10	-2.21	116.82	120.18
2	F	203	2AN	C3-C2-C1	2.21	123.54	120.05
2	j	201	2AN	C4-C3-C2	2.21	124.39	121.00
2	R	202	2AN	C2-C1-C10	-2.21	118.17	120.21
2	T	203	2AN	C6-C5-C4	-2.21	117.98	123.01
6	a	205	FLC	OA1-CAC-CA	-2.20	116.71	122.95
2	P	201	2AN	C13-C12-C11	2.20	122.27	119.73
2	M	201	2AN	C6-C5-C4	-2.20	117.98	123.01
2	V	206	2AN	C16-C11-C12	-2.20	116.12	119.04
2	j	203	2AN	C6-C5-C4	-2.20	117.99	123.01
2	Z	205	2AN	O1-S-C9	2.20	112.74	106.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	204	2AN	C1-C10-C5	-2.20	115.97	118.91
2	F	203	2AN	C2-C1-C10	-2.20	118.18	120.21
2	Q	203	2AN	O2-S-C9	2.20	112.74	106.37
2	j	205	2AN	C9-C10-C5	2.19	120.69	115.98
2	D	203	2AN	C2-C1-C10	-2.19	118.18	120.21
2	I	205	2AN	C3-C2-C1	2.19	123.51	120.05
2	I	204	2AN	C16-C11-C12	-2.19	116.14	119.04
2	S	202	2AN	O2-S-C9	2.19	112.71	106.37
2	Z	203	2AN	C7-C8-C9	2.19	122.80	120.37
2	Z	201	2AN	C12-C11-N	2.18	128.01	120.61
6	a	206	FLC	OA2-CAC-CA	2.18	121.27	114.35
2	V	203	2AN	C6-C5-C10	2.18	122.60	118.27
2	D	201	2AN	C8-C9-C10	-2.18	116.86	120.18
2	T	205	2AN	O1-S-C9	2.18	112.69	106.37
2	T	204	2AN	C6-C5-C10	2.18	122.59	118.27
2	G	201	2AN	C6-C5-C4	-2.18	118.03	123.01
2	D	204	2AN	C4-C5-C10	2.18	122.59	118.27
2	M	203	2AN	C1-C10-C5	-2.18	116.00	118.91
2	j	202	2AN	C4-C5-C10	2.17	122.58	118.27
2	V	206	2AN	C6-C5-C4	-2.17	118.06	123.01
2	f	205	2AN	C11-N-C1	-2.17	121.62	126.36
2	c	206	2AN	C11-N-C1	-2.17	121.63	126.36
2	h	204	2AN	C3-C2-C1	2.17	123.48	120.05
2	j	202	2AN	C6-C5-C4	-2.17	118.06	123.01
2	X	201	2AN	C16-C11-C12	-2.17	116.17	119.04
2	F	204	2AN	C3-C2-C1	2.16	123.47	120.05
2	j	204	2AN	C15-C16-C11	2.16	122.22	119.73
2	Y	202	2AN	C6-C5-C4	-2.16	118.08	123.01
2	Z	202	2AN	C16-C11-C12	-2.16	116.18	119.04
2	N	202	2AN	C1-C10-C5	-2.15	116.03	118.91
2	N	201	2AN	O1-S-C9	2.15	112.61	106.37
2	O	202	2AN	O2-S-C9	2.15	112.60	106.37
2	G	205	2AN	C12-C11-N	2.15	127.90	120.61
2	I	206	2AN	C7-C8-C9	2.15	122.76	120.37
2	j	207	2AN	O2-S-C9	2.15	112.59	106.37
2	V	204	2AN	O2-S-C9	2.15	112.59	106.37
2	g	202	2AN	C11-N-C1	-2.15	121.68	126.36
2	F	202	2AN	C12-C11-N	2.14	127.88	120.61
2	Z	205	2AN	C2-C1-N	2.14	128.89	123.47
2	J	203	2AN	C7-C8-C9	2.14	122.75	120.37
2	T	204	2AN	C15-C16-C11	2.14	122.20	119.73
2	Y	203	2AN	C8-C9-C10	-2.14	116.92	120.18

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	T	203	2AN	C4-C3-C2	2.14	124.29	121.00
2	B	201	2AN	C16-C11-N	-2.14	113.36	120.61
2	c	205	2AN	C7-C8-C9	2.14	122.75	120.37
2	Q	201	2AN	C16-C11-N	2.14	127.86	120.61
2	f	201	2AN	C11-N-C1	-2.14	121.69	126.36
2	Z	202	2AN	C13-C12-C11	2.14	122.19	119.73
6	e	202	FLC	OA1-CAC-CA	-2.14	116.89	122.95
2	X	205	2AN	C7-C8-C9	2.14	122.75	120.37
2	T	204	2AN	C7-C8-C9	2.14	122.75	120.37
6	j	208	FLC	OG1-CGC-CG	-2.13	116.91	122.95
2	h	203	2AN	C16-C11-C12	2.13	121.87	119.04
2	Y	203	2AN	C6-C5-C4	-2.13	118.15	123.01
2	B	203	2AN	C11-N-C1	-2.13	121.72	126.36
2	c	202	2AN	C8-C9-C10	-2.13	116.95	120.18
2	F	201	2AN	C1-C10-C5	-2.12	116.07	118.91
2	A	202	2AN	C7-C8-C9	2.12	122.73	120.37
2	I	202	2AN	C2-C1-N	-2.12	118.10	123.47
2	A	201	2AN	C4-C5-C10	2.12	122.47	118.27
2	N	202	2AN	C6-C5-C4	-2.12	118.18	123.01
2	D	204	2AN	C13-C12-C11	2.12	122.17	119.73
2	V	202	2AN	C16-C11-N	2.12	127.78	120.61
2	A	203	2AN	C1-C10-C5	-2.12	116.08	118.91
2	h	201	2AN	C3-C2-C1	2.12	123.39	120.05
2	S	203	2AN	C11-N-C1	-2.11	121.75	126.36
2	V	201	2AN	C7-C8-C9	2.11	122.72	120.37
2	I	202	2AN	C6-C5-C4	-2.11	118.19	123.01
2	g	201	2AN	C6-C5-C10	2.11	122.45	118.27
2	L	202	2AN	O2-S-C9	2.11	112.49	106.37
2	R	201	2AN	C2-C1-C10	-2.11	118.26	120.21
2	N	204	2AN	C3-C4-C5	-2.11	117.55	120.48
2	P	202	2AN	C6-C5-C4	-2.11	118.20	123.01
2	I	207	2AN	C2-C1-N	-2.11	118.13	123.47
2	I	205	2AN	C15-C14-C13	-2.11	116.98	119.87
2	i	201	2AN	C6-C5-C4	-2.11	118.20	123.01
2	F	204	2AN	C6-C5-C4	-2.11	118.20	123.01
2	G	204	2AN	O2-S-C9	2.11	112.47	106.37
2	X	204	2AN	C16-C11-C12	-2.11	116.25	119.04
2	T	205	2AN	C4-C5-C10	2.10	122.44	118.27
2	T	204	2AN	O2-S-C9	2.10	112.46	106.37
2	h	201	2AN	C1-C10-C5	-2.10	116.10	118.91
2	I	206	2AN	C12-C11-N	-2.10	113.49	120.61
2	I	203	2AN	C8-C9-C10	-2.10	116.98	120.18

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L	204	2AN	C3-C2-C1	2.10	123.37	120.05
2	Y	203	2AN	O2-S-C9	2.10	112.45	106.37
2	B	201	2AN	C12-C11-N	2.10	127.72	120.61
2	Y	204	2AN	C11-N-C1	-2.10	121.78	126.36
2	Z	205	2AN	C11-N-C1	2.10	130.94	126.36
2	P	201	2AN	O2-S-C9	2.09	112.44	106.37
2	E	202	2AN	O3-S-O2	-2.09	101.84	111.55
2	E	201	2AN	C1-C10-C5	-2.09	116.11	118.91
2	B	205	2AN	C12-C11-N	2.09	127.68	120.61
2	L	203	2AN	C10-C1-N	2.09	123.44	120.39
2	g	201	2AN	C7-C8-C9	2.09	122.69	120.37
2	G	203	2AN	C8-C9-C10	2.09	123.36	120.18
2	D	201	2AN	C6-C5-C4	-2.09	118.25	123.01
2	V	205	2AN	O3-S-O1	-2.09	101.87	111.55
2	G	204	2AN	C16-C11-N	2.09	127.67	120.61
2	E	204	2AN	O1-S-C9	2.08	112.41	106.37
2	f	201	2AN	C6-C5-C4	-2.08	118.26	123.01
2	N	203	2AN	O2-S-C9	2.08	112.40	106.37
2	B	201	2AN	C3-C2-C1	2.08	123.33	120.05
4	P	205	EPE	O3S-S-O2S	-2.08	106.20	111.40
2	j	202	2AN	O1-S-C9	2.08	112.38	106.37
6	i	202	FLC	CG-CB-CA	-2.07	103.99	109.31
2	I	201	2AN	C4-C5-C10	2.07	122.38	118.27
2	Y	202	2AN	O2-S-C9	2.07	112.37	106.37
2	a	202	2AN	O3-S-O2	-2.07	101.95	111.55
6	G	206	FLC	OG2-CGC-CG	2.07	120.90	114.35
2	D	203	2AN	C4-C5-C10	2.07	122.37	118.27
2	G	201	2AN	C3-C2-C1	2.07	123.32	120.05
2	A	204	2AN	C2-C1-C10	-2.07	118.30	120.21
2	I	207	2AN	C15-C16-C11	2.07	122.11	119.73
2	d	201	2AN	C13-C12-C11	2.07	122.11	119.73
2	Z	202	2AN	C3-C2-C1	2.07	123.31	120.05
2	E	203	2AN	C4-C5-C10	2.07	122.36	118.27
2	E	202	2AN	O2-S-C9	-2.07	100.38	106.37
2	T	204	2AN	C12-C11-N	2.07	127.61	120.61
2	b	205	2AN	C3-C2-C1	2.06	123.31	120.05
2	H	202	2AN	O1-S-C9	2.06	112.34	106.37
2	M	203	2AN	C8-C9-C10	-2.06	117.05	120.18
2	N	203	2AN	C14-C15-C16	2.06	122.78	120.24
2	L	203	2AN	C16-C11-N	2.06	127.58	120.61
2	Z	203	2AN	O1-S-C9	2.06	112.33	106.37
2	V	204	2AN	C13-C12-C11	2.05	122.10	119.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	h	203	2AN	C7-C6-C5	-2.05	117.63	120.48
2	I	207	2AN	C13-C12-C11	2.05	122.09	119.73
2	d	204	2AN	C3-C2-C1	2.05	123.29	120.05
2	j	203	2AN	C16-C11-C12	-2.05	116.32	119.04
6	j	208	FLC	CB-CG-CGC	-2.05	108.32	113.92
2	K	201	2AN	C4-C5-C10	2.05	122.33	118.27
2	F	203	2AN	C15-C16-C11	2.05	122.09	119.73
2	X	205	2AN	C15-C16-C11	2.05	122.09	119.73
2	A	201	2AN	C10-C1-N	-2.04	117.41	120.39
2	K	202	2AN	O3-S-O1	-2.04	102.08	111.55
2	F	201	2AN	C4-C5-C10	2.04	122.31	118.27
2	J	202	2AN	C14-C15-C16	2.04	122.75	120.24
2	D	203	2AN	C1-C10-C5	-2.04	116.18	118.91
2	O	202	2AN	C10-C1-N	-2.04	117.42	120.39
2	g	203	2AN	C10-C1-N	2.04	123.36	120.39
2	C	203[A]	2AN	C3-C2-C1	2.03	123.26	120.05
2	T	205	2AN	C14-C15-C16	-2.03	117.73	120.24
6	a	205	FLC	CG-CB-CA	2.03	114.53	109.31
2	V	202	2AN	C12-C11-N	-2.03	113.73	120.61
2	K	202	2AN	O1-S-C9	2.03	112.26	106.37
2	R	204	2AN	C13-C12-C11	2.03	122.07	119.73
2	M	202	2AN	C2-C1-N	-2.03	118.33	123.47
2	X	202	2AN	C16-C11-C12	2.03	121.73	119.04
2	F	202	2AN	C16-C11-N	-2.03	113.74	120.61
2	Y	201	2AN	C4-C5-C10	2.03	122.28	118.27
2	L	201	2AN	O3-S-O2	-2.03	102.15	111.55
2	L	202	2AN	C3-C2-C1	2.03	123.25	120.05
6	a	205	FLC	CB-CA-CAC	-2.03	108.38	113.92
2	B	203	2AN	C14-C13-C12	2.03	122.74	120.24
2	Z	204	2AN	C10-C1-N	-2.03	117.44	120.39
2	Q	203	2AN	C7-C8-C9	2.02	122.62	120.37
2	O	201	2AN	C9-C10-C5	2.02	120.32	115.98
2	G	201	2AN	C7-C8-C9	2.02	122.62	120.37
2	h	201	2AN	C13-C12-C11	2.02	122.06	119.73
2	f	203	2AN	C2-C1-C10	-2.02	118.34	120.21
2	h	203	2AN	C6-C5-C4	-2.02	118.40	123.01
2	X	204	2AN	C15-C16-C11	2.02	122.06	119.73
2	Z	201	2AN	C16-C11-N	-2.02	113.77	120.61
2	G	201	2AN	C1-C10-C5	-2.02	116.21	118.91
2	K	202	2AN	C2-C1-C10	-2.02	118.34	120.21
2	Z	201	2AN	C2-C1-N	-2.02	118.36	123.47
2	H	202	2AN	C7-C8-C9	2.02	122.61	120.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	j	205	2AN	C15-C16-C11	2.02	122.06	119.73
2	X	201	2AN	C12-C11-N	2.01	127.42	120.61
2	X	206	2AN	C2-C1-C10	-2.01	118.35	120.21
2	g	201	2AN	O1-S-C9	2.01	112.19	106.37
2	Z	203	2AN	C6-C5-C4	-2.01	118.42	123.01
2	c	202	2AN	C15-C16-C11	2.01	122.04	119.73
2	I	202	2AN	O2-S-C9	2.00	112.17	106.37
2	T	204	2AN	C16-C11-C12	-2.00	116.39	119.04
2	h	201	2AN	O2-S-O1	-2.00	102.80	112.88
2	c	202	2AN	C4-C5-C10	2.00	122.24	118.27
2	Z	201	2AN	C3-C2-C1	2.00	123.21	120.05
2	V	201	2AN	C6-C5-C10	2.00	122.23	118.27

There are no chirality outliers.

All (404) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	205	2AN	C8-C9-S-O1
2	B	205	2AN	C10-C9-S-O1
2	B	205	2AN	C8-C9-S-O2
2	B	205	2AN	C8-C9-S-O3
2	B	205	2AN	C10-C9-S-O3
2	A	203	2AN	C10-C9-S-O1
2	A	203	2AN	C10-C9-S-O2
2	R	203	2AN	C8-C9-S-O1
2	R	203	2AN	C10-C9-S-O1
2	R	203	2AN	C10-C9-S-O2
2	R	203	2AN	C8-C9-S-O3
2	R	203	2AN	C10-C9-S-O3
2	R	204	2AN	C8-C9-S-O1
2	R	204	2AN	C10-C9-S-O2
2	R	204	2AN	C8-C9-S-O3
2	R	204	2AN	C10-C9-S-O3
2	P	203	2AN	C8-C9-S-O1
2	N	203	2AN	C8-C9-S-O1
2	N	203	2AN	C10-C9-S-O1
2	N	203	2AN	C10-C9-S-O2
2	M	203	2AN	C10-C1-N-C11
2	M	203	2AN	C8-C9-S-O1
2	M	203	2AN	C10-C9-S-O1
2	M	203	2AN	C8-C9-S-O3
2	M	203	2AN	C10-C9-S-O3

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Mol	Chain	Res	Type	Atoms
2	I	205	2AN	C8-C9-S-O1
2	I	205	2AN	C8-C9-S-O2
2	I	205	2AN	C10-C9-S-O2
2	I	205	2AN	C8-C9-S-O3
2	I	205	2AN	C10-C9-S-O3
2	I	207	2AN	C8-C9-S-O1
2	I	207	2AN	C8-C9-S-O3
2	G	205	2AN	C8-C9-S-O1
2	G	205	2AN	C10-C9-S-O1
2	G	205	2AN	C10-C9-S-O2
2	G	205	2AN	C8-C9-S-O3
2	G	205	2AN	C10-C9-S-O3
2	F	201	2AN	C8-C9-S-O3
2	F	201	2AN	C10-C9-S-O3
2	F	202	2AN	C8-C9-S-O1
2	F	202	2AN	C10-C9-S-O2
2	F	202	2AN	C8-C9-S-O3
2	F	202	2AN	C10-C9-S-O3
2	E	204	2AN	C8-C9-S-O2
2	E	204	2AN	C10-C9-S-O2
2	E	204	2AN	C8-C9-S-O3
2	E	204	2AN	C10-C9-S-O3
2	D	203	2AN	C10-C9-S-O1
2	D	203	2AN	C8-C9-S-O2
2	D	203	2AN	C10-C9-S-O2
2	D	203	2AN	C8-C9-S-O3
2	D	203	2AN	C10-C9-S-O3
2	D	204	2AN	C8-C9-S-O1
2	D	204	2AN	C10-C9-S-O2
2	D	204	2AN	C8-C9-S-O3
2	D	204	2AN	C10-C9-S-O3
2	e	201	2AN	C8-C9-S-O3
2	e	201	2AN	C10-C9-S-O3
2	d	202	2AN	C8-C9-S-O3
2	d	202	2AN	C10-C9-S-O3
2	b	203	2AN	C8-C9-S-O1
2	b	203	2AN	C10-C9-S-O1
2	b	203	2AN	C10-C9-S-O2
2	b	203	2AN	C8-C9-S-O3
2	b	203	2AN	C10-C9-S-O3
2	b	206	2AN	C10-C9-S-O1
2	b	206	2AN	C10-C9-S-O2

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Mol	Chain	Res	Type	Atoms
2	Z	206	2AN	C10-C9-S-O3
2	Y	202	2AN	C10-C9-S-O3
2	Y	204	2AN	C8-C9-S-O3
2	W	201	2AN	C10-C9-S-O3
2	V	208	2AN	C2-C1-N-C11
2	V	208	2AN	C10-C1-N-C11
2	V	208	2AN	C8-C9-S-O3
2	V	208	2AN	C10-C9-S-O3
2	U	201	2AN	C8-C9-S-O1
2	U	201	2AN	C10-C9-S-O2
2	U	201	2AN	C8-C9-S-O3
2	U	201	2AN	C10-C9-S-O3
2	U	202	2AN	C8-C9-S-O3
2	T	204	2AN	C10-C9-S-O1
2	T	204	2AN	C8-C9-S-O3
2	T	204	2AN	C10-C9-S-O3
2	T	205	2AN	C10-C9-S-O3
2	S	201	2AN	C10-C9-S-O2
2	S	201	2AN	C8-C9-S-O3
2	S	201	2AN	C10-C9-S-O3
2	S	202	2AN	C8-C9-S-O3
2	S	202	2AN	C10-C9-S-O3
2	S	204	2AN	C10-C9-S-O1
2	S	204	2AN	C8-C9-S-O2
2	S	204	2AN	C10-C9-S-O2
2	S	204	2AN	C8-C9-S-O3
2	S	204	2AN	C10-C9-S-O3
2	j	201	2AN	C8-C9-S-O1
2	j	201	2AN	C10-C9-S-O1
2	j	201	2AN	C8-C9-S-O2
2	j	201	2AN	C8-C9-S-O3
2	j	201	2AN	C10-C9-S-O3
2	j	204	2AN	C8-C9-S-O3
2	i	201	2AN	C8-C9-S-O3
2	h	203	2AN	C10-C9-S-O3
6	G	206	FLC	CAC-CA-CB-CBC
6	G	206	FLC	CAC-CA-CB-CG
6	G	206	FLC	CAC-CA-CB-OHB
6	G	206	FLC	CG-CB-CBC-OB1
6	G	206	FLC	CG-CB-CBC-OB2
6	G	206	FLC	OHB-CB-CBC-OB1
6	G	206	FLC	OHB-CB-CBC-OB2

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Mol	Chain	Res	Type	Atoms
6	G	206	FLC	CA-CB-CG-CGC
6	G	206	FLC	CBC-CB-CG-CGC
6	G	206	FLC	OHB-CB-CG-CGC
6	e	202	FLC	CA-CB-CG-CGC
6	e	202	FLC	CBC-CB-CG-CGC
6	a	205	FLC	CG-CB-CBC-OB1
6	a	205	FLC	CG-CB-CBC-OB2
6	a	205	FLC	OHB-CB-CBC-OB1
6	a	205	FLC	OHB-CB-CBC-OB2
6	a	206	FLC	CA-CB-CBC-OB1
6	a	206	FLC	CA-CB-CBC-OB2
6	a	206	FLC	OHB-CB-CBC-OB1
6	a	206	FLC	OHB-CB-CBC-OB2
6	j	208	FLC	CG-CB-CBC-OB1
6	j	208	FLC	CG-CB-CBC-OB2
6	j	208	FLC	OHB-CB-CBC-OB1
6	j	208	FLC	OHB-CB-CBC-OB2
6	i	202	FLC	CA-CB-CBC-OB2
6	i	202	FLC	OHB-CB-CBC-OB2
6	i	203	FLC	CAC-CA-CB-OHB
6	i	203	FLC	CBC-CB-CG-CGC
6	i	203	FLC	OHB-CB-CG-CGC
6	i	203	FLC	CA-CB-CG-CGC
6	e	202	FLC	OHB-CB-CG-CGC
6	i	203	FLC	CAC-CA-CB-CG
2	I	206	2AN	C10-C1-N-C11
2	g	203	2AN	C10-C1-N-C11
2	B	205	2AN	C10-C9-S-O2
2	R	204	2AN	C10-C9-S-O1
2	P	203	2AN	C10-C9-S-O1
2	P	203	2AN	C10-C9-S-O2
2	O	201	2AN	C10-C9-S-O2
2	O	203	2AN	C10-C9-S-O2
2	M	203	2AN	C10-C9-S-O2
2	L	204	2AN	C10-C9-S-O2
2	K	201	2AN	C10-C9-S-O2
2	I	205	2AN	C10-C9-S-O1
2	I	207	2AN	C10-C9-S-O1
2	H	203	2AN	C10-C9-S-O2
2	F	201	2AN	C10-C9-S-O1
2	F	201	2AN	C10-C9-S-O2
2	F	202	2AN	C10-C9-S-O1

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Mol	Chain	Res	Type	Atoms
2	F	205	2AN	C10-C9-S-O1
2	F	205	2AN	C10-C9-S-O2
2	E	203	2AN	C10-C9-S-O1
2	E	204	2AN	C10-C9-S-O1
2	D	204	2AN	C10-C9-S-O1
2	C	203[A]	2AN	C10-C9-S-O1
2	C	203[A]	2AN	C10-C9-S-O2
2	e	201	2AN	C10-C9-S-O1
2	d	202	2AN	C10-C9-S-O1
2	d	202	2AN	C10-C9-S-O2
2	c	203	2AN	C10-C9-S-O1
2	c	203	2AN	C10-C9-S-O2
2	Z	206	2AN	C10-C9-S-O2
2	Y	202	2AN	C10-C9-S-O1
2	Y	202	2AN	C10-C9-S-O2
2	Y	204	2AN	C10-C9-S-O1
2	W	201	2AN	C10-C9-S-O1
2	W	201	2AN	C10-C9-S-O2
2	U	201	2AN	C10-C9-S-O1
2	U	202	2AN	C10-C9-S-O1
2	U	202	2AN	C10-C9-S-O2
2	T	204	2AN	C10-C9-S-O2
2	T	205	2AN	C10-C9-S-O1
2	S	201	2AN	C10-C9-S-O1
2	S	202	2AN	C10-C9-S-O1
2	j	201	2AN	C10-C9-S-O2
2	j	204	2AN	C10-C9-S-O1
6	e	202	FLC	CAC-CA-CB-OHB
6	a	205	FLC	CAC-CA-CB-OHB
6	j	208	FLC	CBC-CB-CG-CGC
2	Q	203	2AN	C2-C1-N-C11
2	J	203	2AN	C2-C1-N-C11
2	I	206	2AN	C2-C1-N-C11
2	F	202	2AN	C2-C1-N-C11
2	F	206	2AN	C2-C1-N-C11
2	E	204	2AN	C2-C1-N-C11
2	C	203[A]	2AN	C2-C1-N-C11
2	Z	206	2AN	C2-C1-N-C11
2	Y	204	2AN	C2-C1-N-C11
2	S	201	2AN	C2-C1-N-C11
2	A	203	2AN	C8-C9-S-O1
2	A	203	2AN	C8-C9-S-O2

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Mol	Chain	Res	Type	Atoms
2	R	203	2AN	C8-C9-S-O2
2	R	204	2AN	C8-C9-S-O2
2	Q	203	2AN	C8-C9-S-O2
2	O	201	2AN	C8-C9-S-O2
2	M	203	2AN	C8-C9-S-O2
2	L	204	2AN	C8-C9-S-O2
2	H	203	2AN	C8-C9-S-O2
2	F	201	2AN	C8-C9-S-O2
2	F	202	2AN	C8-C9-S-O2
2	E	203	2AN	C8-C9-S-O1
2	E	204	2AN	C8-C9-S-O1
2	e	201	2AN	C8-C9-S-O1
2	d	202	2AN	C8-C9-S-O1
2	Y	202	2AN	C8-C9-S-O2
2	W	201	2AN	C8-C9-S-O1
2	W	201	2AN	C8-C9-S-O2
2	V	201	2AN	C8-C9-S-O2
2	V	203	2AN	C8-C9-S-O1
2	U	201	2AN	C8-C9-S-O2
2	U	202	2AN	C8-C9-S-O1
2	T	204	2AN	C8-C9-S-O2
2	S	201	2AN	C8-C9-S-O1
2	S	202	2AN	C8-C9-S-O1
2	j	204	2AN	C8-C9-S-O1
6	a	205	FLC	CAC-CA-CB-CG
6	e	202	FLC	CG-CB-CBC-OB2
6	i	202	FLC	CA-CB-CBC-OB1
6	e	202	FLC	CAC-CA-CB-CBC
6	e	202	FLC	CAC-CA-CB-CG
6	a	206	FLC	CAC-CA-CB-OHB
2	a	201	2AN	C2-C1-N-C11
2	B	201	2AN	C10-C1-N-C11
2	A	202	2AN	C10-C1-N-C11
2	A	204	2AN	C10-C1-N-C11
2	Q	203	2AN	C10-C1-N-C11
2	P	202	2AN	C10-C1-N-C11
2	N	203	2AN	C10-C1-N-C11
2	M	202	2AN	C10-C1-N-C11
2	L	203	2AN	C10-C1-N-C11
2	J	203	2AN	C10-C1-N-C11
2	I	201	2AN	C10-C1-N-C11
2	H	202	2AN	C10-C1-N-C11

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Mol	Chain	Res	Type	Atoms
2	G	202	2AN	C10-C1-N-C11
2	C	203[A]	2AN	C10-C1-N-C11
2	c	201	2AN	C10-C1-N-C11
2	a	201	2AN	C10-C1-N-C11
2	V	205	2AN	C10-C1-N-C11
2	S	204	2AN	C10-C1-N-C11
2	Q	203	2AN	C10-C9-S-O2
2	O	201	2AN	C10-C9-S-O1
2	O	203	2AN	C10-C9-S-O1
2	L	204	2AN	C10-C9-S-O1
2	K	201	2AN	C10-C9-S-O1
2	I	207	2AN	C10-C9-S-O2
2	H	203	2AN	C10-C9-S-O1
2	H	204	2AN	C10-C9-S-O1
2	H	204	2AN	C10-C9-S-O2
2	F	204	2AN	C10-C9-S-O1
2	F	204	2AN	C10-C9-S-O2
2	c	204	2AN	C10-C9-S-O1
2	Z	206	2AN	C10-C9-S-O1
2	Y	204	2AN	C10-C9-S-O2
2	X	204	2AN	C10-C9-S-O2
2	V	201	2AN	C10-C9-S-O2
2	S	202	2AN	C10-C9-S-O2
2	j	204	2AN	C10-C9-S-O2
2	i	201	2AN	C10-C9-S-O2
2	h	203	2AN	C10-C9-S-O1
2	g	202	2AN	C10-C9-S-O2
6	a	205	FLC	CB-CG-CGC-OG2
6	G	206	FLC	CA-CB-CBC-OB1
6	e	202	FLC	CA-CB-CBC-OB1
6	e	202	FLC	CG-CB-CBC-OB1
6	i	202	FLC	CG-CB-CBC-OB2
2	N	203	2AN	C2-C1-N-C11
2	M	203	2AN	C2-C1-N-C11
2	L	203	2AN	C2-C1-N-C11
2	G	202	2AN	C2-C1-N-C11
2	D	204	2AN	C2-C1-N-C11
2	b	206	2AN	C2-C1-N-C11
2	X	203	2AN	C2-C1-N-C11
2	X	206	2AN	C2-C1-N-C11
6	a	205	FLC	CB-CG-CGC-OG1
2	A	203	2AN	C8-C9-S-O3

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Mol	Chain	Res	Type	Atoms
2	P	203	2AN	C8-C9-S-O3
2	N	203	2AN	C8-C9-S-O3
2	L	204	2AN	C8-C9-S-O3
2	H	203	2AN	C8-C9-S-O3
2	C	203[A]	2AN	C8-C9-S-O3
2	Z	206	2AN	C8-C9-S-O3
2	Y	202	2AN	C8-C9-S-O3
2	X	204	2AN	C8-C9-S-O3
2	W	201	2AN	C8-C9-S-O3
2	T	205	2AN	C8-C9-S-O3
2	h	203	2AN	C8-C9-S-O3
2	g	202	2AN	C8-C9-S-O3
6	a	205	FLC	CAC-CA-CB-CBC
2	A	203	2AN	C10-C9-S-O3
2	P	203	2AN	C10-C9-S-O3
2	O	201	2AN	C10-C9-S-O3
2	N	203	2AN	C10-C9-S-O3
2	I	207	2AN	C10-C9-S-O3
2	H	203	2AN	C10-C9-S-O3
2	Y	204	2AN	C10-C9-S-O3
2	X	204	2AN	C10-C9-S-O3
2	U	202	2AN	C10-C9-S-O3
2	j	204	2AN	C10-C9-S-O3
2	i	201	2AN	C10-C9-S-O3
2	g	202	2AN	C10-C9-S-O3
2	O	203	2AN	C8-C9-S-O2
2	N	203	2AN	C8-C9-S-O2
2	G	205	2AN	C8-C9-S-O2
2	D	204	2AN	C8-C9-S-O2
2	C	203[A]	2AN	C8-C9-S-O1
2	b	206	2AN	C8-C9-S-O1
2	Y	204	2AN	C8-C9-S-O1
2	T	204	2AN	C8-C9-S-O1
2	S	201	2AN	C8-C9-S-O2
2	Q	201	2AN	C10-C1-N-C11
2	E	204	2AN	C10-C1-N-C11
2	f	206	2AN	C10-C1-N-C11
2	Z	206	2AN	C10-C1-N-C11
2	Y	204	2AN	C10-C1-N-C11
2	X	203	2AN	C10-C1-N-C11
2	S	201	2AN	C10-C1-N-C11
2	A	204	2AN	C2-C1-N-C11

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Mol	Chain	Res	Type	Atoms
2	R	202	2AN	C2-C1-N-C11
2	d	203	2AN	C2-C1-N-C11
2	g	203	2AN	C2-C1-N-C11
6	i	202	FLC	OHB-CB-CBC-OB1
6	G	206	FLC	CA-CB-CBC-OB2
6	e	202	FLC	CA-CB-CBC-OB2
6	j	208	FLC	CA-CB-CBC-OB2
6	i	202	FLC	CG-CB-CBC-OB1
2	A	204	2AN	C10-C9-S-O1
2	Q	203	2AN	C10-C9-S-O1
2	M	202	2AN	C10-C9-S-O2
2	c	204	2AN	C10-C9-S-O2
2	T	205	2AN	C10-C9-S-O2
2	B	201	2AN	C2-C1-N-C11
2	P	202	2AN	C2-C1-N-C11
2	M	202	2AN	C2-C1-N-C11
2	f	203	2AN	C2-C1-N-C11
2	S	204	2AN	C2-C1-N-C11
2	B	205	2AN	C10-C1-N-C11
2	R	202	2AN	C10-C1-N-C11
2	P	204	2AN	C10-C1-N-C11
2	O	203	2AN	C10-C1-N-C11
2	N	202	2AN	C10-C1-N-C11
2	F	202	2AN	C10-C1-N-C11
2	E	202	2AN	C10-C1-N-C11
2	D	202	2AN	C10-C1-N-C11
2	D	204	2AN	C10-C1-N-C11
2	C	201	2AN	C10-C1-N-C11
2	f	203	2AN	C10-C1-N-C11
2	d	203	2AN	C10-C1-N-C11
2	b	206	2AN	C10-C1-N-C11
2	Z	201	2AN	C10-C1-N-C11
2	X	206	2AN	C10-C1-N-C11
2	V	202	2AN	C10-C1-N-C11
2	j	202	2AN	C10-C1-N-C11
6	i	203	FLC	CA-CB-CBC-OB1
6	i	203	FLC	CA-CB-CBC-OB2
4	P	205	EPE	C9-C10-S-O2S
2	P	203	2AN	C8-C9-S-O2
2	O	203	2AN	C8-C9-S-O1
2	L	204	2AN	C8-C9-S-O1
2	K	201	2AN	C8-C9-S-O2

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Mol	Chain	Res	Type	Atoms
2	H	203	2AN	C8-C9-S-O1
2	F	201	2AN	C8-C9-S-O1
2	F	205	2AN	C8-C9-S-O2
2	D	203	2AN	C8-C9-S-O1
2	C	203[A]	2AN	C8-C9-S-O2
2	d	202	2AN	C8-C9-S-O2
2	c	203	2AN	C8-C9-S-O2
2	b	203	2AN	C8-C9-S-O2
2	b	206	2AN	C8-C9-S-O2
2	Y	202	2AN	C8-C9-S-O1
2	S	202	2AN	C8-C9-S-O2
2	S	204	2AN	C8-C9-S-O1
4	P	205	EPE	C8-C7-N4-C3
6	i	202	FLC	CB-CG-CGC-OG2
6	i	203	FLC	CB-CG-CGC-OG1
2	A	204	2AN	C10-C9-S-O2
2	E	203	2AN	C10-C9-S-O2
6	i	202	FLC	CB-CG-CGC-OG1
6	i	203	FLC	CB-CG-CGC-OG2
6	j	208	FLC	CA-CB-CBC-OB1
2	B	206	2AN	C10-C1-N-C11
2	K	201	2AN	C10-C1-N-C11
2	G	201	2AN	C10-C1-N-C11
2	F	206	2AN	C10-C1-N-C11
2	f	202	2AN	C10-C1-N-C11
2	T	202	2AN	C10-C1-N-C11
2	T	205	2AN	C10-C1-N-C11
2	j	205	2AN	C10-C1-N-C11
2	g	202	2AN	C10-C1-N-C11
6	a	206	FLC	CB-CA-CAC-OA1
2	A	202	2AN	C2-C1-N-C11
2	I	201	2AN	C2-C1-N-C11
2	H	202	2AN	C2-C1-N-C11
2	c	201	2AN	C2-C1-N-C11
2	Z	201	2AN	C2-C1-N-C11
2	V	205	2AN	C2-C1-N-C11
6	G	206	FLC	CB-CA-CAC-OA1
2	O	201	2AN	C8-C9-S-O3
2	O	203	2AN	C8-C9-S-O3
2	b	206	2AN	C8-C9-S-O3
6	G	206	FLC	CB-CA-CAC-OA2
6	e	202	FLC	CB-CG-CGC-OG2

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Mol	Chain	Res	Type	Atoms
6	a	206	FLC	CB-CA-CAC-OA2

There are no ring outliers.

167 monomers are involved in 1144 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	e	201	2AN	4	0
2	T	202	2AN	5	0
2	a	202	2AN	3	0
3	A	205	SO4	6	0
2	J	203	2AN	5	0
2	T	205	2AN	5	0
2	Z	204	2AN	3	0
2	a	204	2AN	19	0
4	P	205	EPE	6	0
2	E	203	2AN	5	0
2	Q	201	2AN	3	0
2	V	208	2AN	21	0
2	d	201	2AN	19	0
2	a	203	2AN	8	0
2	d	202	2AN	7	0
2	j	201	2AN	8	0
2	d	204	2AN	13	0
5	N	206	DMS	2	0
2	f	204	2AN	8	0
2	W	201	2AN	6	0
2	h	206	2AN	6	0
2	N	205	2AN	8	0
2	F	203	2AN	9	0
2	I	202	2AN	6	0
2	I	207	2AN	5	0
2	E	202	2AN	3	0
2	f	205	2AN	10	0
2	M	202	2AN	2	0
2	c	205	2AN	1	0
2	c	206	2AN	7	0
2	Y	203	2AN	6	0
2	D	203	2AN	12	0
2	j	203	2AN	7	0
2	A	202	2AN	7	0
2	h	204	2AN	17	0
6	G	206	FLC	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	F	202	2AN	20	0
2	Z	206	2AN	14	0
2	I	201	2AN	3	0
2	X	206	2AN	56	0
2	D	201	2AN	8	0
2	V	201	2AN	15	0
2	P	201	2AN	6	0
2	K	201	2AN	4	0
2	J	201	2AN	6	0
2	F	206	2AN	14	0
2	X	205	2AN	4	0
2	f	203	2AN	5	0
2	c	202	2AN	7	0
2	R	201	2AN	8	0
2	c	203	2AN	5	0
2	Y	204	2AN	10	0
2	f	202	2AN	8	0
2	F	204	2AN	8	0
2	Z	201	2AN	2	0
2	A	203	2AN	4	0
2	C	202	2AN	11	0
2	h	202	2AN	7	0
2	O	203	2AN	5	0
2	T	204	2AN	3	0
2	b	201	2AN	11	0
2	I	204	2AN	8	0
2	S	202	2AN	4	0
2	P	204	2AN	4	0
2	O	201	2AN	12	0
2	g	201	2AN	4	0
2	P	203	2AN	9	0
3	g	204	SO4	1	0
2	E	204	2AN	3	0
2	M	201	2AN	6	0
6	j	208	FLC	9	0
2	h	205	2AN	3	0
2	G	202	2AN	4	0
2	B	201	2AN	7	0
2	R	203	2AN	10	0
2	X	202	2AN	9	0
2	Y	202	2AN	5	0
2	L	202	2AN	6	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	202	2AN	5	0
2	V	202	2AN	3	0
2	j	205	2AN	9	0
2	b	206	2AN	5	0
2	K	203	2AN	6	0
2	Q	202	2AN	6	0
2	B	204	2AN	8	0
2	S	203	2AN	2	0
2	R	204	2AN	10	0
2	H	203	2AN	5	0
2	K	202	2AN	12	0
2	J	202	2AN	8	0
2	f	206	2AN	9	0
2	E	201	2AN	5	0
2	a	201	2AN	3	0
2	M	203	2AN	2	0
2	G	207	2AN	6	0
2	R	202	2AN	4	0
2	j	207	2AN	4	0
3	c	207	SO4	1	0
2	g	203	2AN	4	0
2	V	205	2AN	12	0
2	b	205	2AN	8	0
2	N	201	2AN	10	0
2	B	202	2AN	8	0
2	H	201	2AN	5	0
2	g	202	2AN	10	0
2	U	201	2AN	7	0
2	S	204	2AN	17	0
5	G	208	DMS	1	0
2	c	204	2AN	4	0
2	f	201	2AN	4	0
2	Q	203	2AN	3	0
2	T	201	2AN	13	0
2	h	201	2AN	3	0
6	i	203	FLC	3	0
2	B	206	2AN	6	0
2	Y	201	2AN	9	0
2	j	202	2AN	4	0
2	b	202	2AN	11	0
2	Z	205	2AN	5	0
2	X	203	2AN	7	0

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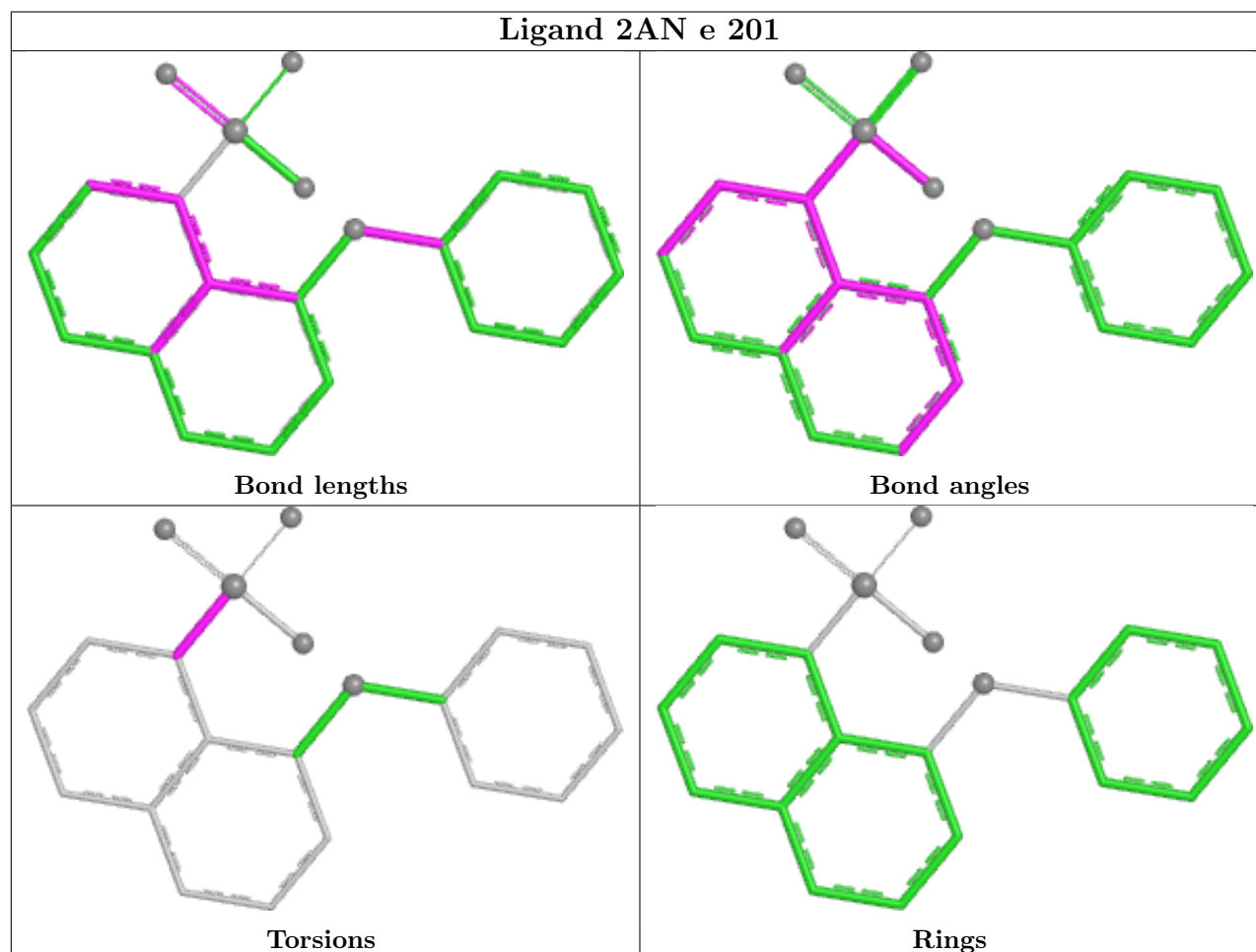
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	V	204	2AN	11	0
6	e	202	FLC	1	0
2	I	203	2AN	7	0
2	V	207	2AN	5	0
2	A	201	2AN	4	0
2	D	204	2AN	6	0
2	V	203	2AN	11	0
2	h	203	2AN	3	0
2	O	202	2AN	5	0
2	G	203	2AN	9	0
2	Z	202	2AN	4	0
2	c	201	2AN	7	0
2	N	202	2AN	4	0
2	H	202	2AN	4	0
2	G	201	2AN	3	0
2	j	206	2AN	5	0
2	P	202	2AN	4	0
2	C	201	2AN	4	0
2	B	205	2AN	6	0
2	X	201	2AN	3	0
2	N	204	2AN	5	0
2	I	205	2AN	13	0
2	L	204	2AN	10	0
2	b	204	2AN	9	0
6	a	205	FLC	1	0
2	d	203	2AN	6	0
2	F	201	2AN	11	0
2	Z	203	2AN	10	0
2	G	204	2AN	6	0
2	j	204	2AN	7	0
2	N	203	2AN	3	0
2	X	204	2AN	4	0
2	R	205	2AN	9	0
2	S	201	2AN	4	0
2	U	202	2AN	5	0
2	C	203[A]	2AN	3	0
2	H	204	2AN	10	0
2	L	203	2AN	4	0
2	b	203	2AN	9	0
2	F	205	2AN	4	0
2	T	203	2AN	12	0
3	Y	205	SO4	2	0

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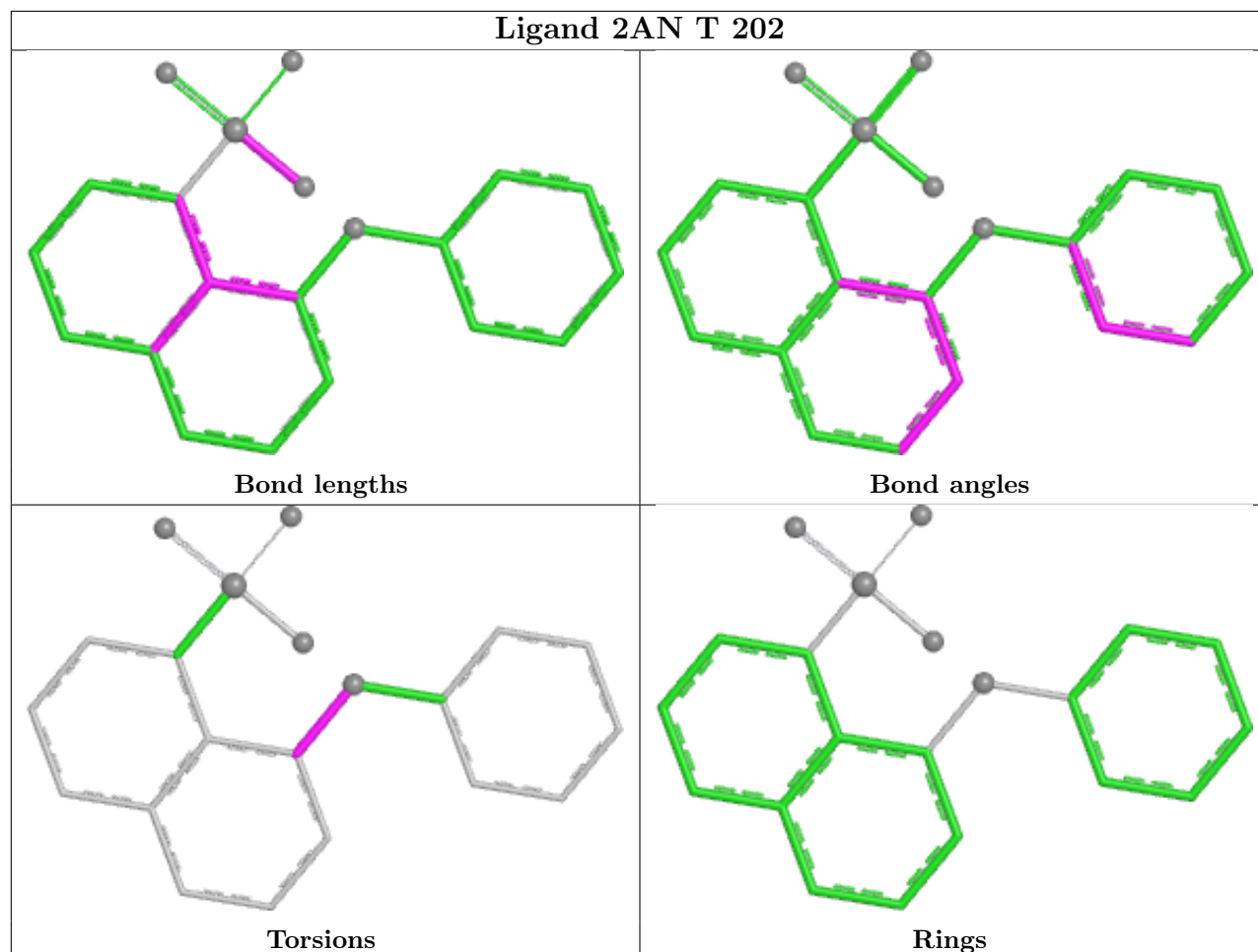
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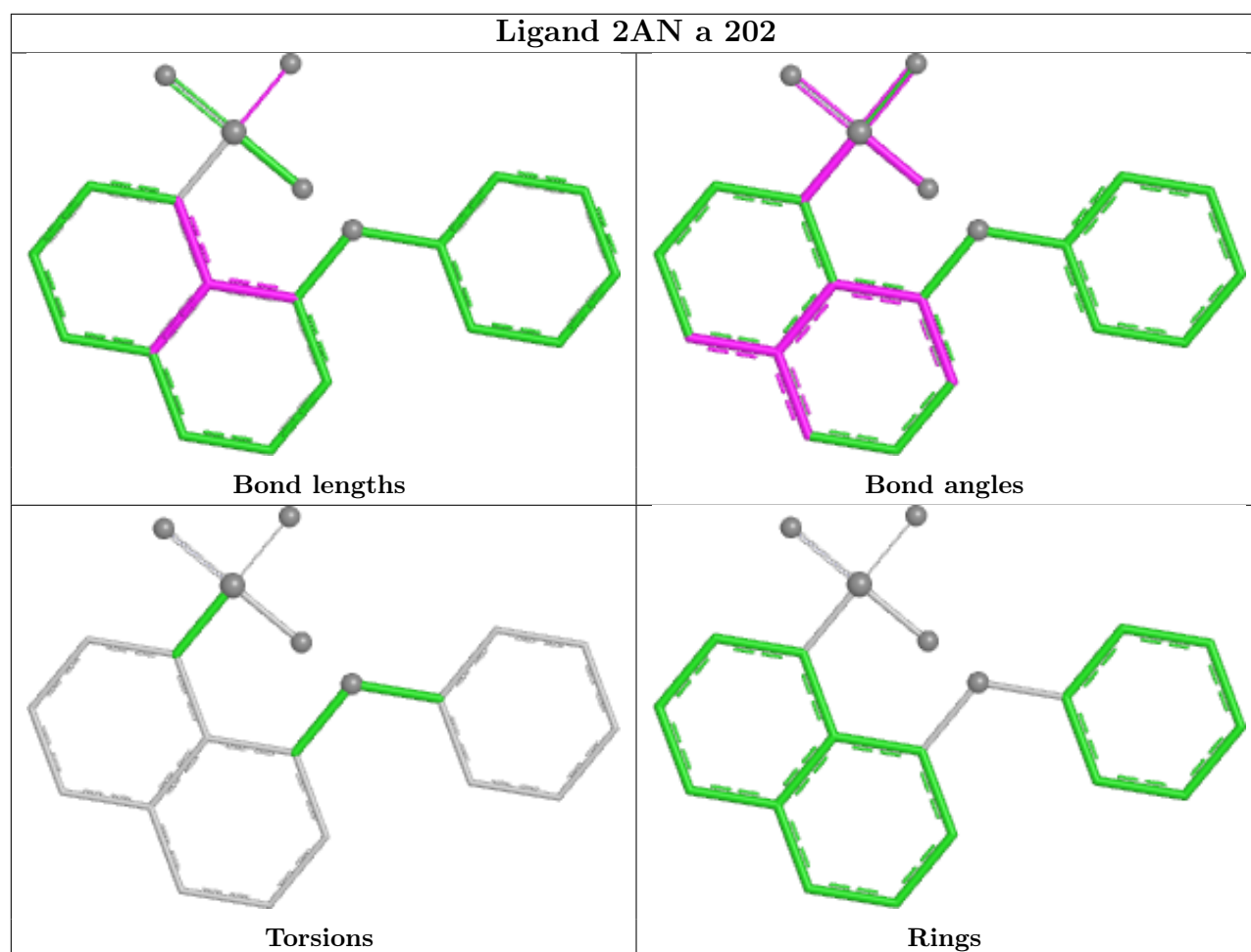
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	203	2AN	9	0
2	L	201	2AN	7	0
2	I	206	2AN	4	0
2	V	206	2AN	4	0
2	i	201	2AN	3	0

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

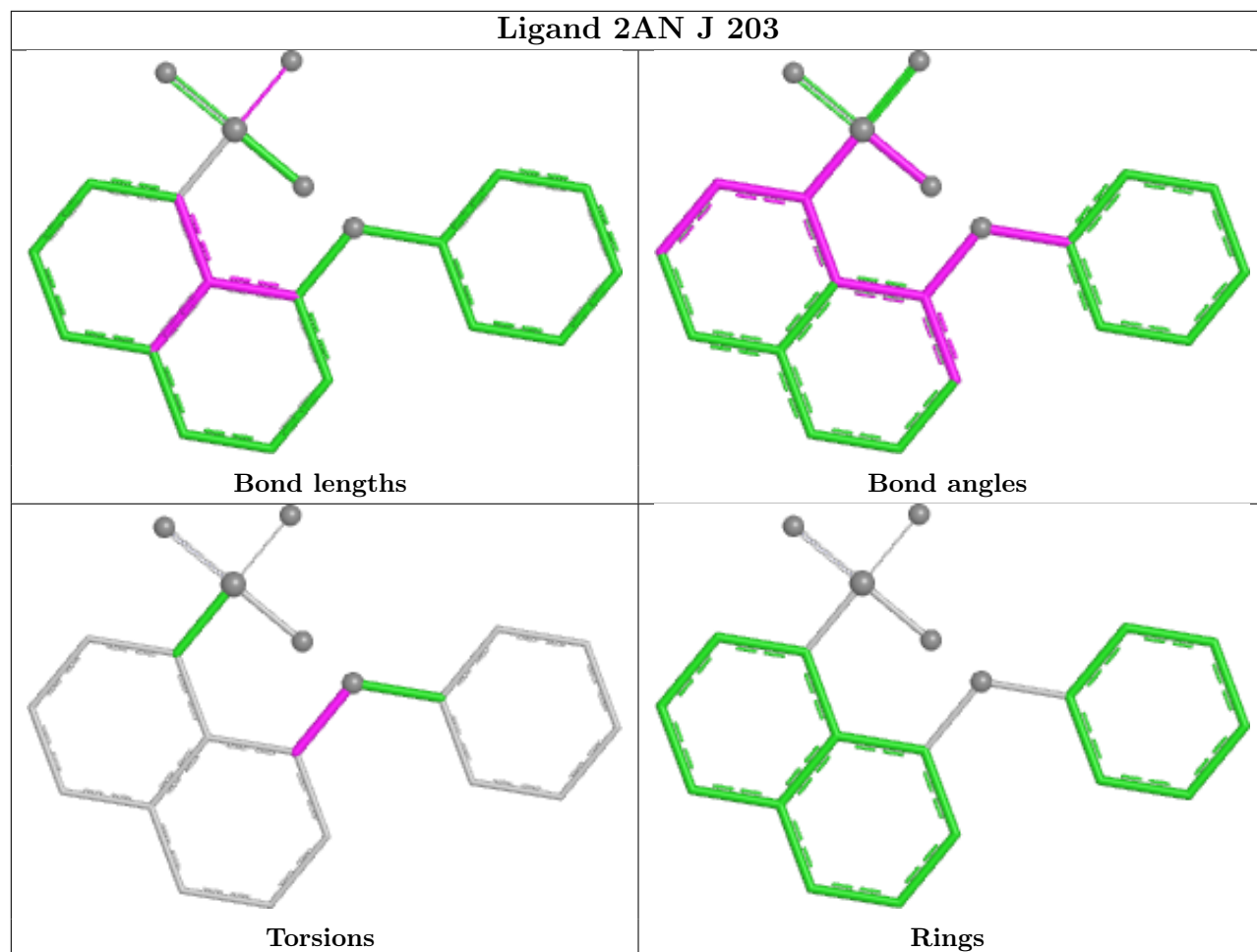


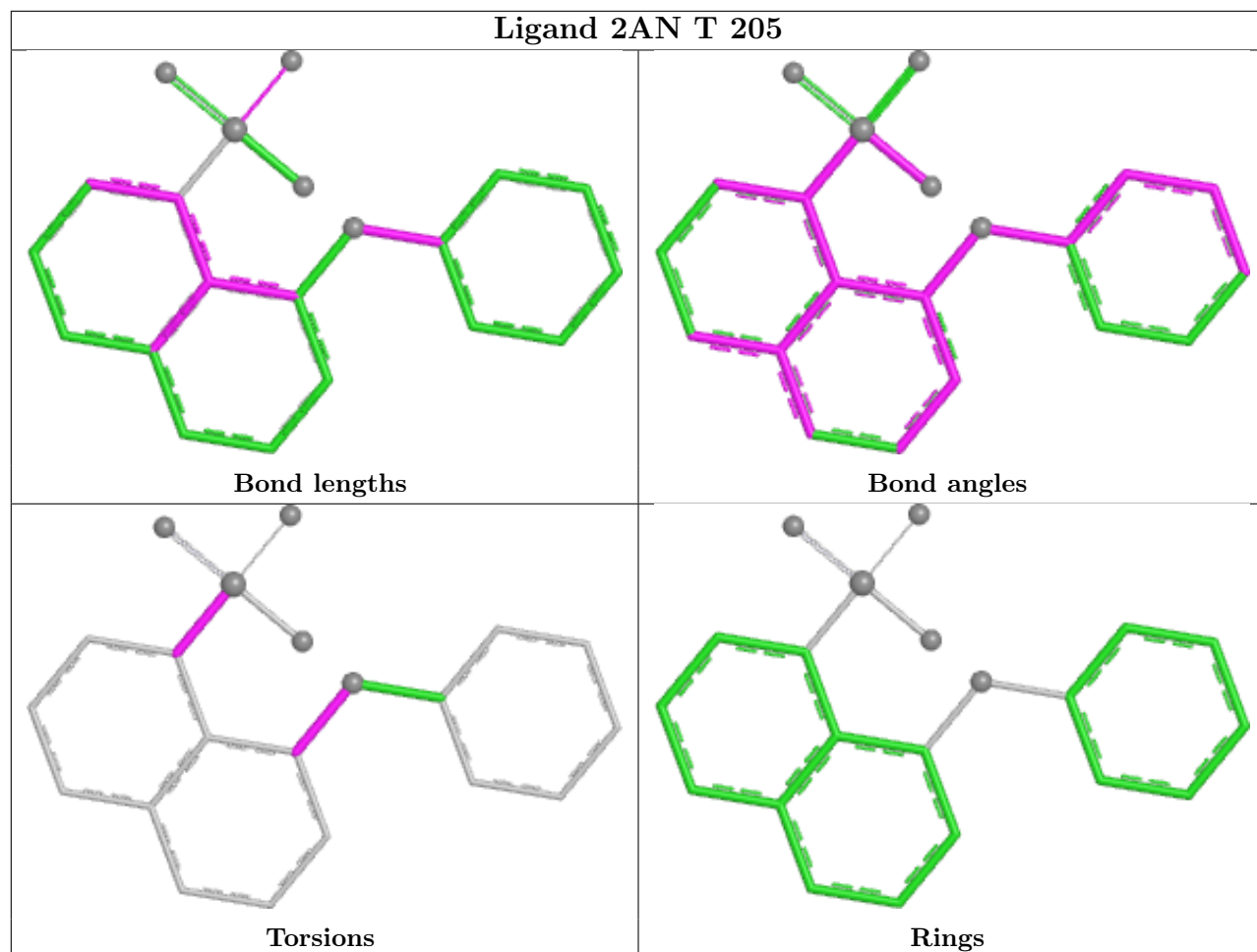
Ligand 2AN T 202

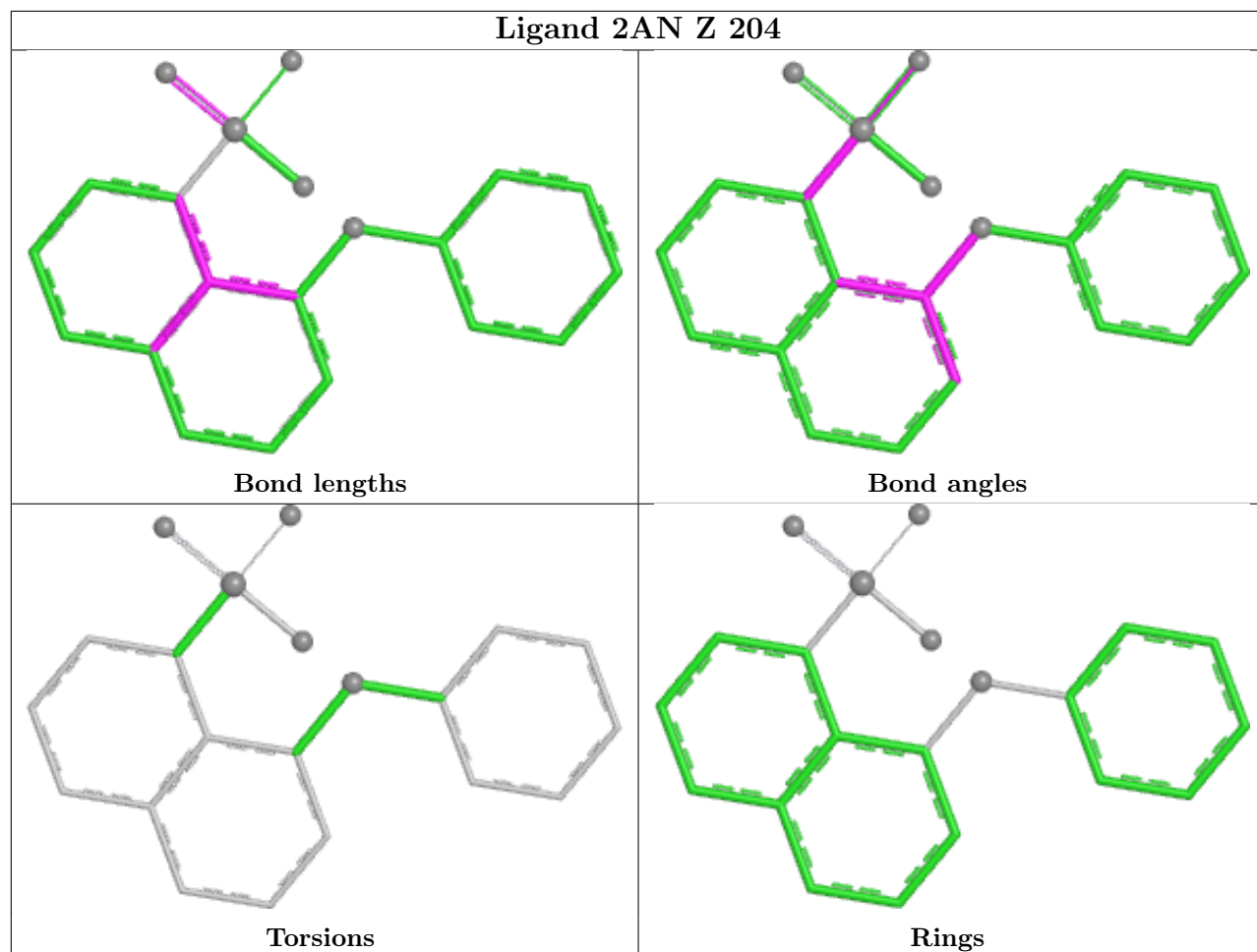




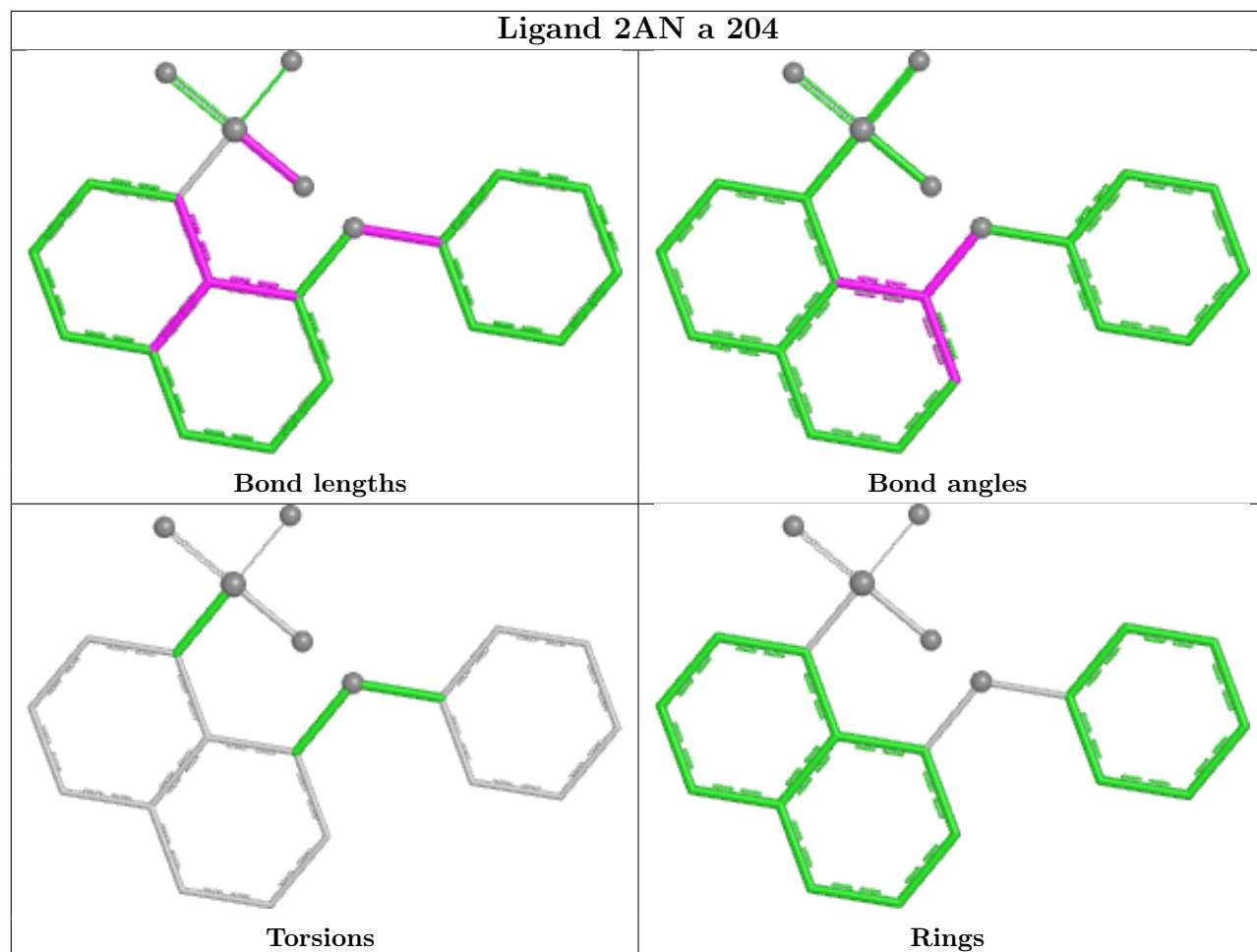
Ligand 2AN J 203



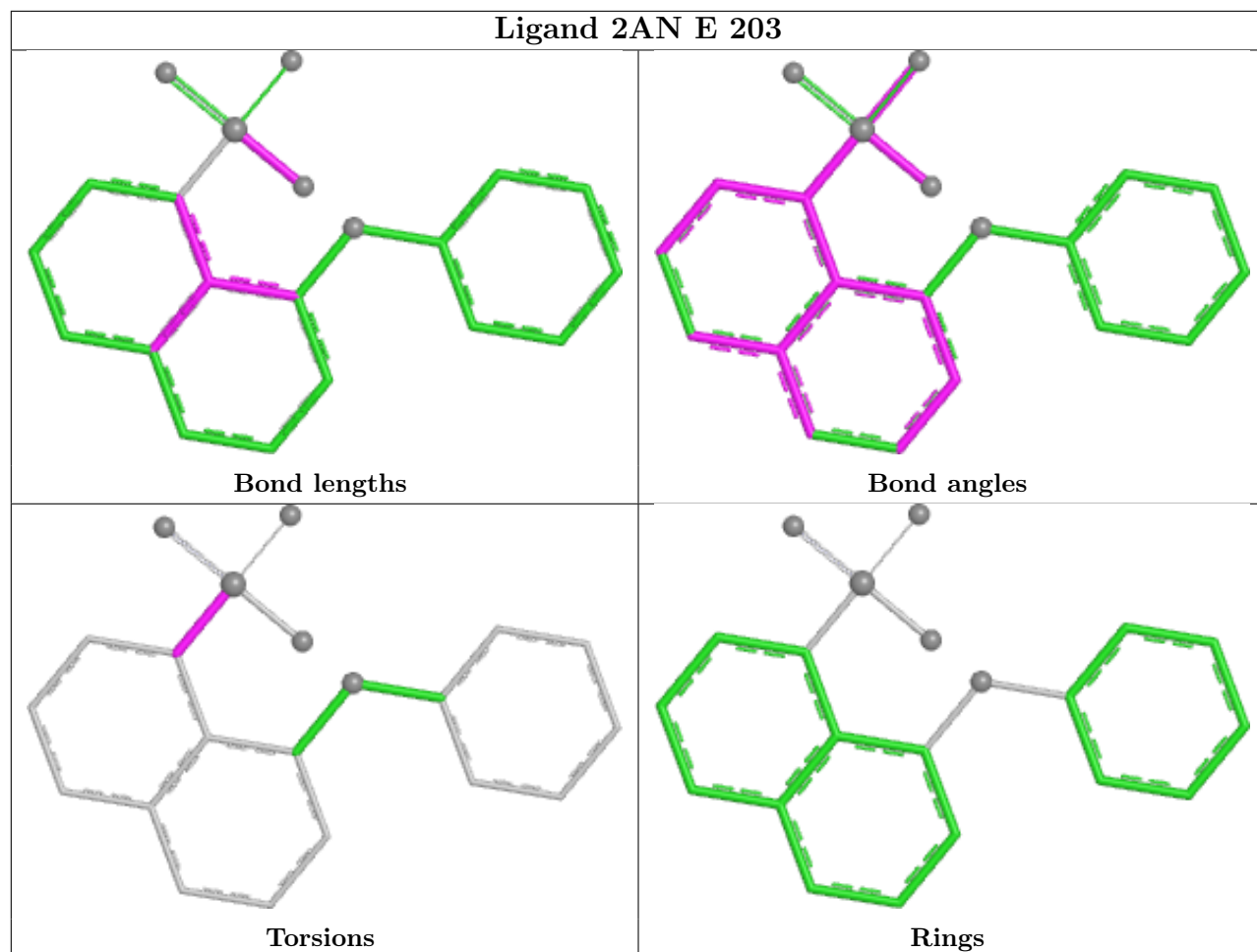




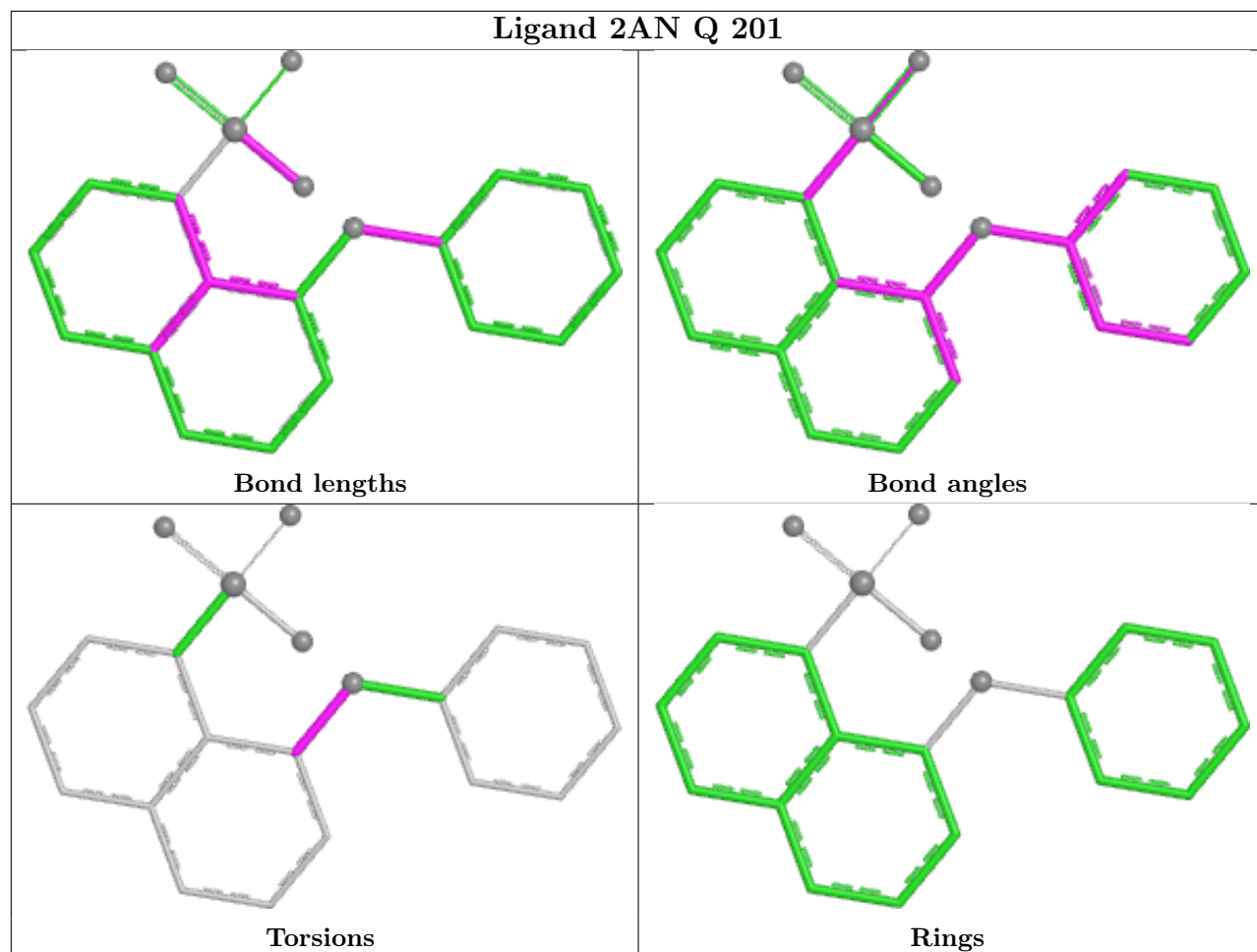
Ligand 2AN a 204



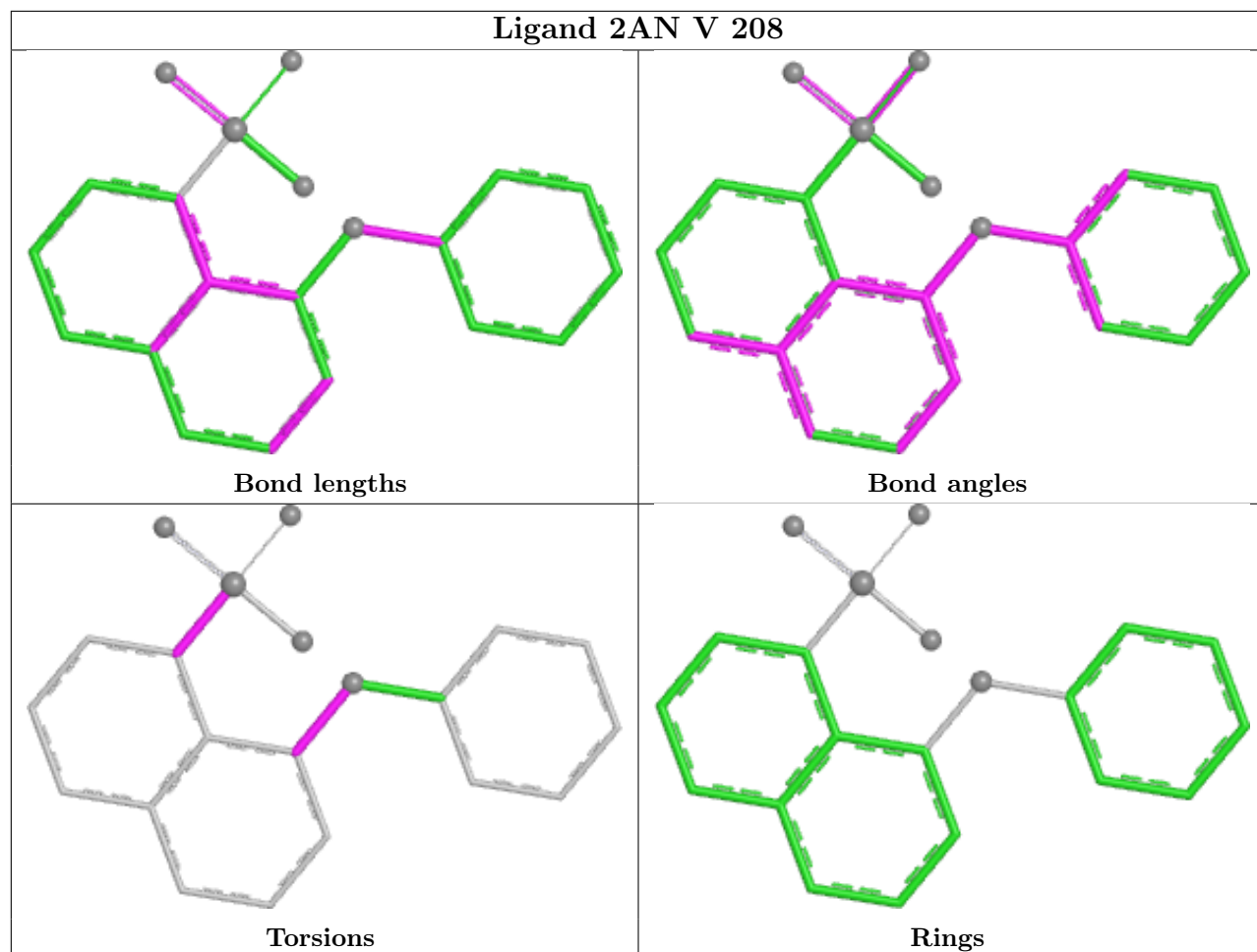
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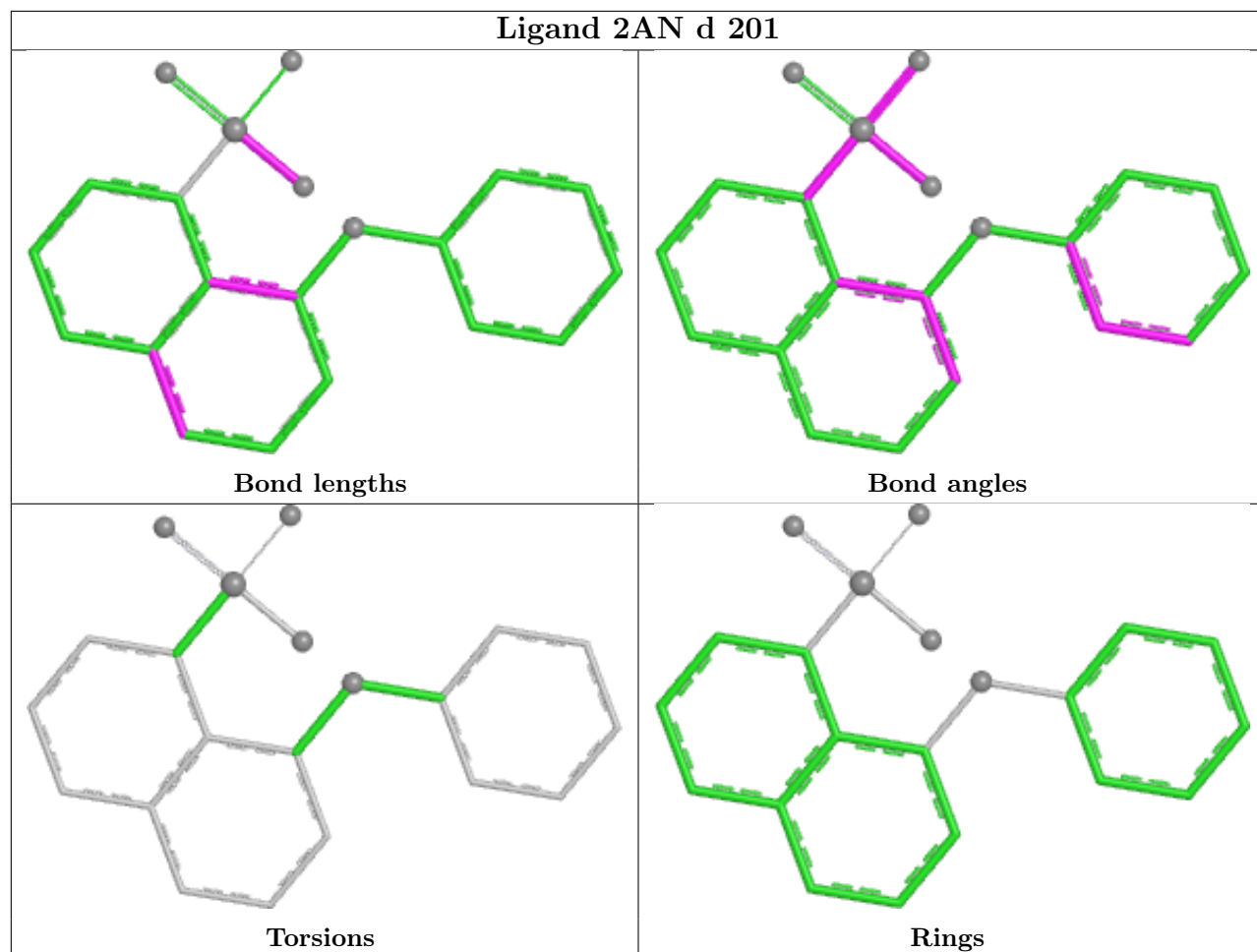


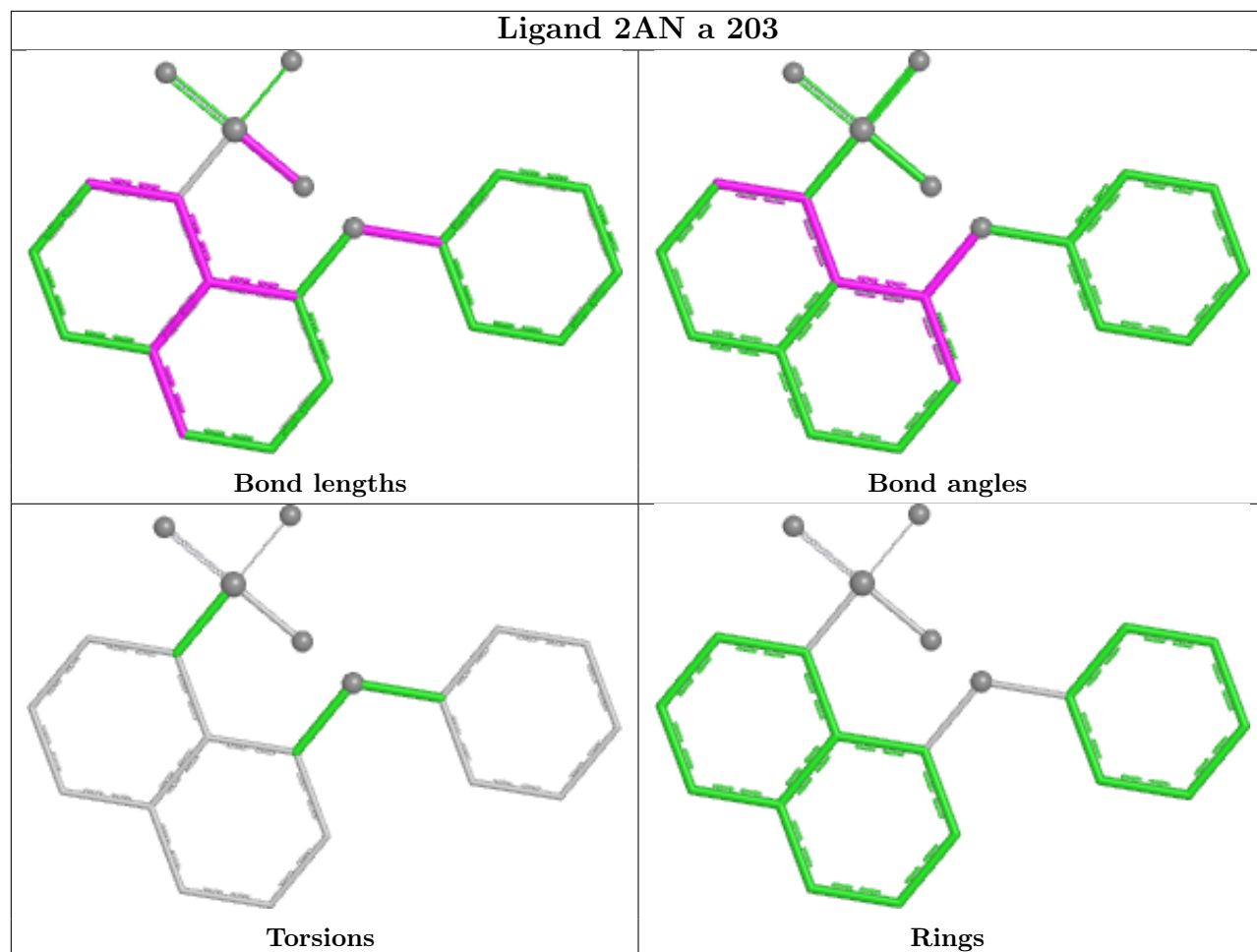
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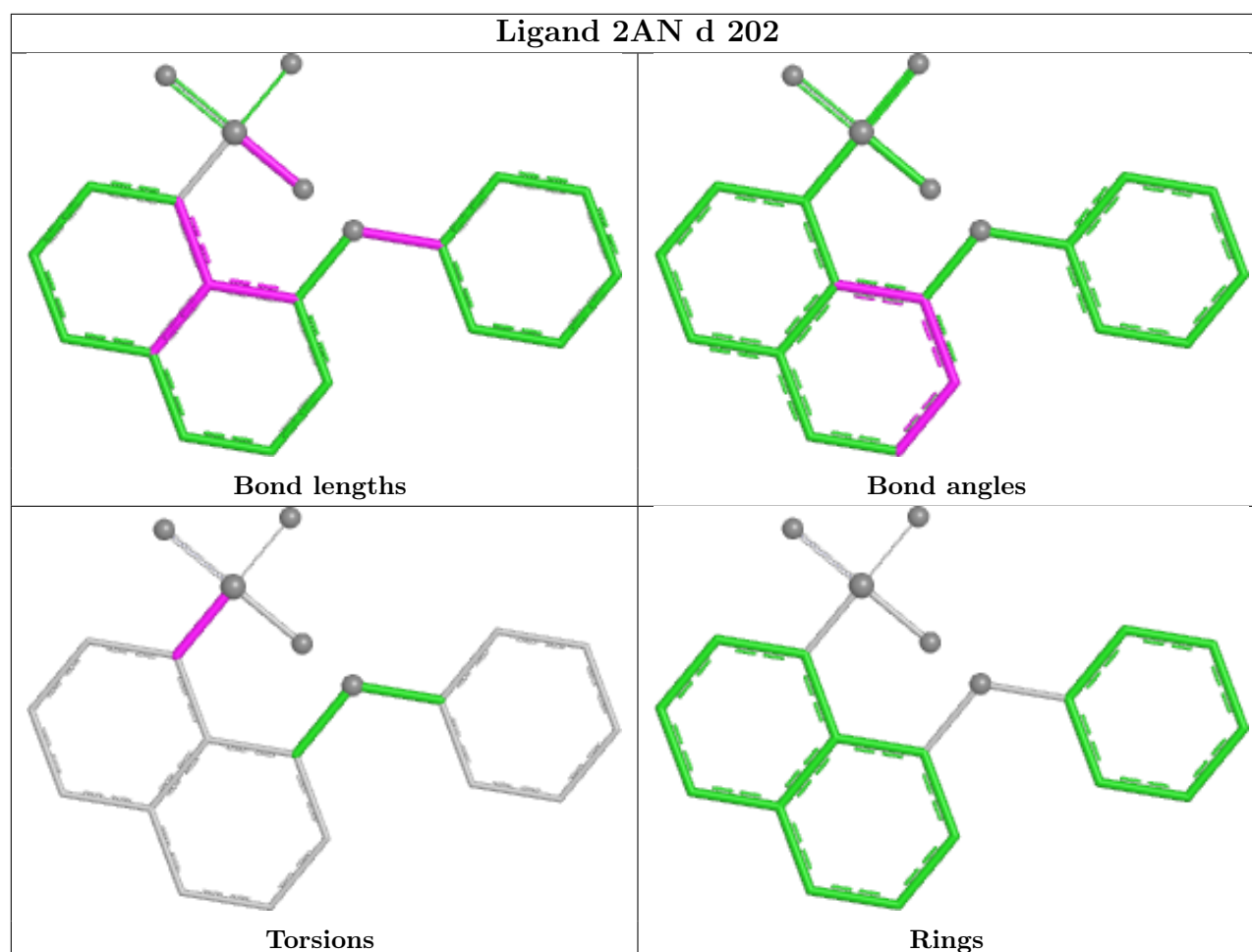


Ligand 2AN V 208

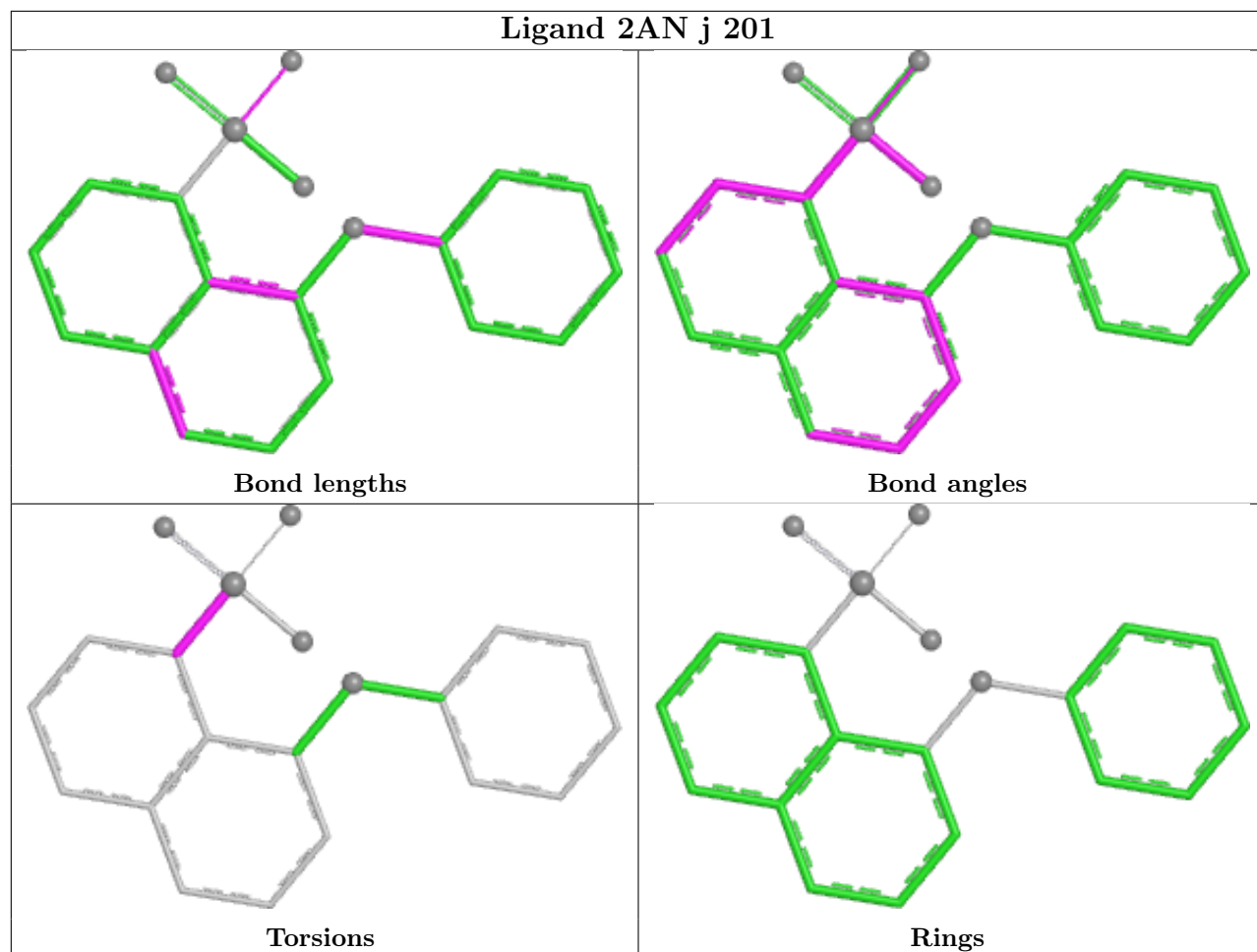




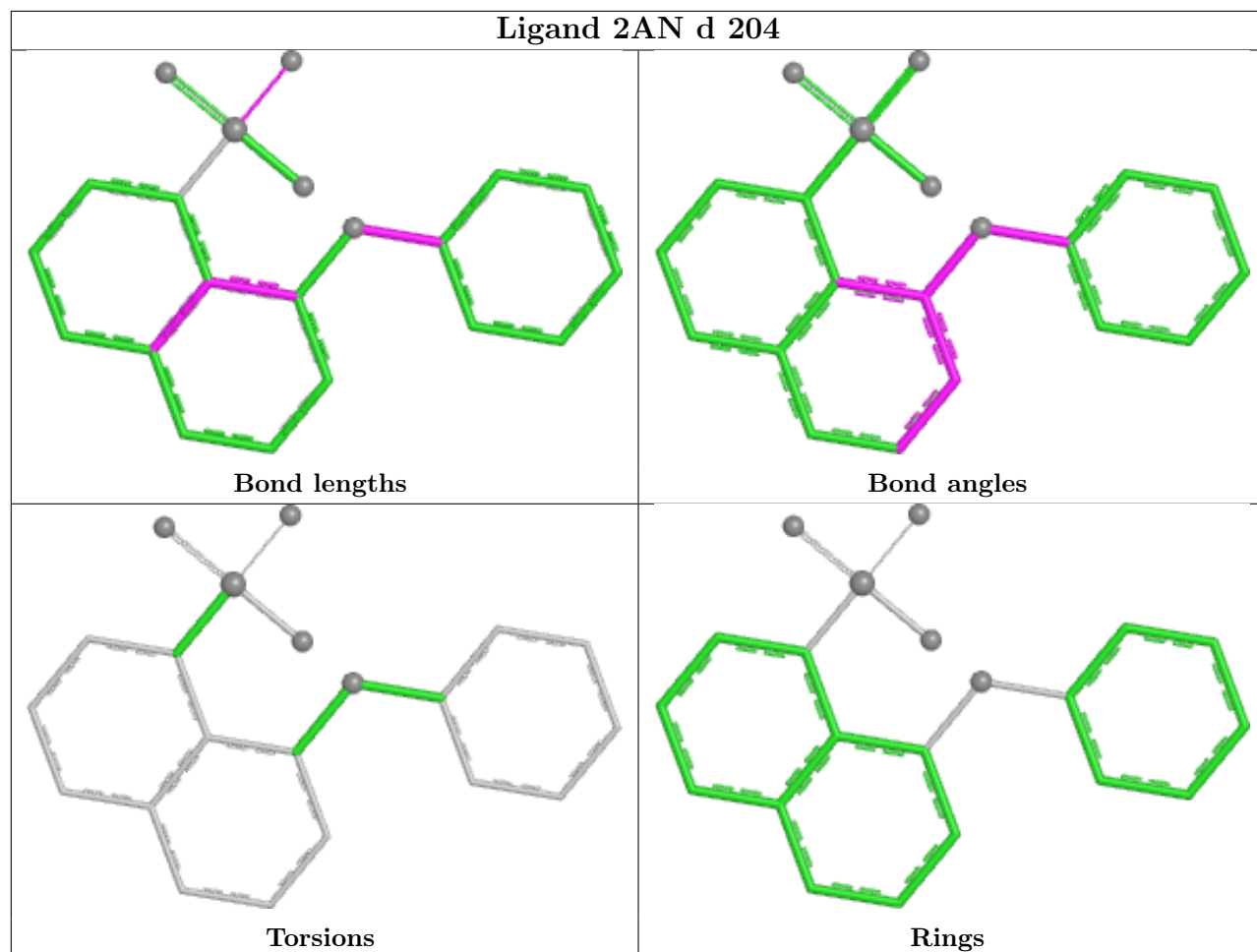




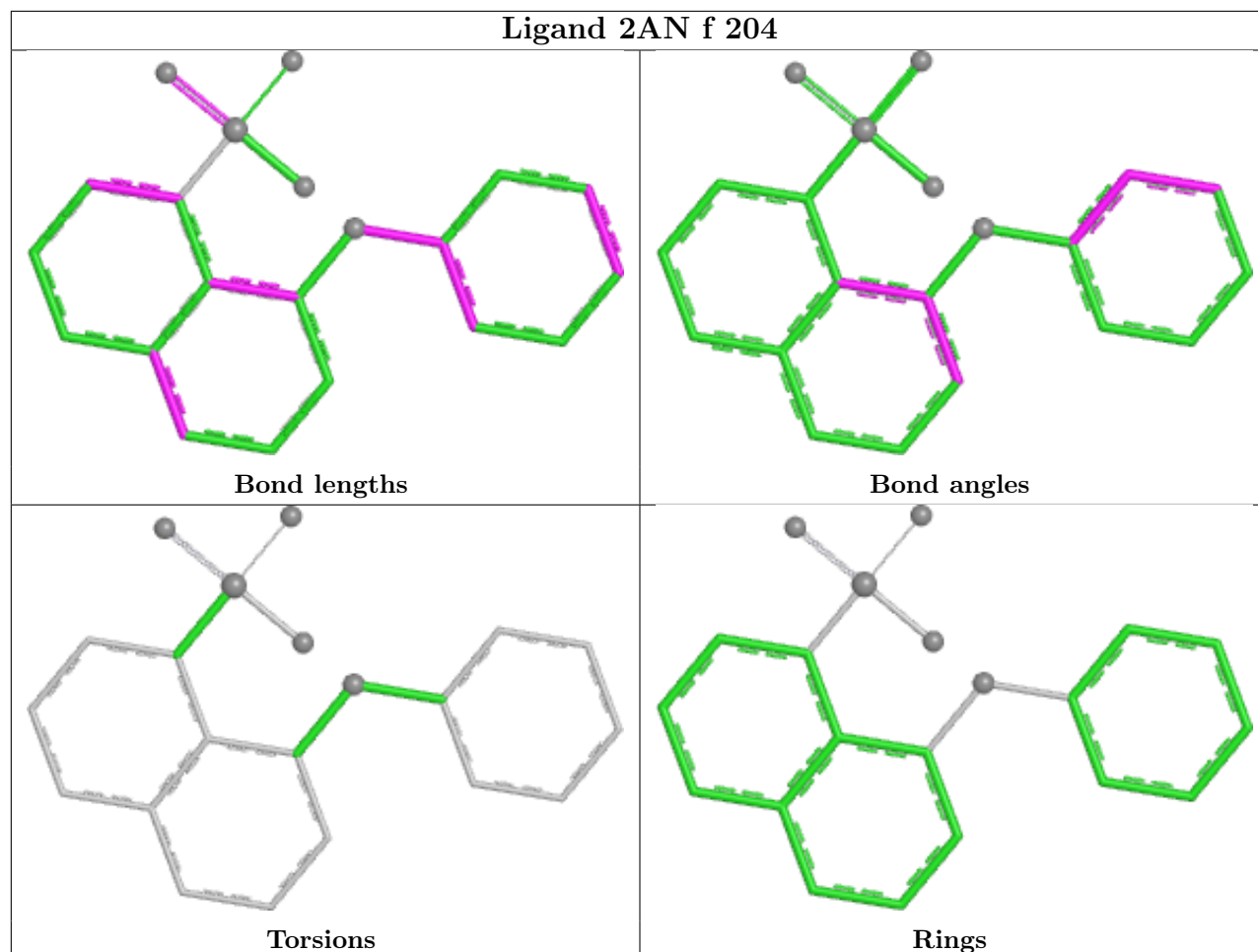
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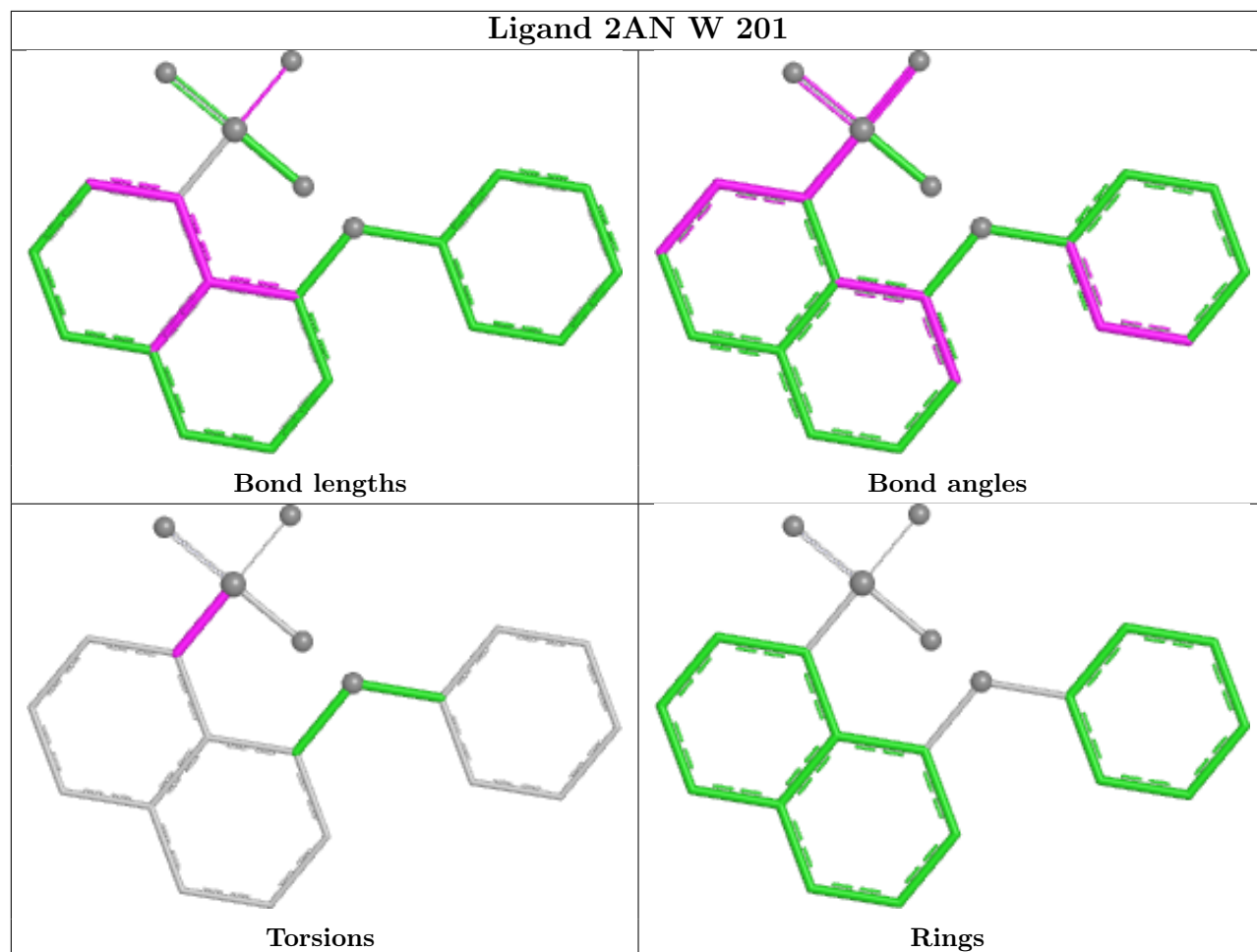


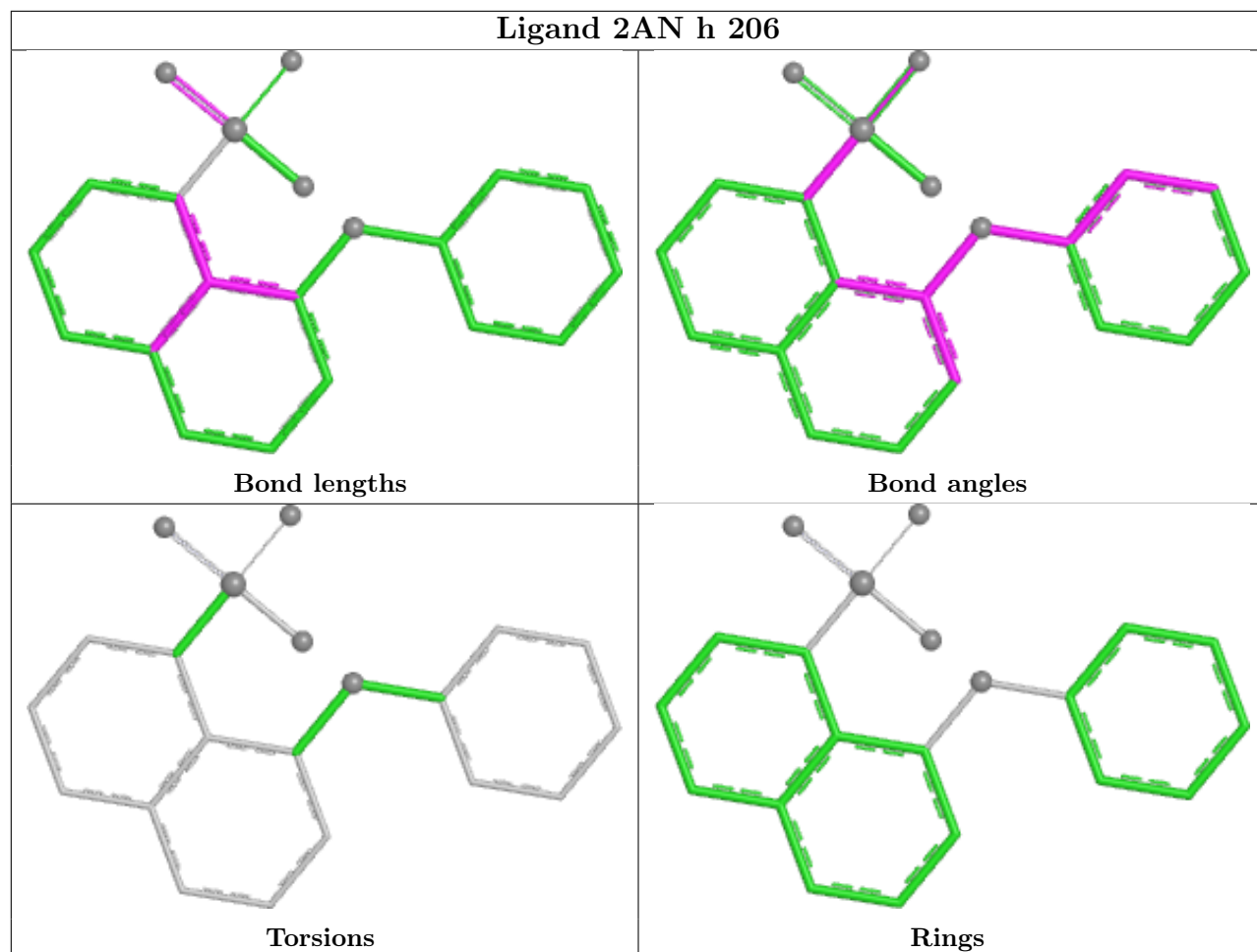
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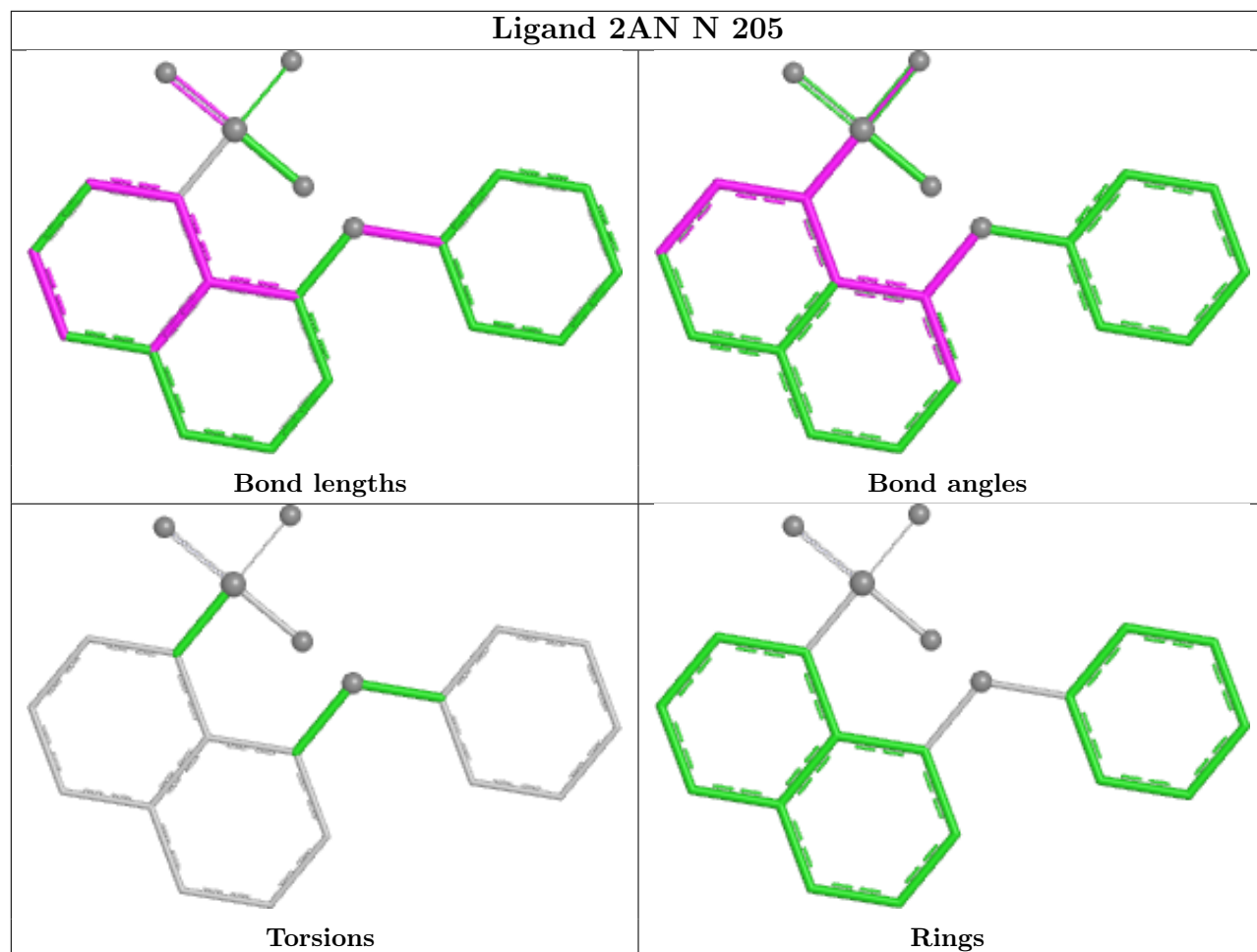


Ligand 2AN f 204

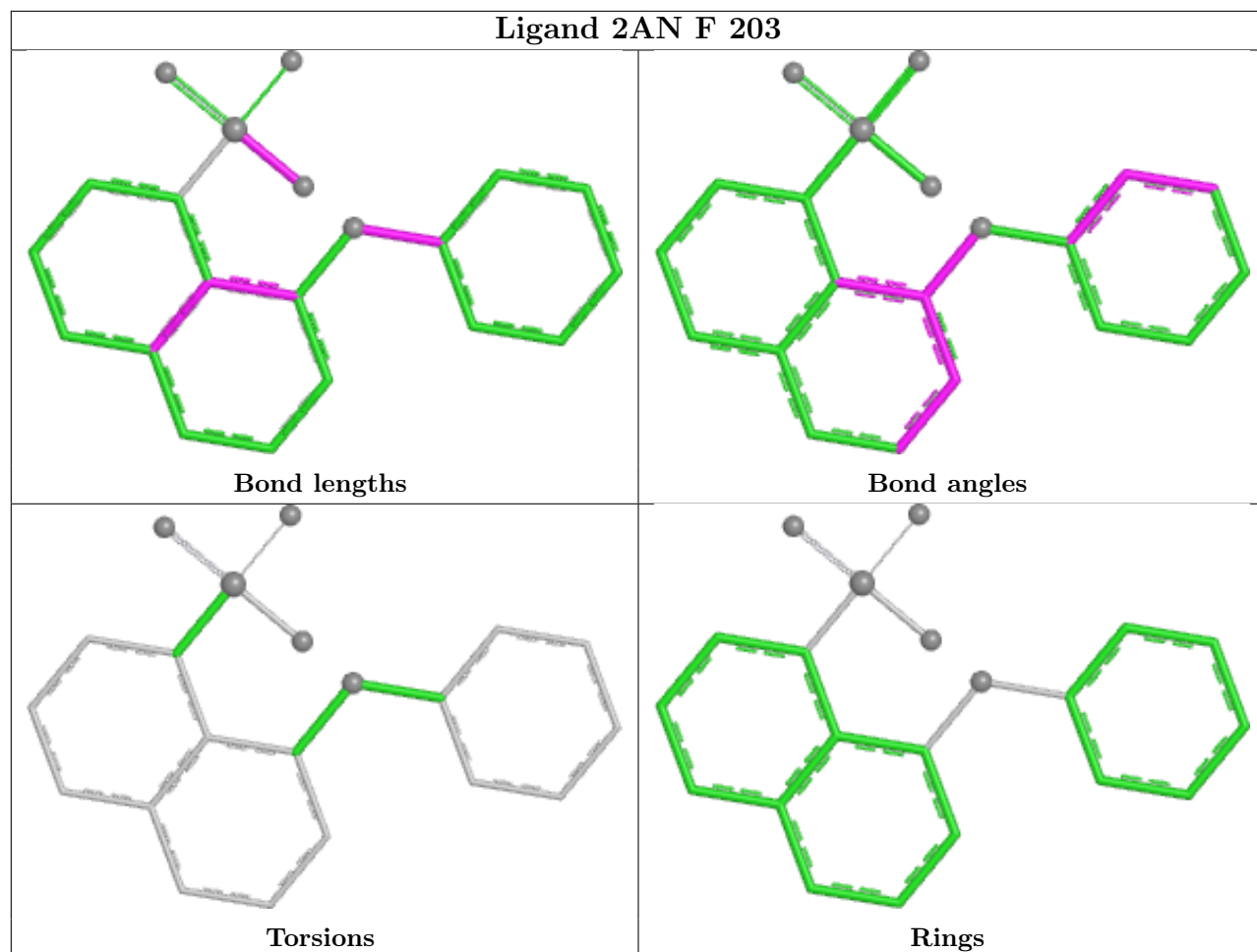




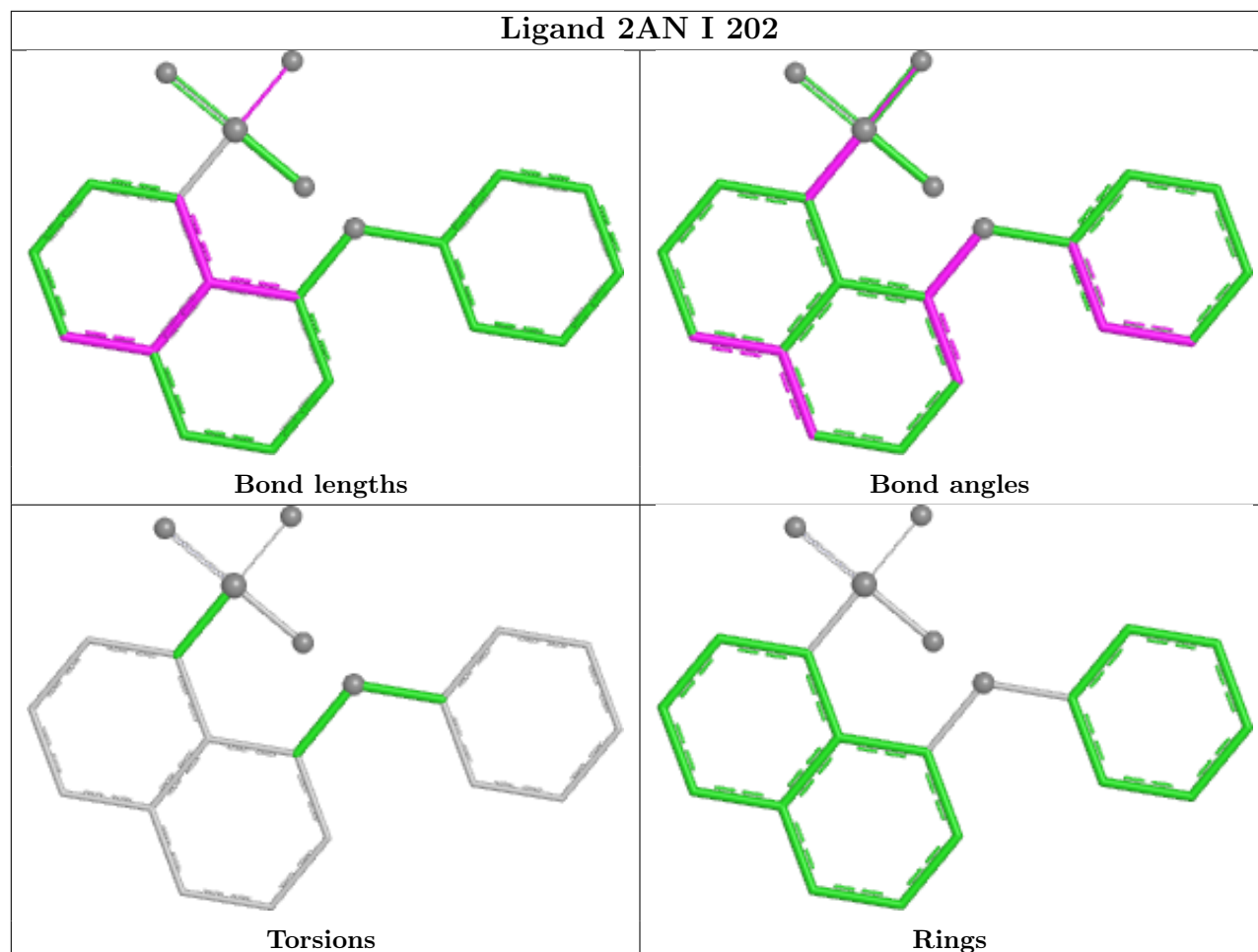




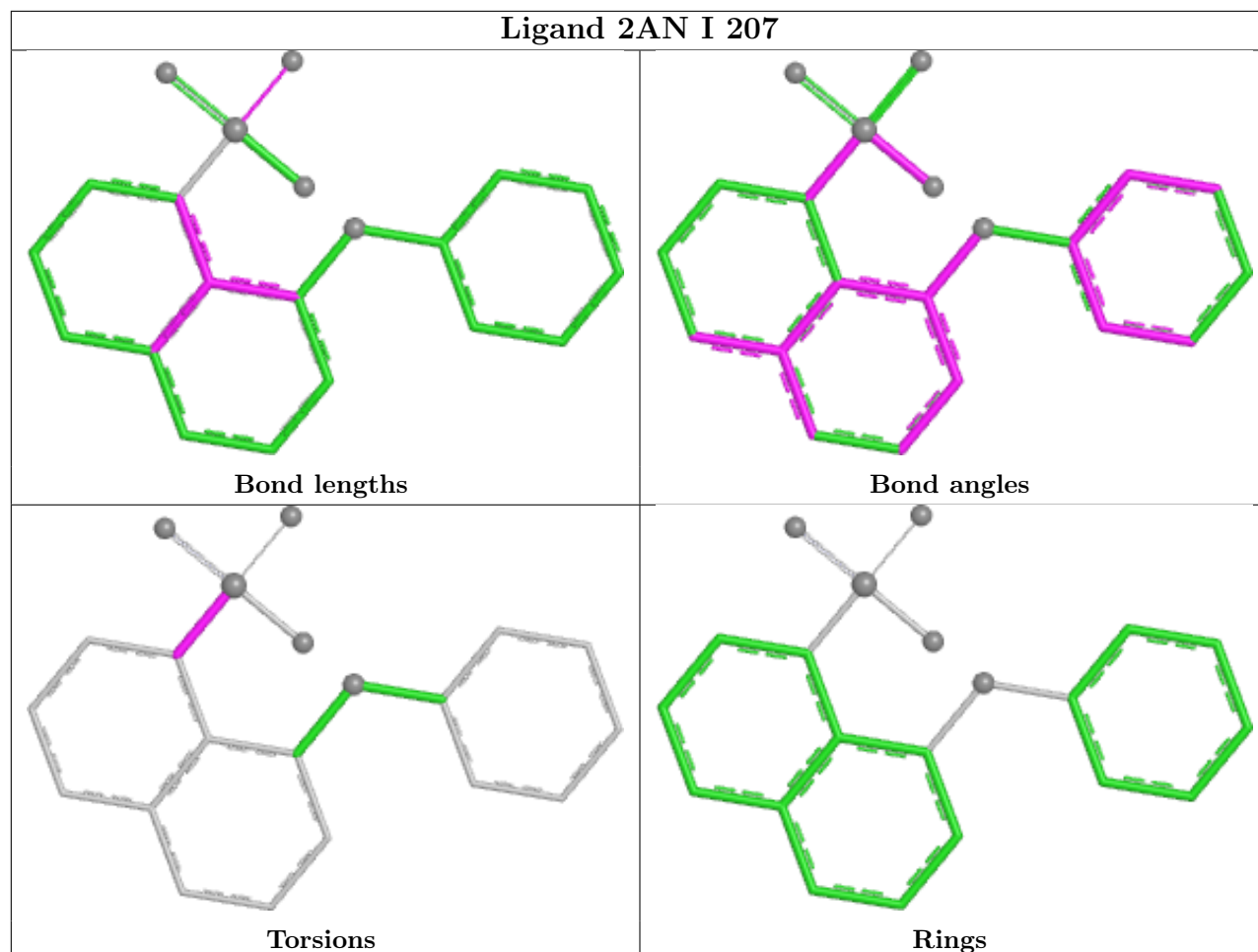
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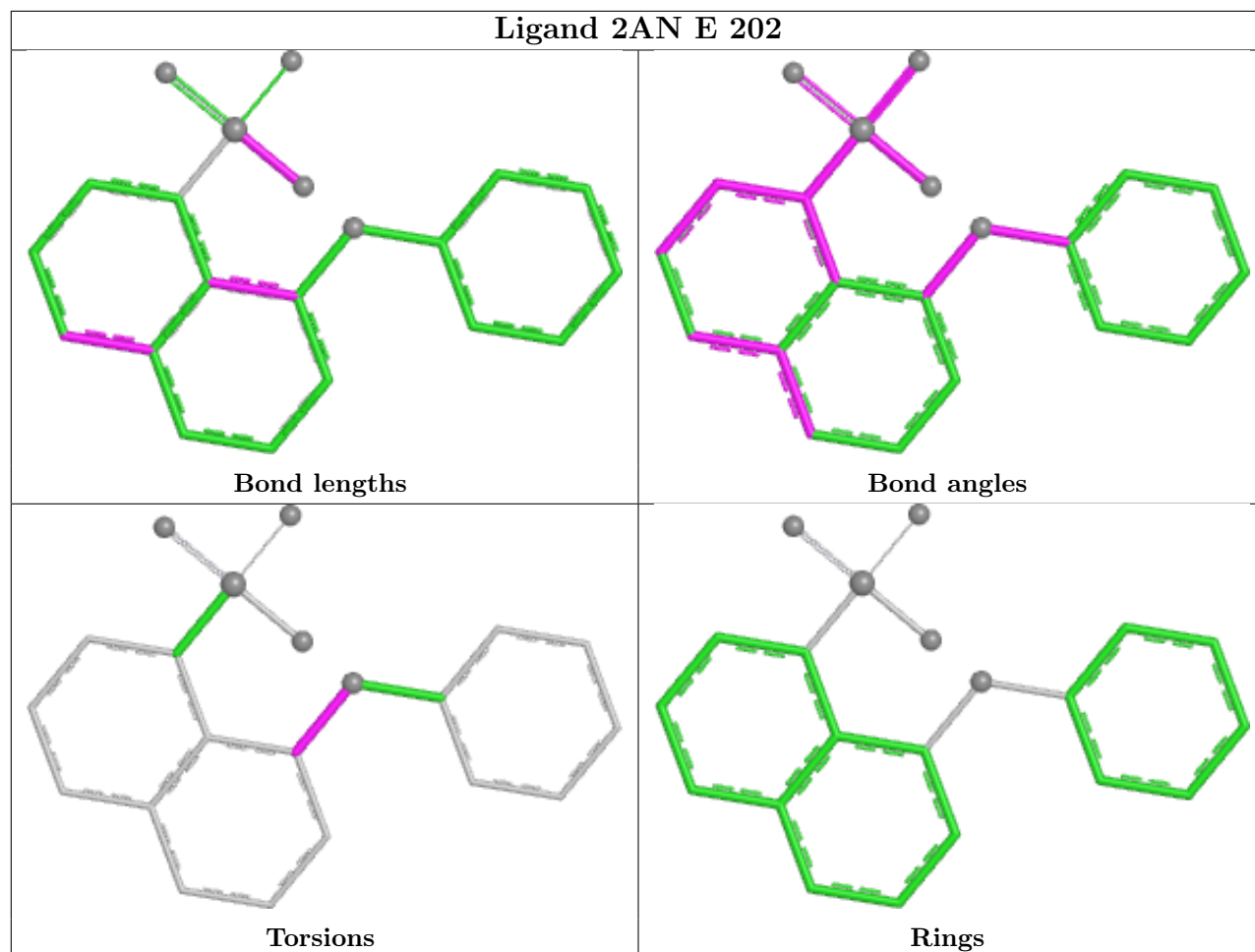


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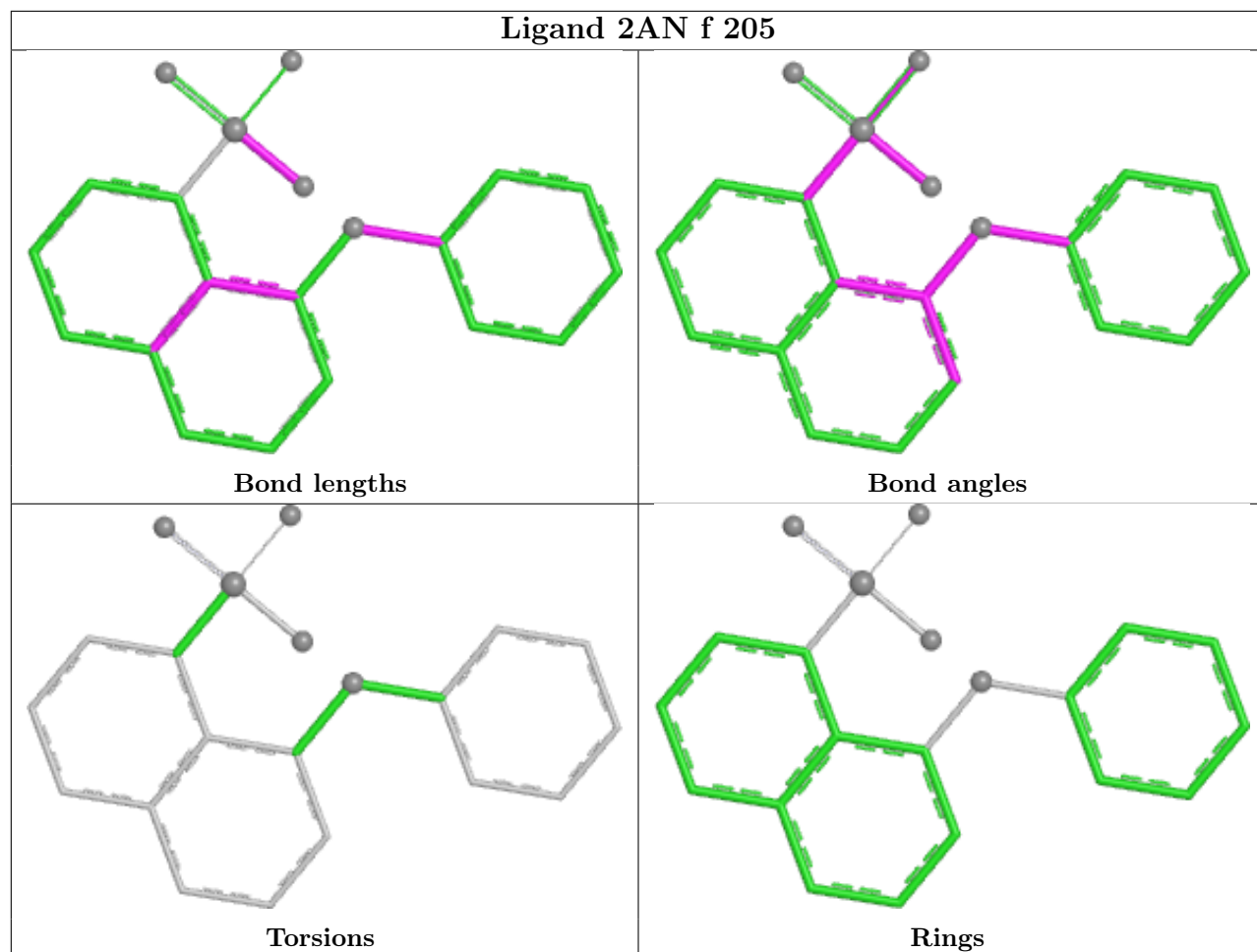


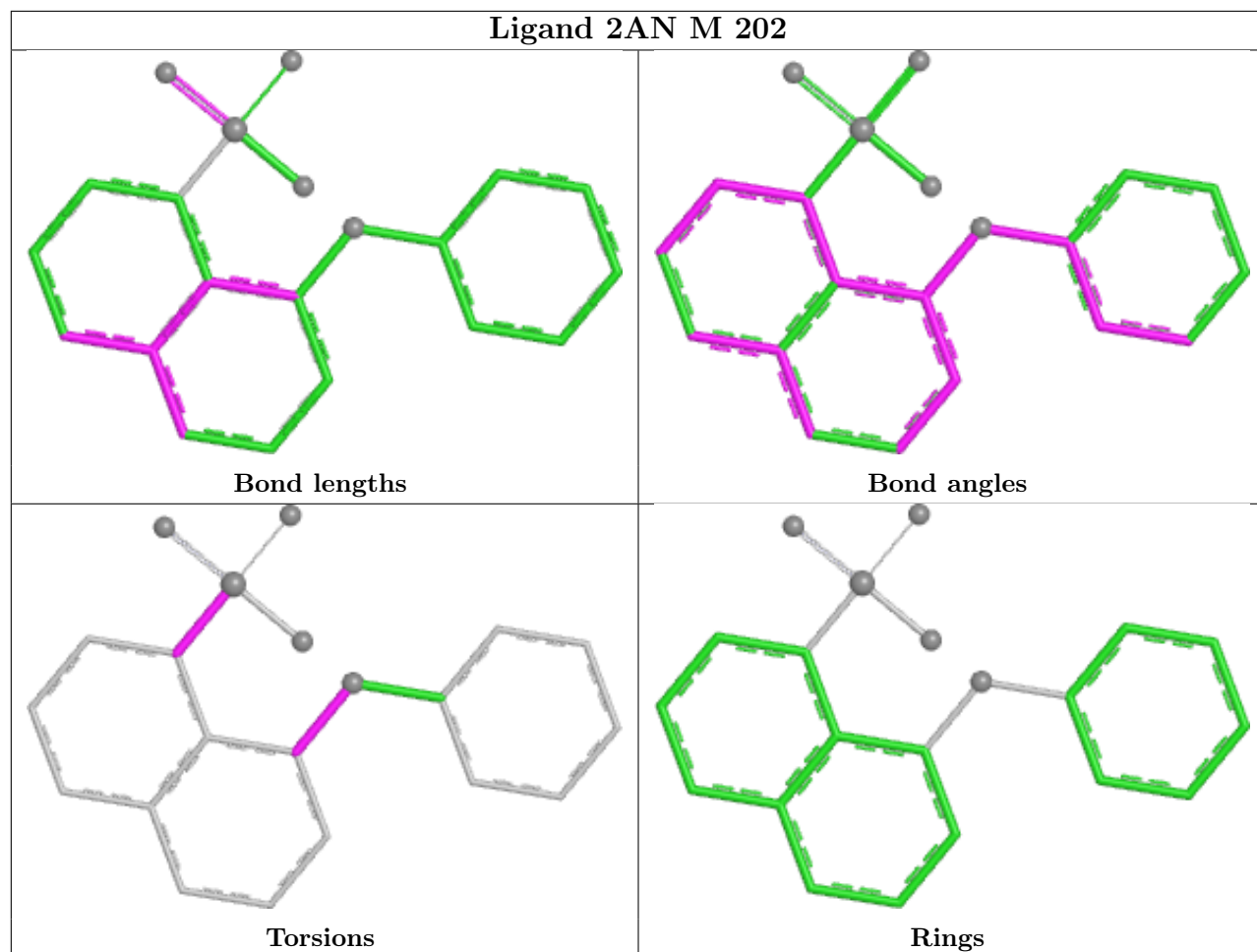
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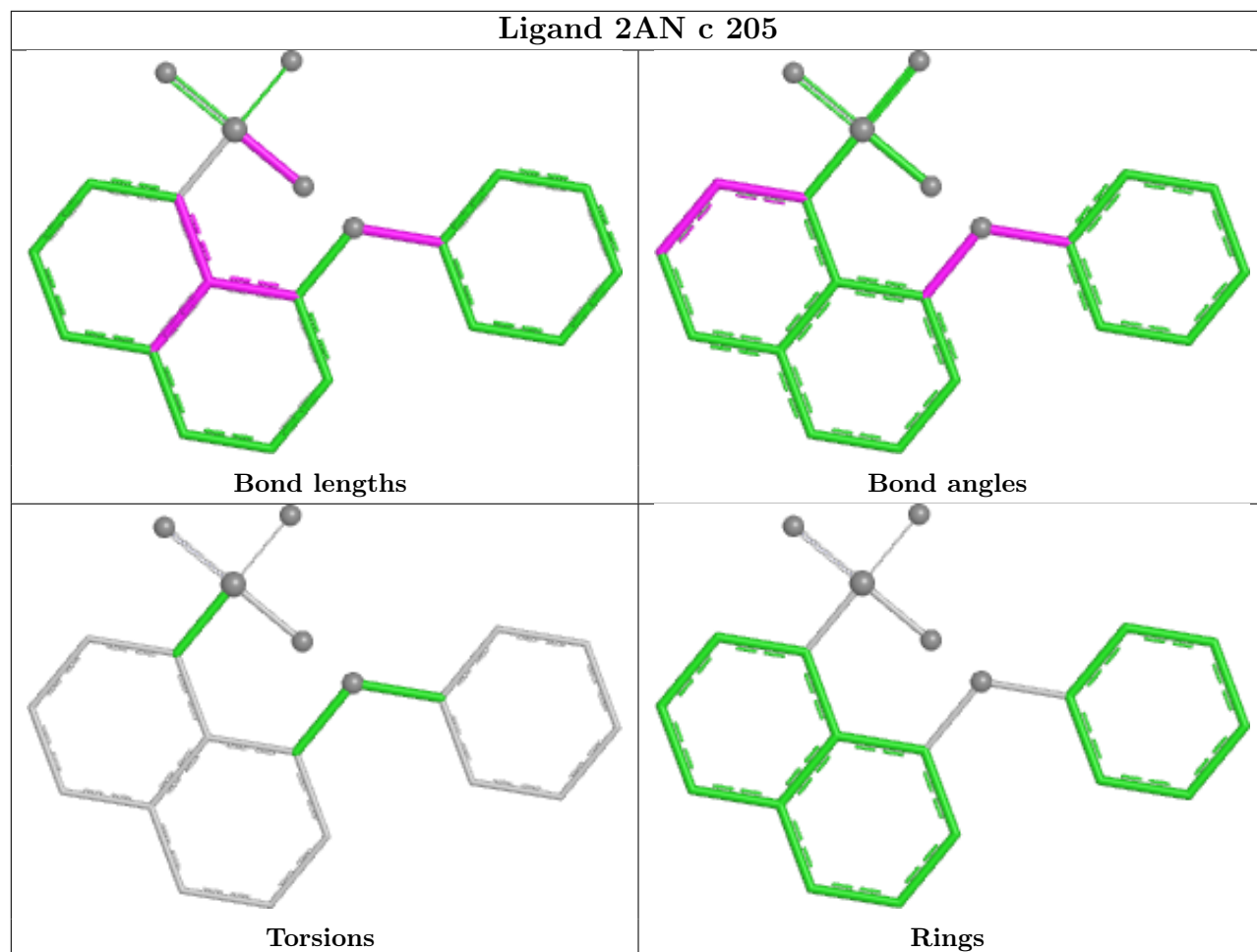




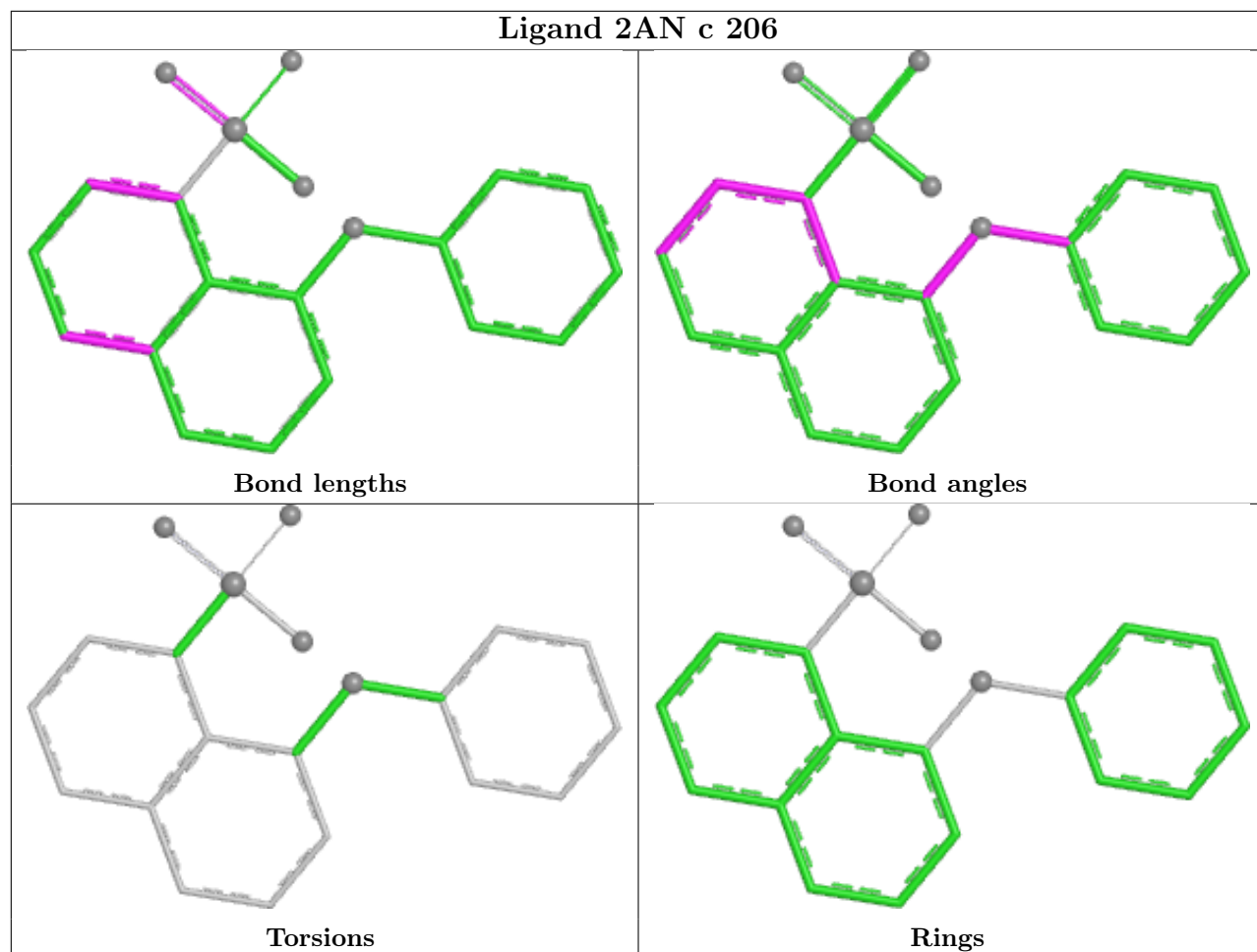
Ligand 2AN f 205

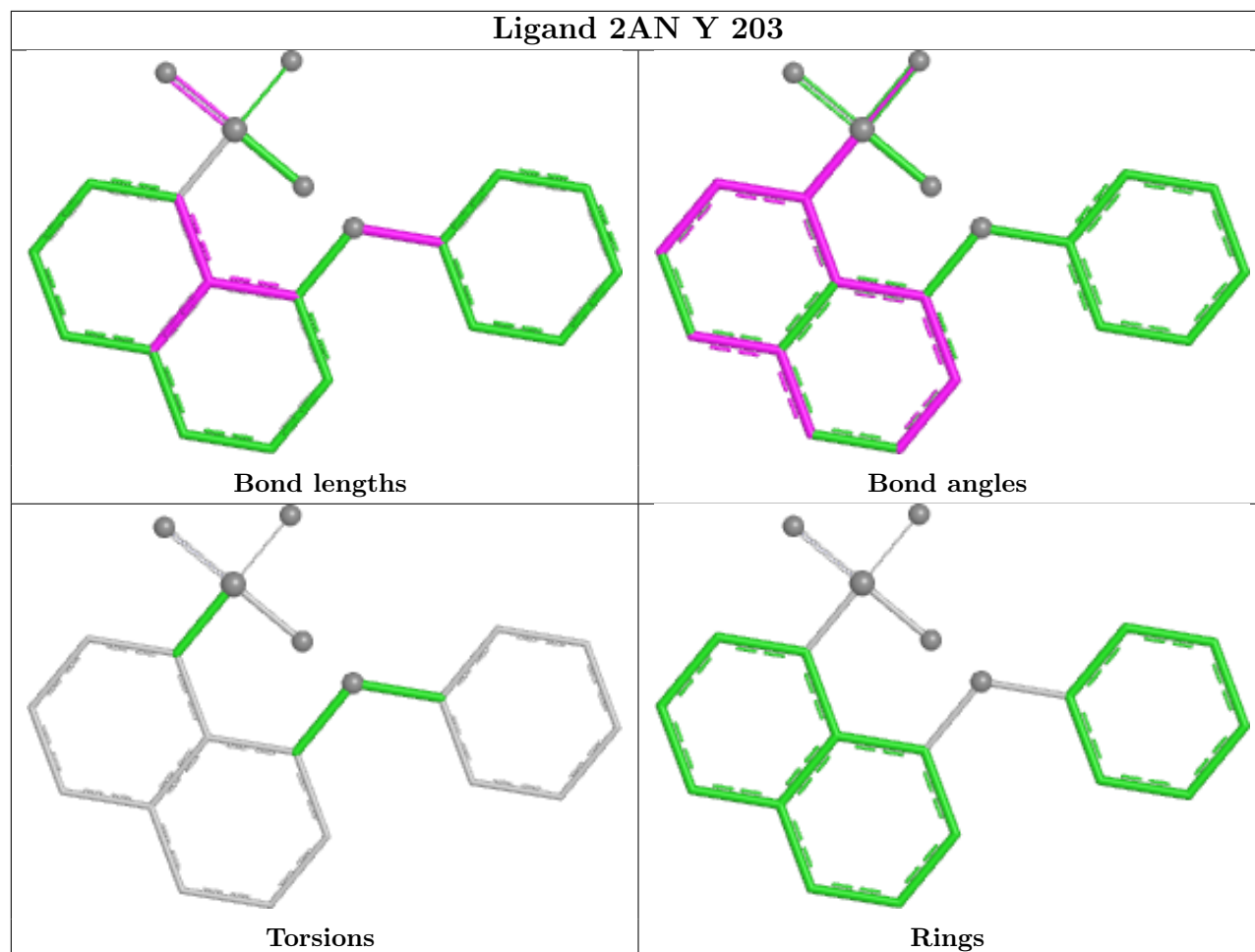




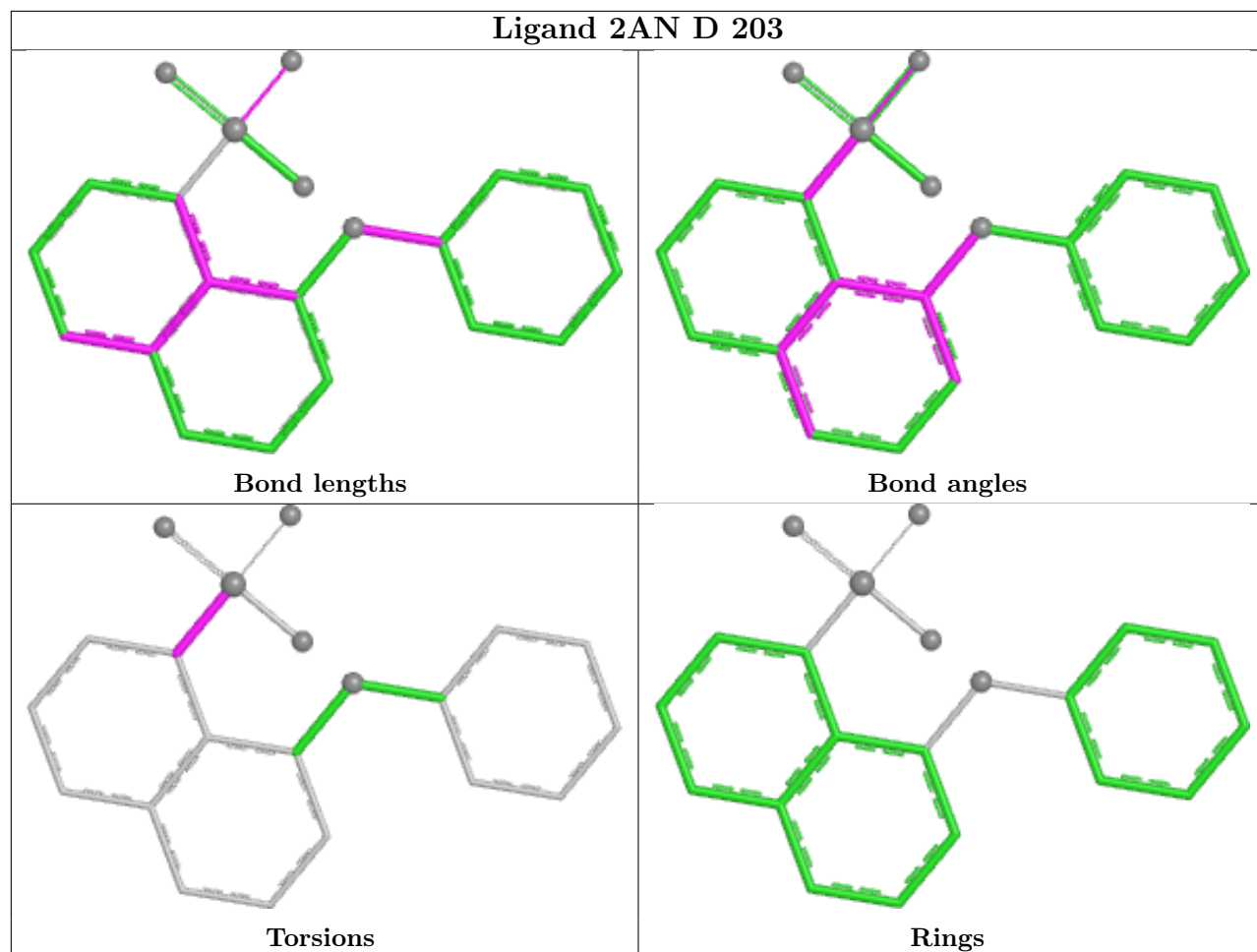


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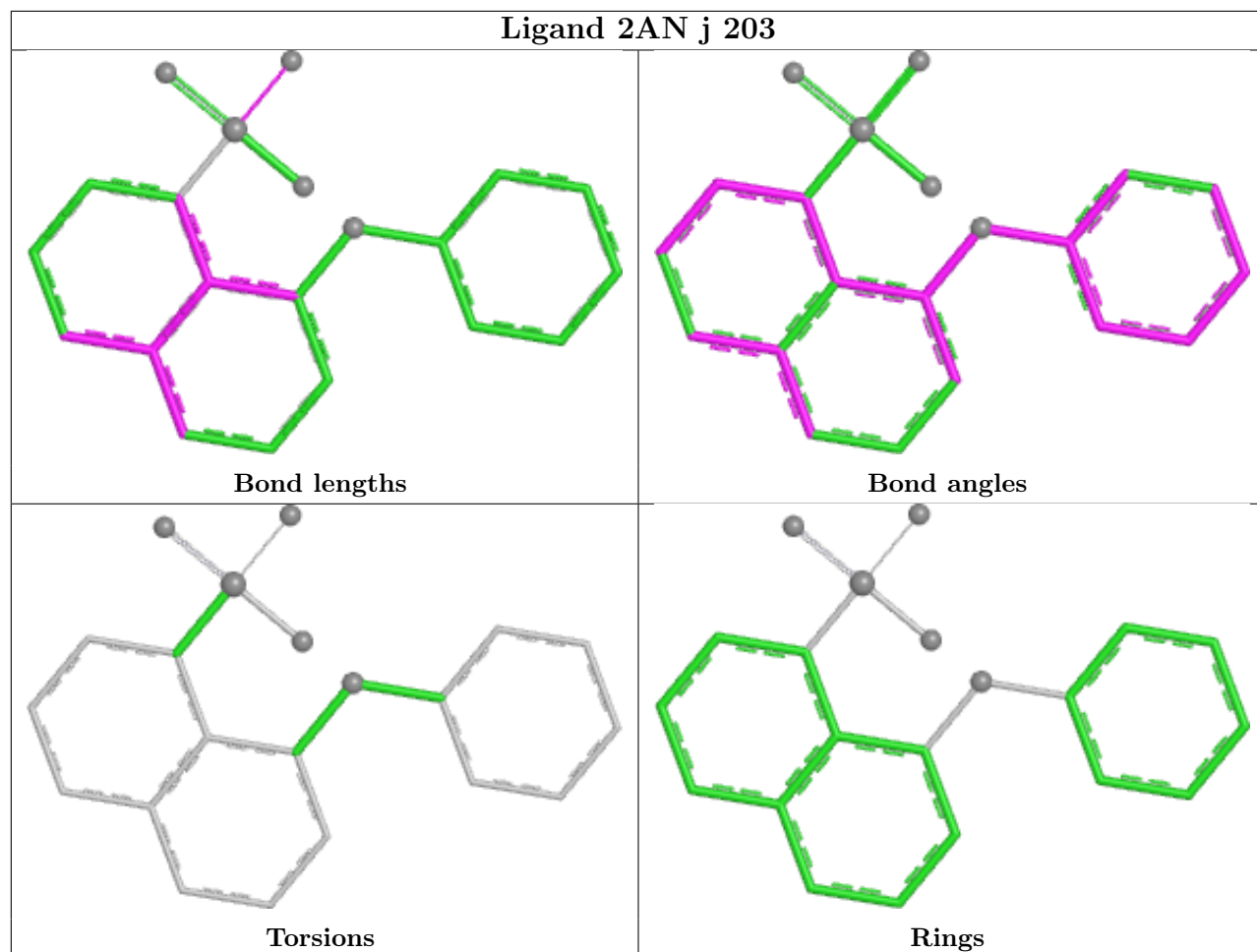




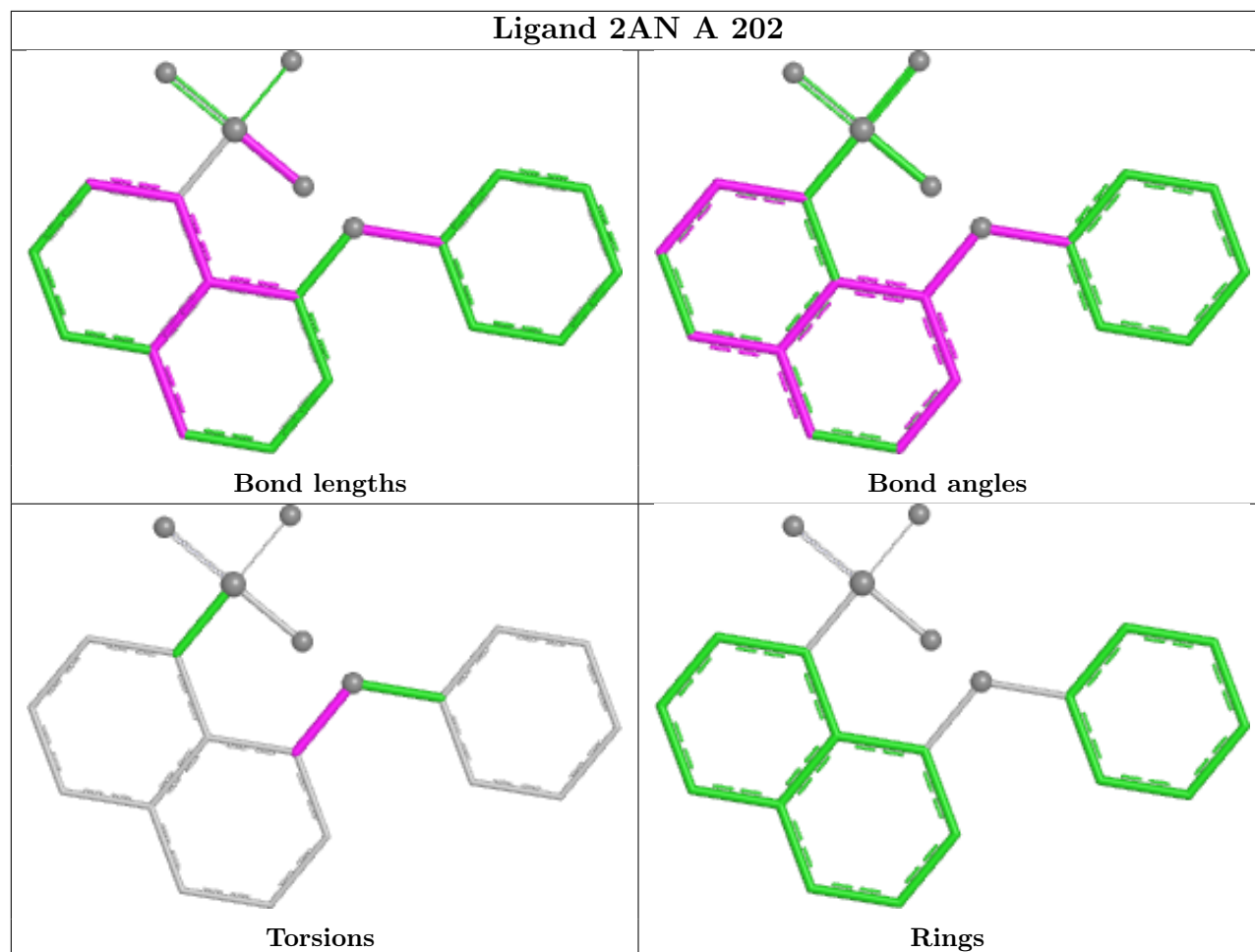
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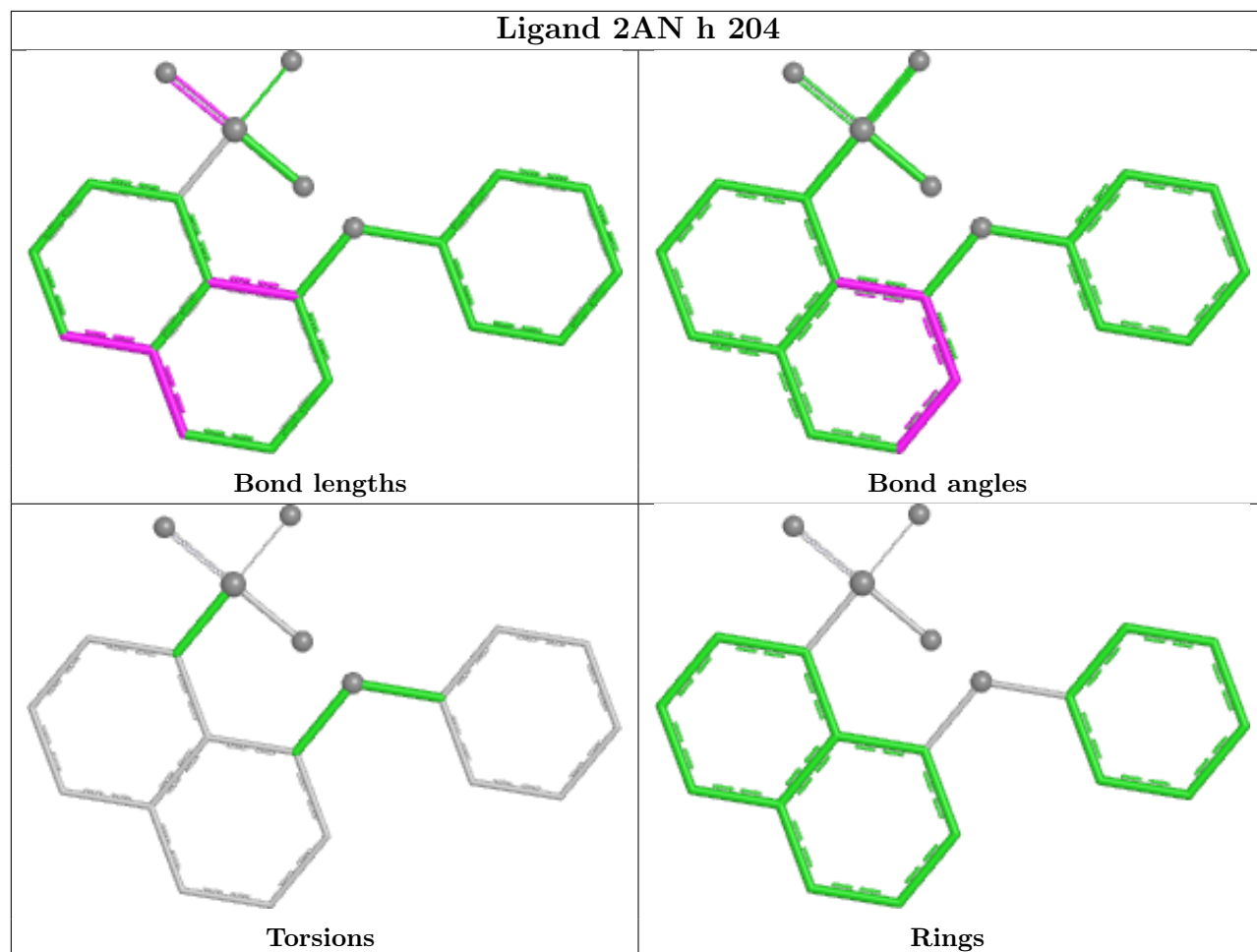
Ligand 2AN j 203



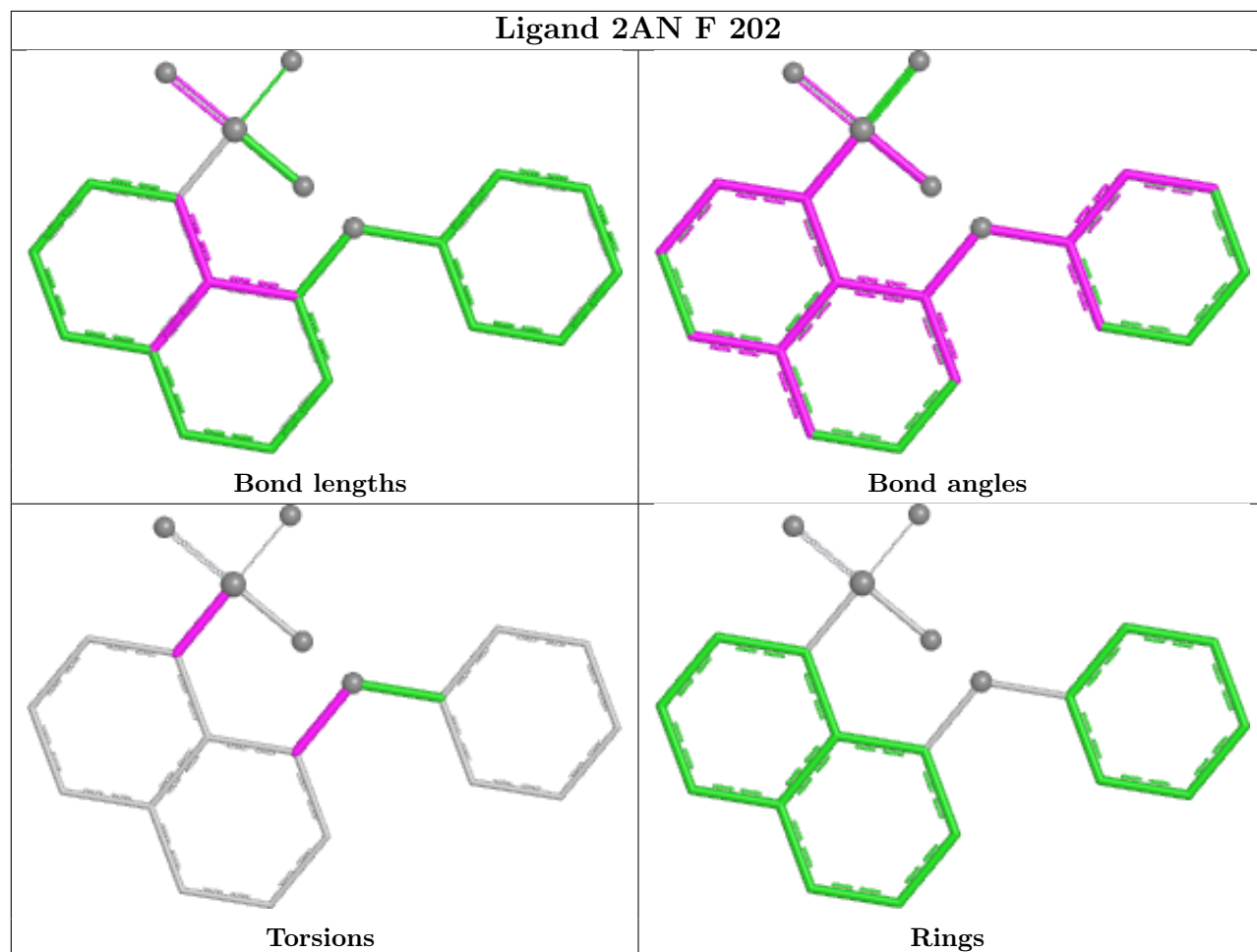
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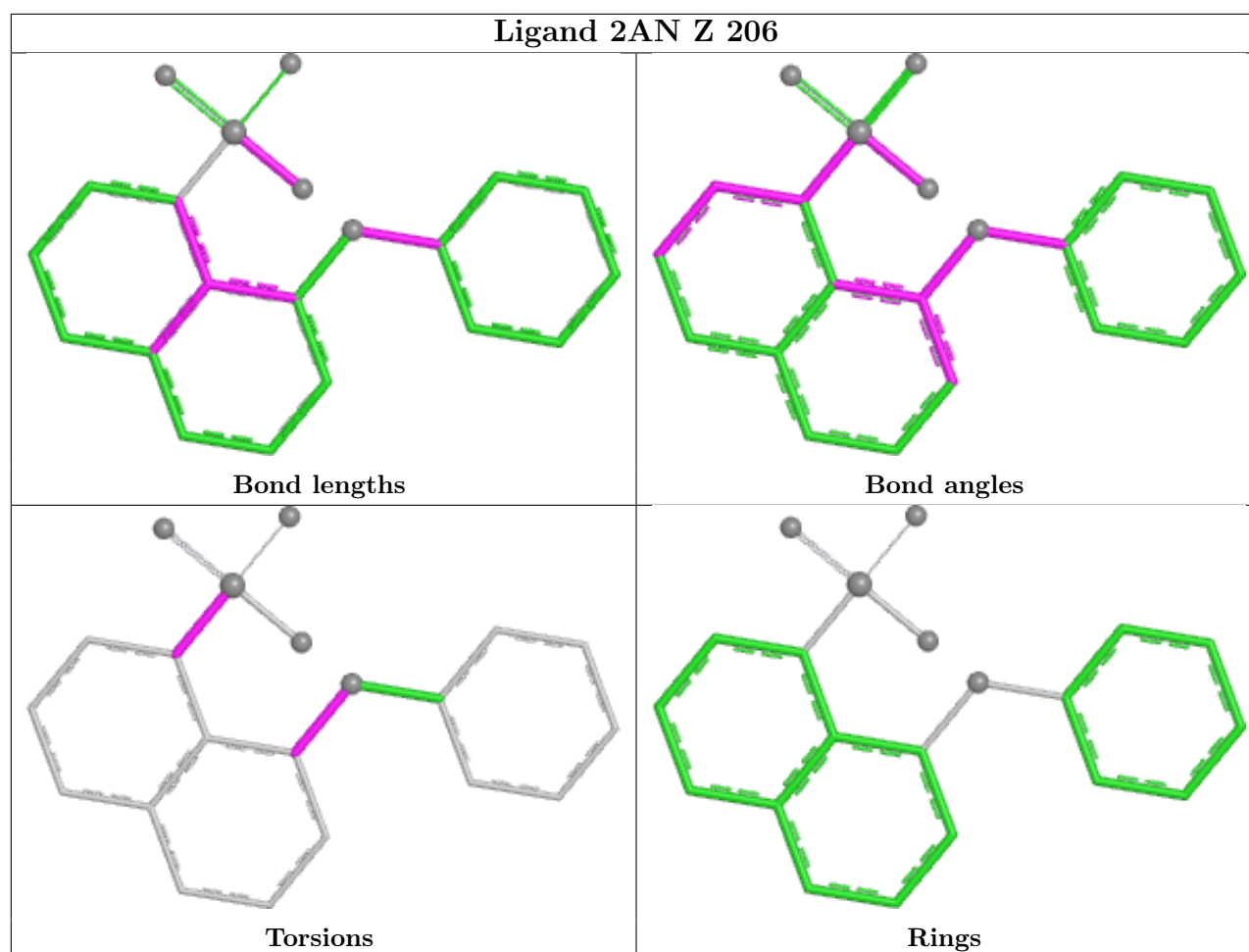


Ligand 2AN h 204

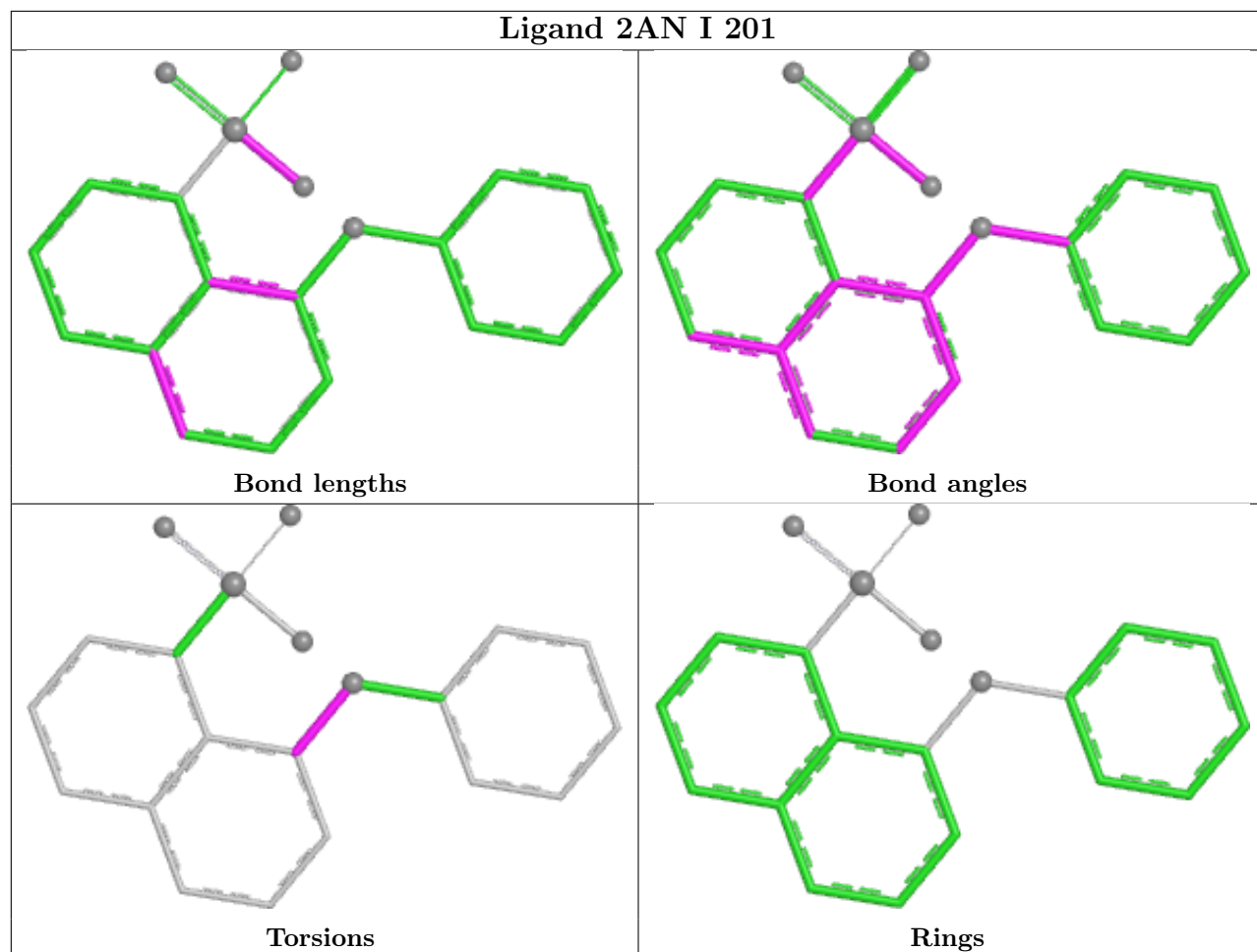


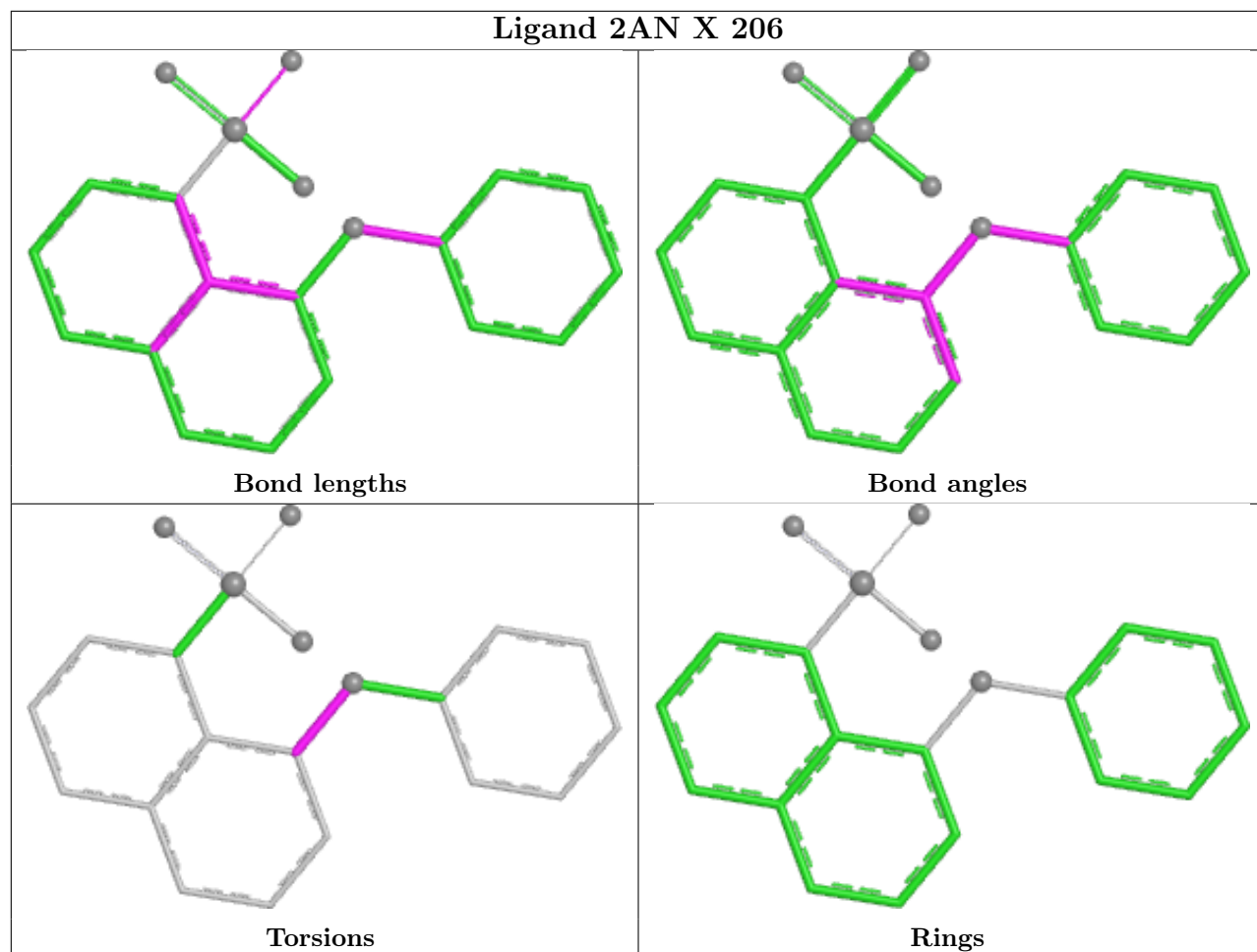
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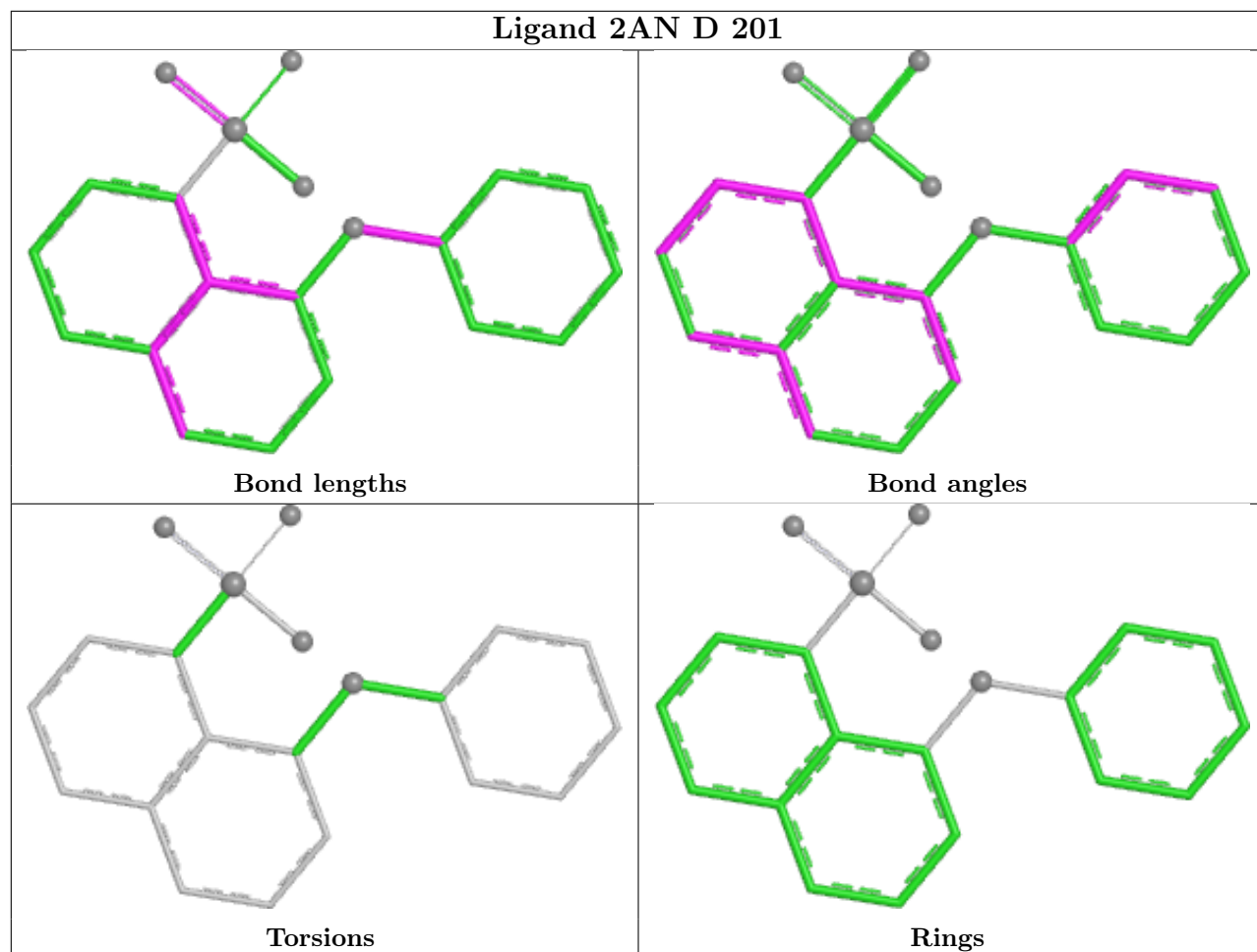


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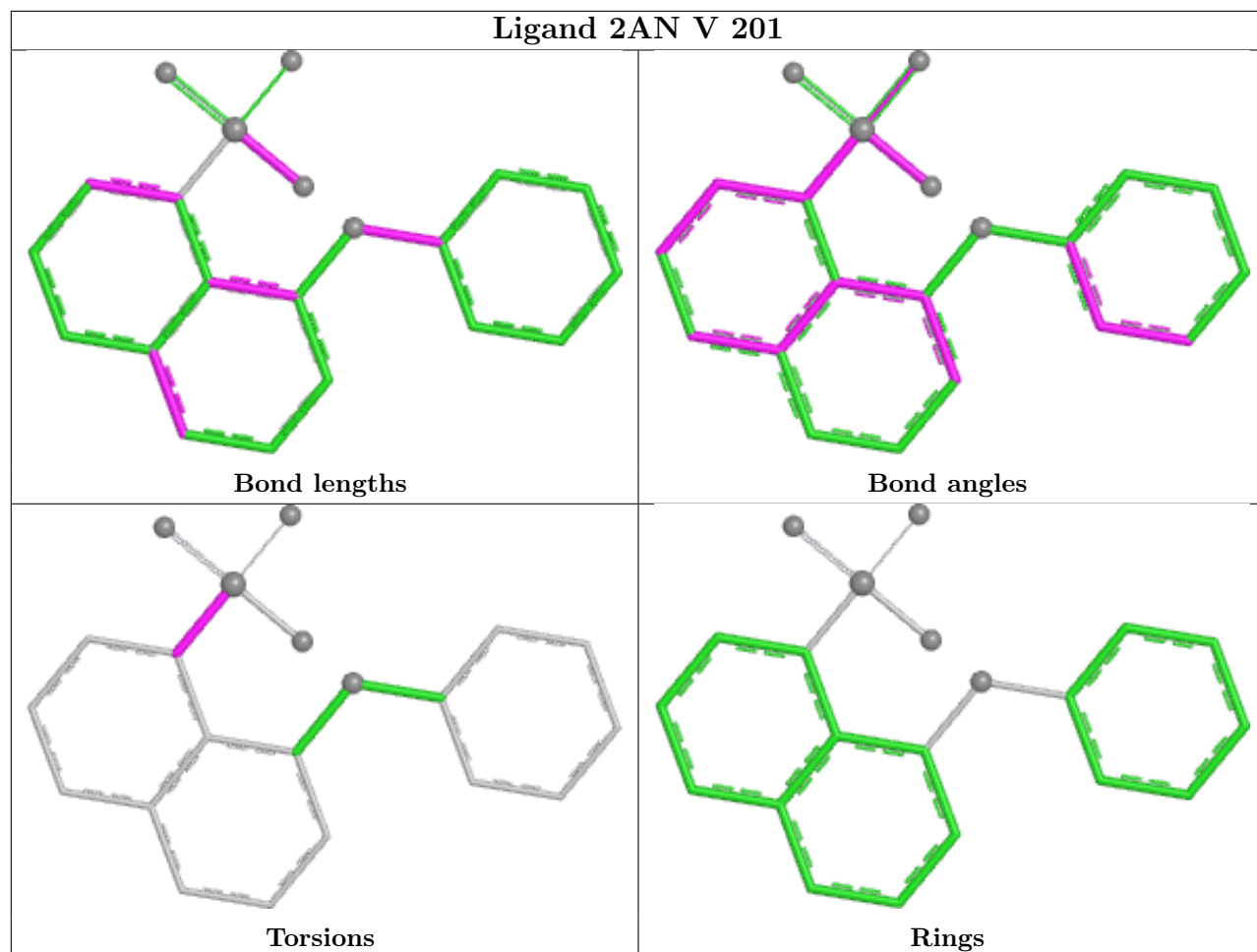




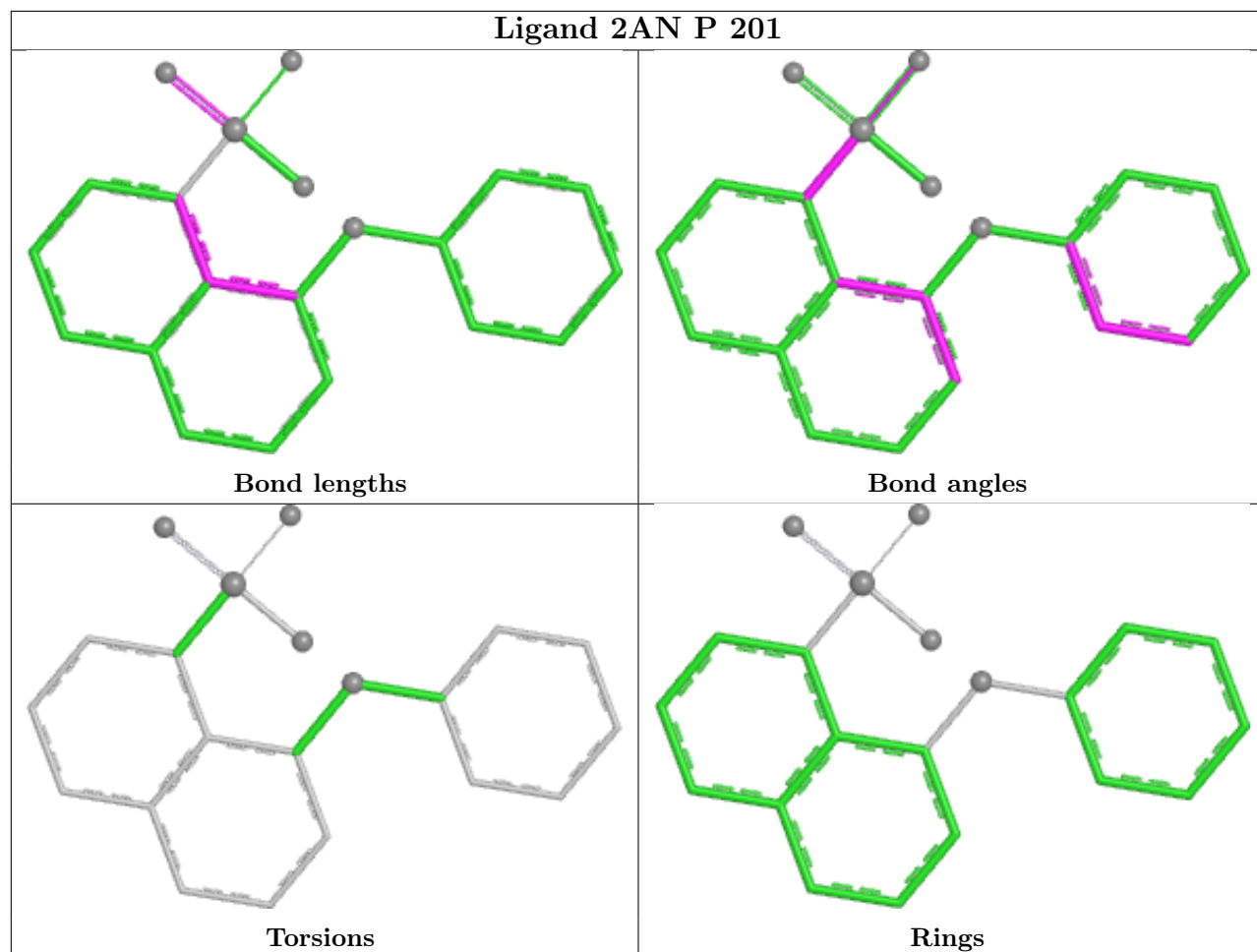
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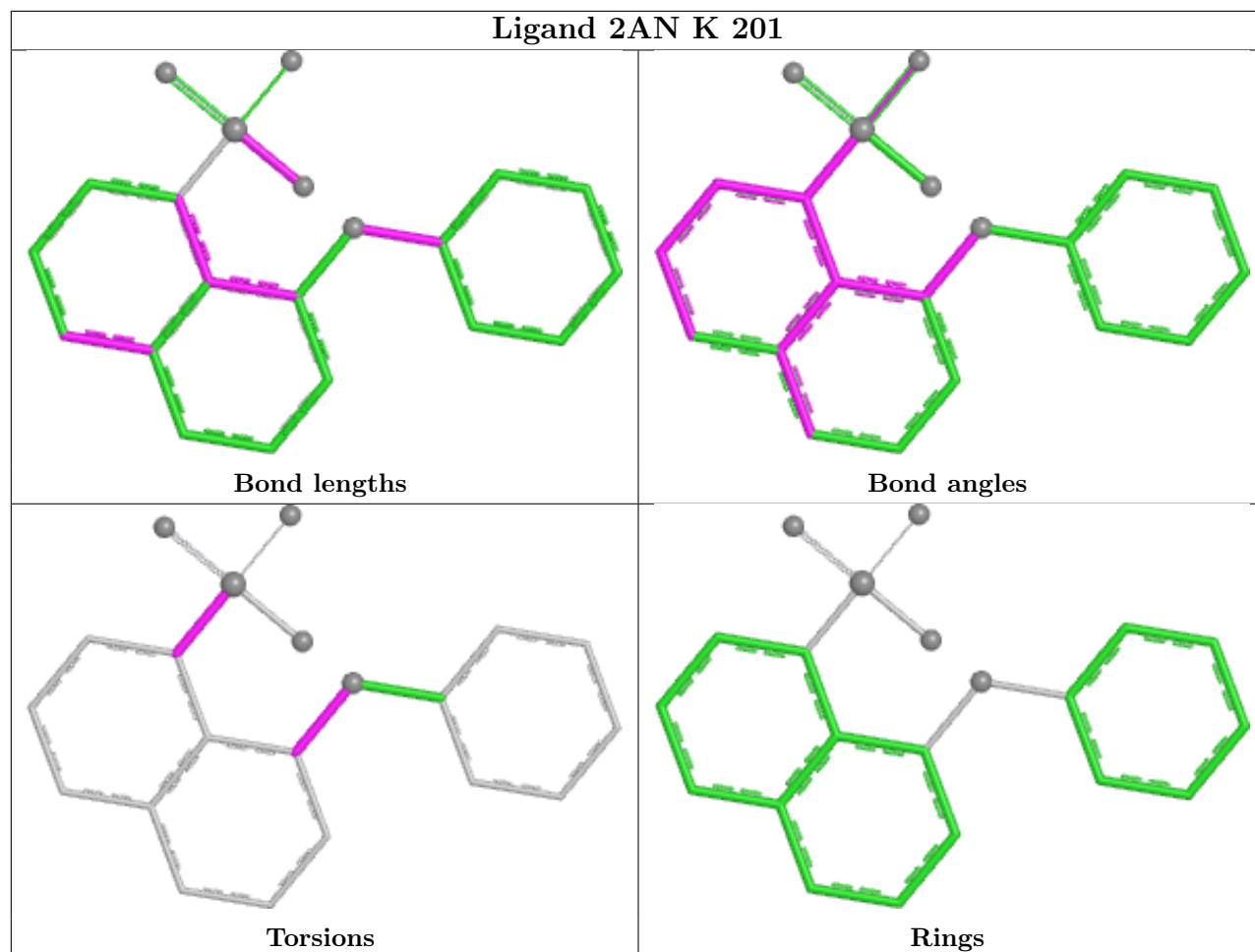
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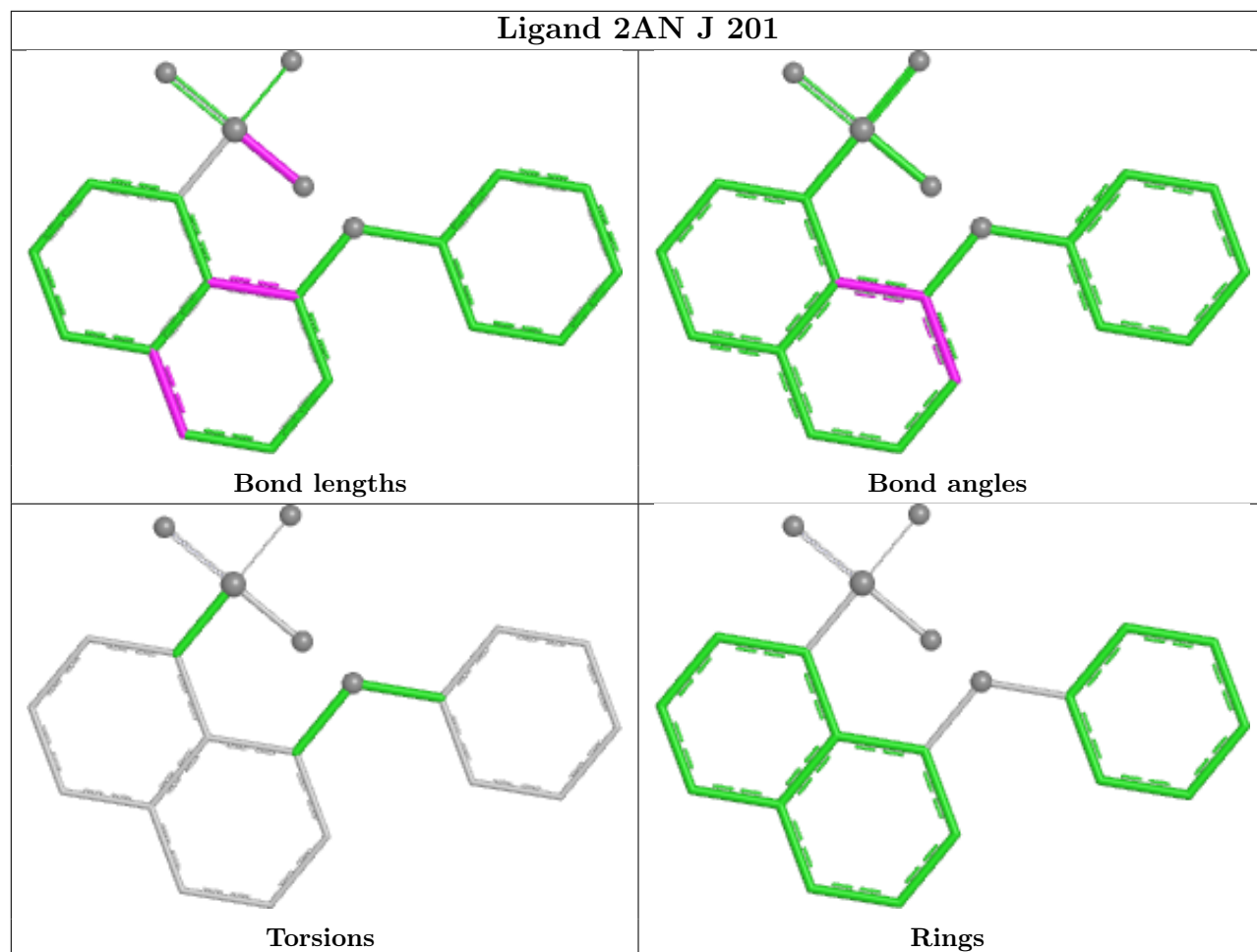
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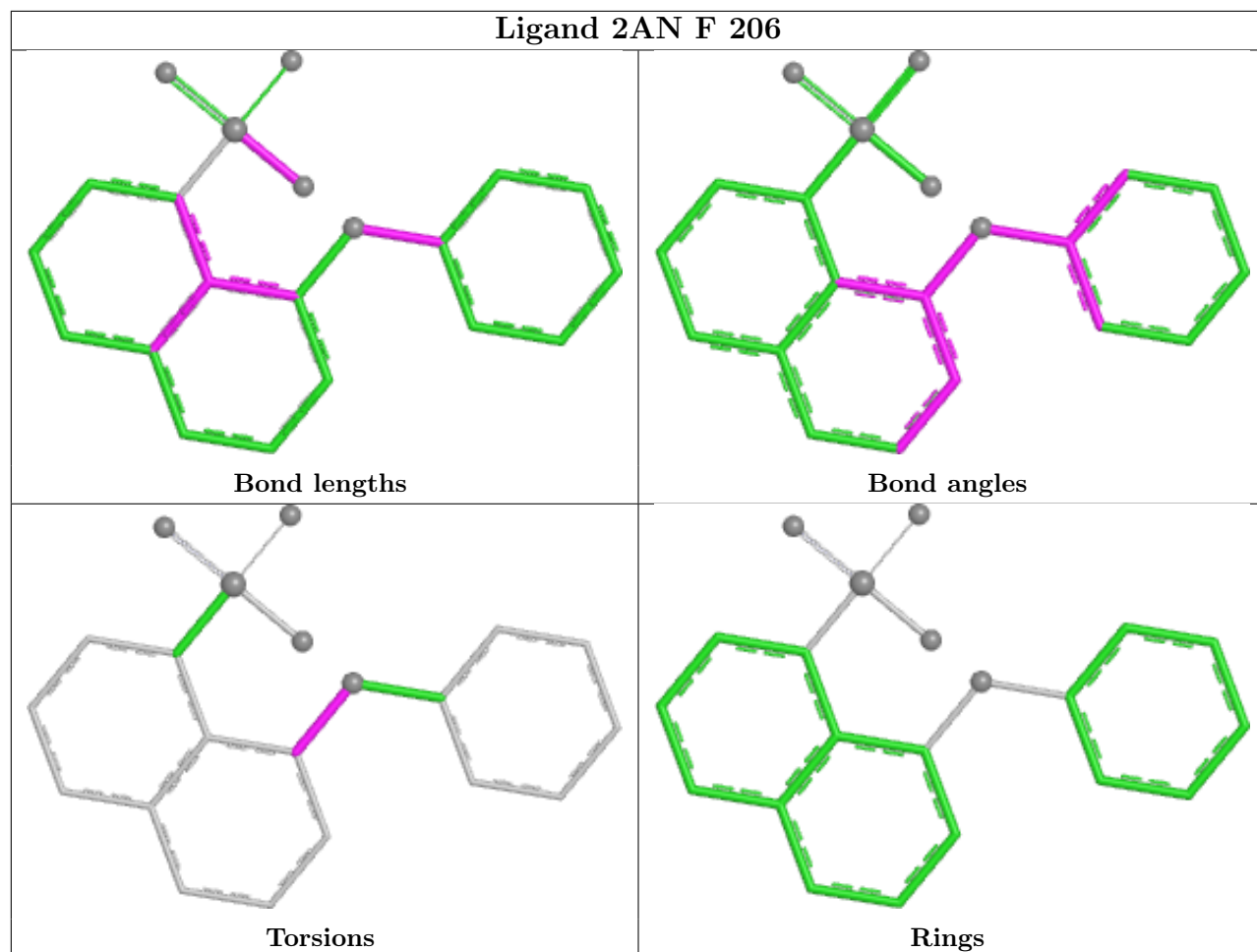
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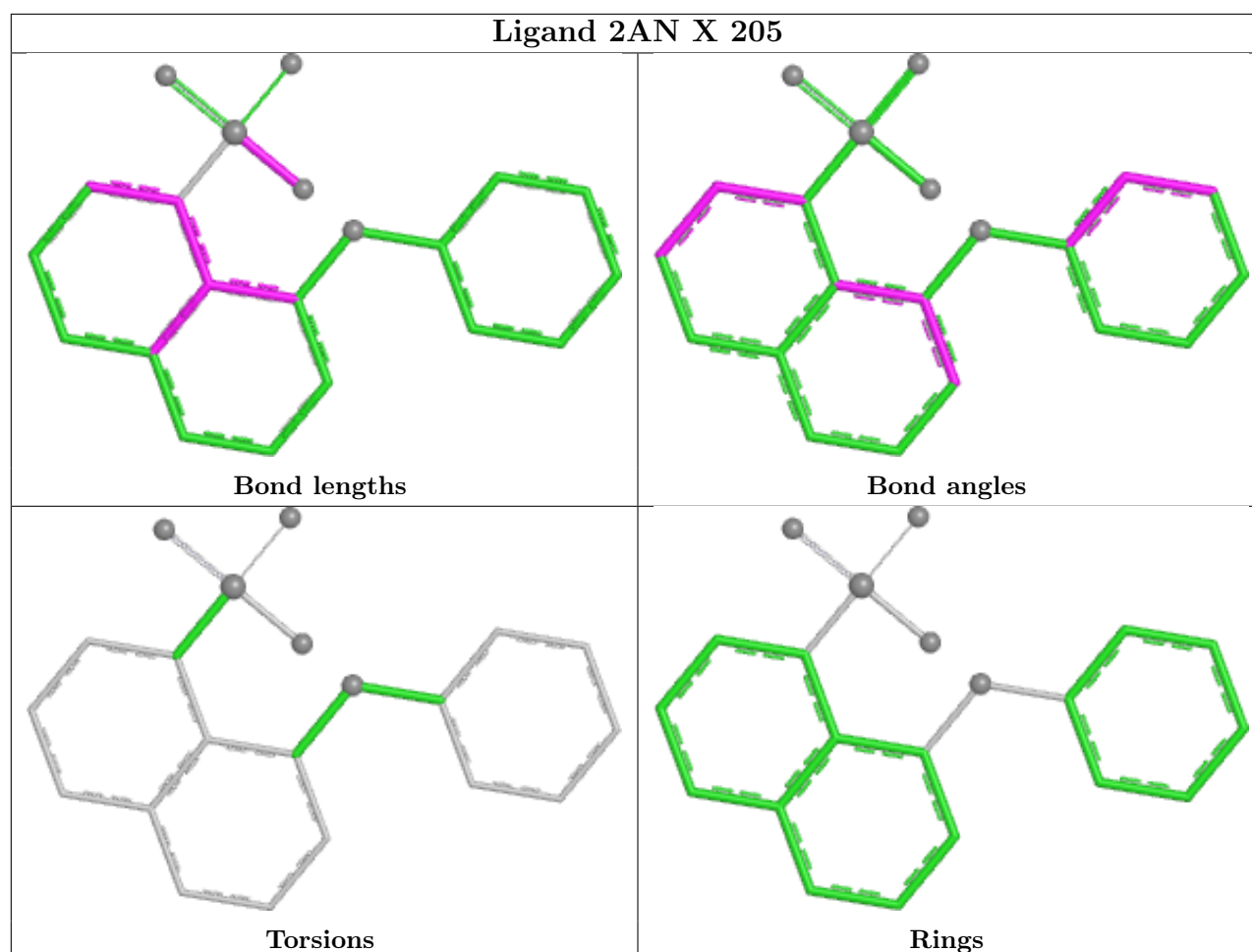


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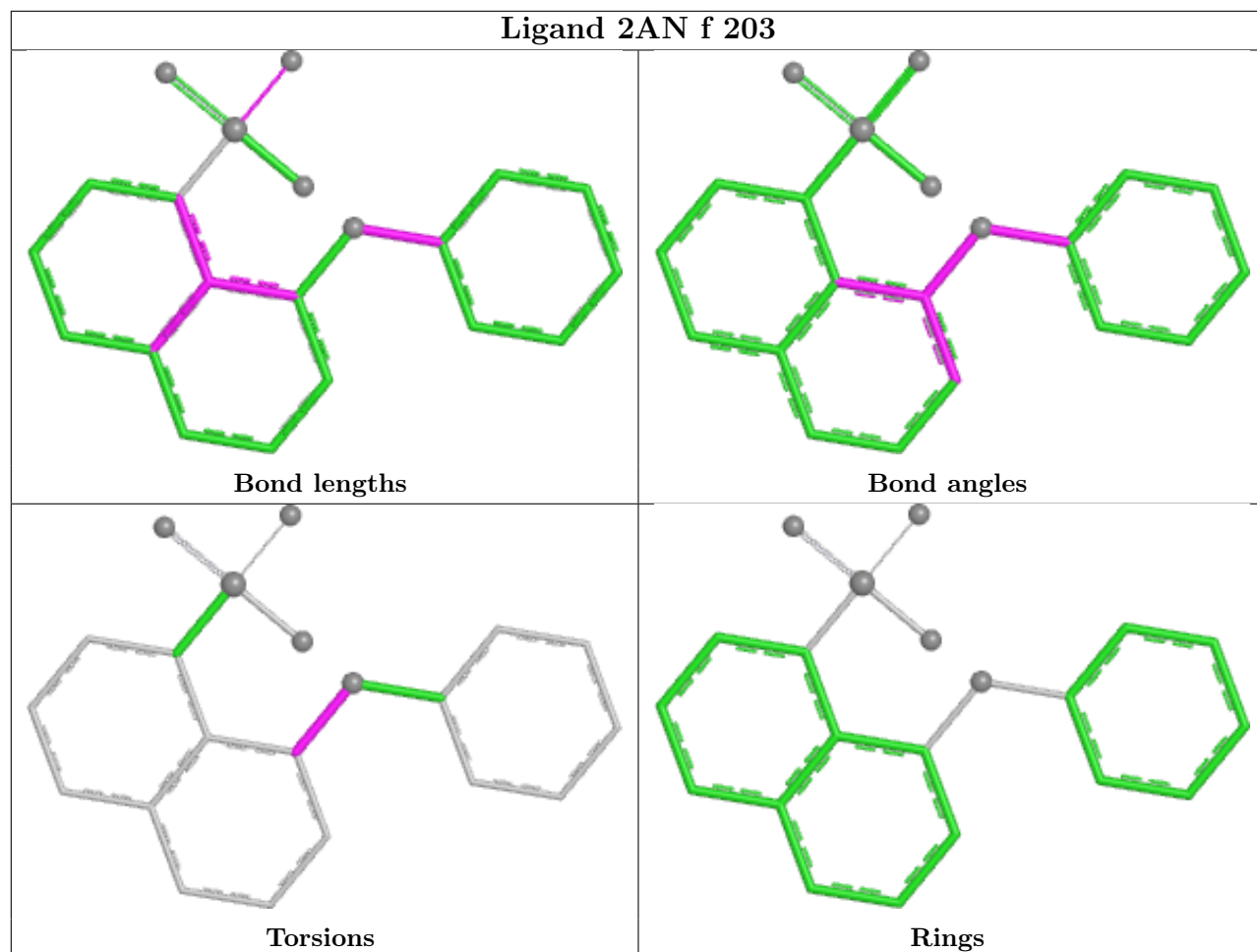


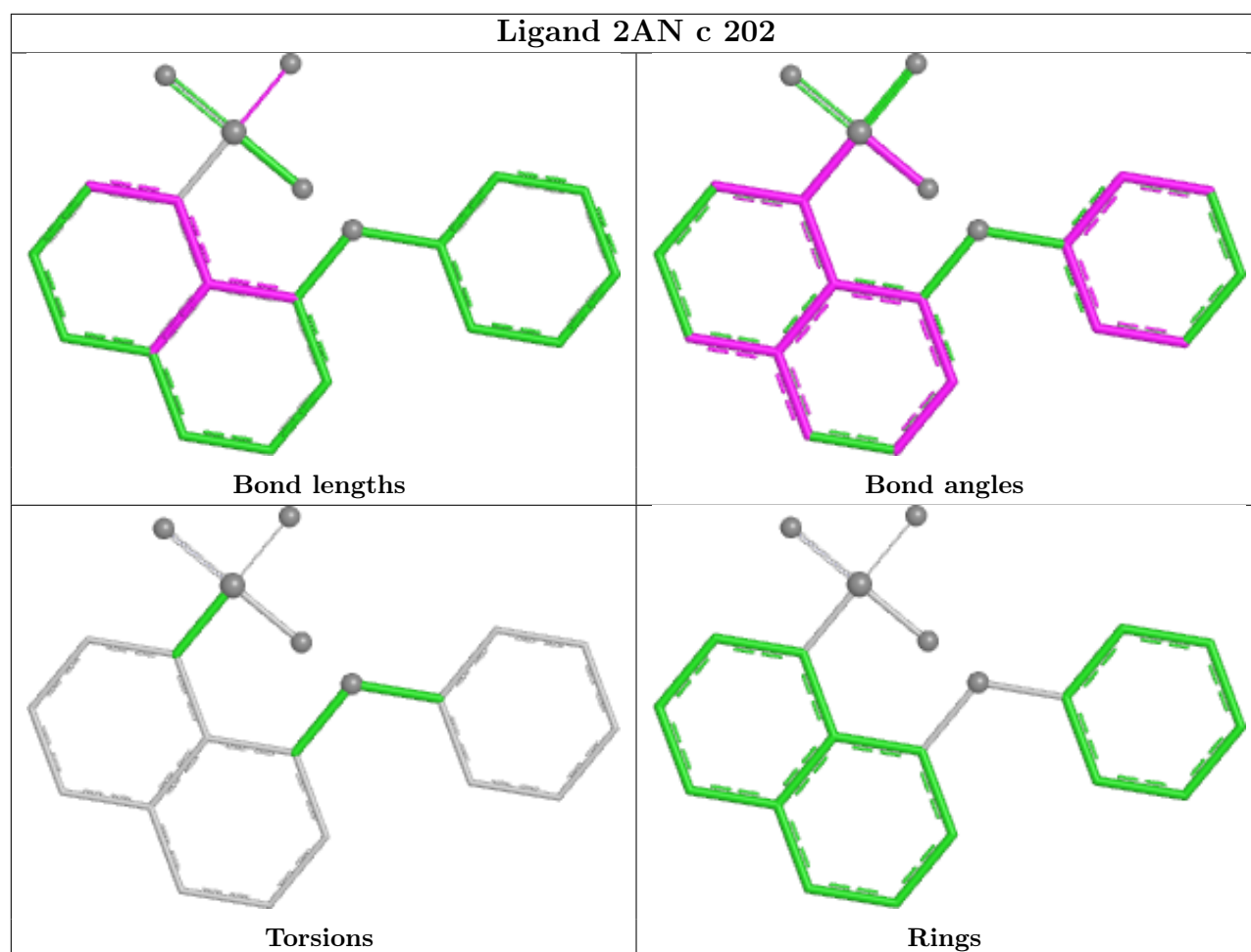
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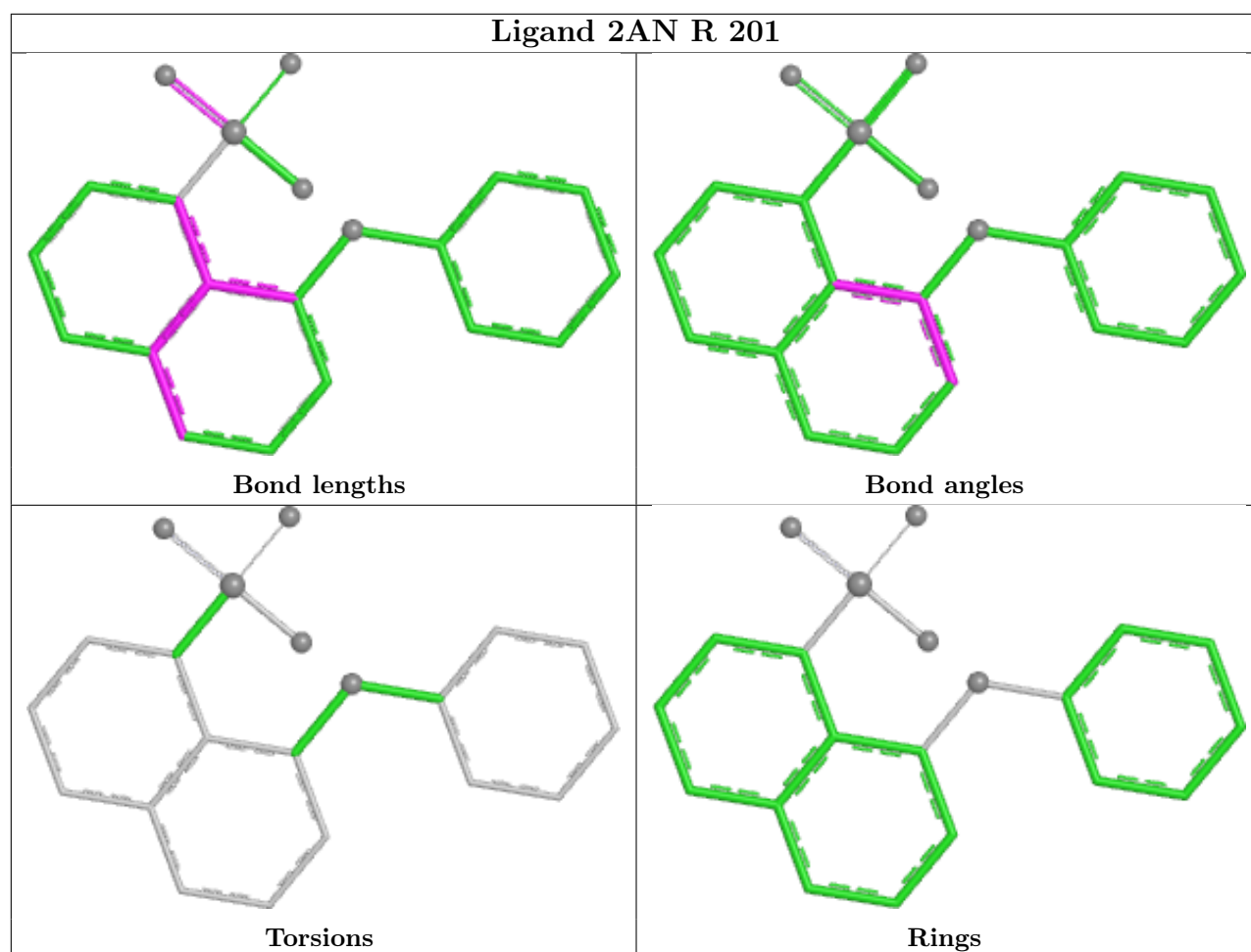


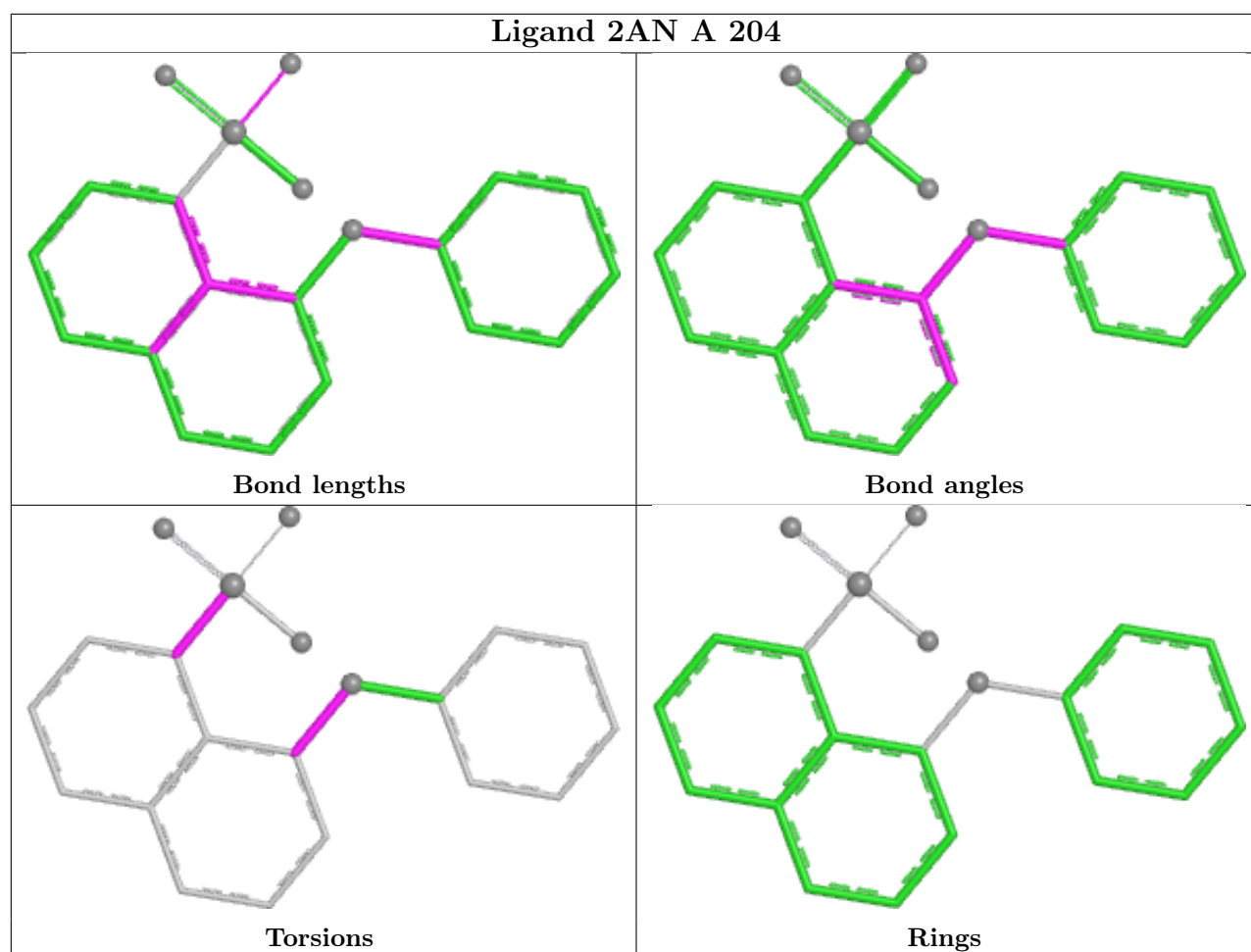


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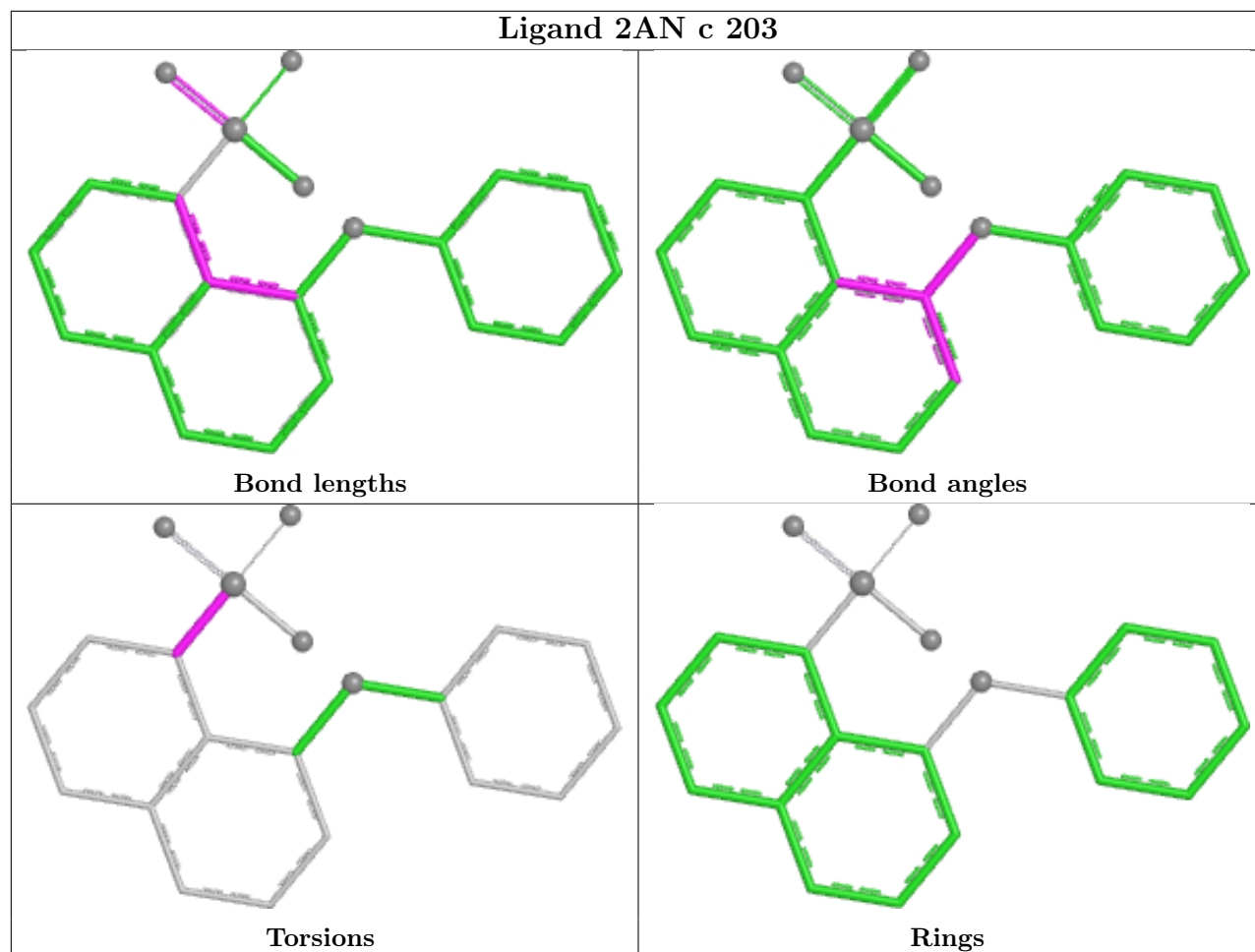


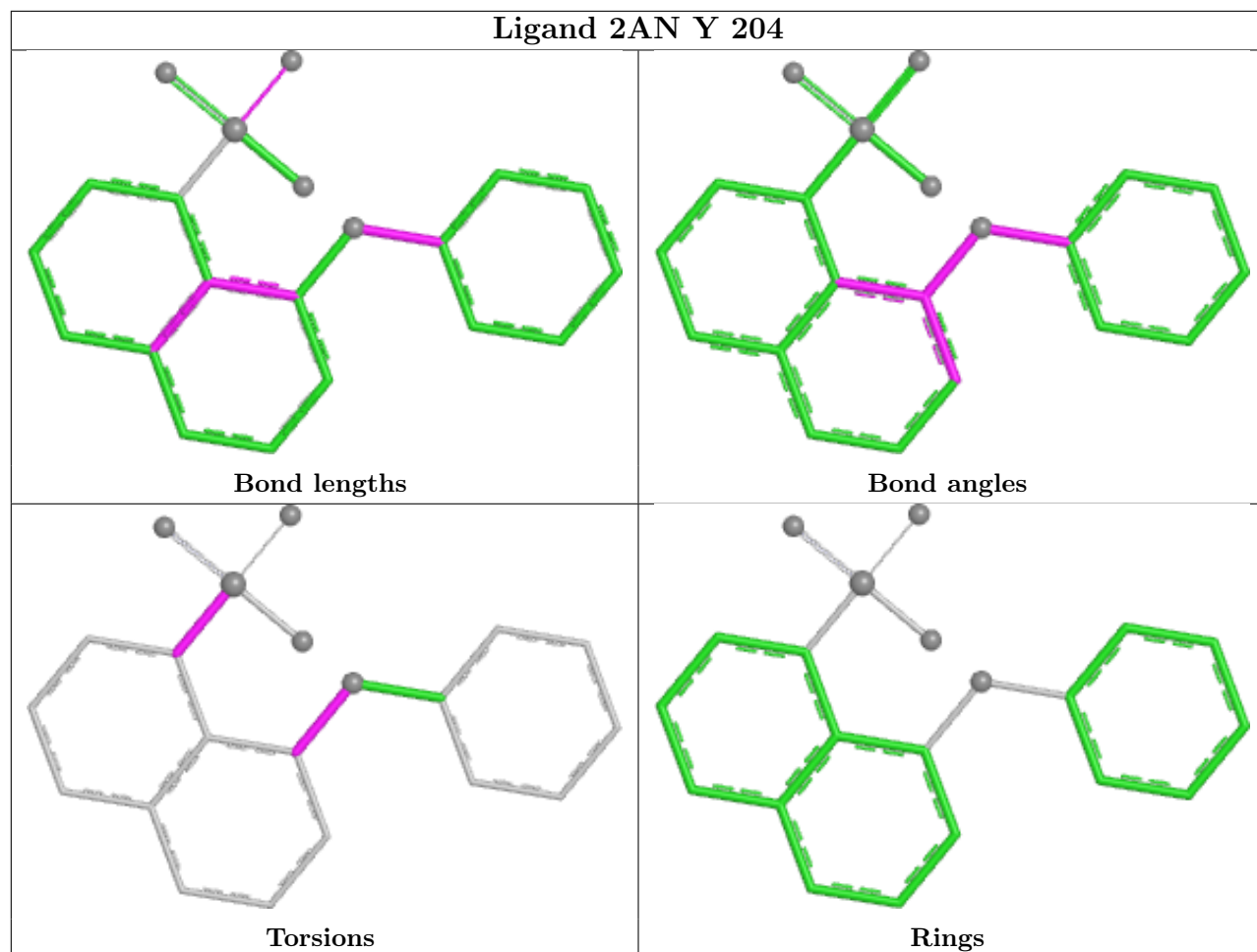




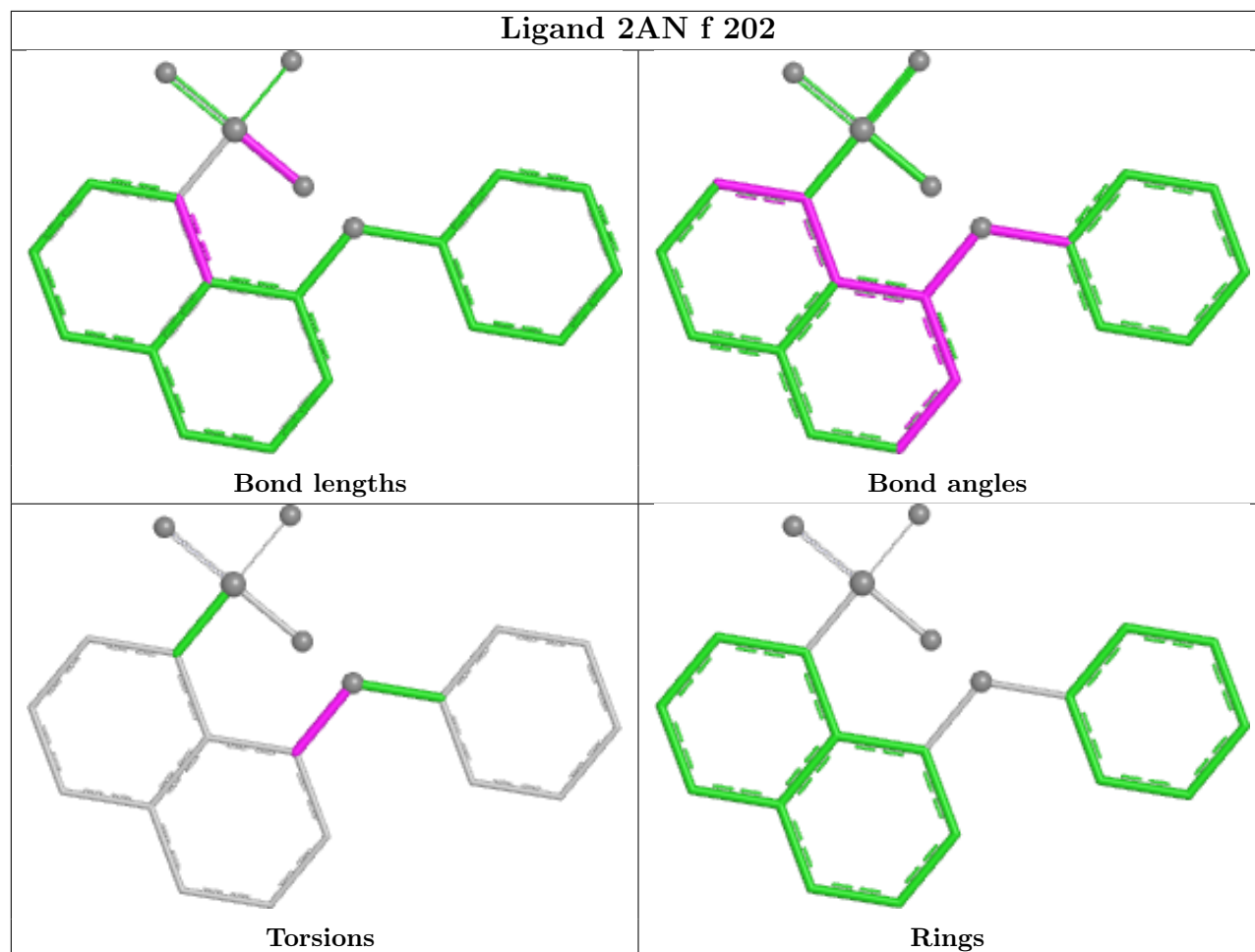


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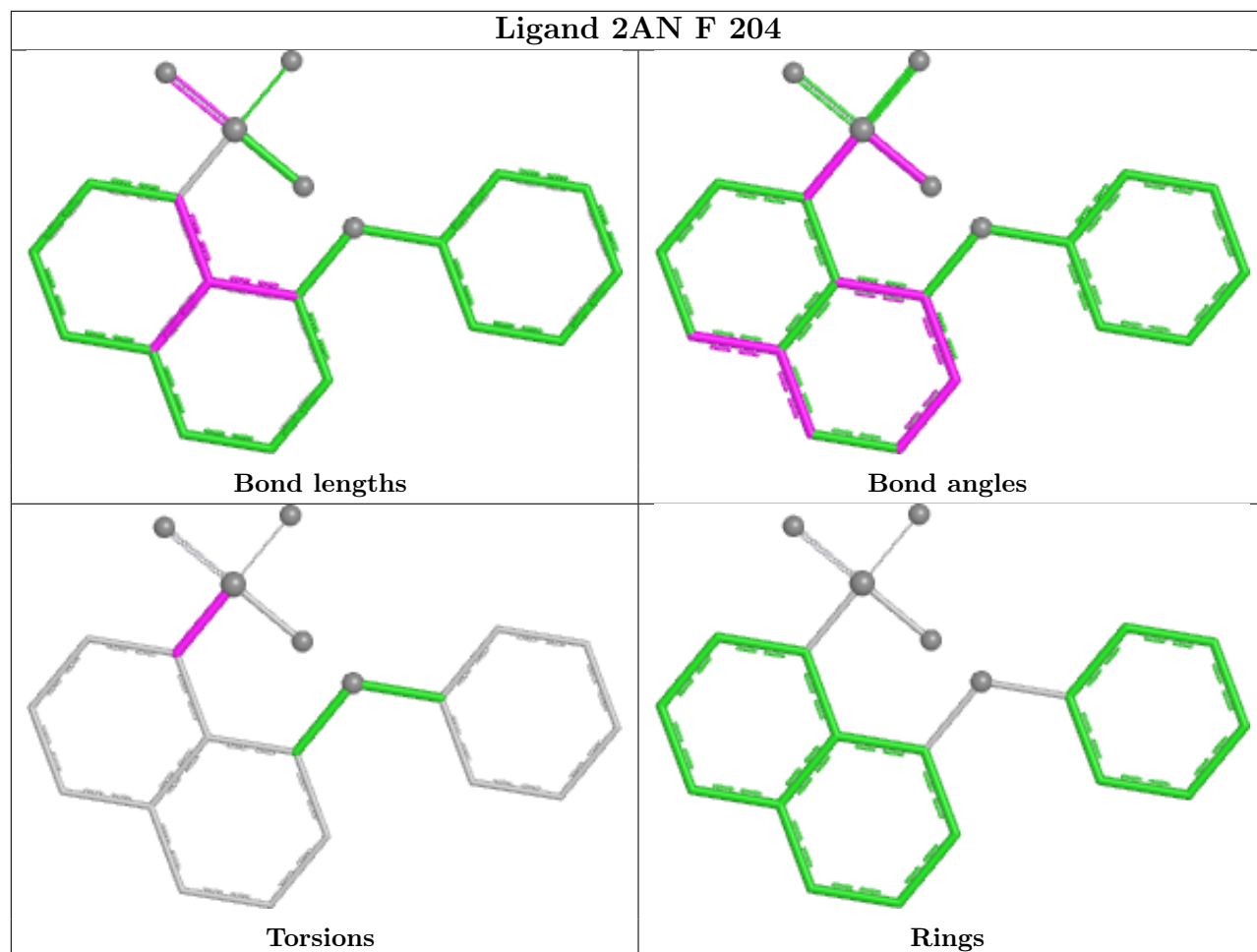


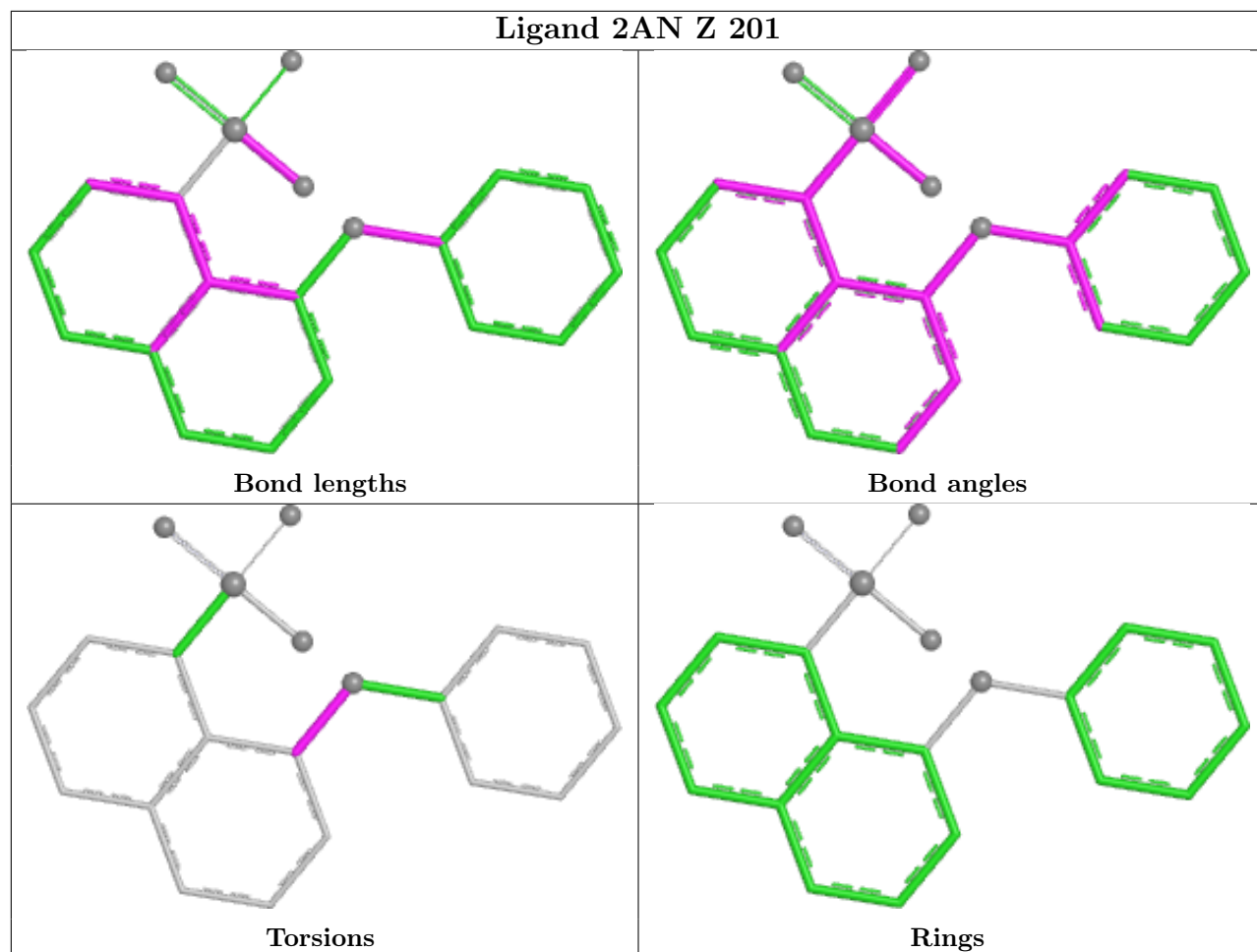


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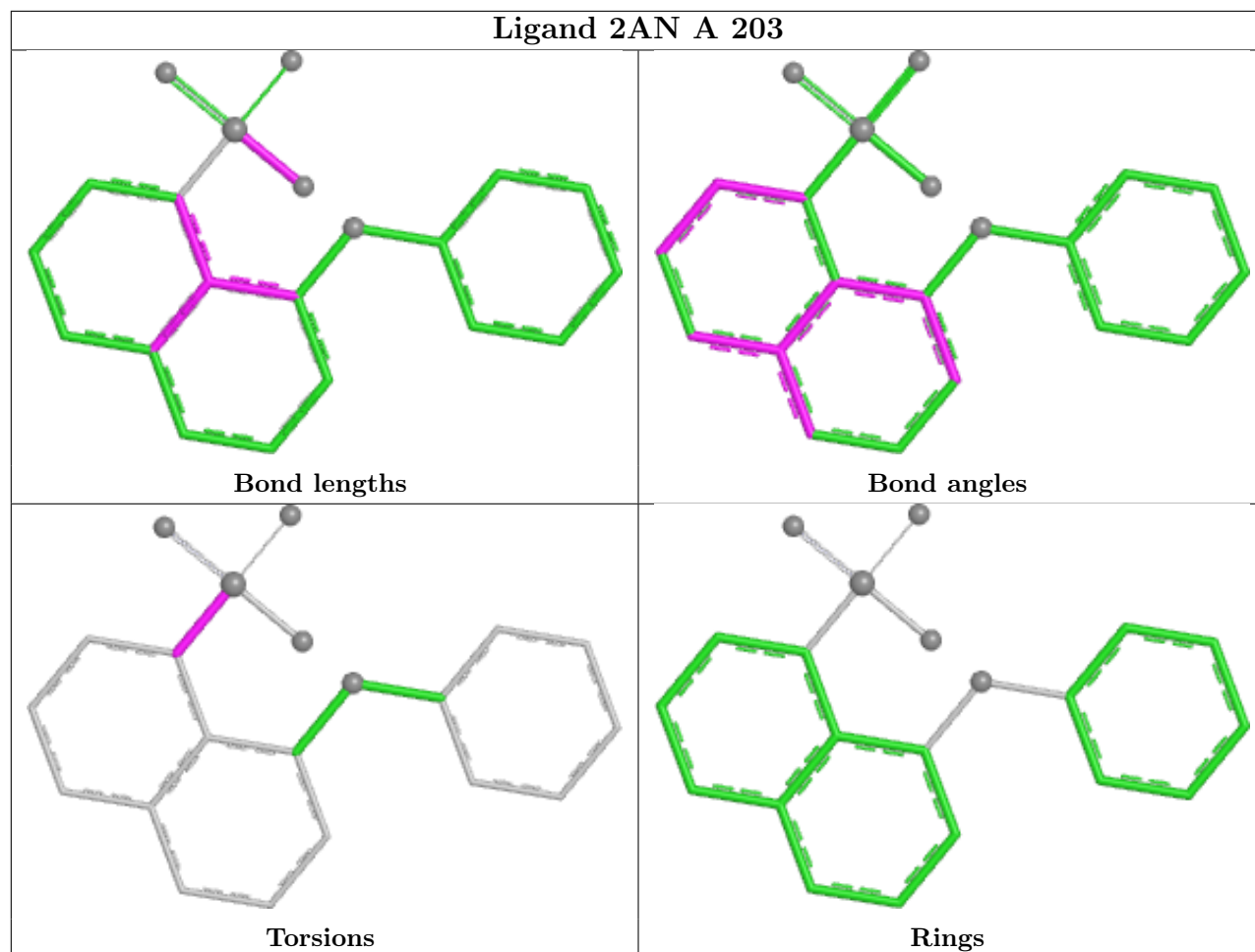


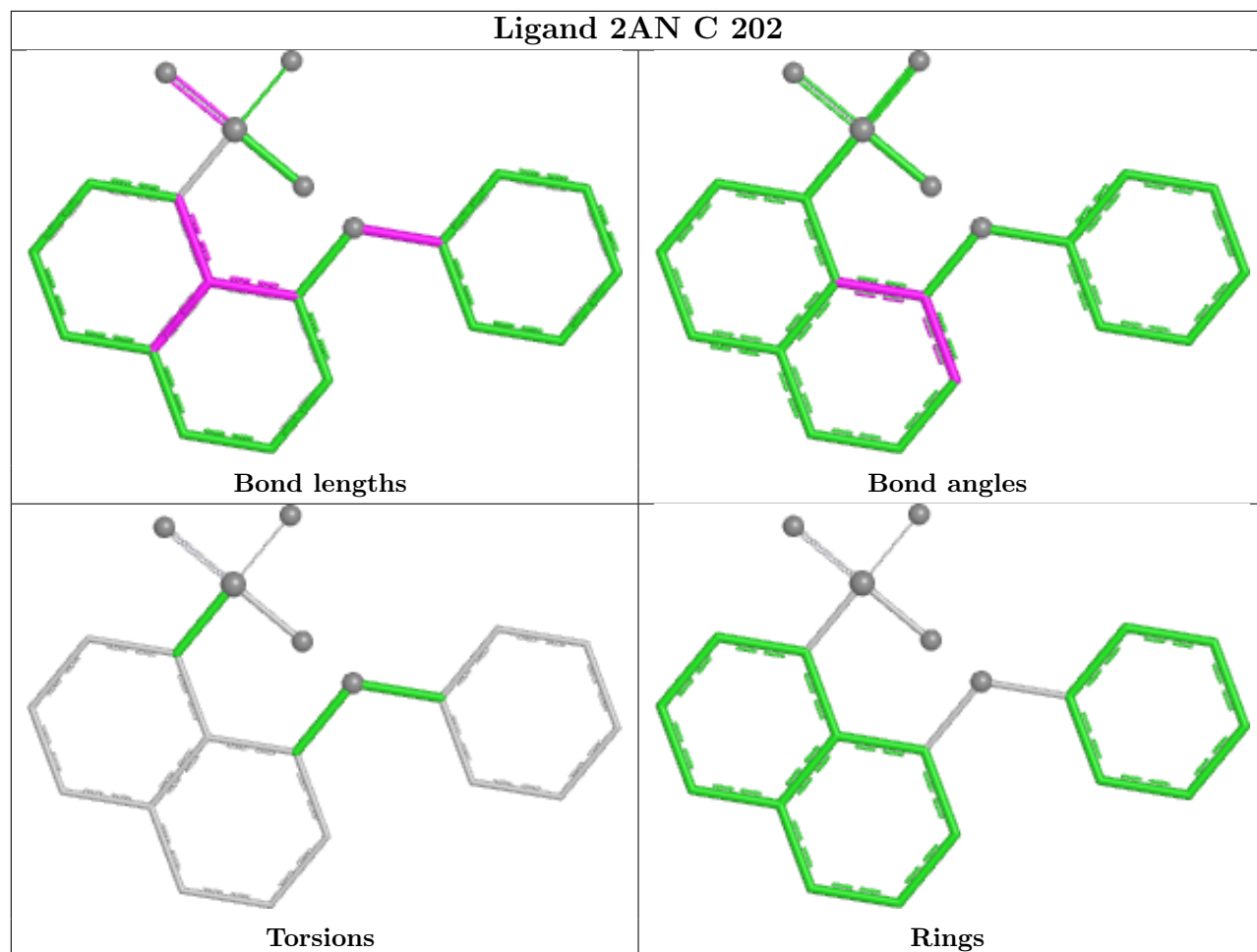
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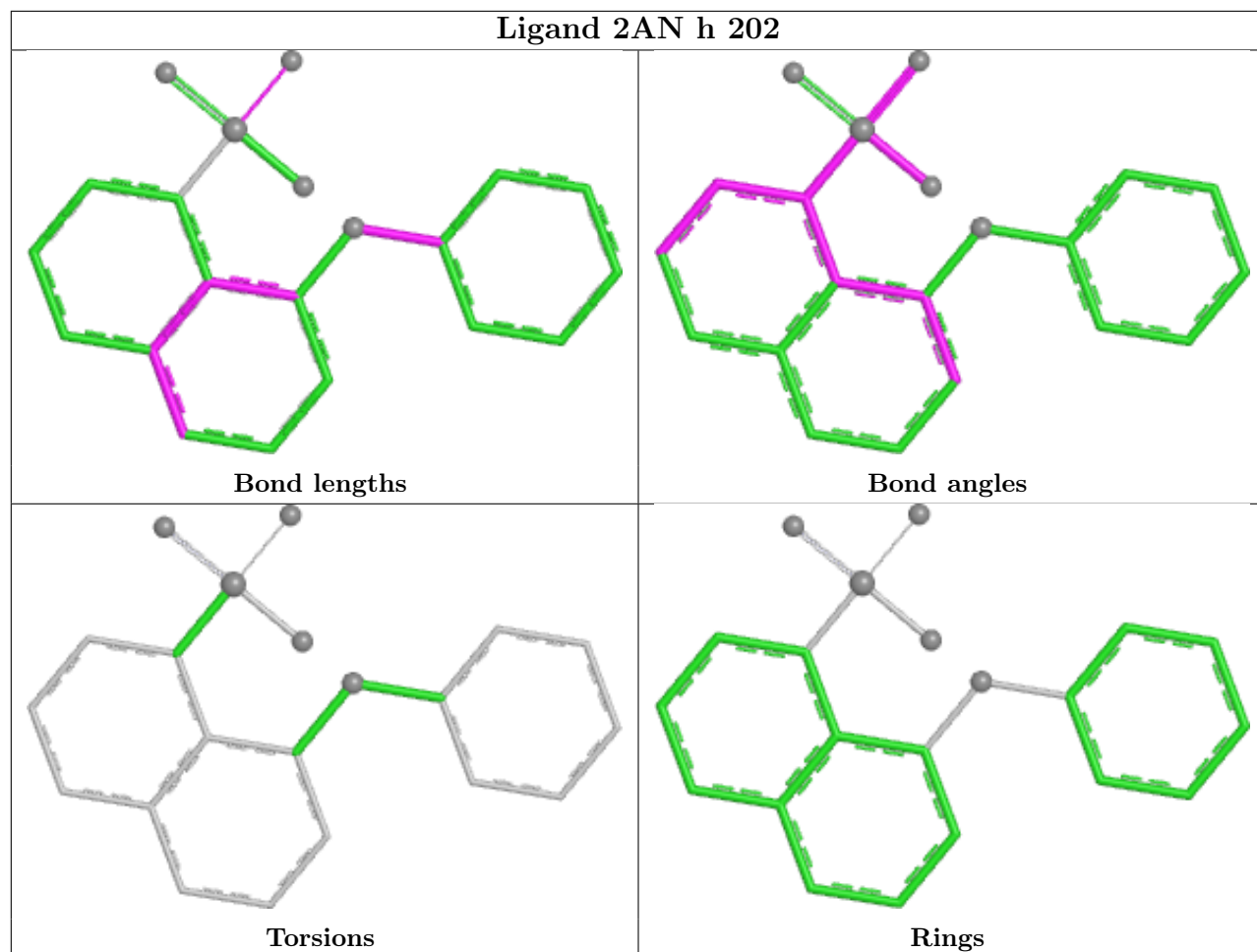


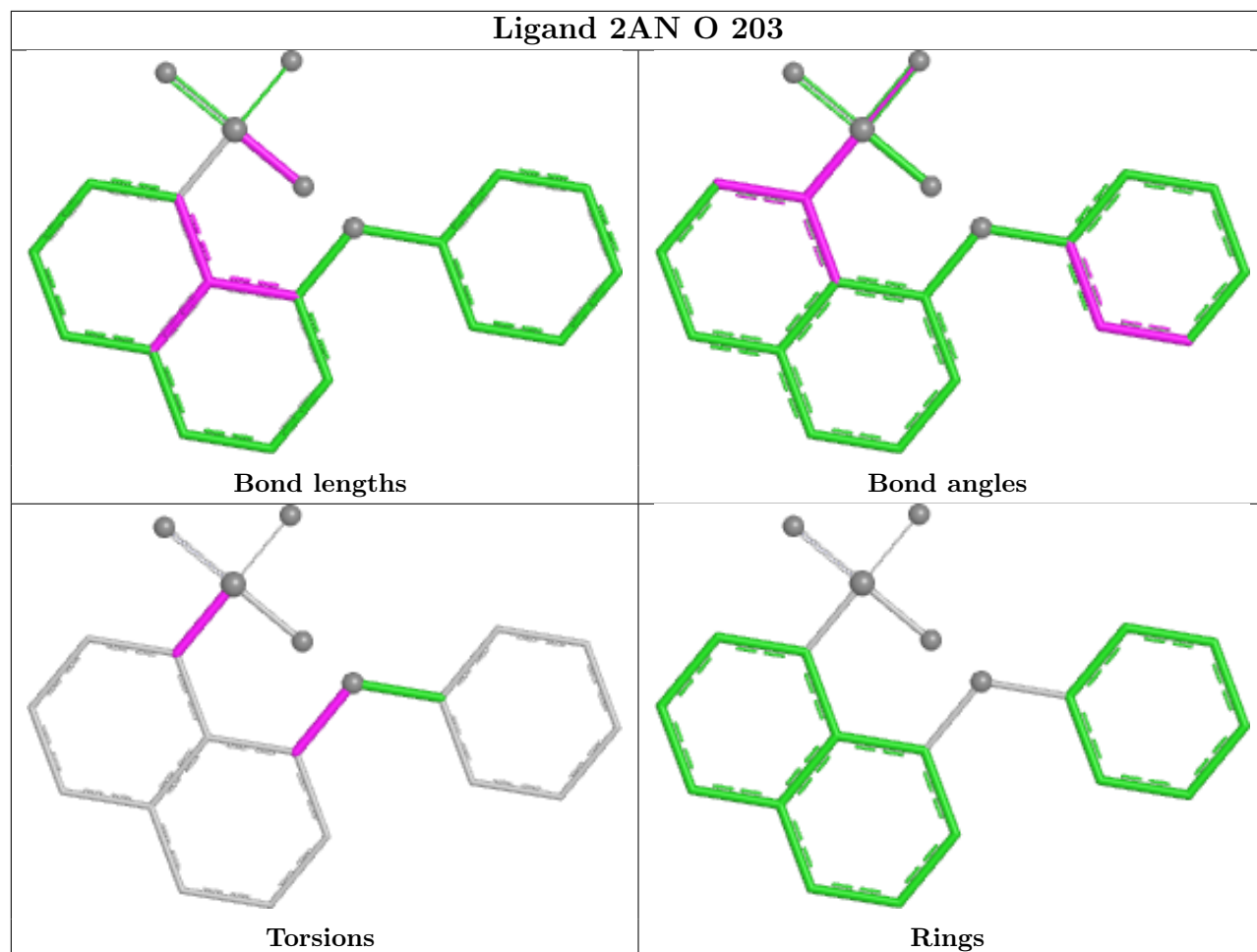


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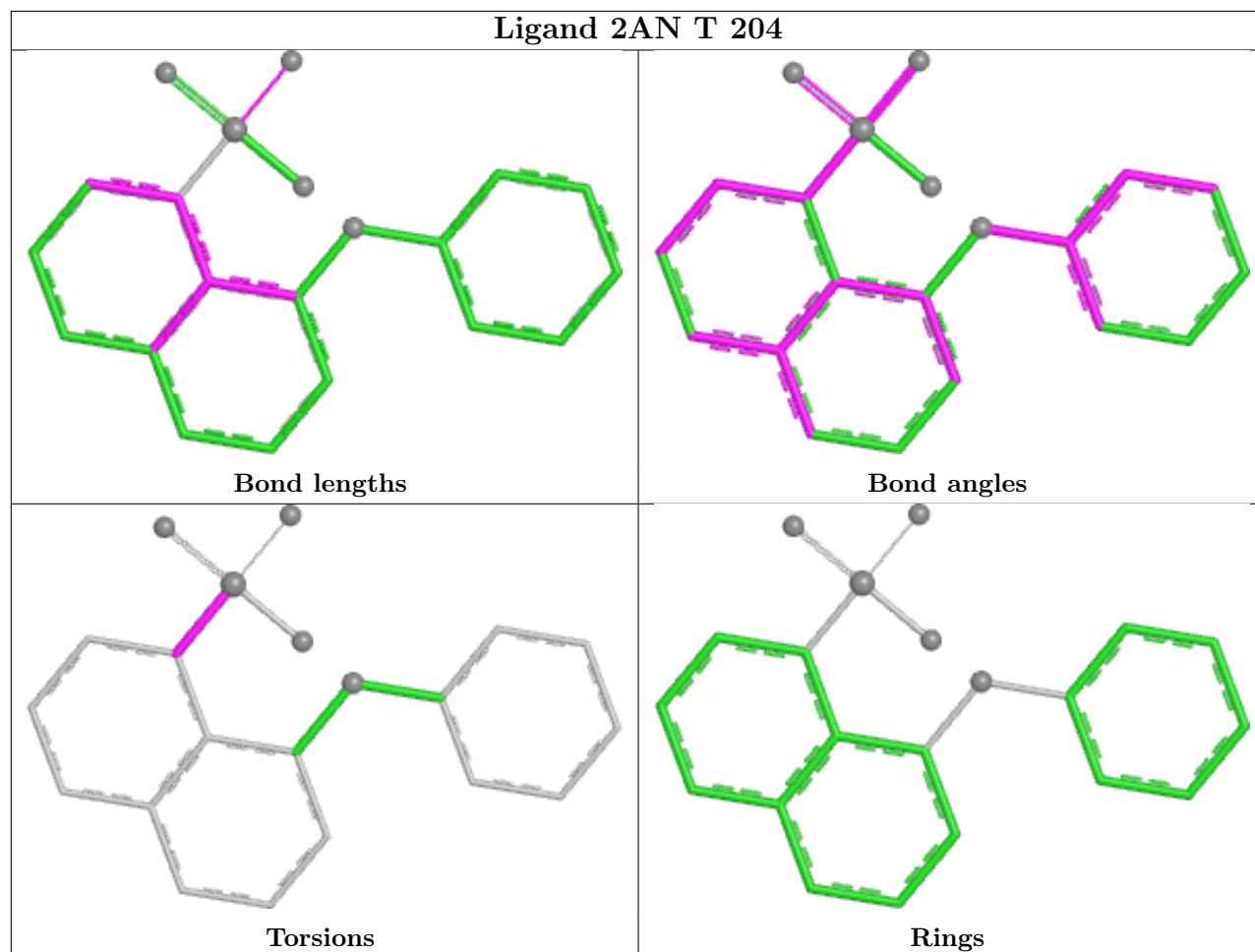




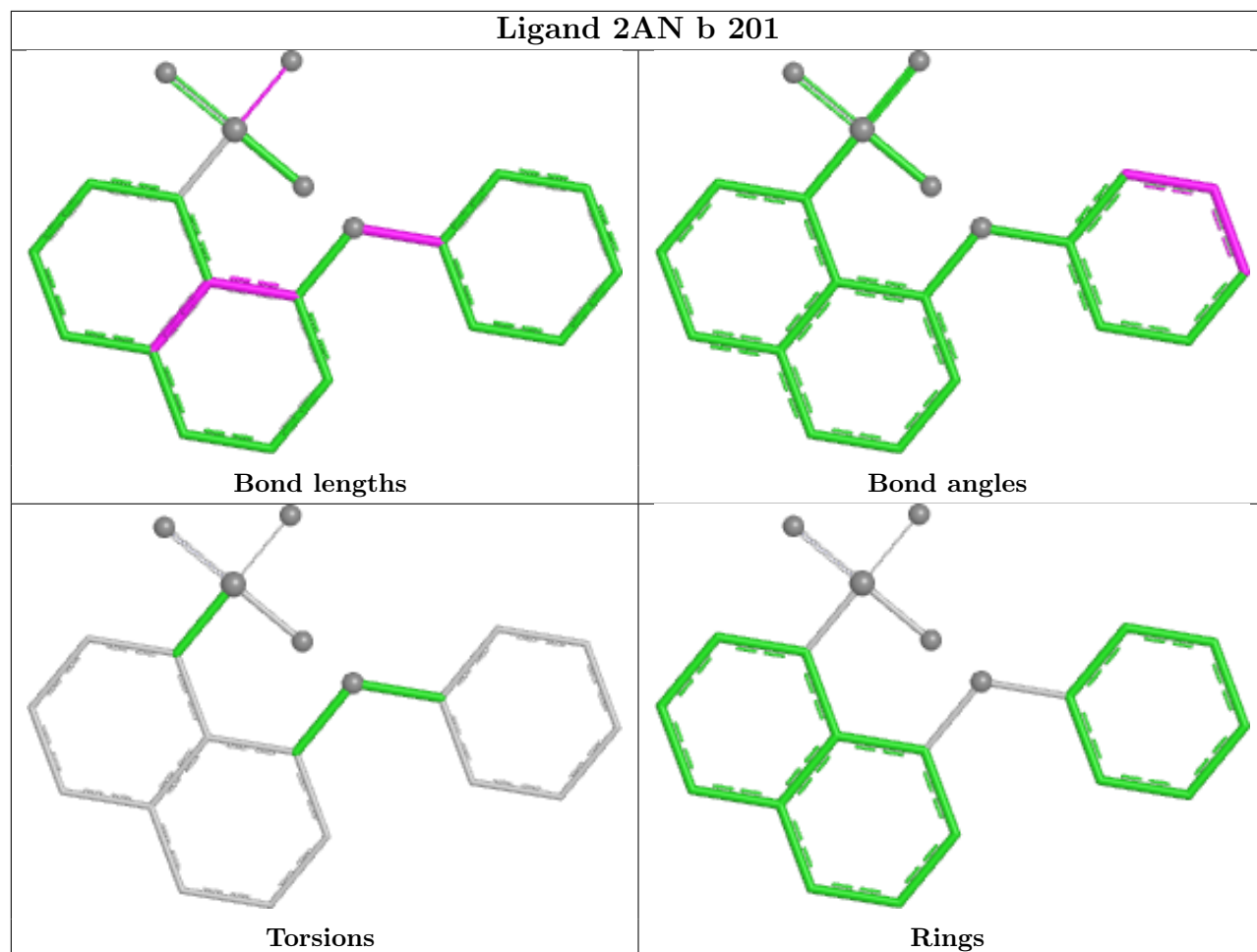




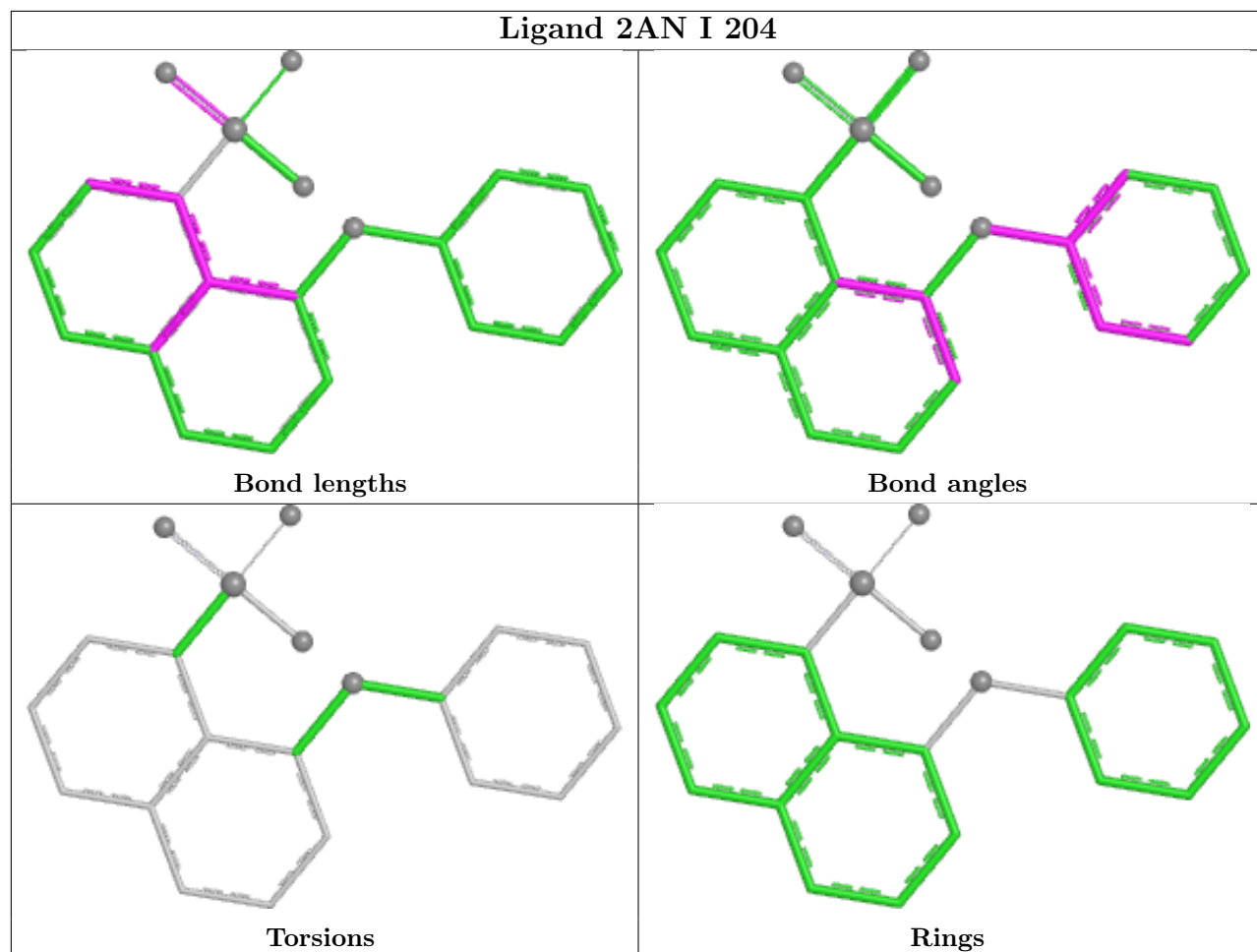
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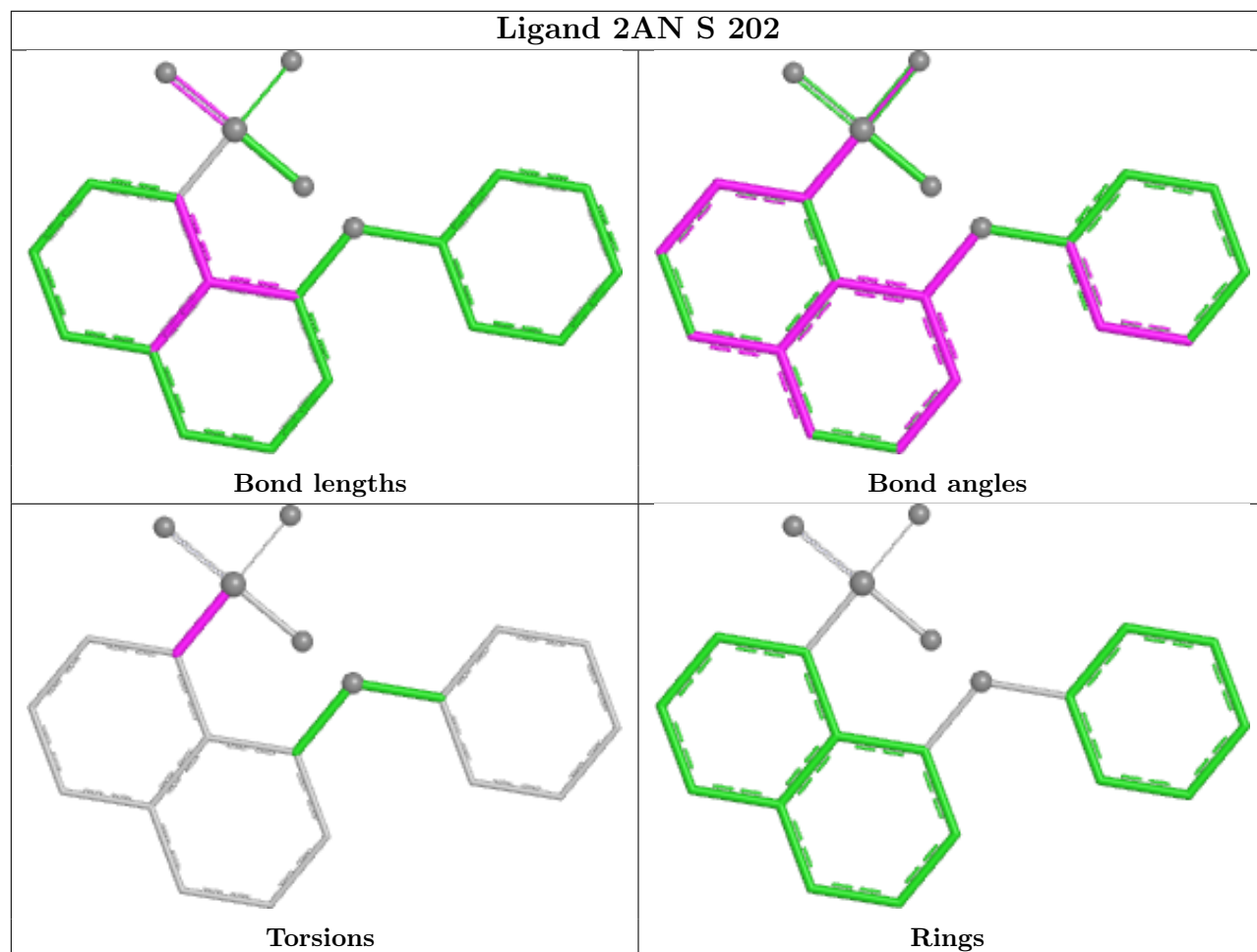
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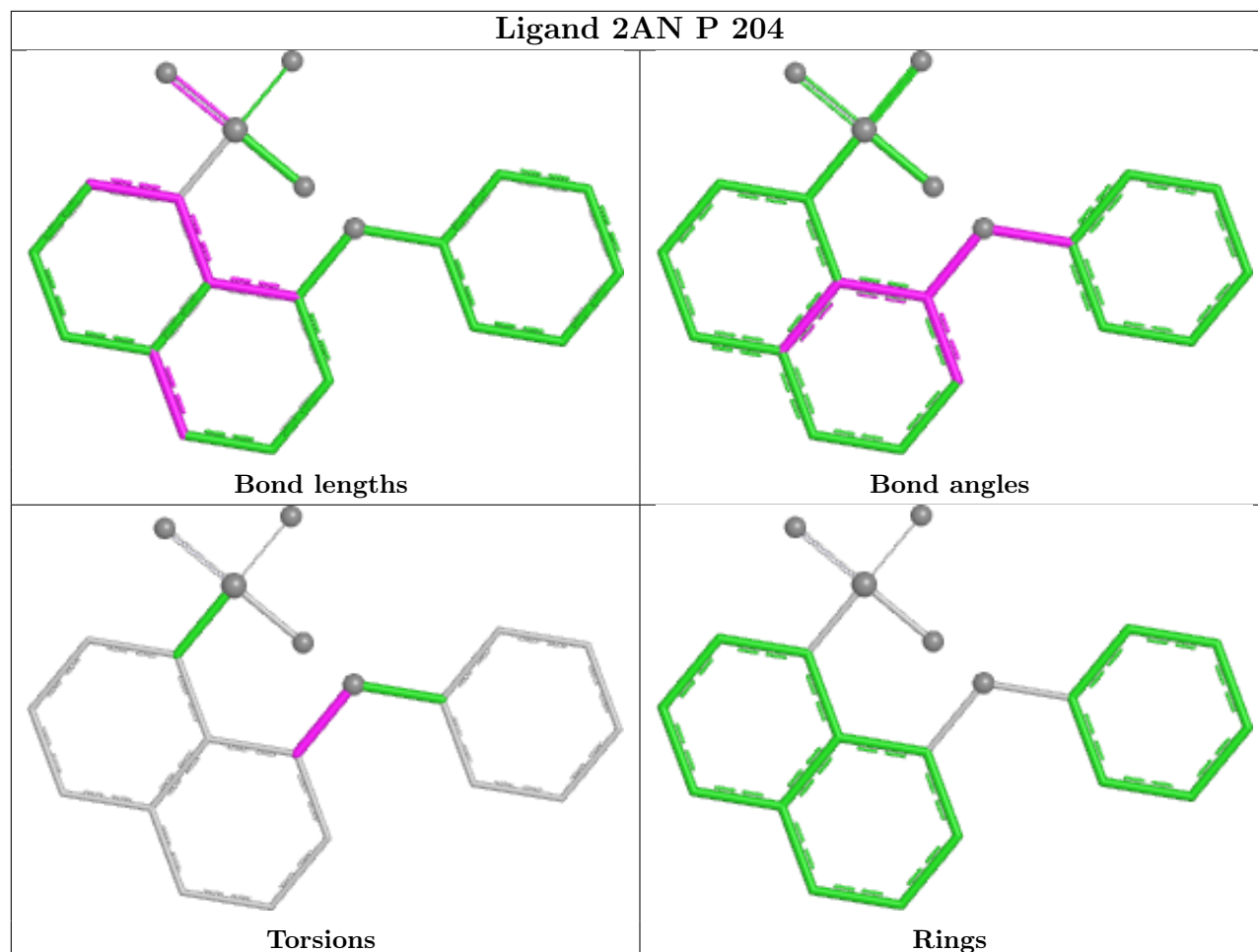
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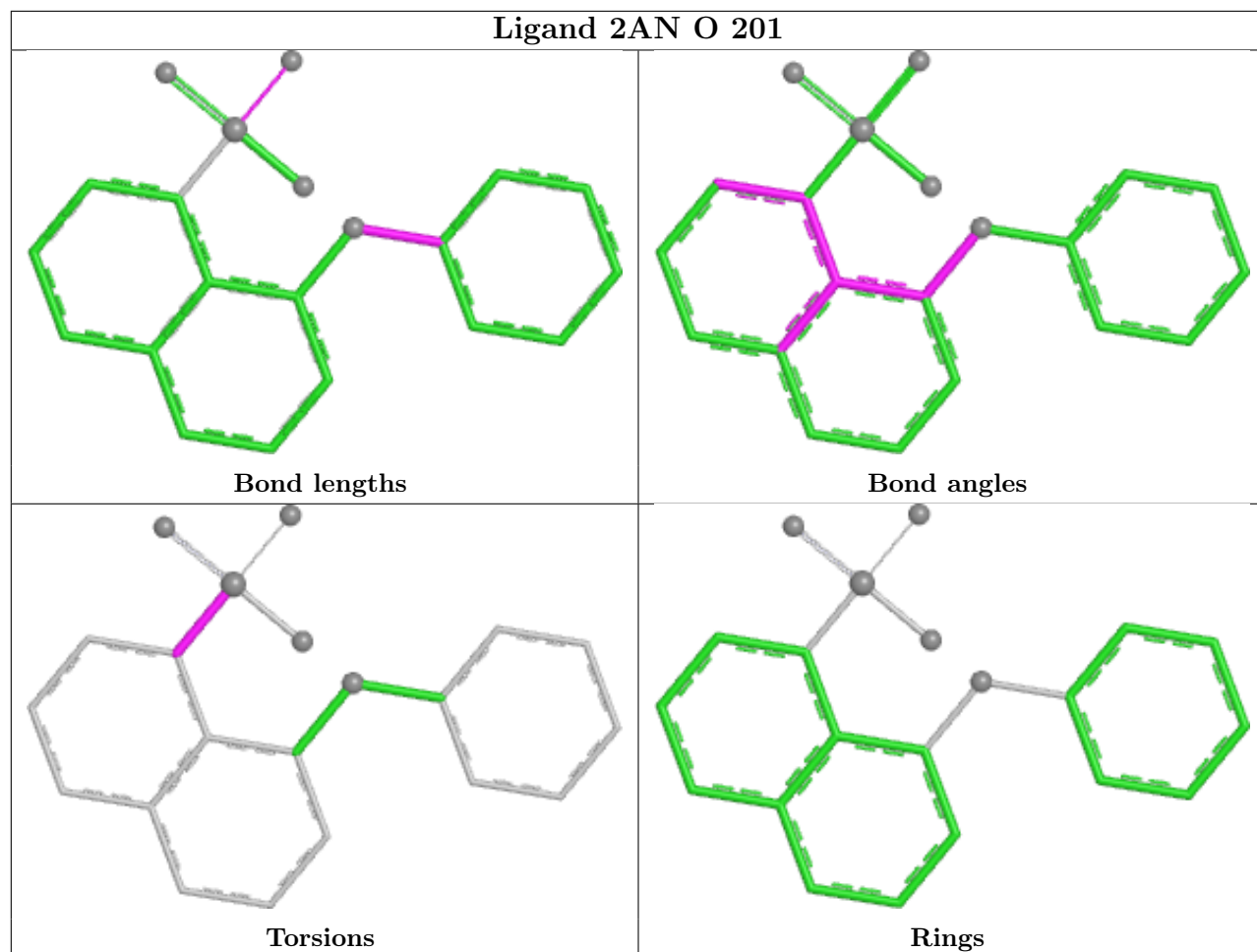


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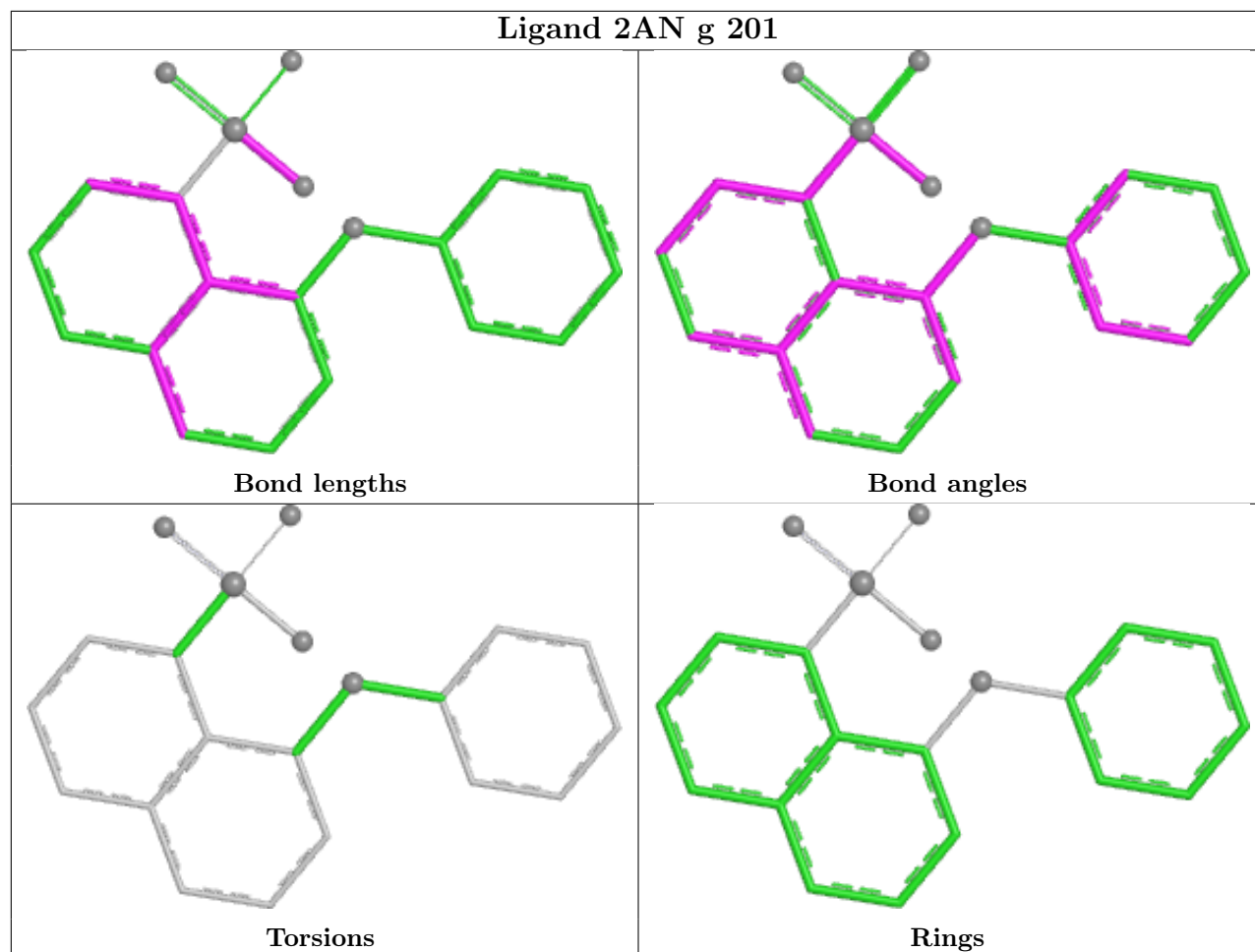


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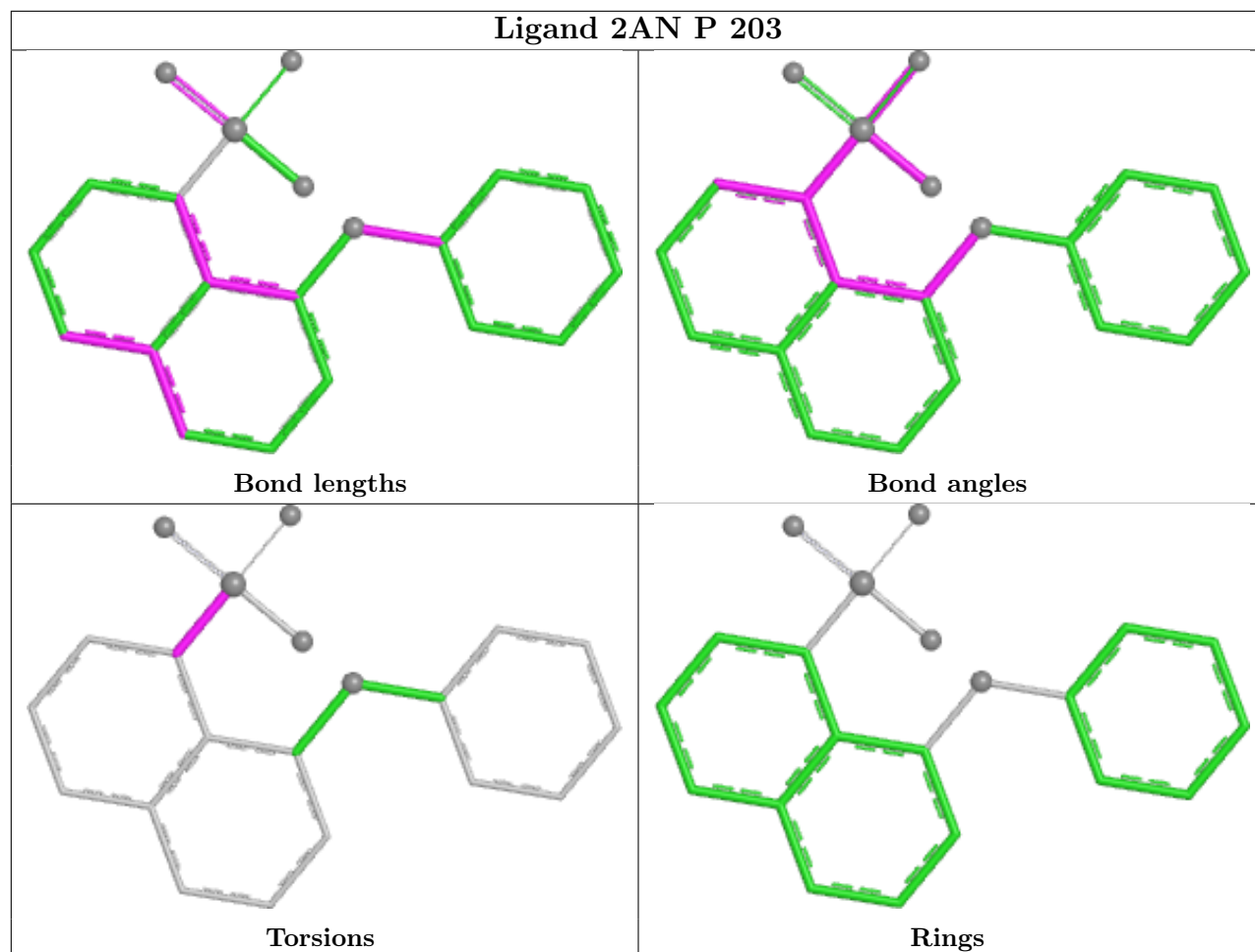




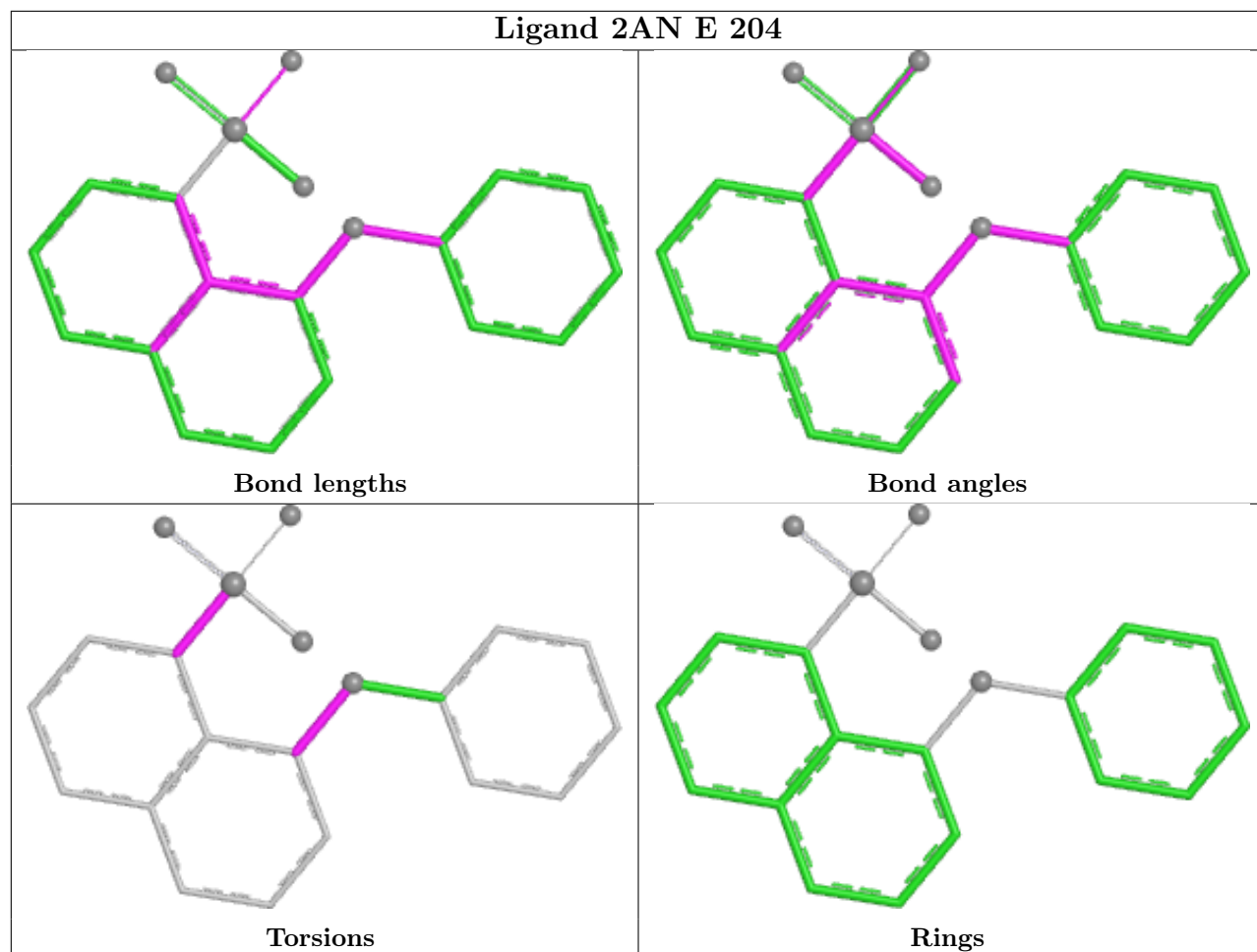
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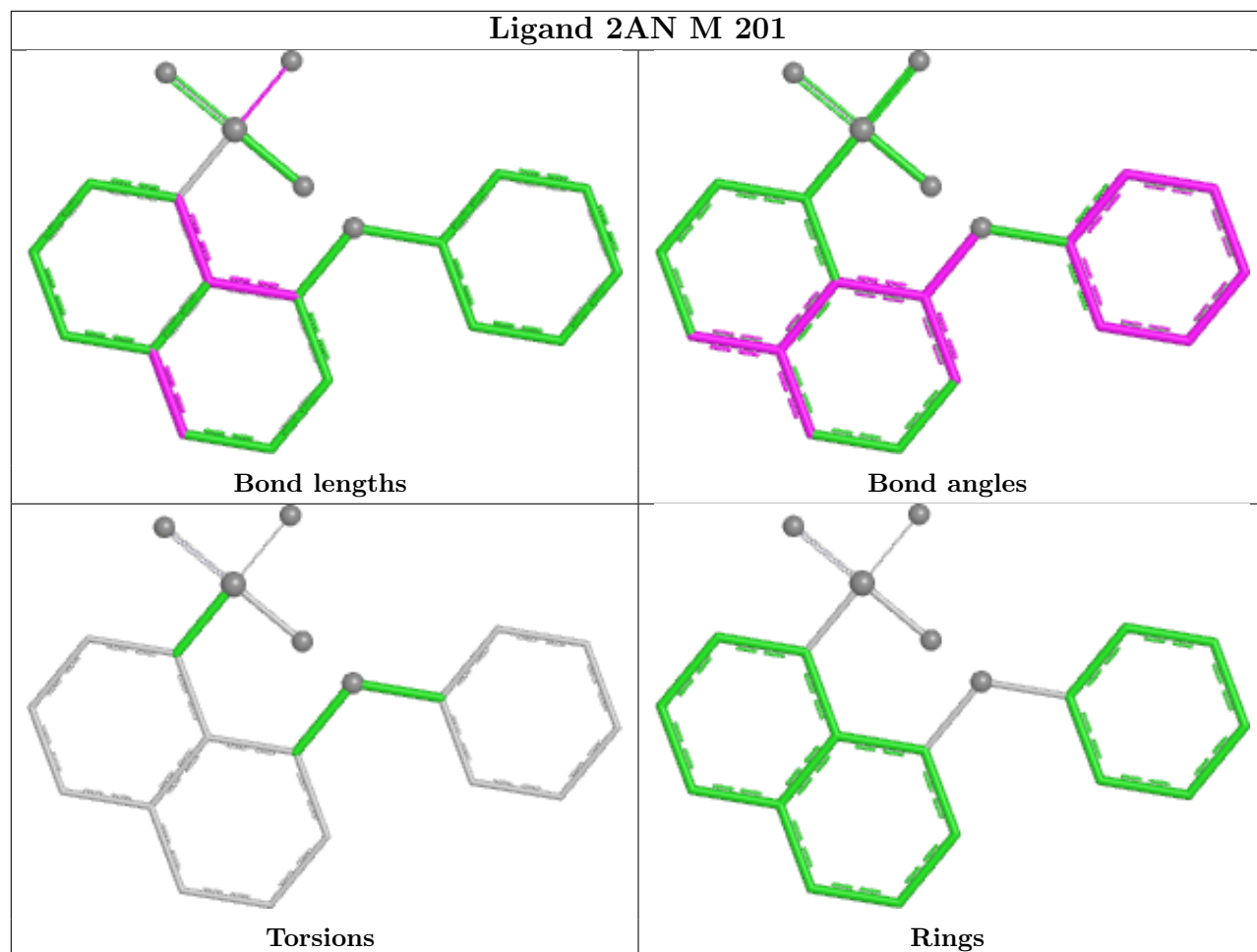


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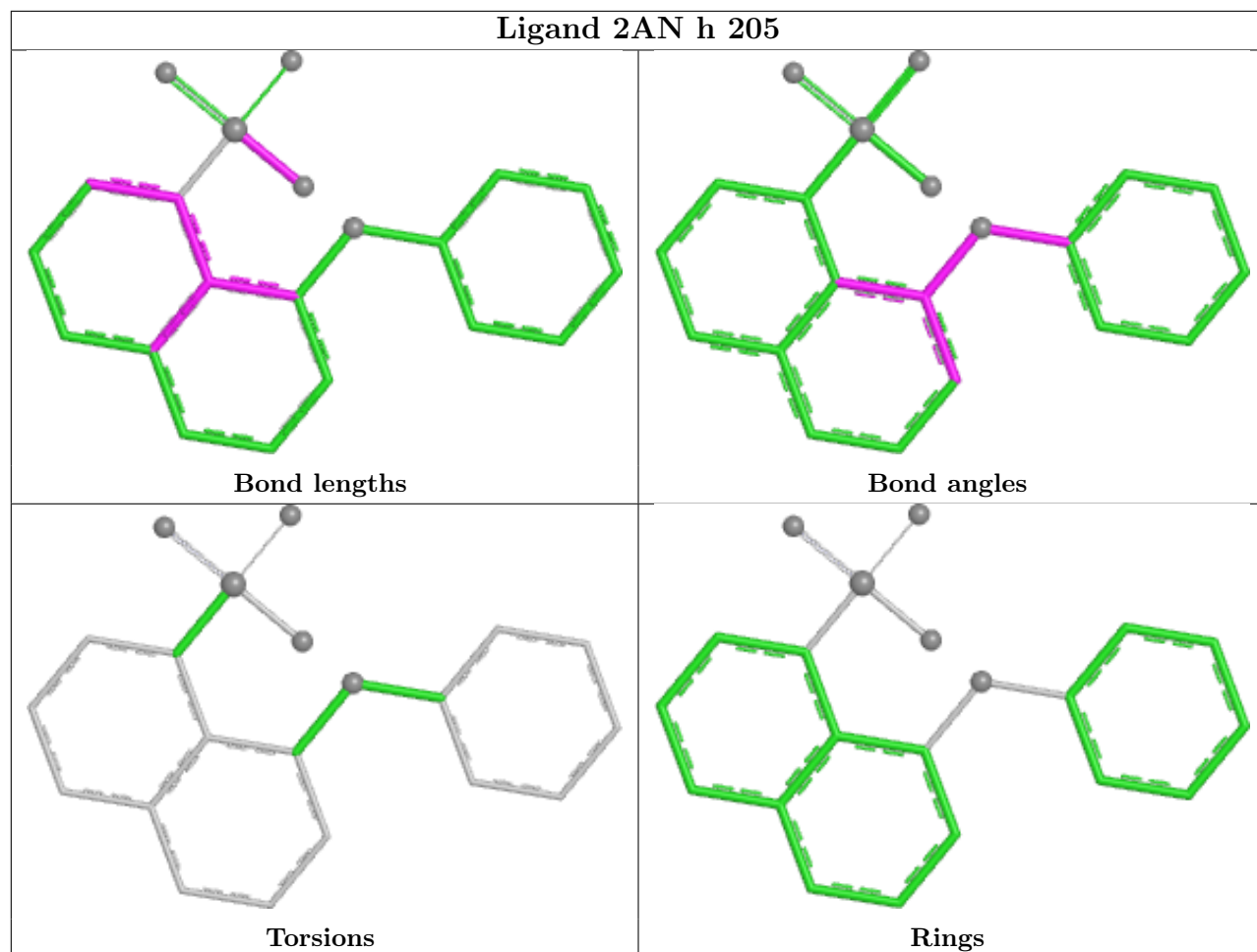


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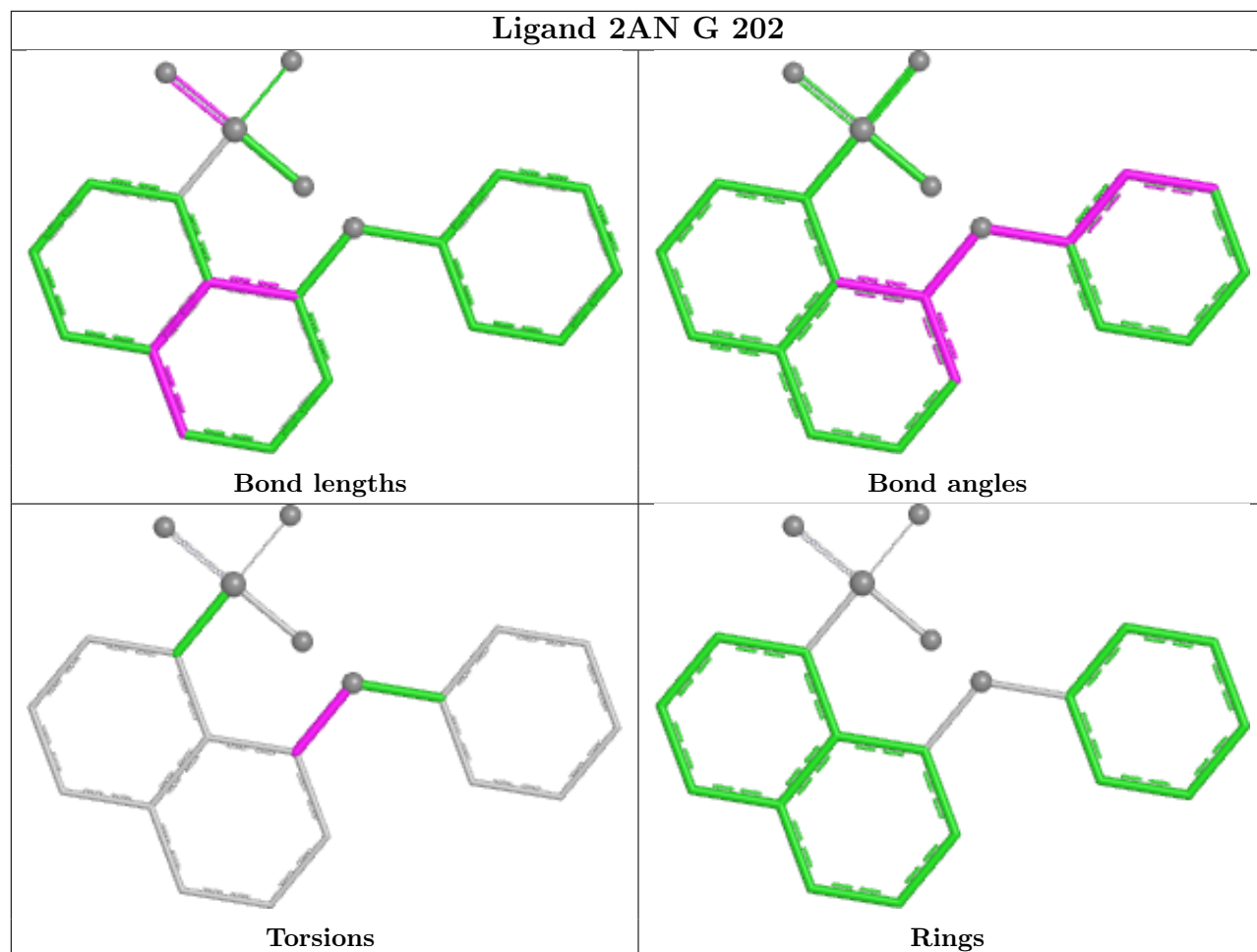




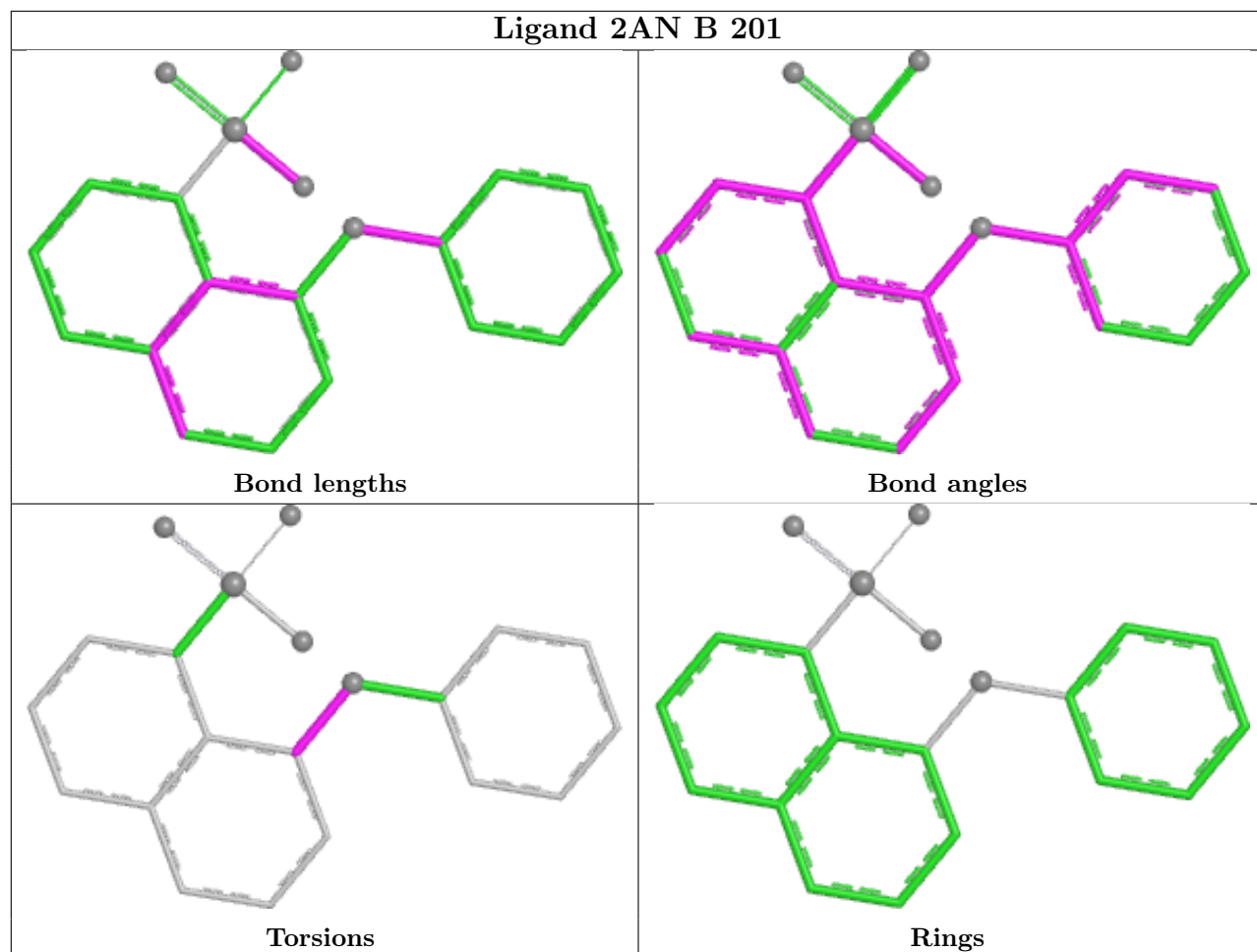
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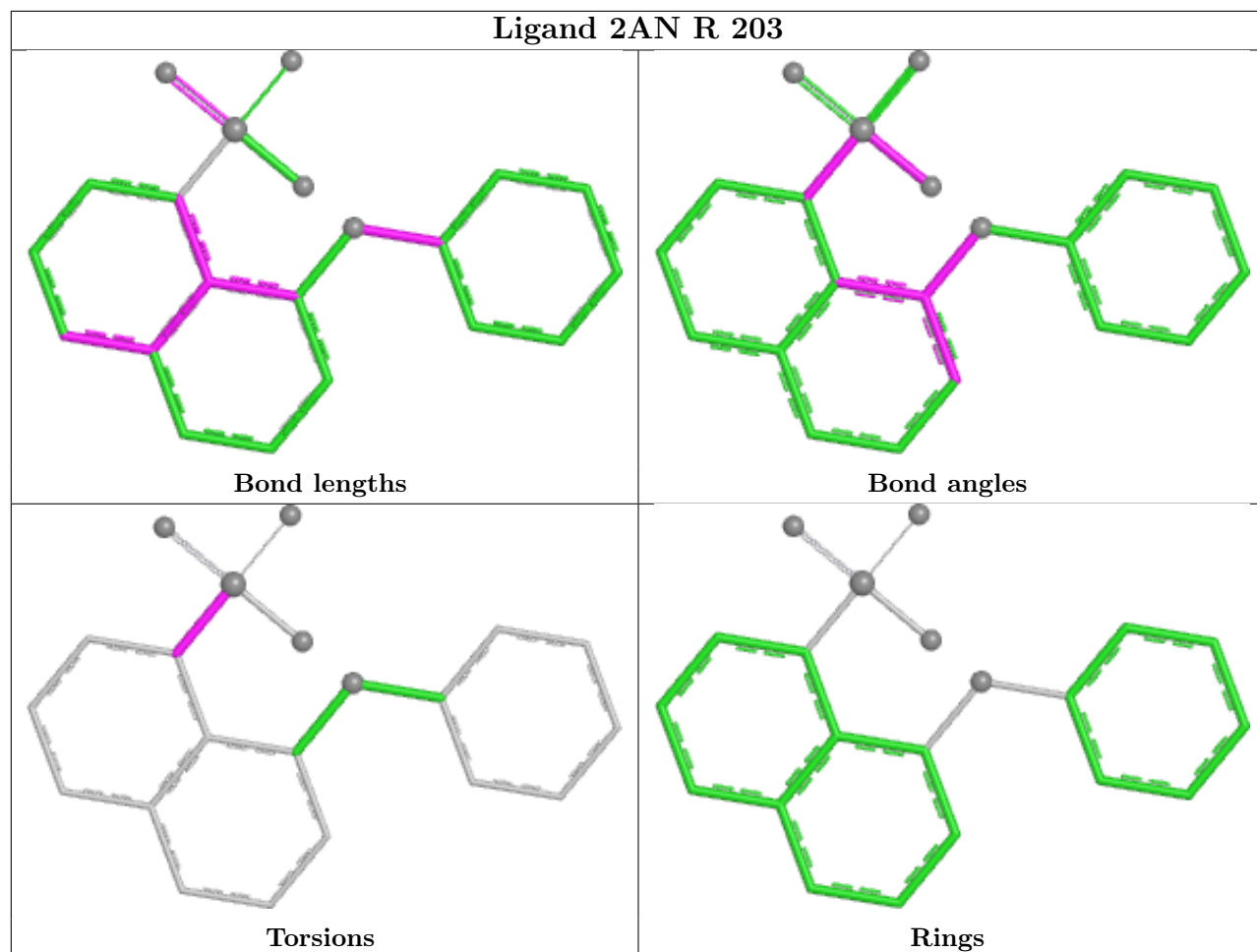
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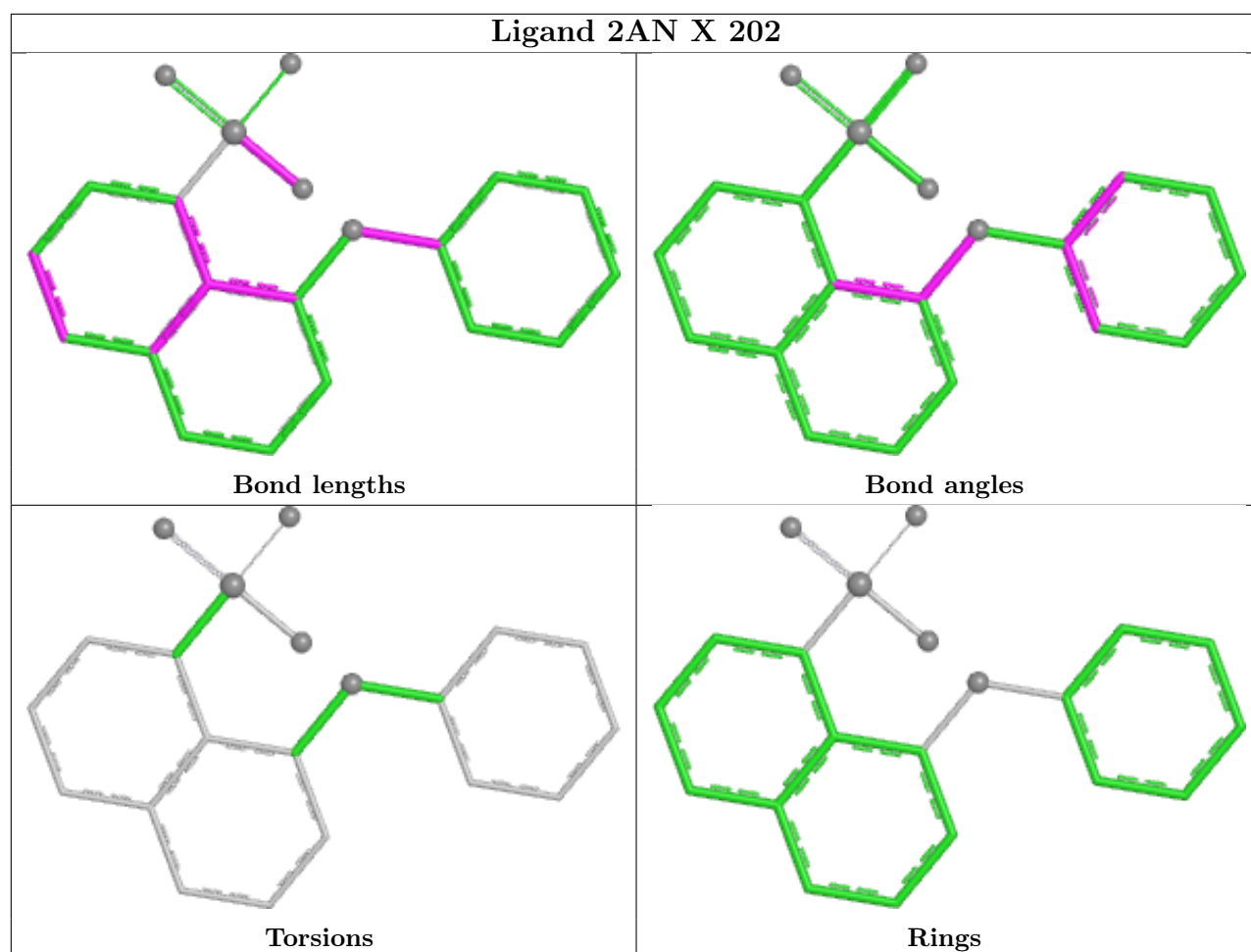


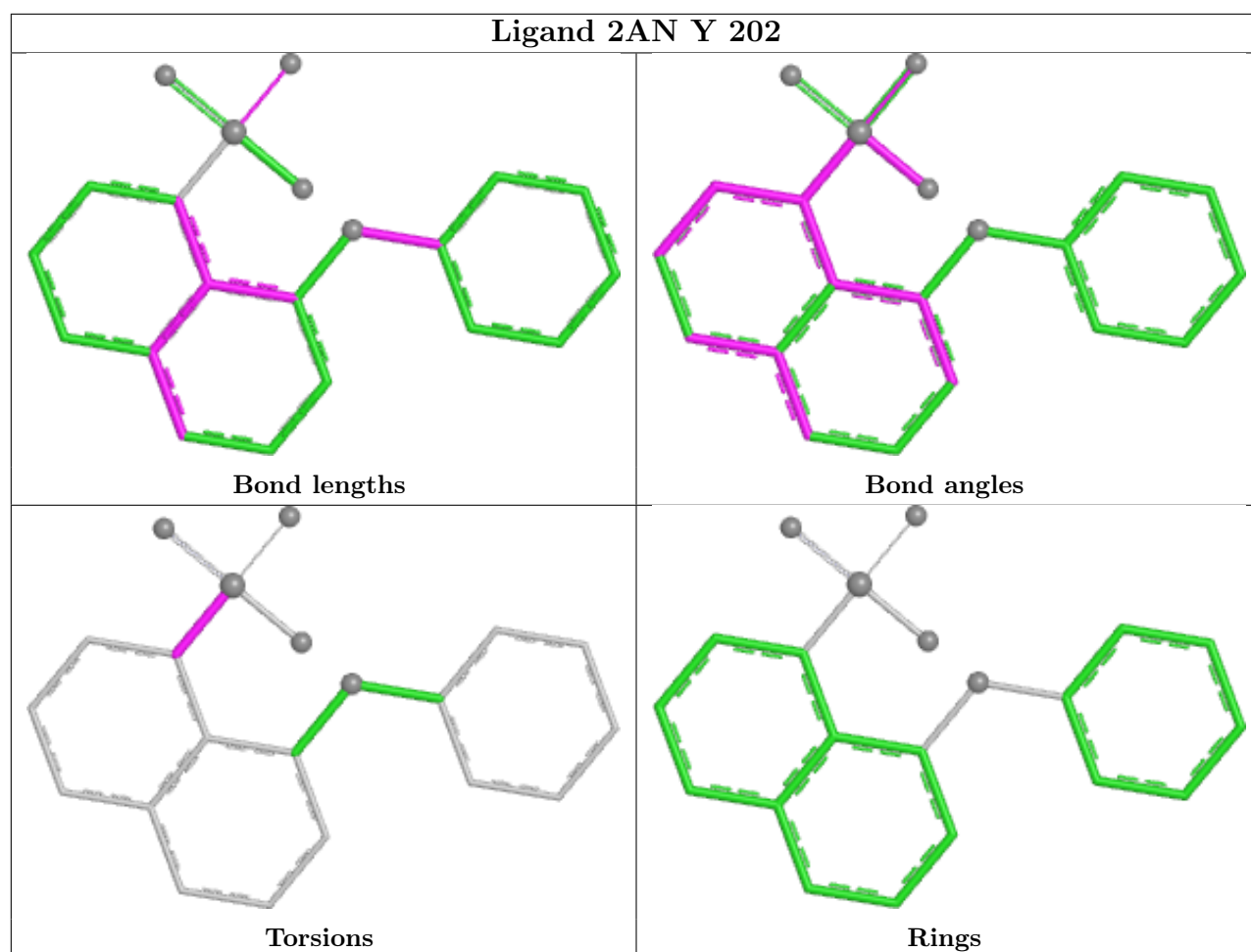
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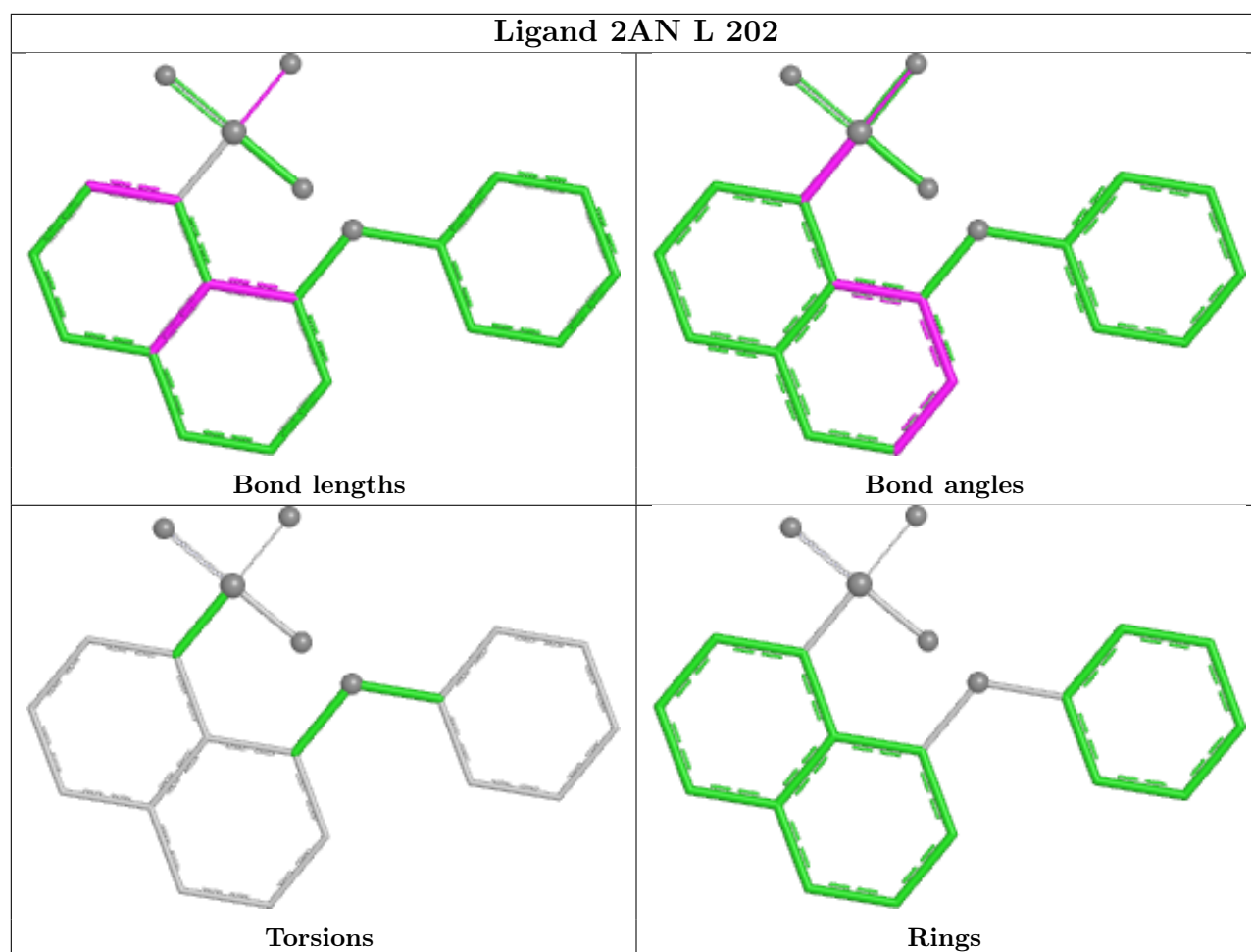


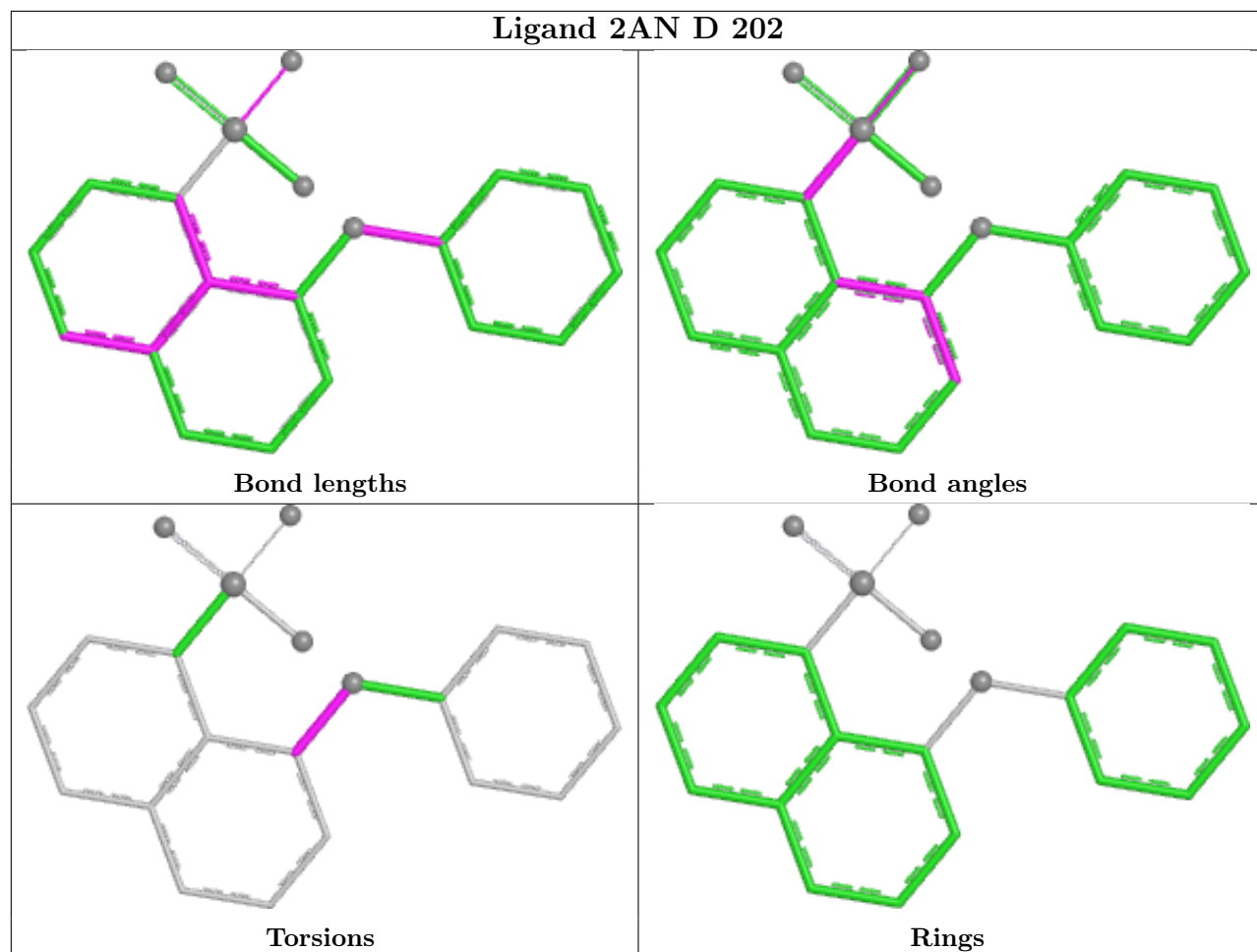
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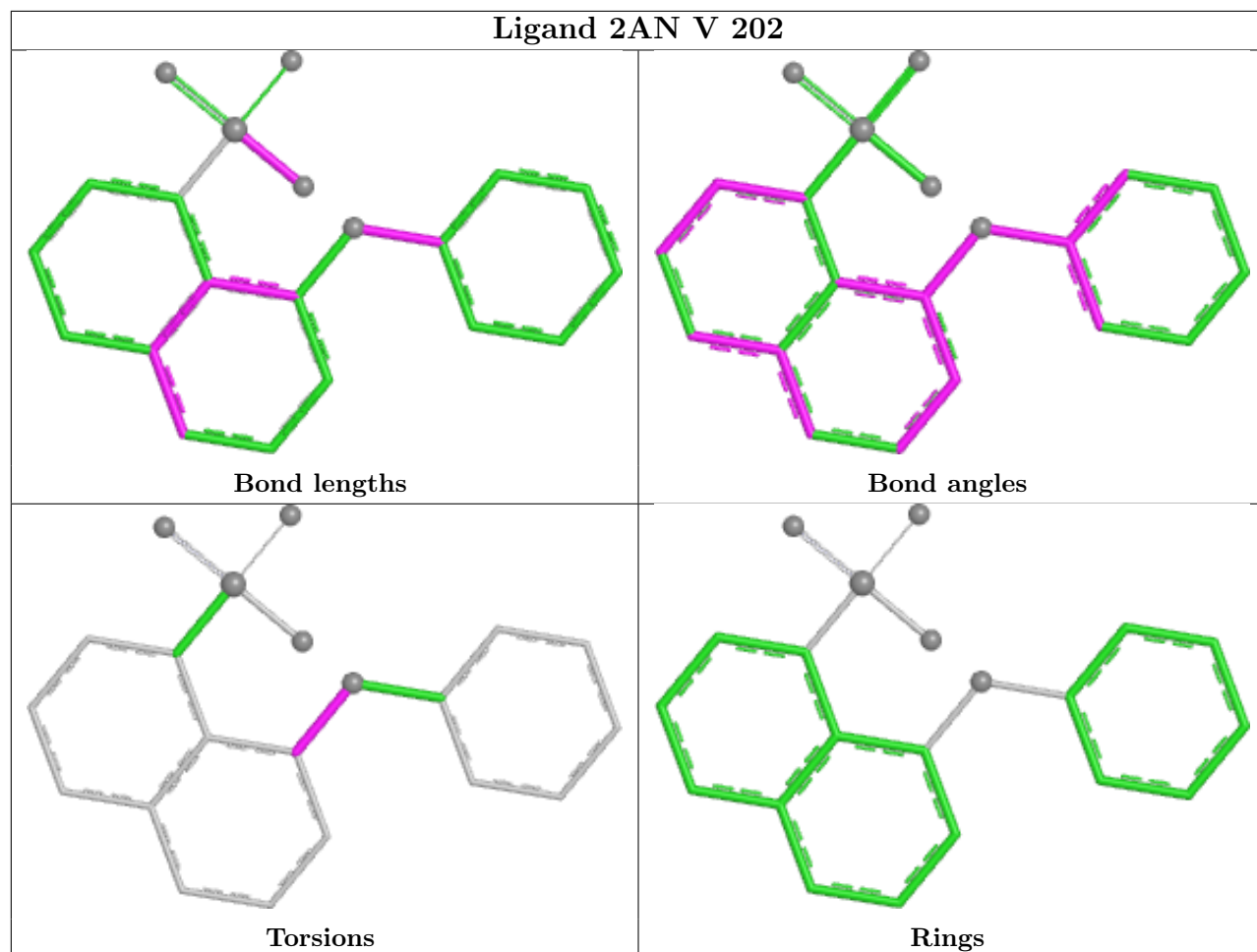




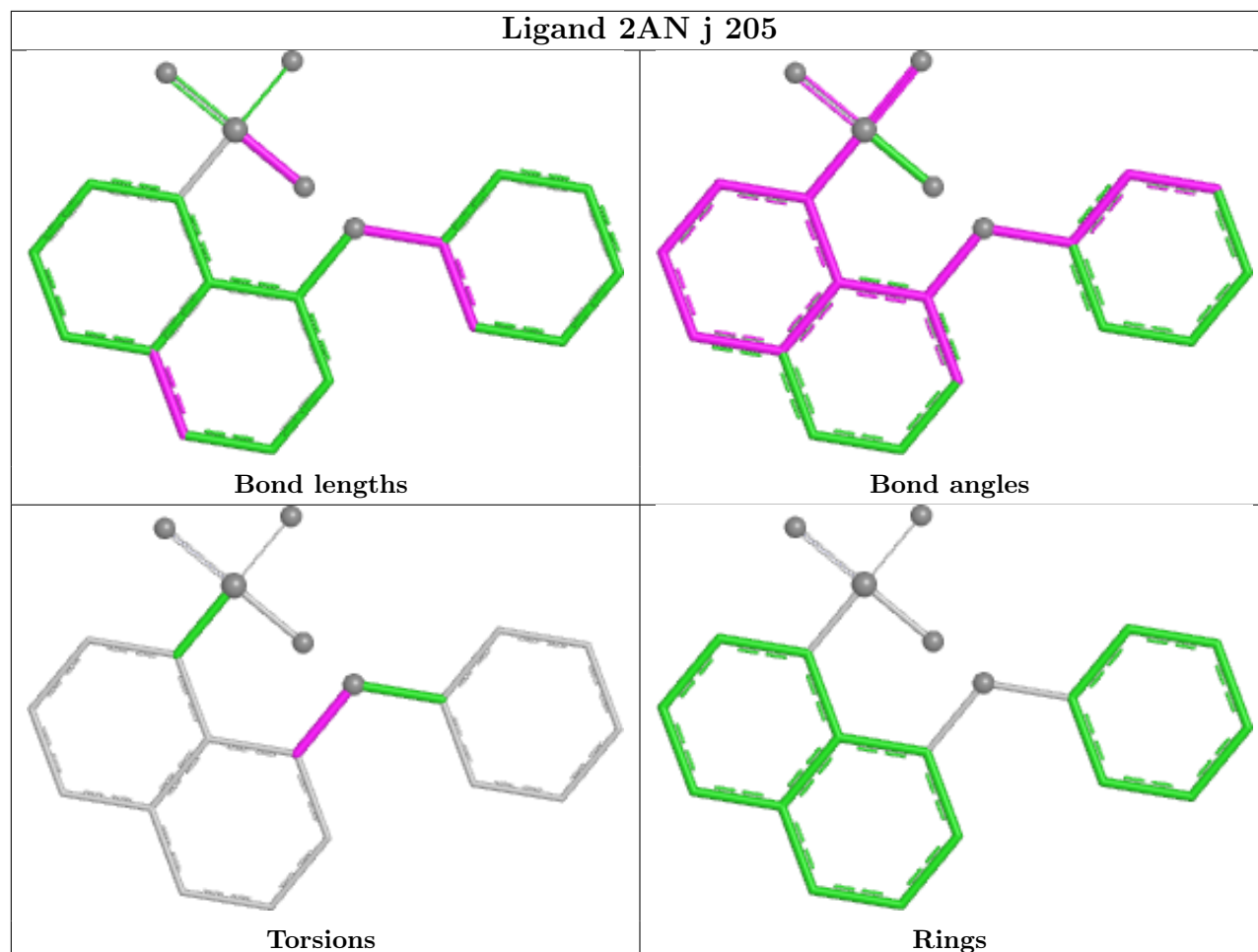




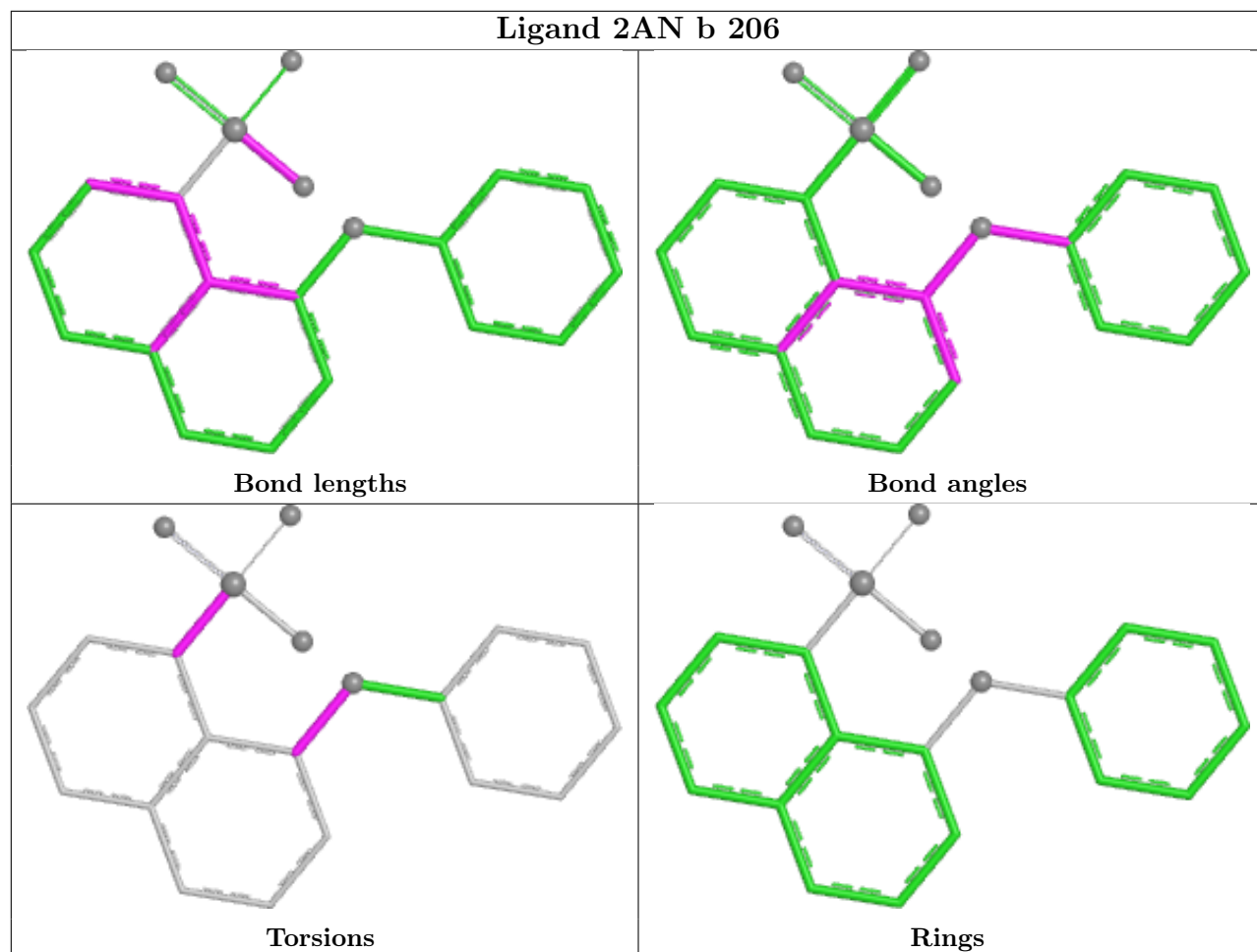


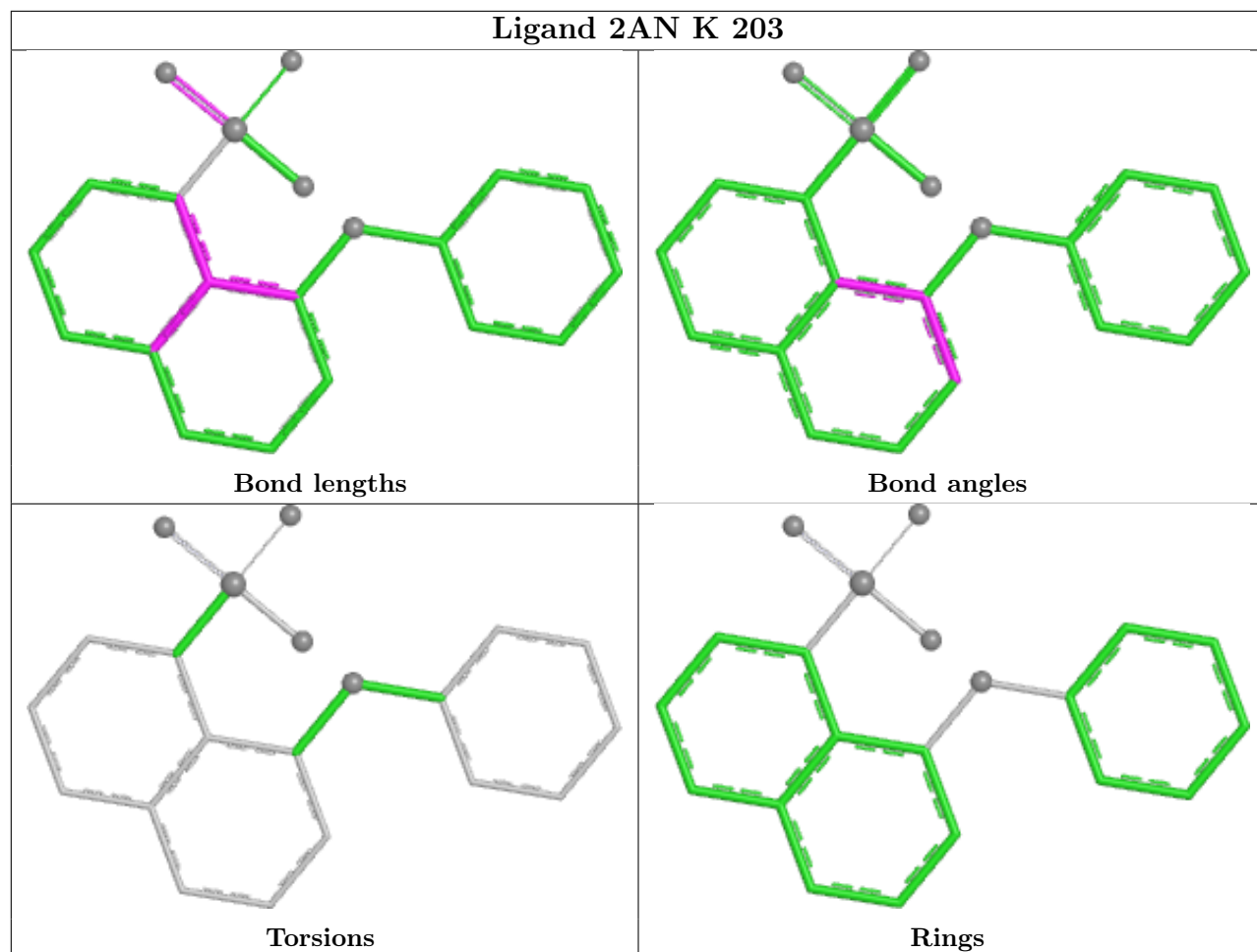


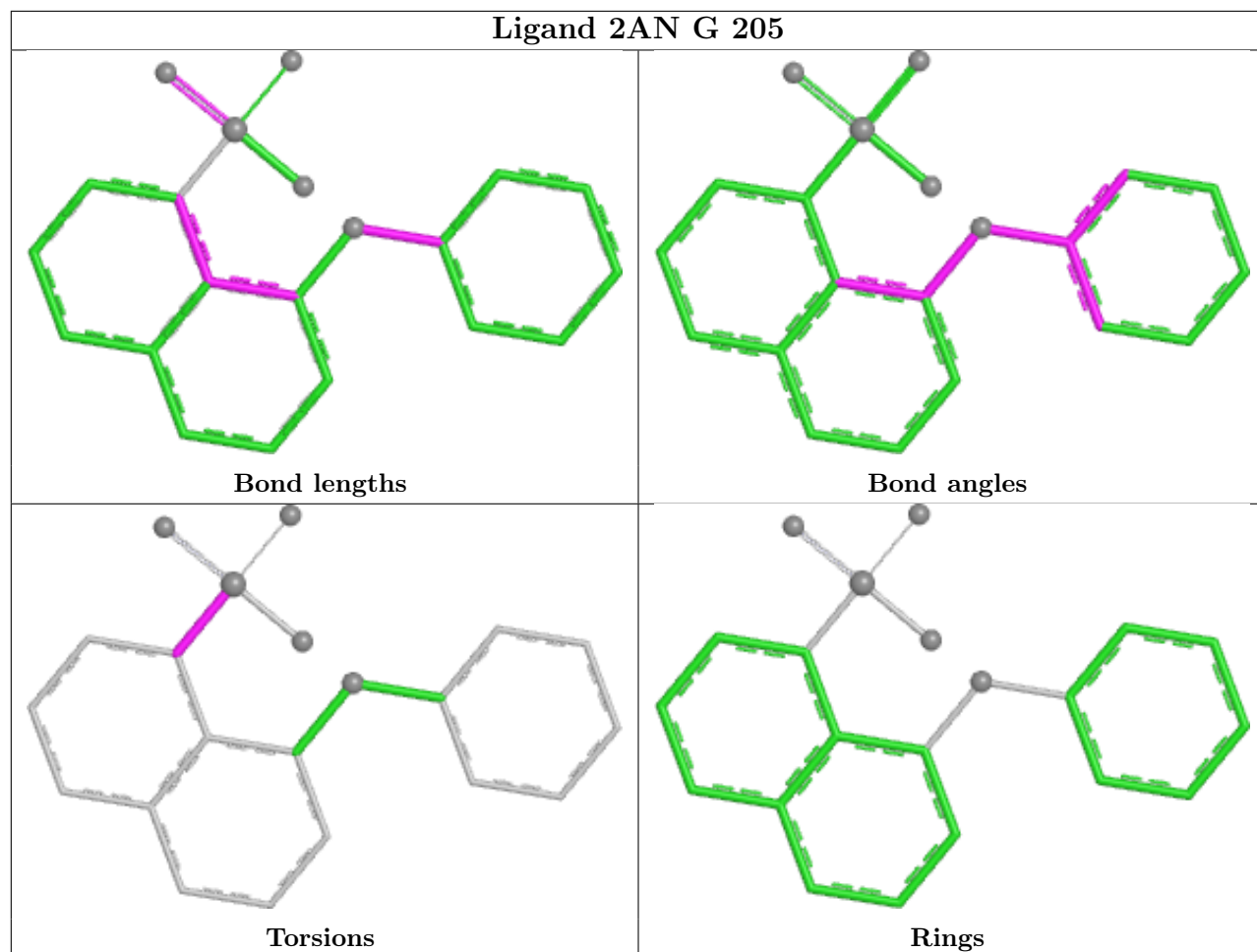
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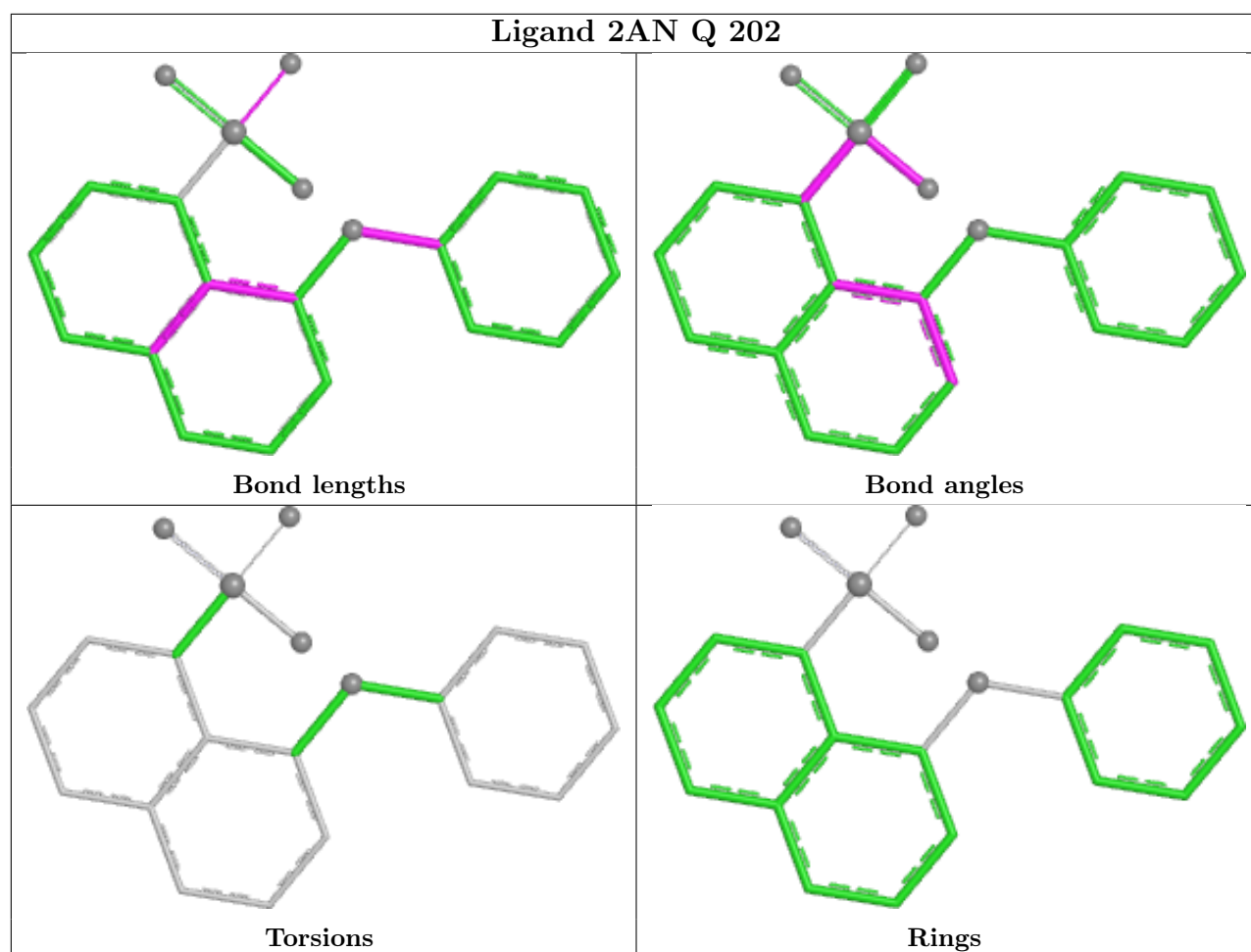


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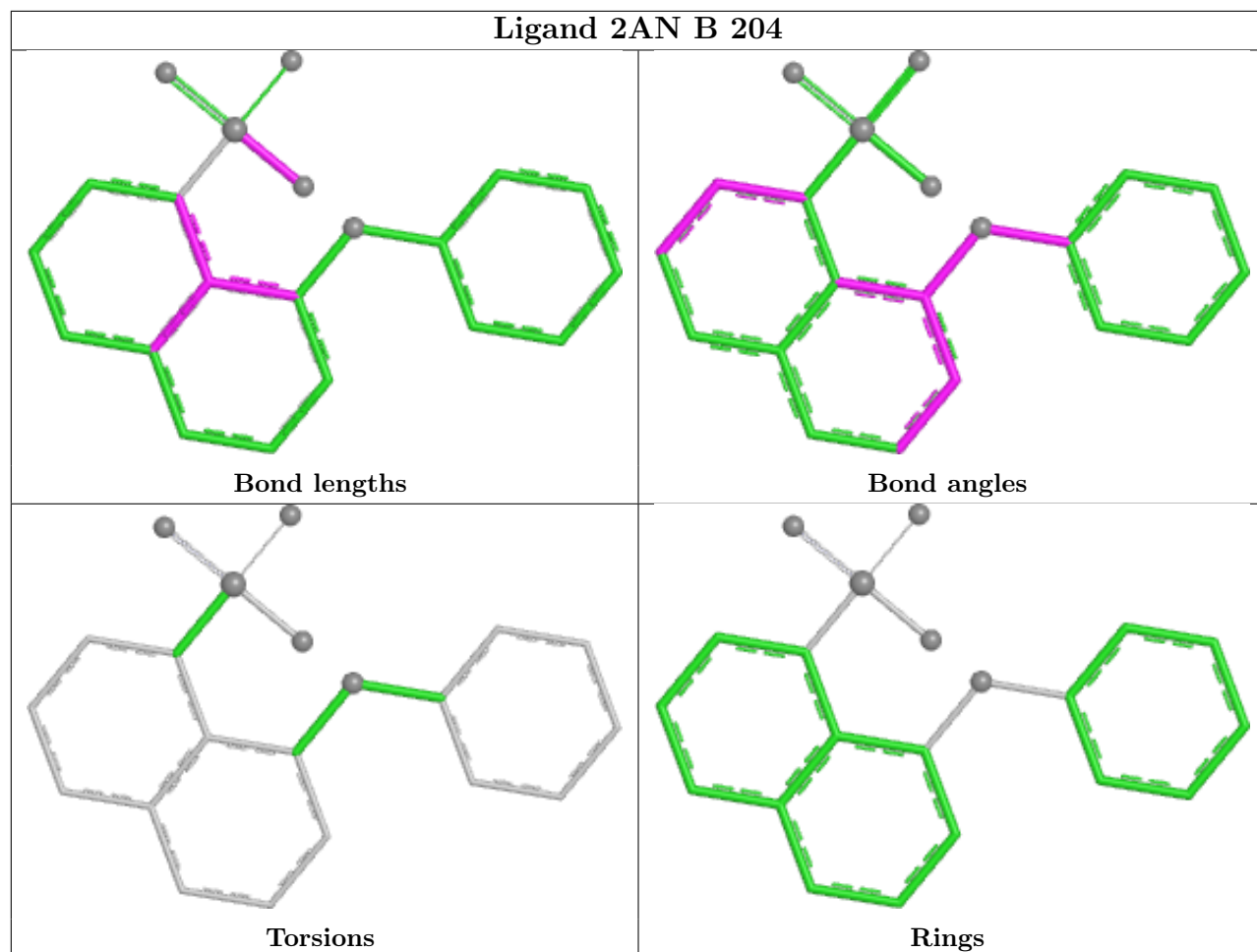




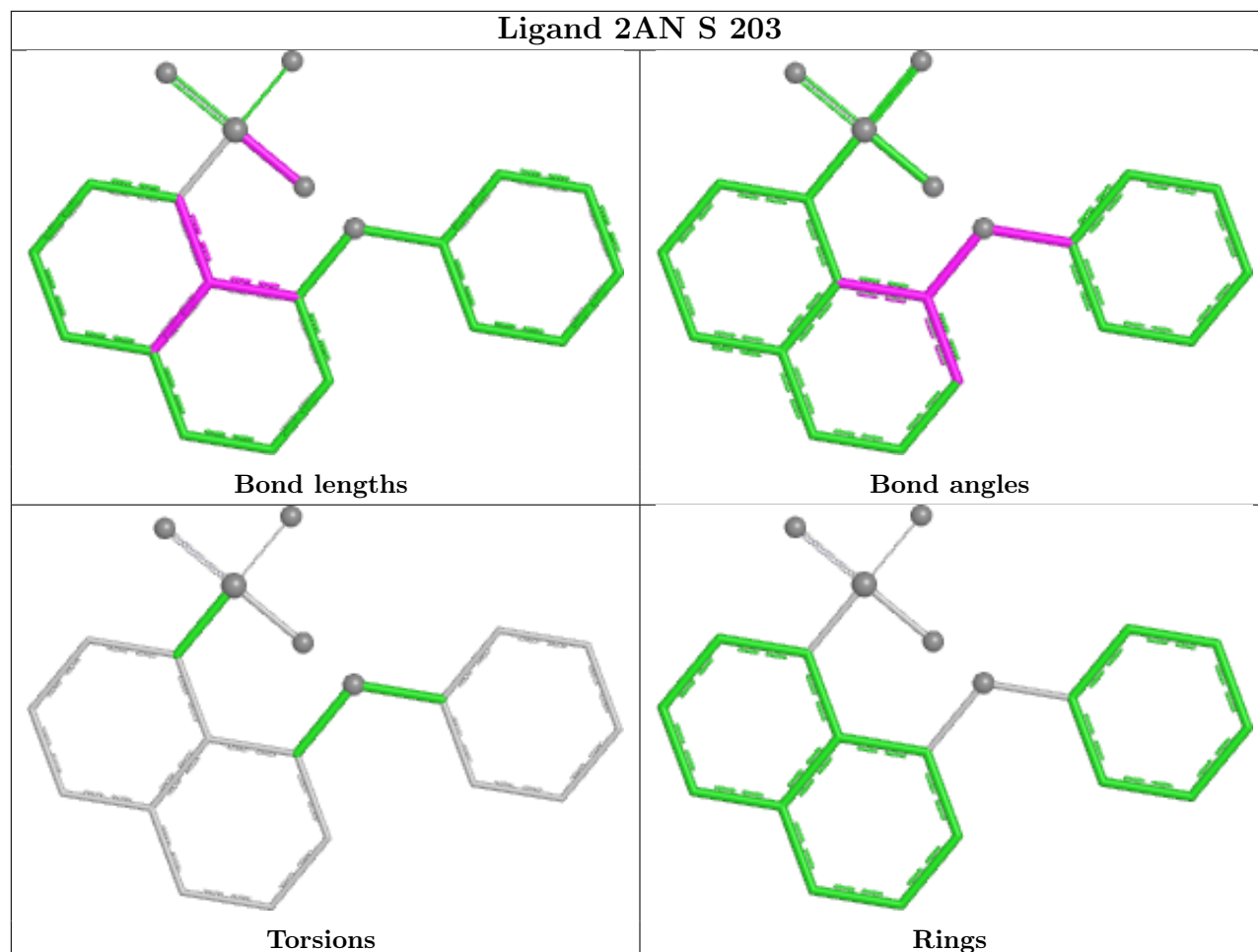




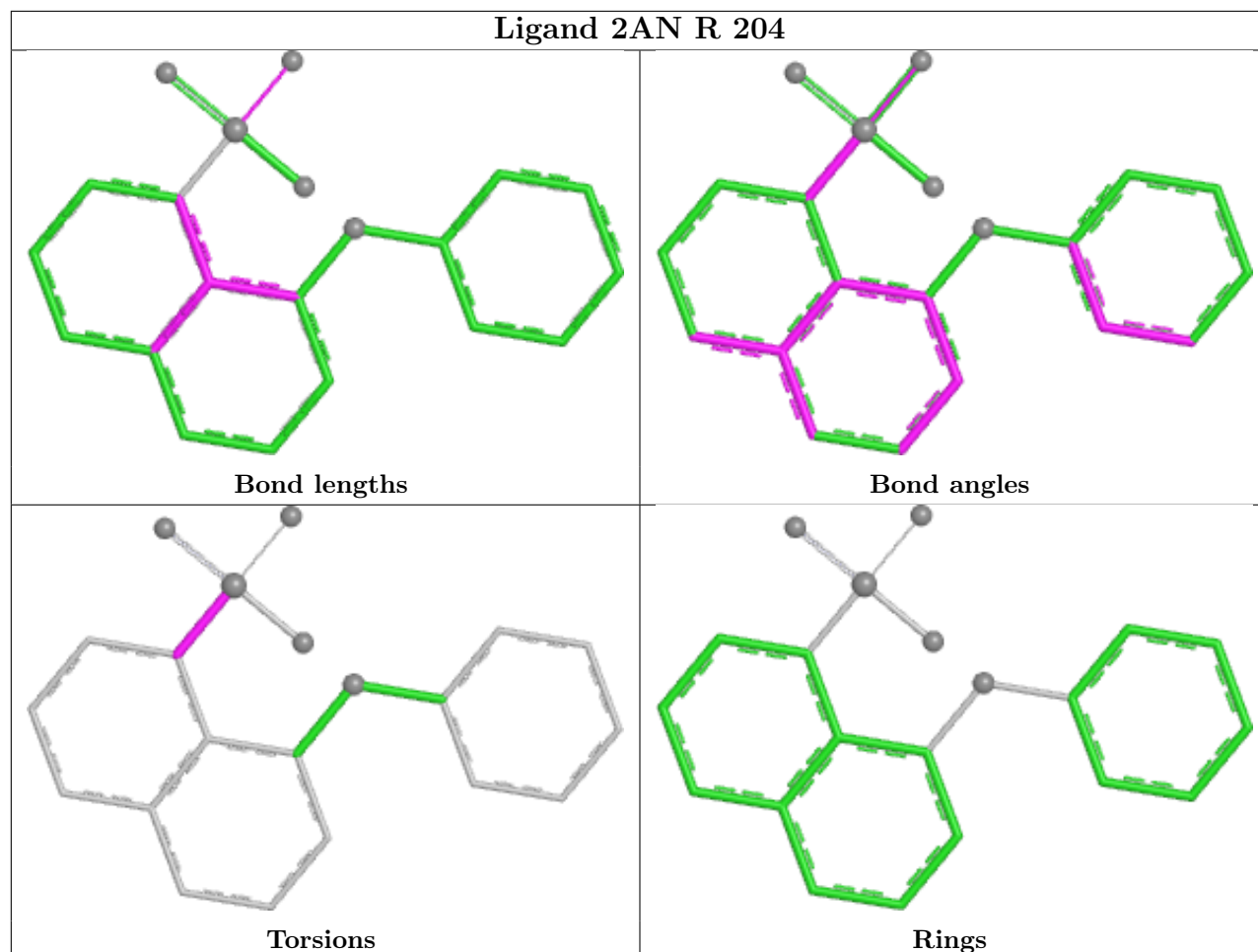
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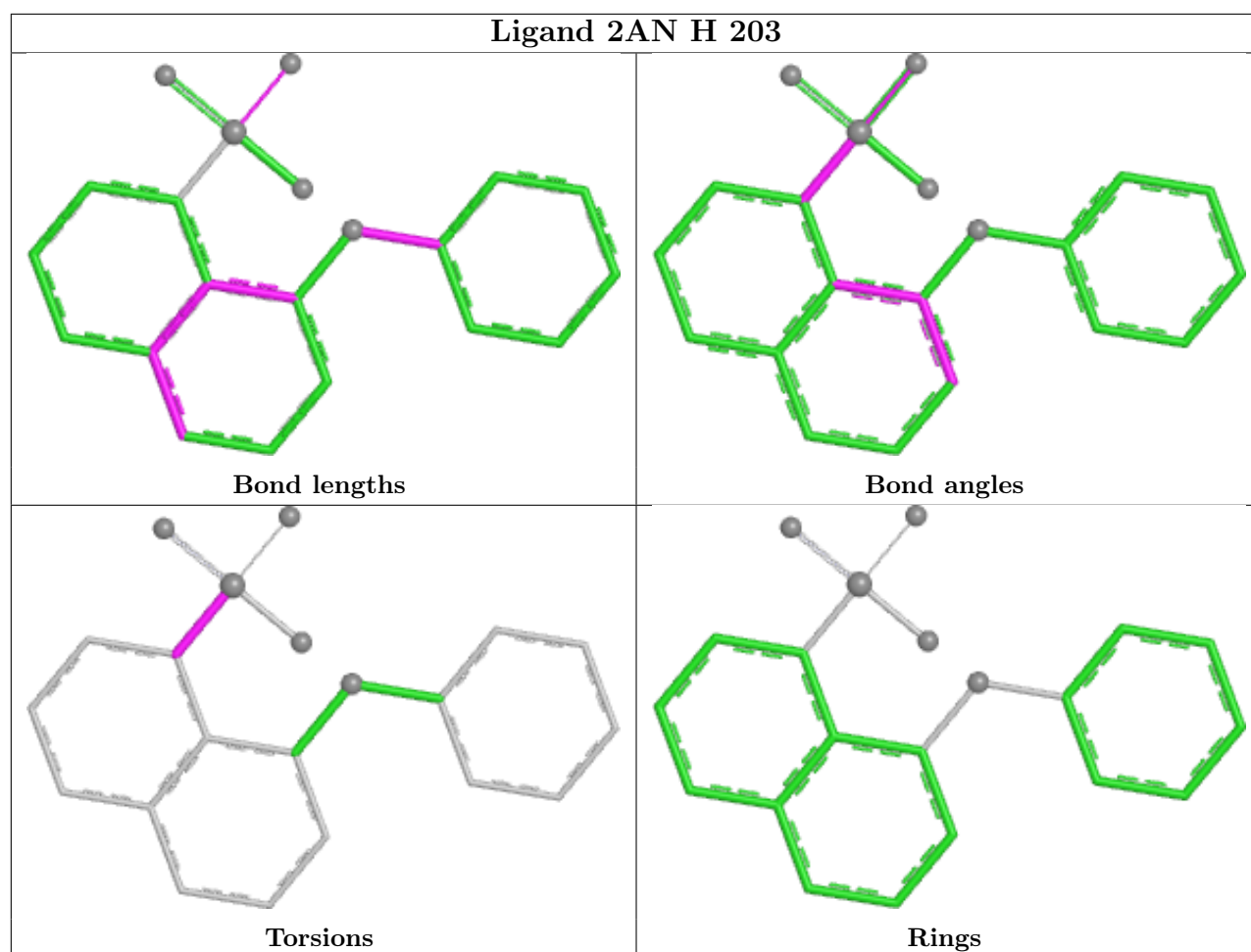


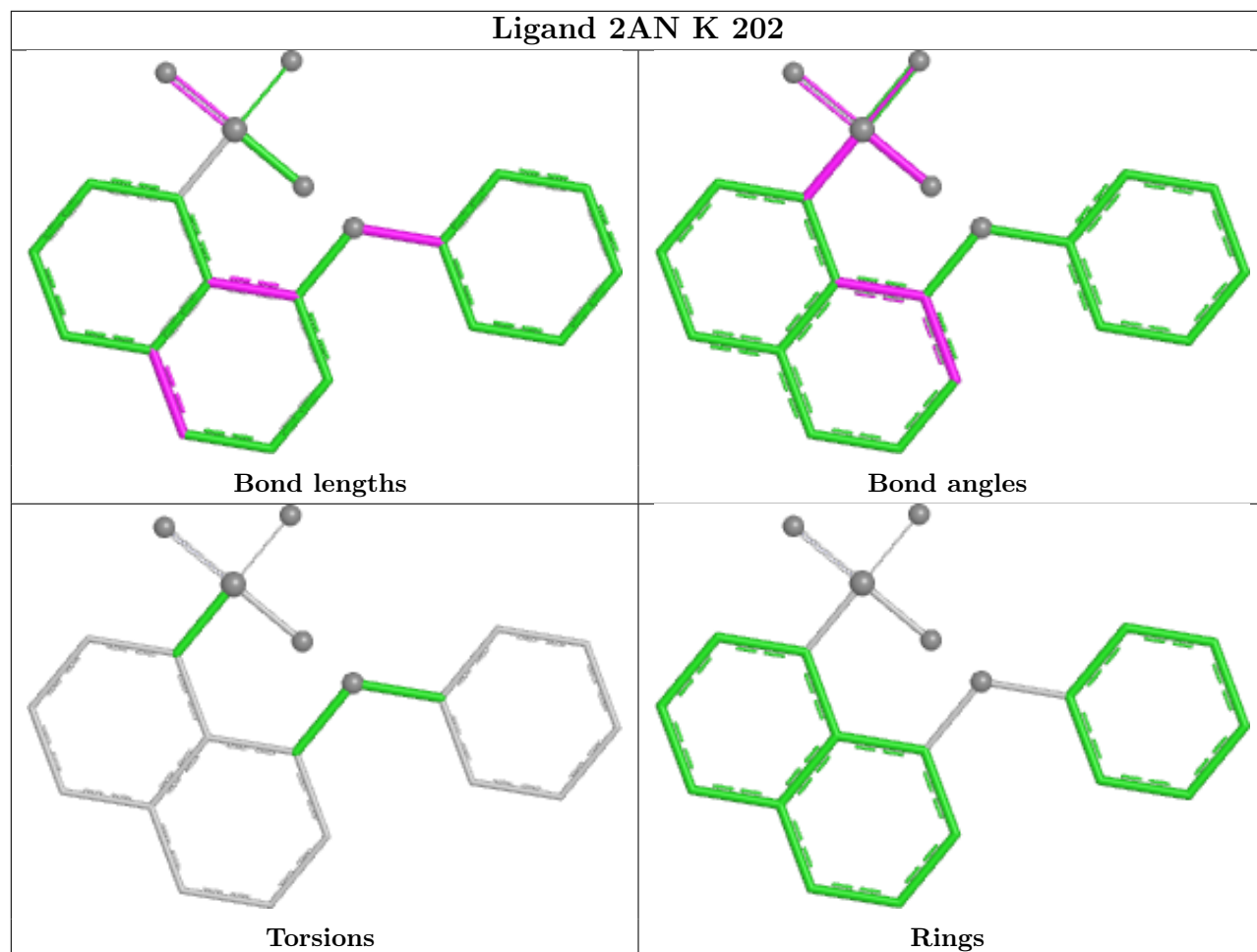
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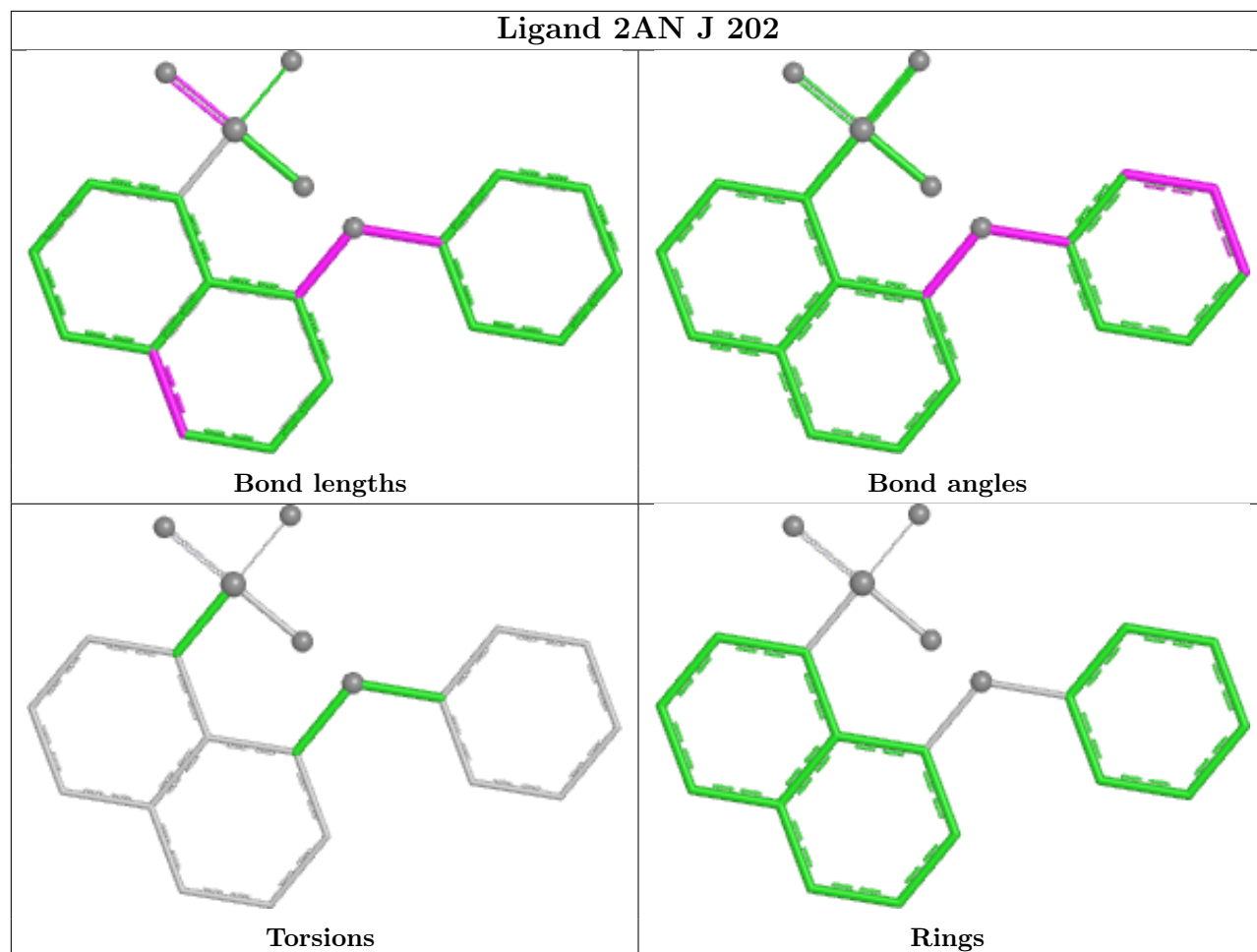


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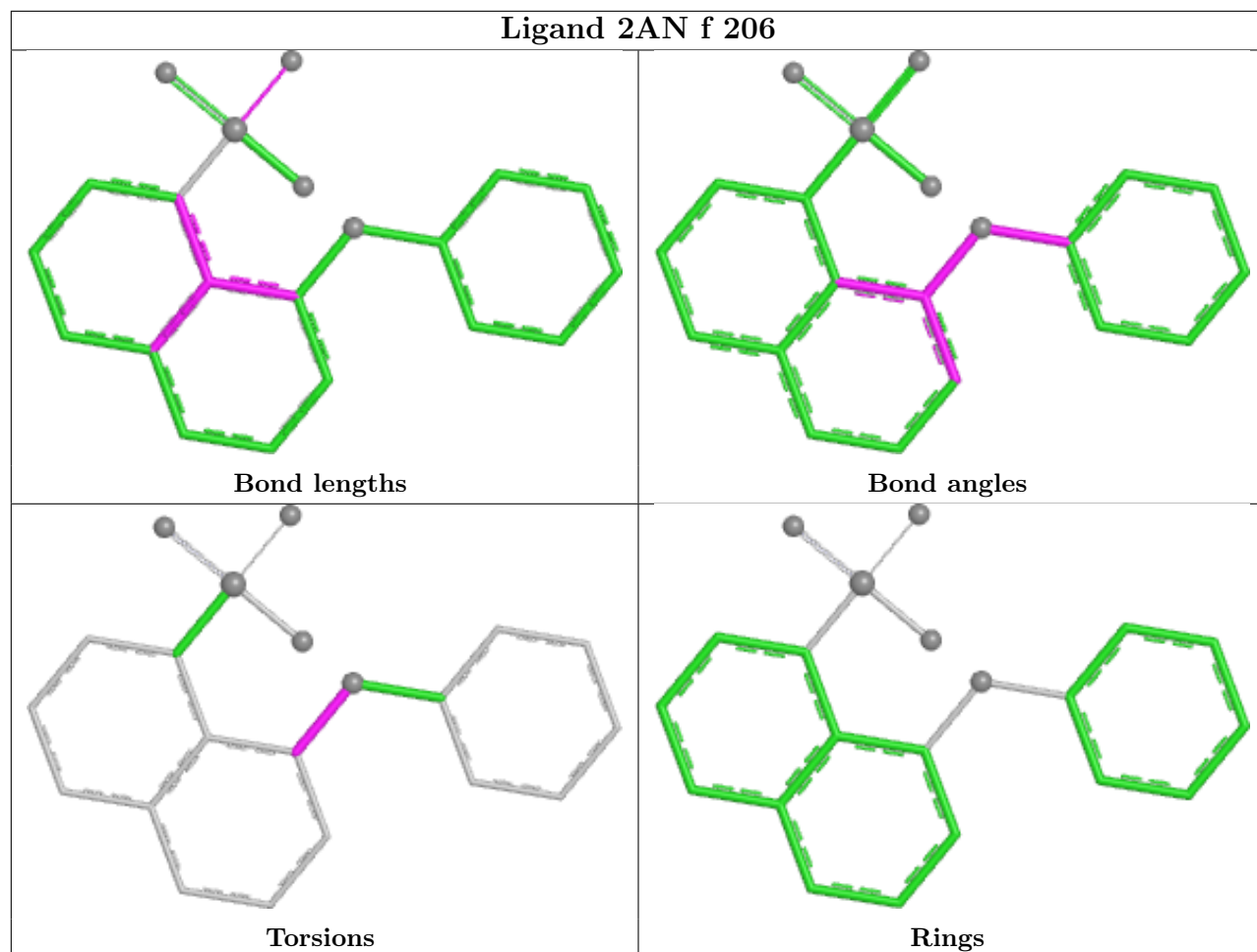


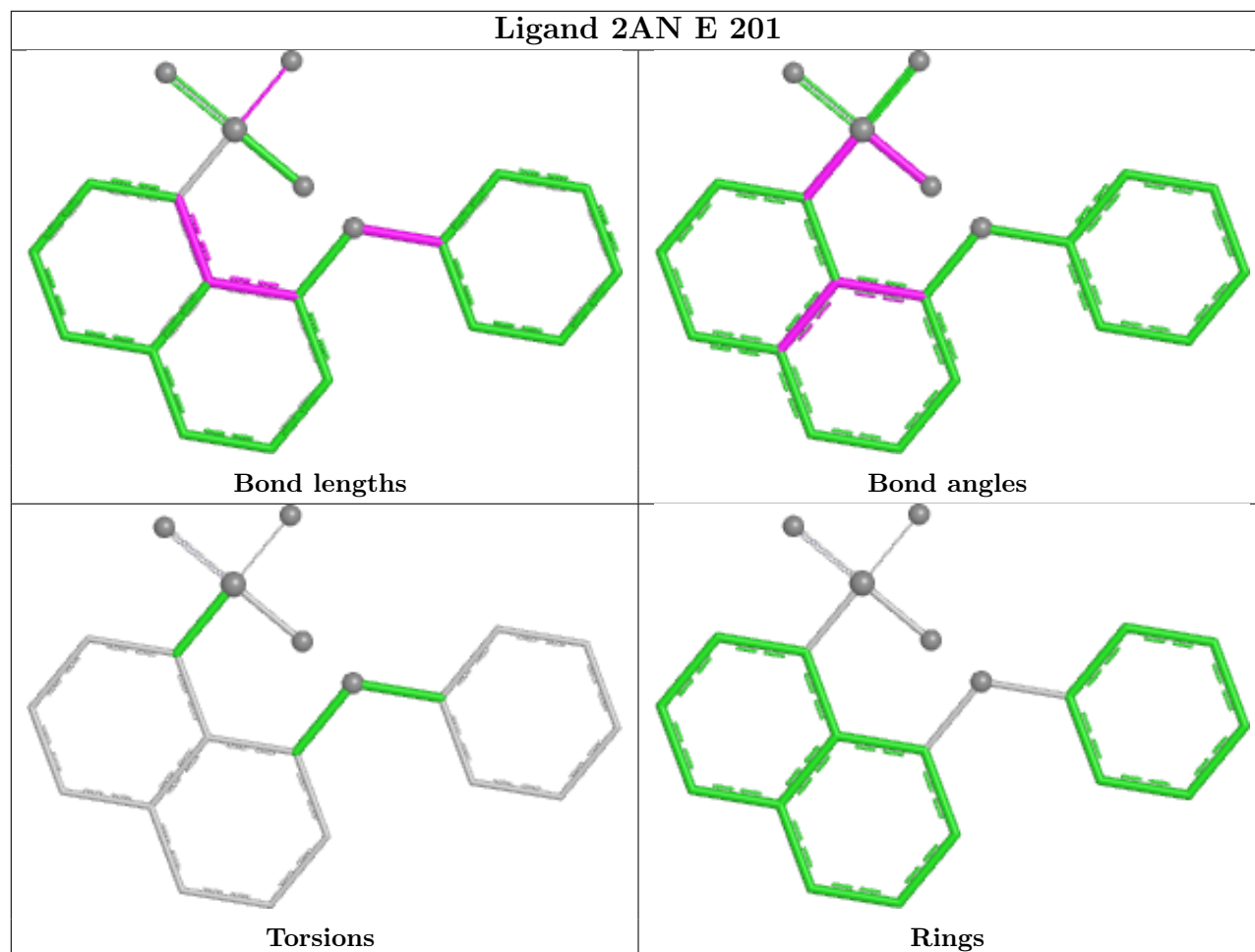




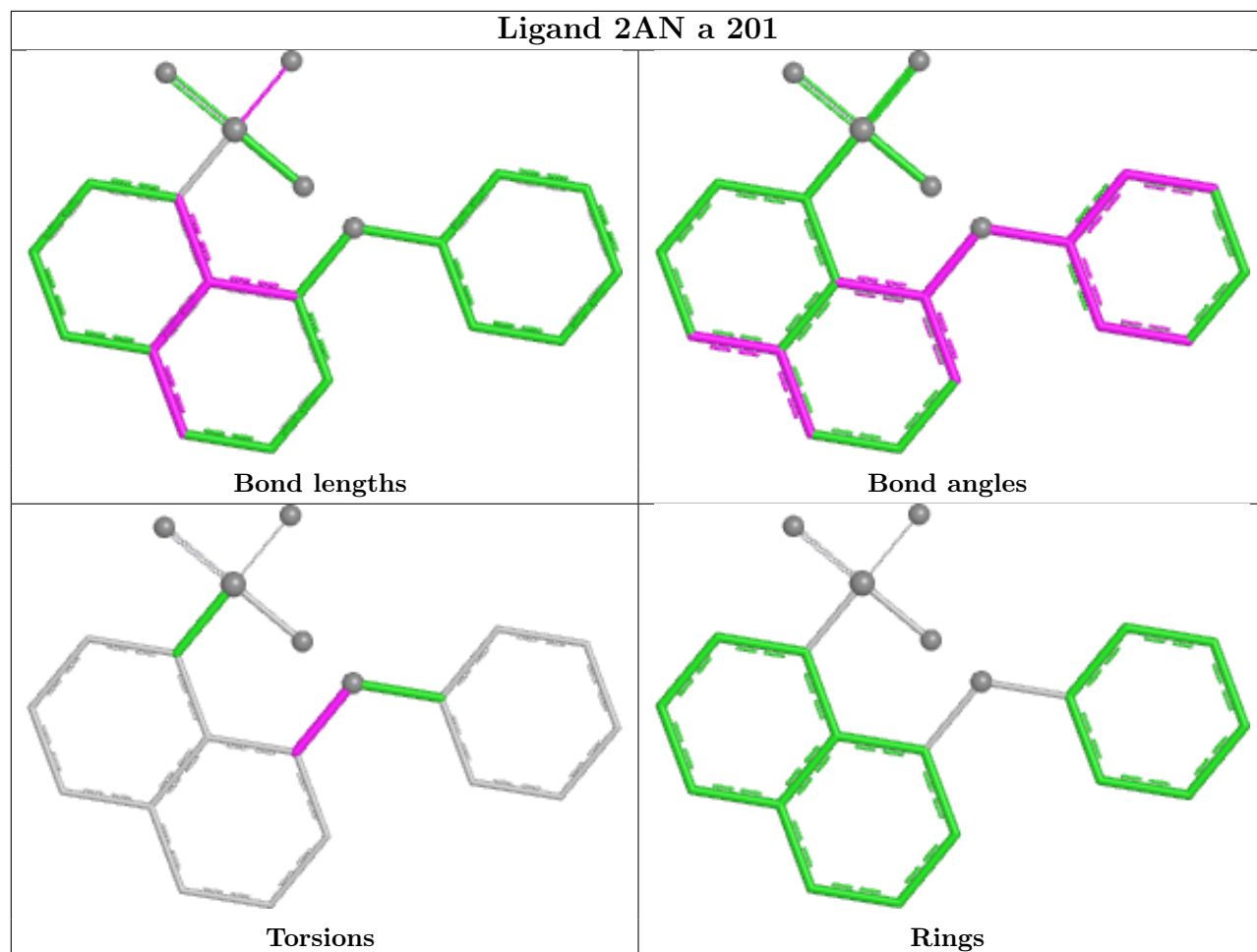


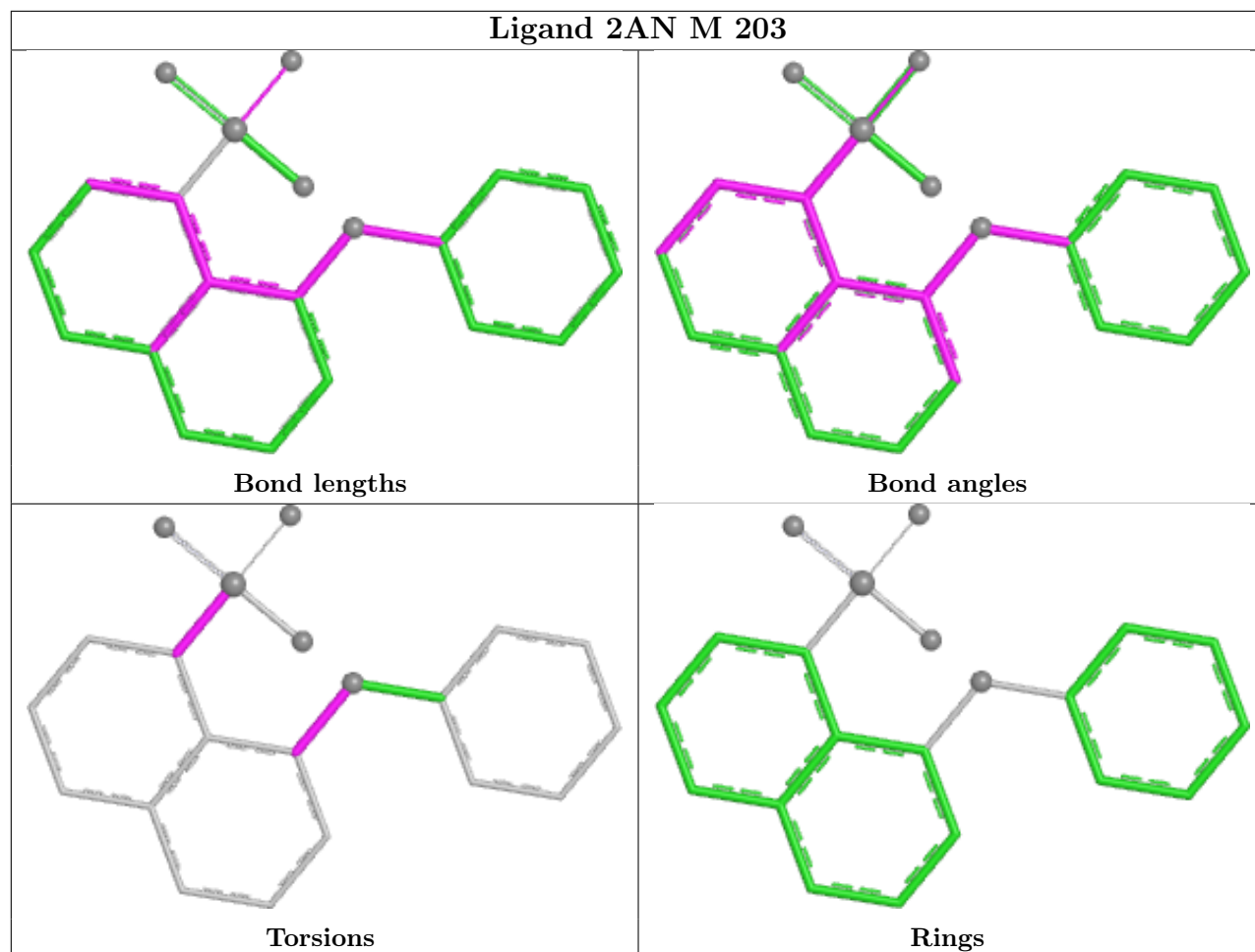
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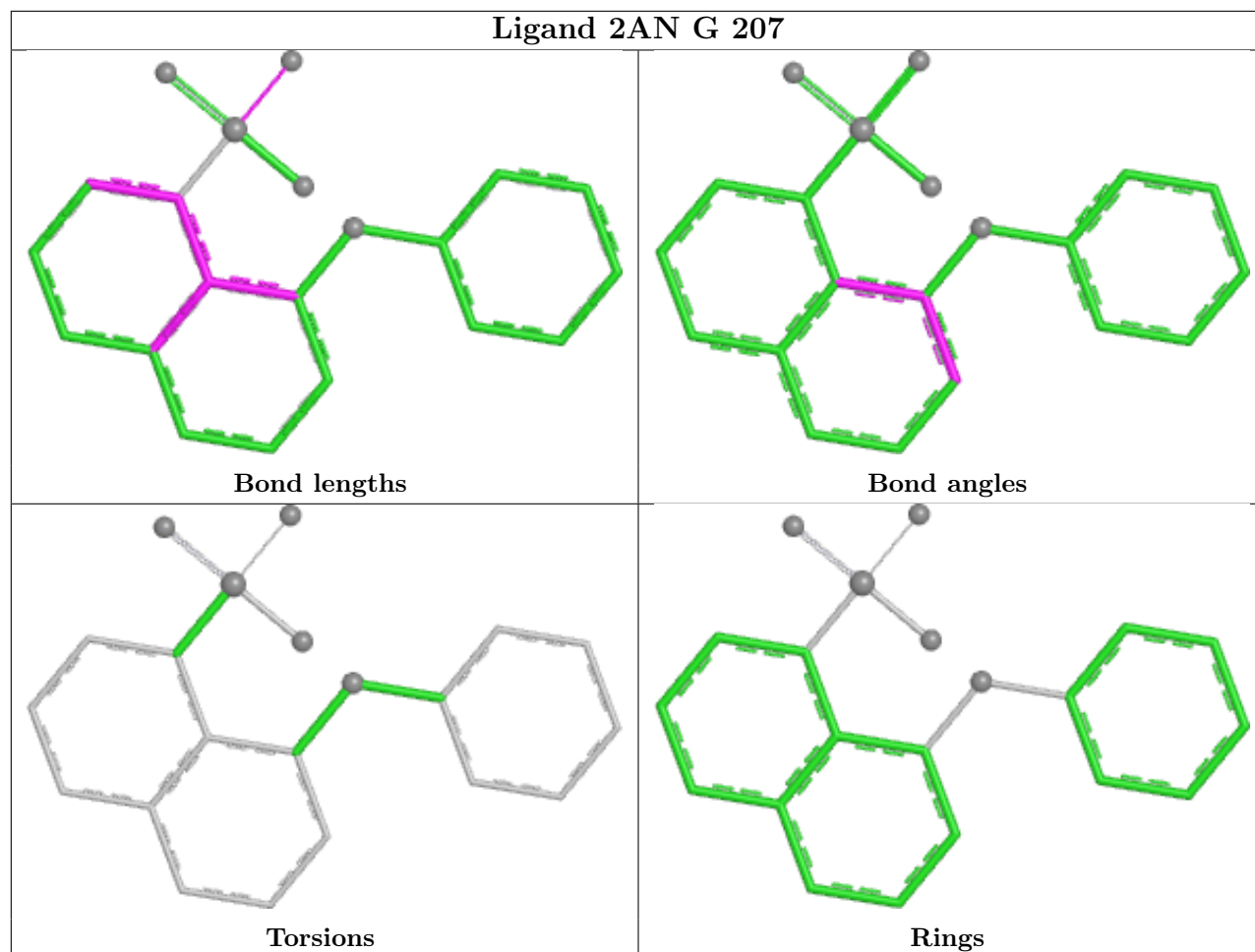




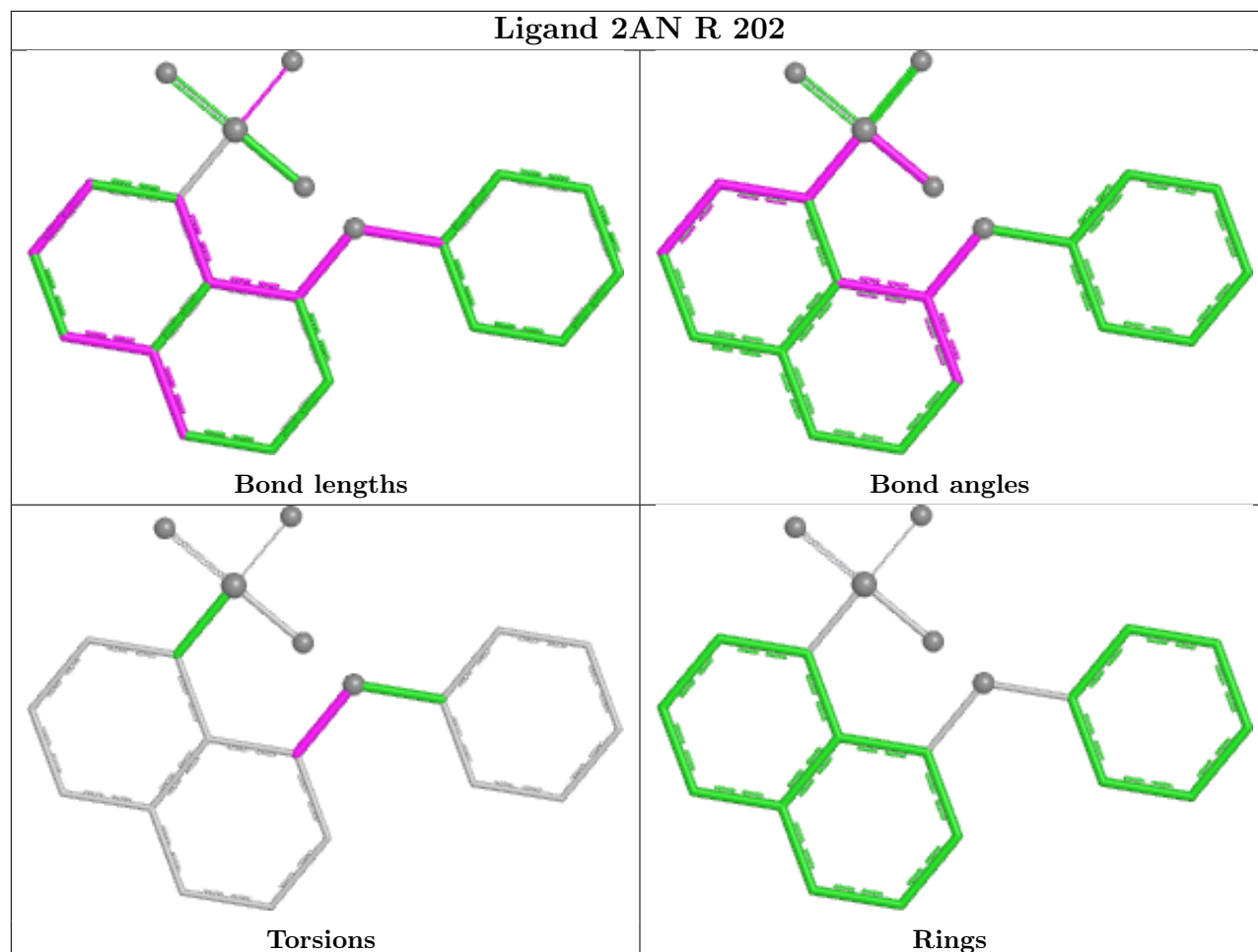
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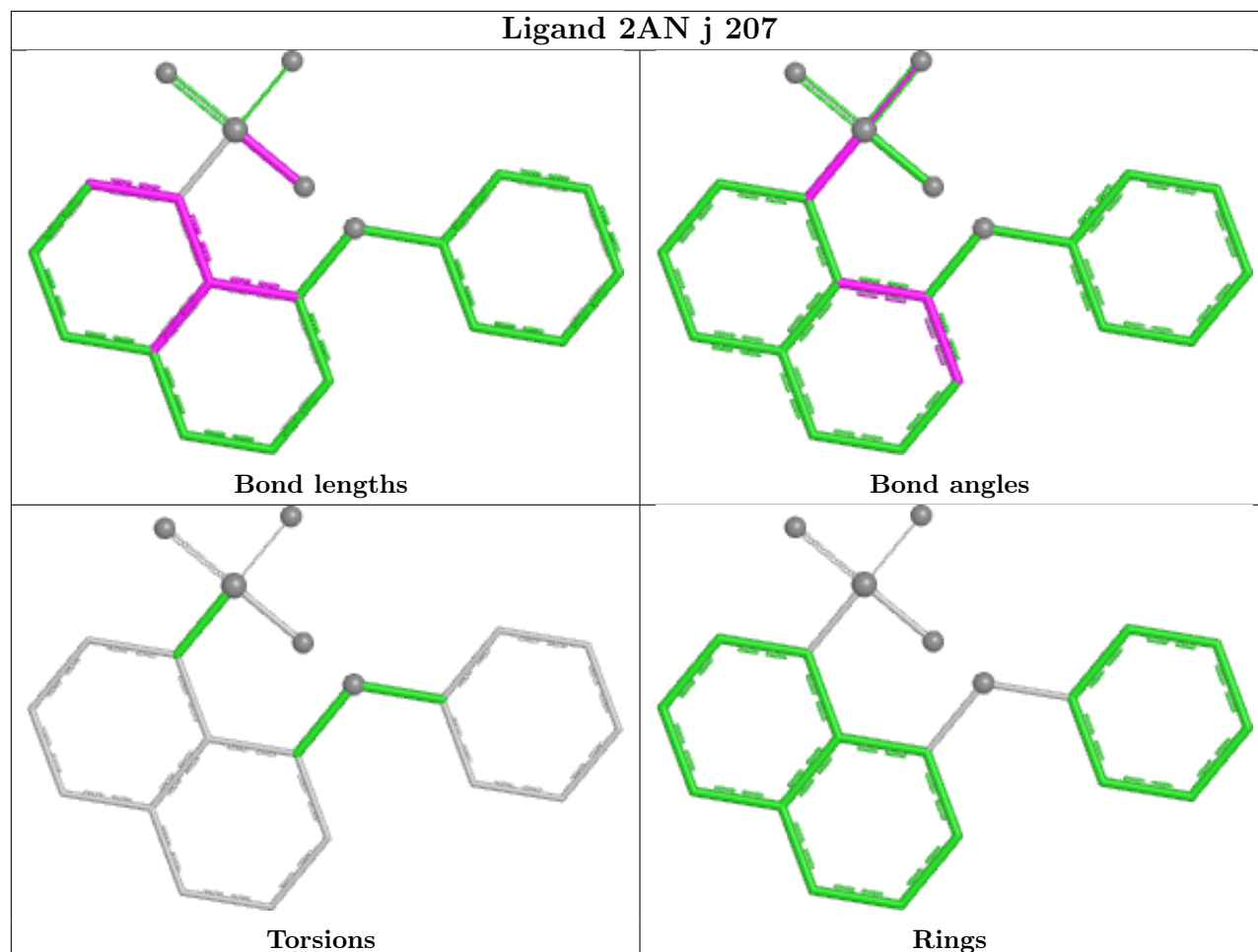




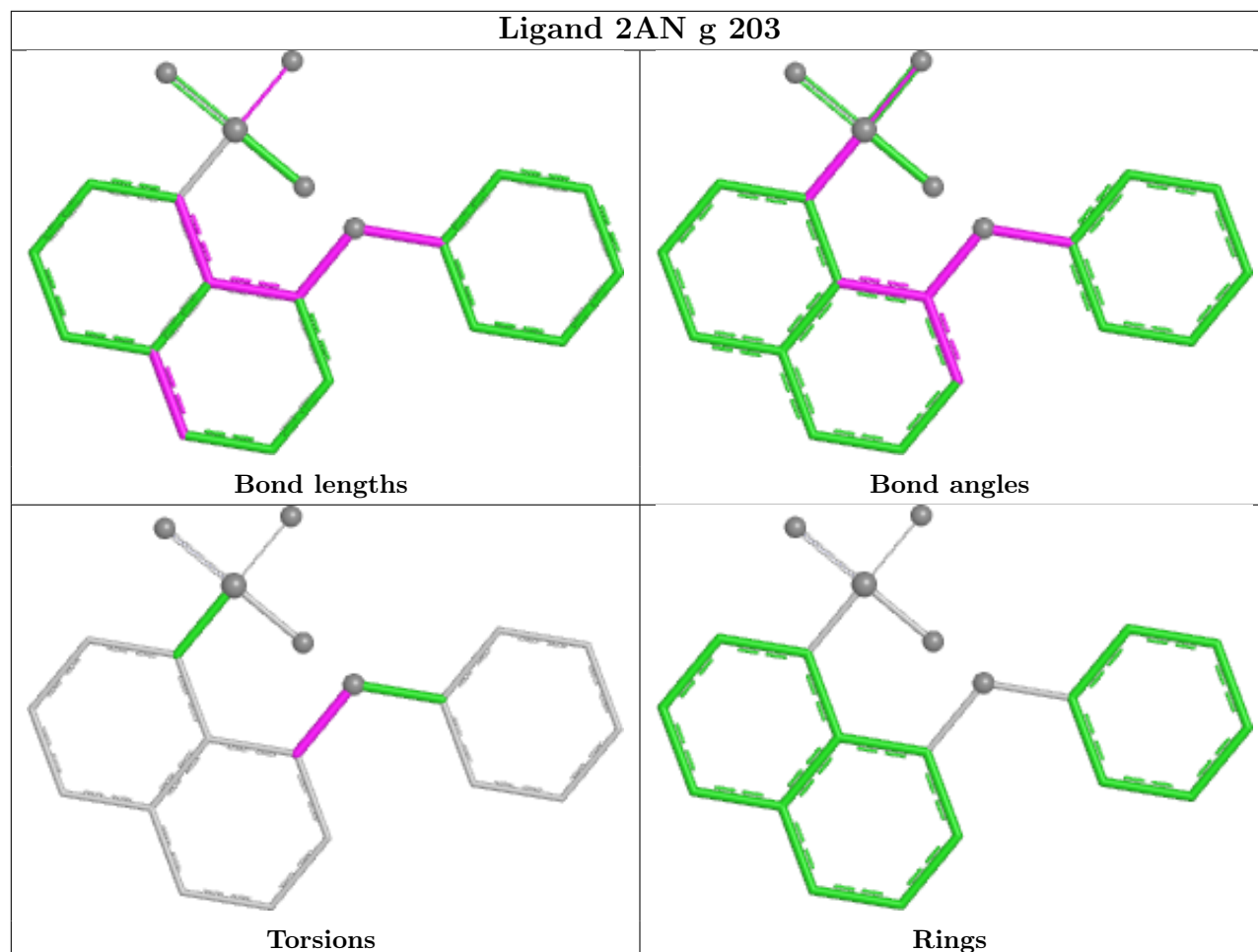
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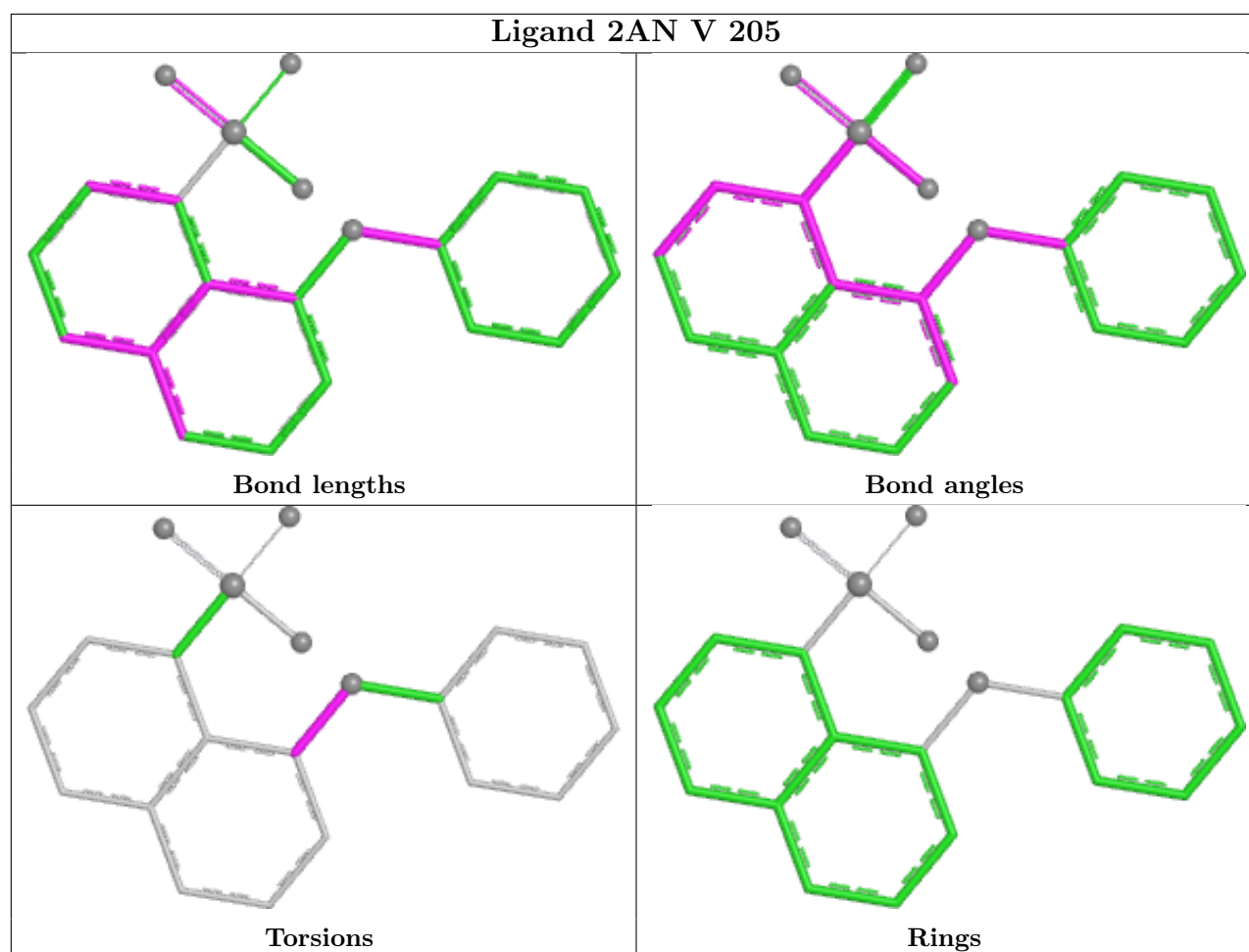


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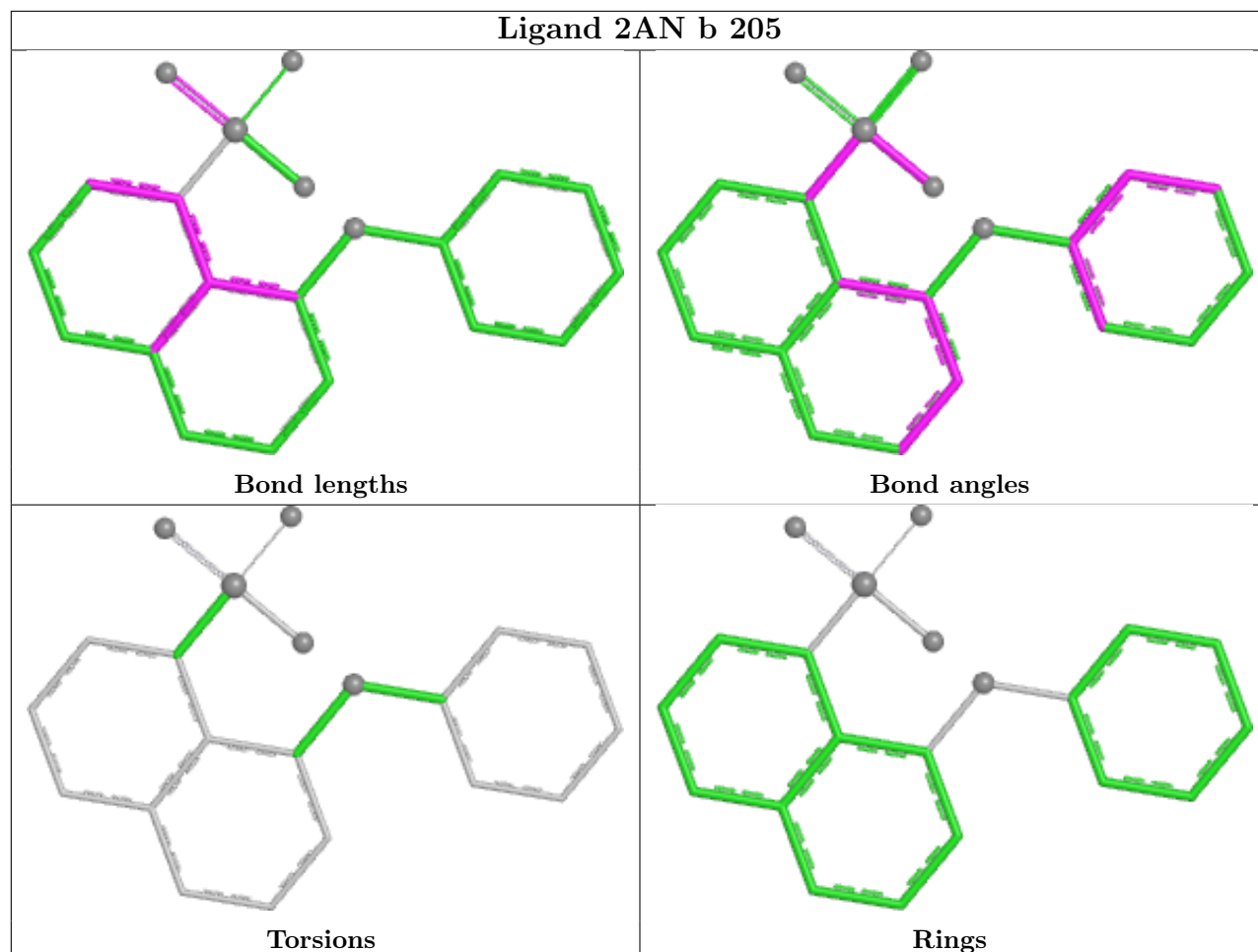


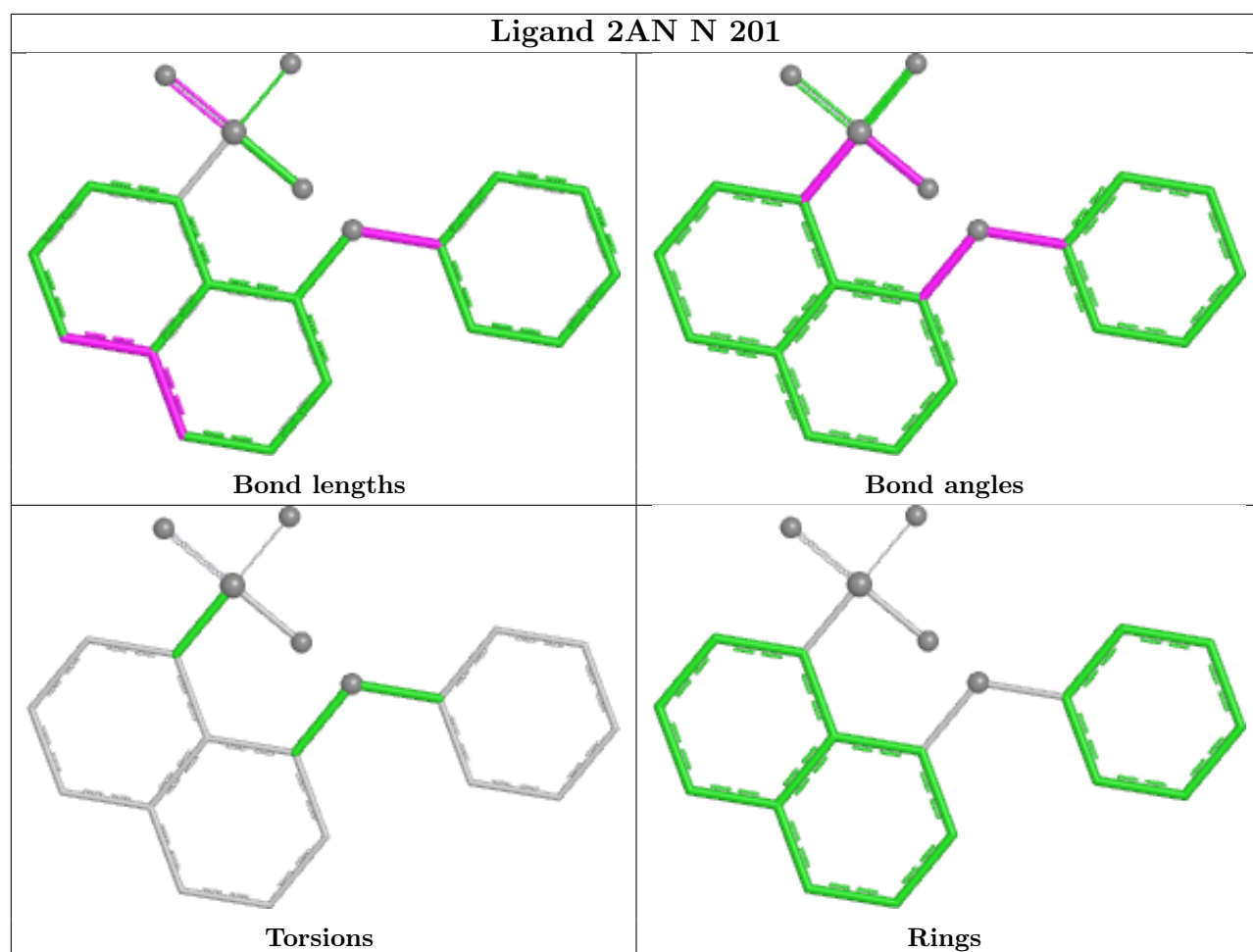
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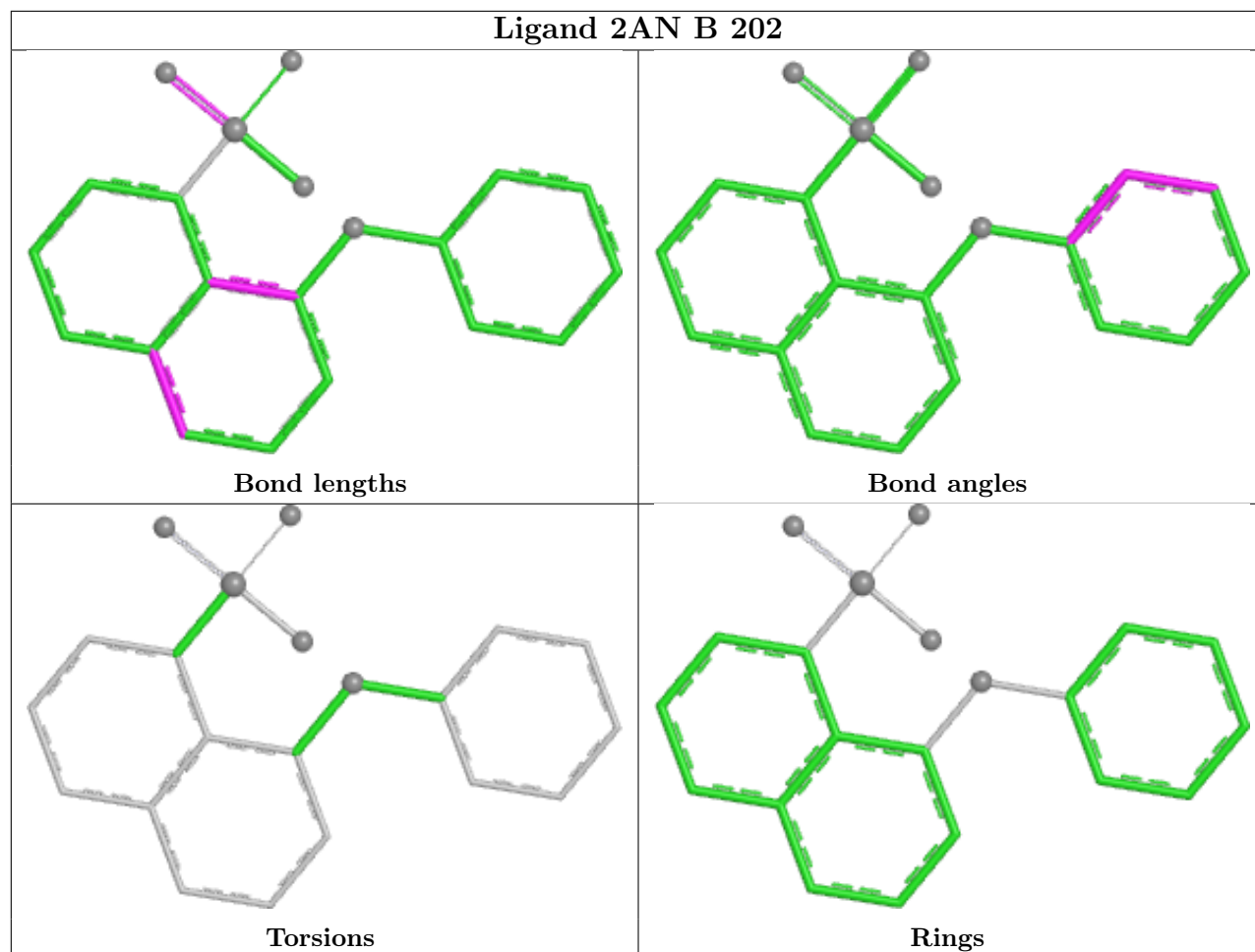




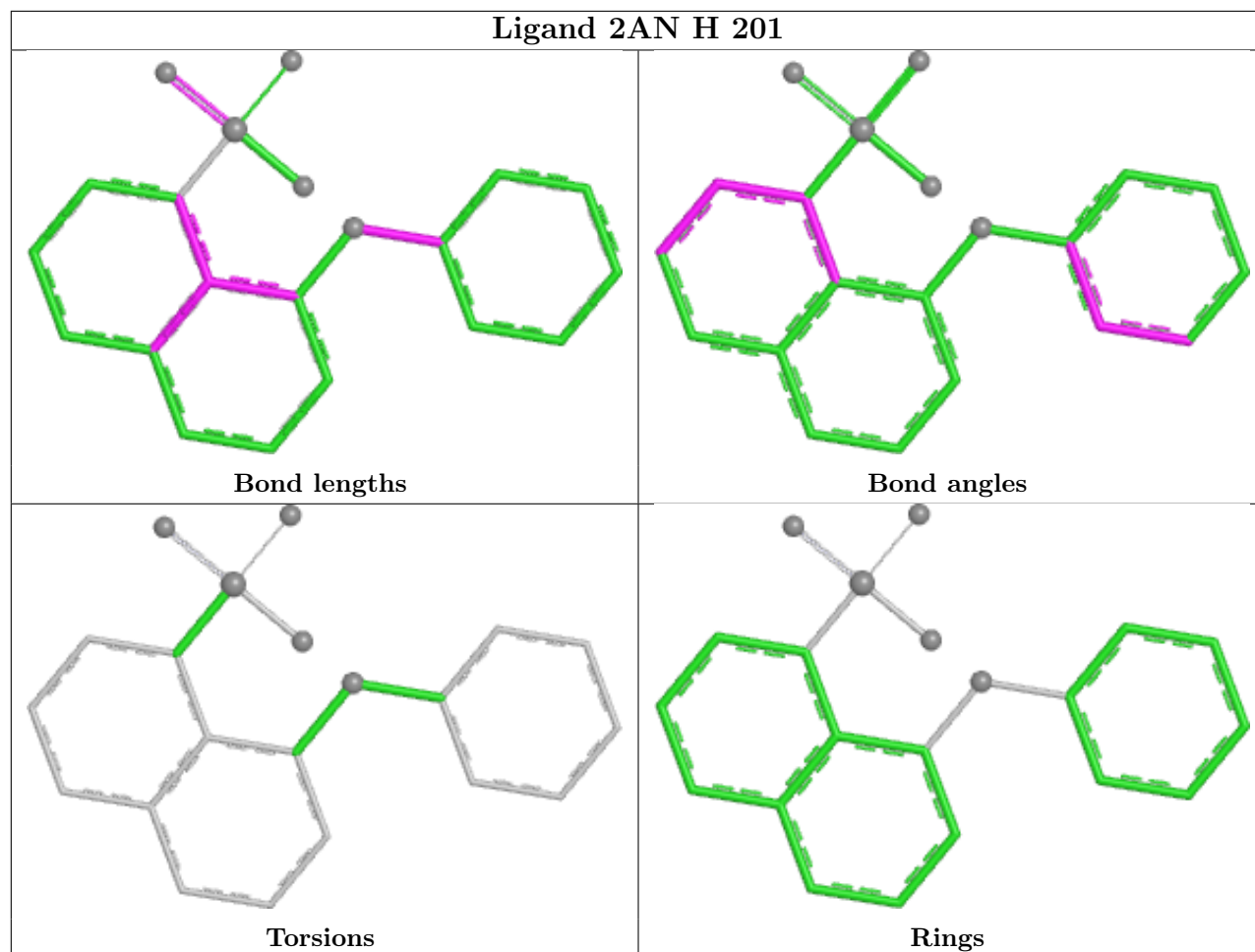
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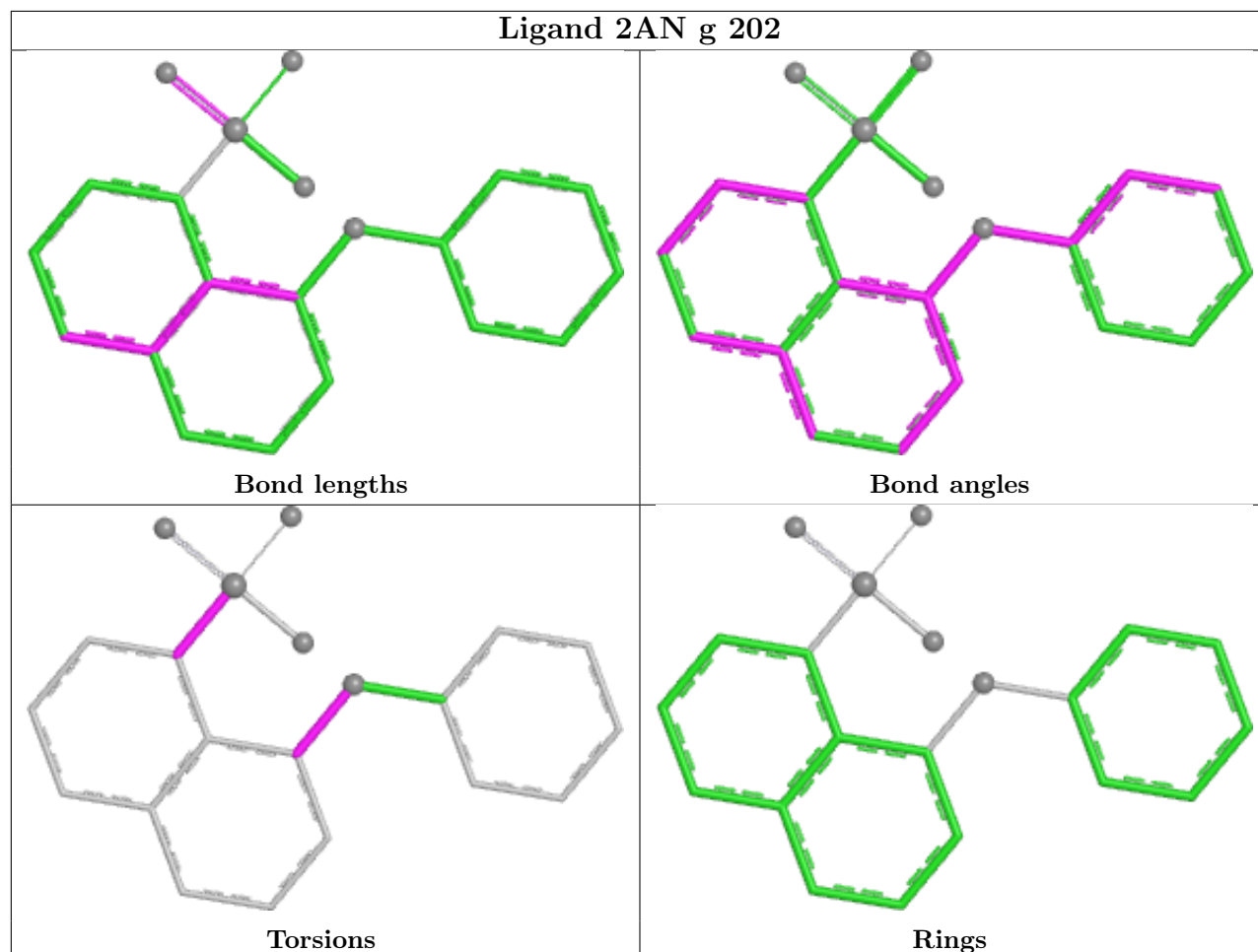


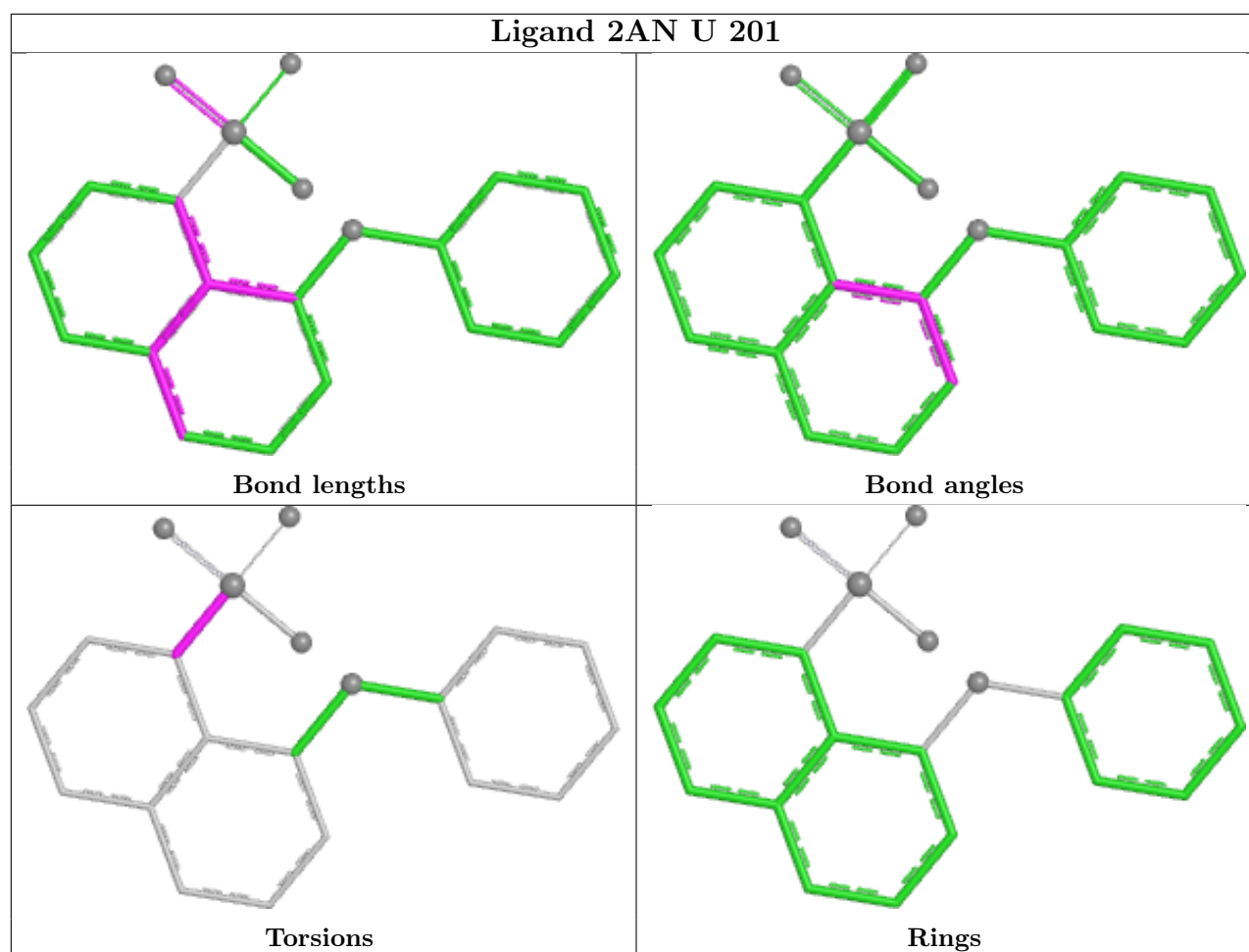


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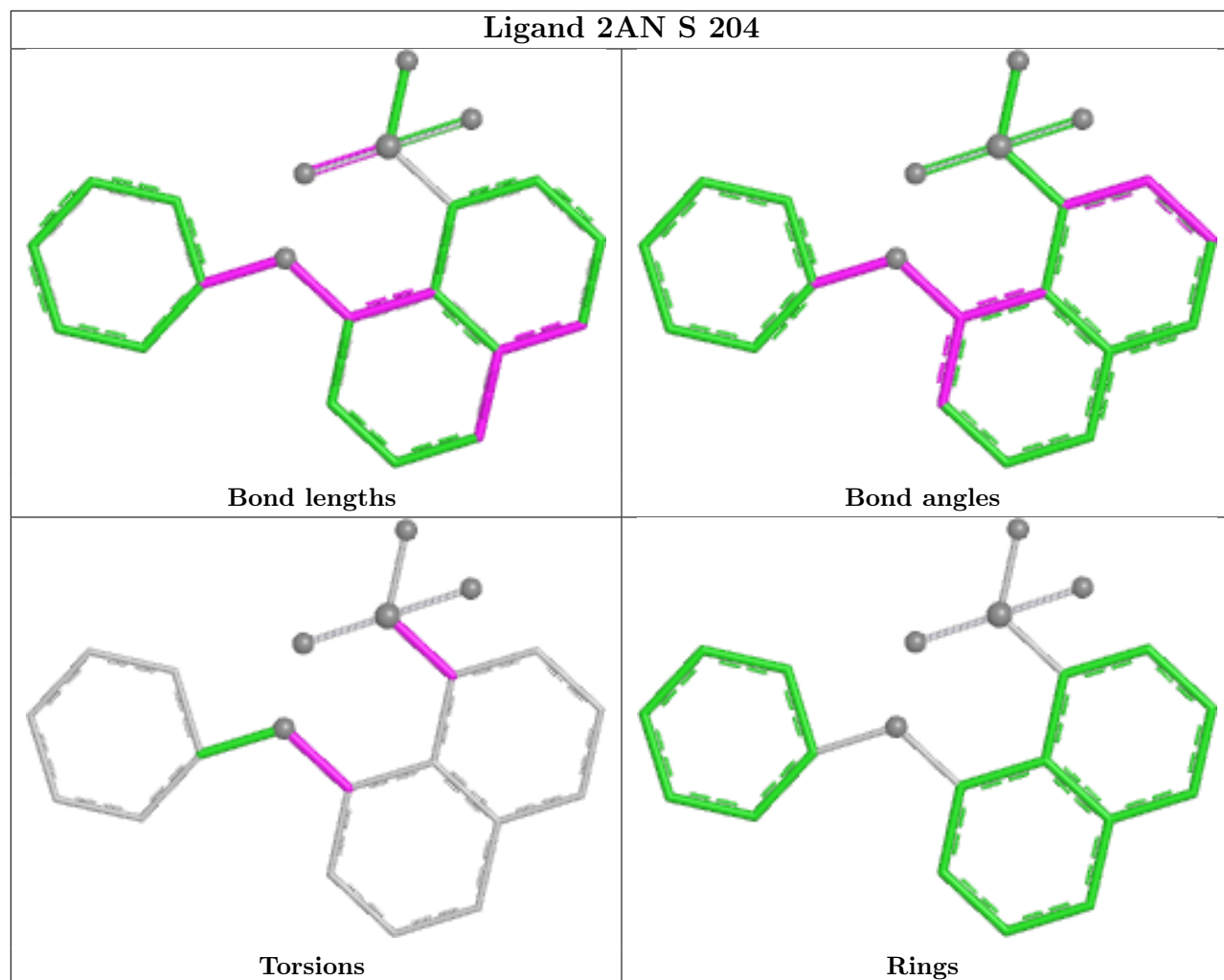


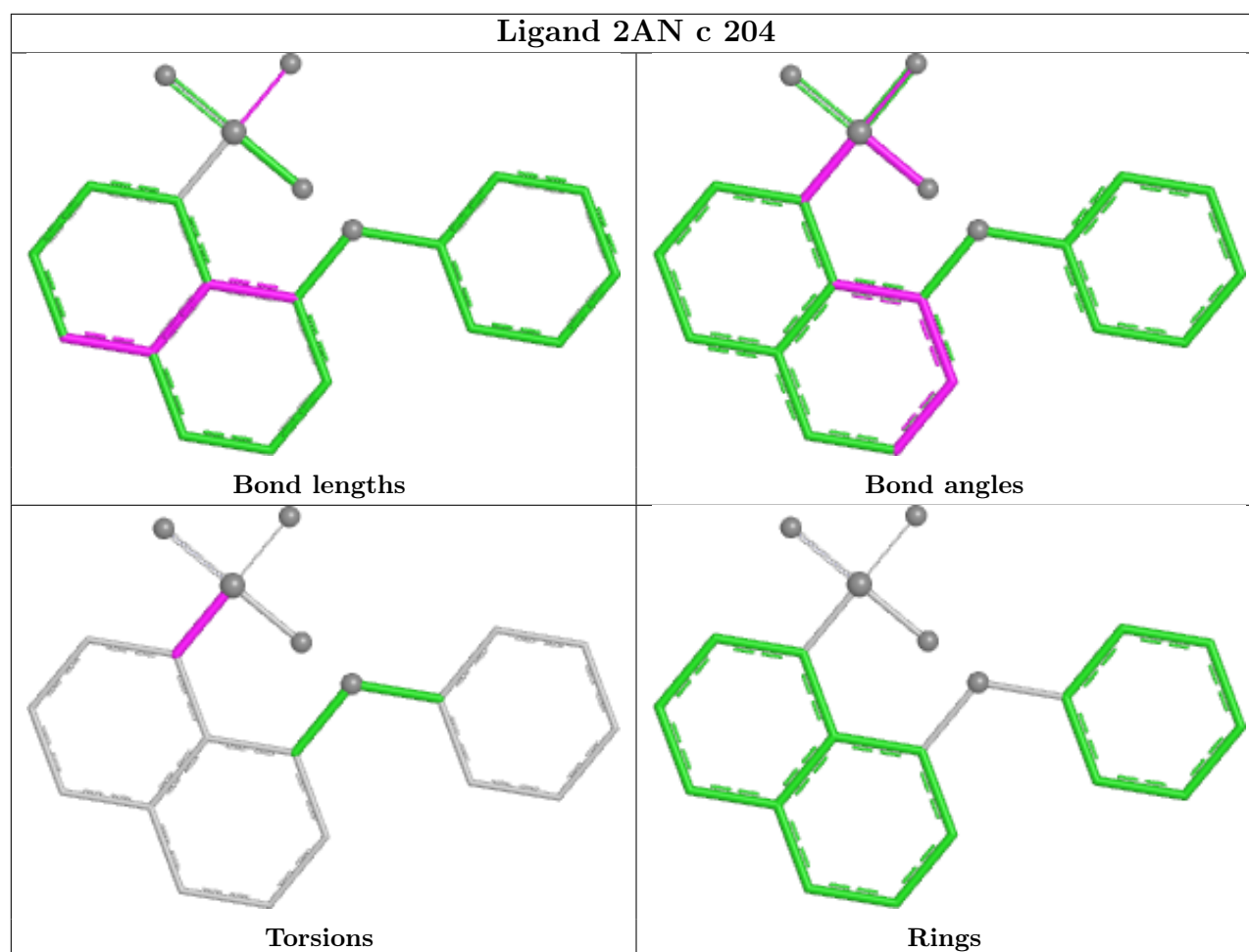
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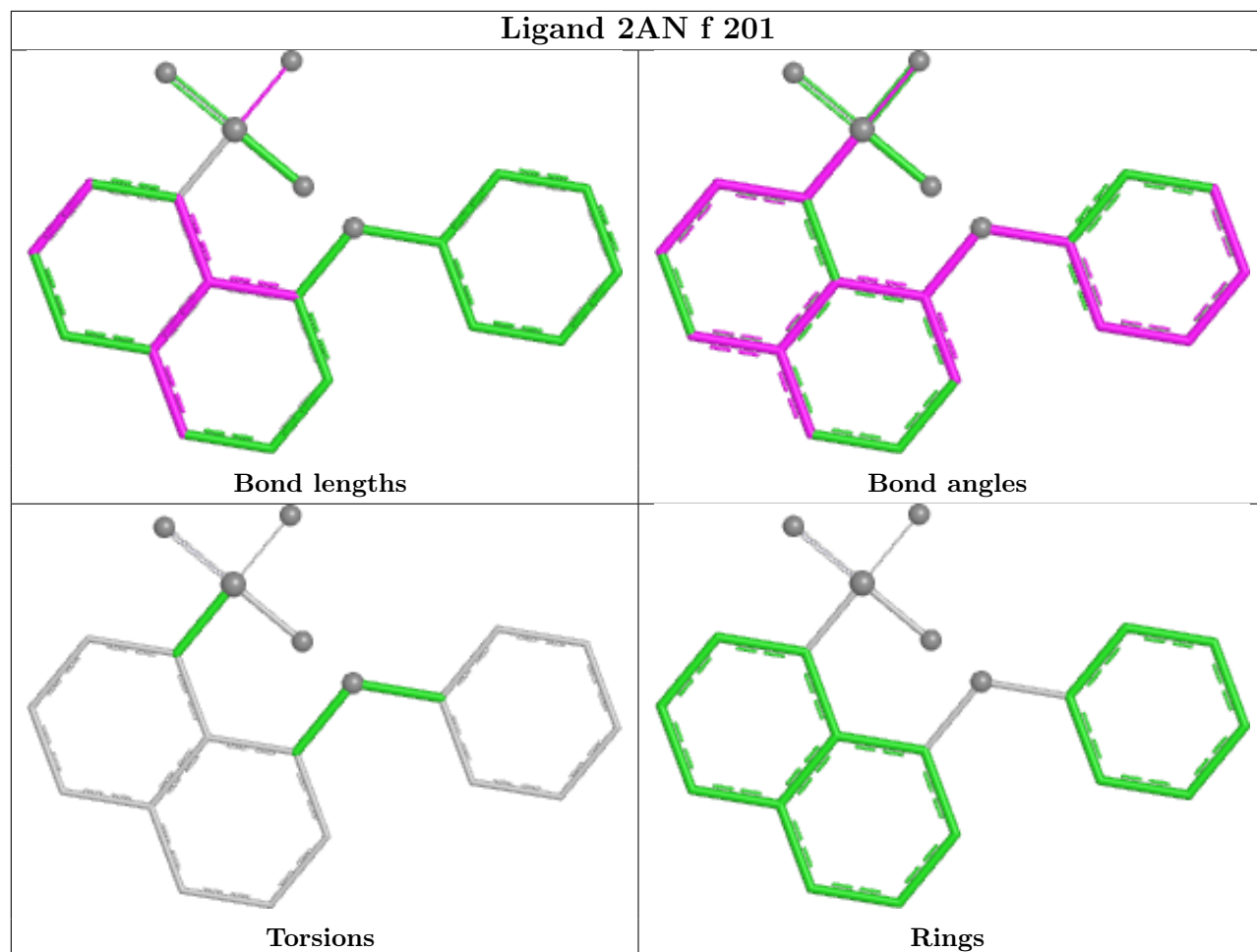


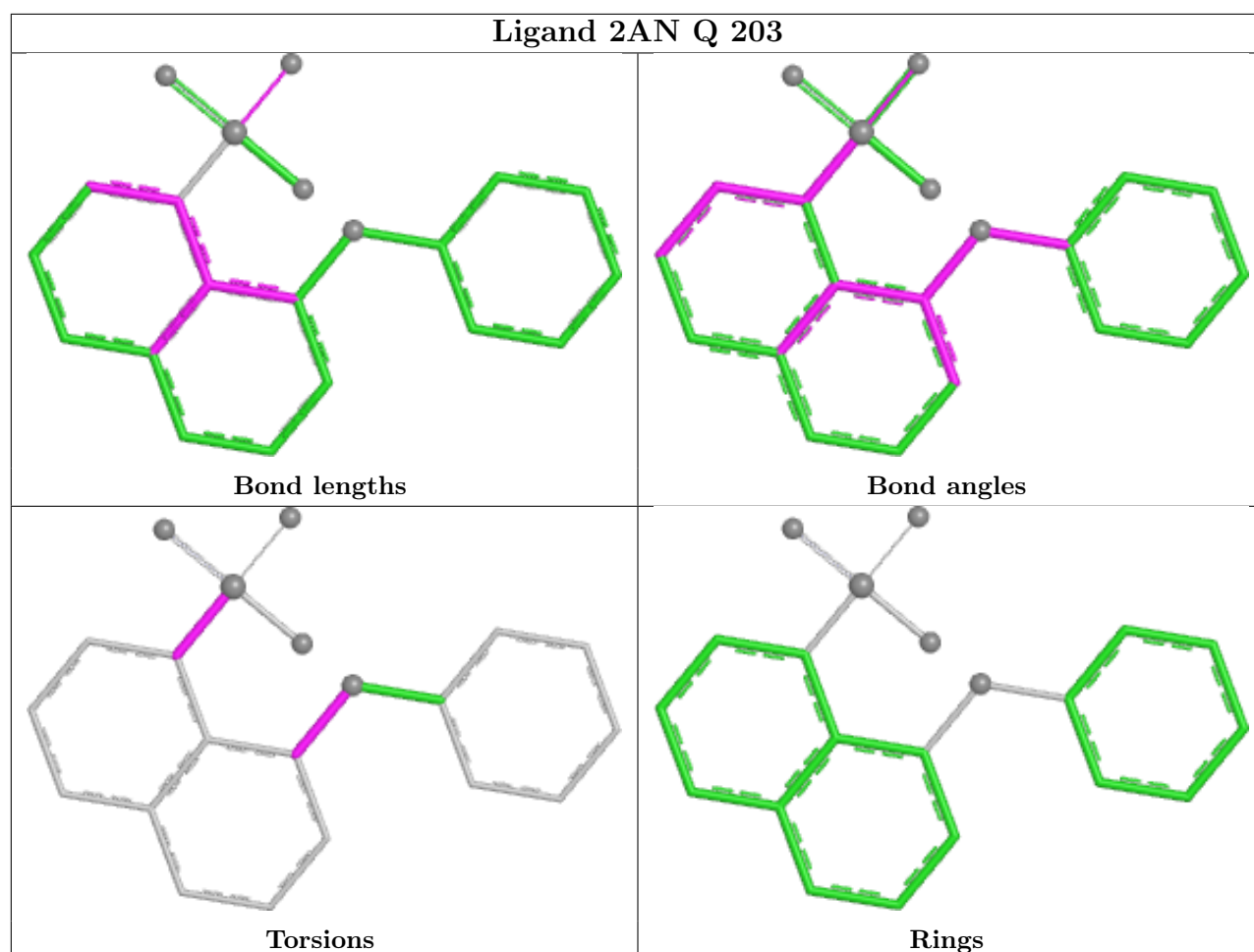
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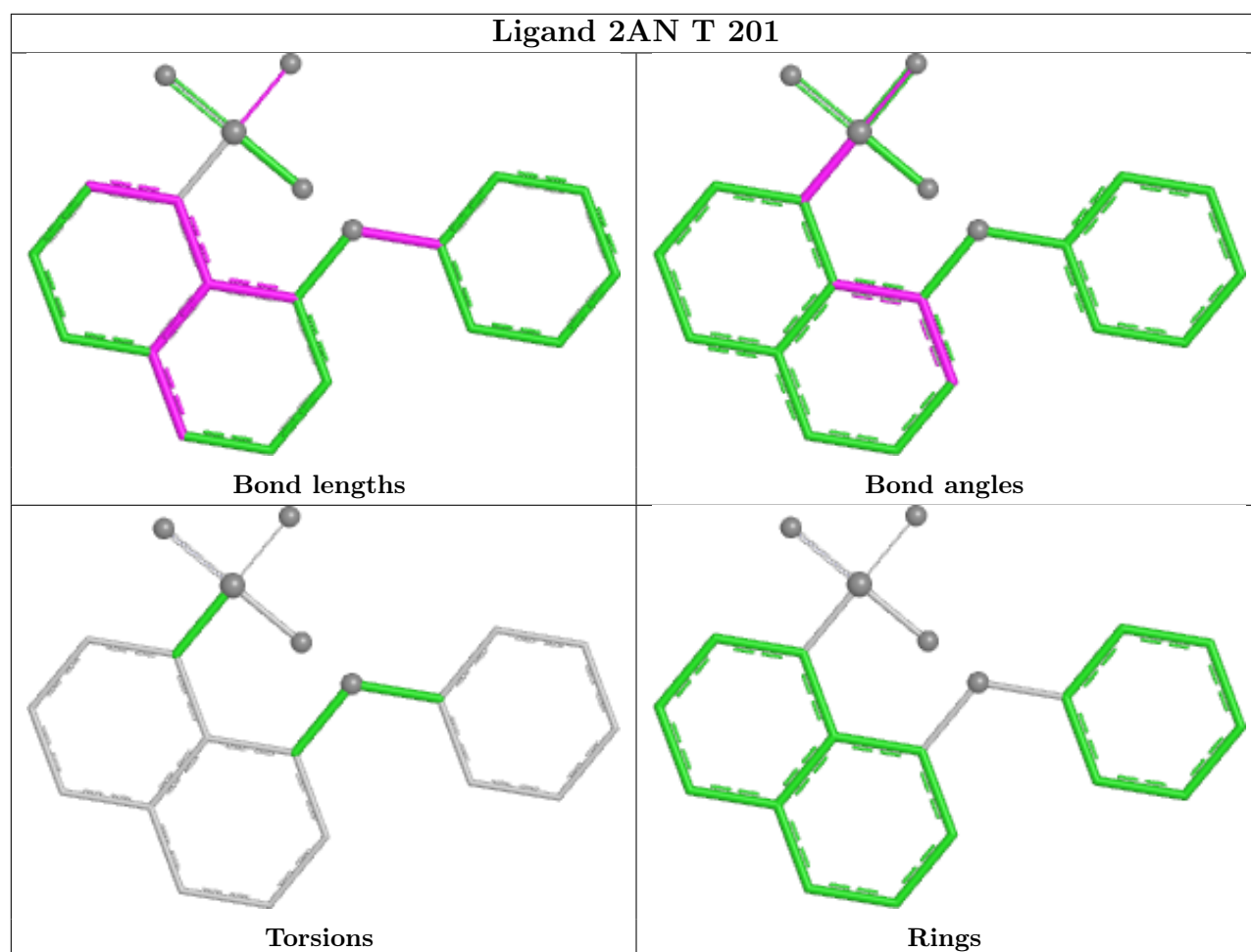




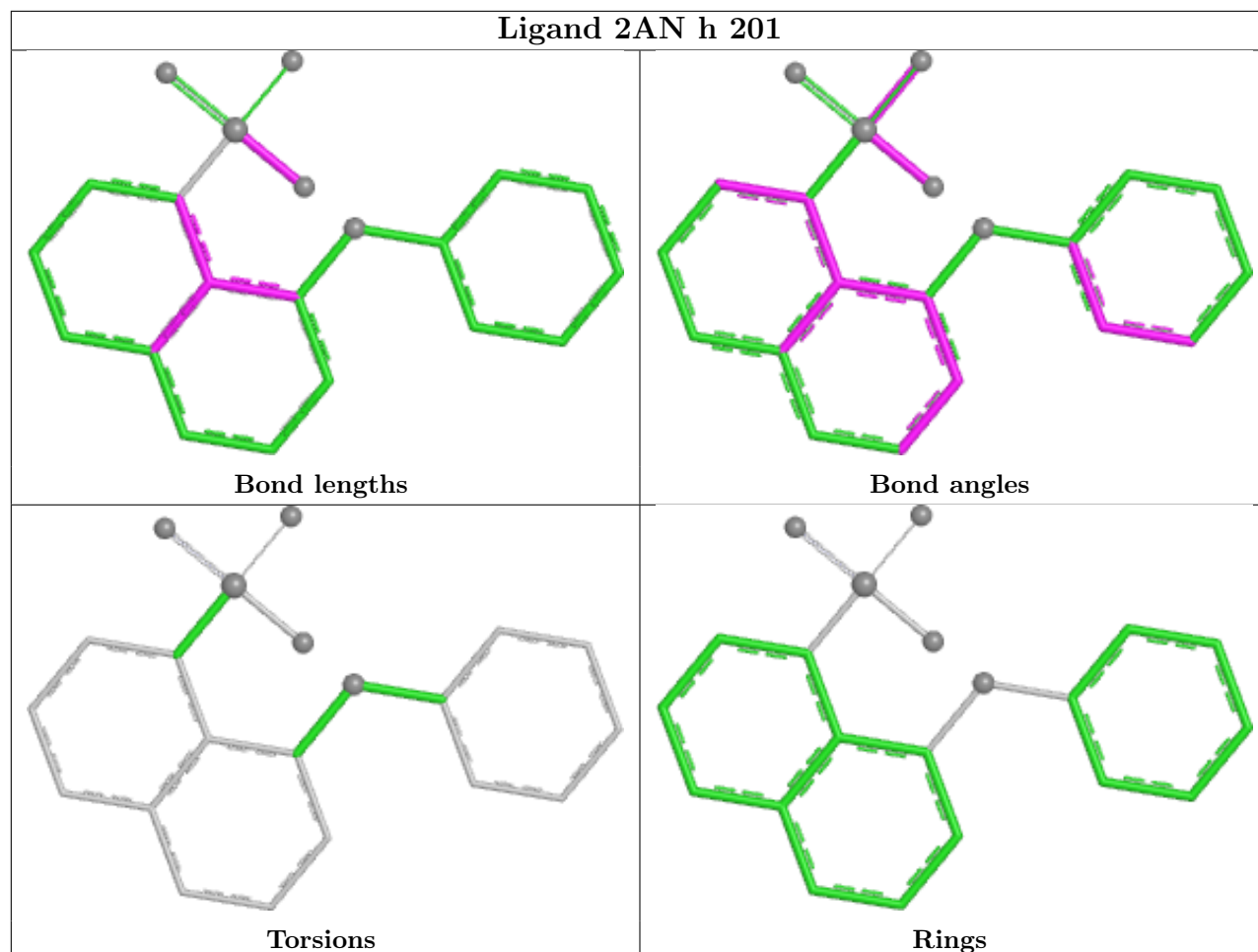
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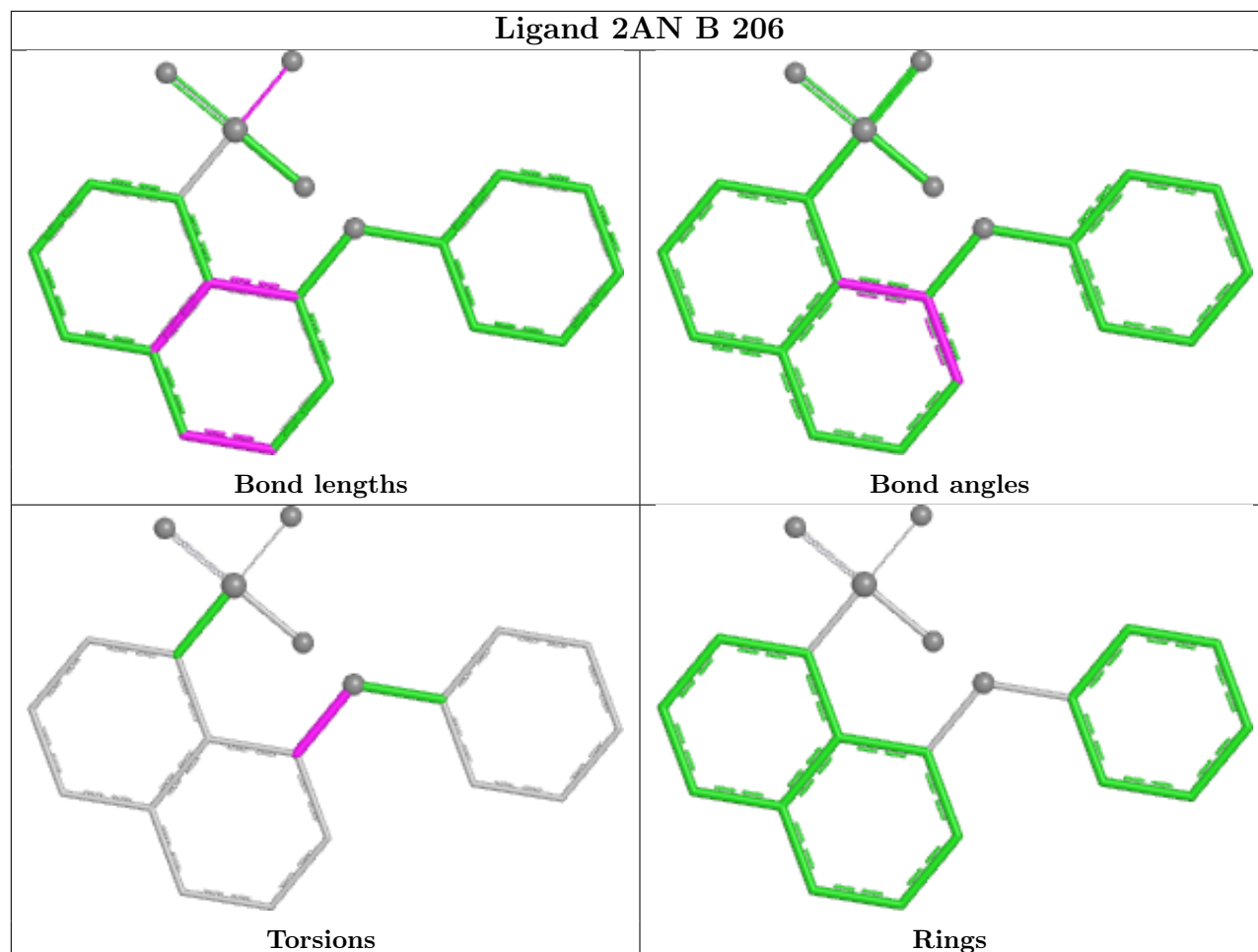




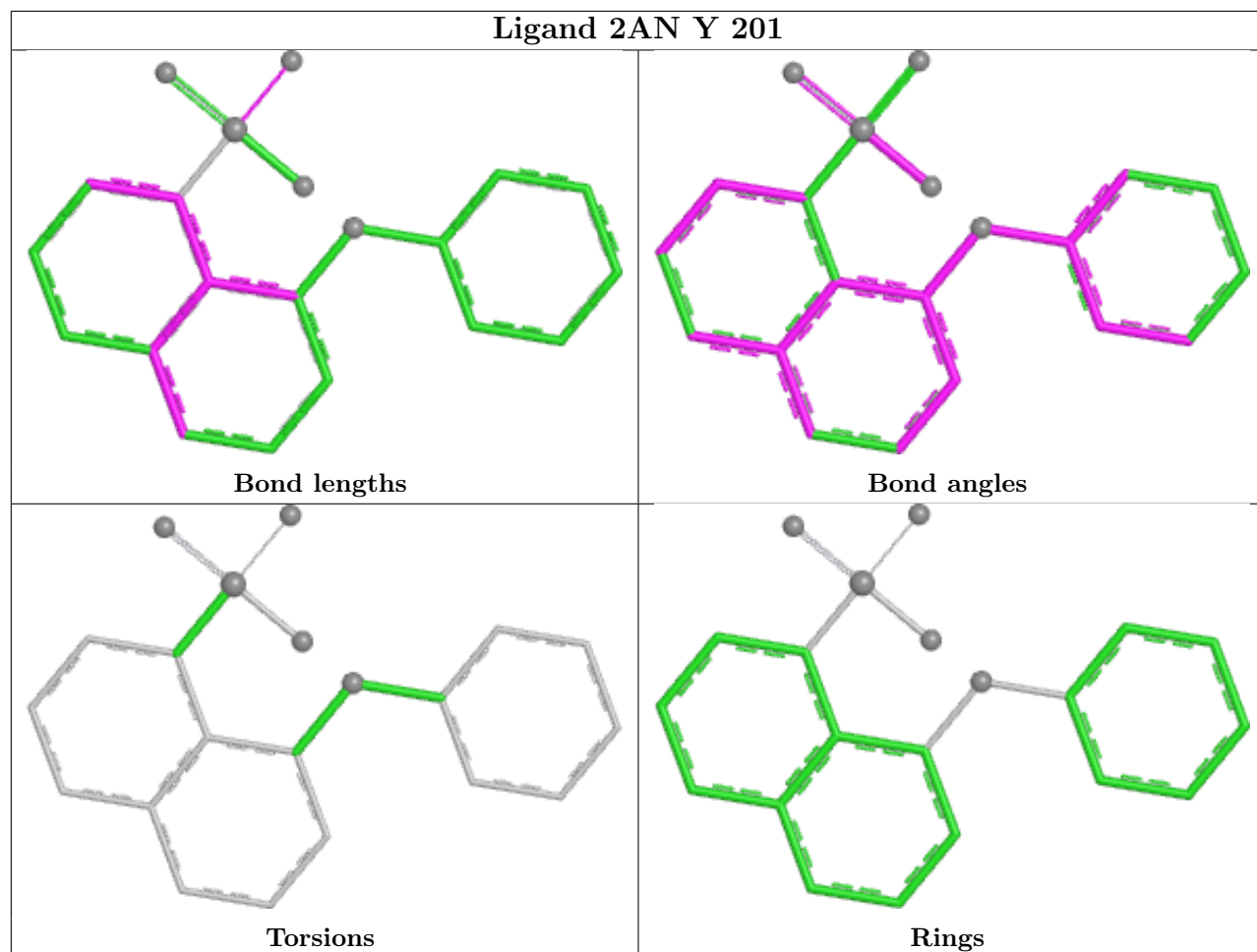
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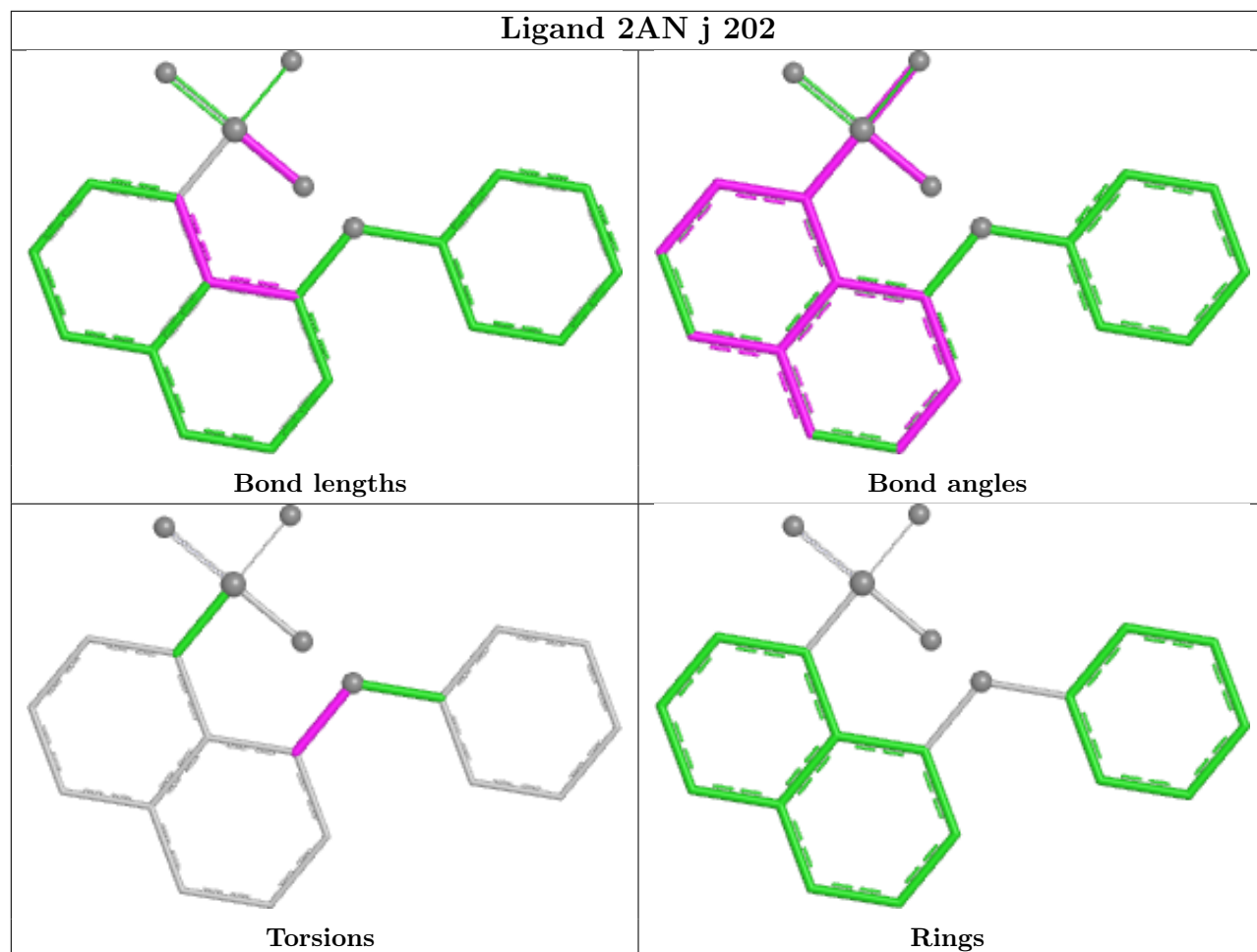
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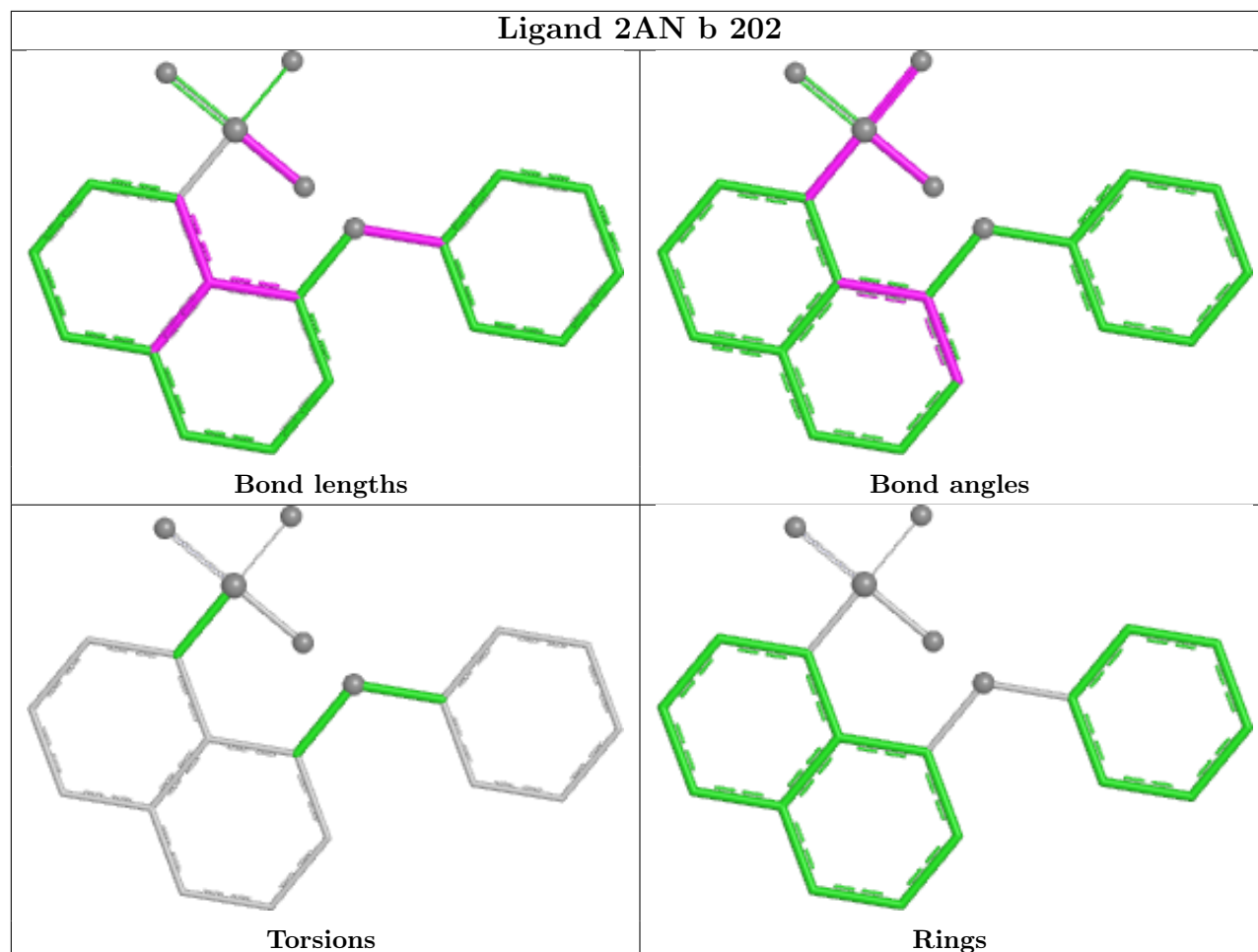
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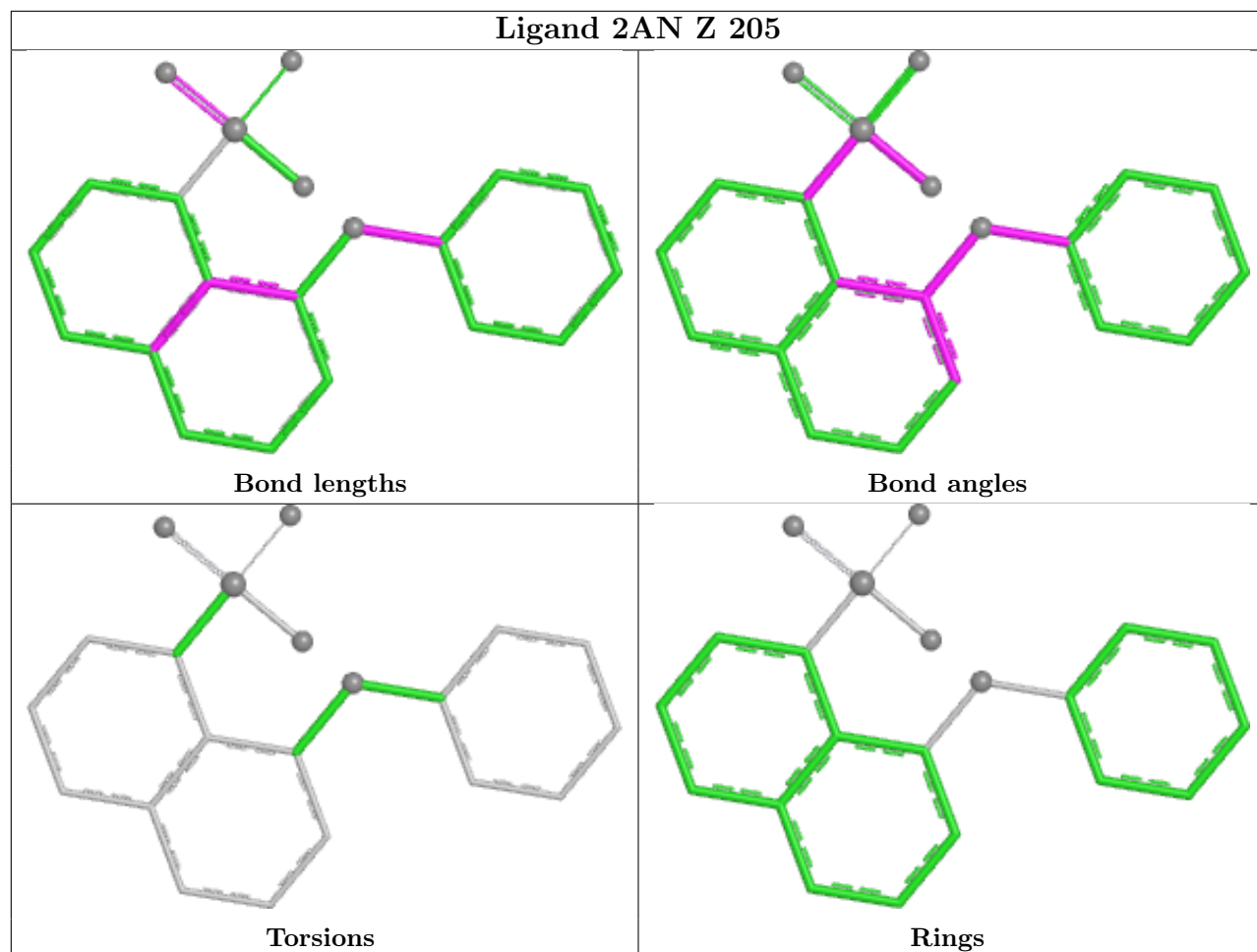
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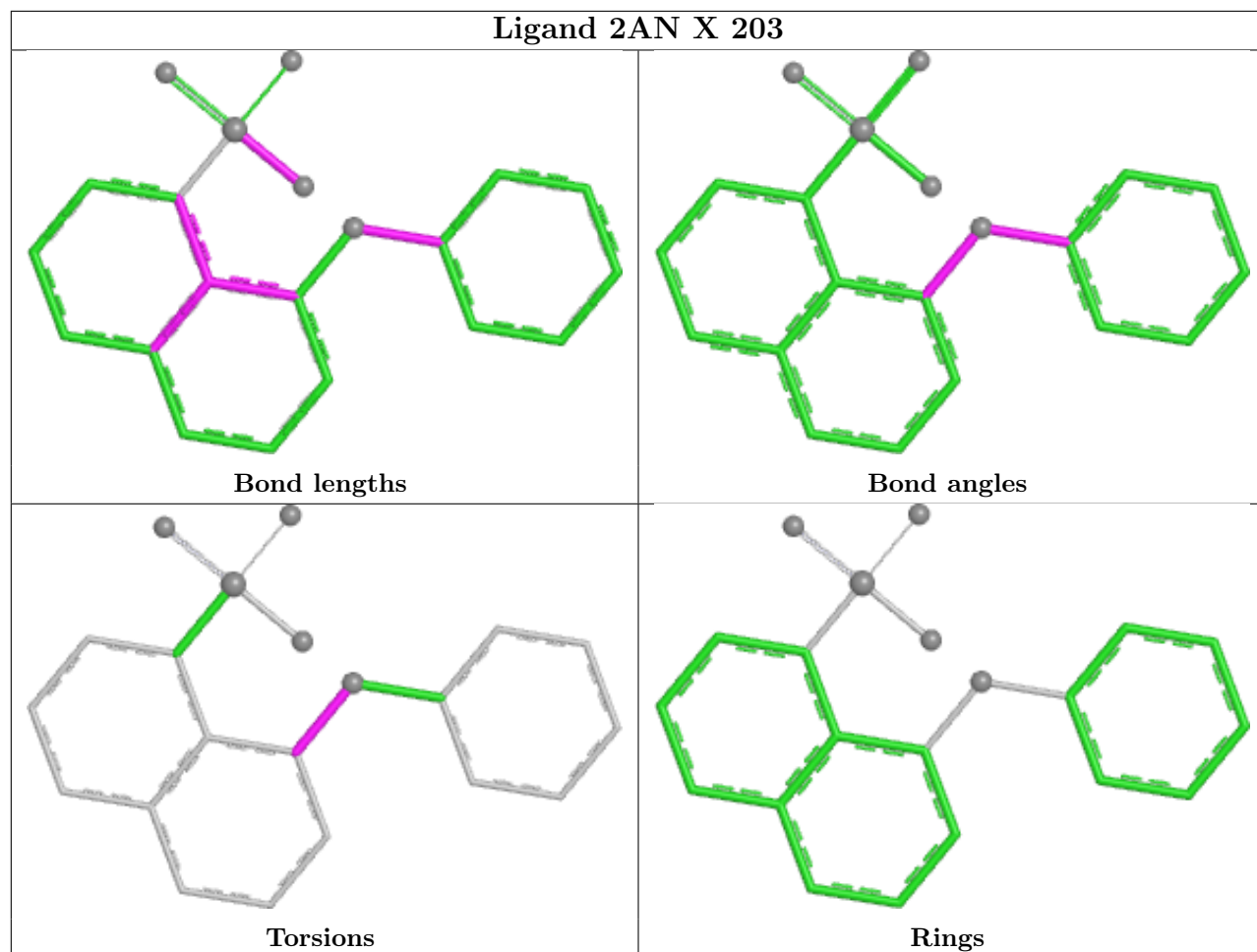


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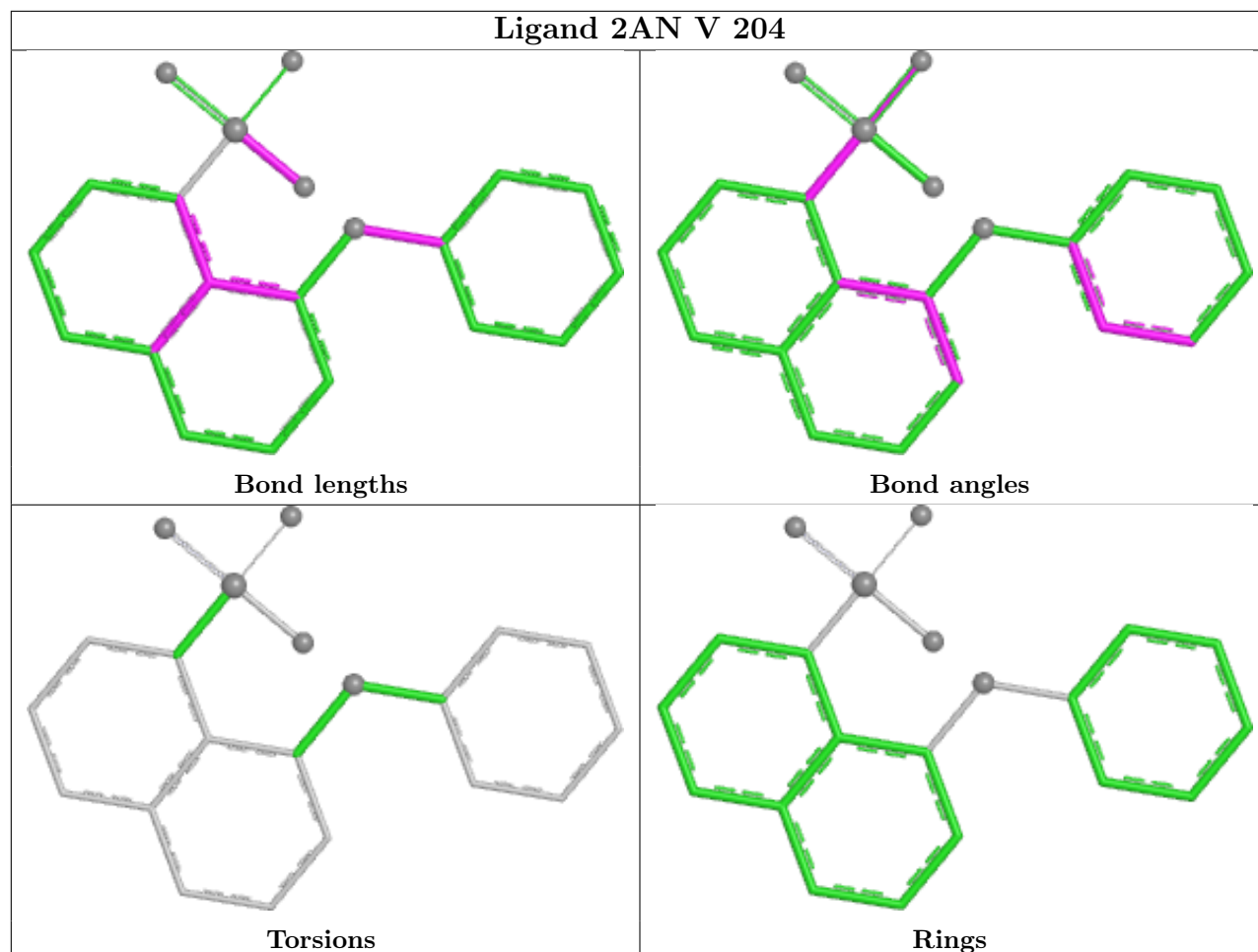


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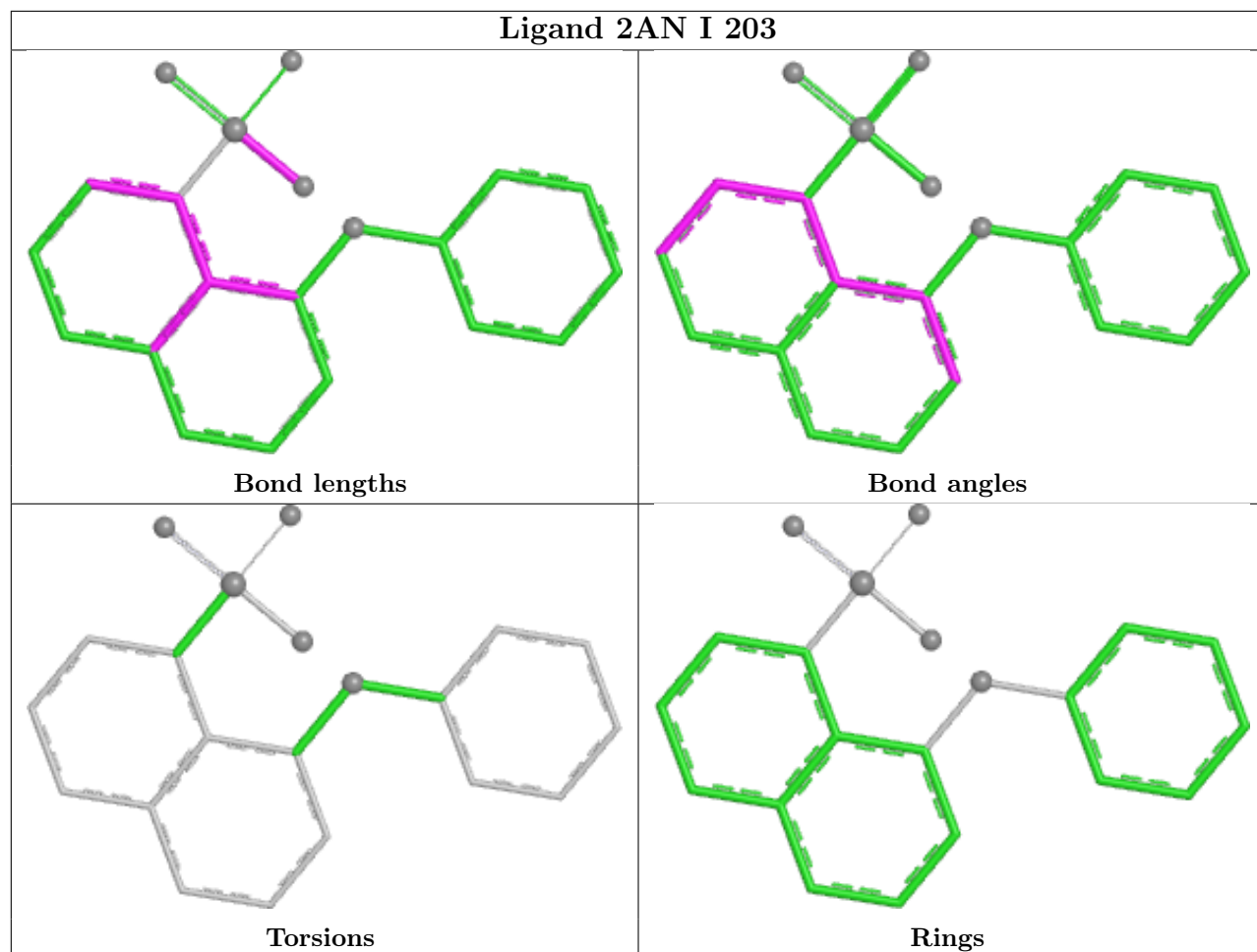


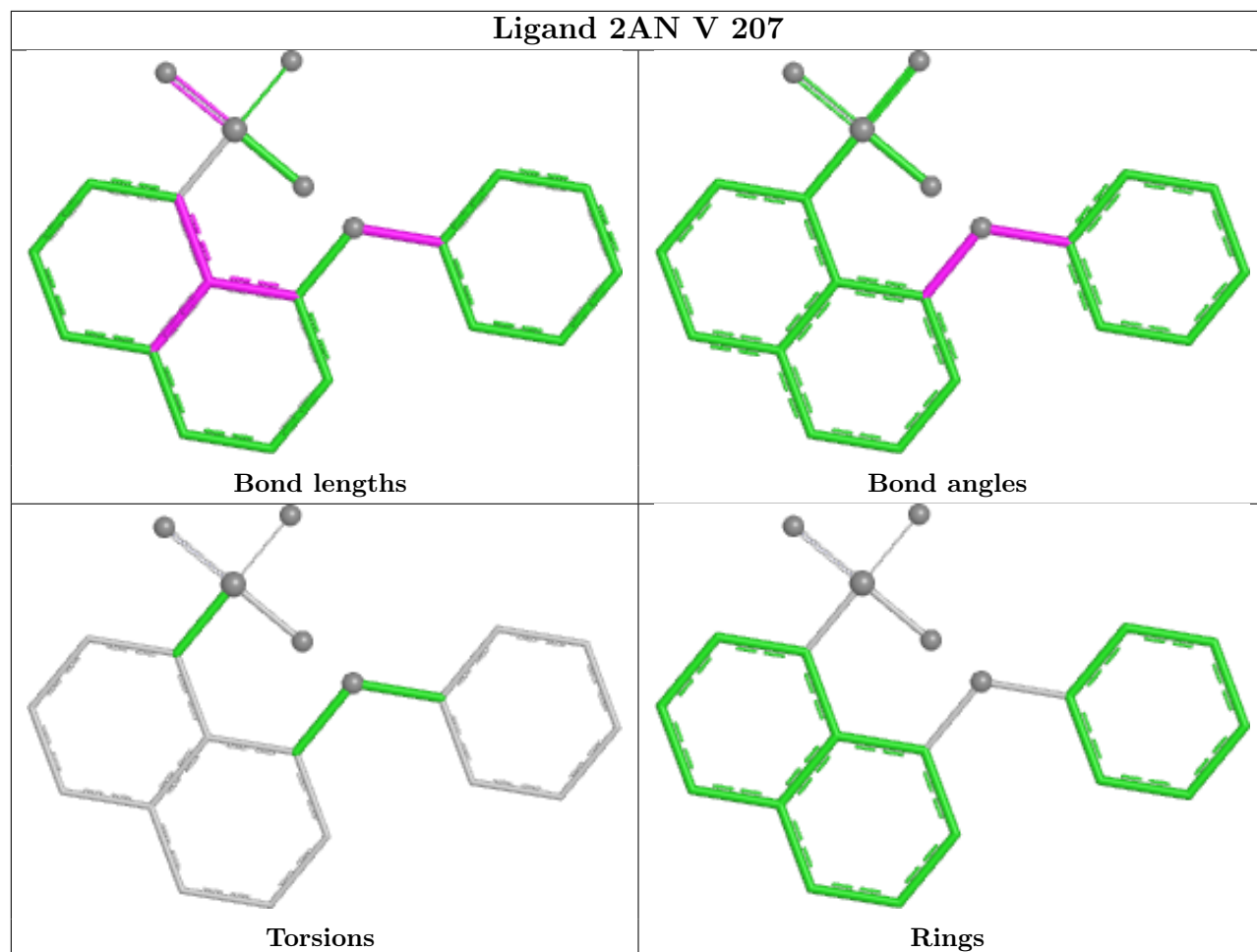


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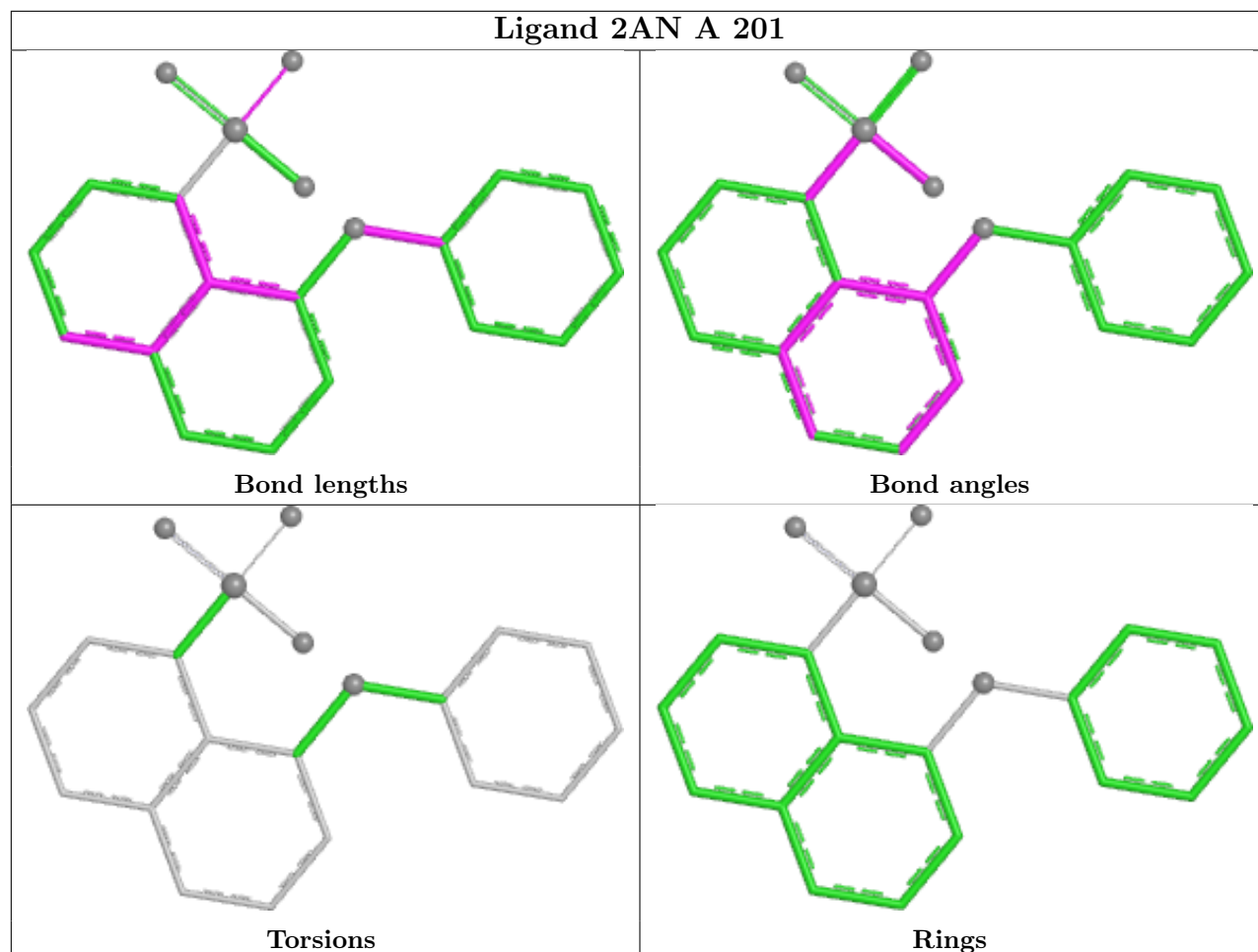


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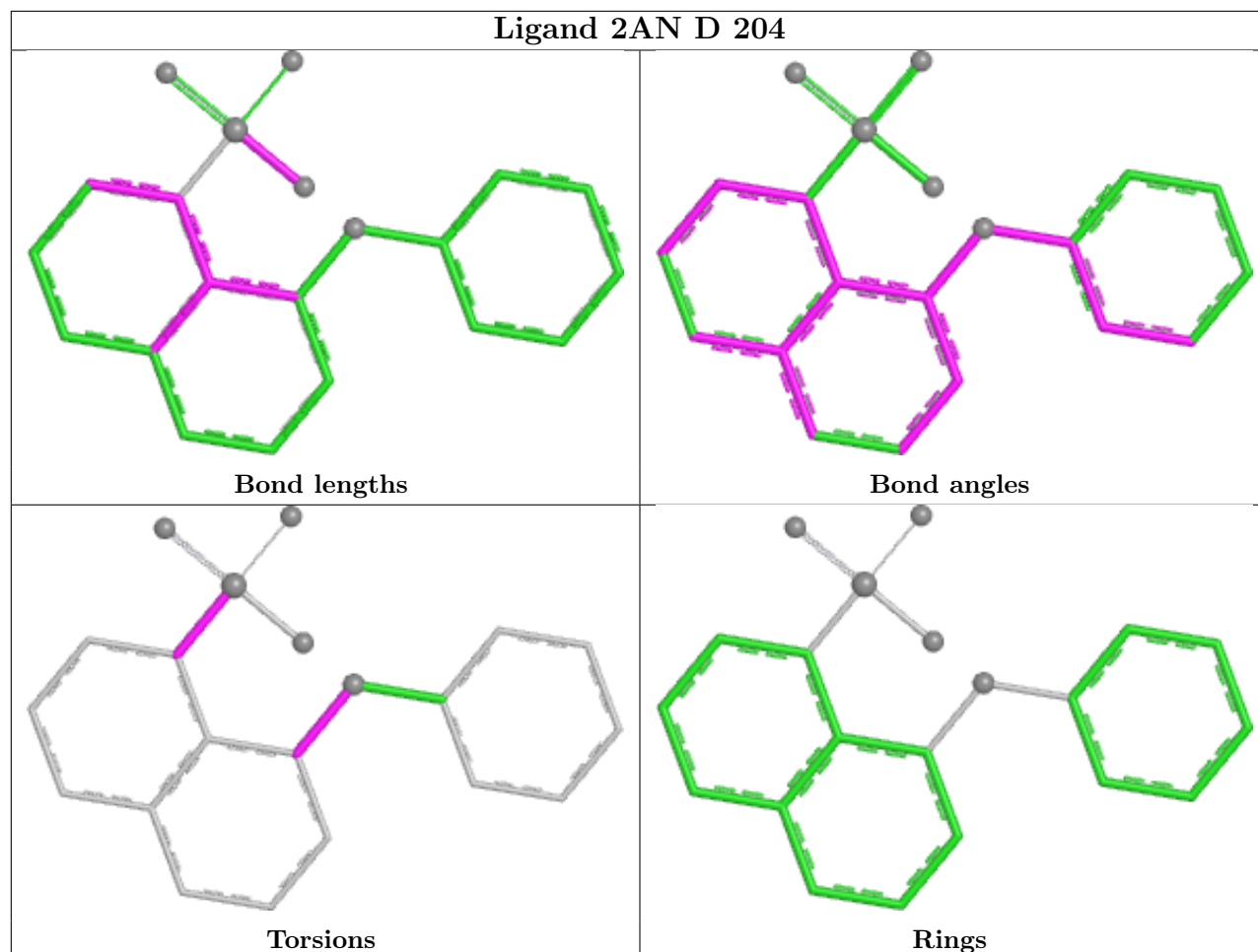




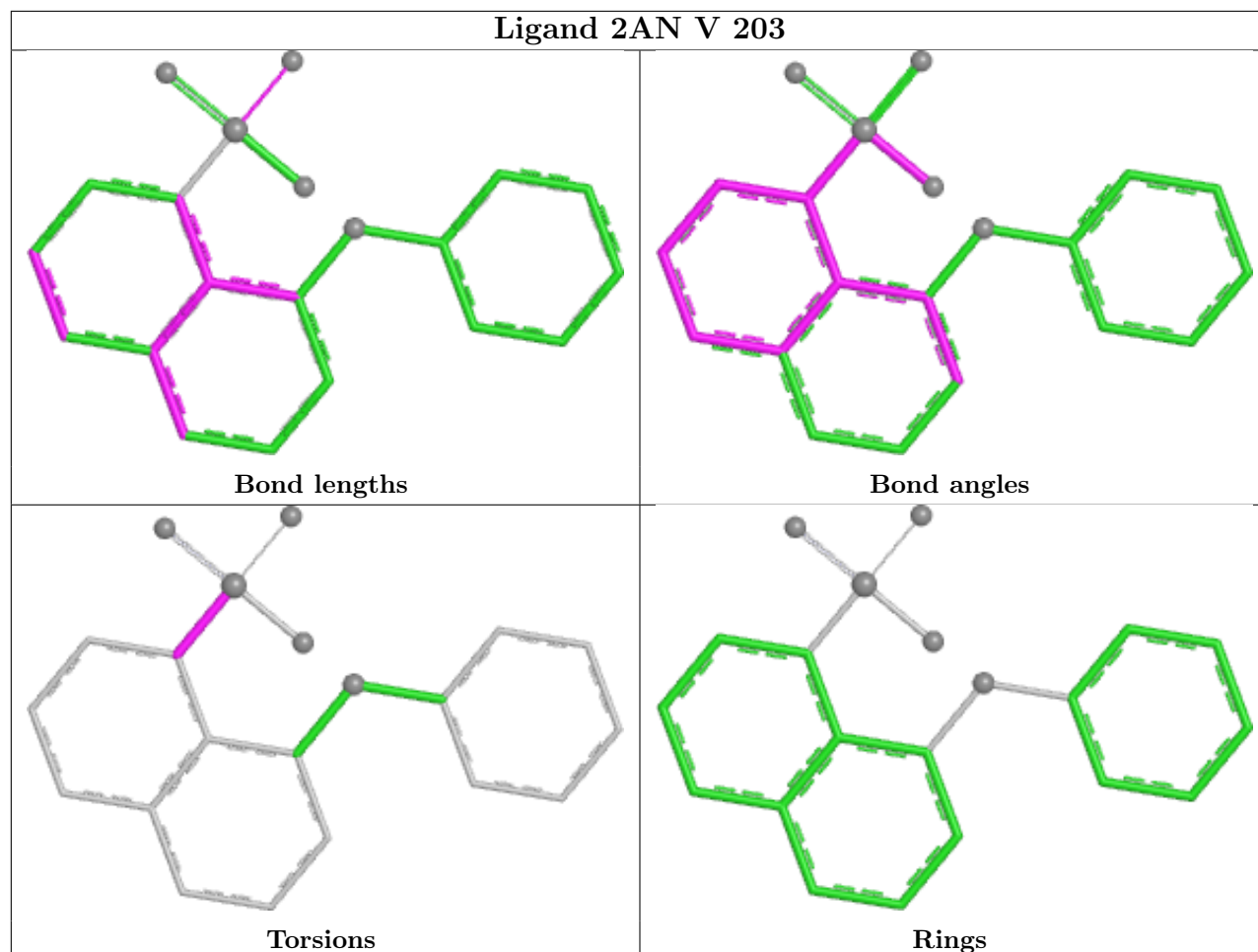
Ligand 2AN A 201



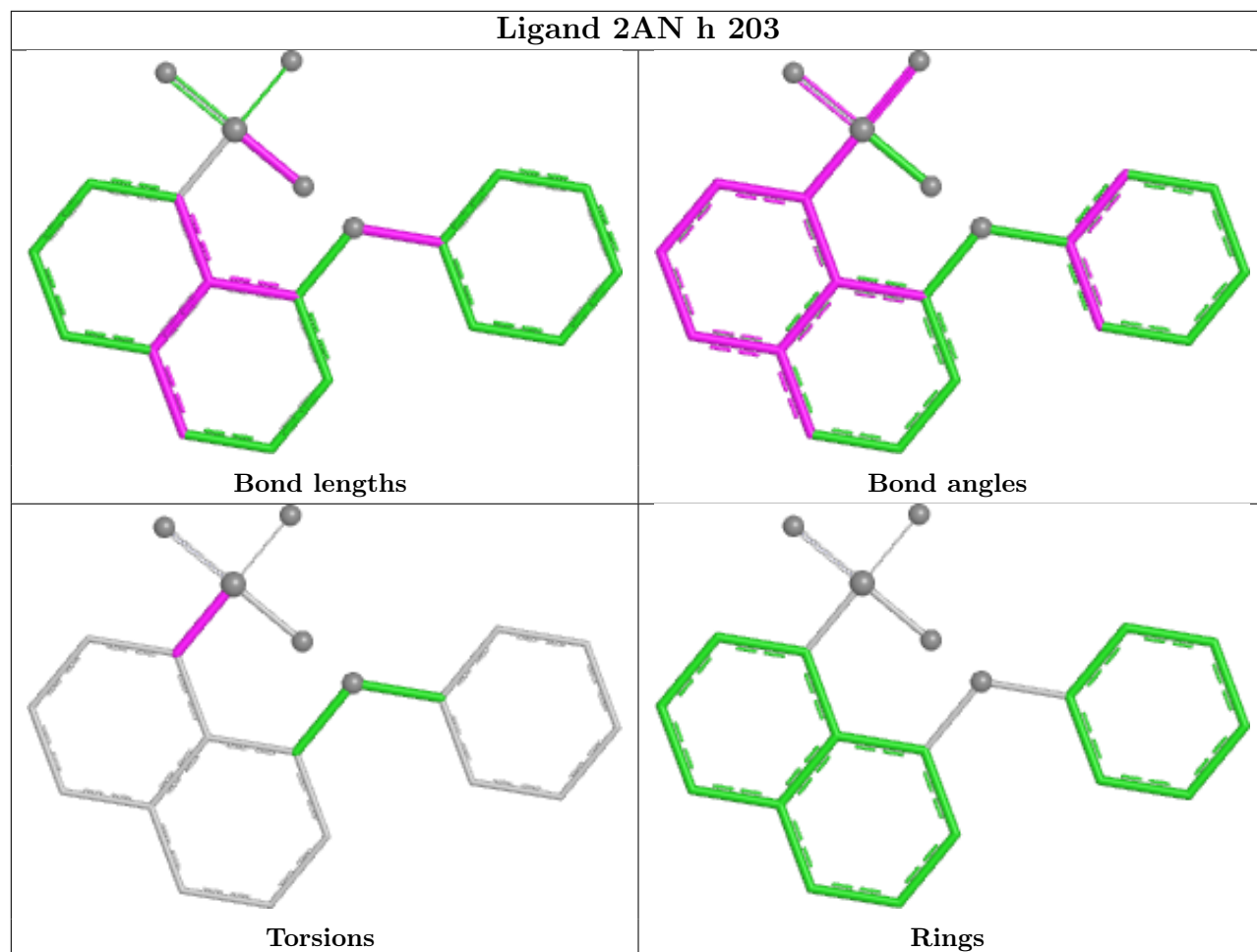
Ligand 2AN D 204

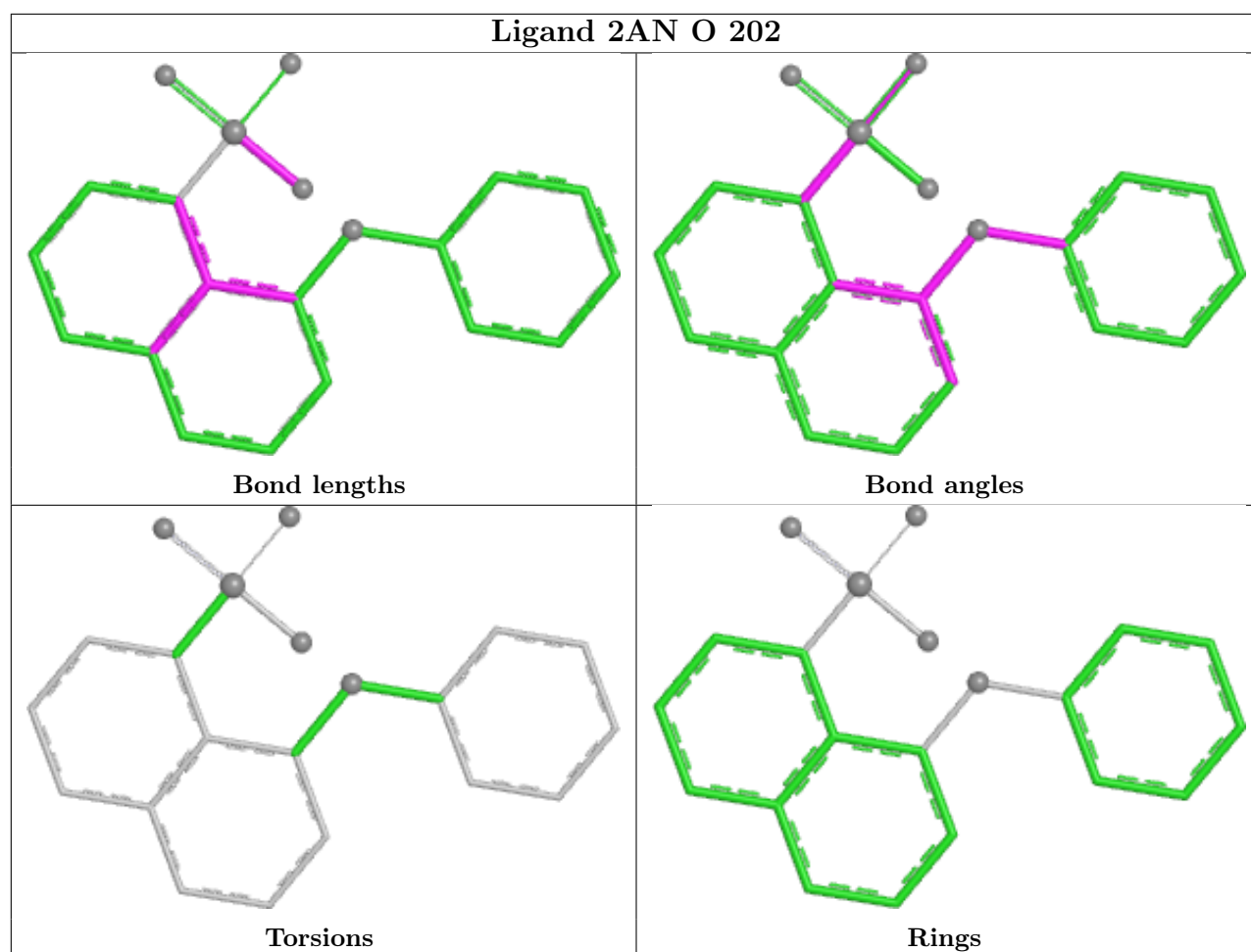


Ligand 2AN V 203

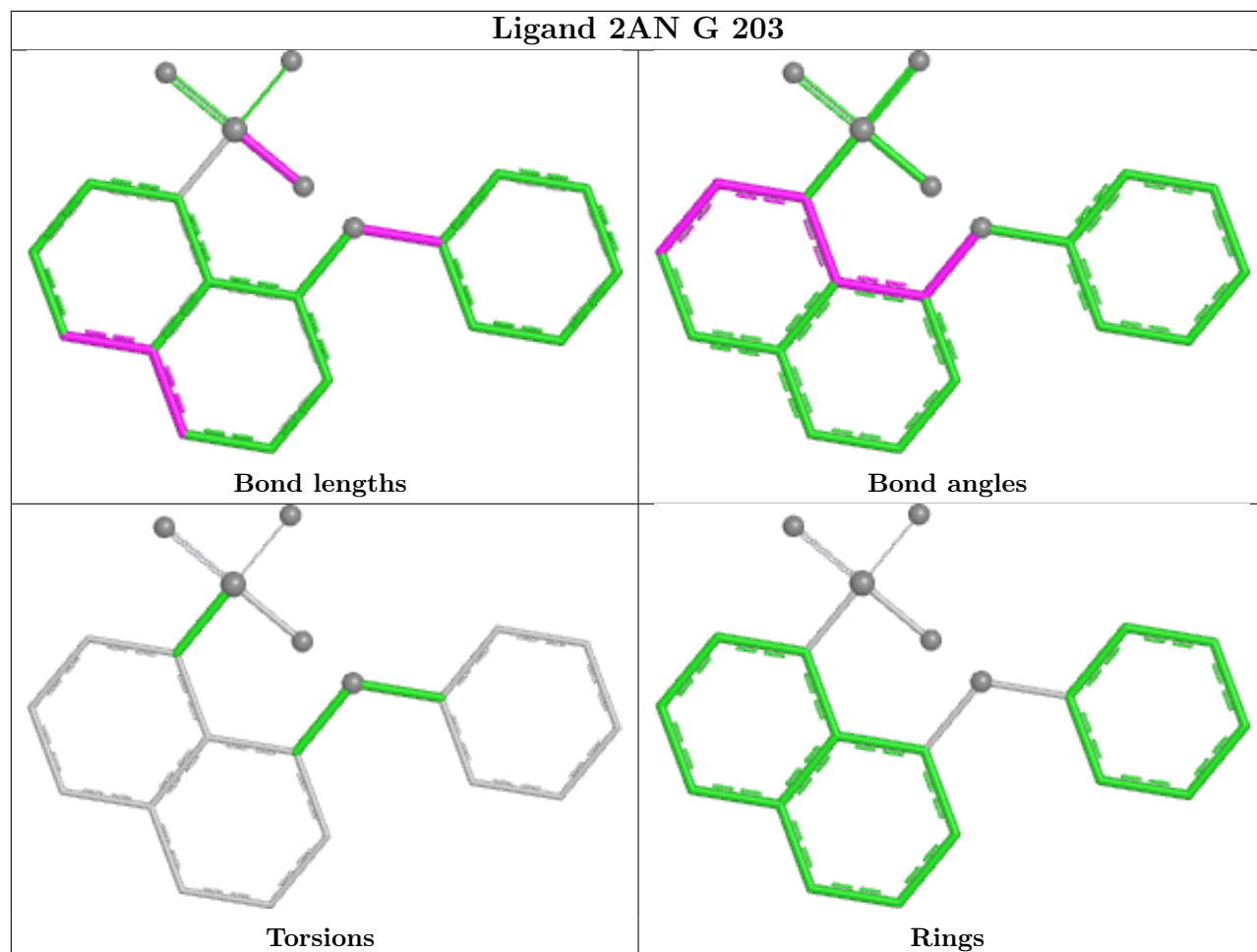


Ligand 2AN h 203

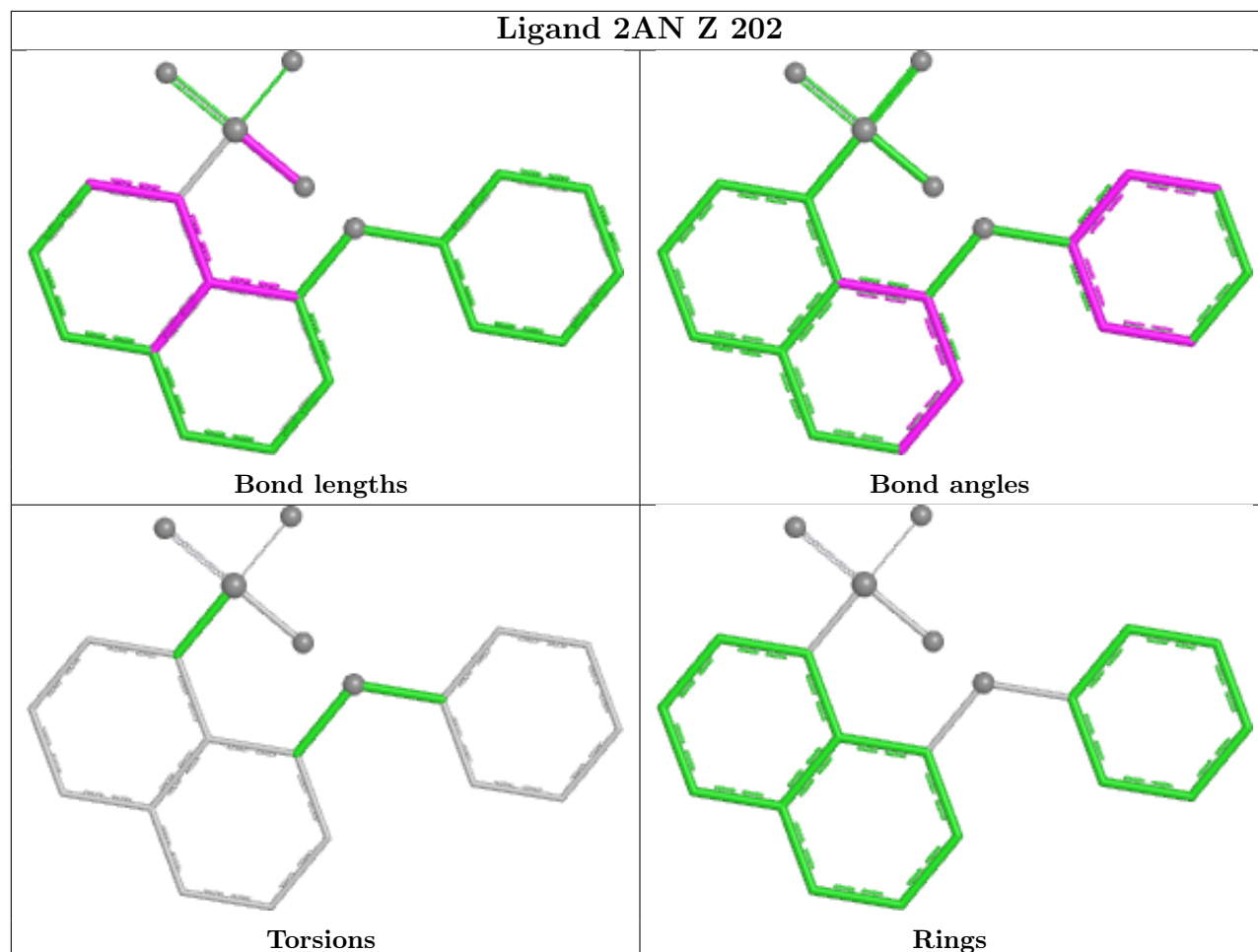




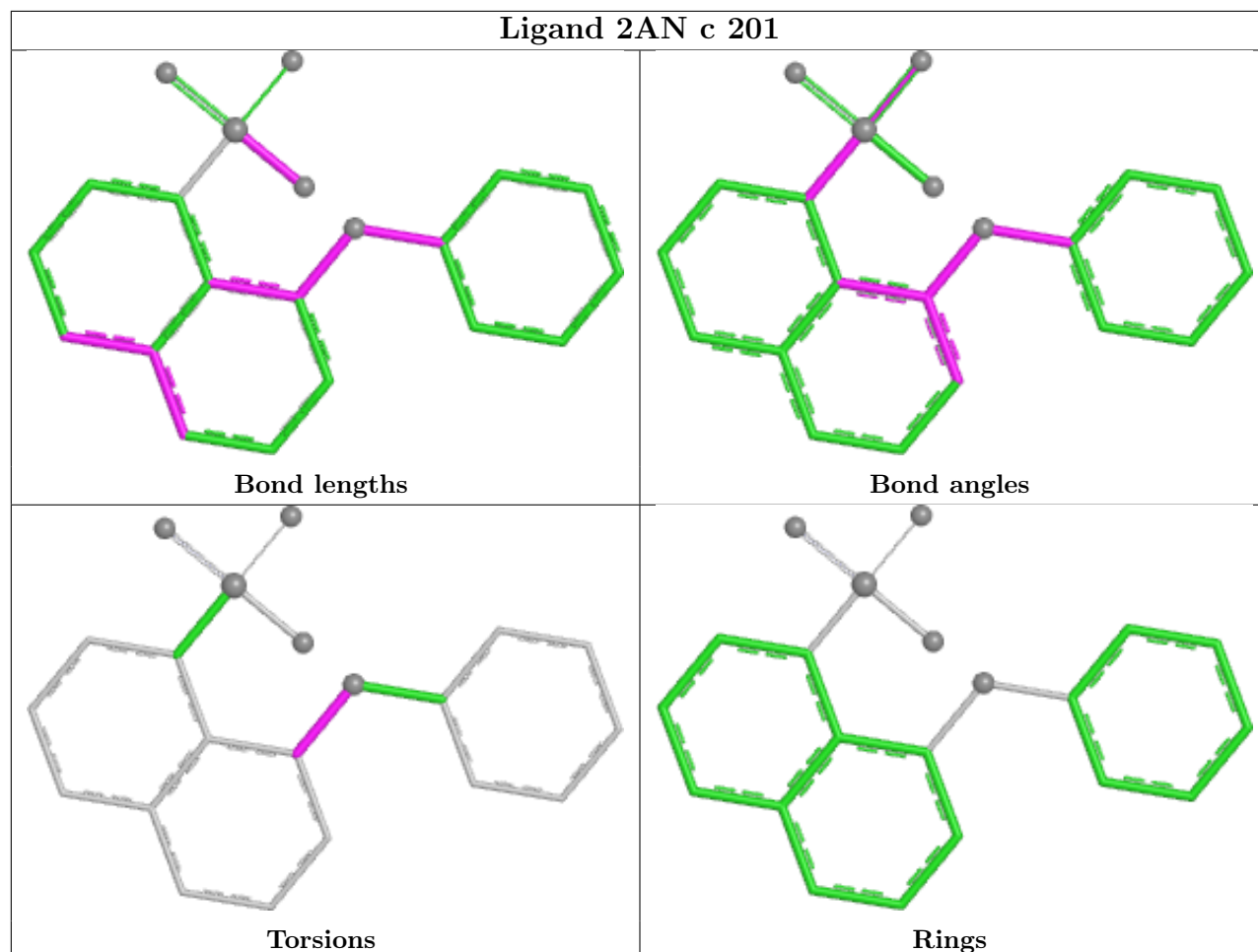
Ligand 2AN G 203

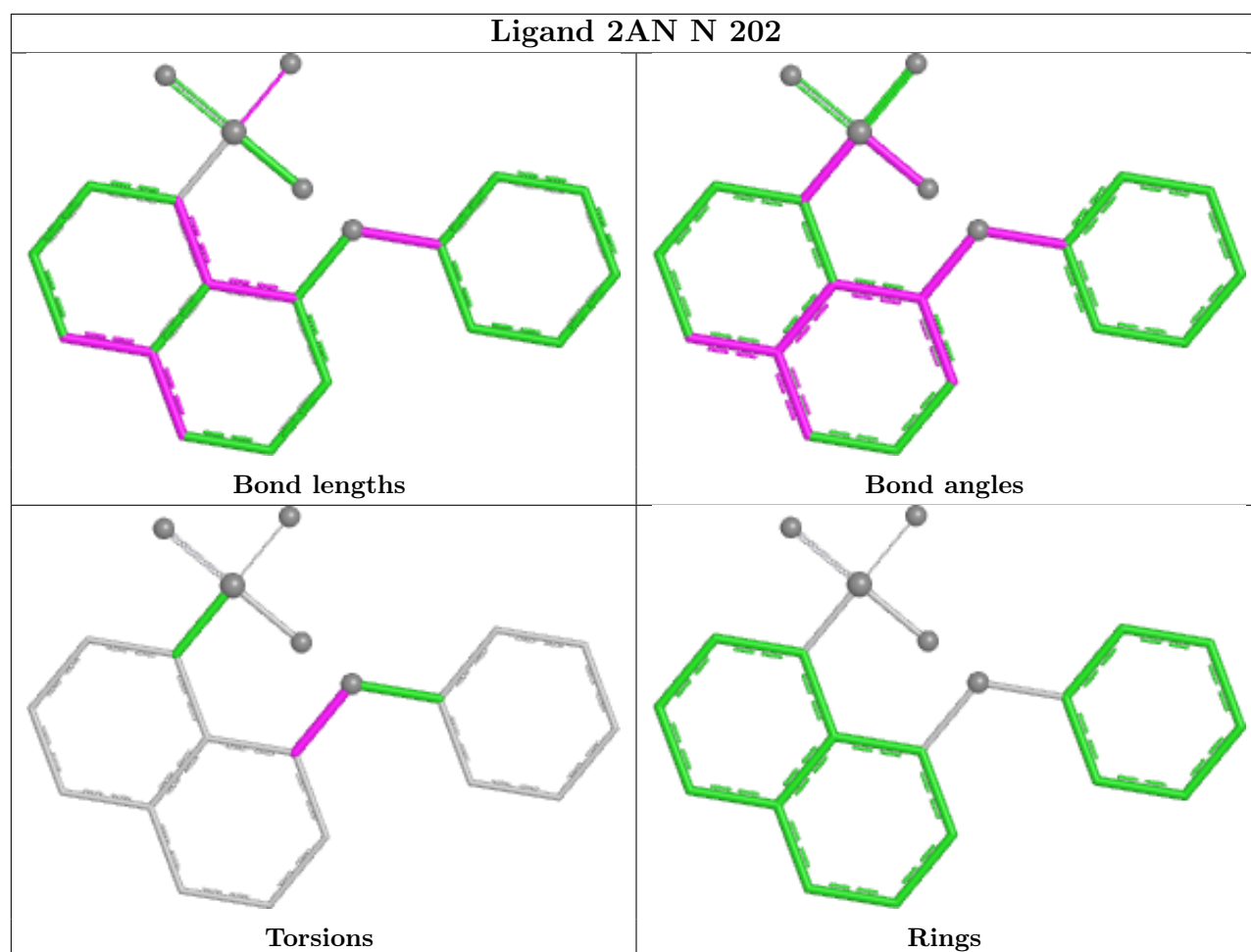


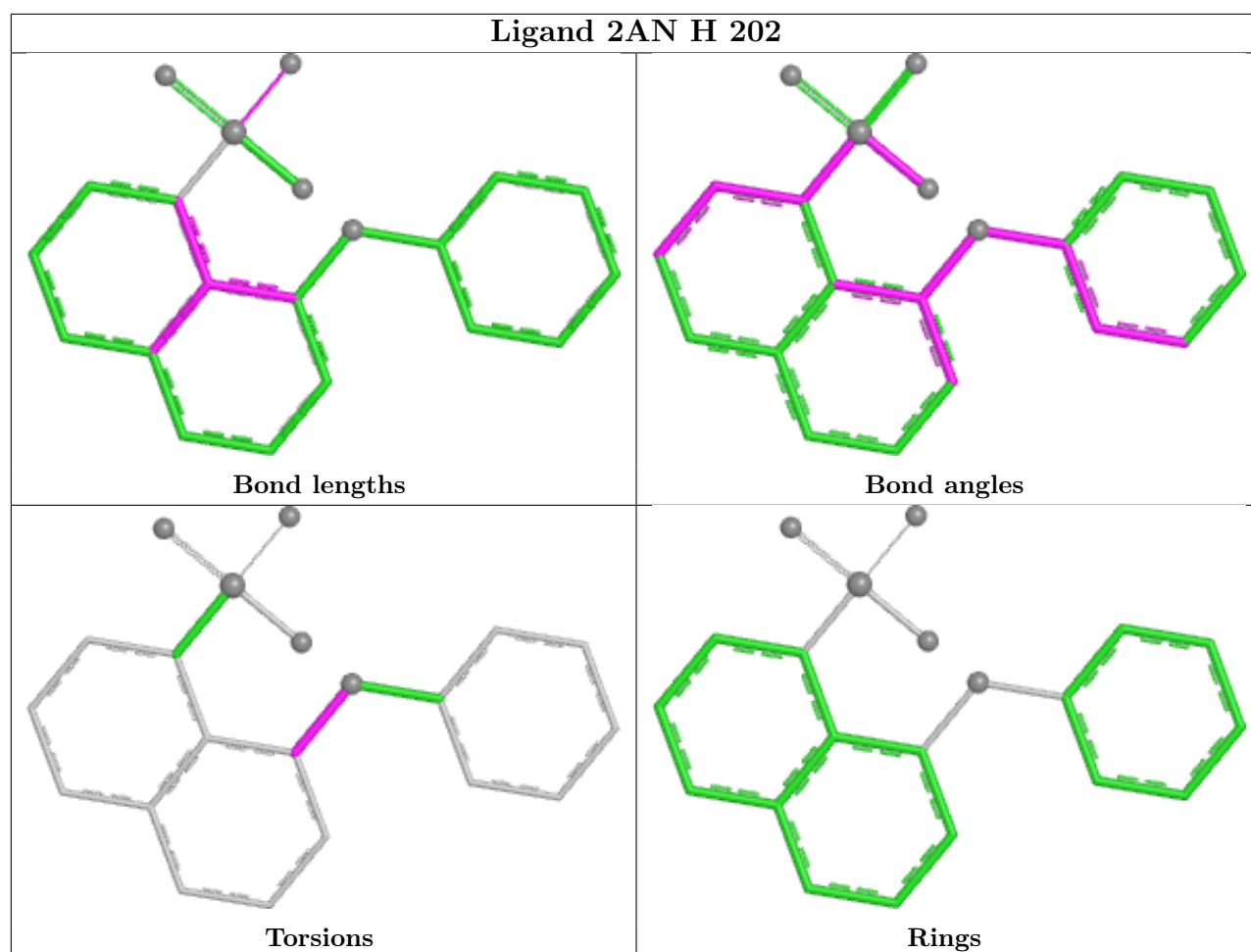
Ligand 2AN Z 202



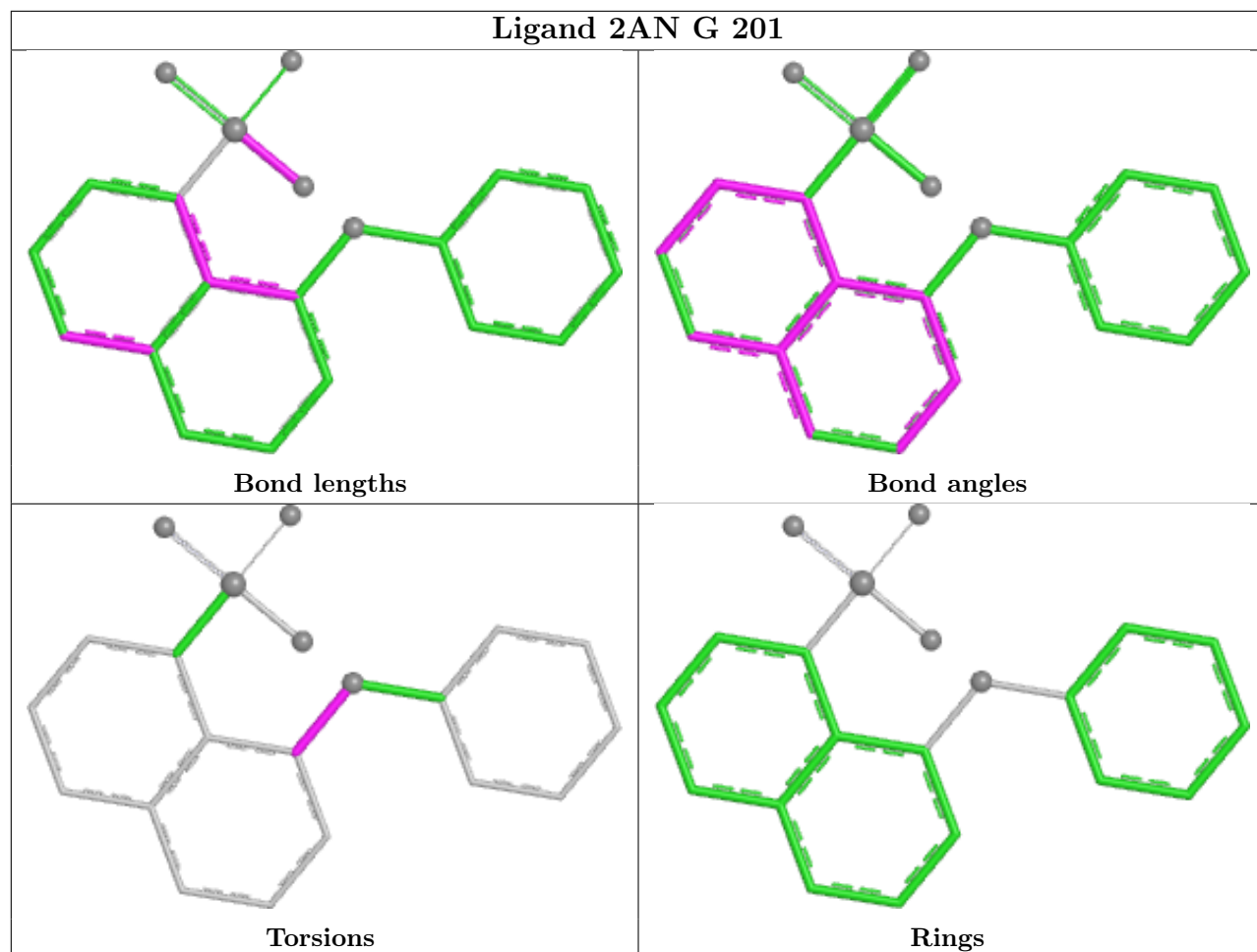
Ligand 2AN c 201



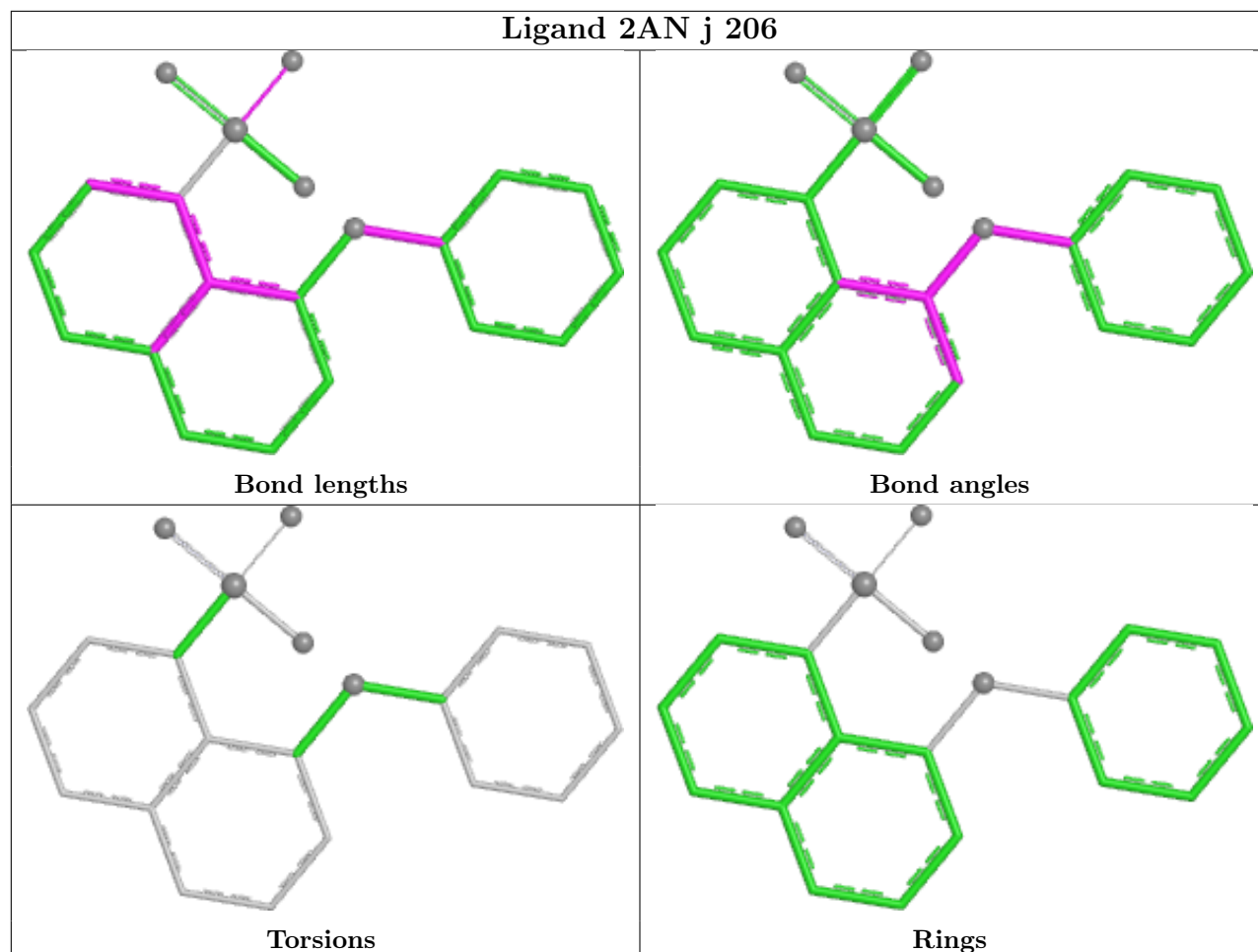




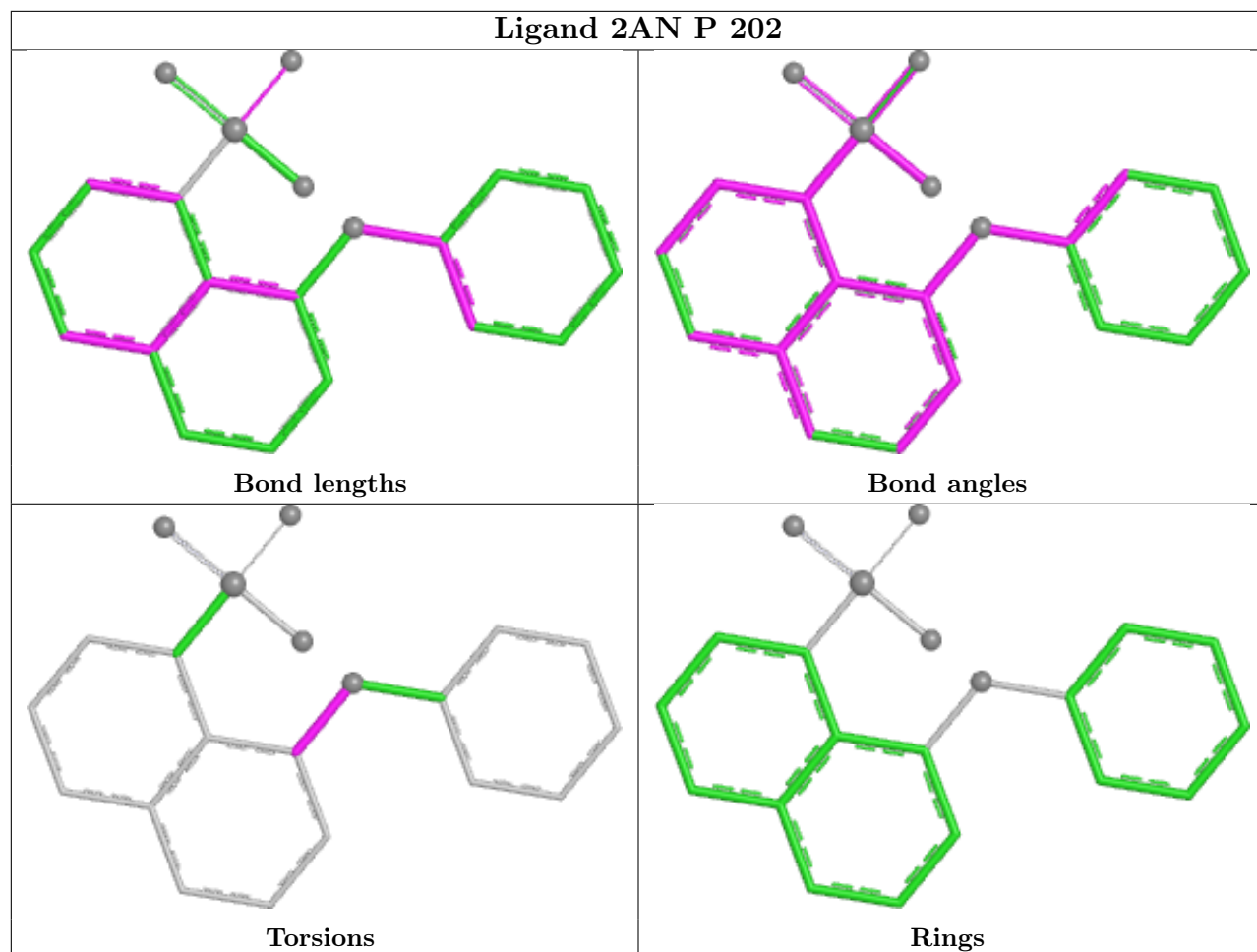
Ligand 2AN G 201



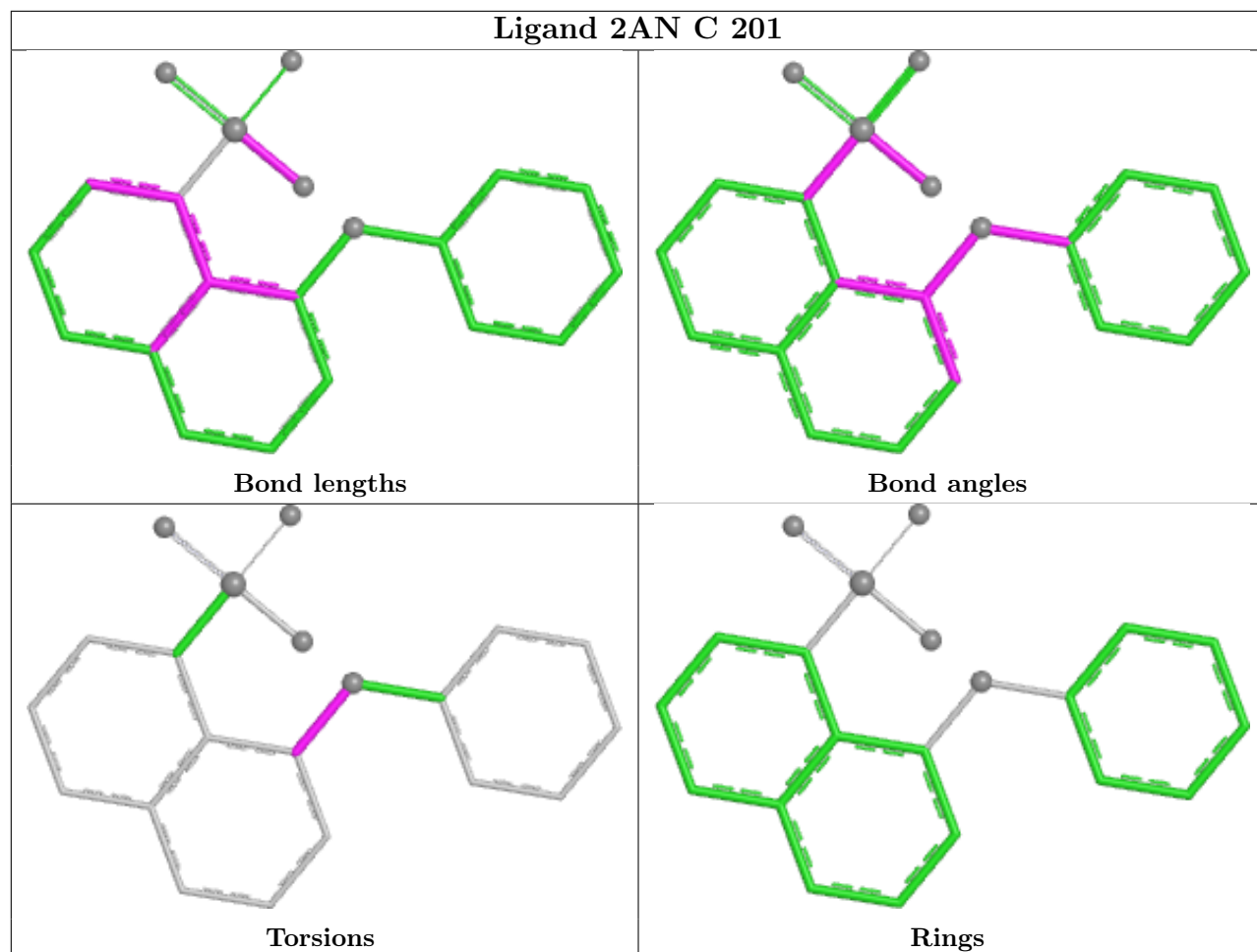
Ligand 2AN j 206



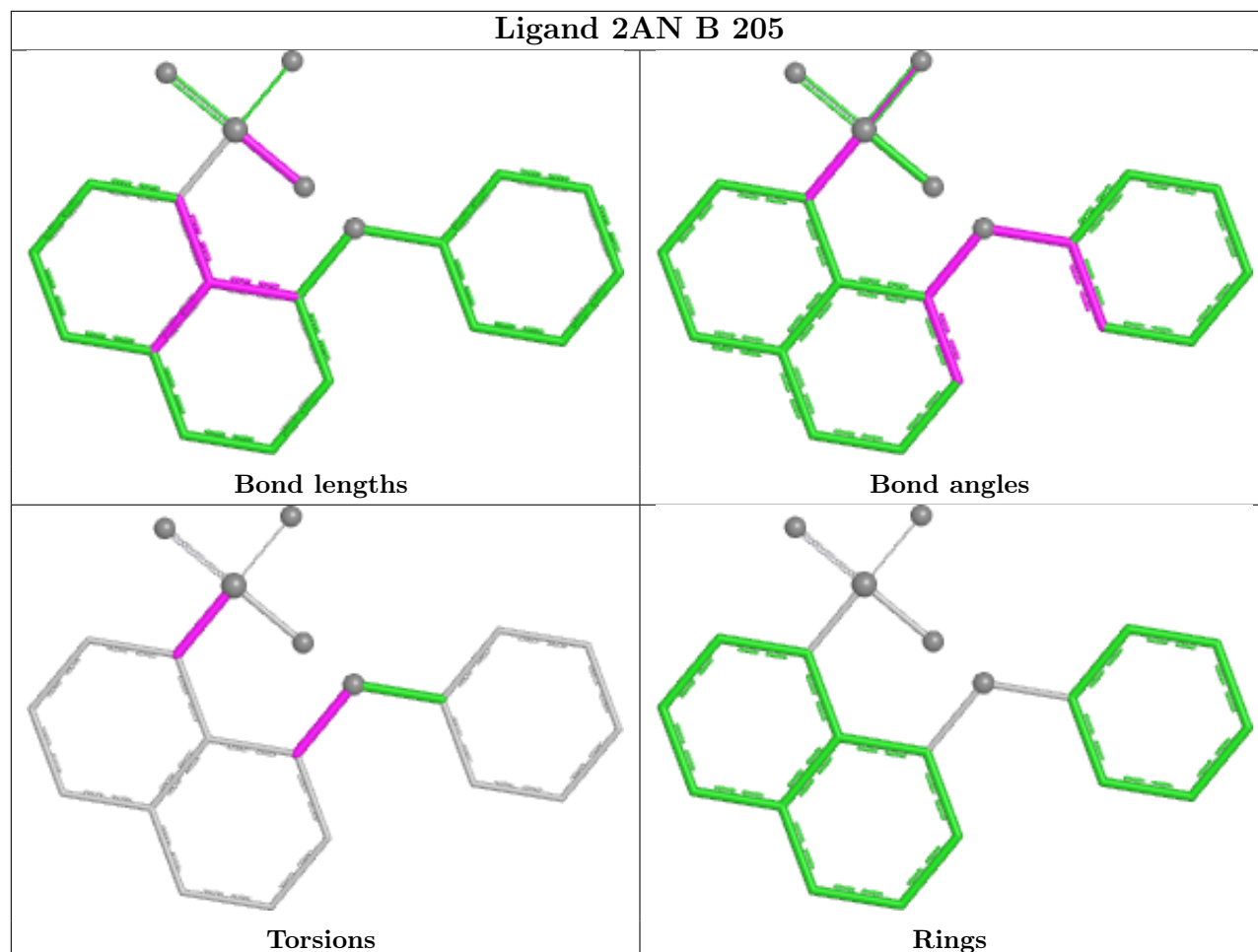
Ligand 2AN P 202

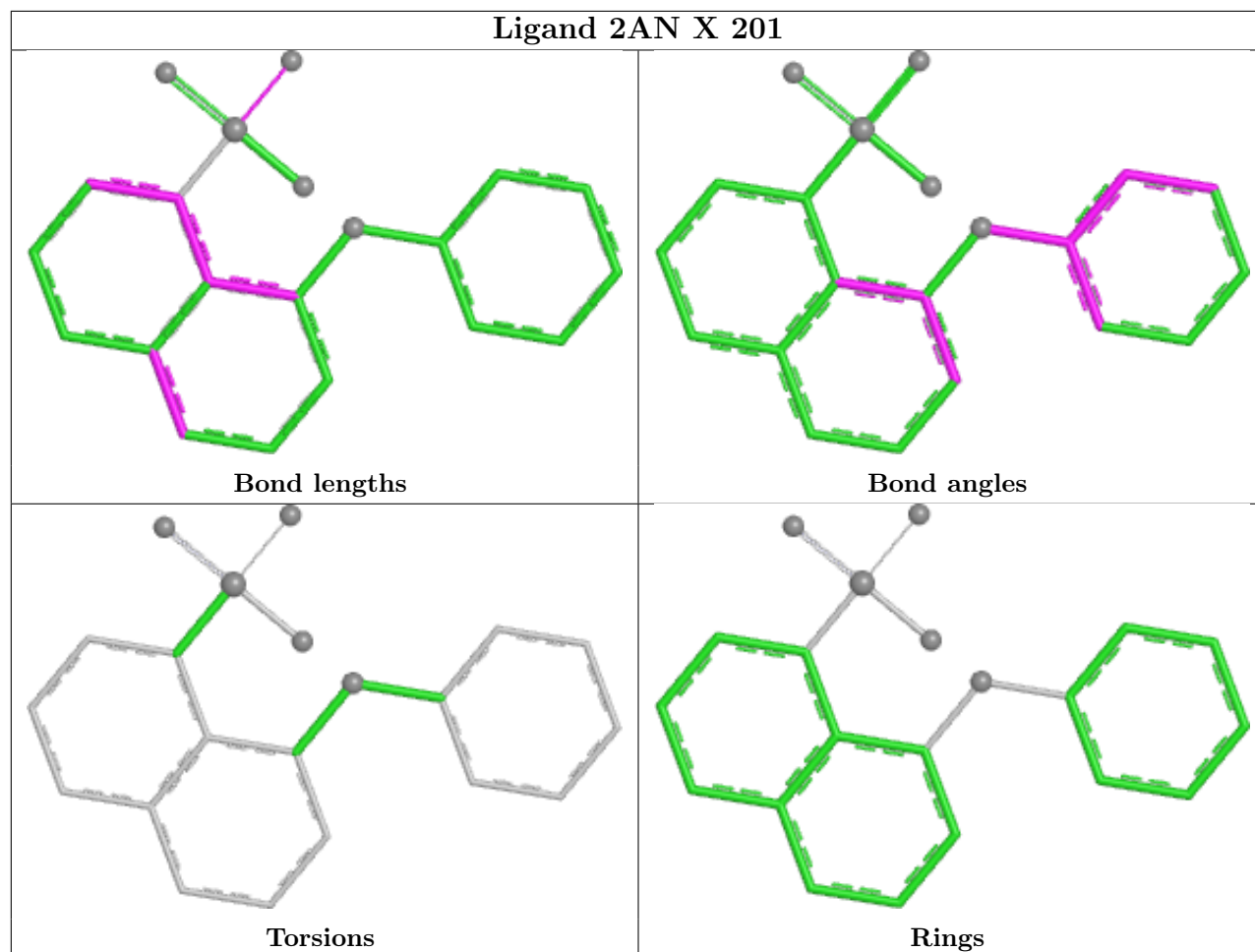


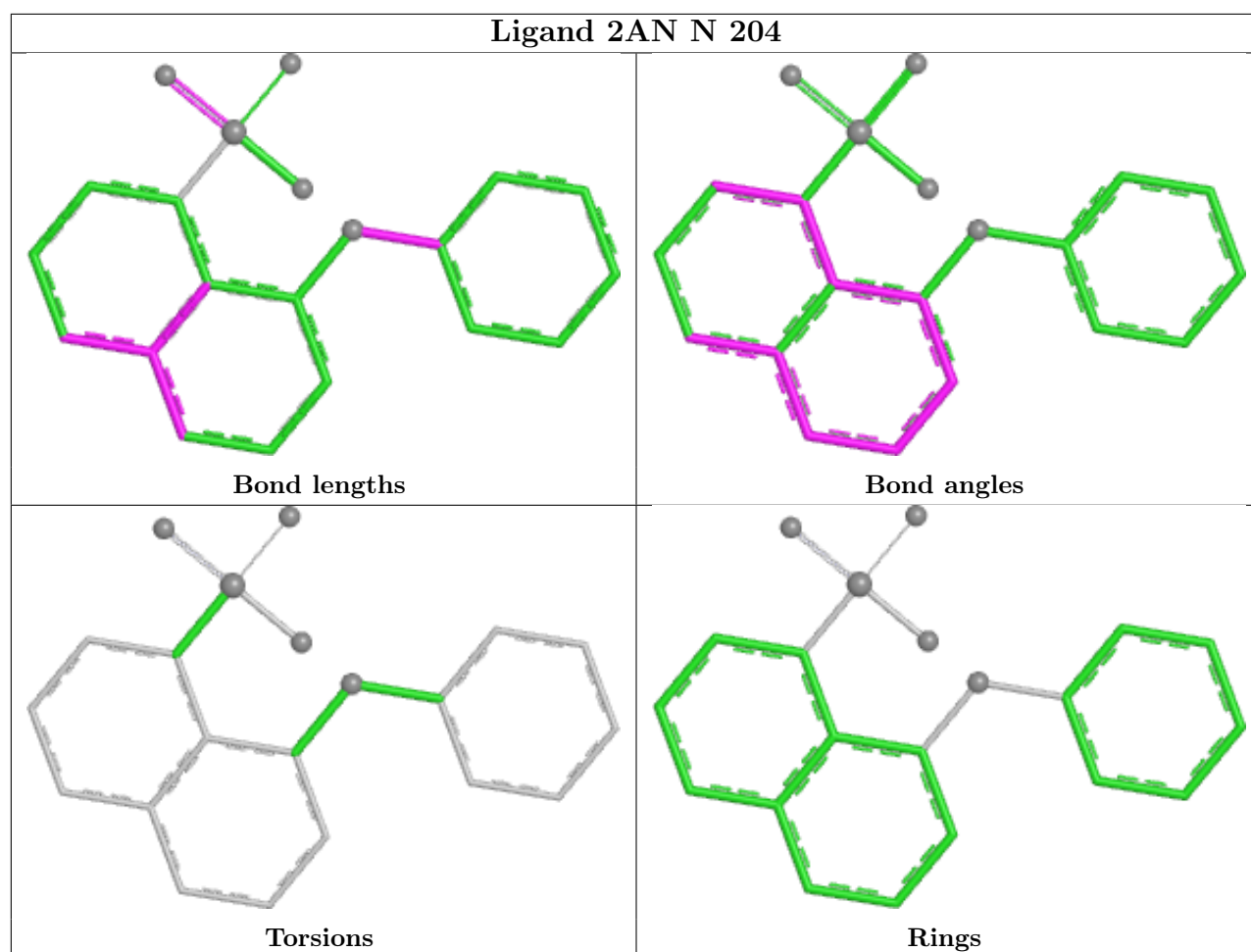
Ligand 2AN C 201



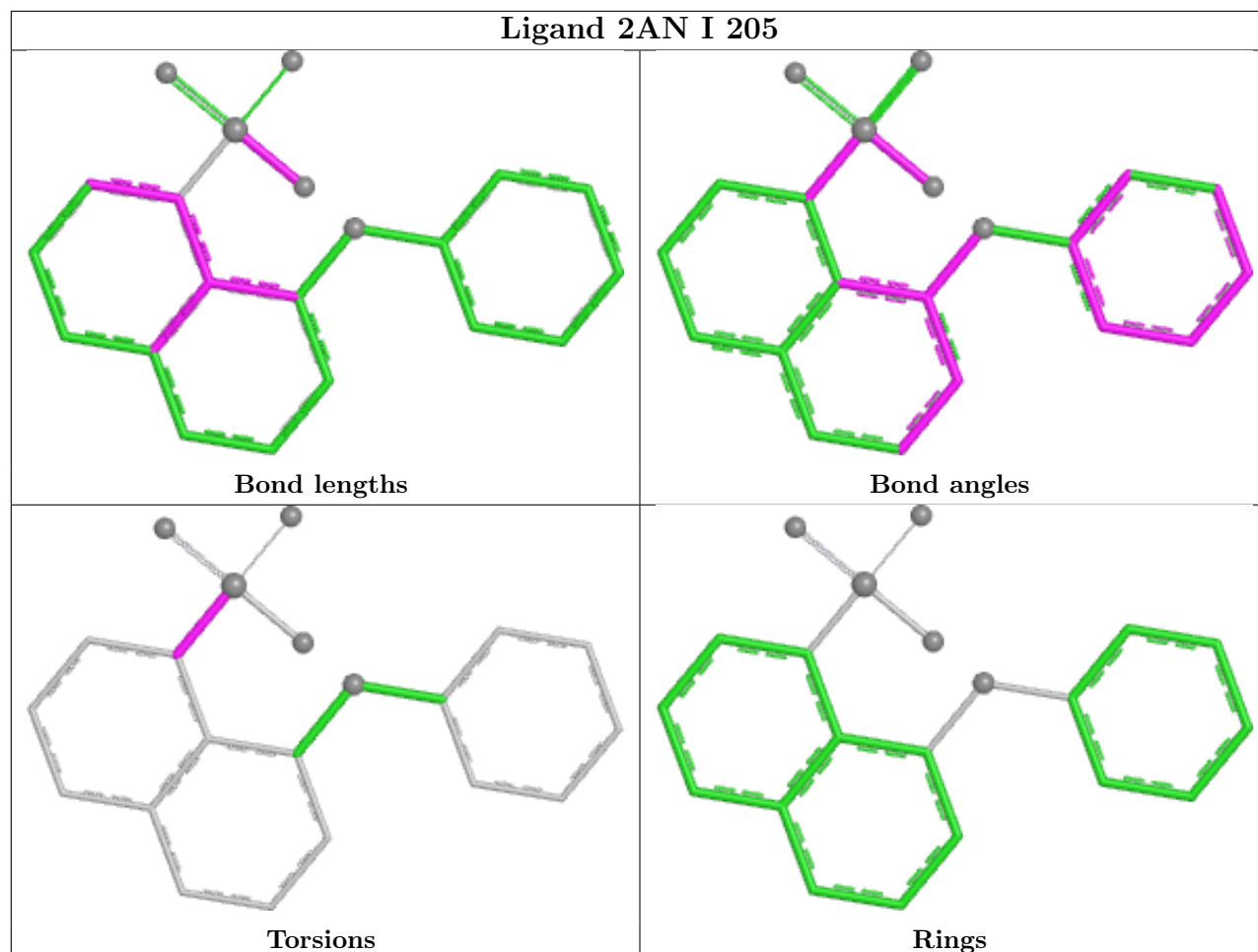
Ligand 2AN B 205



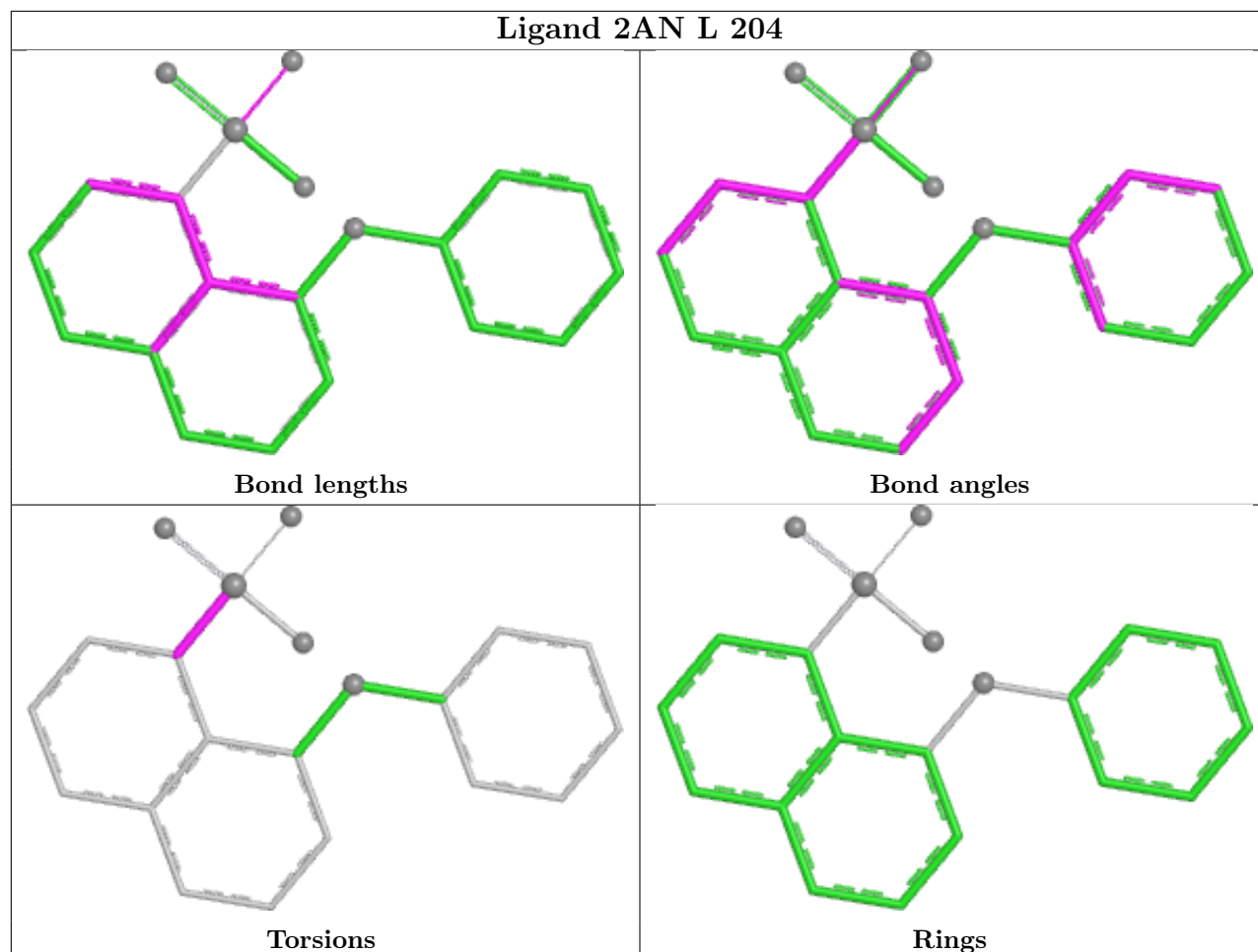




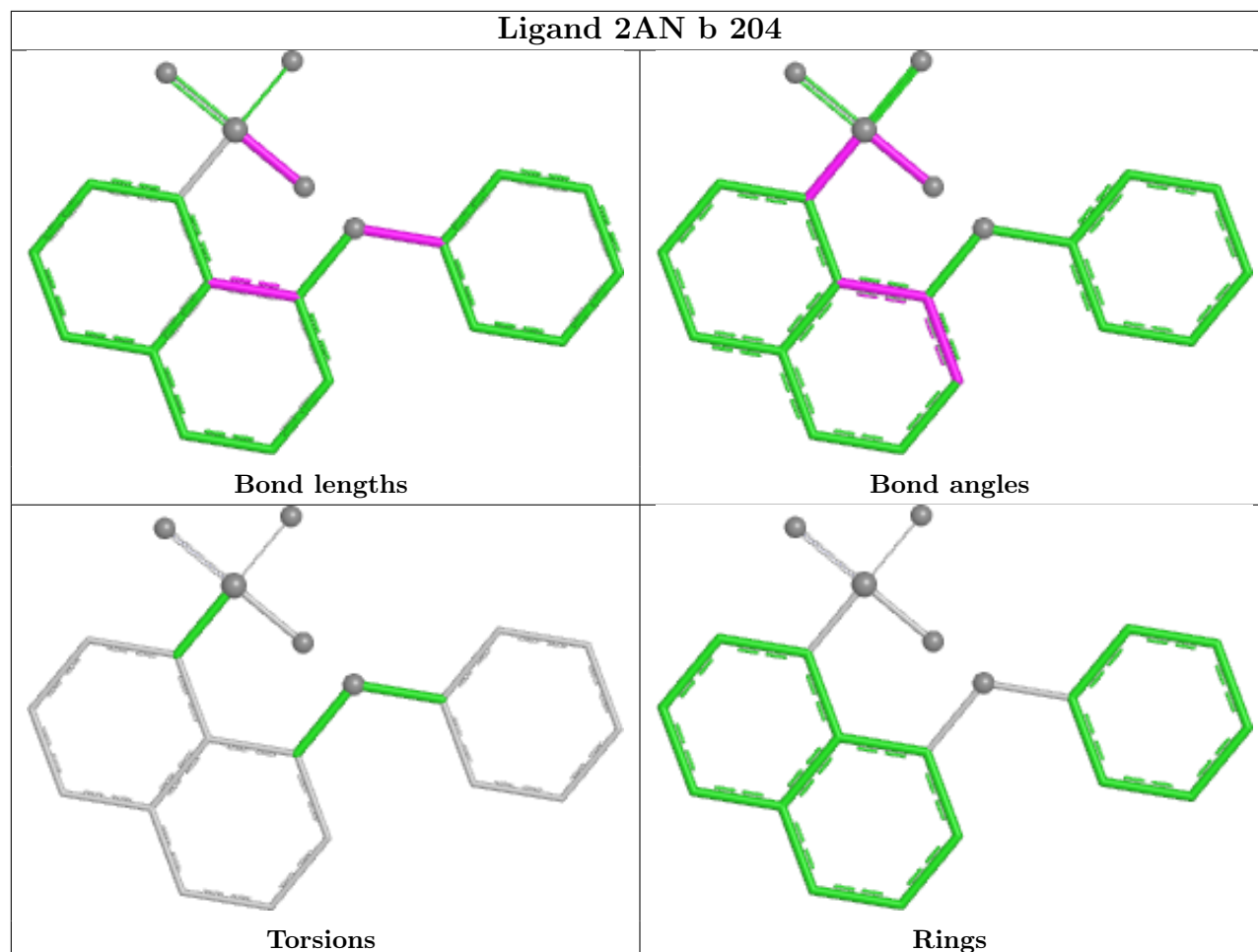
Ligand 2AN I 205



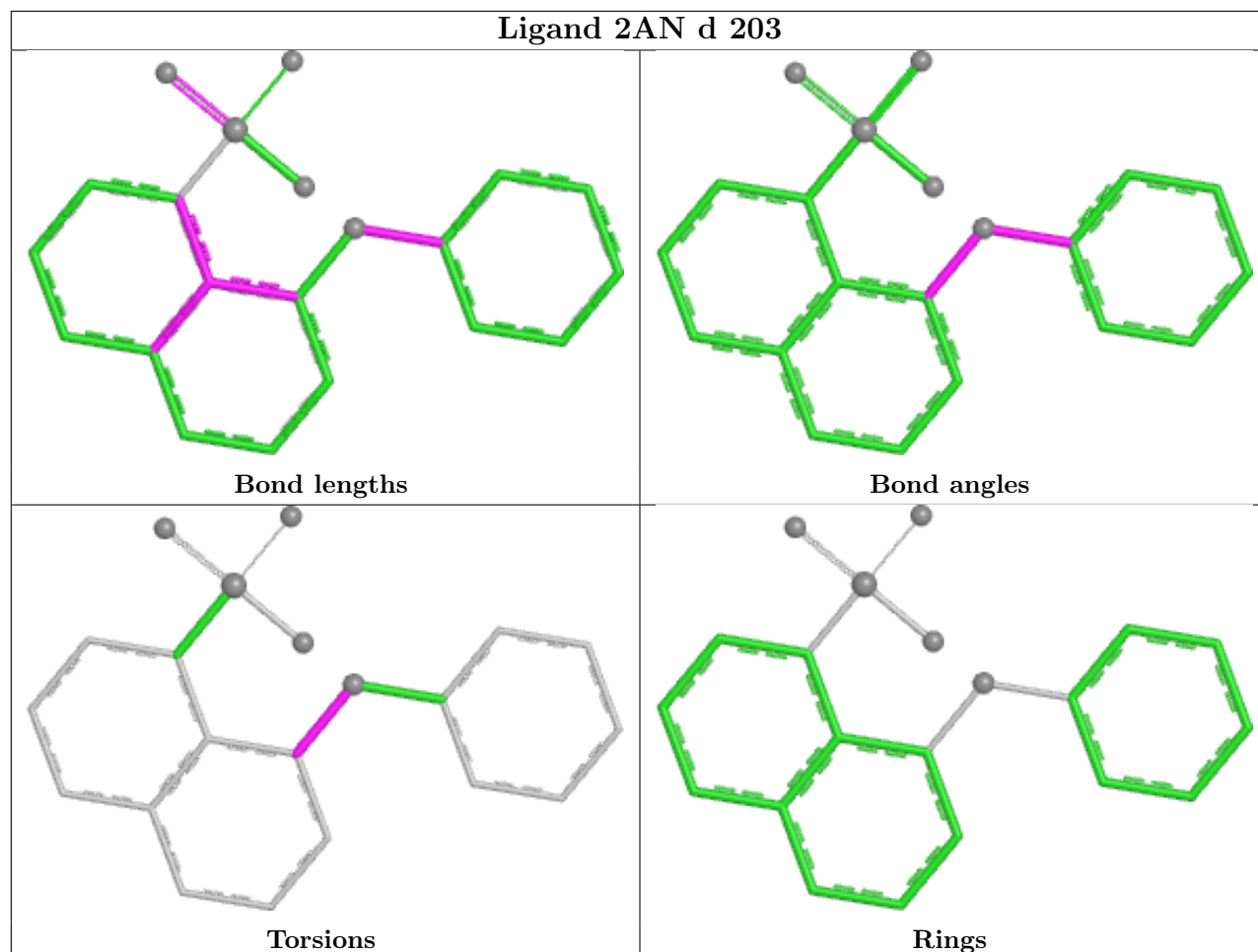
Ligand 2AN L 204



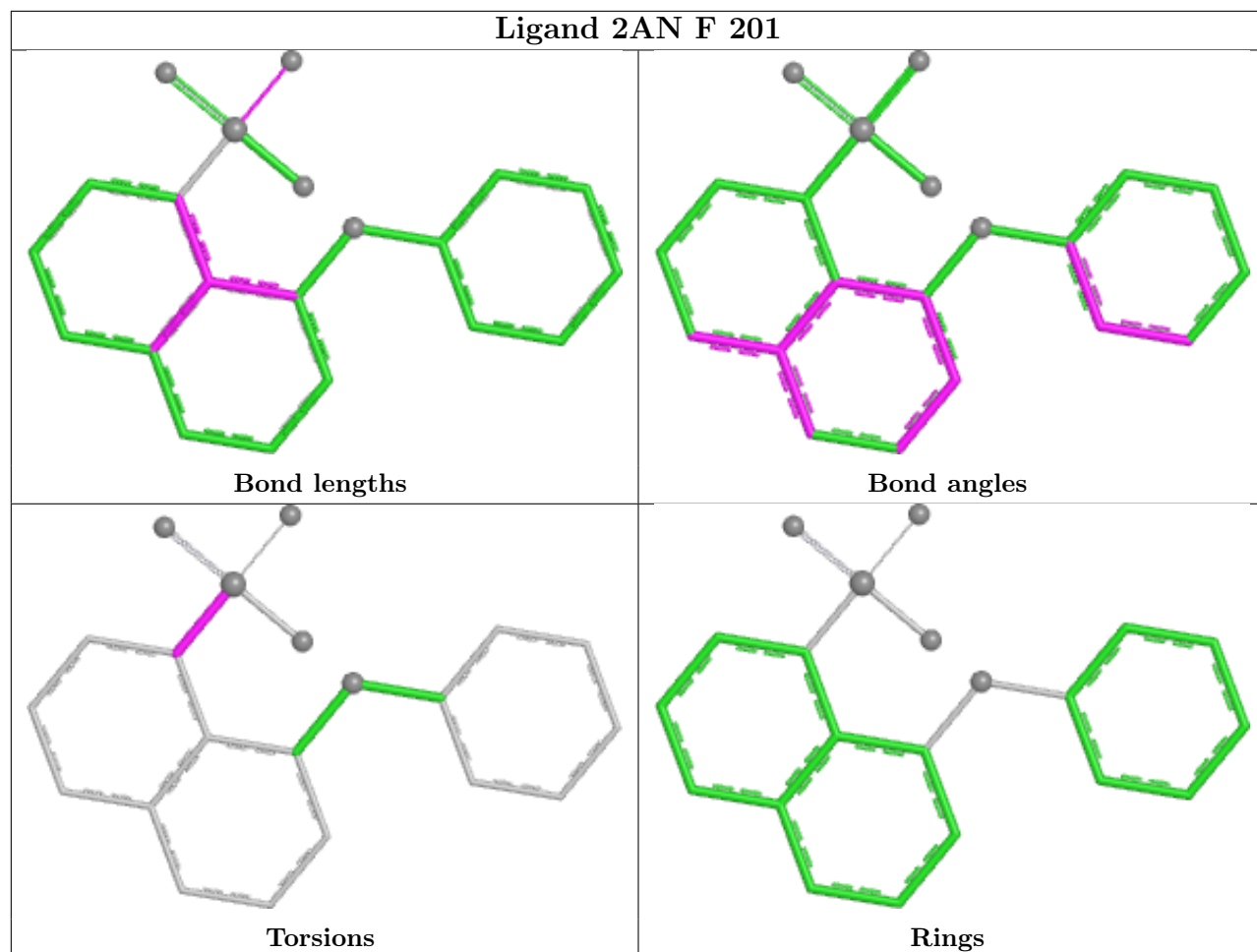
Ligand 2AN b 204



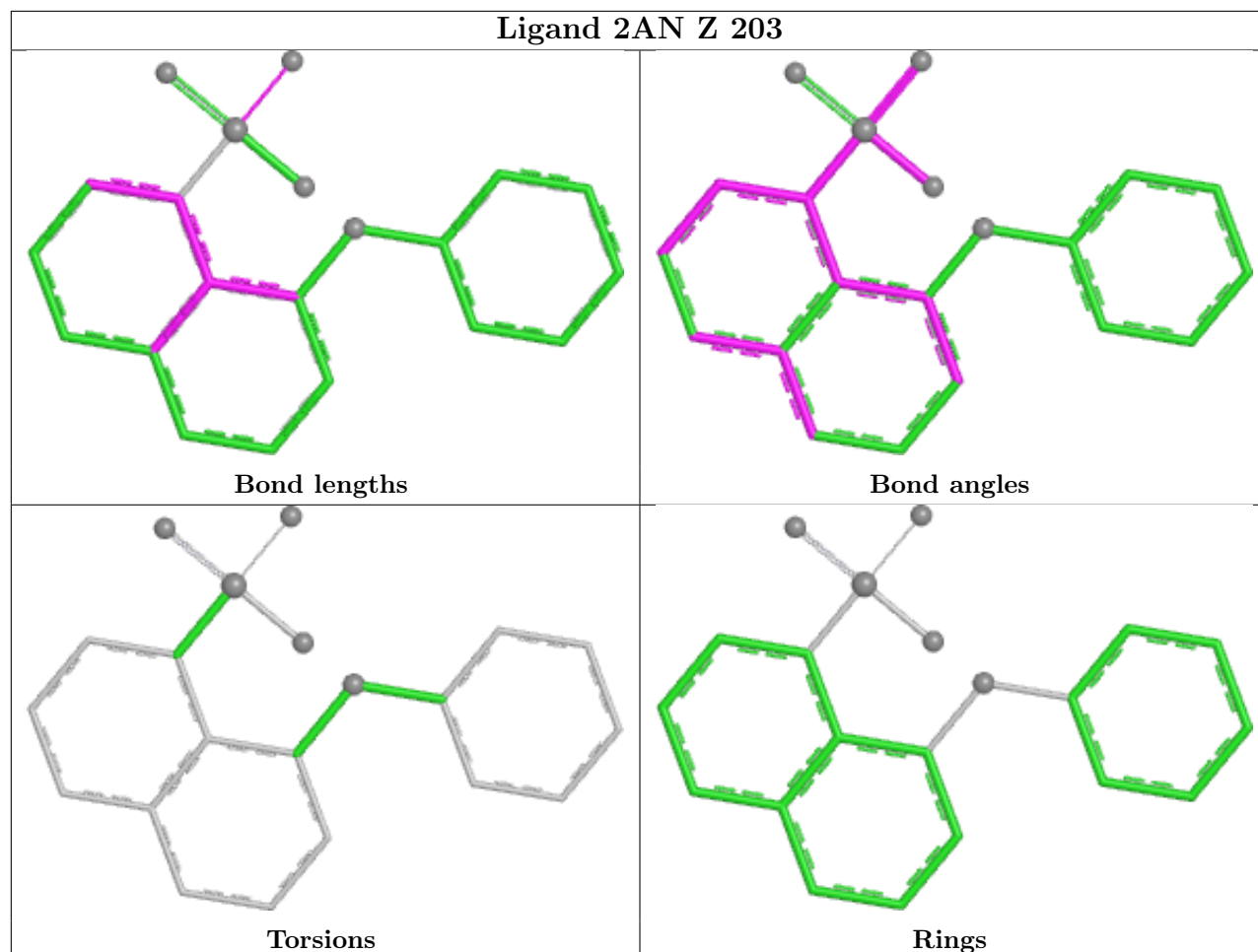
Ligand 2AN d 203



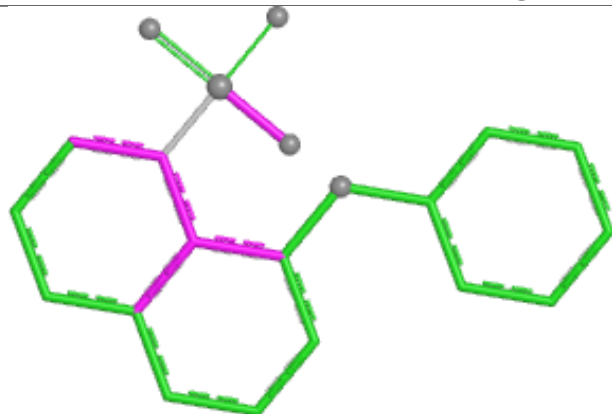
Ligand 2AN F 201



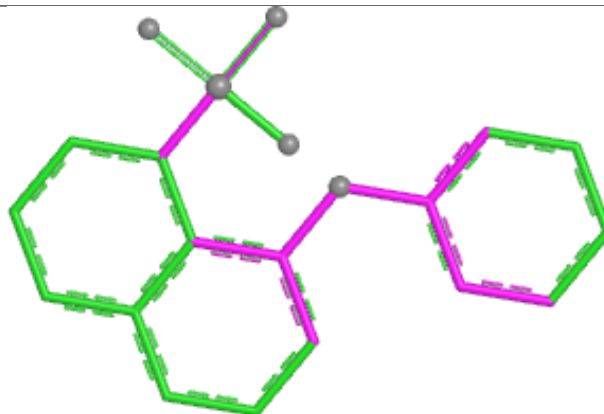
Ligand 2AN Z 203



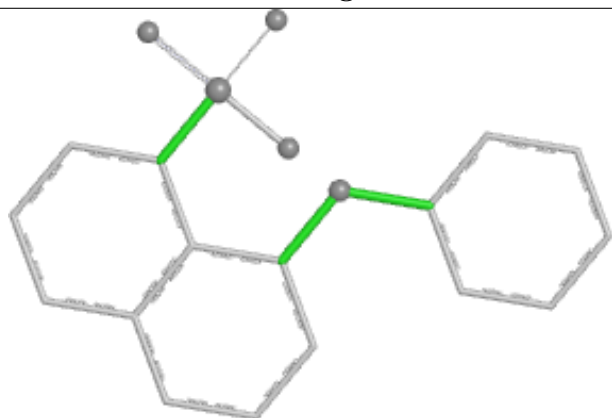
Ligand 2AN G 204



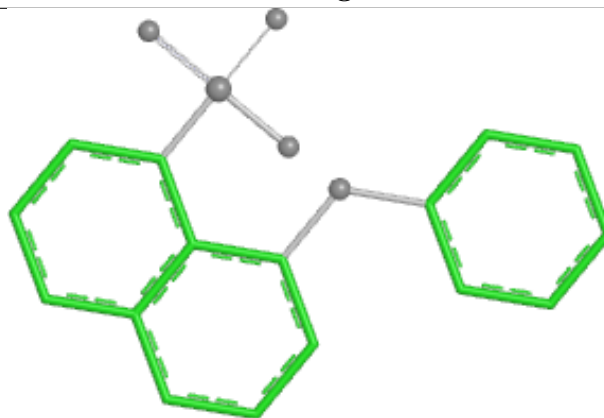
Bond lengths



Bond angles

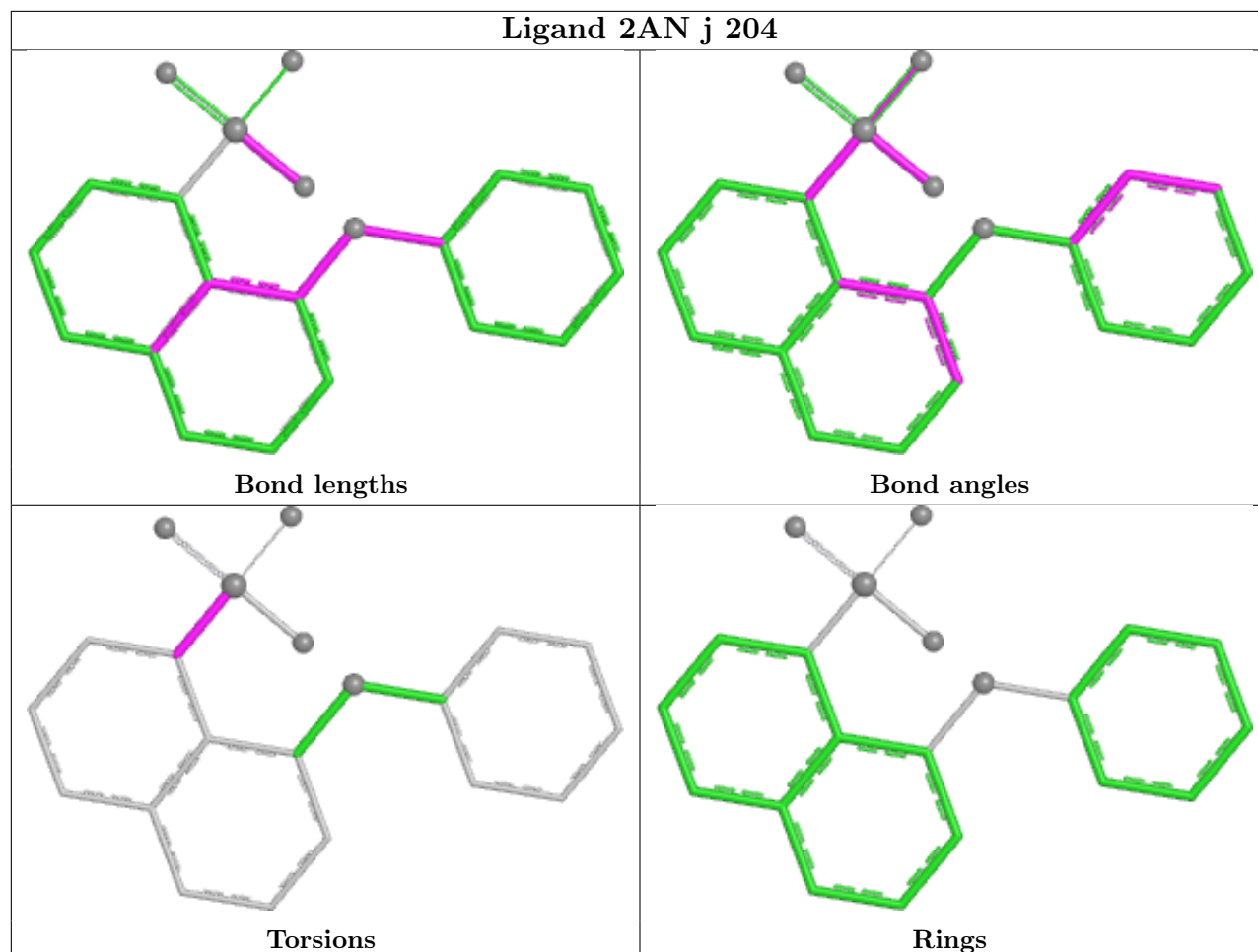


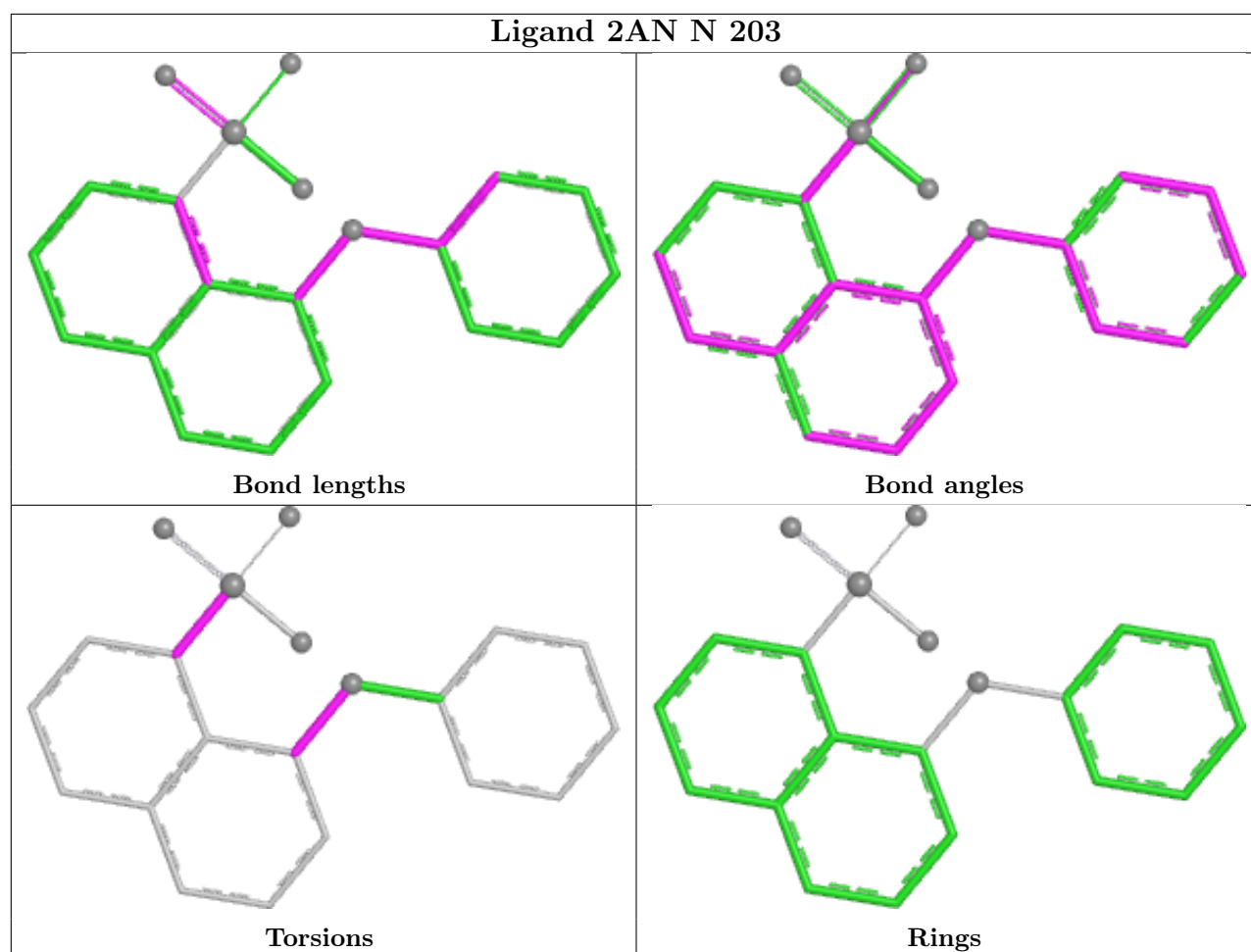
Torsions



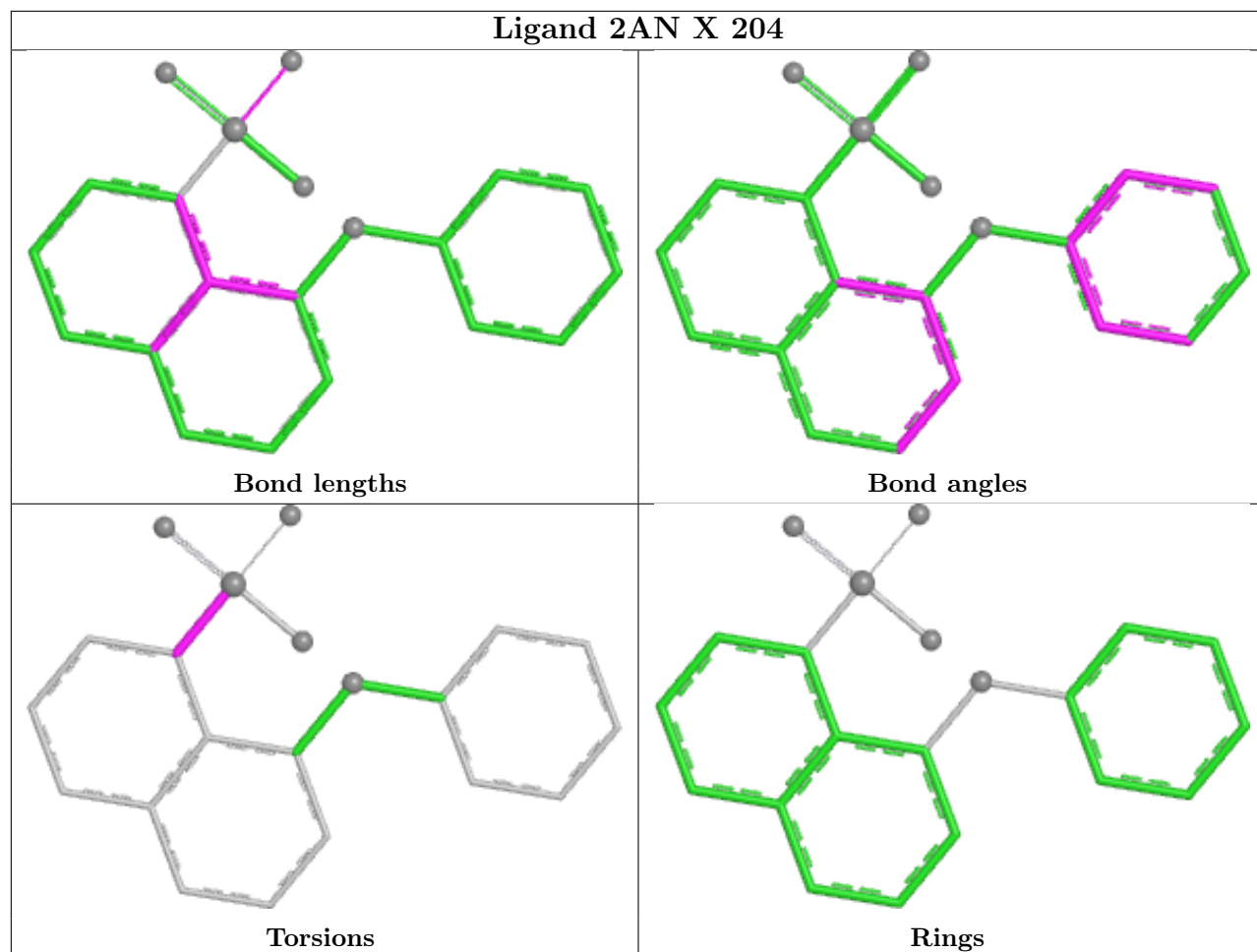
Rings

Ligand 2AN j 204

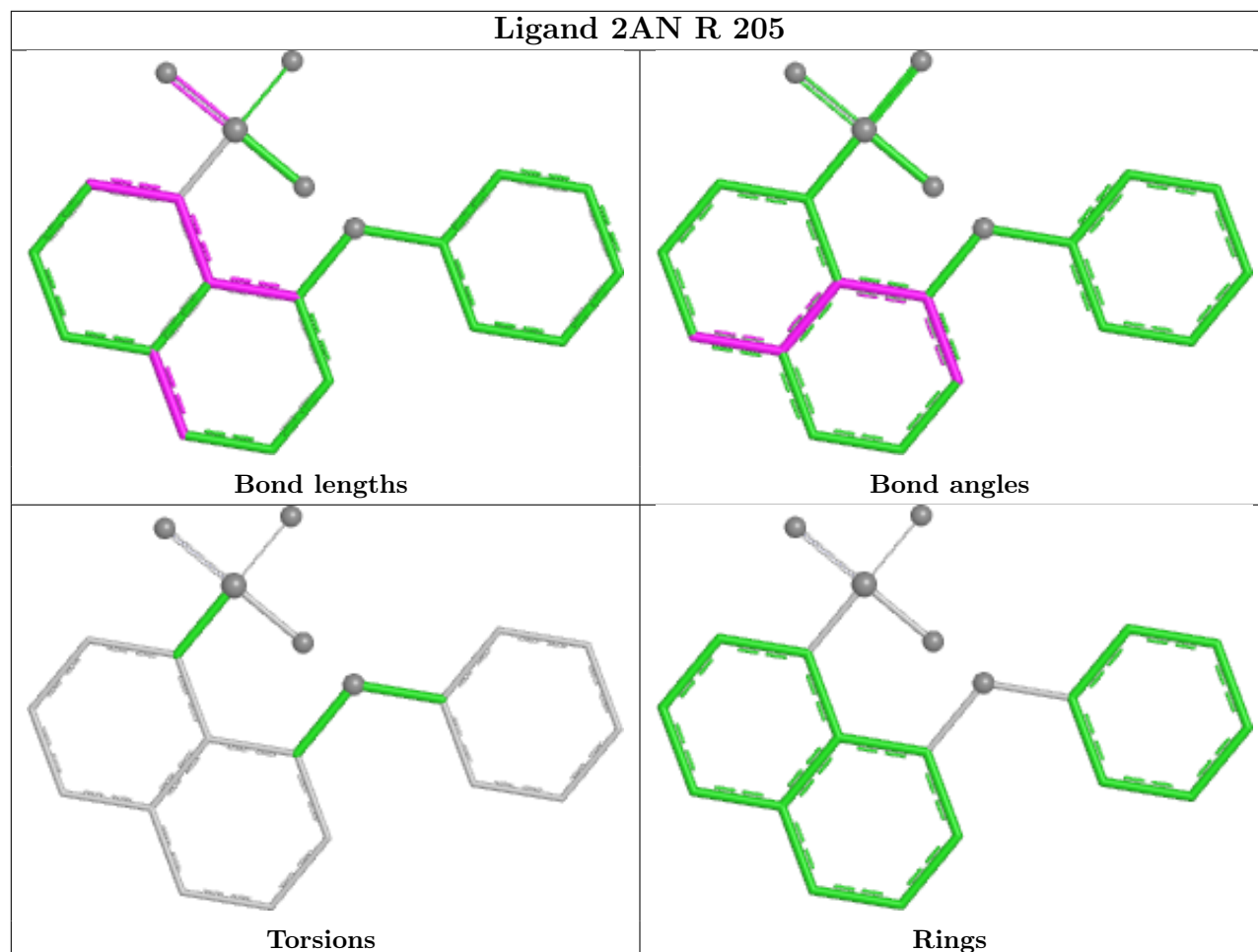




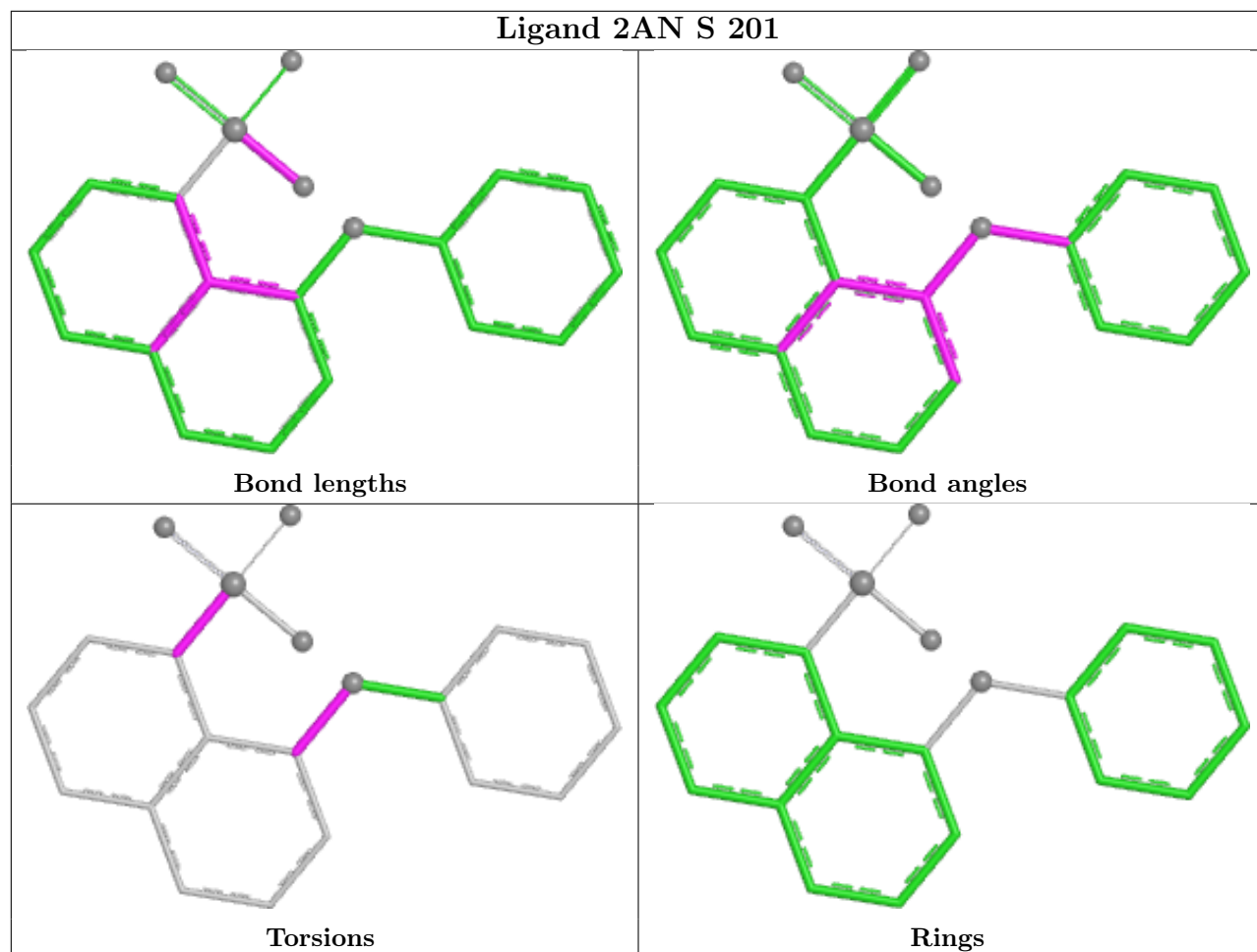
Ligand 2AN X 204

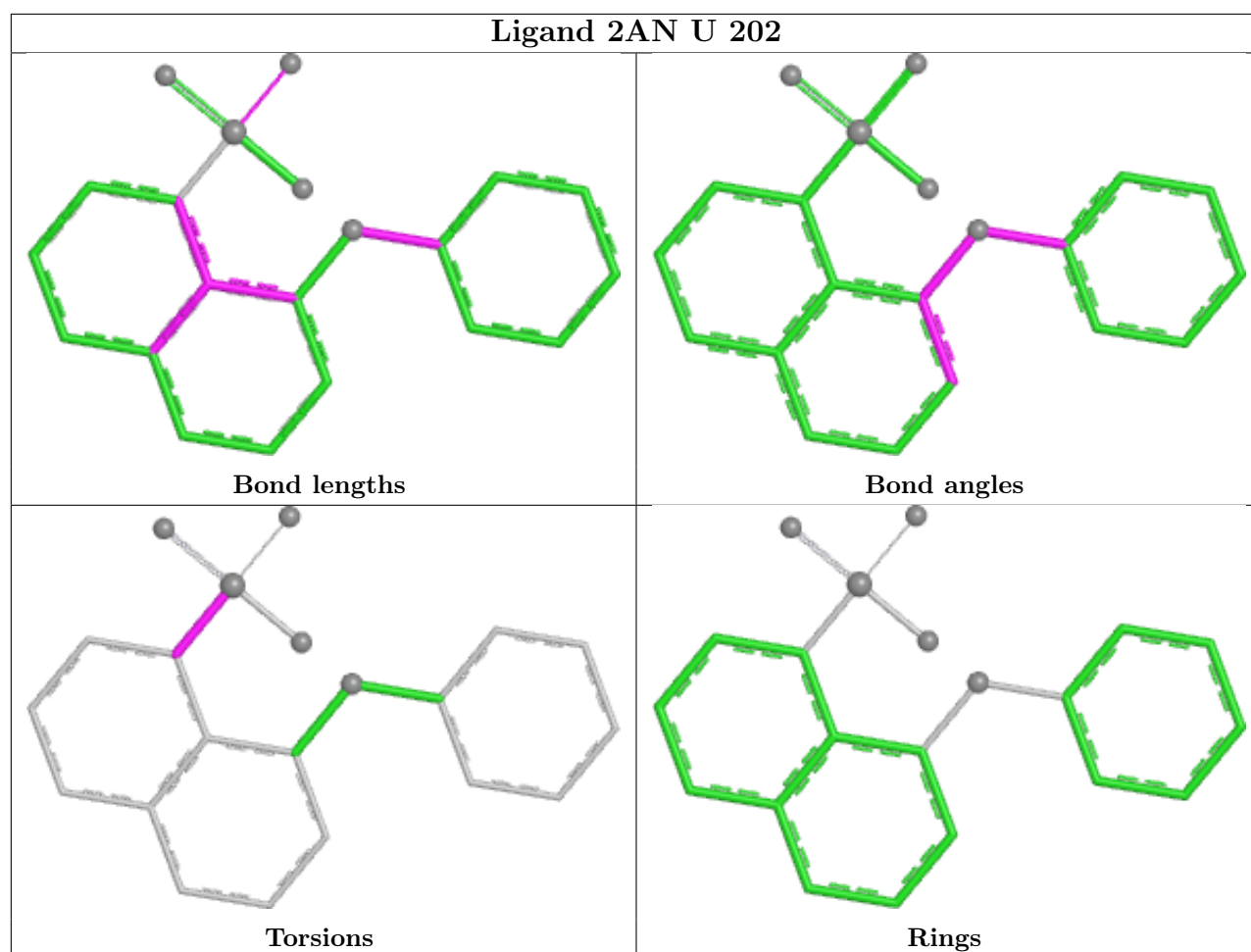


Ligand 2AN R 205

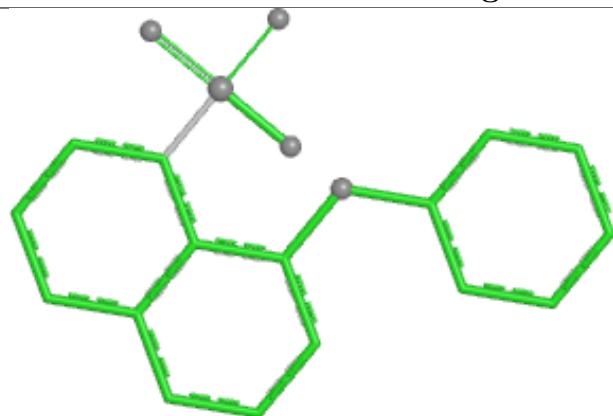


Ligand 2AN S 201

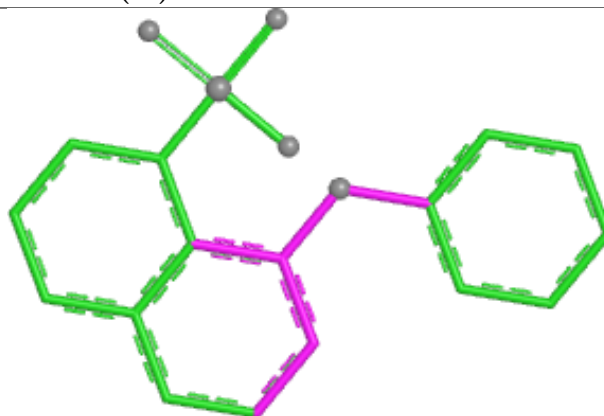




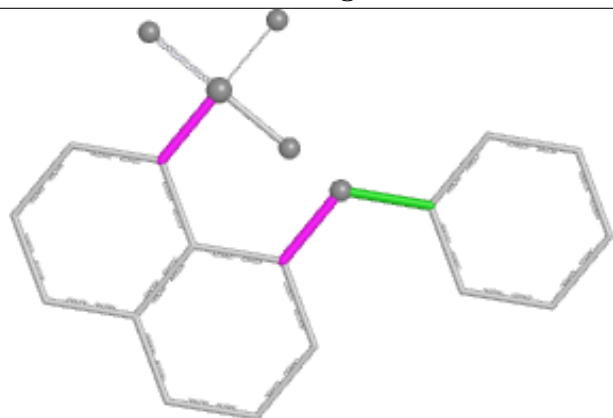
Ligand 2AN C 203 (A)



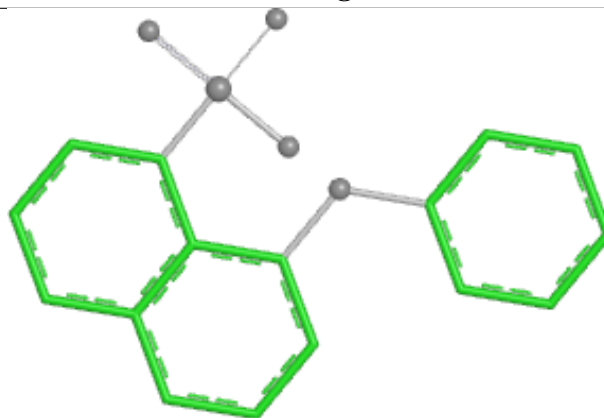
Bond lengths



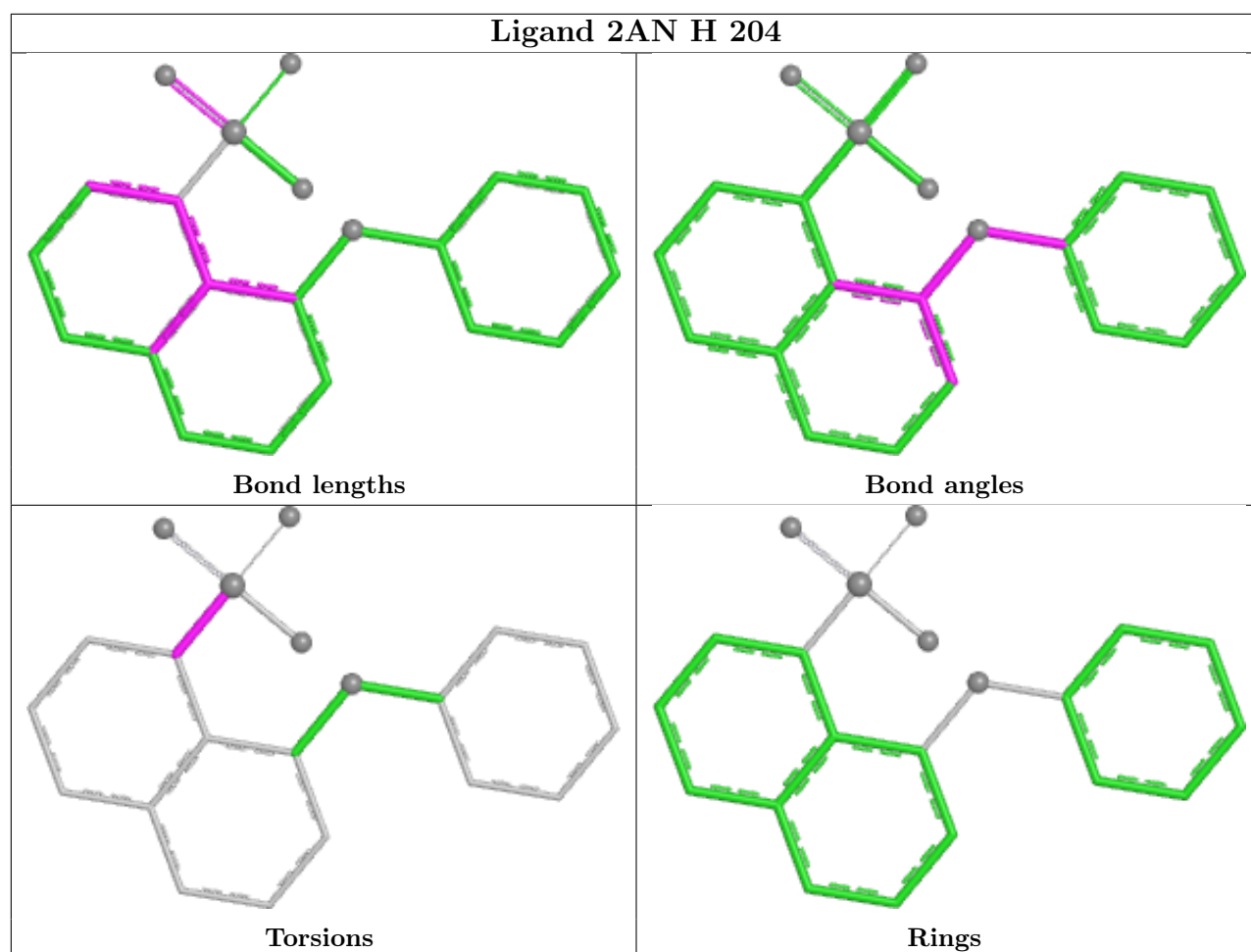
Bond angles



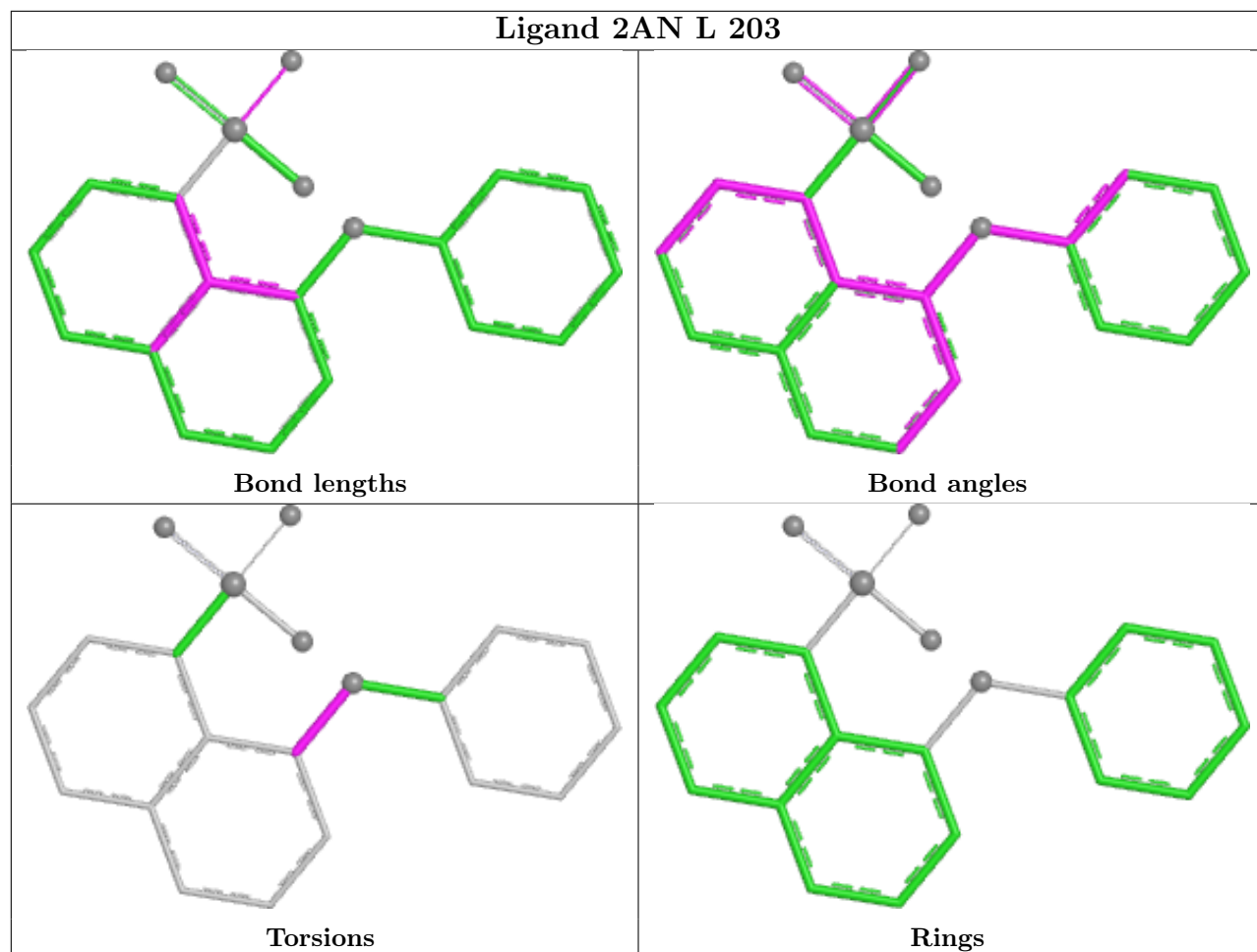
Torsions



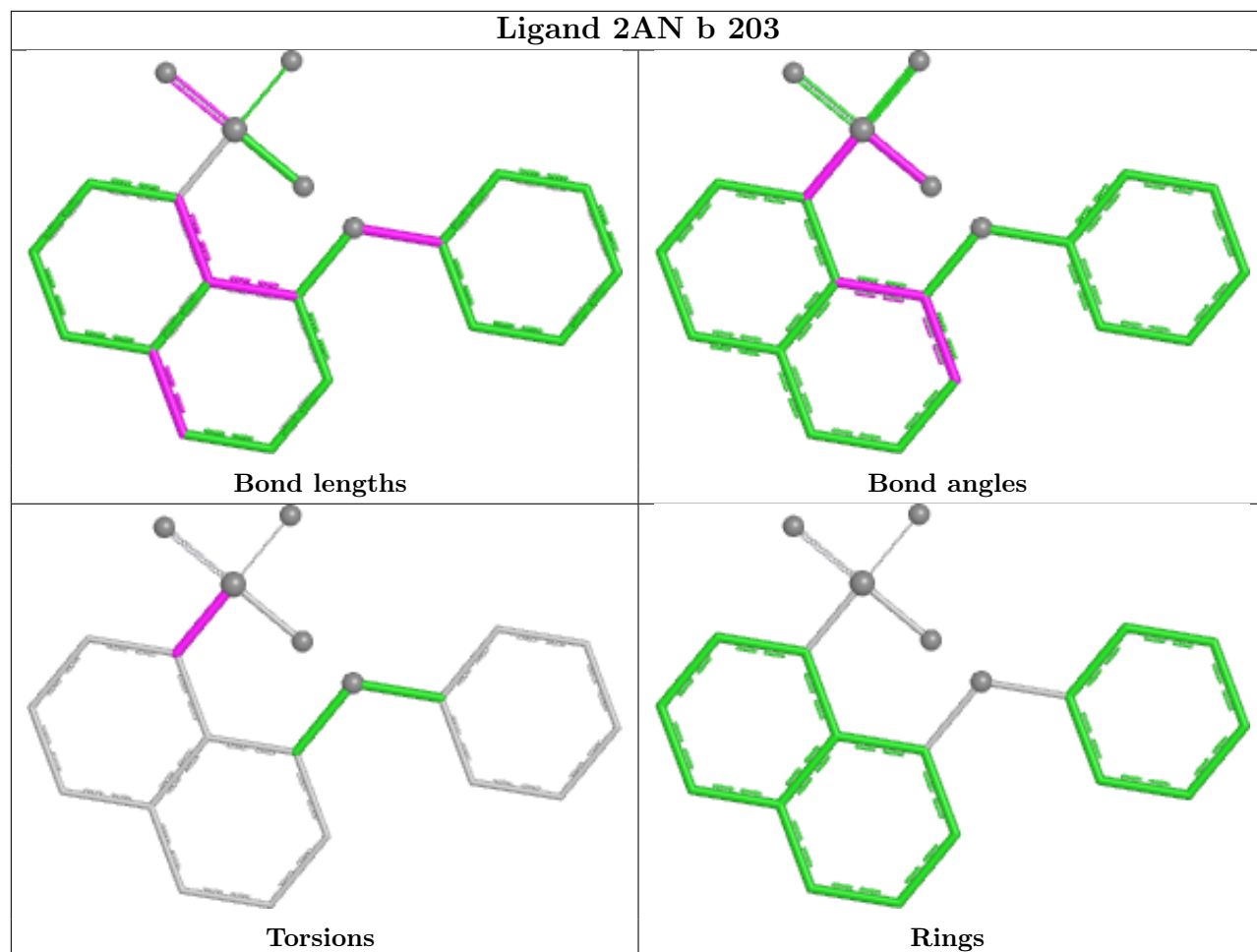
Rings



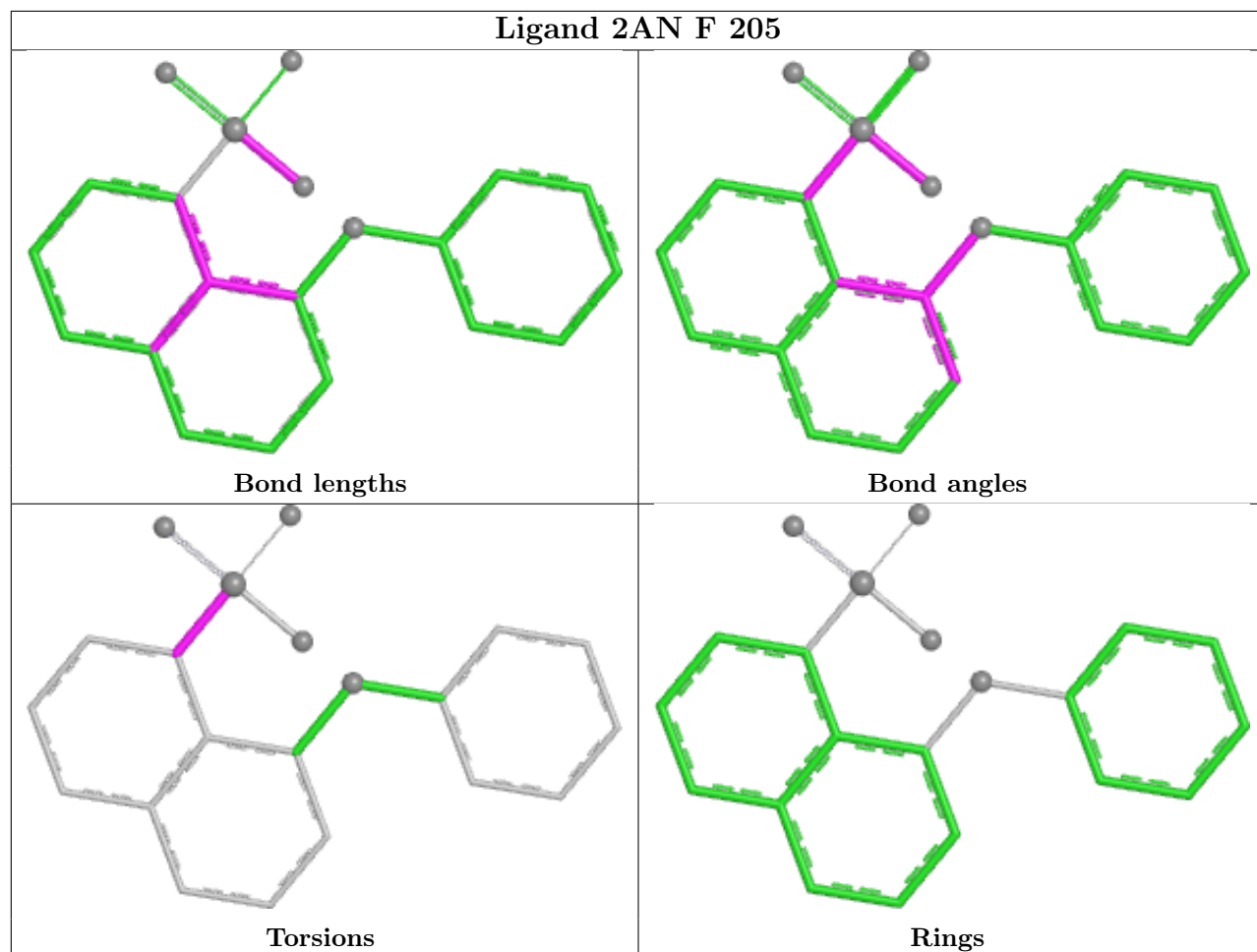
Ligand 2AN L 203



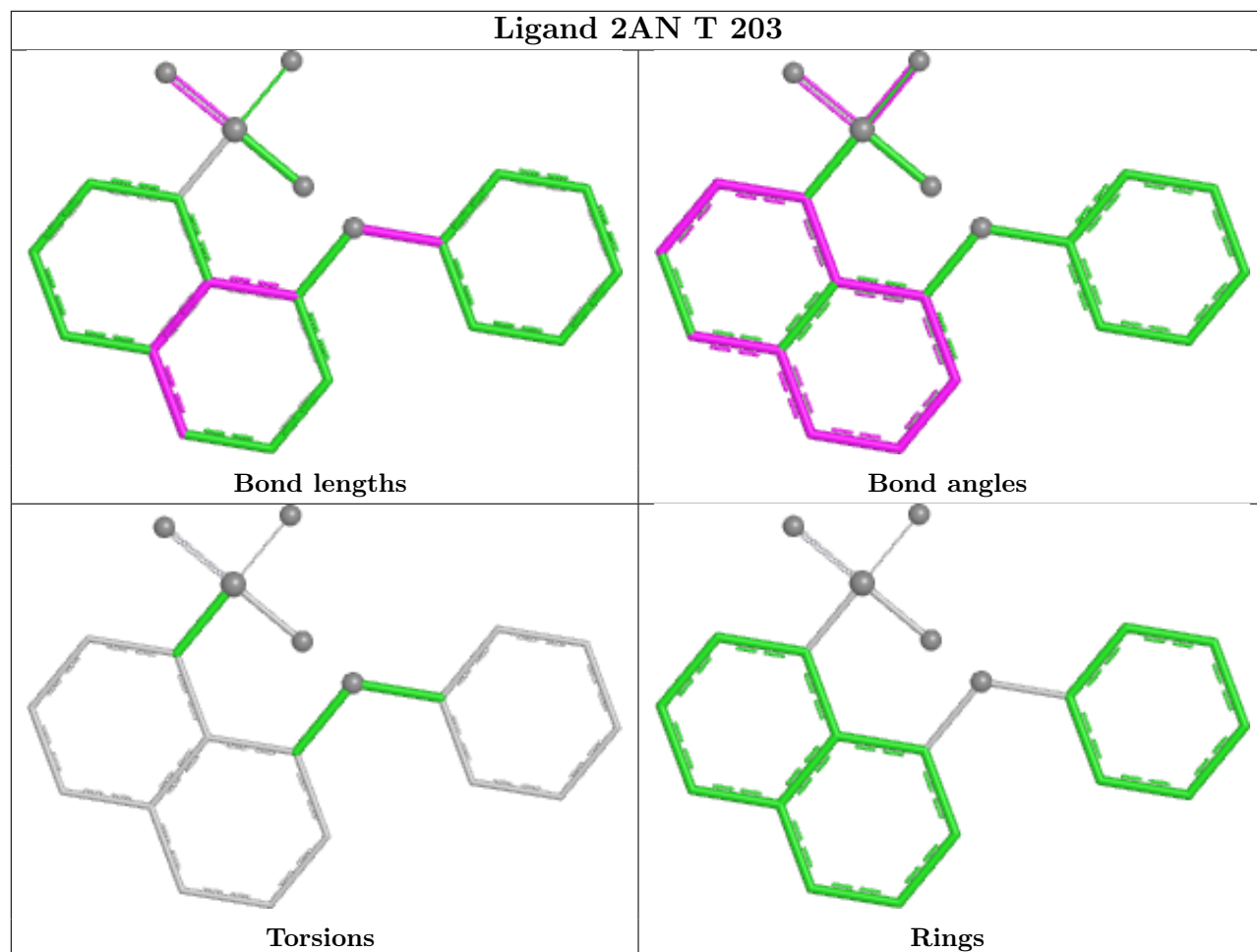
Ligand 2AN b 203



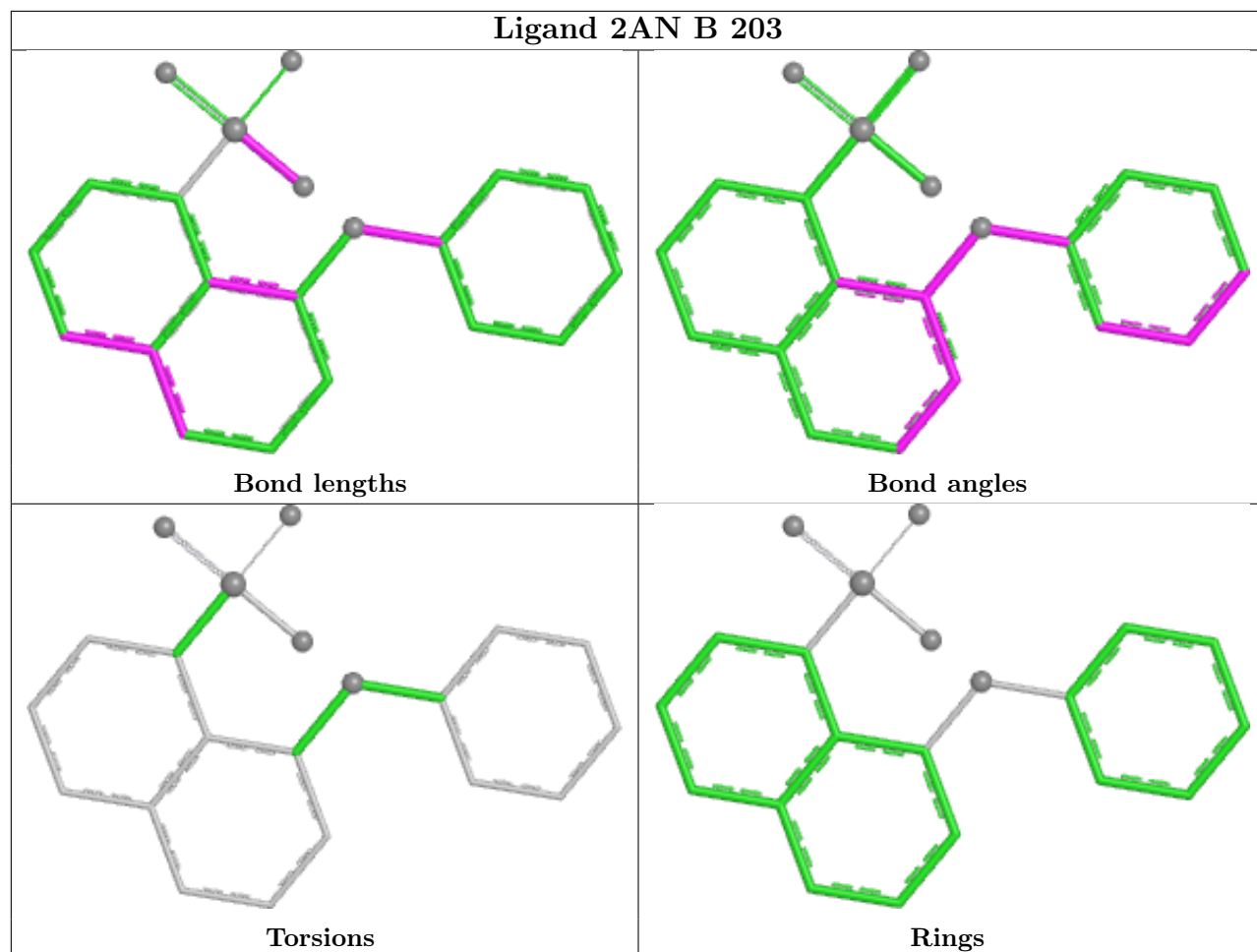
Ligand 2AN F 205



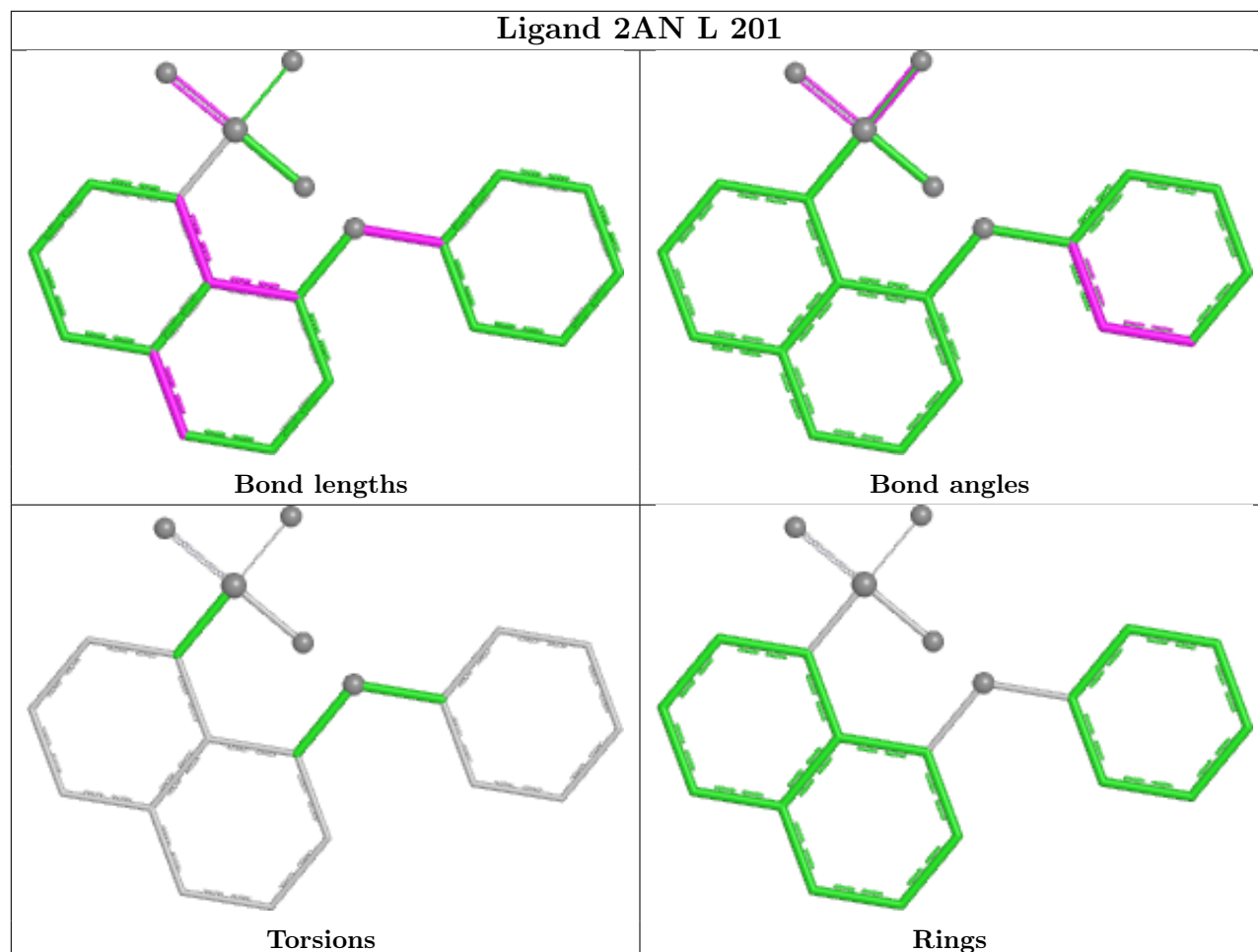
Ligand 2AN T 203



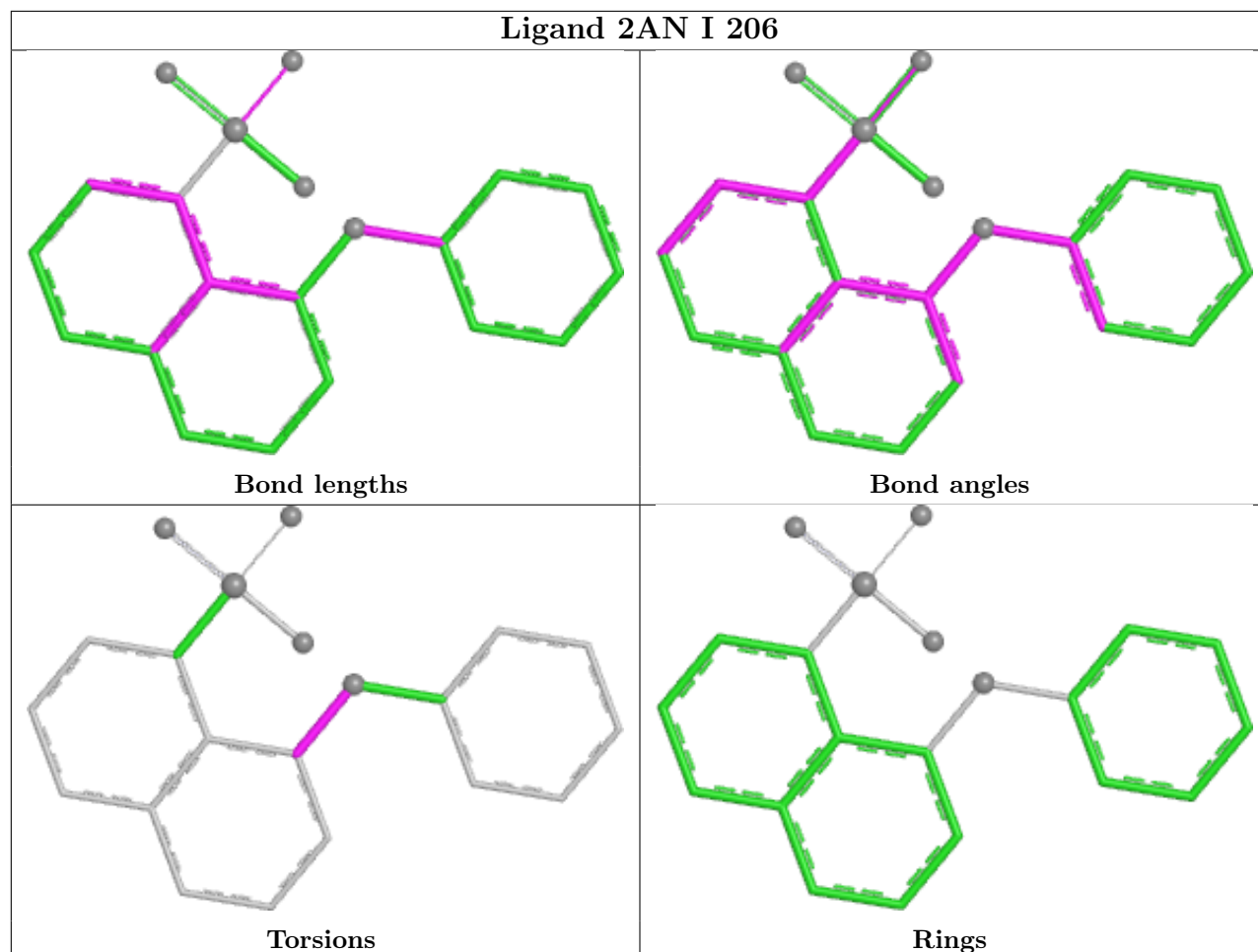
Ligand 2AN B 203



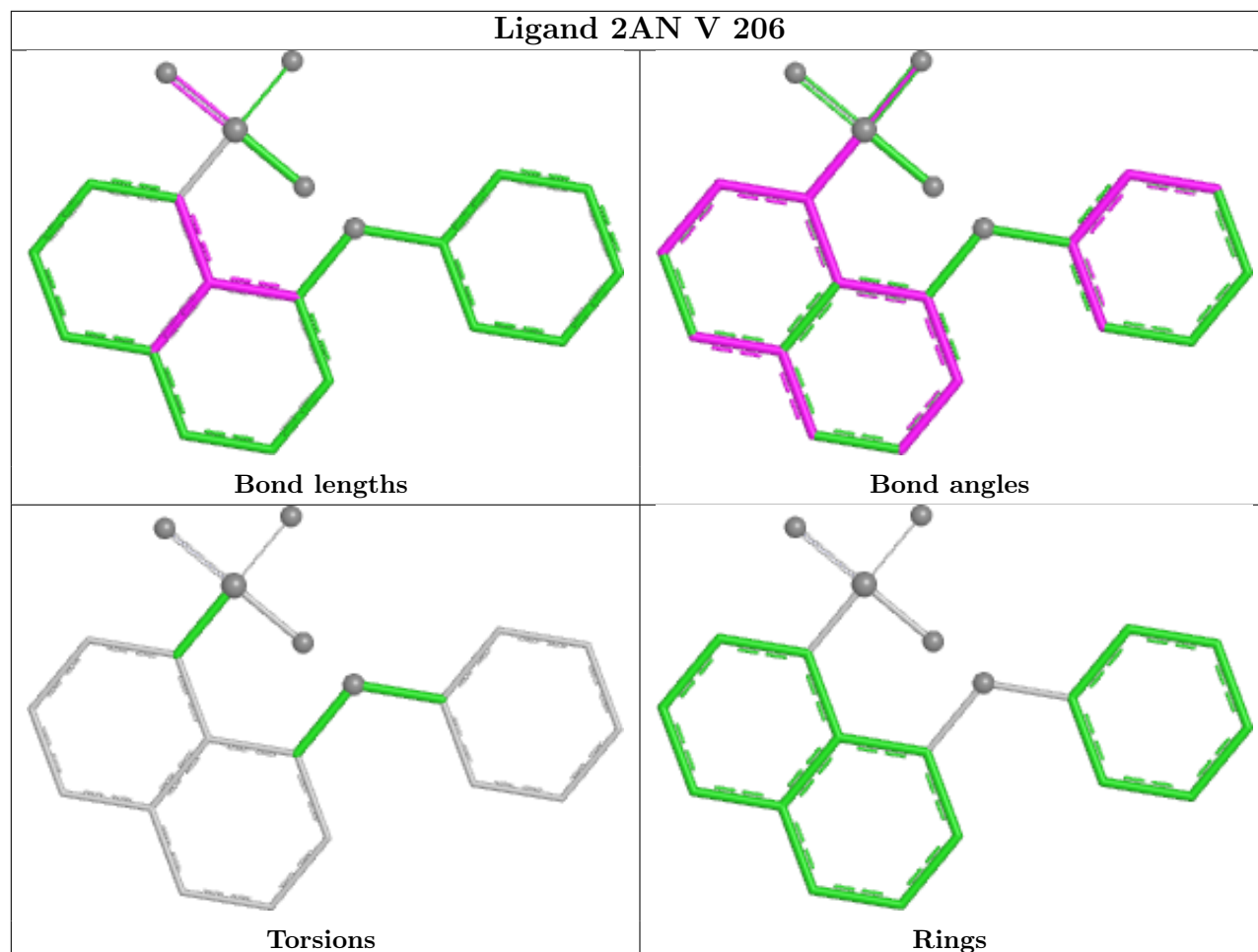
Ligand 2AN L 201

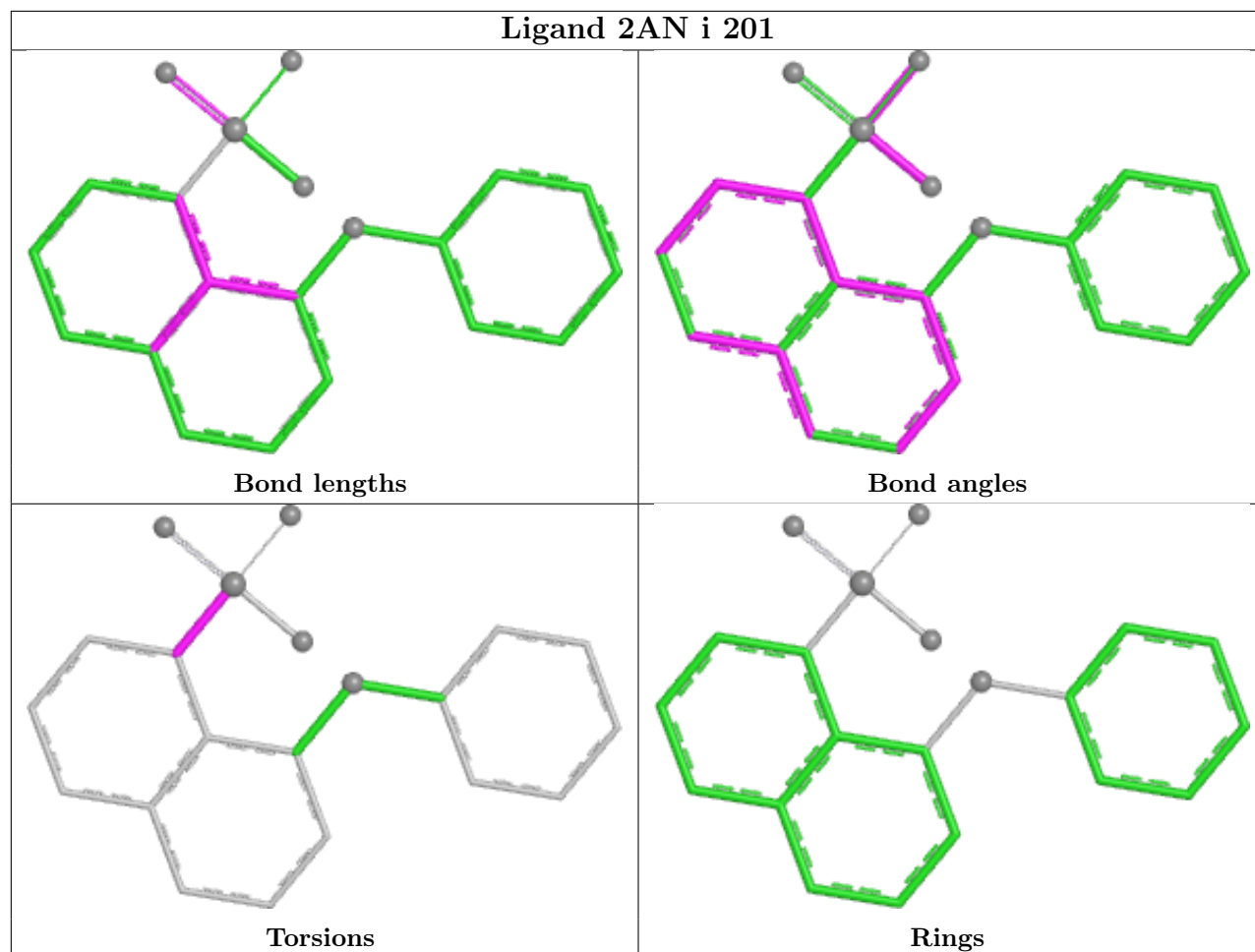


Ligand 2AN I 206



Ligand 2AN V 206





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	162/163 (99%)	2.11	71 (43%) 0 0	56, 78, 120, 132	0
1	B	159/163 (97%)	1.57	40 (25%) 1 2	28, 62, 107, 131	2 (1%)
1	C	161/163 (98%)	2.11	78 (48%) 0 0	58, 82, 114, 139	0
1	D	159/163 (97%)	1.94	64 (40%) 0 0	46, 76, 120, 146	0
1	E	161/163 (98%)	1.67	55 (34%) 1 1	42, 63, 96, 114	0
1	F	159/163 (97%)	2.31	89 (55%) 0 0	50, 80, 115, 147	2 (1%)
1	G	162/163 (99%)	2.03	72 (44%) 0 0	37, 72, 103, 119	3 (1%)
1	H	160/163 (98%)	1.92	60 (37%) 1 1	45, 70, 112, 153	1 (0%)
1	I	161/163 (98%)	1.65	49 (30%) 1 1	39, 62, 90, 108	0
1	J	163/163 (100%)	1.93	66 (40%) 0 0	47, 72, 98, 259	1 (0%)
1	K	162/163 (99%)	1.73	50 (30%) 1 1	26, 63, 88, 111	2 (1%)
1	L	160/163 (98%)	1.50	37 (23%) 2 2	39, 61, 97, 124	4 (2%)
1	M	162/163 (99%)	1.60	44 (27%) 1 1	41, 64, 89, 131	1 (0%)
1	N	163/163 (100%)	1.62	45 (27%) 1 1	38, 61, 91, 131	0
1	O	161/163 (98%)	2.22	82 (50%) 0 0	58, 81, 105, 123	1 (0%)
1	P	159/163 (97%)	1.42	33 (20%) 2 3	22, 56, 89, 106	0
1	Q	162/163 (99%)	1.49	41 (25%) 1 2	40, 67, 100, 140	0
1	R	161/163 (98%)	1.66	46 (28%) 1 1	43, 65, 99, 120	0
1	S	160/163 (98%)	1.42	35 (21%) 2 2	35, 62, 95, 120	0
1	T	161/163 (98%)	1.60	47 (29%) 1 1	37, 61, 93, 146	3 (1%)
1	U	159/163 (97%)	2.22	81 (50%) 0 0	50, 85, 123, 163	0
1	V	159/163 (97%)	1.49	33 (20%) 2 3	34, 58, 88, 121	0
1	W	159/163 (97%)	1.95	58 (36%) 1 1	20, 73, 118, 148	7 (4%)
1	X	159/163 (97%)	2.02	74 (46%) 0 0	52, 79, 113, 135	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å ²)	Q<0.9
1	Y	159/163 (97%)	1.83	60 (37%)	1	0	46, 72, 102, 124	1 (0%)
1	Z	159/163 (97%)	2.20	80 (50%)	0	0	50, 78, 104, 126	2 (1%)
1	a	159/163 (97%)	1.98	72 (45%)	0	0	40, 71, 104, 180	1 (0%)
1	b	161/163 (98%)	1.79	55 (34%)	1	1	49, 74, 102, 122	1 (0%)
1	c	159/163 (97%)	1.37	35 (22%)	2	2	36, 59, 89, 122	1 (0%)
1	d	162/163 (99%)	2.23	84 (51%)	0	0	26, 75, 108, 161	3 (1%)
1	e	161/163 (98%)	1.35	29 (18%)	3	4	32, 58, 85, 104	1 (0%)
1	f	161/163 (98%)	1.47	40 (24%)	2	2	33, 60, 91, 118	0
1	g	160/163 (98%)	1.38	33 (20%)	2	3	38, 60, 86, 115	0
1	h	162/163 (99%)	1.48	36 (22%)	2	2	25, 58, 86, 121	3 (1%)
1	i	161/163 (98%)	1.54	43 (26%)	1	1	40, 65, 93, 134	1 (0%)
1	j	159/163 (97%)	1.04	22 (13%)	6	7	30, 54, 78, 129	1 (0%)
All	All	5777/5868 (98%)	1.75	1939 (33%)	1	1	20, 68, 105, 259	42 (0%)

All (1939) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	59	PHE	11.8
1	R	95	ASN	9.4
1	V	130	GLU	8.9
1	R	60	VAL	8.4
1	V	129	ASN	8.4
1	H	57	ILE	8.1
1	R	58	THR	8.1
1	H	58	THR	7.6
1	J	-3	ASP	7.5
1	F	10	GLU	7.3
1	W	96	ILE	7.2
1	N	-3	ASP	7.1
1	Z	3	ALA	7.1
1	D	4	TYR	6.9
1	U	128	VAL	6.7
1	F	144	TYR	6.7
1	B	6	ILE	6.7
1	H	138	LYS	6.6
1	g	90	ASP	6.5
1	X	67	TYR	6.3
1	G	80	PHE	6.3

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Mol	Chain	Res	Type	RSRZ
1	h	17	HIS	6.3
1	R	59	PHE	6.3
1	G	121	HIS	6.3
1	U	10	GLU	6.2
1	K	4	TYR	6.2
1	C	67	TYR	6.2
1	A	18	ARG	6.2
1	E	95	ASN	6.2
1	E	133	VAL	6.1
1	B	4	TYR	6.1
1	h	110	GLY	6.0
1	L	92	LEU	6.0
1	Z	15	ALA	6.0
1	N	40	LYS	6.0
1	R	96	ILE	5.9
1	A	140	ALA	5.9
1	Z	136	GLY	5.8
1	N	39	PHE	5.8
1	O	67	TYR	5.7
1	P	51	VAL	5.7
1	f	2	ALA	5.7
1	A	6	ILE	5.7
1	N	60	VAL	5.7
1	F	86	LEU	5.7
1	h	93	ARG	5.6
1	Z	140	ALA	5.6
1	e	125	GLY	5.6
1	f	0	THR	5.6
1	Y	65	LEU	5.5
1	H	91	VAL	5.5
1	T	97	GLU	5.5
1	D	2	ALA	5.5
1	f	-1	PHE	5.4
1	U	60	VAL	5.4
1	R	61	ASP	5.4
1	f	132	GLU	5.4
1	W	2	ALA	5.4
1	B	120	TYR	5.4
1	d	126	CYS	5.4
1	d	133	VAL	5.4
1	F	7	VAL	5.3
1	A	3	ALA	5.3

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Mol	Chain	Res	Type	RSRZ
1	T	17	HIS	5.3
1	X	45	ILE	5.3
1	h	125	GLY	5.3
1	G	87	PHE	5.2
1	h	1	MET	5.2
1	Z	2	ALA	5.2
1	C	60	VAL	5.2
1	I	133	VAL	5.2
1	a	124	PRO	5.2
1	D	159	ALA	5.2
1	d	142	GLU	5.2
1	d	4	TYR	5.1
1	Z	146	GLN	5.1
1	O	51	VAL	5.1
1	F	57	ILE	5.1
1	F	101	TYR	5.1
1	I	55	THR	5.1
1	O	65	LEU	5.1
1	G	43	GLU	5.0
1	R	159	ALA	5.0
1	J	120	TYR	5.0
1	F	99	VAL	5.0
1	P	6	ILE	5.0
1	V	131	GLU	5.0
1	a	125	GLY	4.9
1	A	133	VAL	4.9
1	U	24	VAL	4.9
1	d	92	LEU	4.9
1	A	78	ALA	4.9
1	A	47	GLY	4.9
1	O	52	GLY	4.9
1	R	4	TYR	4.9
1	O	66	THR	4.9
1	Z	32	VAL	4.8
1	W	72	PHE	4.8
1	a	92	LEU	4.8
1	j	122	PRO	4.8
1	e	135	ILE	4.8
1	b	81	TYR	4.8
1	B	42	GLY	4.8
1	J	91	VAL	4.8
1	d	60	VAL	4.8

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Mol	Chain	Res	Type	RSRZ
1	F	85	THR	4.7
1	W	86	LEU	4.7
1	f	4	TYR	4.7
1	A	118	VAL	4.7
1	W	92	LEU	4.7
1	N	59	PHE	4.7
1	V	122	PRO	4.7
1	d	139	LYS	4.7
1	Q	91	VAL	4.7
1	A	120	TYR	4.7
1	b	67	TYR	4.7
1	N	125	GLY	4.7
1	F	50	GLY	4.7
1	b	62	GLY	4.7
1	K	1	MET	4.6
1	U	50	GLY	4.6
1	T	128	VAL	4.6
1	D	122	PRO	4.6
1	X	87	PHE	4.6
1	G	52	GLY	4.6
1	b	2	ALA	4.6
1	W	120	TYR	4.6
1	i	148	GLU	4.6
1	W	127	THR	4.6
1	O	38	VAL	4.6
1	U	159	ALA	4.5
1	O	37	HIS	4.5
1	W	61	ASP	4.5
1	O	44	ILE	4.5
1	W	139	LYS	4.5
1	B	10	GLU	4.5
1	P	131	GLU	4.5
1	R	69	LEU	4.5
1	B	122	PRO	4.4
1	L	133	VAL	4.4
1	d	109	GLY	4.4
1	O	3	ALA	4.4
1	L	0	THR	4.4
1	F	4	TYR	4.4
1	O	60	VAL	4.4
1	R	132	GLU	4.4
1	M	142	GLU	4.4

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Mol	Chain	Res	Type	RSRZ
1	X	62	GLY	4.4
1	A	158	PHE	4.4
1	O	20	PHE	4.4
1	U	77	ALA	4.4
1	b	0	THR	4.4
1	A	100	VAL	4.4
1	G	60	VAL	4.4
1	X	133	VAL	4.4
1	d	62	GLY	4.4
1	A	4	TYR	4.4
1	O	-1	PHE	4.4
1	B	2	ALA	4.3
1	H	2	ALA	4.3
1	M	57	ILE	4.3
1	G	81	TYR	4.3
1	H	124	PRO	4.3
1	G	62	GLY	4.3
1	F	125	GLY	4.3
1	C	91	VAL	4.3
1	K	131	GLU	4.3
1	H	72	PHE	4.3
1	X	139	LYS	4.3
1	g	92	LEU	4.3
1	D	1	MET	4.3
1	W	60	VAL	4.3
1	d	94	ASP	4.3
1	d	138	LYS	4.2
1	d	80	PHE	4.2
1	O	62	GLY	4.2
1	Y	6	ILE	4.2
1	D	60	VAL	4.2
1	j	131	GLU	4.2
1	K	120	TYR	4.2
1	d	141	TYR	4.2
1	U	120	TYR	4.2
1	O	68	MET	4.2
1	G	89	GLY	4.2
1	X	52	GLY	4.2
1	C	135	ILE	4.2
1	J	157	VAL	4.2
1	U	133	VAL	4.2
1	C	64	PRO	4.2

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Mol	Chain	Res	Type	RSRZ
1	B	43	GLU	4.2
1	C	90	ASP	4.2
1	J	67	TYR	4.2
1	a	4	TYR	4.2
1	H	92	LEU	4.2
1	H	125	GLY	4.1
1	A	135	ILE	4.1
1	P	4	TYR	4.1
1	S	141	TYR	4.1
1	Q	69	LEU	4.1
1	C	158	PHE	4.1
1	Y	96	ILE	4.1
1	T	6	ILE	4.1
1	a	87	PHE	4.1
1	Y	127	THR	4.1
1	a	73	ASP	4.1
1	N	91	VAL	4.1
1	b	-1	PHE	4.1
1	N	44	ILE	4.1
1	G	51	VAL	4.1
1	h	126	CYS	4.1
1	Y	4	TYR	4.0
1	G	41	SER	4.0
1	d	96	ILE	4.0
1	U	51	VAL	4.0
1	Q	86	LEU	4.0
1	W	67	TYR	4.0
1	A	73	ASP	4.0
1	W	75	ILE	4.0
1	E	118	VAL	4.0
1	C	103	VAL	4.0
1	C	15	ALA	4.0
1	J	72	PHE	4.0
1	I	-1	PHE	4.0
1	F	20	PHE	4.0
1	U	158	PHE	4.0
1	b	44	ILE	4.0
1	M	56	LYS	4.0
1	d	108	VAL	4.0
1	D	34	ALA	4.0
1	i	43	GLU	4.0
1	e	75	ILE	4.0

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Mol	Chain	Res	Type	RSRZ
1	W	135	ILE	4.0
1	a	51	VAL	3.9
1	B	136	GLY	3.9
1	d	49	GLY	3.9
1	a	132	GLU	3.9
1	h	43	GLU	3.9
1	I	72	PHE	3.9
1	g	158	PHE	3.9
1	N	4	TYR	3.9
1	J	4	TYR	3.9
1	G	4	TYR	3.9
1	F	6	ILE	3.9
1	Y	120	TYR	3.9
1	Q	133	VAL	3.9
1	M	133	VAL	3.9
1	U	65	LEU	3.9
1	Z	62	GLY	3.9
1	D	53	THR	3.9
1	c	90	ASP	3.9
1	A	96	ILE	3.9
1	P	122	PRO	3.9
1	Z	116	ILE	3.9
1	T	122	PRO	3.9
1	A	119	THR	3.9
1	G	66	THR	3.9
1	c	8	LYS	3.9
1	S	63	HIS	3.9
1	O	158	PHE	3.9
1	L	93	ARG	3.9
1	E	158	PHE	3.9
1	B	44	ILE	3.9
1	R	57	ILE	3.9
1	I	57	ILE	3.9
1	F	135	ILE	3.9
1	T	150	TYR	3.9
1	j	4	TYR	3.9
1	J	68	MET	3.9
1	O	109	GLY	3.9
1	C	47	GLY	3.9
1	O	159	ALA	3.9
1	X	15	ALA	3.9
1	G	73	ASP	3.8

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Mol	Chain	Res	Type	RSRZ
1	J	122	PRO	3.8
1	W	122	PRO	3.8
1	S	6	ILE	3.8
1	X	81	TYR	3.8
1	g	67	TYR	3.8
1	I	7	VAL	3.8
1	d	30	VAL	3.8
1	F	110	GLY	3.8
1	C	25	LEU	3.8
1	U	22	ALA	3.8
1	U	153	ALA	3.8
1	i	159	ALA	3.8
1	Z	73	ASP	3.8
1	Q	88	GLU	3.8
1	O	135	ILE	3.8
1	X	25	LEU	3.8
1	H	55	THR	3.8
1	b	94	ASP	3.8
1	B	29	GLN	3.8
1	L	46	GLU	3.8
1	Q	126	CYS	3.8
1	C	72	PHE	3.8
1	U	59	PHE	3.8
1	g	139	LYS	3.8
1	c	45	ILE	3.8
1	d	24	VAL	3.8
1	a	67	TYR	3.8
1	L	49	GLY	3.8
1	F	136	GLY	3.8
1	g	51	VAL	3.8
1	d	78	ALA	3.8
1	D	64	PRO	3.8
1	K	80	PHE	3.8
1	d	143	PHE	3.8
1	Y	87	PHE	3.8
1	E	6	ILE	3.8
1	V	14	ILE	3.8
1	V	45	ILE	3.8
1	g	63	HIS	3.8
1	P	92	LEU	3.8
1	A	107	ALA	3.7
1	F	78	ALA	3.7

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Mol	Chain	Res	Type	RSRZ
1	J	158	PHE	3.7
1	H	126	CYS	3.7
1	H	63	HIS	3.7
1	b	52	GLY	3.7
1	b	92	LEU	3.7
1	I	30	VAL	3.7
1	F	60	VAL	3.7
1	U	91	VAL	3.7
1	X	1	MET	3.7
1	Z	72	PHE	3.7
1	H	17	HIS	3.7
1	Z	135	ILE	3.7
1	D	52	GLY	3.7
1	C	86	LEU	3.7
1	Z	65	LEU	3.7
1	X	65	LEU	3.7
1	W	62	GLY	3.7
1	W	100	VAL	3.7
1	h	128	VAL	3.7
1	a	55	THR	3.7
1	d	41	SER	3.7
1	a	28	HIS	3.7
1	Y	45	ILE	3.7
1	Y	47	GLY	3.7
1	G	1	MET	3.7
1	M	120	TYR	3.7
1	e	77	ALA	3.7
1	d	152	ALA	3.7
1	W	4	TYR	3.7
1	V	77	ALA	3.7
1	a	122	PRO	3.7
1	O	75	ILE	3.6
1	a	6	ILE	3.6
1	Z	20	PHE	3.6
1	X	75	ILE	3.6
1	V	44	ILE	3.6
1	Z	125	GLY	3.6
1	C	1	MET	3.6
1	O	32	VAL	3.6
1	J	51	VAL	3.6
1	E	100	VAL	3.6
1	W	95	ASN	3.6

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Mol	Chain	Res	Type	RSRZ
1	i	60	VAL	3.6
1	h	0	THR	3.6
1	Q	4	TYR	3.6
1	N	-2	PRO	3.6
1	d	17	HIS	3.6
1	E	131	GLU	3.6
1	W	26	GLU	3.6
1	A	20	PHE	3.6
1	X	59	PHE	3.6
1	B	119	THR	3.6
1	O	24	VAL	3.6
1	f	7	VAL	3.6
1	U	32	VAL	3.6
1	U	127	THR	3.6
1	O	16	PRO	3.6
1	L	2	ALA	3.6
1	J	-2	PRO	3.6
1	X	34	ALA	3.6
1	S	159	ALA	3.6
1	J	101	TYR	3.6
1	D	120	TYR	3.6
1	T	4	TYR	3.6
1	T	46	GLU	3.6
1	i	158	PHE	3.6
1	a	47	GLY	3.6
1	M	91	VAL	3.6
1	J	60	VAL	3.6
1	C	32	VAL	3.6
1	j	51	VAL	3.6
1	O	152	ALA	3.6
1	d	116	ILE	3.6
1	I	158	PHE	3.6
1	F	59	PHE	3.6
1	D	48	ASP	3.6
1	S	0	THR	3.6
1	H	128	VAL	3.6
1	V	128	VAL	3.6
1	O	2	ALA	3.6
1	H	27	ARG	3.5
1	Z	75	ILE	3.5
1	h	6	ILE	3.5
1	d	42	GLY	3.5

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Mol	Chain	Res	Type	RSRZ
1	a	59	PHE	3.5
1	i	80	PHE	3.5
1	W	37	HIS	3.5
1	F	58	THR	3.5
1	A	99	VAL	3.5
1	a	60	VAL	3.5
1	F	2	ALA	3.5
1	V	2	ALA	3.5
1	D	141	TYR	3.5
1	K	136	GLY	3.5
1	D	89	GLY	3.5
1	U	92	LEU	3.5
1	O	28	HIS	3.5
1	a	126	CYS	3.5
1	f	44	ILE	3.5
1	G	158	PHE	3.5
1	F	92	LEU	3.5
1	c	158	PHE	3.5
1	S	92	LEU	3.5
1	S	94	ASP	3.5
1	W	5	THR	3.5
1	A	60	VAL	3.5
1	G	30	VAL	3.5
1	K	135	ILE	3.5
1	H	6	ILE	3.5
1	F	14	ILE	3.5
1	C	14	ILE	3.5
1	X	6	ILE	3.5
1	U	45	ILE	3.5
1	S	135	ILE	3.5
1	A	25	LEU	3.5
1	K	48	ASP	3.5
1	a	69	LEU	3.5
1	Z	46	GLU	3.5
1	W	43	GLU	3.5
1	a	93	ARG	3.5
1	B	58	THR	3.4
1	M	55	THR	3.4
1	J	64	PRO	3.4
1	E	117	THR	3.4
1	U	64	PRO	3.4
1	T	0	THR	3.4

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Mol	Chain	Res	Type	RSRZ
1	J	133	VAL	3.4
1	a	54	VAL	3.4
1	C	41	SER	3.4
1	O	111	GLY	3.4
1	d	136	GLY	3.4
1	Y	125	GLY	3.4
1	O	57	ILE	3.4
1	M	6	ILE	3.4
1	b	93	ARG	3.4
1	d	150	TYR	3.4
1	T	61	ASP	3.4
1	T	94	ASP	3.4
1	i	129	ASN	3.4
1	O	87	PHE	3.4
1	L	59	PHE	3.4
1	d	58	THR	3.4
1	U	13	PRO	3.4
1	D	103	VAL	3.4
1	X	38	VAL	3.4
1	P	46	GLU	3.4
1	O	42	GLY	3.4
1	Z	49	GLY	3.4
1	G	94	ASP	3.4
1	c	25	LEU	3.4
1	C	120	TYR	3.4
1	b	59	PHE	3.4
1	Q	7	VAL	3.4
1	P	91	VAL	3.4
1	D	51	VAL	3.4
1	W	103	VAL	3.4
1	P	2	ALA	3.4
1	F	112	SER	3.4
1	E	2	ALA	3.4
1	h	9	GLU	3.4
1	T	62	GLY	3.4
1	L	44	ILE	3.4
1	a	75	ILE	3.4
1	W	1	MET	3.4
1	S	72	PHE	3.4
1	E	85	THR	3.4
1	W	117	THR	3.4
1	f	133	VAL	3.4

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Mol	Chain	Res	Type	RSRZ
1	Y	133	VAL	3.4
1	W	91	VAL	3.4
1	V	15	ALA	3.4
1	K	42	GLY	3.4
1	h	136	GLY	3.4
1	H	48	ASP	3.4
1	G	79	ASN	3.4
1	X	86	LEU	3.3
1	U	31	LEU	3.3
1	a	1	MET	3.3
1	A	87	PHE	3.3
1	B	5	THR	3.3
1	Q	120	TYR	3.3
1	F	81	TYR	3.3
1	E	119	THR	3.3
1	S	43	GLU	3.3
1	d	128	VAL	3.3
1	V	1	MET	3.3
1	F	124	PRO	3.3
1	d	16	PRO	3.3
1	I	87	PHE	3.3
1	H	0	THR	3.3
1	O	131	GLU	3.3
1	E	97	GLU	3.3
1	C	84	TYR	3.3
1	Y	131	GLU	3.3
1	B	7	VAL	3.3
1	A	2	ALA	3.3
1	E	78	ALA	3.3
1	D	153	ALA	3.3
1	a	108	VAL	3.3
1	T	77	ALA	3.3
1	A	86	LEU	3.3
1	K	6	ILE	3.3
1	U	11	GLU	3.3
1	R	-1	PHE	3.3
1	G	127	THR	3.3
1	D	87	PHE	3.3
1	B	144	TYR	3.3
1	V	120	TYR	3.3
1	J	118	VAL	3.3
1	G	24	VAL	3.3

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Mol	Chain	Res	Type	RSRZ
1	Z	133	VAL	3.3
1	X	128	VAL	3.3
1	N	50	GLY	3.3
1	c	95	ASN	3.3
1	B	92	LEU	3.3
1	f	92	LEU	3.3
1	e	93	ARG	3.3
1	d	-2	PRO	3.3
1	a	135	ILE	3.3
1	Z	14	ILE	3.3
1	Y	75	ILE	3.3
1	a	56	LYS	3.3
1	X	134	LYS	3.3
1	C	143	PHE	3.3
1	R	101	TYR	3.3
1	O	4	TYR	3.3
1	T	67	TYR	3.3
1	N	157	VAL	3.3
1	K	51	VAL	3.3
1	F	22	ALA	3.2
1	b	3	ALA	3.2
1	b	60	VAL	3.3
1	a	15	ALA	3.2
1	Y	91	VAL	3.3
1	H	49	GLY	3.2
1	F	42	GLY	3.2
1	C	62	GLY	3.2
1	M	86	LEU	3.2
1	G	132	GLU	3.2
1	N	6	ILE	3.2
1	a	57	ILE	3.2
1	X	17	HIS	3.2
1	R	53	THR	3.2
1	A	80	PHE	3.2
1	D	59	PHE	3.2
1	O	103	VAL	3.2
1	d	118	VAL	3.2
1	Z	128	VAL	3.2
1	F	49	GLY	3.2
1	A	92	LEU	3.2
1	Z	69	LEU	3.2
1	Y	105	LEU	3.2

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Mol	Chain	Res	Type	RSRZ
1	U	25	LEU	3.2
1	H	64	PRO	3.2
1	H	96	ILE	3.2
1	O	82	CYS	3.2
1	E	126	CYS	3.2
1	M	5	THR	3.2
1	g	39	PHE	3.2
1	Z	1	MET	3.2
1	P	78	ALA	3.2
1	K	2	ALA	3.2
1	A	52	GLY	3.2
1	D	62	GLY	3.2
1	d	125	GLY	3.2
1	i	51	VAL	3.2
1	i	157	VAL	3.2
1	L	94	ASP	3.2
1	D	46	GLU	3.2
1	d	105	LEU	3.2
1	H	122	PRO	3.2
1	X	64	PRO	3.2
1	D	45	ILE	3.2
1	U	135	ILE	3.2
1	I	1	MET	3.2
1	C	87	PHE	3.2
1	d	20	PHE	3.2
1	X	41	SER	3.2
1	R	125	GLY	3.2
1	L	4	TYR	3.2
1	L	91	VAL	3.2
1	C	144	TYR	3.2
1	d	84	TYR	3.2
1	Z	101	TYR	3.2
1	Z	120	TYR	3.2
1	Y	60	VAL	3.2
1	X	77	ALA	3.2
1	W	129	ASN	3.2
1	M	65	LEU	3.2
1	W	124	PRO	3.2
1	U	23	LEU	3.2
1	L	75	ILE	3.2
1	D	44	ILE	3.2
1	h	135	ILE	3.2

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Mol	Chain	Res	Type	RSRZ
1	Y	5	THR	3.2
1	F	72	PHE	3.1
1	D	97	GLU	3.1
1	D	3	ALA	3.1
1	A	157	VAL	3.1
1	b	4	TYR	3.1
1	F	64	PRO	3.1
1	D	65	LEU	3.1
1	I	6	ILE	3.1
1	F	116	ILE	3.1
1	e	45	ILE	3.1
1	V	6	ILE	3.1
1	b	18	ARG	3.1
1	S	1	MET	3.1
1	N	43	GLU	3.1
1	U	9	GLU	3.1
1	F	111	GLY	3.1
1	B	3	ALA	3.1
1	A	152	ALA	3.1
1	Y	77	ALA	3.1
1	R	51	VAL	3.1
1	G	103	VAL	3.1
1	O	23	LEU	3.1
1	D	67	TYR	3.1
1	U	19	LEU	3.1
1	M	44	ILE	3.1
1	K	134	LYS	3.1
1	a	58	THR	3.1
1	V	46	GLU	3.1
1	h	137	GLU	3.1
1	Z	12	SER	3.1
1	M	143	PHE	3.1
1	G	-1	PHE	3.1
1	A	91	VAL	3.1
1	M	128	VAL	3.1
1	X	100	VAL	3.1
1	O	25	LEU	3.1
1	C	19	LEU	3.1
1	K	141	TYR	3.1
1	a	84	TYR	3.1
1	Z	139	LYS	3.1
1	c	1	MET	3.1

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Mol	Chain	Res	Type	RSRZ
1	Z	57	ILE	3.1
1	S	75	ILE	3.1
1	G	53	THR	3.1
1	a	53	THR	3.1
1	f	111	GLY	3.1
1	U	87	PHE	3.1
1	T	-1	PHE	3.1
1	W	94	ASP	3.1
1	P	103	VAL	3.1
1	O	118	VAL	3.1
1	E	98	LYS	3.1
1	C	133	VAL	3.1
1	i	133	VAL	3.1
1	O	69	LEU	3.1
1	J	69	LEU	3.1
1	D	23	LEU	3.1
1	U	105	LEU	3.1
1	M	150	TYR	3.0
1	C	81	TYR	3.0
1	Z	67	TYR	3.0
1	D	74	GLU	3.0
1	d	46	GLU	3.0
1	J	53	THR	3.0
1	V	121	HIS	3.0
1	g	61	ASP	3.0
1	H	153	ALA	3.0
1	F	122	PRO	3.0
1	O	151	LEU	3.0
1	G	25	LEU	3.0
1	X	60	VAL	3.0
1	S	51	VAL	3.0
1	B	132	GLU	3.0
1	I	132	GLU	3.0
1	B	101	TYR	3.0
1	R	120	TYR	3.0
1	F	84	TYR	3.0
1	F	120	TYR	3.0
1	Y	116	ILE	3.0
1	G	0	THR	3.0
1	X	66	THR	3.0
1	W	119	THR	3.0
1	W	112	SER	3.0

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Mol	Chain	Res	Type	RSRZ
1	a	61	ASP	3.0
1	O	13	PRO	3.0
1	E	15	ALA	3.0
1	E	159	ALA	3.0
1	V	78	ALA	3.0
1	U	15	ALA	3.0
1	T	15	ALA	3.0
1	A	32	VAL	3.0
1	M	131	GLU	3.0
1	M	157	VAL	3.0
1	J	65	LEU	3.0
1	f	128	VAL	3.0
1	d	23	LEU	3.0
1	S	7	VAL	3.0
1	A	45	ILE	3.0
1	D	101	TYR	3.0
1	Y	101	TYR	3.0
1	d	93	ARG	3.0
1	K	52	GLY	3.0
1	G	42	GLY	3.0
1	f	47	GLY	3.0
1	Z	52	GLY	3.0
1	U	111	GLY	3.0
1	C	-1	PHE	3.0
1	L	78	ALA	3.0
1	F	77	ALA	3.0
1	P	126	CYS	3.0
1	K	25	LEU	3.0
1	H	23	LEU	3.0
1	C	31	LEU	3.0
1	a	7	VAL	3.0
1	Z	91	VAL	3.0
1	Z	92	LEU	3.0
1	U	157	VAL	3.0
1	i	108	VAL	3.0
1	d	44	ILE	3.0
1	L	123	LYS	3.0
1	A	141	TYR	3.0
1	d	127	THR	3.0
1	c	127	THR	3.0
1	g	0	THR	3.0
1	R	129	ASN	3.0

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Mol	Chain	Res	Type	RSRZ
1	O	110	GLY	3.0
1	K	62	GLY	3.0
1	Q	131	GLU	3.0
1	a	106	GLU	3.0
1	U	131	GLU	3.0
1	U	20	PHE	2.9
1	N	3	ALA	2.9
1	K	77	ALA	2.9
1	d	153	ALA	2.9
1	Y	2	ALA	2.9
1	S	140	ALA	2.9
1	J	31	LEU	2.9
1	F	23	LEU	2.9
1	d	19	LEU	2.9
1	b	65	LEU	2.9
1	X	19	LEU	2.9
1	R	91	VAL	2.9
1	U	139	LYS	2.9
1	A	116	ILE	2.9
1	I	44	ILE	2.9
1	G	44	ILE	2.9
1	U	14	ILE	2.9
1	j	14	ILE	2.9
1	B	127	THR	2.9
1	K	67	TYR	2.9
1	G	144	TYR	2.9
1	D	61	ASP	2.9
1	f	89	GLY	2.9
1	V	50	GLY	2.9
1	U	94	ASP	2.9
1	A	124	PRO	2.9
1	K	-1	PHE	2.9
1	N	69	LEU	2.9
1	V	3	ALA	2.9
1	B	133	VAL	2.9
1	K	99	VAL	2.9
1	H	133	VAL	2.9
1	F	133	VAL	2.9
1	C	128	VAL	2.9
1	e	24	VAL	2.9
1	X	51	VAL	2.9
1	T	51	VAL	2.9

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Mol	Chain	Res	Type	RSRZ
1	i	30	VAL	2.9
1	L	45	ILE	2.9
1	a	44	ILE	2.9
1	g	135	ILE	2.9
1	L	53	THR	2.9
1	S	5	THR	2.9
1	K	101	TYR	2.9
1	f	81	TYR	2.9
1	d	9	GLU	2.9
1	Q	125	GLY	2.9
1	G	61	ASP	2.9
1	T	52	GLY	2.9
1	R	122	PRO	2.9
1	A	77	ALA	2.9
1	R	2	ALA	2.9
1	O	22	ALA	2.9
1	M	92	LEU	2.9
1	K	87	PHE	2.9
1	H	123	LYS	2.9
1	G	72	PHE	2.9
1	D	69	LEU	2.9
1	b	22	ALA	2.9
1	W	159	ALA	2.9
1	J	147	VAL	2.9
1	U	116	ILE	2.9
1	C	88	GLU	2.9
1	C	149	GLU	2.9
1	f	1	MET	2.9
1	g	43	GLU	2.9
1	d	52	GLY	2.9
1	T	73	ASP	2.9
1	D	144	TYR	2.9
1	a	101	TYR	2.9
1	T	120	TYR	2.9
1	A	56	LYS	2.9
1	G	-2	PRO	2.9
1	d	64	PRO	2.9
1	X	40	LYS	2.9
1	U	21	LYS	2.9
1	O	39	PHE	2.9
1	O	59	PHE	2.9
1	O	146	GLN	2.9

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Mol	Chain	Res	Type	RSRZ
1	N	65	LEU	2.9
1	L	152	ALA	2.9
1	K	3	ALA	2.9
1	I	65	LEU	2.9
1	G	78	ALA	2.9
1	Q	128	VAL	2.9
1	O	30	VAL	2.9
1	O	99	VAL	2.9
1	d	147	VAL	2.9
1	d	157	VAL	2.9
1	b	128	VAL	2.9
1	S	24	VAL	2.9
1	A	88	GLU	2.9
1	M	132	GLU	2.9
1	Q	5	THR	2.9
1	Y	1	MET	2.9
1	U	1	MET	2.9
1	i	44	ILE	2.9
1	Q	145	LYS	2.8
1	C	33	LYS	2.8
1	Z	110	GLY	2.8
1	U	112	SER	2.8
1	O	141	TYR	2.8
1	L	122	PRO	2.8
1	W	141	TYR	2.8
1	Z	31	LEU	2.8
1	F	153	ALA	2.8
1	f	59	PHE	2.8
1	G	133	VAL	2.8
1	U	30	VAL	2.8
1	U	103	VAL	2.8
1	X	148	GLU	2.8
1	F	117	THR	2.8
1	C	82	CYS	2.8
1	a	45	ILE	2.8
1	Y	85	THR	2.8
1	V	127	THR	2.8
1	g	127	THR	2.8
1	A	48	ASP	2.8
1	F	61	ASP	2.8
1	P	52	GLY	2.8
1	R	37	HIS	2.8

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Mol	Chain	Res	Type	RSRZ
1	F	36	PRO	2.8
1	V	4	TYR	2.8
1	e	92	LEU	2.8
1	K	158	PHE	2.8
1	I	78	ALA	2.8
1	J	46	GLU	2.8
1	F	128	VAL	2.8
1	b	7	VAL	2.8
1	b	24	VAL	2.8
1	N	58	THR	2.8
1	M	93	ARG	2.8
1	M	135	ILE	2.8
1	I	18	ARG	2.8
1	d	14	ILE	2.8
1	Y	66	THR	2.8
1	E	49	GLY	2.8
1	i	16	PRO	2.8
1	H	144	TYR	2.8
1	U	67	TYR	2.8
1	Q	92	LEU	2.8
1	G	105	LEU	2.8
1	j	92	LEU	2.8
1	N	26	GLU	2.8
1	E	130	GLU	2.8
1	X	97	GLU	2.8
1	U	43	GLU	2.8
1	K	159	ALA	2.8
1	g	159	ALA	2.8
1	d	72	PHE	2.8
1	b	20	PHE	2.8
1	c	139	LYS	2.8
1	Y	98	LYS	2.8
1	K	32	VAL	2.8
1	X	157	VAL	2.8
1	V	51	VAL	2.8
1	F	127	THR	2.8
1	c	57	ILE	2.8
1	K	41	SER	2.8
1	X	35	GLN	2.8
1	U	122	PRO	2.8
1	H	132	GLU	2.8
1	C	132	GLU	2.8

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Mol	Chain	Res	Type	RSRZ
1	G	65	LEU	2.8
1	a	65	LEU	2.8
1	V	92	LEU	2.8
1	G	3	ALA	2.8
1	F	159	ALA	2.8
1	f	39	PHE	2.8
1	Z	18	ARG	2.8
1	G	32	VAL	2.8
1	E	108	VAL	2.8
1	e	60	VAL	2.8
1	d	38	VAL	2.8
1	b	100	VAL	2.8
1	Z	118	VAL	2.8
1	Q	96	ILE	2.7
1	P	53	THR	2.7
1	D	55	THR	2.7
1	h	116	ILE	2.7
1	g	57	ILE	2.7
1	i	47	GLY	2.7
1	B	126	CYS	2.7
1	Y	21	LYS	2.7
1	N	86	LEU	2.7
1	C	151	LEU	2.7
1	O	81	TYR	2.7
1	O	101	TYR	2.7
1	d	67	TYR	2.7
1	b	120	TYR	2.7
1	Y	159	ALA	2.7
1	f	87	PHE	2.7
1	Q	32	VAL	2.7
1	K	103	VAL	2.7
1	C	17	HIS	2.7
1	C	24	VAL	2.7
1	Z	38	VAL	2.7
1	X	7	VAL	2.7
1	C	85	THR	2.7
1	U	58	THR	2.7
1	i	29	GLN	2.7
1	P	95	ASN	2.7
1	J	44	ILE	2.7
1	I	75	ILE	2.7
1	G	45	ILE	2.7

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Mol	Chain	Res	Type	RSRZ
1	f	96	ILE	2.7
1	Y	61	ASP	2.7
1	S	95	ASN	2.7
1	F	89	GLY	2.7
1	Y	49	GLY	2.7
1	C	131	GLU	2.7
1	P	123	LYS	2.7
1	R	1	MET	2.7
1	J	1	MET	2.7
1	G	68	MET	2.7
1	R	65	LEU	2.7
1	A	67	TYR	2.7
1	P	3	ALA	2.7
1	N	101	TYR	2.7
1	c	4	TYR	2.7
1	G	17	HIS	2.7
1	D	70	HIS	2.7
1	Z	59	PHE	2.7
1	M	24	VAL	2.7
1	L	51	VAL	2.7
1	c	118	VAL	2.7
1	a	118	VAL	2.7
1	Y	100	VAL	2.7
1	F	55	THR	2.7
1	C	58	THR	2.7
1	a	117	THR	2.7
1	X	94	ASP	2.7
1	A	125	GLY	2.7
1	O	14	ILE	2.7
1	M	89	GLY	2.7
1	d	75	ILE	2.7
1	b	42	GLY	2.7
1	V	75	ILE	2.7
1	P	132	GLU	2.7
1	I	134	LYS	2.7
1	F	65	LEU	2.7
1	f	78	ALA	2.7
1	Z	159	ALA	2.7
1	d	120	TYR	2.7
1	X	120	TYR	2.7
1	A	143	PHE	2.7
1	Q	143	PHE	2.7

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Mol	Chain	Res	Type	RSRZ
1	K	54	VAL	2.7
1	J	99	VAL	2.7
1	H	54	VAL	2.7
1	E	157	VAL	2.7
1	b	51	VAL	2.7
1	Z	147	VAL	2.7
1	a	26	GLU	2.7
1	J	62	GLY	2.7
1	E	96	ILE	2.7
1	f	49	GLY	2.7
1	K	-2	PRO	2.7
1	Y	124	PRO	2.7
1	i	18	ARG	2.7
1	F	1	MET	2.7
1	F	105	LEU	2.7
1	C	92	LEU	2.7
1	Z	107	ALA	2.6
1	W	15	ALA	2.6
1	W	22	ALA	2.6
1	W	146	GLN	2.6
1	U	78	ALA	2.6
1	Q	141	TYR	2.6
1	N	72	PHE	2.6
1	J	134	LYS	2.6
1	I	56	LYS	2.6
1	F	67	TYR	2.6
1	E	113	LYS	2.6
1	D	84	TYR	2.6
1	J	30	VAL	2.6
1	F	24	VAL	2.6
1	E	99	VAL	2.6
1	D	99	VAL	2.6
1	X	103	VAL	2.6
1	C	55	THR	2.6
1	Z	127	THR	2.6
1	F	114	GLY	2.6
1	C	96	ILE	2.6
1	f	62	GLY	2.6
1	K	18	ARG	2.6
1	G	27	ARG	2.6
1	L	112	SER	2.6
1	Z	41	SER	2.6

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Mol	Chain	Res	Type	RSRZ
1	U	124	PRO	2.6
1	T	64	PRO	2.6
1	Y	121	HIS	2.6
1	J	113	LYS	2.6
1	Q	2	ALA	2.6
1	C	22	ALA	2.6
1	A	142	GLU	2.6
1	Y	43	GLU	2.6
1	Y	88	GLU	2.6
1	X	137	GLU	2.6
1	W	88	GLU	2.6
1	S	142	GLU	2.6
1	M	94	ASP	2.6
1	G	67	TYR	2.6
1	F	38	VAL	2.6
1	C	7	VAL	2.6
1	e	127	THR	2.6
1	U	147	VAL	2.6
1	b	50	GLY	2.6
1	b	89	GLY	2.6
1	Z	89	GLY	2.6
1	S	127	THR	2.6
1	h	49	GLY	2.6
1	h	127	THR	2.6
1	I	135	ILE	2.6
1	c	16	PRO	2.6
1	Z	16	PRO	2.6
1	i	45	ILE	2.6
1	D	37	HIS	2.6
1	a	37	HIS	2.6
1	K	65	LEU	2.6
1	J	23	LEU	2.6
1	d	69	LEU	2.6
1	R	3	ALA	2.6
1	I	15	ALA	2.6
1	H	93	ARG	2.6
1	F	129	ASN	2.6
1	U	79	ASN	2.6
1	h	61	ASP	2.6
1	M	20	PHE	2.6
1	X	72	PHE	2.6
1	B	118	VAL	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	103	VAL	2.6
1	H	100	VAL	2.6
1	G	99	VAL	2.6
1	D	124	PRO	2.6
1	D	133	VAL	2.6
1	f	51	VAL	2.6
1	f	64	PRO	2.6
1	b	103	VAL	2.6
1	Z	141	TYR	2.6
1	Y	103	VAL	2.6
1	X	54	VAL	2.6
1	W	81	TYR	2.6
1	S	91	VAL	2.6
1	h	-2	PRO	2.6
1	U	57	ILE	2.6
1	d	37	HIS	2.6
1	D	86	LEU	2.6
1	a	105	LEU	2.6
1	Z	151	LEU	2.6
1	K	43	GLU	2.6
1	b	137	GLU	2.6
1	R	126	CYS	2.6
1	T	126	CYS	2.6
1	J	2	ALA	2.6
1	d	15	ALA	2.6
1	Z	77	ALA	2.6
1	U	2	ALA	2.6
1	P	61	ASP	2.6
1	R	52	GLY	2.6
1	Q	127	THR	2.6
1	K	0	THR	2.6
1	G	50	GLY	2.6
1	Z	64	PRO	2.6
1	Y	72	PHE	2.6
1	X	42	GLY	2.6
1	V	72	PHE	2.6
1	T	125	GLY	2.6
1	E	60	VAL	2.6
1	b	54	VAL	2.6
1	a	24	VAL	2.6
1	Z	103	VAL	2.6
1	Y	108	VAL	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	116	ILE	2.6
1	Q	41	SER	2.6
1	Q	144	TYR	2.6
1	K	44	ILE	2.6
1	H	120	TYR	2.6
1	G	120	TYR	2.6
1	F	75	ILE	2.6
1	E	14	ILE	2.6
1	d	101	TYR	2.6
1	b	45	ILE	2.6
1	Z	45	ILE	2.6
1	C	121	HIS	2.6
1	D	83	LYS	2.6
1	C	134	LYS	2.6
1	Q	23	LEU	2.5
1	I	92	LEU	2.5
1	M	77	ALA	2.5
1	C	34	ALA	2.5
1	C	126	CYS	2.5
1	B	1	MET	2.5
1	K	94	ASP	2.5
1	B	49	GLY	2.5
1	R	143	PHE	2.5
1	N	122	PRO	2.5
1	K	55	THR	2.5
1	J	125	GLY	2.5
1	G	122	PRO	2.5
1	X	89	GLY	2.5
1	U	5	THR	2.5
1	T	110	GLY	2.5
1	j	49	GLY	2.5
1	E	87	PHE	2.5
1	B	121	HIS	2.5
1	J	21	LYS	2.5
1	J	24	VAL	2.5
1	E	91	VAL	2.5
1	f	91	VAL	2.5
1	b	30	VAL	2.5
1	b	157	VAL	2.5
1	Z	54	VAL	2.5
1	D	57	ILE	2.5
1	d	57	ILE	2.5

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Mol	Chain	Res	Type	RSRZ
1	E	137	GLU	2.5
1	T	132	GLU	2.5
1	H	69	LEU	2.5
1	E	1	MET	2.5
1	U	68	MET	2.5
1	A	76	ASP	2.5
1	K	95	ASN	2.5
1	H	3	ALA	2.5
1	G	48	ASP	2.5
1	F	79	ASN	2.5
1	E	77	ALA	2.5
1	c	77	ALA	2.5
1	a	22	ALA	2.5
1	Z	22	ALA	2.5
1	Y	76	ASP	2.5
1	Y	126	CYS	2.5
1	W	153	ALA	2.5
1	U	152	ALA	2.5
1	A	98	LYS	2.5
1	I	50	GLY	2.5
1	a	155	PRO	2.5
1	Z	109	GLY	2.5
1	X	125	GLY	2.5
1	L	85	THR	2.5
1	J	117	THR	2.5
1	D	17	HIS	2.5
1	a	5	THR	2.5
1	Q	20	PHE	2.5
1	C	39	PHE	2.5
1	L	108	VAL	2.5
1	F	32	VAL	2.5
1	F	100	VAL	2.5
1	D	118	VAL	2.5
1	f	24	VAL	2.5
1	e	128	VAL	2.5
1	g	24	VAL	2.5
1	O	45	ILE	2.5
1	P	10	GLU	2.5
1	S	97	GLU	2.5
1	G	18	ARG	2.5
1	O	19	LEU	2.5
1	M	69	LEU	2.5

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Mol	Chain	Res	Type	RSRZ
1	C	69	LEU	2.5
1	e	25	LEU	2.5
1	a	31	LEU	2.5
1	h	25	LEU	2.5
1	M	78	ALA	2.5
1	E	104	LYS	2.5
1	d	77	ALA	2.5
1	d	159	ALA	2.5
1	h	129	ASN	2.5
1	g	78	ALA	2.5
1	A	49	GLY	2.5
1	L	62	GLY	2.5
1	D	50	GLY	2.5
1	C	28	HIS	2.5
1	f	42	GLY	2.5
1	Y	64	PRO	2.5
1	M	117	THR	2.5
1	Y	117	THR	2.5
1	B	135	ILE	2.5
1	A	54	VAL	2.5
1	O	7	VAL	2.5
1	H	7	VAL	2.5
1	H	106	GLU	2.5
1	D	75	ILE	2.5
1	C	30	VAL	2.5
1	e	133	VAL	2.5
1	d	51	VAL	2.5
1	a	128	VAL	2.5
1	Z	112	SER	2.5
1	Z	157	VAL	2.5
1	X	14	ILE	2.5
1	X	30	VAL	2.5
1	i	93	ARG	2.5
1	h	7	VAL	2.5
1	h	46	GLU	2.5
1	G	84	TYR	2.5
1	Z	4	TYR	2.5
1	X	92	LEU	2.5
1	X	98	LYS	2.5
1	R	78	ALA	2.5
1	J	22	ALA	2.5
1	I	152	ALA	2.5

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Mol	Chain	Res	Type	RSRZ
1	D	77	ALA	2.5
1	C	152	ALA	2.5
1	X	121	HIS	2.5
1	g	52	GLY	2.5
1	A	55	THR	2.4
1	G	26	GLU	2.4
1	W	58	THR	2.4
1	i	127	THR	2.4
1	h	130	GLU	2.4
1	L	57	ILE	2.4
1	D	7	VAL	2.4
1	b	91	VAL	2.4
1	Y	118	VAL	2.4
1	X	57	ILE	2.4
1	X	91	VAL	2.4
1	W	51	VAL	2.4
1	U	96	ILE	2.4
1	g	96	ILE	2.4
1	A	19	LEU	2.4
1	E	92	LEU	2.4
1	c	144	TYR	2.4
1	Z	23	LEU	2.4
1	G	56	LYS	2.4
1	e	1	MET	2.4
1	F	48	ASP	2.4
1	i	79	ASN	2.4
1	I	2	ALA	2.4
1	I	159	ALA	2.4
1	F	152	ALA	2.4
1	a	152	ALA	2.4
1	O	88	GLU	2.4
1	G	47	GLY	2.4
1	i	50	GLY	2.4
1	h	52	GLY	2.4
1	h	62	GLY	2.4
1	J	85	THR	2.4
1	d	0	THR	2.4
1	T	85	THR	2.4
1	F	82	CYS	2.4
1	E	12	SER	2.4
1	A	7	VAL	2.4
1	P	133	VAL	2.4

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Mol	Chain	Res	Type	RSRZ
1	O	100	VAL	2.4
1	N	96	ILE	2.4
1	K	60	VAL	2.4
1	H	75	ILE	2.4
1	G	135	ILE	2.4
1	G	143	PHE	2.4
1	E	72	PHE	2.4
1	D	24	VAL	2.4
1	C	147	VAL	2.4
1	f	14	ILE	2.4
1	e	59	PHE	2.4
1	c	133	VAL	2.4
1	c	157	VAL	2.4
1	b	14	ILE	2.4
1	b	133	VAL	2.4
1	W	38	VAL	2.4
1	U	108	VAL	2.4
1	j	72	PHE	2.4
1	j	96	ILE	2.4
1	i	6	ILE	2.4
1	h	157	VAL	2.4
1	O	115	LYS	2.4
1	N	71	LYS	2.4
1	j	1	MET	2.4
1	O	105	LEU	2.4
1	J	25	LEU	2.4
1	T	65	LEU	2.4
1	I	144	TYR	2.4
1	A	121	HIS	2.4
1	K	17	HIS	2.4
1	C	37	HIS	2.4
1	U	17	HIS	2.4
1	C	61	ASP	2.4
1	Z	48	ASP	2.4
1	H	142	GLU	2.4
1	T	148	GLU	2.4
1	R	47	GLY	2.4
1	O	15	ALA	2.4
1	C	42	GLY	2.4
1	c	15	ALA	2.4
1	i	22	ALA	2.4
1	H	5	THR	2.4

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Mol	Chain	Res	Type	RSRZ
1	J	112	SER	2.4
1	B	100	VAL	2.4
1	O	72	PHE	2.4
1	J	32	VAL	2.4
1	J	59	PHE	2.4
1	J	103	VAL	2.4
1	J	143	PHE	2.4
1	G	75	ILE	2.4
1	D	56	LYS	2.4
1	M	32	VAL	2.4
1	F	54	VAL	2.4
1	E	32	VAL	2.4
1	d	45	ILE	2.4
1	b	39	PHE	2.4
1	j	75	ILE	2.4
1	J	19	LEU	2.4
1	T	86	LEU	2.4
1	A	146	GLN	2.4
1	N	120	TYR	2.4
1	D	63	HIS	2.4
1	C	150	TYR	2.4
1	i	146	GLN	2.4
1	C	137	GLU	2.4
1	c	61	ASP	2.4
1	X	155	PRO	2.4
1	g	64	PRO	2.4
1	N	159	ALA	2.4
1	G	77	ALA	2.4
1	d	110	GLY	2.4
1	S	153	ALA	2.4
1	j	111	GLY	2.4
1	O	12	SER	2.4
1	Q	157	VAL	2.4
1	N	24	VAL	2.4
1	N	108	VAL	2.4
1	N	158	PHE	2.4
1	M	1	MET	2.4
1	K	75	ILE	2.4
1	I	24	VAL	2.4
1	G	6	ILE	2.4
1	G	14	ILE	2.4
1	F	51	VAL	2.4

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Mol	Chain	Res	Type	RSRZ
1	c	91	VAL	2.4
1	Z	6	ILE	2.4
1	X	39	PHE	2.4
1	T	45	ILE	2.4
1	h	133	VAL	2.4
1	g	157	VAL	2.4
1	C	65	LEU	2.4
1	C	105	LEU	2.4
1	O	121	HIS	2.4
1	F	63	HIS	2.4
1	D	146	GLN	2.4
1	A	106	GLU	2.4
1	R	84	TYR	2.3
1	H	4	TYR	2.3
1	d	48	ASP	2.3
1	d	144	TYR	2.3
1	Z	144	TYR	2.3
1	U	73	ASP	2.3
1	U	144	TYR	2.3
1	J	89	GLY	2.3
1	a	62	GLY	2.3
1	V	52	GLY	2.3
1	I	77	ALA	2.3
1	E	107	ALA	2.3
1	Y	3	ALA	2.3
1	U	107	ALA	2.3
1	h	2	ALA	2.3
1	B	117	THR	2.3
1	R	0	THR	2.3
1	H	127	THR	2.3
1	C	5	THR	2.3
1	R	128	VAL	2.3
1	P	118	VAL	2.3
1	M	54	VAL	2.3
1	L	128	VAL	2.3
1	E	-1	PHE	2.3
1	f	6	ILE	2.3
1	f	108	VAL	2.3
1	d	135	ILE	2.3
1	b	72	PHE	2.3
1	V	32	VAL	2.3
1	S	39	PHE	2.3

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Mol	Chain	Res	Type	RSRZ
1	S	44	ILE	2.3
1	i	118	VAL	2.3
1	i	128	VAL	2.3
1	g	59	PHE	2.3
1	d	65	LEU	2.3
1	b	86	LEU	2.3
1	G	88	GLU	2.3
1	F	74	GLU	2.3
1	f	131	GLU	2.3
1	A	84	TYR	2.3
1	J	36	PRO	2.3
1	I	150	TYR	2.3
1	H	81	TYR	2.3
1	E	144	TYR	2.3
1	e	155	PRO	2.3
1	X	145	LYS	2.3
1	U	101	TYR	2.3
1	R	50	GLY	2.3
1	F	109	GLY	2.3
1	C	89	GLY	2.3
1	b	47	GLY	2.3
1	a	52	GLY	2.3
1	I	107	ALA	2.3
1	U	34	ALA	2.3
1	U	140	ALA	2.3
1	S	2	ALA	2.3
1	S	77	ALA	2.3
1	X	55	THR	2.3
1	N	41	SER	2.3
1	A	57	ILE	2.3
1	P	14	ILE	2.3
1	c	63	HIS	2.3
1	g	45	ILE	2.3
1	M	51	VAL	2.3
1	L	72	PHE	2.3
1	K	133	VAL	2.3
1	F	88	GLU	2.3
1	E	128	VAL	2.3
1	d	59	PHE	2.3
1	d	103	VAL	2.3
1	Z	80	PHE	2.3
1	W	118	VAL	2.3

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Mol	Chain	Res	Type	RSRZ
1	i	7	VAL	2.3
1	i	24	VAL	2.3
1	I	69	LEU	2.3
1	I	126	CYS	2.3
1	C	23	LEU	2.3
1	e	23	LEU	2.3
1	X	151	LEU	2.3
1	W	65	LEU	2.3
1	H	40	LYS	2.3
1	F	76	ASP	2.3
1	c	94	ASP	2.3
1	b	139	LYS	2.3
1	a	21	LYS	2.3
1	A	81	TYR	2.3
1	M	110	GLY	2.3
1	J	110	GLY	2.3
1	I	84	TYR	2.3
1	e	67	TYR	2.3
1	a	50	GLY	2.3
1	Z	111	GLY	2.3
1	G	107	ALA	2.3
1	d	34	ALA	2.3
1	H	41	SER	2.3
1	T	93	ARG	2.3
1	M	121	HIS	2.3
1	Y	97	GLU	2.3
1	X	9	GLU	2.3
1	Q	75	ILE	2.3
1	O	96	ILE	2.3
1	C	6	ILE	2.3
1	O	143	PHE	2.3
1	M	7	VAL	2.3
1	G	39	PHE	2.3
1	e	108	VAL	2.3
1	d	158	PHE	2.3
1	Z	100	VAL	2.3
1	Z	108	VAL	2.3
1	W	7	VAL	2.3
1	W	87	PHE	2.3
1	h	72	PHE	2.3
1	A	23	LEU	2.3
1	Q	105	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
1	N	134	LYS	2.3
1	I	105	LEU	2.3
1	Y	123	LYS	2.3
1	Q	94	ASP	2.3
1	N	129	ASN	2.3
1	M	129	ASN	2.3
1	T	129	ASN	2.3
1	b	124	PRO	2.3
1	Q	52	GLY	2.3
1	O	125	GLY	2.3
1	I	62	GLY	2.3
1	D	49	GLY	2.3
1	Y	62	GLY	2.3
1	X	49	GLY	2.3
1	U	62	GLY	2.3
1	U	110	GLY	2.3
1	S	89	GLY	2.3
1	j	110	GLY	2.3
1	d	68	MET	2.3
1	N	84	TYR	2.3
1	E	101	TYR	2.3
1	Z	84	TYR	2.3
1	A	159	ALA	2.3
1	N	2	ALA	2.3
1	a	2	ALA	2.3
1	J	58	THR	2.3
1	H	66	THR	2.3
1	A	74	GLU	2.3
1	P	11	GLU	2.3
1	L	11	GLU	2.3
1	G	70	HIS	2.3
1	F	121	HIS	2.3
1	b	63	HIS	2.3
1	Z	17	HIS	2.3
1	i	41	SER	2.3
1	W	137	GLU	2.3
1	T	44	ILE	2.3
1	B	91	VAL	2.3
1	B	103	VAL	2.3
1	O	86	LEU	2.2
1	N	100	VAL	2.3
1	J	105	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
1	G	59	PHE	2.2
1	F	143	PHE	2.2
1	E	23	LEU	2.2
1	E	80	PHE	2.2
1	D	32	VAL	2.3
1	e	158	PHE	2.2
1	d	32	VAL	2.3
1	Z	24	VAL	2.3
1	T	25	LEU	2.2
1	i	-1	PHE	2.2
1	i	87	PHE	2.2
1	Q	90	ASP	2.2
1	K	154	ASN	2.2
1	j	79	ASN	2.2
1	T	155	PRO	2.2
1	A	136	GLY	2.2
1	Y	52	GLY	2.2
1	U	18	ARG	2.2
1	U	49	GLY	2.2
1	R	153	ALA	2.2
1	O	153	ALA	2.2
1	C	107	ALA	2.2
1	e	131	GLU	2.2
1	a	107	ALA	2.2
1	X	84	TYR	2.2
1	X	156	GLU	2.2
1	V	22	ALA	2.2
1	H	53	THR	2.2
1	b	5	THR	2.2
1	N	123	LYS	2.2
1	P	96	ILE	2.2
1	O	116	ILE	2.2
1	e	6	ILE	2.2
1	c	96	ILE	2.2
1	X	44	ILE	2.2
1	V	135	ILE	2.2
1	d	99	VAL	2.2
1	Z	60	VAL	2.2
1	V	19	LEU	2.2
1	U	151	LEU	2.2
1	F	80	PHE	2.2
1	U	72	PHE	2.2

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Mol	Chain	Res	Type	RSRZ
1	P	129	ASN	2.2
1	a	154	ASN	2.2
1	b	1	MET	2.2
1	b	68	MET	2.2
1	Z	155	PRO	2.2
1	P	110	GLY	2.2
1	F	47	GLY	2.2
1	C	136	GLY	2.2
1	O	142	GLU	2.2
1	L	17	HIS	2.2
1	I	131	GLU	2.2
1	F	130	GLU	2.2
1	a	130	GLU	2.2
1	Z	63	HIS	2.2
1	Y	63	HIS	2.2
1	N	8	LYS	2.2
1	J	56	LYS	2.2
1	F	29	GLN	2.2
1	F	71	LYS	2.2
1	f	77	ALA	2.2
1	d	2	ALA	2.2
1	Z	66	THR	2.2
1	c	150	TYR	2.2
1	X	144	TYR	2.2
1	W	150	TYR	2.2
1	H	116	ILE	2.2
1	C	75	ILE	2.2
1	Y	57	ILE	2.2
1	T	14	ILE	2.2
1	A	65	LEU	2.2
1	R	86	LEU	2.2
1	U	69	LEU	2.2
1	Q	38	VAL	2.2
1	J	128	VAL	2.2
1	H	60	VAL	2.2
1	F	118	VAL	2.2
1	a	32	VAL	2.2
1	X	32	VAL	2.2
1	T	7	VAL	2.2
1	T	59	PHE	2.2
1	M	48	ASP	2.2
1	T	95	ASN	2.2

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Mol	Chain	Res	Type	RSRZ
1	X	122	PRO	2.2
1	L	126	CYS	2.2
1	c	125	GLY	2.2
1	R	102	GLU	2.2
1	M	130	GLU	2.2
1	J	63	HIS	2.2
1	G	74	GLU	2.2
1	a	131	GLU	2.2
1	Y	142	GLU	2.2
1	W	97	GLU	2.2
1	O	134	LYS	2.2
1	H	139	LYS	2.2
1	e	123	LYS	2.2
1	b	123	LYS	2.2
1	U	33	LYS	2.2
1	i	28	HIS	2.2
1	R	117	THR	2.2
1	R	152	ALA	2.2
1	Q	3	ALA	2.2
1	F	3	ALA	2.2
1	E	127	THR	2.2
1	c	159	ALA	2.2
1	j	152	ALA	2.2
1	i	140	ALA	2.2
1	d	112	SER	2.2
1	d	81	TYR	2.2
1	B	96	ILE	2.2
1	F	25	LEU	2.2
1	E	25	LEU	2.2
1	b	19	LEU	2.2
1	Y	135	ILE	2.2
1	h	23	LEU	2.2
1	I	99	VAL	2.2
1	G	100	VAL	2.2
1	W	128	VAL	2.2
1	V	103	VAL	2.2
1	L	1	MET	2.2
1	b	158	PHE	2.2
1	a	158	PHE	2.2
1	e	124	PRO	2.2
1	a	64	PRO	2.2
1	K	46	GLU	2.2

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Mol	Chain	Res	Type	RSRZ
1	X	132	GLU	2.2
1	Y	136	GLY	2.2
1	A	153	ALA	2.2
1	P	119	THR	2.2
1	J	153	ALA	2.2
1	H	34	ALA	2.2
1	E	0	THR	2.2
1	C	2	ALA	2.2
1	c	112	SER	2.2
1	i	15	ALA	2.2
1	g	66	THR	2.2
1	I	4	TYR	2.1
1	f	101	TYR	2.1
1	h	120	TYR	2.1
1	P	75	ILE	2.1
1	J	57	ILE	2.1
1	H	86	LEU	2.1
1	Z	86	LEU	2.1
1	i	92	LEU	2.1
1	i	105	LEU	2.1
1	h	92	LEU	2.1
1	O	1	MET	2.1
1	N	128	VAL	2.1
1	N	133	VAL	2.1
1	I	147	VAL	2.1
1	D	95	ASN	2.1
1	C	118	VAL	2.1
1	a	91	VAL	2.1
1	Z	129	ASN	2.1
1	Y	95	ASN	2.1
1	g	60	VAL	2.1
1	O	33	LYS	2.1
1	L	64	PRO	2.1
1	H	20	PHE	2.1
1	d	13	PRO	2.1
1	X	20	PHE	2.1
1	W	158	PHE	2.1
1	i	131	GLU	2.1
1	E	121	HIS	2.1
1	d	146	GLN	2.1
1	L	50	GLY	2.1
1	X	111	GLY	2.1

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Mol	Chain	Res	Type	RSRZ
1	D	126	CYS	2.1
1	O	41	SER	2.1
1	O	55	THR	2.1
1	K	5	THR	2.1
1	K	127	THR	2.1
1	I	153	ALA	2.1
1	H	112	SER	2.1
1	G	153	ALA	2.1
1	i	77	ALA	2.1
1	Q	93	ARG	2.1
1	Z	93	ARG	2.1
1	W	93	ARG	2.1
1	A	144	TYR	2.1
1	L	120	TYR	2.1
1	J	81	TYR	2.1
1	a	144	TYR	2.1
1	g	4	TYR	2.1
1	R	45	ILE	2.1
1	O	92	LEU	2.1
1	M	33	LYS	2.1
1	I	14	ILE	2.1
1	I	96	ILE	2.1
1	H	31	LEU	2.1
1	E	71	LYS	2.1
1	f	65	LEU	2.1
1	c	6	ILE	2.1
1	a	40	LYS	2.1
1	a	116	ILE	2.1
1	U	75	ILE	2.1
1	P	94	ASP	2.1
1	F	73	ASP	2.1
1	Q	100	VAL	2.1
1	R	39	PHE	2.1
1	O	64	PRO	2.1
1	G	54	VAL	2.1
1	J	146	GLN	2.1
1	I	80	PHE	2.1
1	H	146	GLN	2.1
1	G	64	PRO	2.1
1	F	155	PRO	2.1
1	C	122	PRO	2.1
1	C	124	PRO	2.1

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Mol	Chain	Res	Type	RSRZ
1	e	51	VAL	2.1
1	e	91	VAL	2.1
1	c	103	VAL	2.1
1	X	118	VAL	2.1
1	i	32	VAL	2.1
1	K	114	GLY	2.1
1	J	50	GLY	2.1
1	Y	109	GLY	2.1
1	W	42	GLY	2.1
1	O	27	ARG	2.1
1	G	126	CYS	2.1
1	Z	82	CYS	2.1
1	H	77	ALA	2.1
1	G	112	SER	2.1
1	F	119	THR	2.1
1	W	77	ALA	2.1
1	U	12	SER	2.1
1	T	127	THR	2.1
1	N	78	ALA	2.1
1	A	68	MET	2.1
1	Q	1	MET	2.1
1	H	1	MET	2.1
1	F	21	LYS	2.1
1	D	8	LYS	2.1
1	U	123	LYS	2.1
1	H	74	GLU	2.1
1	D	92	LEU	2.1
1	e	43	GLU	2.1
1	f	45	ILE	2.1
1	c	105	LEU	2.1
1	W	105	LEU	2.1
1	W	106	GLU	2.1
1	S	31	LEU	2.1
1	Q	129	ASN	2.1
1	J	141	TYR	2.1
1	J	150	TYR	2.1
1	E	67	TYR	2.1
1	a	129	ASN	2.1
1	a	141	TYR	2.1
1	S	61	ASP	2.1
1	S	67	TYR	2.1
1	D	35	GLN	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	108	VAL	2.1
1	B	124	PRO	2.1
1	O	108	VAL	2.1
1	O	157	VAL	2.1
1	J	7	VAL	2.1
1	F	13	PRO	2.1
1	F	16	PRO	2.1
1	F	91	VAL	2.1
1	E	24	VAL	2.1
1	j	100	VAL	2.1
1	M	72	PHE	2.1
1	L	39	PHE	2.1
1	h	80	PHE	2.1
1	P	93	ARG	2.1
1	U	93	ARG	2.1
1	c	85	THR	2.1
1	U	66	THR	2.1
1	Q	107	ALA	2.1
1	C	21	LYS	2.1
1	a	140	ALA	2.1
1	a	159	ALA	2.1
1	Z	71	LYS	2.1
1	X	78	ALA	2.1
1	j	3	ALA	2.1
1	R	74	GLU	2.1
1	O	132	GLU	2.1
1	C	43	GLU	2.1
1	B	86	LEU	2.1
1	J	86	LEU	2.1
1	c	92	LEU	2.1
1	b	121	HIS	2.1
1	a	146	GLN	2.1
1	S	86	LEU	2.1
1	L	116	ILE	2.1
1	J	6	ILE	2.1
1	E	75	ILE	2.1
1	E	94	ASP	2.1
1	Z	44	ILE	2.1
1	S	96	ILE	2.1
1	E	4	TYR	2.1
1	C	101	TYR	2.1
1	f	120	TYR	2.1

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Mol	Chain	Res	Type	RSRZ
1	e	122	PRO	2.1
1	E	7	VAL	2.1
1	f	103	VAL	2.1
1	Y	7	VAL	2.1
1	j	133	VAL	2.1
1	h	60	VAL	2.1
1	R	89	GLY	2.1
1	Q	47	GLY	2.1
1	M	87	PHE	2.1
1	H	158	PHE	2.1
1	Y	20	PHE	2.1
1	X	143	PHE	2.1
1	U	80	PHE	2.1
1	T	49	GLY	2.1
1	O	138	LYS	2.0
1	K	40	LYS	2.0
1	b	33	LYS	2.0
1	b	134	LYS	2.0
1	T	139	LYS	2.0
1	N	119	THR	2.0
1	a	127	THR	2.0
1	h	112	SER	2.0
1	P	159	ALA	2.0
1	L	132	GLU	2.0
1	I	26	GLU	2.0
1	d	3	ALA	2.0
1	j	2	ALA	2.0
1	j	130	GLU	2.0
1	g	2	ALA	2.0
1	i	17	HIS	2.0
1	B	151	LEU	2.0
1	A	31	LEU	2.0
1	R	94	ASP	2.0
1	P	69	LEU	2.0
1	J	154	ASN	2.0
1	I	23	LEU	2.0
1	I	25	LEU	2.0
1	I	94	ASP	2.0
1	D	73	ASP	2.0
1	f	48	ASP	2.0
1	a	86	LEU	2.0
1	X	23	LEU	2.0

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Mol	Chain	Res	Type	RSRZ
1	i	19	LEU	2.0
1	D	116	ILE	2.0
1	f	135	ILE	2.0
1	b	6	ILE	2.0
1	T	135	ILE	2.0
1	g	44	ILE	2.0
1	S	36	PRO	2.0
1	A	150	TYR	2.0
1	R	144	TYR	2.0
1	Y	81	TYR	2.0
1	X	101	TYR	2.0
1	V	144	TYR	2.0
1	S	4	TYR	2.0
1	B	128	VAL	2.0
1	A	38	VAL	2.0
1	N	7	VAL	2.0
1	N	32	VAL	2.0
1	M	30	VAL	2.0
1	C	38	VAL	2.0
1	C	93	ARG	2.0
1	b	118	VAL	2.0
1	Z	30	VAL	2.0
1	W	99	VAL	2.0
1	V	133	VAL	2.0
1	i	91	VAL	2.0
1	g	103	VAL	2.0
1	O	136	GLY	2.0
1	J	111	GLY	2.0
1	I	49	GLY	2.0
1	Y	50	GLY	2.0
1	T	136	GLY	2.0
1	j	136	GLY	2.0
1	A	72	PHE	2.0
1	c	87	PHE	2.0
1	X	158	PHE	2.0
1	T	87	PHE	2.0
1	Y	139	LYS	2.0
1	T	104	LYS	2.0
1	A	85	THR	2.0
1	R	46	GLU	2.0
1	J	148	GLU	2.0
1	c	142	GLU	2.0

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Mol	Chain	Res	Type	RSRZ
1	X	68	MET	2.0
1	W	66	THR	2.0
1	g	148	GLU	2.0
1	B	78	ALA	2.0
1	Y	107	ALA	2.0
1	Q	70	HIS	2.0
1	N	17	HIS	2.0
1	M	146	GLN	2.0
1	K	126	CYS	2.0
1	A	151	LEU	2.0
1	F	31	LEU	2.0
1	D	31	LEU	2.0
1	d	86	LEU	2.0
1	d	154	ASN	2.0
1	Z	19	LEU	2.0
1	g	31	LEU	2.0
1	g	86	LEU	2.0
1	Q	6	ILE	2.0
1	E	93	ARG	2.0
1	D	6	ILE	2.0
1	f	75	ILE	2.0
1	e	96	ILE	2.0
1	c	14	ILE	2.0
1	T	116	ILE	2.0
1	j	6	ILE	2.0
1	O	123	LYS	2.0
1	F	138	LYS	2.0
1	g	40	LYS	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 oligosaccharides 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(Å ²)	Q<0.9
2	2AN	N	203	21/21	0.39	0.45	56,74,126,131	0
5	DMS	X	207	4/4	0.49	0.62	68,68,69,71	4
2	2AN	f	203	21/21	0.56	0.30	60,68,80,86	0
2	2AN	j	207	21/21	0.63	0.29	87,134,147,162	0
2	2AN	X	203	21/21	0.63	0.29	53,62,71,76	0
6	FLC	e	202	13/13	0.66	0.23	62,69,75,77	0
2	2AN	h	205	21/21	0.67	0.34	127,179,191,208	0
2	2AN	d	203	21/21	0.69	0.29	66,79,115,120	0
2	2AN	D	204	21/21	0.69	0.31	68,98,111,114	0
2	2AN	b	206	21/21	0.73	0.32	57,86,103,108	21
2	2AN	X	206	21/21	0.74	0.25	48,61,70,74	0
2	2AN	G	207	21/21	0.75	0.28	62,68,79,90	21
2	2AN	a	204	21/21	0.75	0.38	54,112,142,163	21
2	2AN	I	207	21/21	0.76	0.36	68,96,114,116	21
2	2AN	S	204	21/21	0.77	0.43	50,62,75,79	21
5	DMS	G	208	4/4	0.77	0.30	61,61,63,75	4
4	EPE	P	205	15/15	0.78	0.27	57,75,92,109	0
2	2AN	j	205	21/21	0.78	0.24	31,43,51,57	0
2	2AN	R	205	21/21	0.79	0.25	77,99,112,117	0
2	2AN	d	204	21/21	0.79	0.40	50,68,80,82	21
2	2AN	c	202	21/21	0.79	0.25	56,68,103,110	0
2	2AN	b	205	21/21	0.79	0.29	114,123,138,168	0
2	2AN	I	205	21/21	0.80	0.25	57,74,84,86	21
3	SO4	Q	204	5/5	0.80	0.18	47,67,73,75	5
2	2AN	A	204	21/21	0.80	0.58	58,79,92,95	21
2	2AN	R	204	21/21	0.80	0.22	61,75,82,83	0
2	2AN	F	206	21/21	0.80	0.34	49,63,97,104	21
2	2AN	Y	204	21/21	0.80	0.30	47,58,66,70	21
6	FLC	a	206	13/13	0.80	0.14	60,76,89,90	13
2	2AN	I	204	21/21	0.81	0.29	57,71,83,89	21
2	2AN	G	204	21/21	0.82	0.23	47,66,102,109	21
2	2AN	T	203	21/21	0.82	0.23	45,60,101,108	0
2	2AN	Y	201	21/21	0.83	0.21	63,72,89,91	0
5	DMS	N	206	4/4	0.83	0.28	36,47,47,48	4
2	2AN	U	202	21/21	0.83	0.46	76,90,110,117	21
6	FLC	i	202	13/13	0.83	0.17	47,60,64,70	13
2	2AN	f	206	21/21	0.84	0.23	62,76,97,101	21
2	2AN	T	204	21/21	0.84	0.20	50,64,70,85	0
2	2AN	S	203	21/21	0.84	0.28	46,51,80,83	21
2	2AN	H	204	21/21	0.84	0.23	71,79,107,109	21
6	FLC	j	208	13/13	0.84	0.27	30,38,45,59	13

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	2AN	G	205	21/21	0.84	0.23	32,40,50,55	21
2	2AN	j	206	21/21	0.85	0.20	52,69,105,107	0
2	2AN	I	203	21/21	0.85	0.20	63,75,83,91	21
2	2AN	F	204	21/21	0.86	0.27	74,96,127,138	0
2	2AN	O	202	21/21	0.86	0.21	74,83,90,94	21
2	2AN	c	203	21/21	0.86	0.19	58,78,115,123	0
2	2AN	F	202	21/21	0.86	0.19	50,81,108,112	0
6	FLC	i	203	13/13	0.86	0.08	45,52,60,62	0
3	SO4	Y	205	5/5	0.87	0.26	29,31,38,41	5
2	2AN	S	201	21/21	0.87	0.18	81,103,116,120	0
2	2AN	a	201	21/21	0.87	0.22	58,96,117,123	0
2	2AN	C	203[A]	21/21	0.87	0.30	51,60,72,76	21
2	2AN	V	208	21/21	0.87	0.25	54,67,114,129	21
6	FLC	G	206	13/13	0.87	0.24	45,60,64,69	13
2	2AN	Z	206	21/21	0.87	0.17	55,78,100,109	0
2	2AN	E	204	21/21	0.87	0.29	48,69,105,112	21
2	2AN	N	205	21/21	0.87	0.18	53,68,76,88	0
2	2AN	T	205	21/21	0.87	0.17	54,60,75,78	0
3	SO4	G	209	5/5	0.87	0.12	52,59,68,70	5
2	2AN	V	207	21/21	0.88	0.21	48,62,88,96	0
6	FLC	a	205	13/13	0.88	0.18	55,64,75,77	13
3	SO4	A	205	5/5	0.88	0.28	23,24,27,29	5
2	2AN	Z	202	21/21	0.88	0.18	88,99,106,119	0
2	2AN	I	206	21/21	0.88	0.19	54,78,87,90	0
2	2AN	W	201	21/21	0.88	0.20	45,60,69,73	21
2	2AN	X	202	21/21	0.89	0.17	70,81,106,111	0
2	2AN	h	203	21/21	0.89	0.16	36,44,58,66	0
2	2AN	A	202	21/21	0.89	0.16	54,71,83,94	0
2	2AN	c	205	21/21	0.89	0.23	38,48,57,61	21
2	2AN	Z	204	21/21	0.89	0.15	69,80,92,97	0
2	2AN	B	206	21/21	0.89	0.21	65,80,111,114	0
2	2AN	Q	203	21/21	0.89	0.17	81,100,118,121	0
2	2AN	U	201	21/21	0.89	0.21	89,112,138,139	0
2	2AN	K	203	21/21	0.89	0.20	45,61,72,73	21
2	2AN	V	206	21/21	0.90	0.16	50,64,84,93	0
2	2AN	a	203	21/21	0.90	0.17	58,67,76,81	0
2	2AN	j	204	21/21	0.90	0.16	44,54,66,71	0
2	2AN	Y	203	21/21	0.90	0.15	52,68,87,92	0
2	2AN	A	203	21/21	0.90	0.19	61,67,94,98	21
2	2AN	X	201	21/21	0.90	0.17	40,49,81,90	0
2	2AN	h	201	21/21	0.90	0.20	34,48,53,62	21
2	2AN	E	203	21/21	0.90	0.18	44,52,76,79	21

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	2AN	O	203	21/21	0.90	0.14	53,63,74,92	0
2	2AN	g	201	21/21	0.90	0.20	46,57,79,83	21
2	2AN	g	203	21/21	0.90	0.16	48,76,86,88	0
2	2AN	Z	205	21/21	0.90	0.17	68,75,126,139	0
2	2AN	D	203	21/21	0.90	0.16	72,78,87,91	0
2	2AN	P	203	21/21	0.91	0.17	44,55,68,85	0
2	2AN	F	205	21/21	0.91	0.18	67,91,99,104	0
2	2AN	Z	201	21/21	0.91	0.14	54,62,71,78	0
2	2AN	X	204	21/21	0.91	0.14	63,74,85,91	0
3	SO4	c	207	5/5	0.91	0.20	27,27,32,36	5
3	SO4	c	208	5/5	0.91	0.18	32,36,36,41	5
2	2AN	d	201	21/21	0.91	0.15	46,61,68,72	0
2	2AN	j	201	21/21	0.91	0.13	34,48,58,61	0
2	2AN	d	202	21/21	0.91	0.15	50,61,76,81	0
2	2AN	R	202	21/21	0.92	0.12	36,49,57,62	0
2	2AN	C	201	21/21	0.92	0.13	46,57,67,84	0
2	2AN	B	204	21/21	0.92	0.15	43,52,59,59	21
2	2AN	b	202	21/21	0.92	0.14	54,68,80,85	0
2	2AN	b	204	21/21	0.92	0.15	65,72,87,92	0
2	2AN	Y	202	21/21	0.92	0.18	45,53,56,59	21
2	2AN	G	201	21/21	0.92	0.14	48,55,82,93	0
2	2AN	B	205	21/21	0.92	0.15	48,62,80,82	0
2	2AN	h	206	21/21	0.92	0.13	39,57,75,82	0
2	2AN	M	203	21/21	0.92	0.17	57,73,80,81	0
2	2AN	L	204	21/21	0.92	0.12	65,75,91,95	0
2	2AN	D	202	21/21	0.92	0.13	50,59,76,79	0
2	2AN	F	201	21/21	0.92	0.17	61,70,79,84	0
2	2AN	X	205	21/21	0.92	0.13	55,66,81,86	0
2	2AN	f	204	21/21	0.93	0.14	38,50,60,72	0
2	2AN	J	201	21/21	0.93	0.18	53,69,97,103	0
2	2AN	b	203	21/21	0.93	0.11	47,55,66,72	0
2	2AN	B	203	21/21	0.93	0.16	38,49,74,80	0
2	2AN	i	201	21/21	0.93	0.16	40,48,51,52	21
2	2AN	N	204	21/21	0.93	0.17	53,64,92,95	0
2	2AN	V	201	21/21	0.93	0.14	46,58,79,93	0
2	2AN	c	204	21/21	0.94	0.16	39,46,53,55	21
2	2AN	P	204	21/21	0.94	0.16	36,52,60,62	0
2	2AN	b	201	21/21	0.94	0.14	44,52,58,60	0
2	2AN	T	202	21/21	0.94	0.16	31,39,49,52	21
2	2AN	J	202	21/21	0.94	0.16	44,52,71,73	0
2	2AN	G	203	21/21	0.94	0.18	42,52,92,100	0
2	2AN	f	205	21/21	0.94	0.13	41,54,66,68	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	2AN	O	201	21/21	0.94	0.14	42,62,79,92	0
3	SO4	c	209	5/5	0.94	0.12	47,52,58,61	5
2	2AN	S	202	21/21	0.94	0.13	46,56,69,70	21
2	2AN	e	201	21/21	0.94	0.14	39,50,52,57	0
2	2AN	Q	202	21/21	0.94	0.15	46,64,70,74	0
2	2AN	a	202	21/21	0.94	0.14	46,52,60,66	0
2	2AN	L	203	21/21	0.94	0.12	33,53,64,65	0
2	2AN	B	202	21/21	0.94	0.13	45,59,67,68	0
2	2AN	A	201	21/21	0.94	0.17	46,57,80,91	0
2	2AN	F	203	21/21	0.94	0.17	51,61,81,84	0
2	2AN	V	204	21/21	0.94	0.12	50,63,75,86	0
2	2AN	V	205	21/21	0.94	0.14	42,59,68,72	0
2	2AN	Z	203	21/21	0.94	0.14	60,69,82,90	0
2	2AN	C	202	21/21	0.94	0.16	66,99,110,116	0
2	2AN	P	202	21/21	0.95	0.12	29,43,52,57	0
2	2AN	L	202	21/21	0.95	0.13	46,54,67,71	0
3	SO4	I	208	5/5	0.95	0.10	35,36,41,46	5
2	2AN	H	202	21/21	0.95	0.12	48,67,79,83	0
2	2AN	V	203	21/21	0.95	0.12	44,52,61,62	0
2	2AN	f	202	21/21	0.95	0.12	33,49,57,62	0
2	2AN	H	203	21/21	0.95	0.13	53,66,79,84	0
2	2AN	B	201	21/21	0.95	0.12	35,51,62,63	0
2	2AN	J	203	21/21	0.95	0.12	43,69,75,80	0
2	2AN	E	201	21/21	0.95	0.13	40,49,68,76	0
2	2AN	E	202	21/21	0.95	0.12	34,41,50,65	0
2	2AN	G	202	21/21	0.95	0.13	56,64,68,75	0
2	2AN	T	201	21/21	0.95	0.12	38,49,58,65	0
2	2AN	h	204	21/21	0.95	0.15	48,67,91,97	0
2	2AN	I	202	21/21	0.95	0.15	37,47,59,69	0
2	2AN	R	203	21/21	0.95	0.14	54,73,82,84	0
2	2AN	K	201	21/21	0.95	0.11	38,44,66,82	0
2	2AN	g	202	21/21	0.95	0.11	37,51,60,64	0
2	2AN	K	202	21/21	0.95	0.19	45,54,83,89	0
2	2AN	V	202	21/21	0.96	0.12	26,40,56,62	0
2	2AN	h	202	21/21	0.96	0.12	37,52,59,61	0
2	2AN	D	201	21/21	0.96	0.13	38,69,79,84	0
3	SO4	g	204	5/5	0.96	0.11	24,30,34,38	5
2	2AN	N	201	21/21	0.96	0.12	36,44,54,58	0
2	2AN	H	201	21/21	0.96	0.14	44,58,62,65	0
2	2AN	M	201	21/21	0.96	0.15	40,49,59,60	0
2	2AN	c	206	21/21	0.96	0.13	30,44,58,62	0
2	2AN	N	202	21/21	0.96	0.14	37,52,61,64	0

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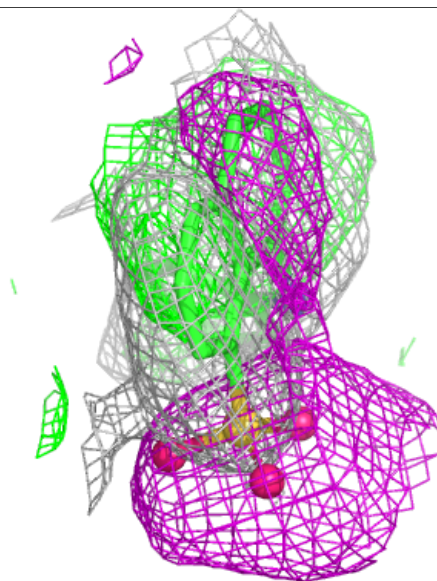
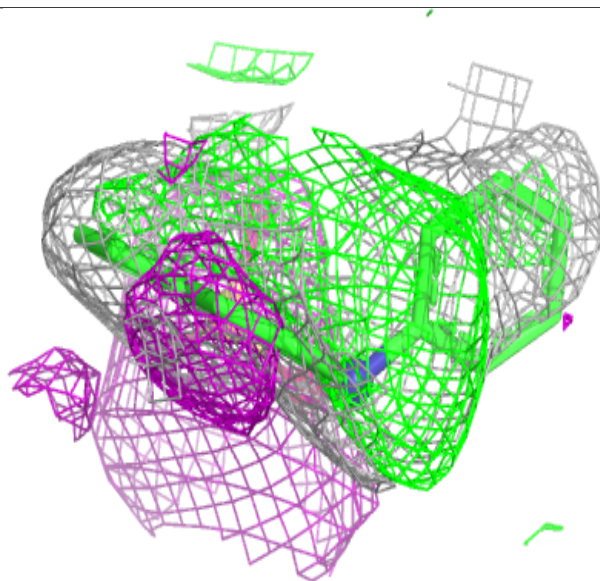
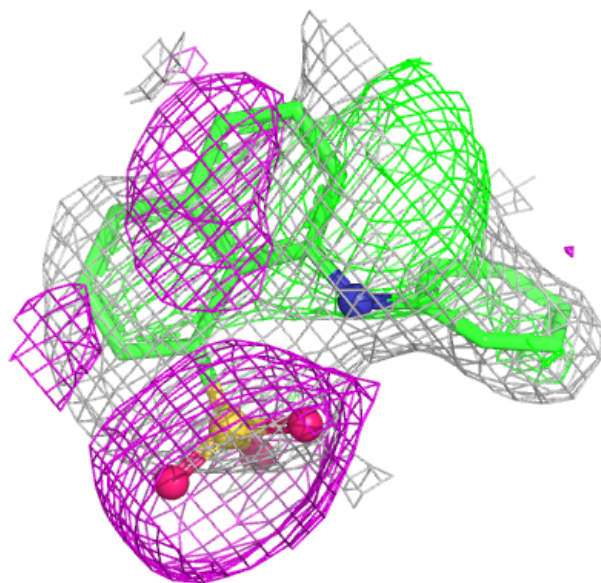
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	2AN	j	202	21/21	0.96	0.11	26,40,57,58	0
2	2AN	L	201	21/21	0.96	0.13	37,47,56,57	0
2	2AN	Q	201	21/21	0.96	0.12	40,50,60,67	0
2	2AN	f	201	21/21	0.96	0.12	34,40,48,49	0
2	2AN	P	201	21/21	0.96	0.10	38,50,59,61	0
2	2AN	c	201	21/21	0.96	0.12	35,45,58,59	0
2	2AN	M	202	21/21	0.97	0.10	38,48,54,56	0
2	2AN	I	201	21/21	0.97	0.11	28,39,57,62	0
2	2AN	j	203	21/21	0.97	0.11	32,40,49,58	0
3	SO4	E	205	5/5	0.97	0.12	34,41,51,56	5
2	2AN	R	201	21/21	0.98	0.10	29,52,60,61	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.

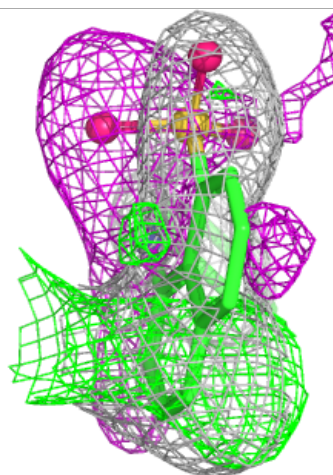
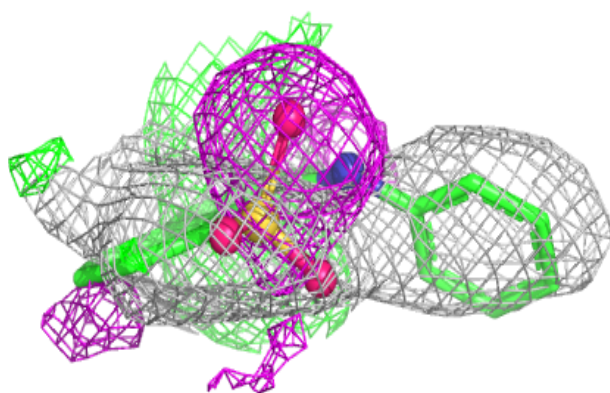
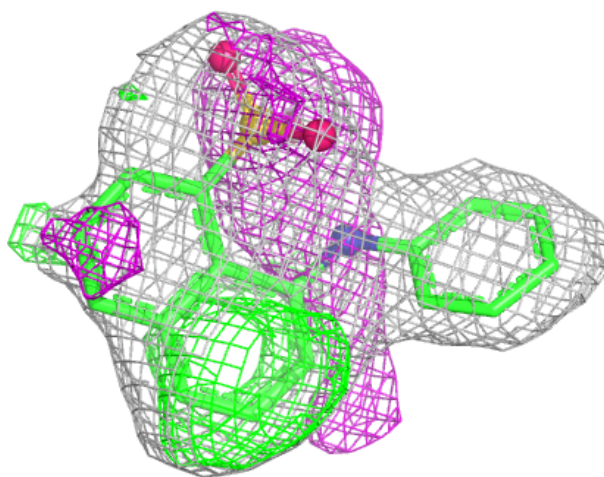
Electron density around 2AN N 203:

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



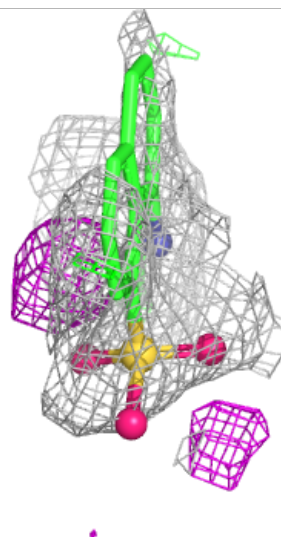
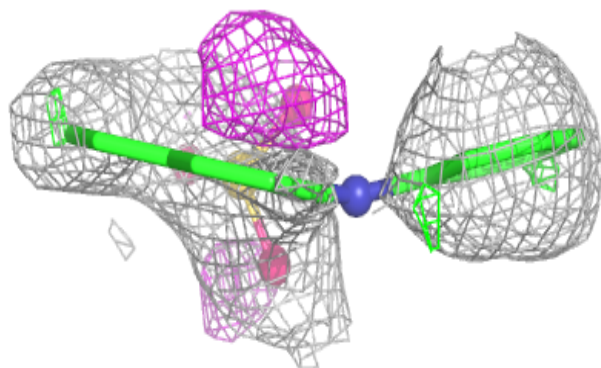
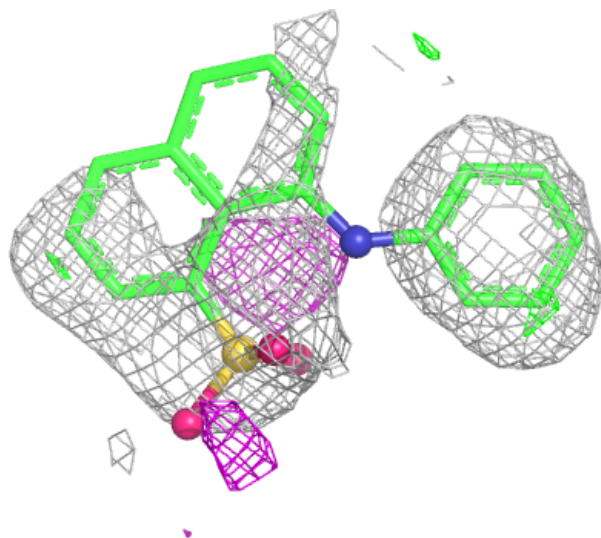
Electron density around 2AN f 203:

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



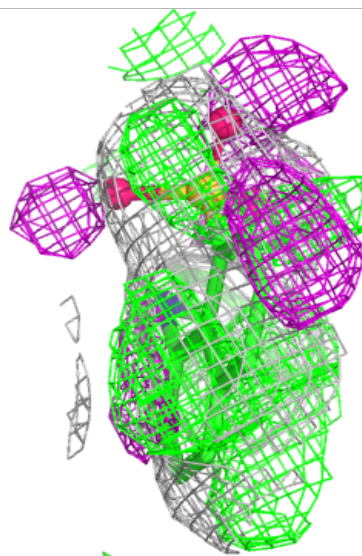
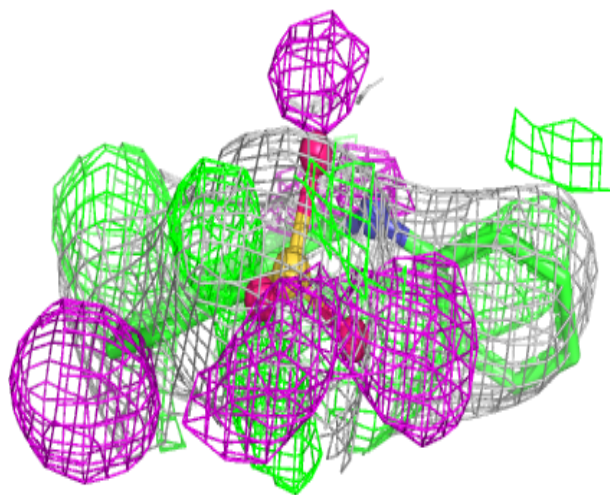
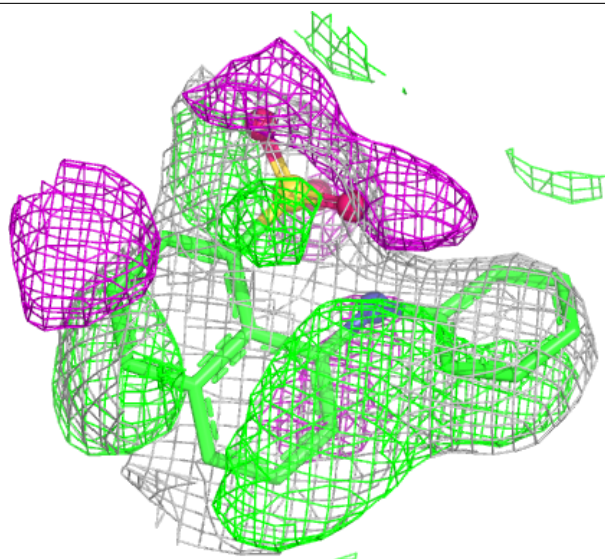
Electron density around 2AN j 207:

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



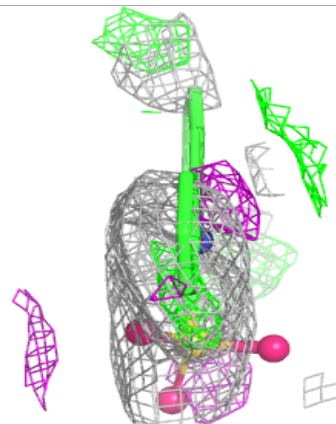
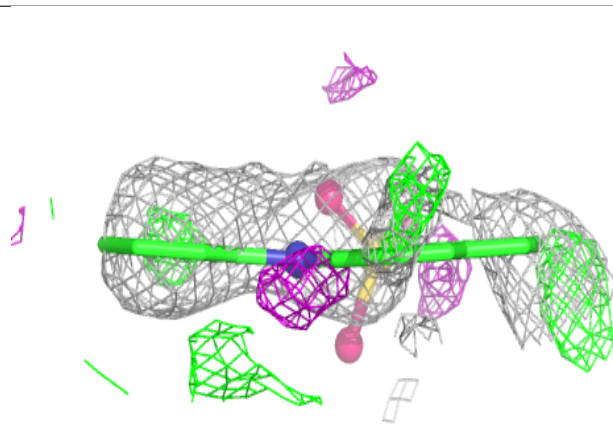
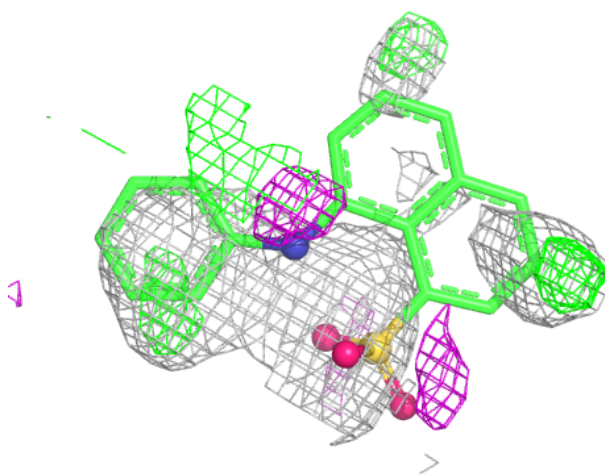
Electron density around 2AN X 203:

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



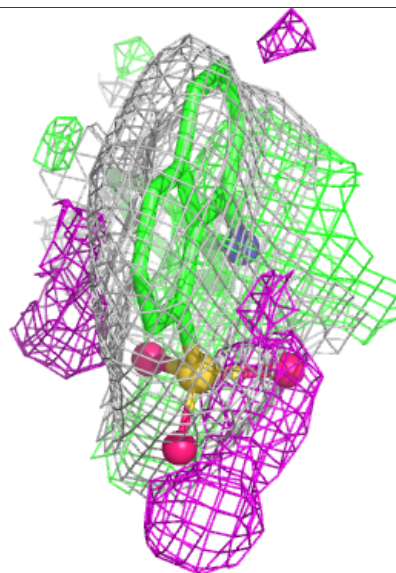
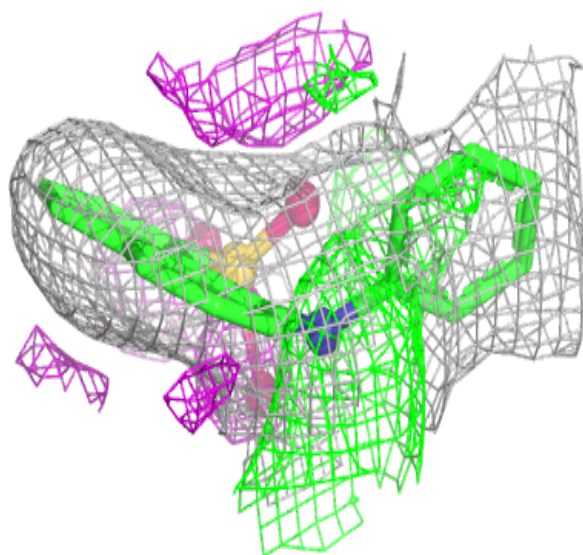
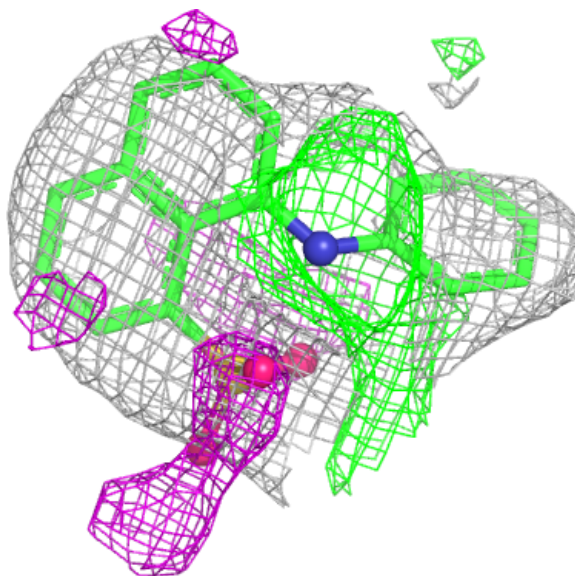
Electron density around 2AN h 205:

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



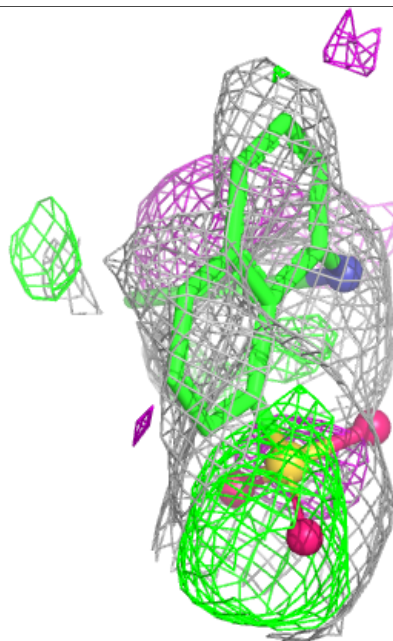
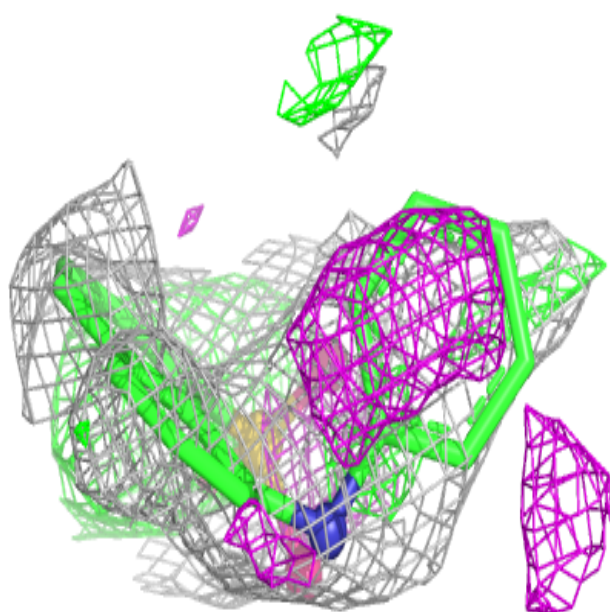
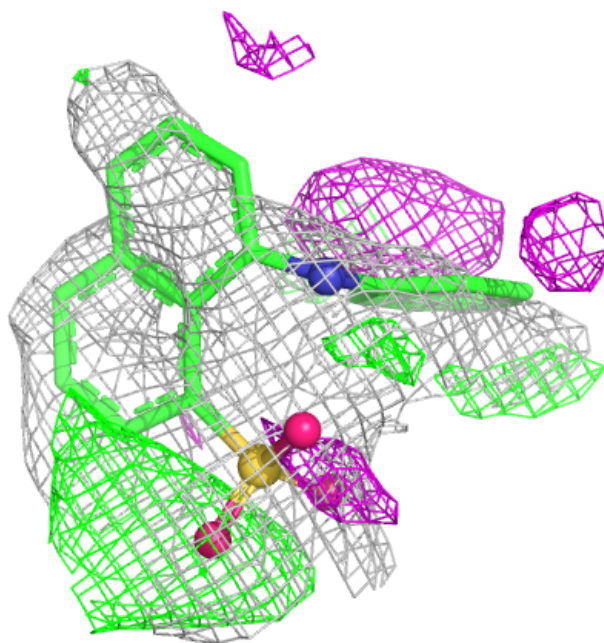
Electron density around 2AN d 203:

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



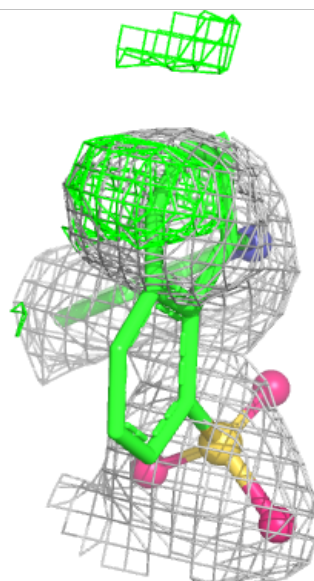
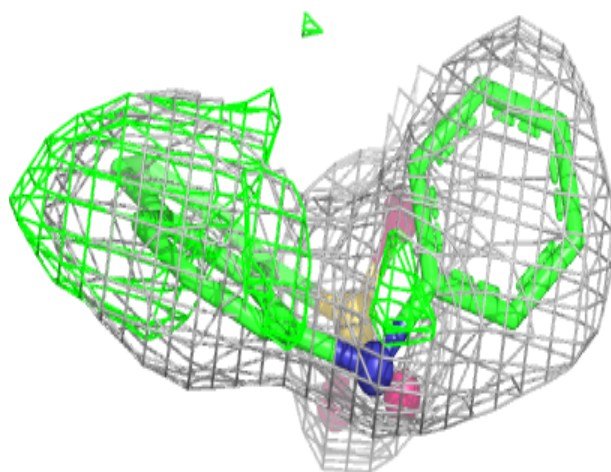
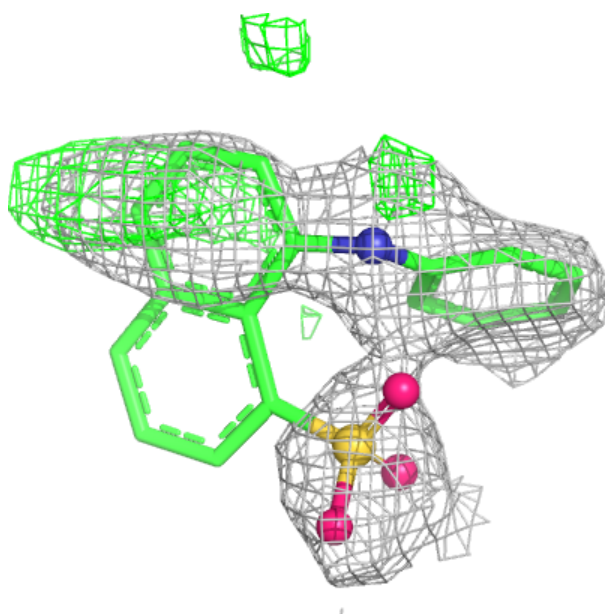
Electron density around 2AN D 204:

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



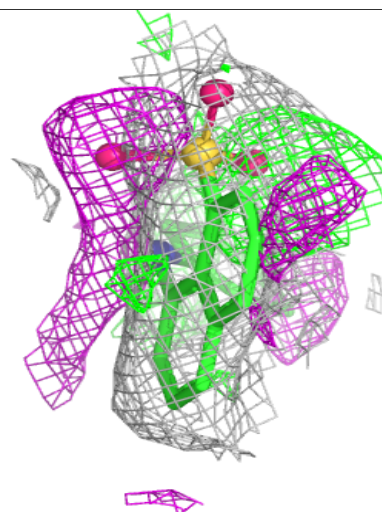
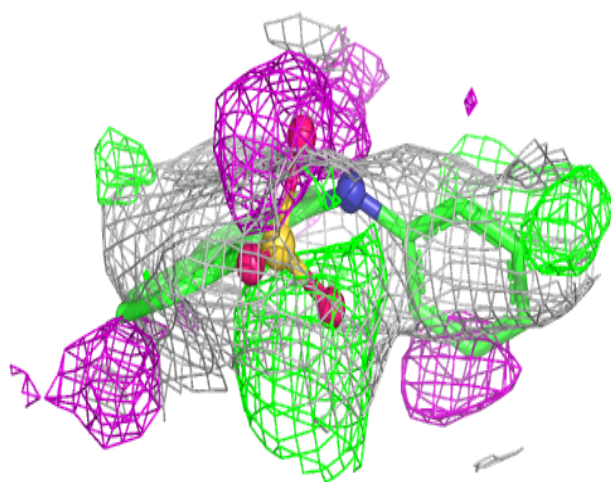
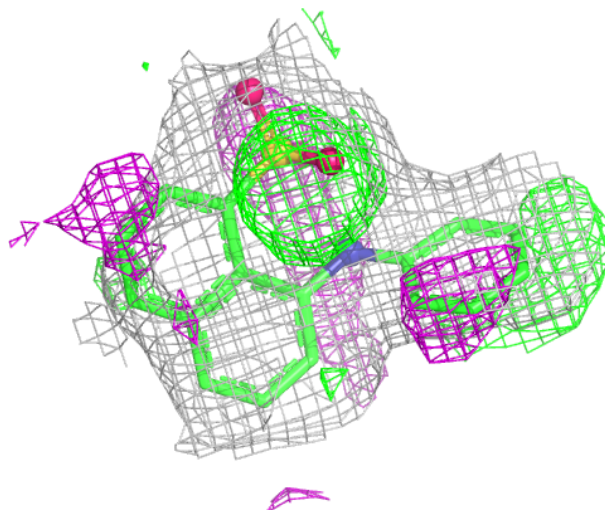
Electron density around 2AN b 206:

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



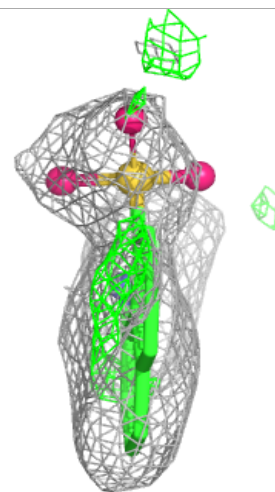
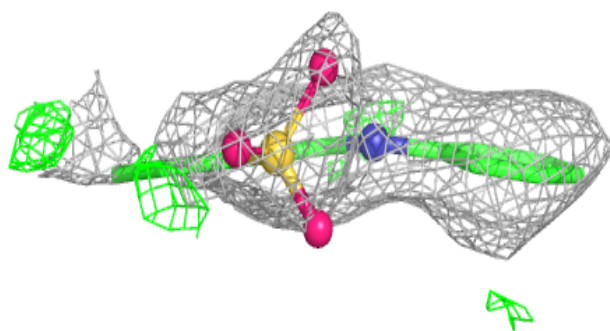
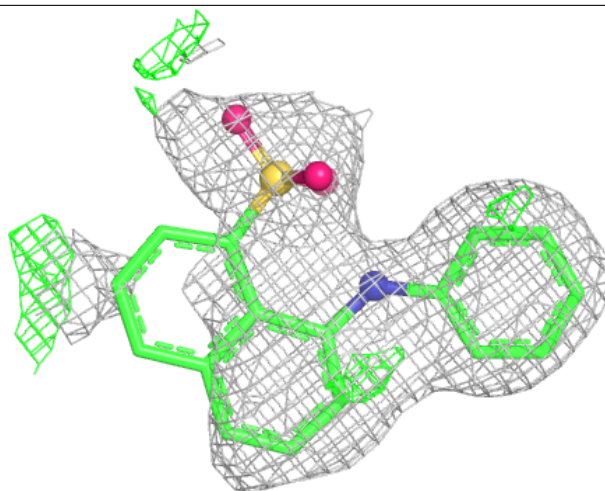
Electron density around 2AN X 206:

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



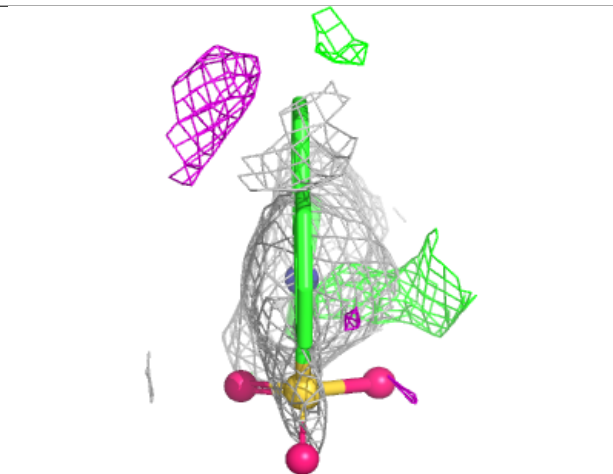
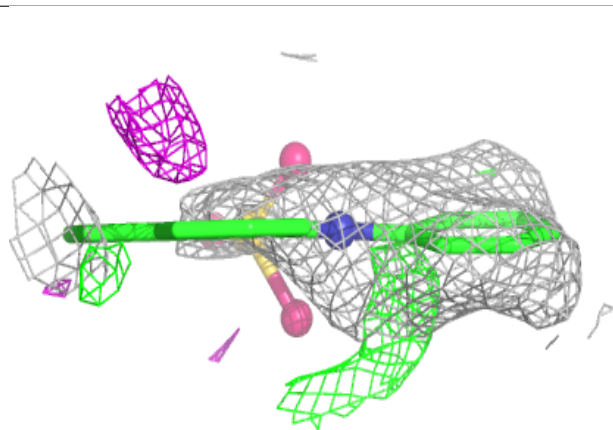
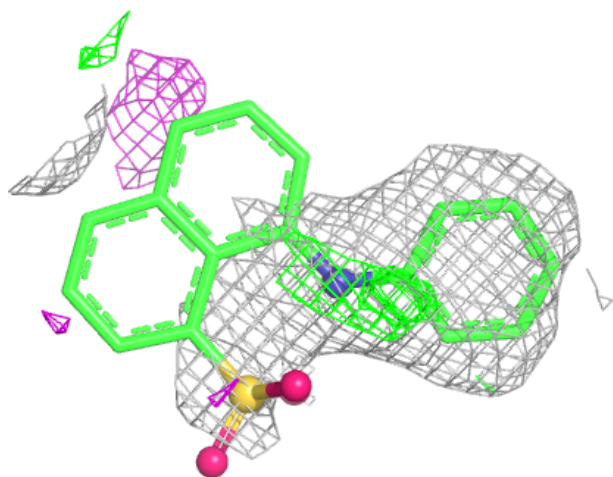
Electron density around 2AN G 207:

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



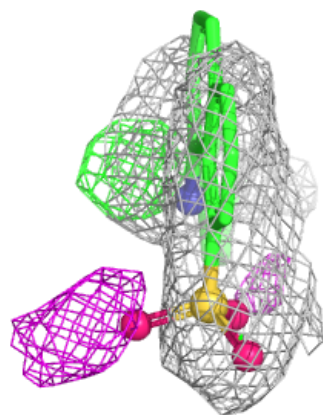
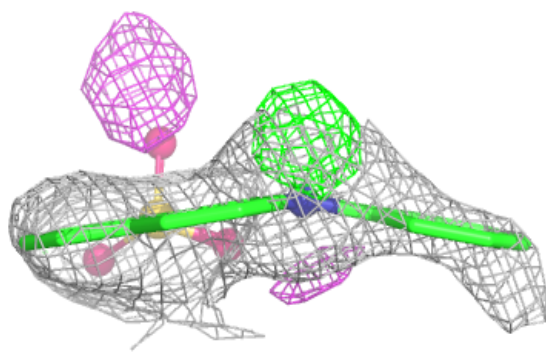
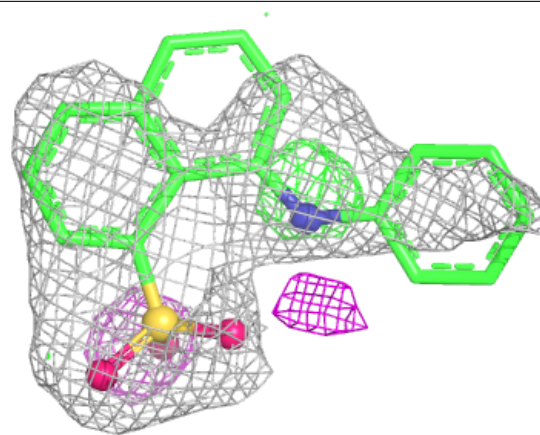
Electron density around 2AN a 204:

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



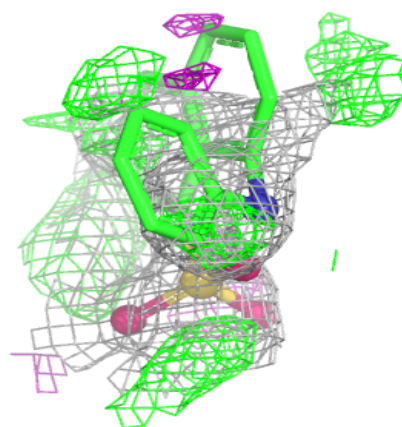
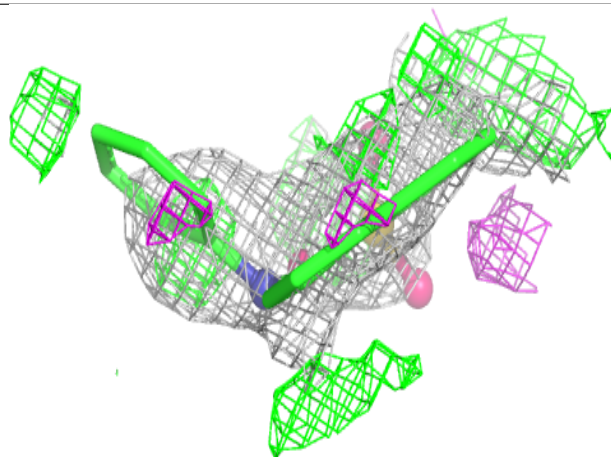
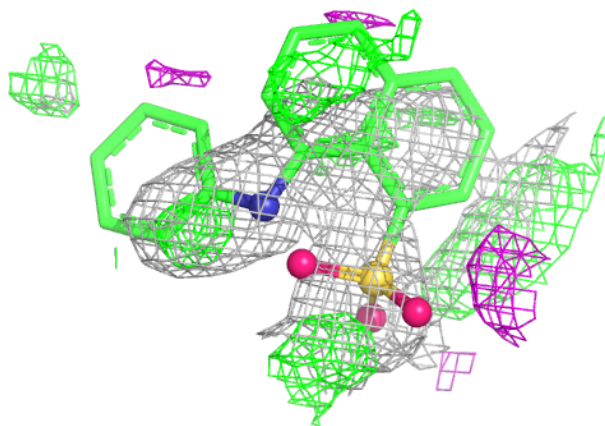
Electron density around 2AN I 207:

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



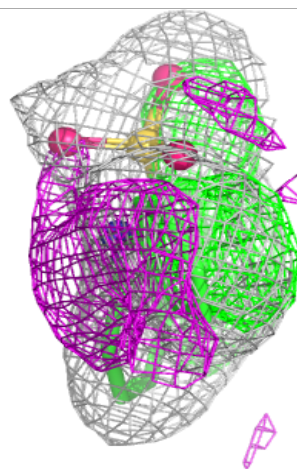
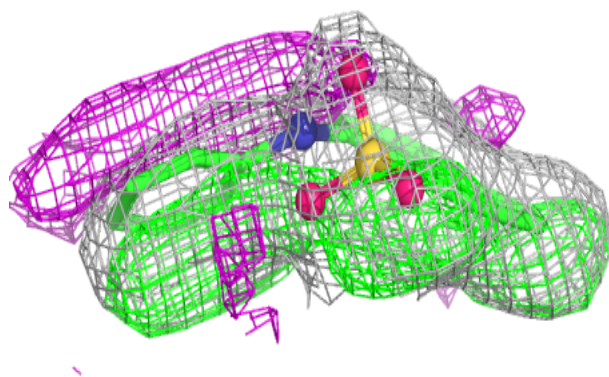
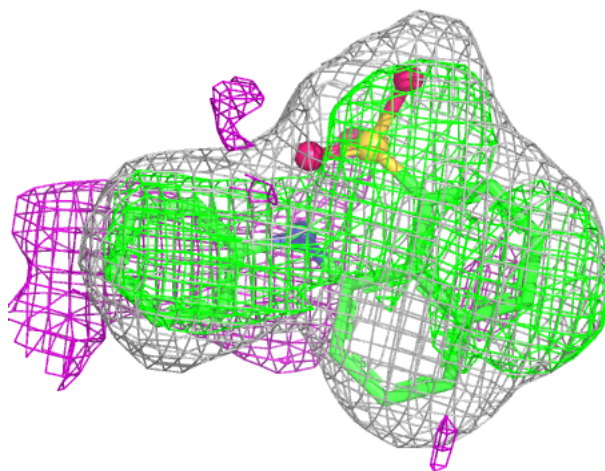
Electron density around 2AN S 204:

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



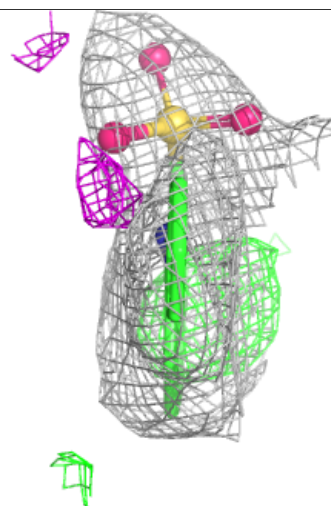
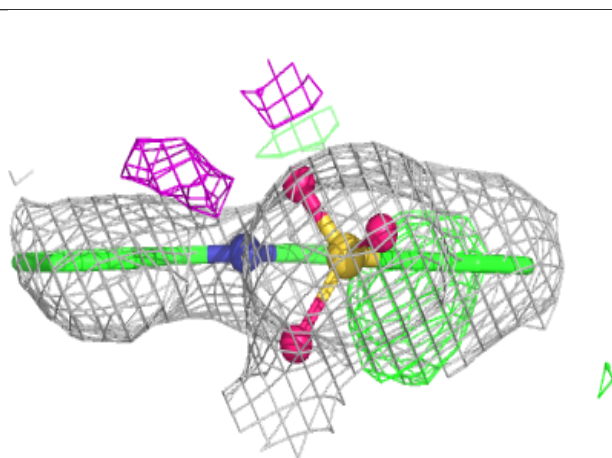
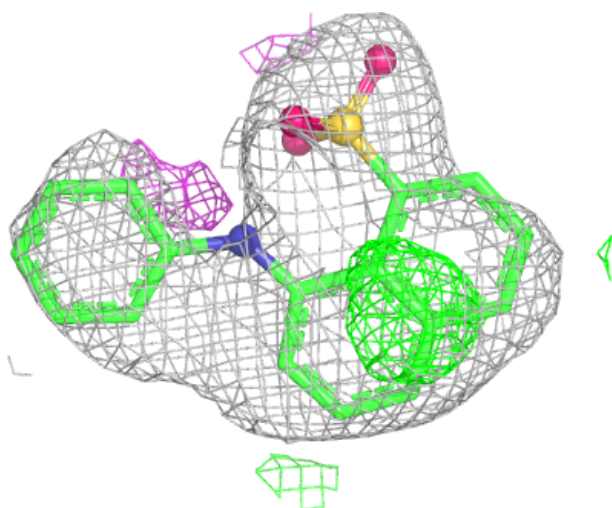
Electron density around 2AN j 205:

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



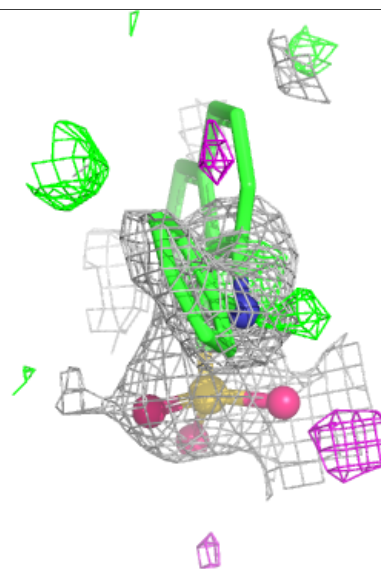
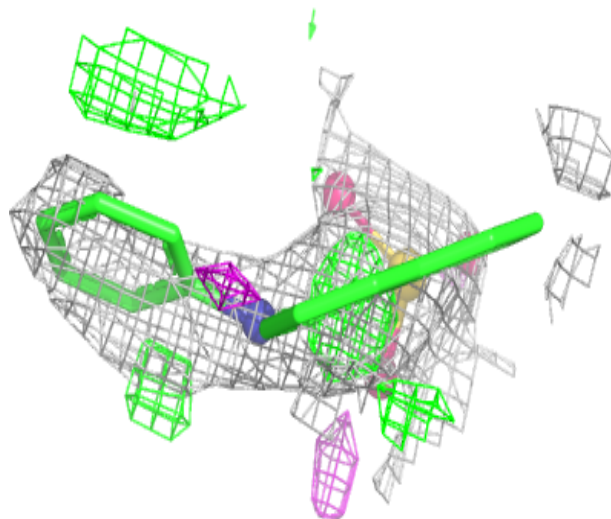
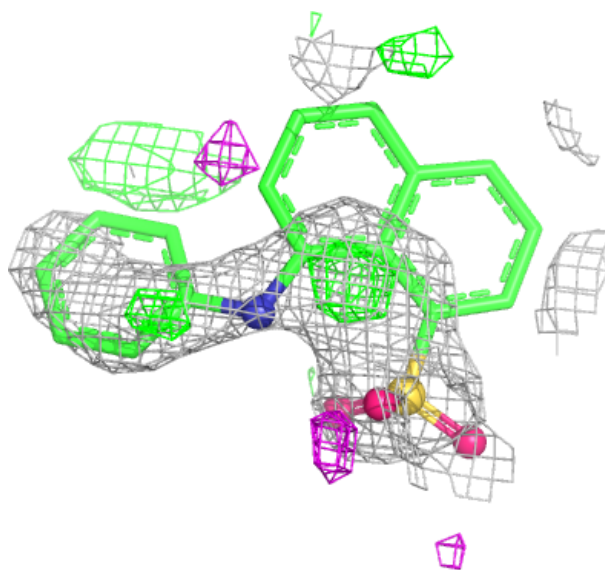
Electron density around 2AN R 205:

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



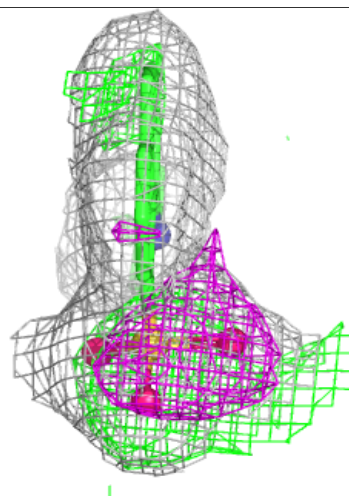
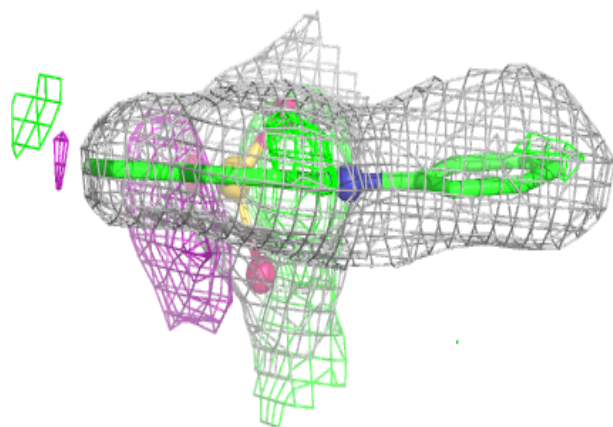
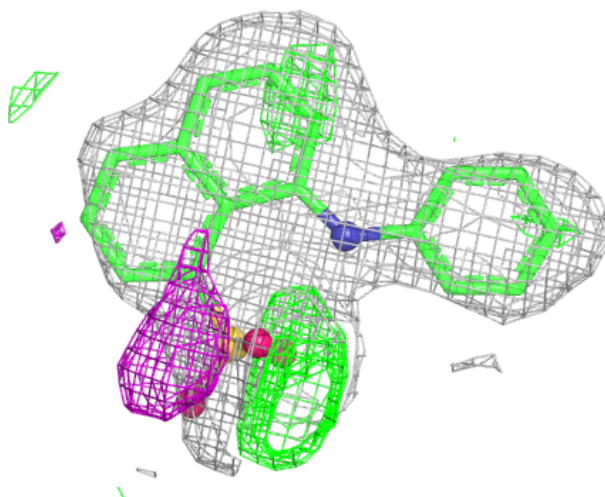
Electron density around 2AN d 204:

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



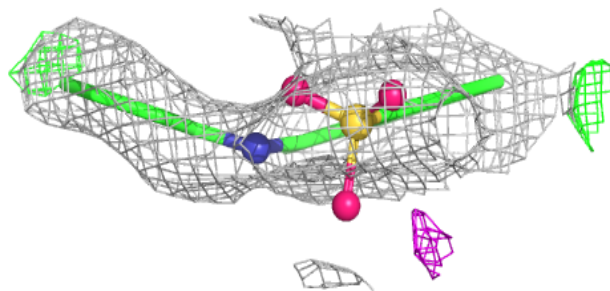
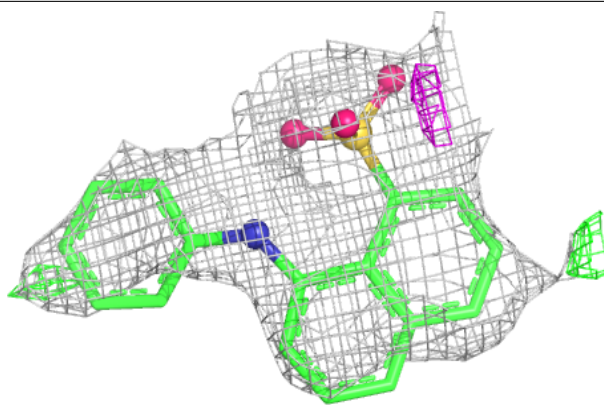
Electron density around 2AN c 202:

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



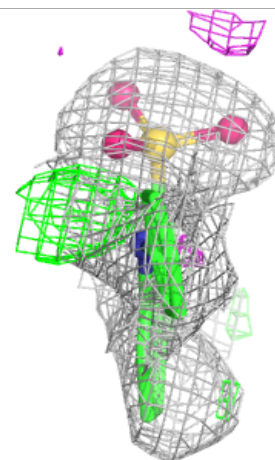
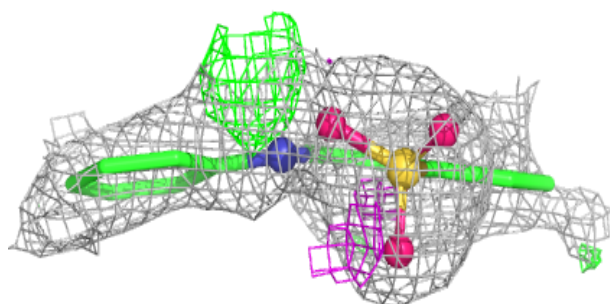
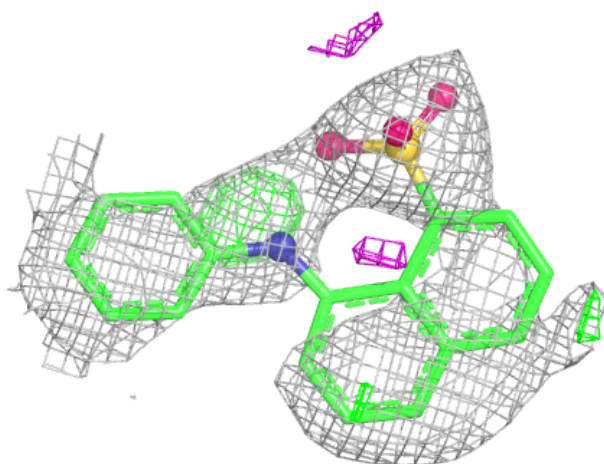
Electron density around 2AN b 205:

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



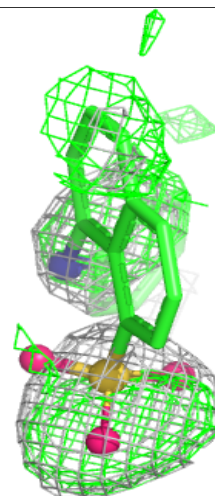
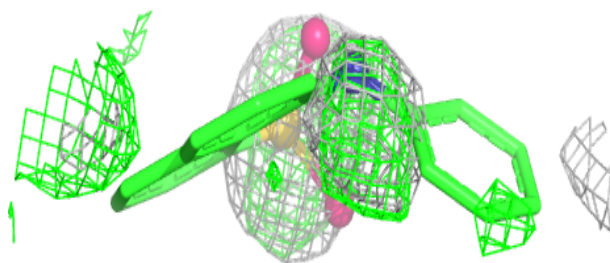
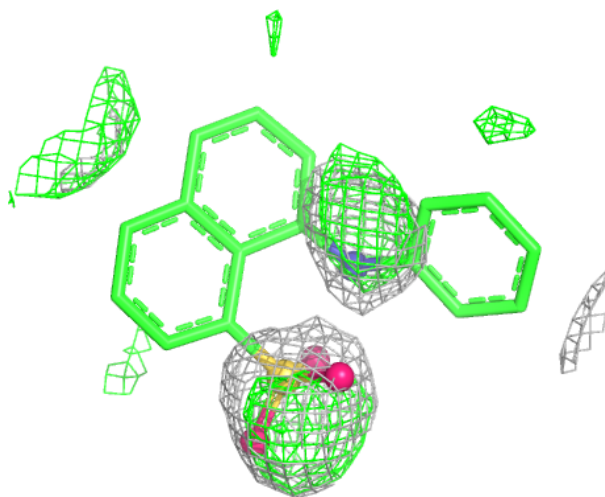
Electron density around 2AN I 205:

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



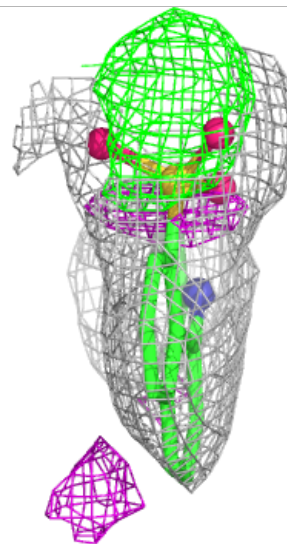
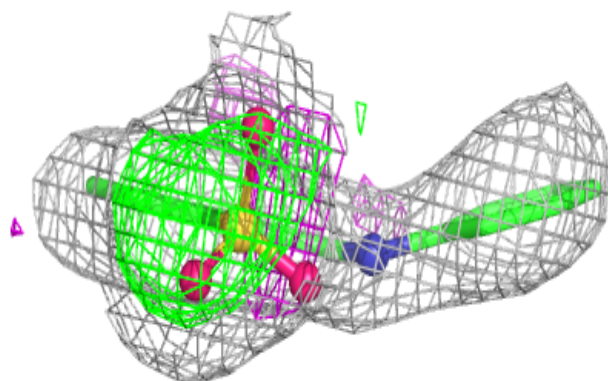
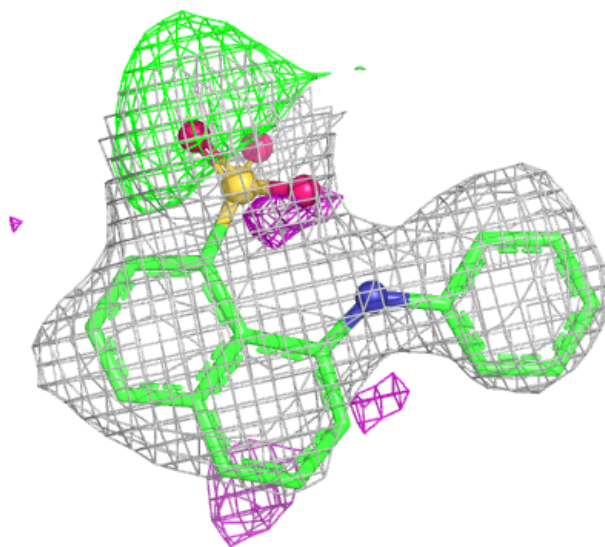
Electron density around 2AN A 204:

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



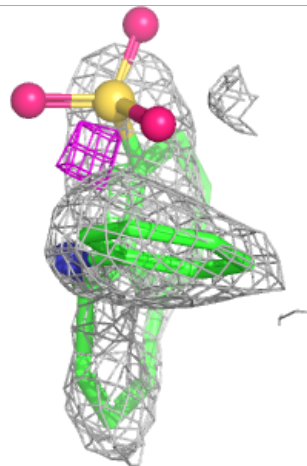
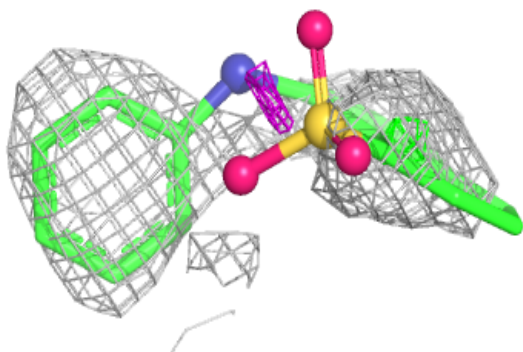
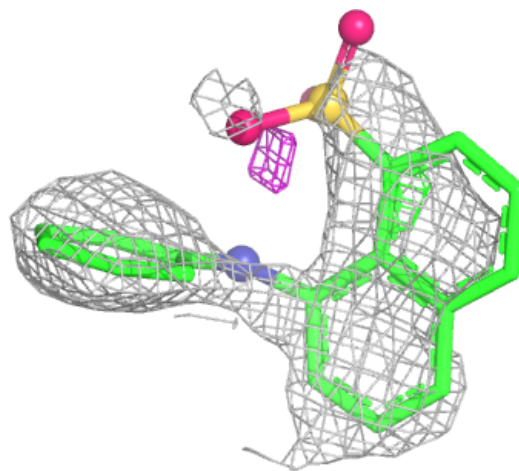
Electron density around 2AN R 204:

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



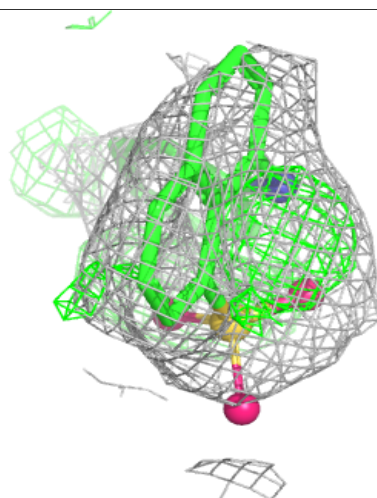
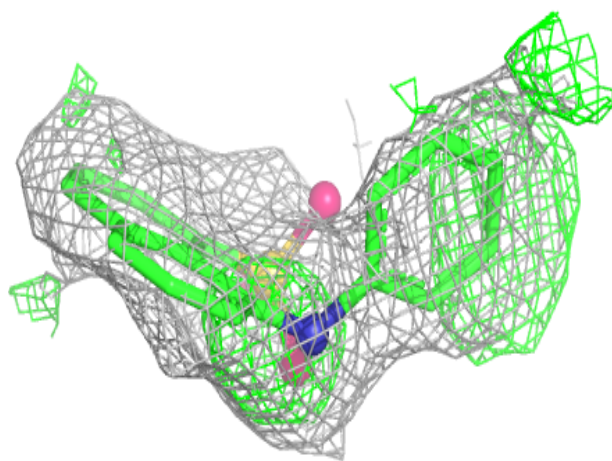
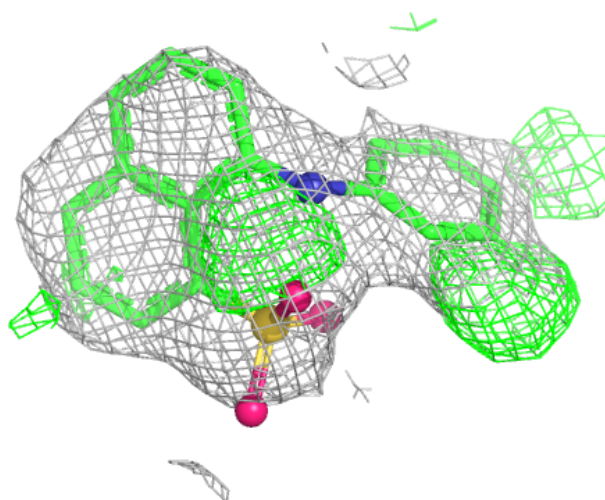
Electron density around 2AN F 206:

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



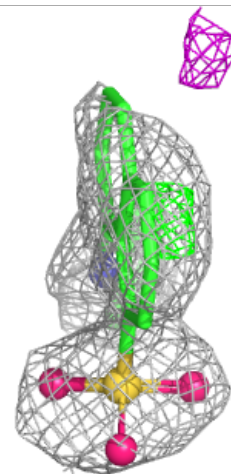
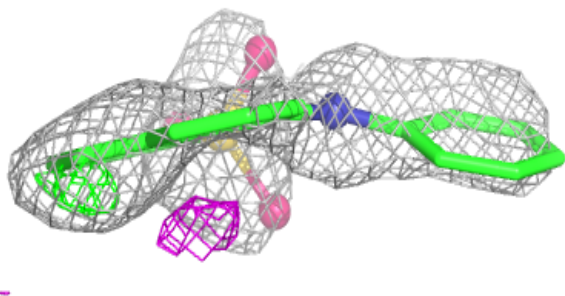
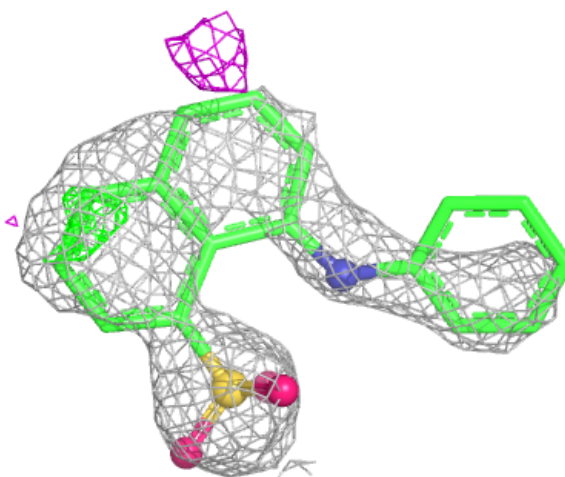
Electron density around 2AN Y 204:

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



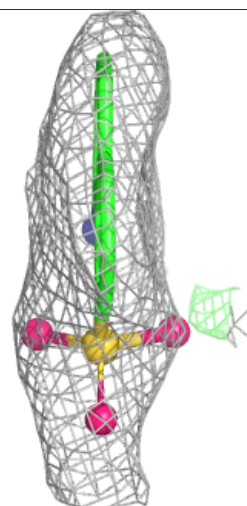
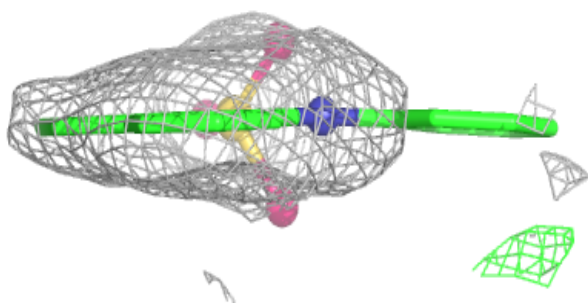
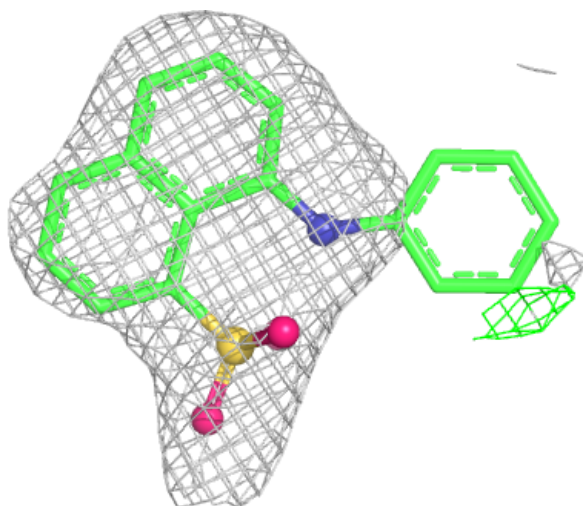
Electron density around 2AN I 204:

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



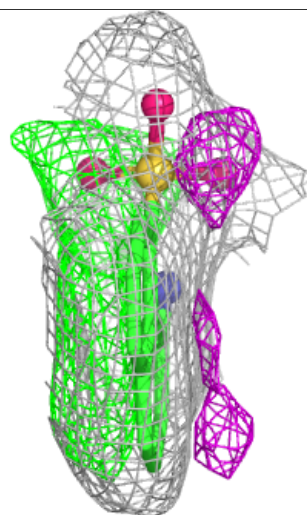
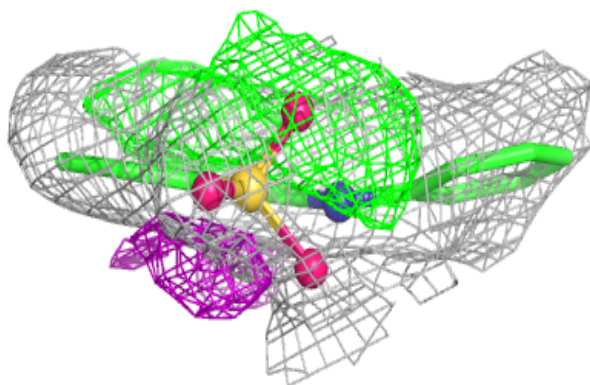
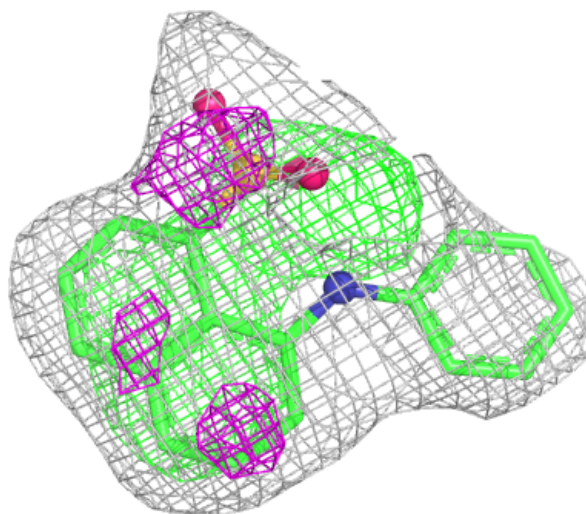
Electron density around 2AN G 204:

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



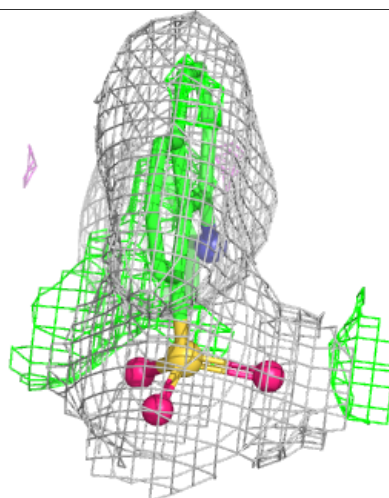
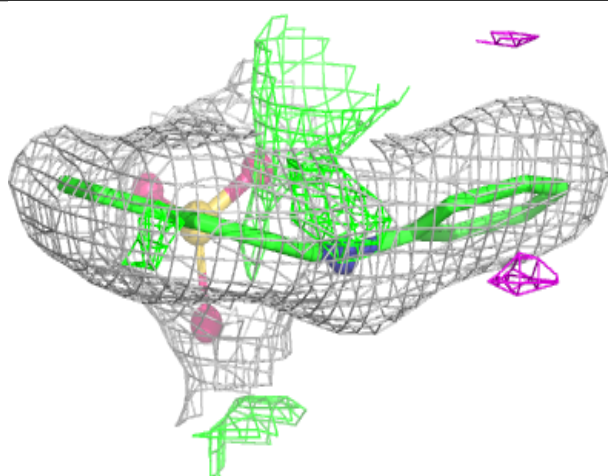
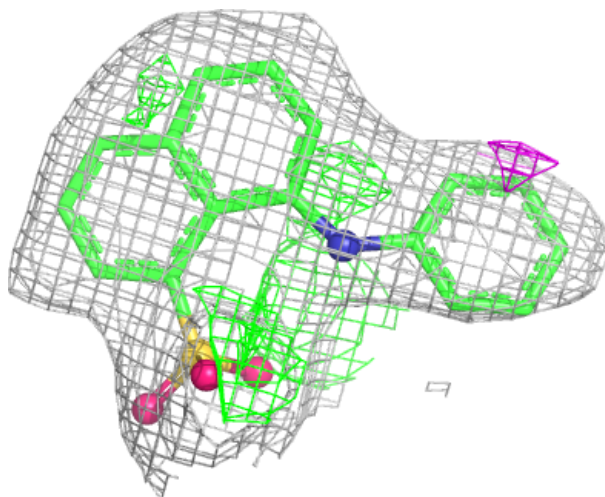
Electron density around 2AN T 203:

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



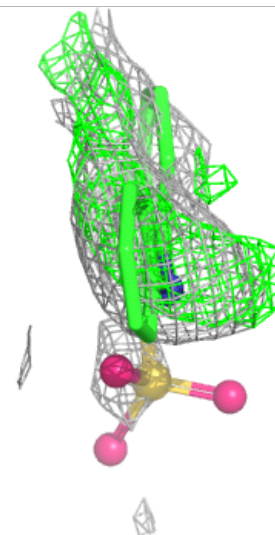
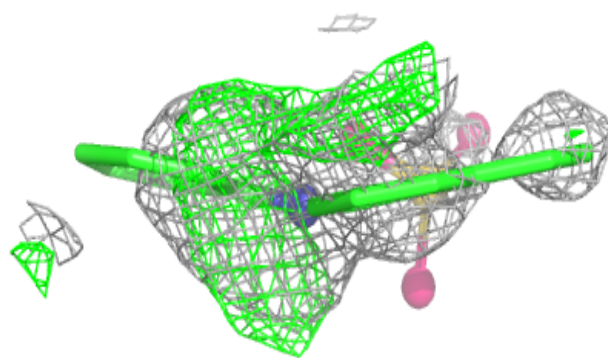
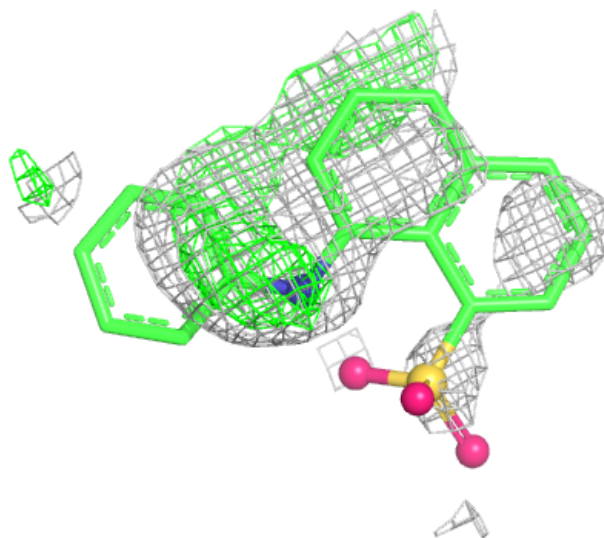
Electron density around 2AN Y 201:

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



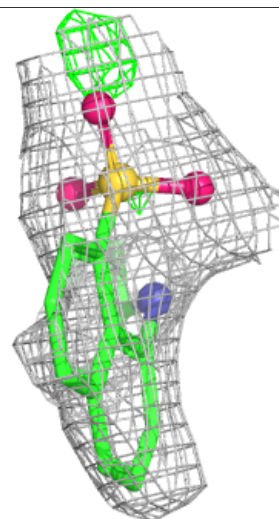
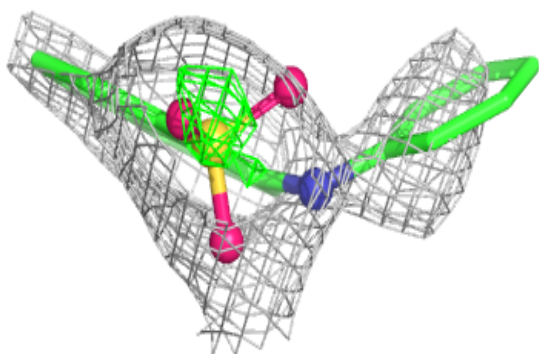
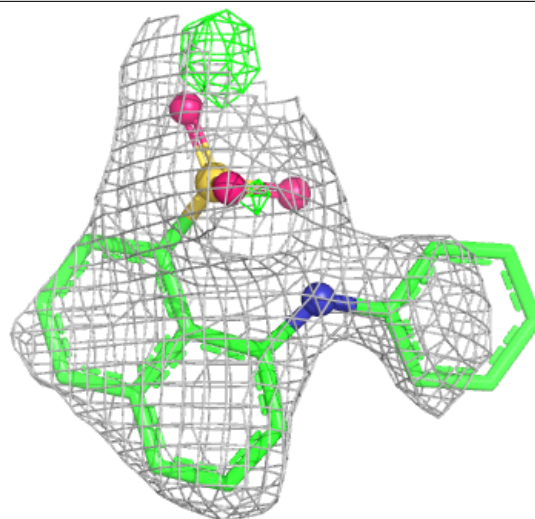
Electron density around 2AN U 202:

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



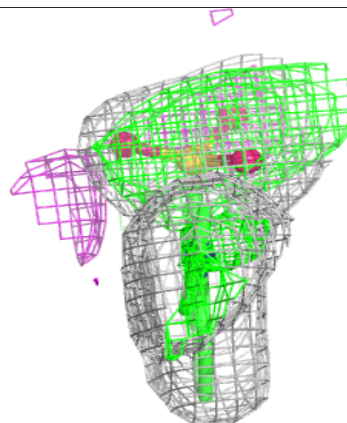
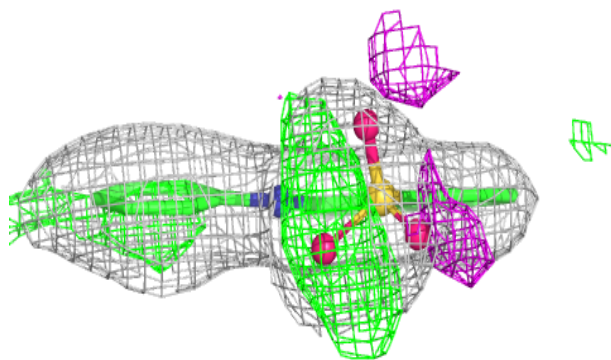
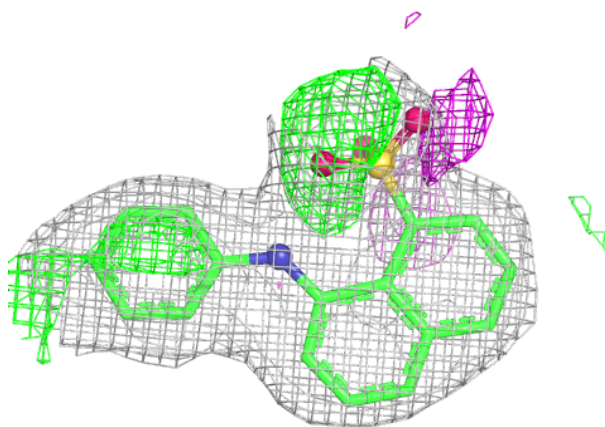
Electron density around 2AN f 206:

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



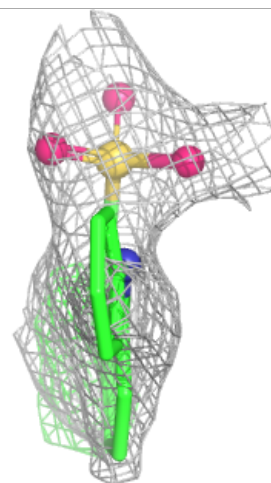
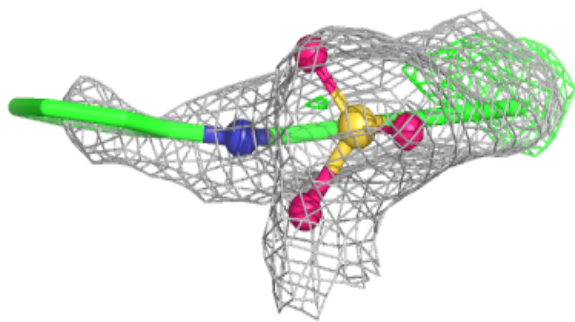
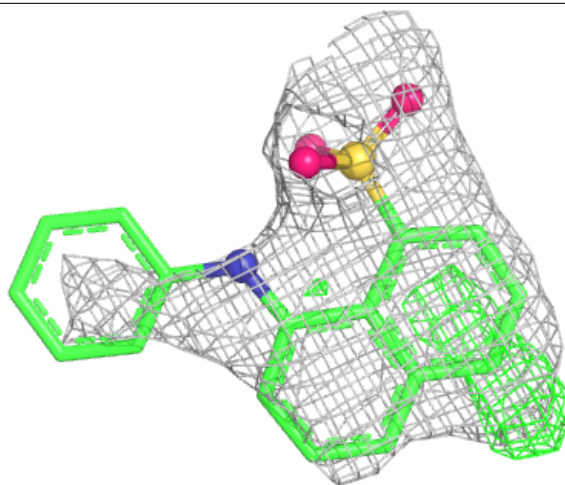
Electron density around 2AN T 204:

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



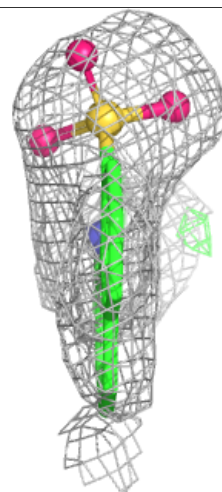
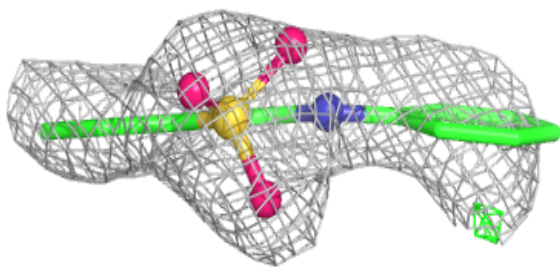
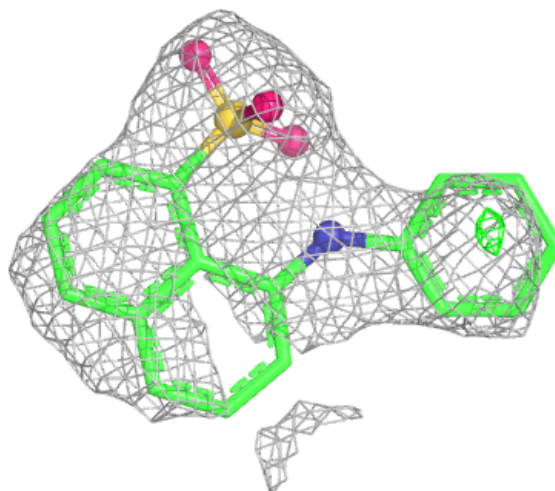
Electron density around 2AN S 203:

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



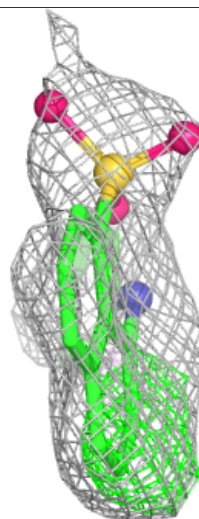
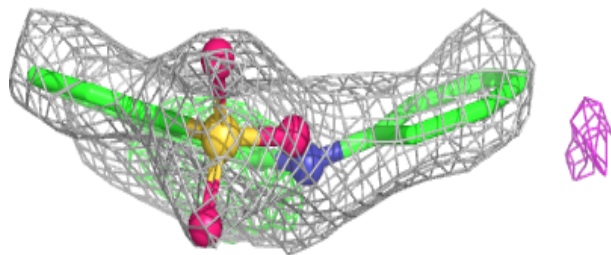
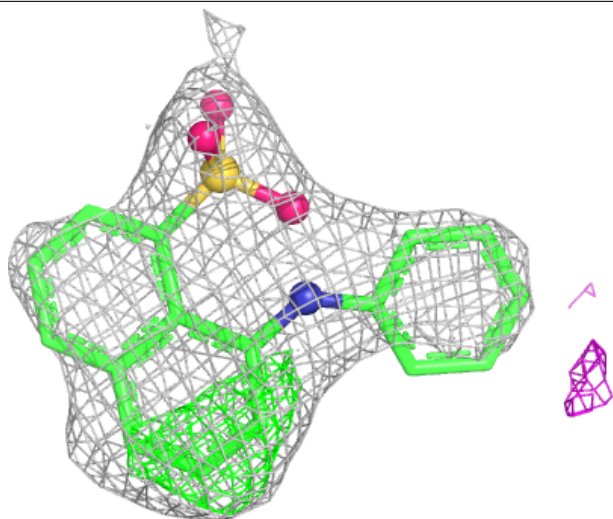
Electron density around 2AN H 204:

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



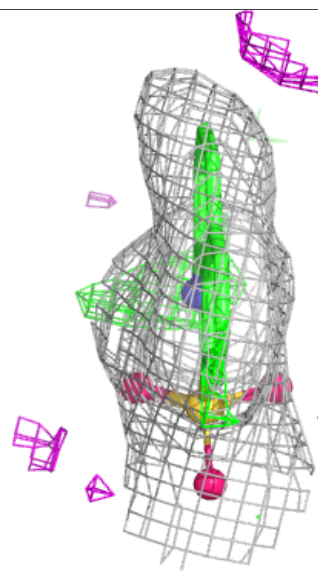
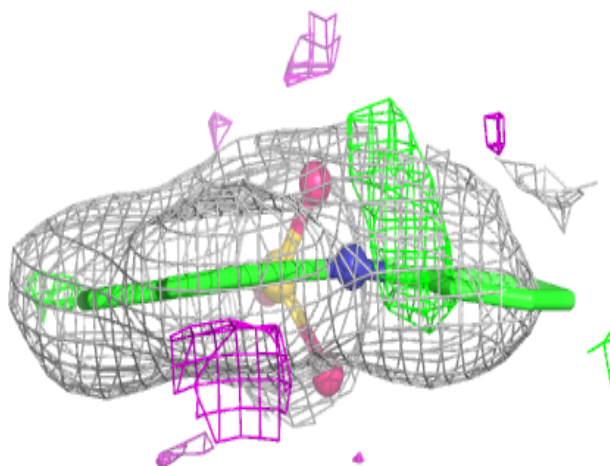
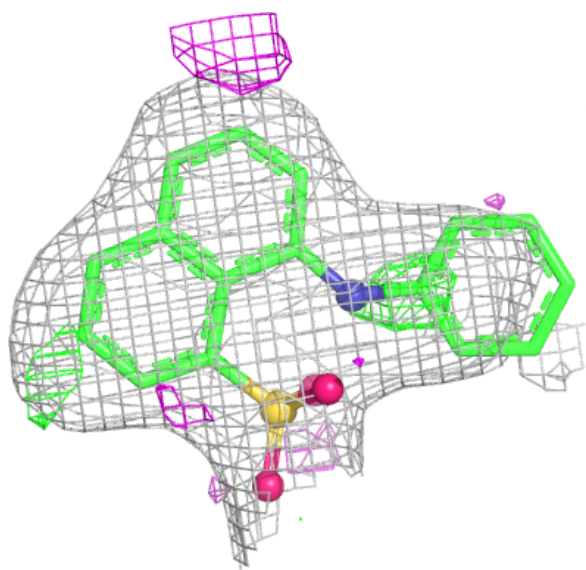
Electron density around 2AN G 205:

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



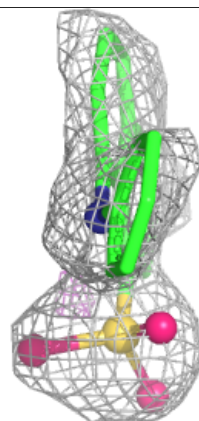
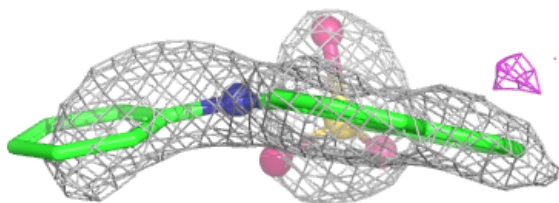
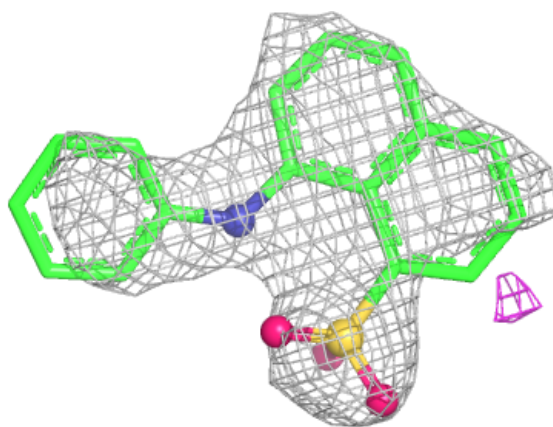
Electron density around 2AN j 206:

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



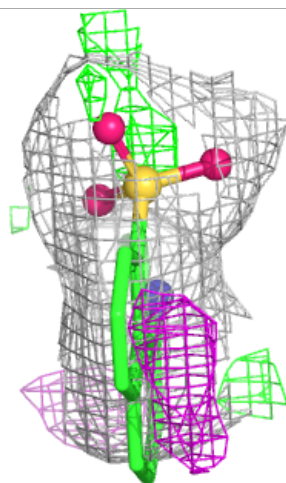
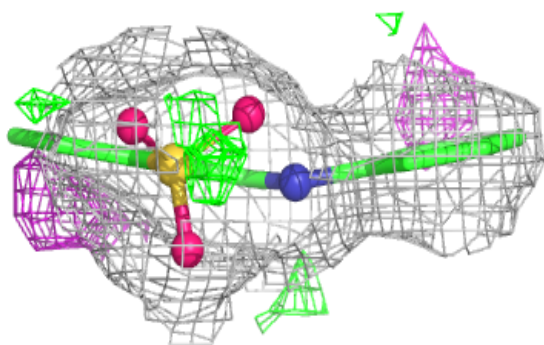
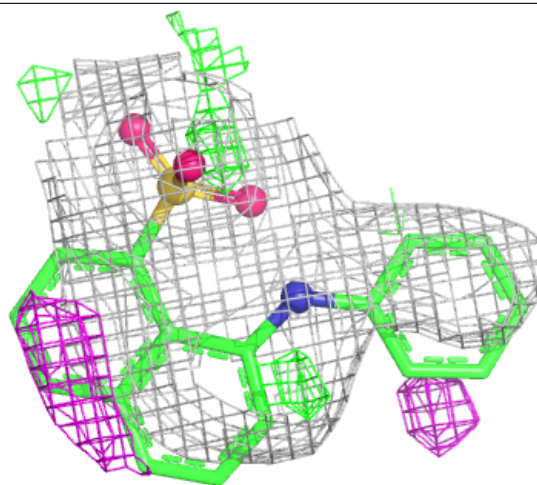
Electron density around 2AN I 203:

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



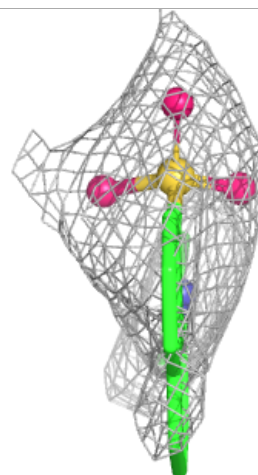
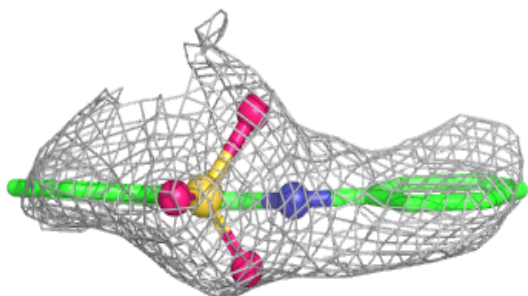
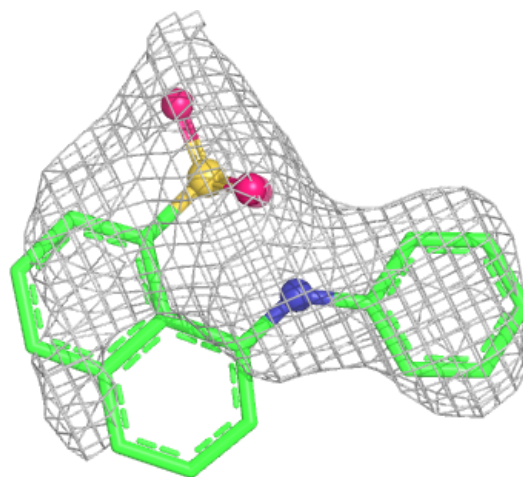
Electron density around 2AN F 204:

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



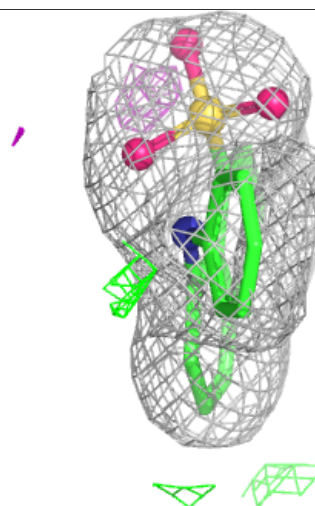
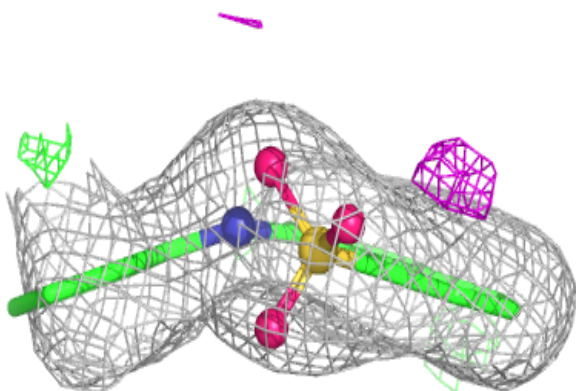
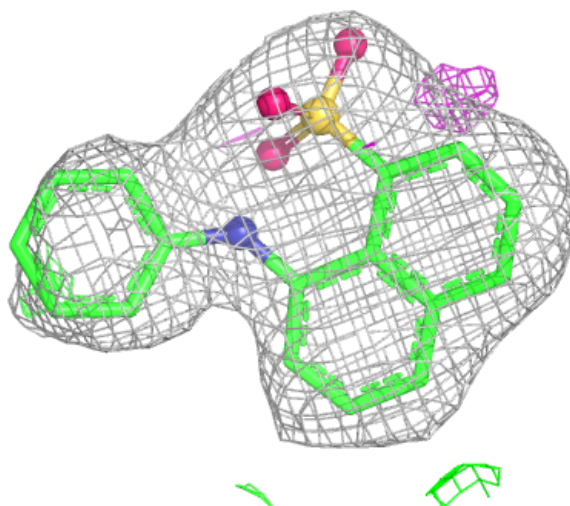
Electron density around 2AN O 202:

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



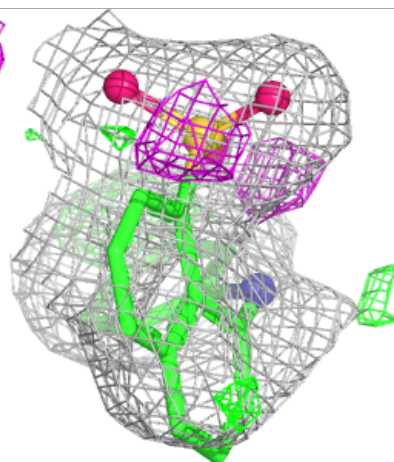
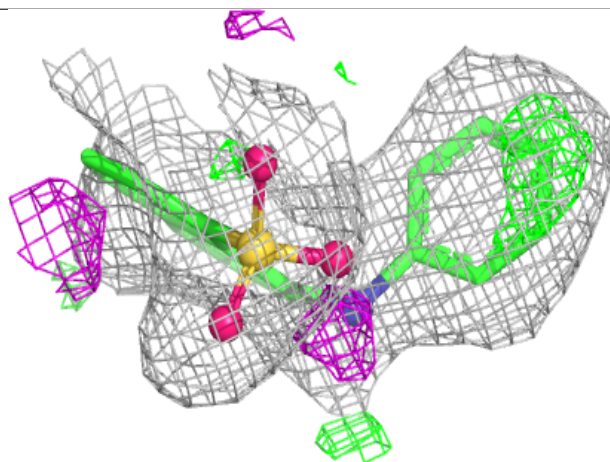
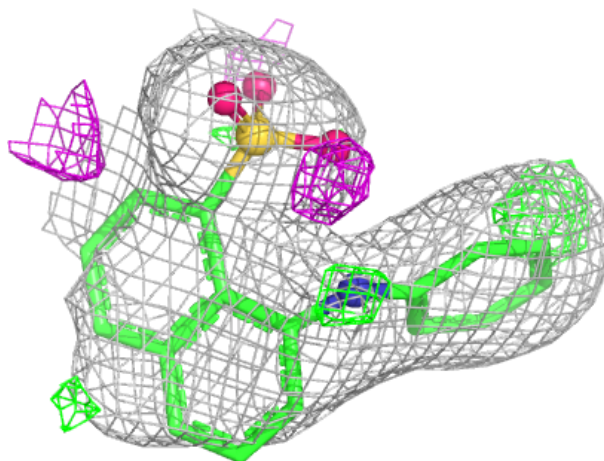
Electron density around 2AN c 203:

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



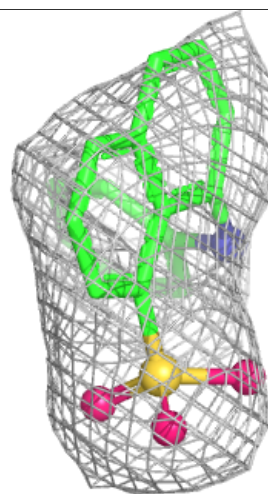
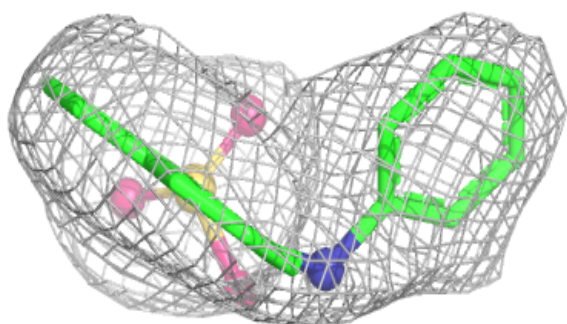
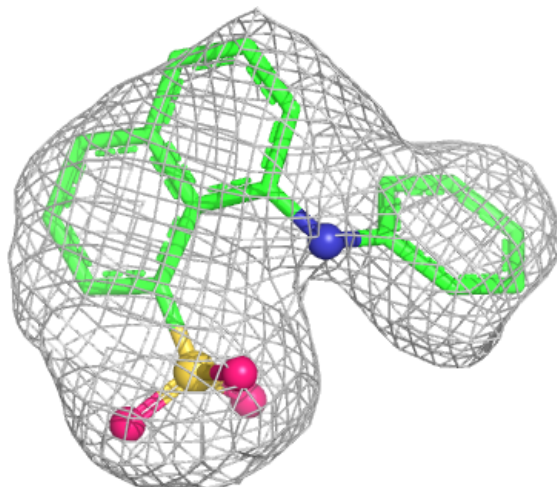
Electron density around 2AN F 202:

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



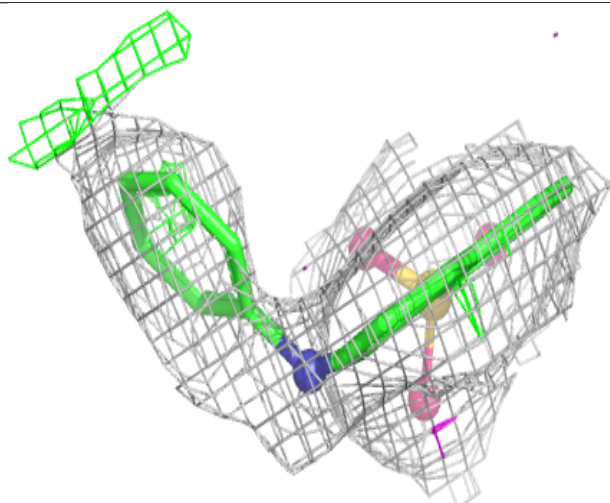
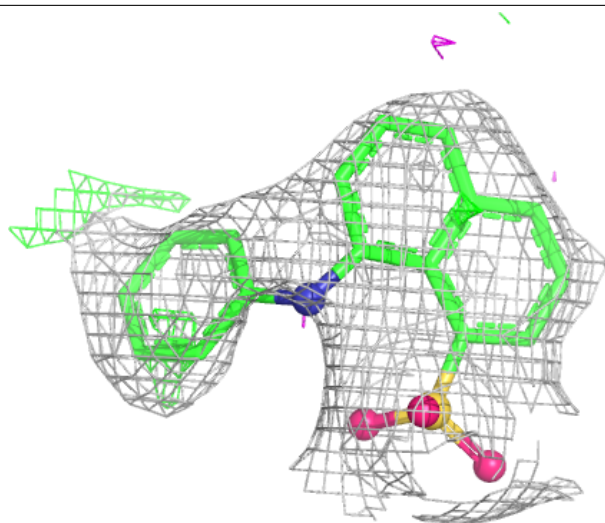
Electron density around 2AN S 201:

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



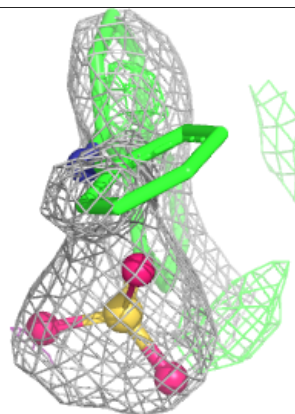
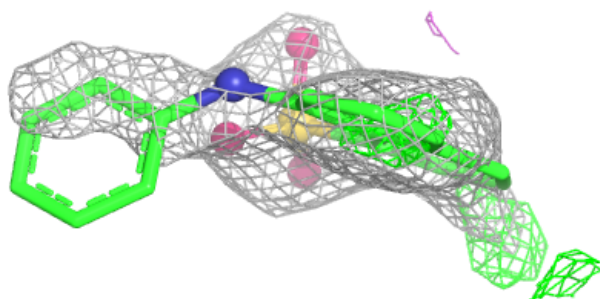
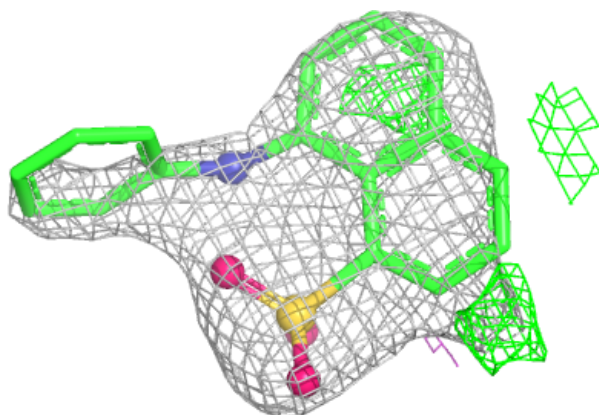
Electron density around 2AN a 201:

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



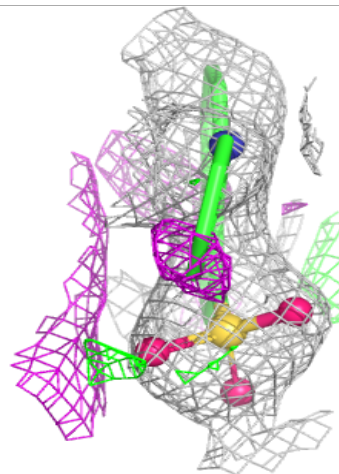
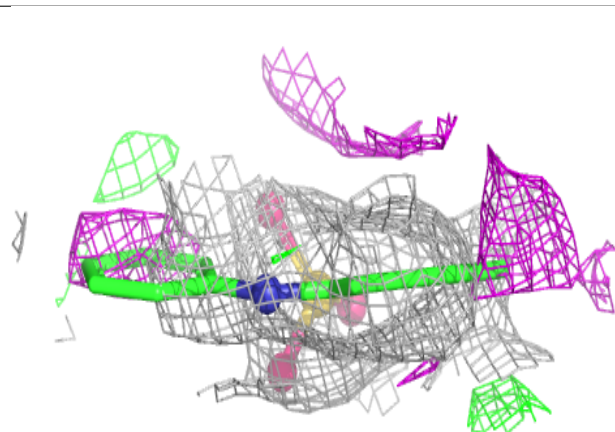
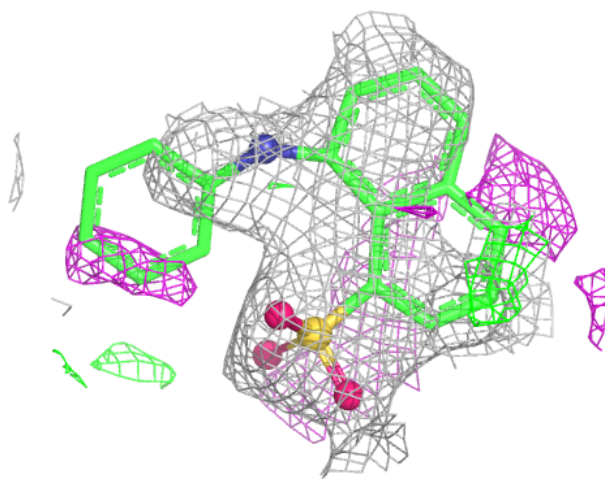
Electron density around 2AN C 203 (A):

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



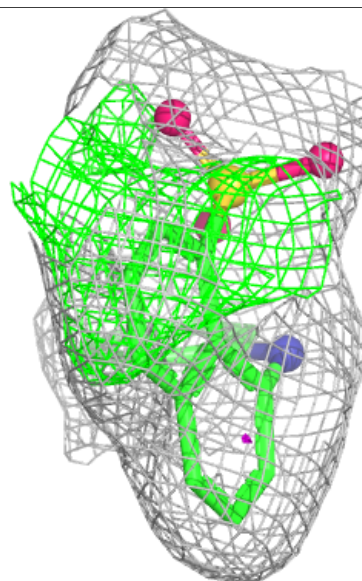
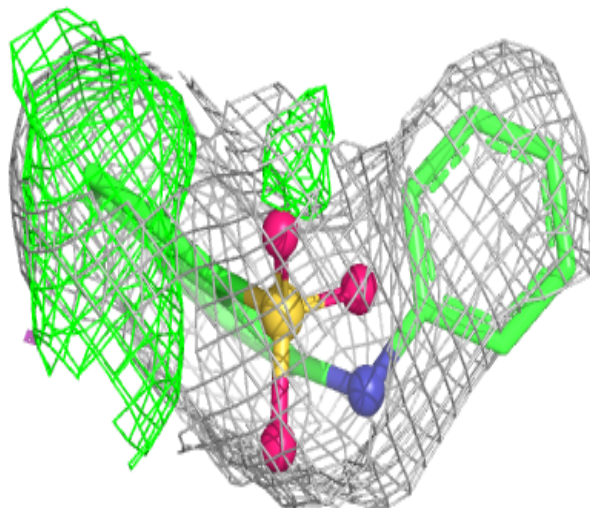
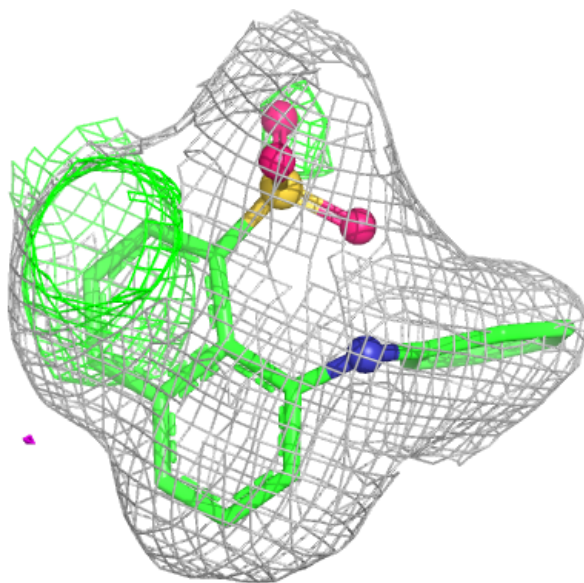
Electron density around 2AN V 208:

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



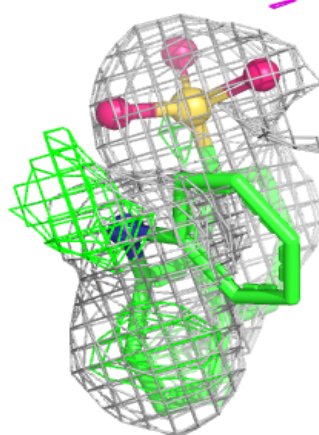
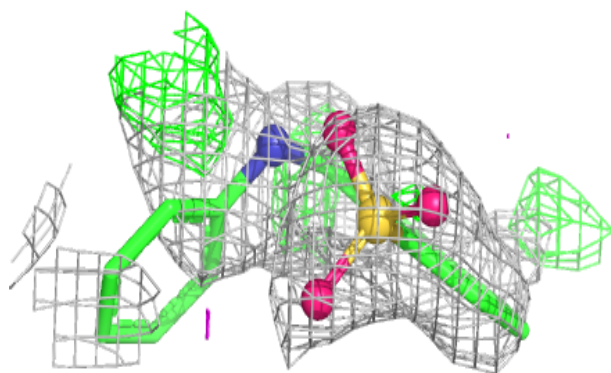
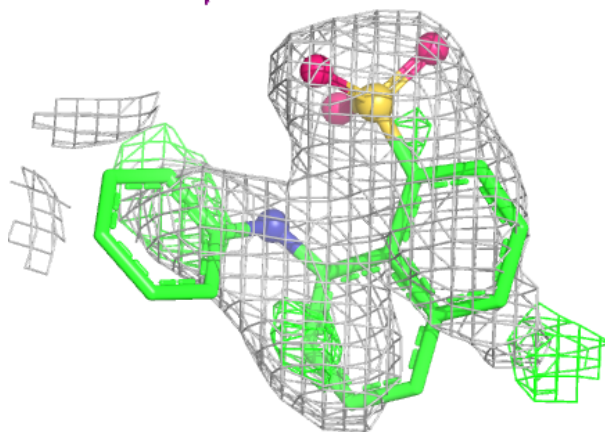
Electron density around 2AN Z 206:

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



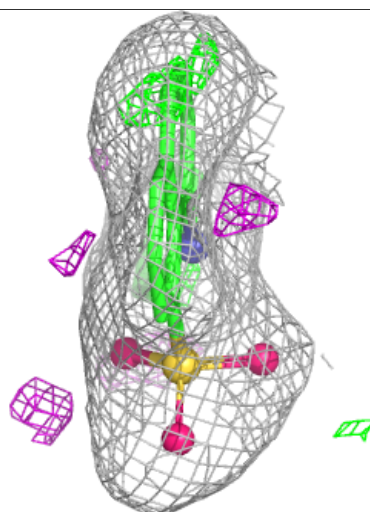
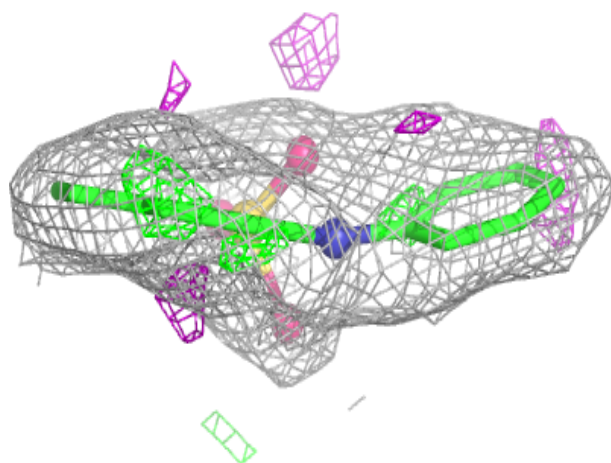
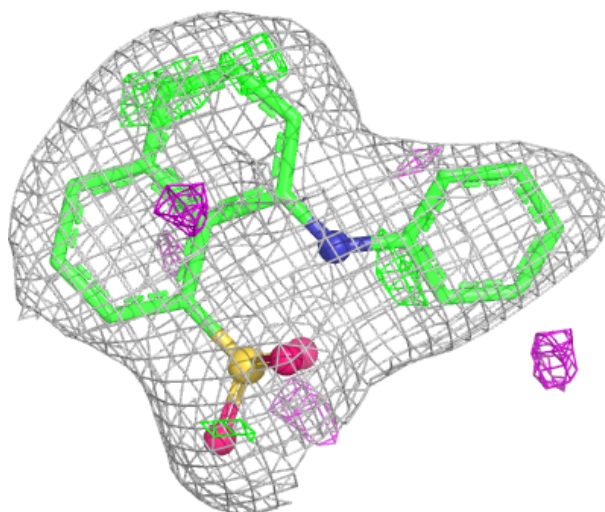
Electron density around 2AN E 204:

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



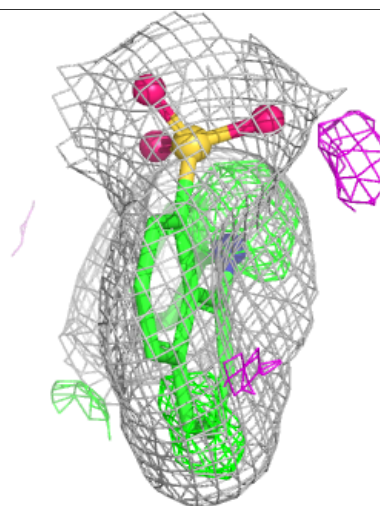
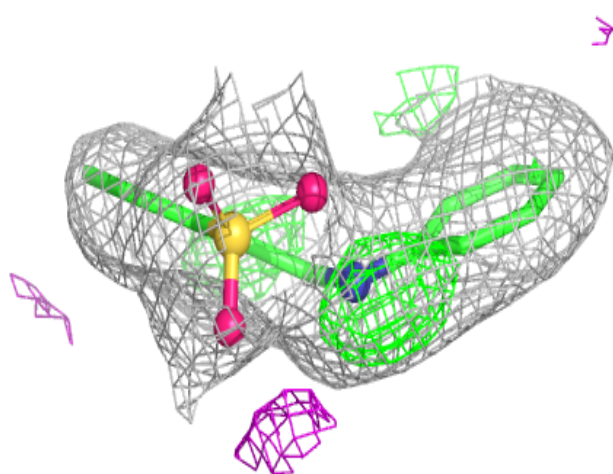
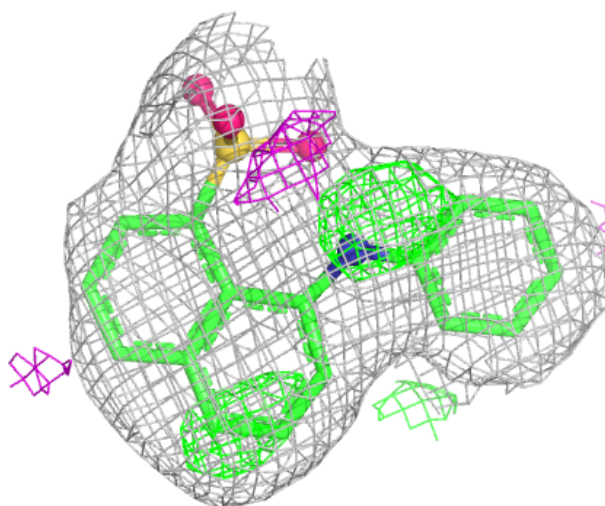
Electron density around 2AN N 205:

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



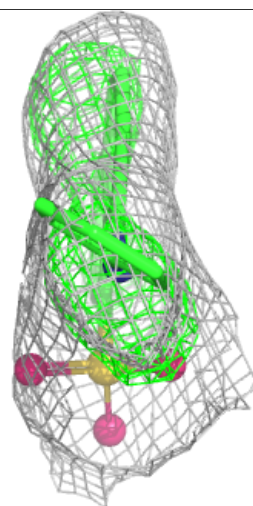
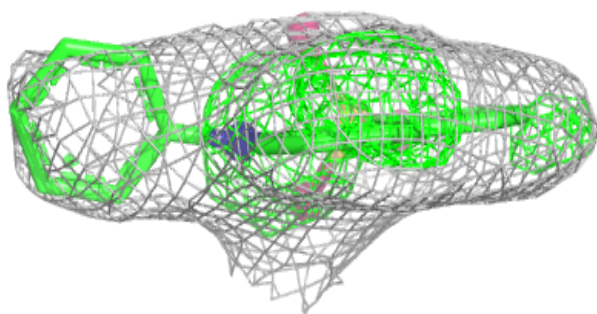
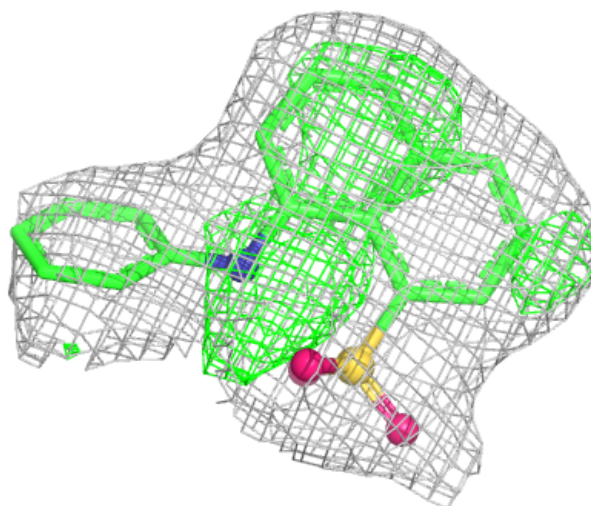
Electron density around 2AN T 205:

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



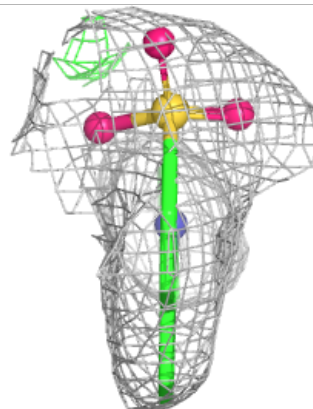
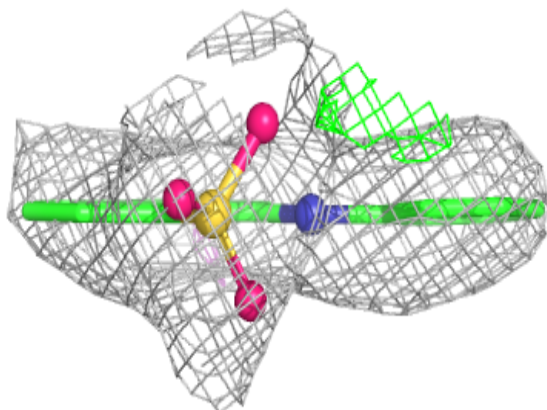
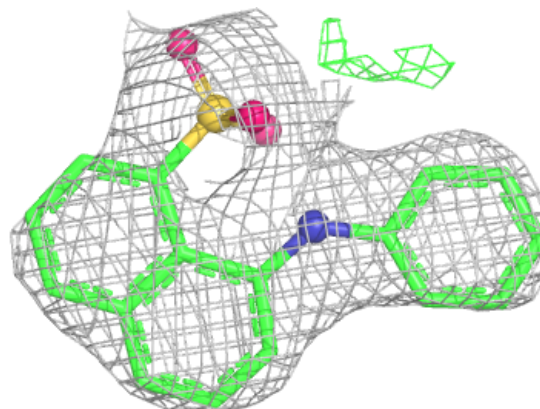
Electron density around 2AN V 207:

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



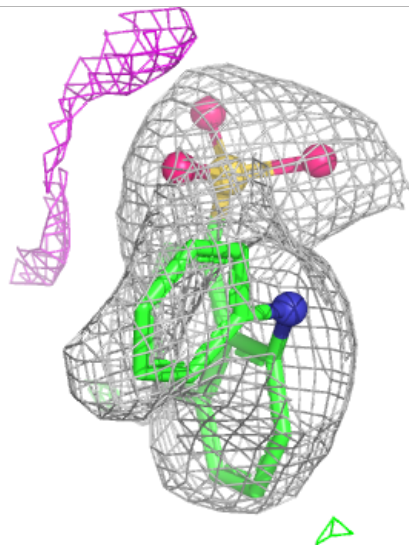
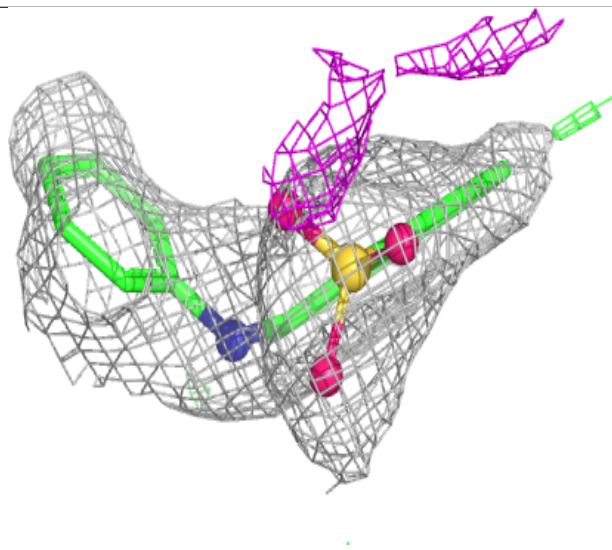
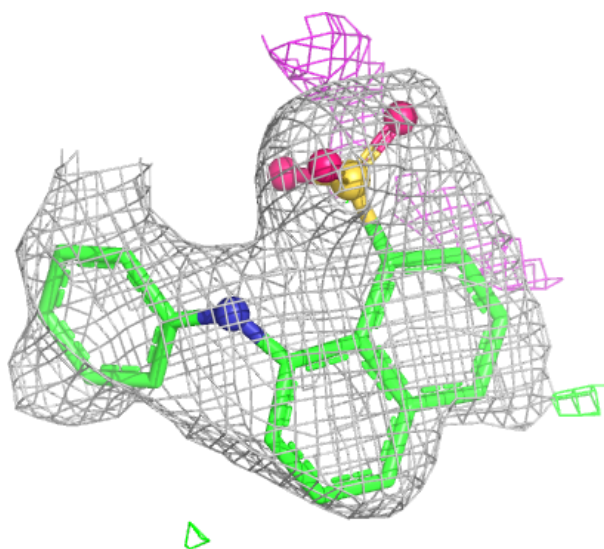
Electron density around 2AN Z 202:

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



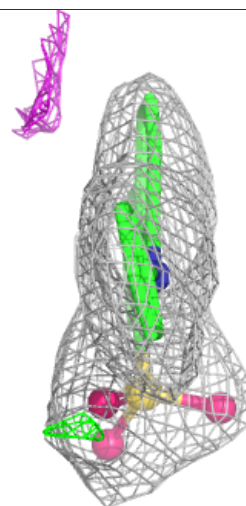
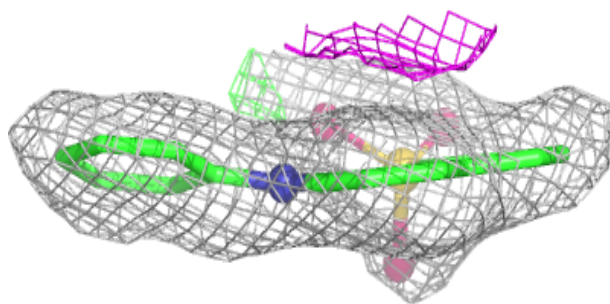
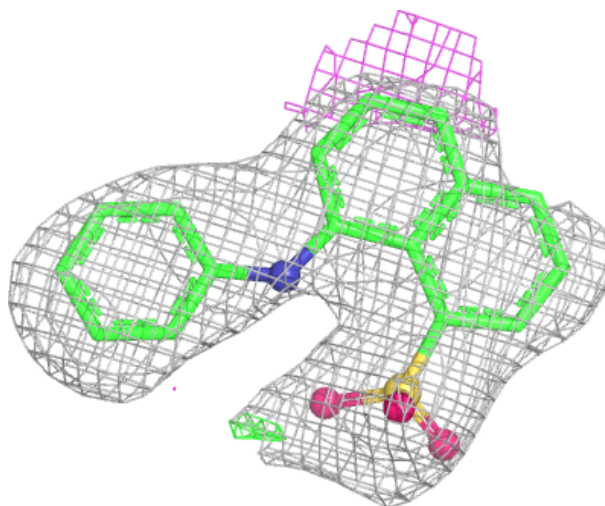
Electron density around 2AN I 206:

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



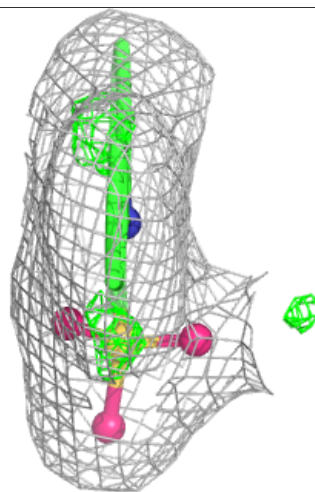
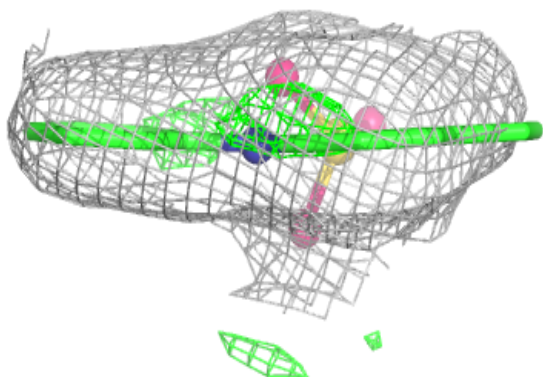
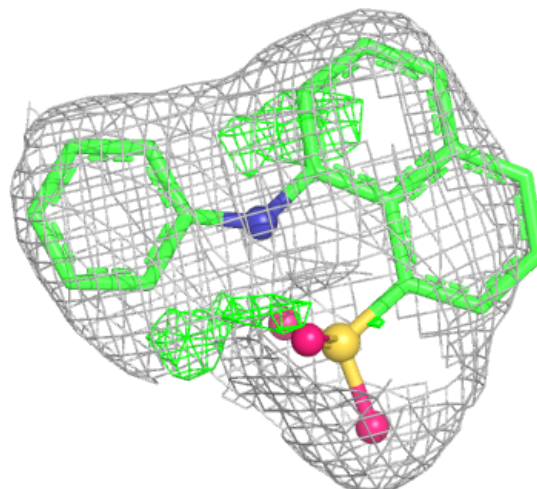
Electron density around 2AN W 201:

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



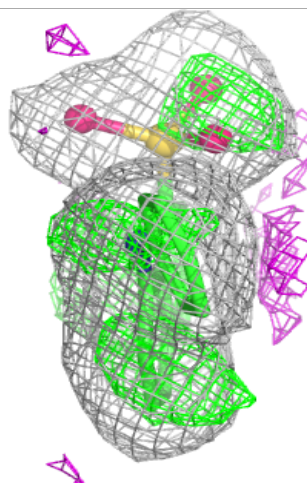
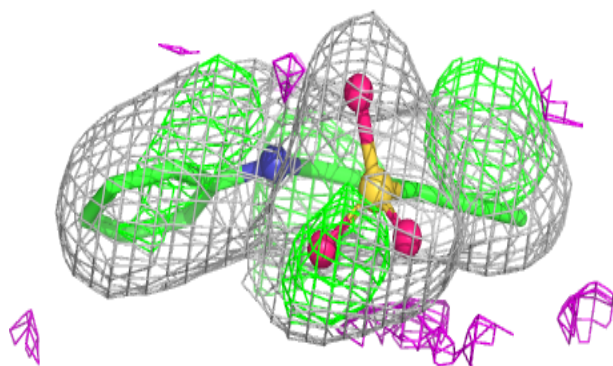
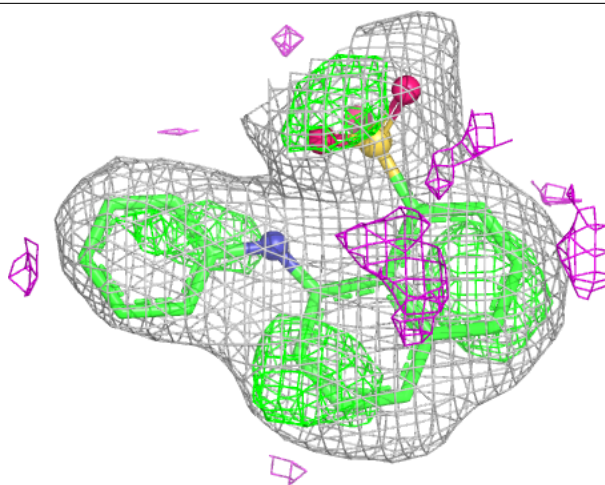
Electron density around 2AN X 202:

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



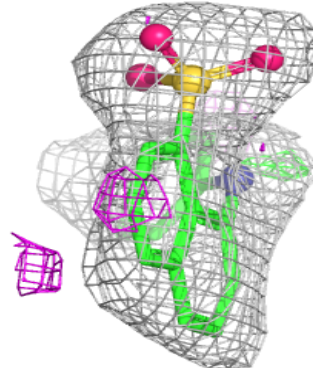
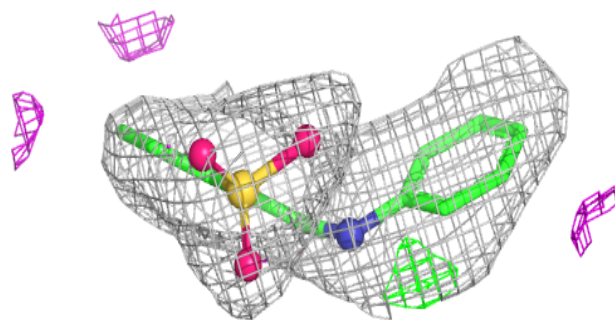
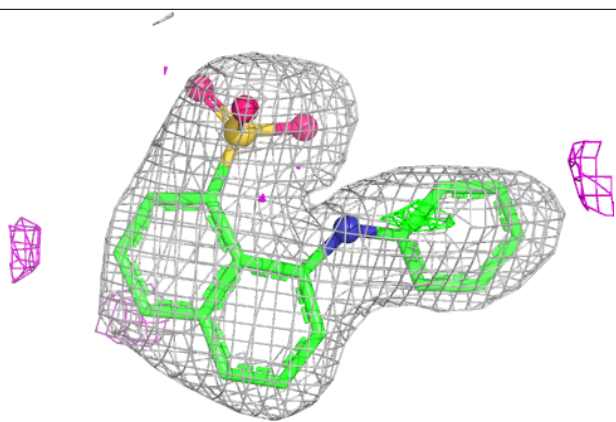
Electron density around 2AN h 203:

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



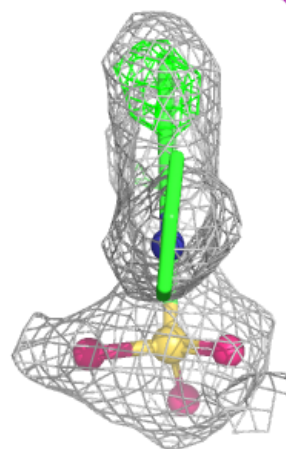
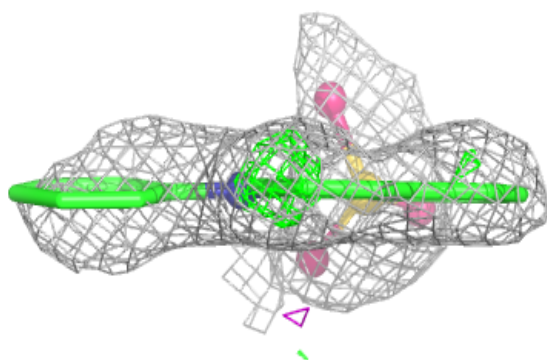
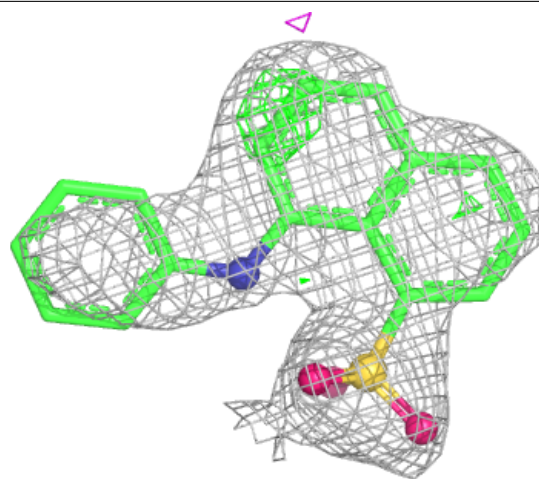
Electron density around 2AN A 202:

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



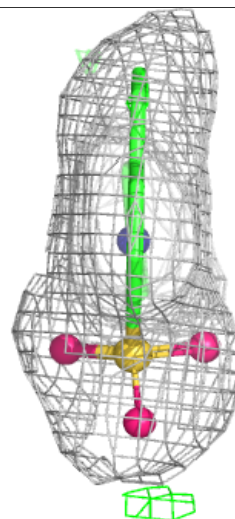
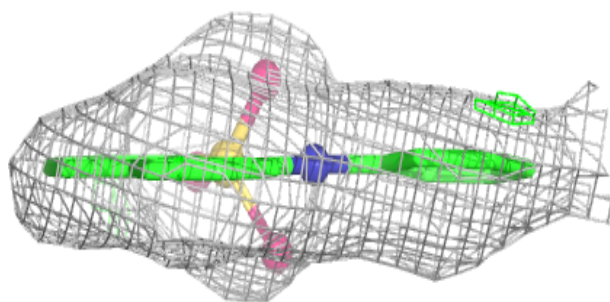
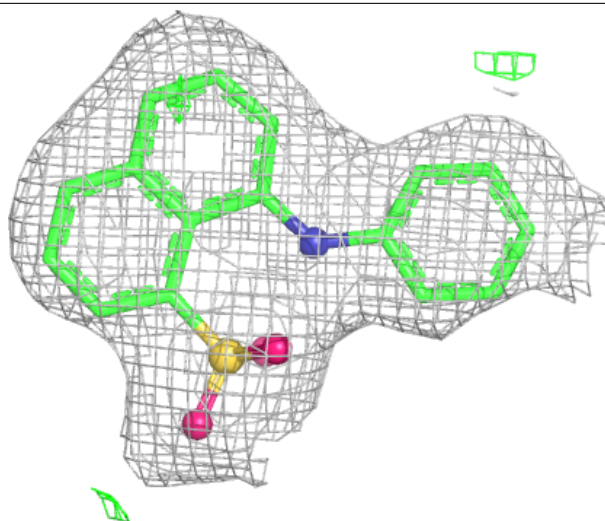
Electron density around 2AN c 205:

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



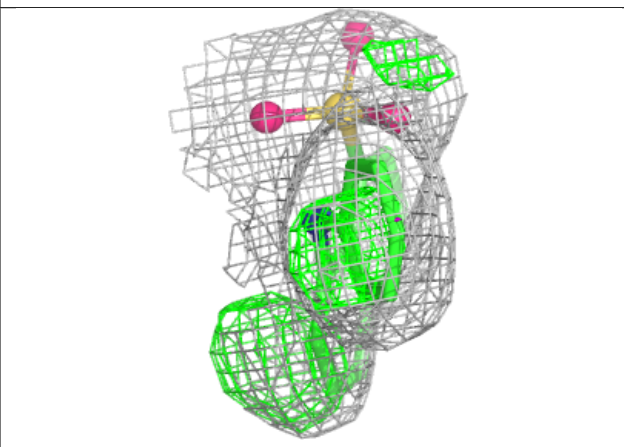
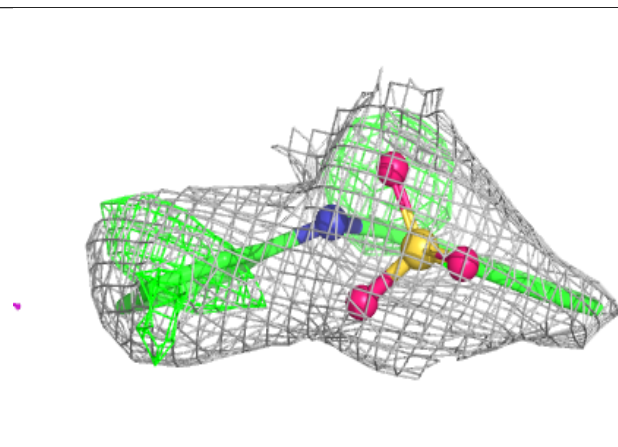
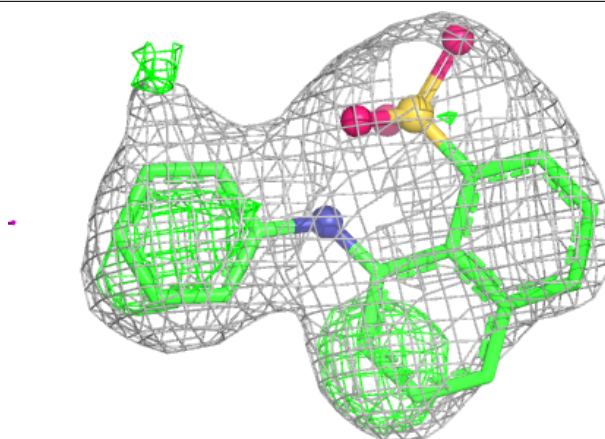
Electron density around 2AN Z 204:

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



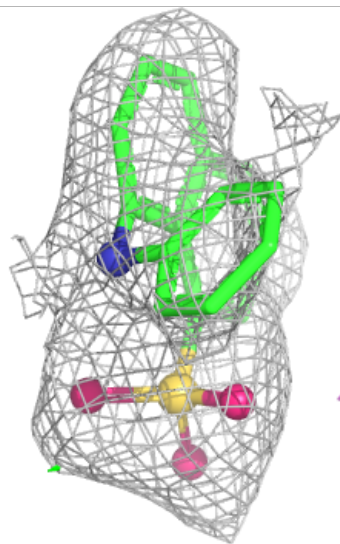
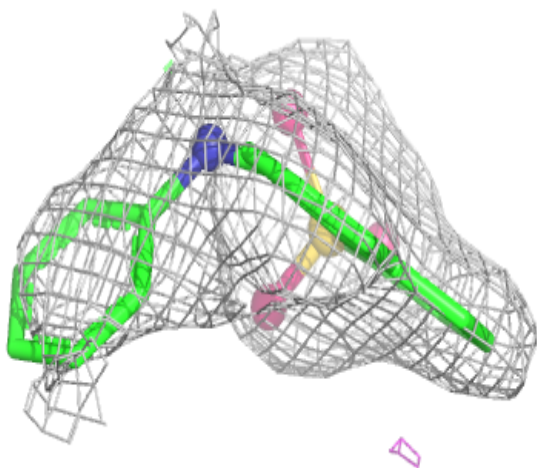
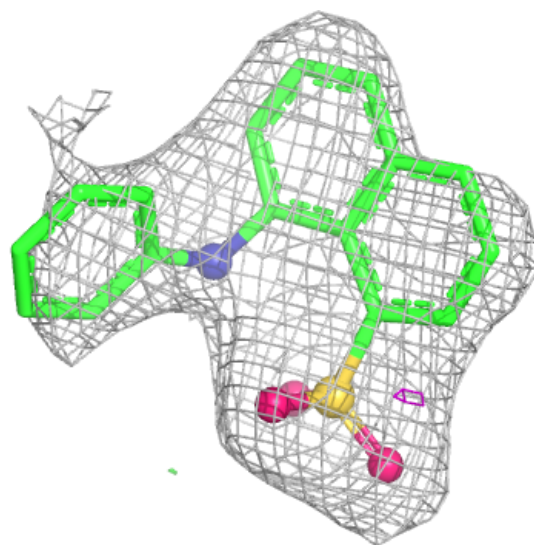
Electron density around 2AN B 206:

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



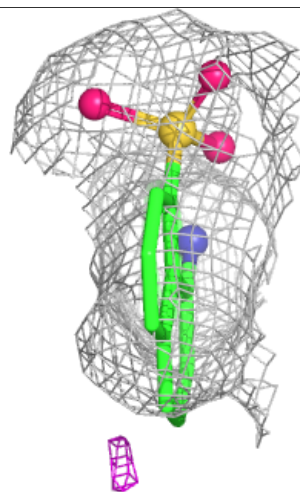
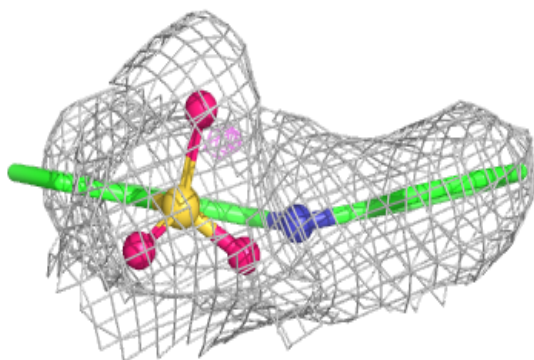
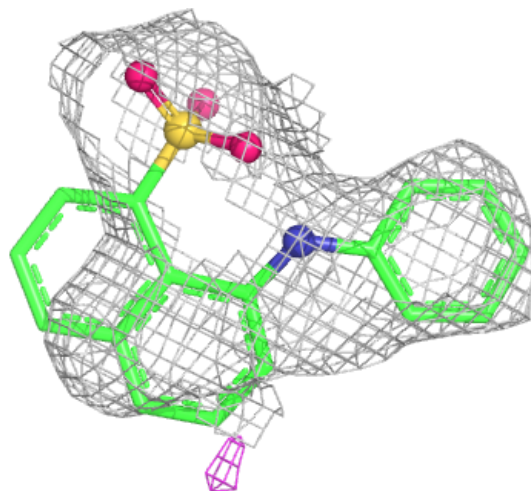
Electron density around 2AN Q 203:

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



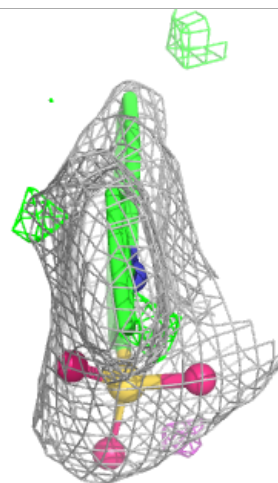
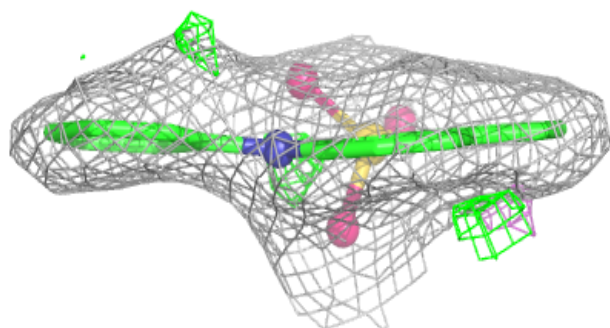
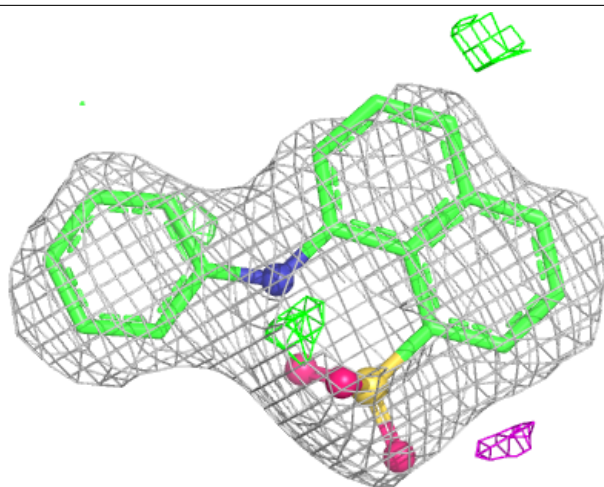
Electron density around 2AN U 201:

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



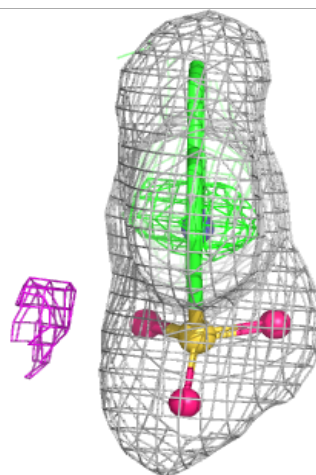
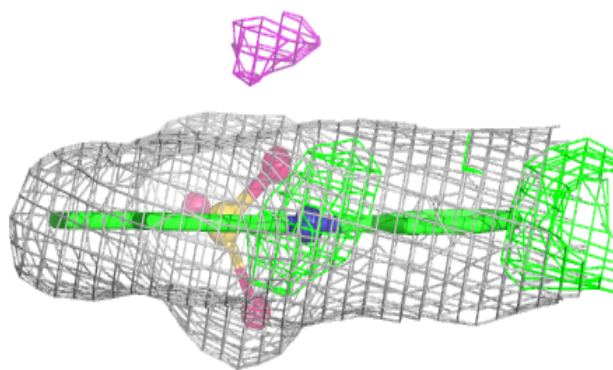
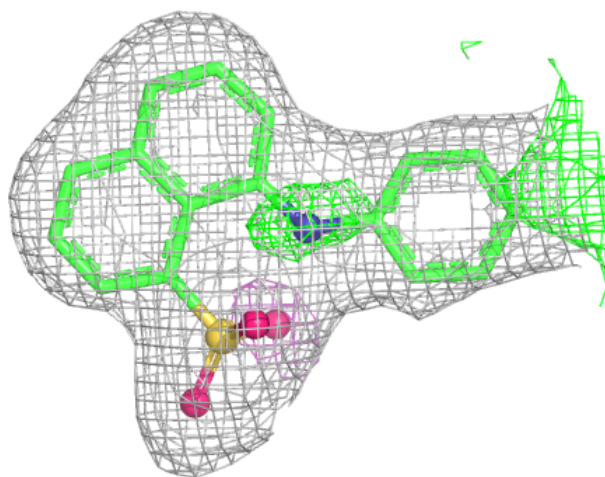
Electron density around 2AN K 203:

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



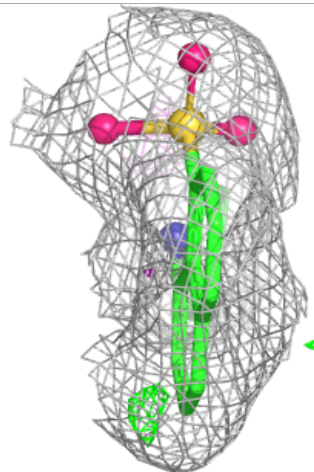
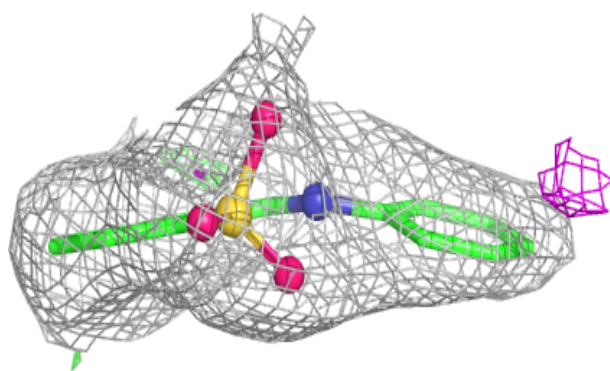
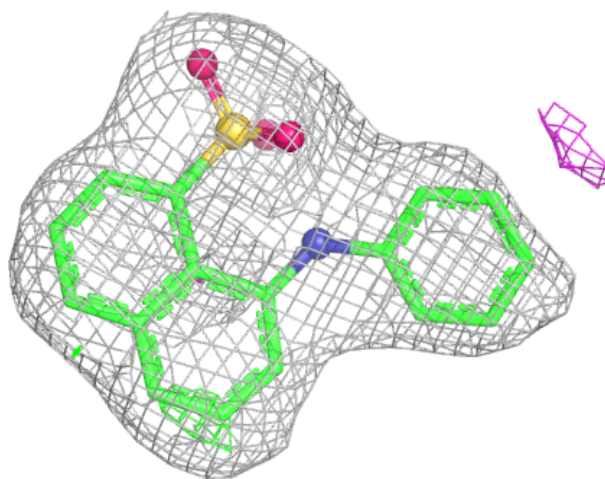
Electron density around 2AN V 206:

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



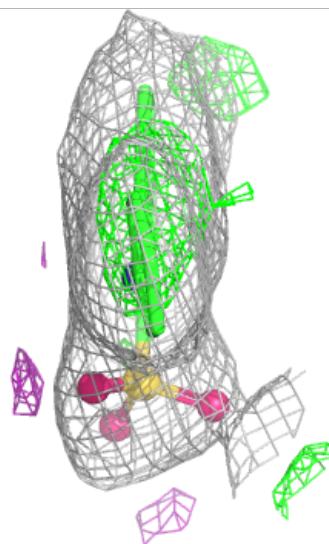
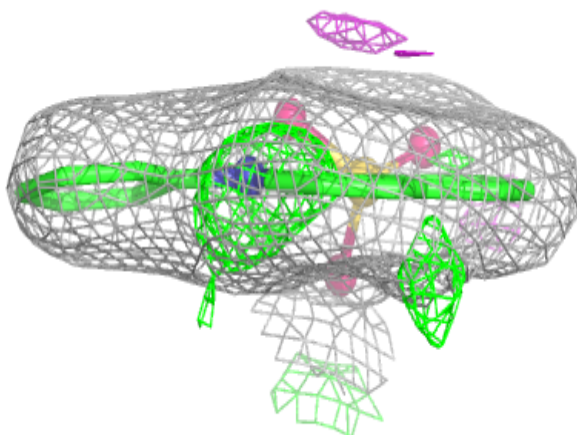
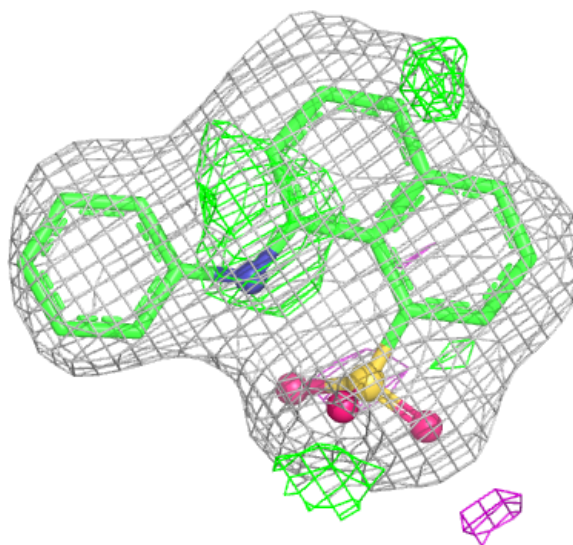
Electron density around 2AN a 203:

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



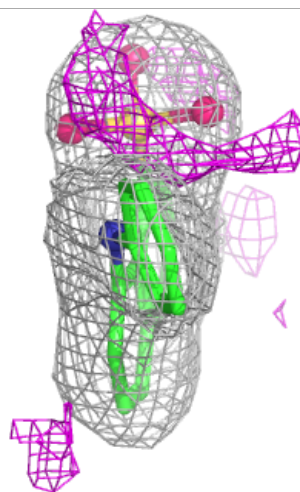
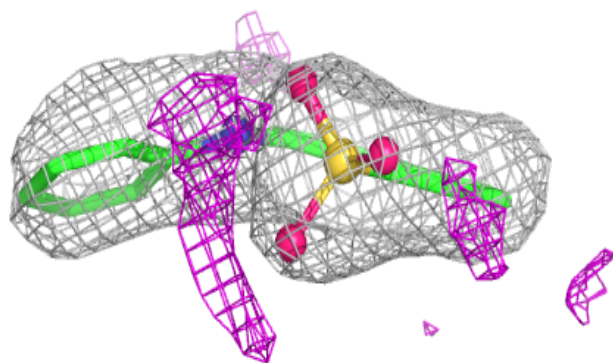
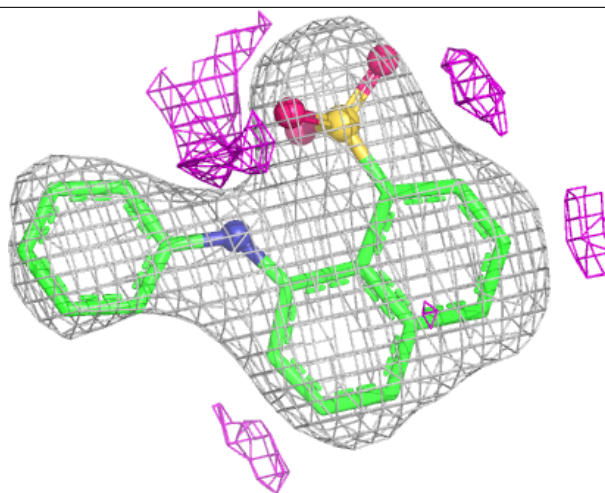
Electron density around 2AN j 204:

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



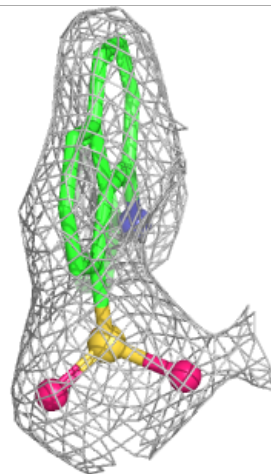
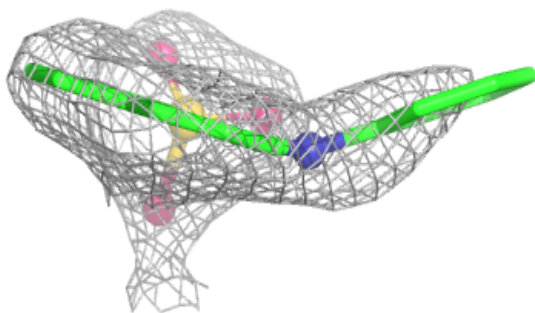
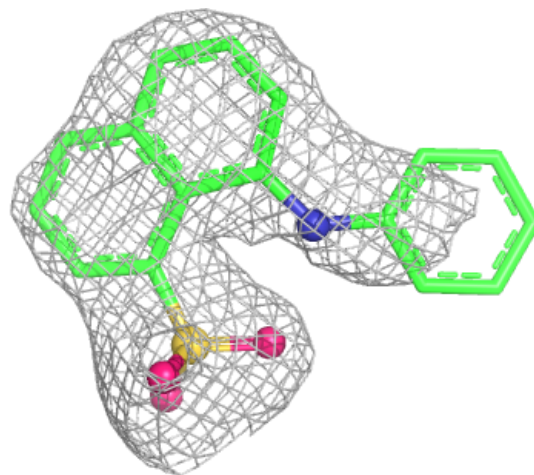
Electron density around 2AN Y 203:

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



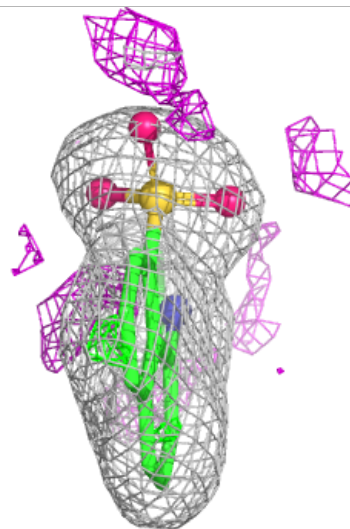
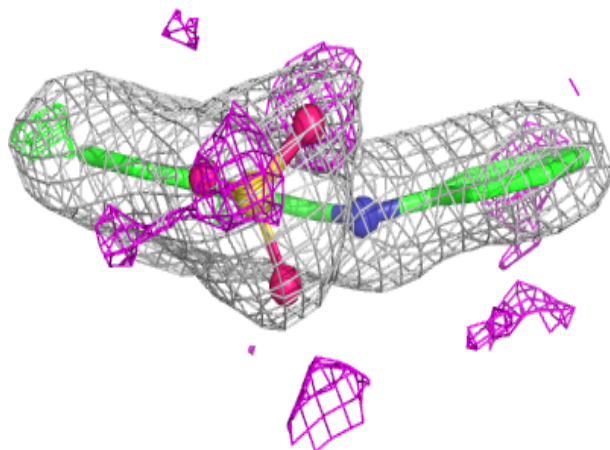
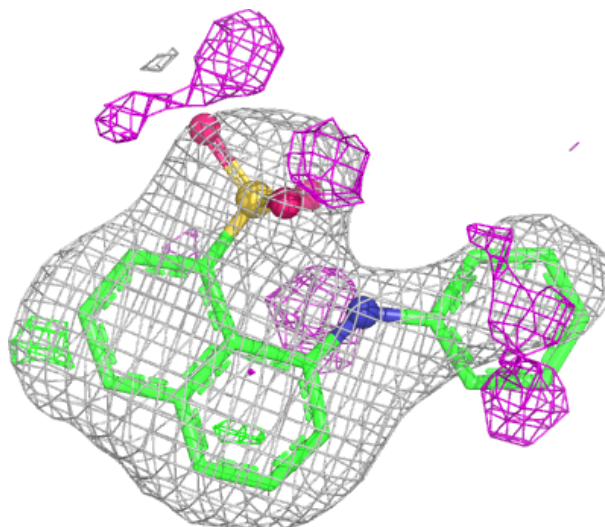
Electron density around 2AN A 203:

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



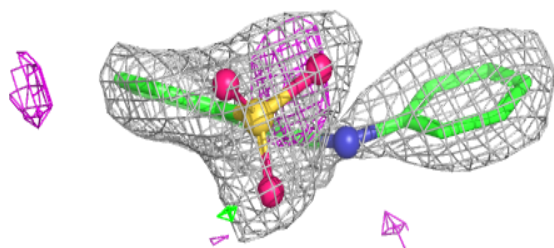
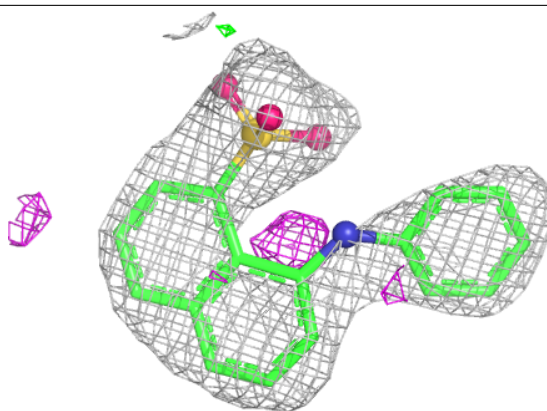
Electron density around 2AN X 201:

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



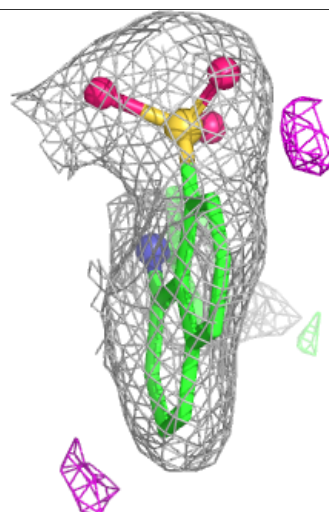
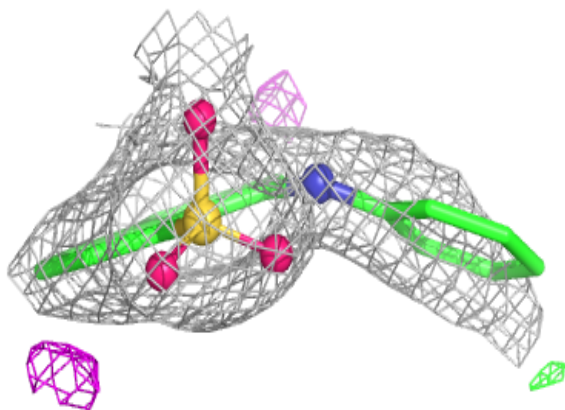
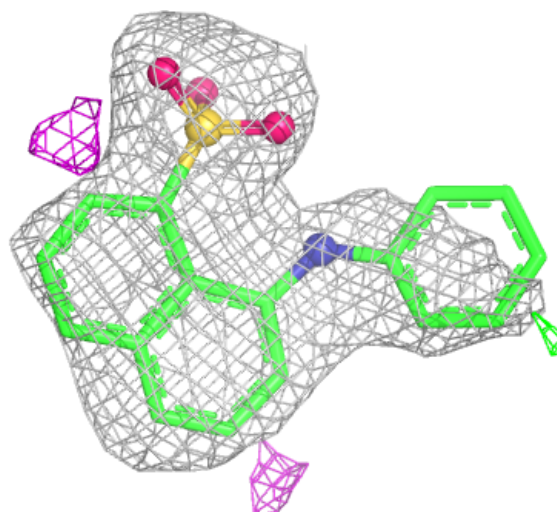
Electron density around 2AN h 201:

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



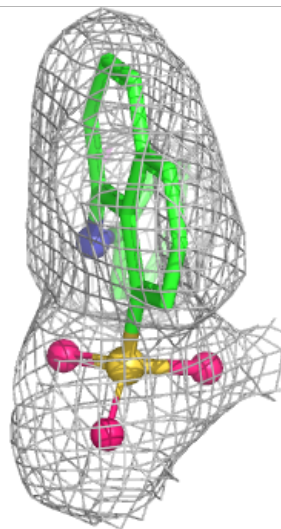
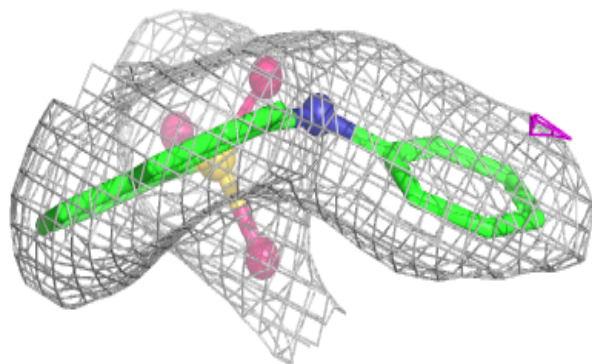
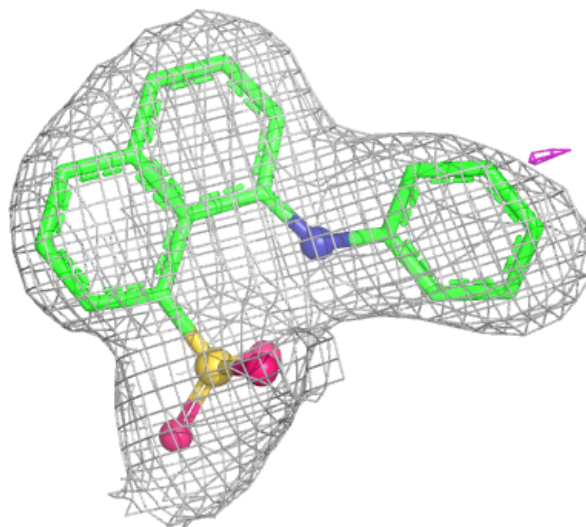
Electron density around 2AN E 203:

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



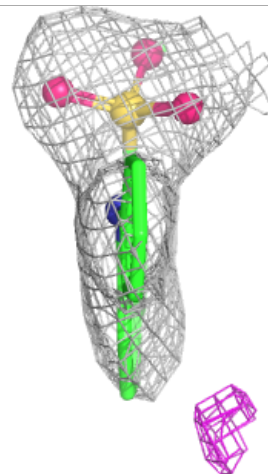
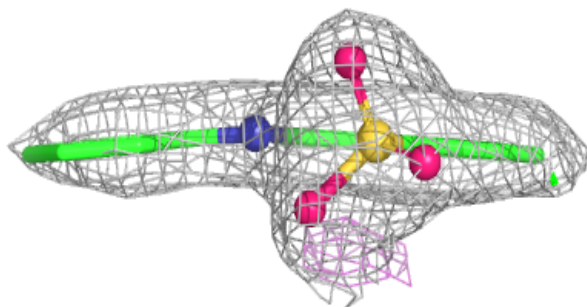
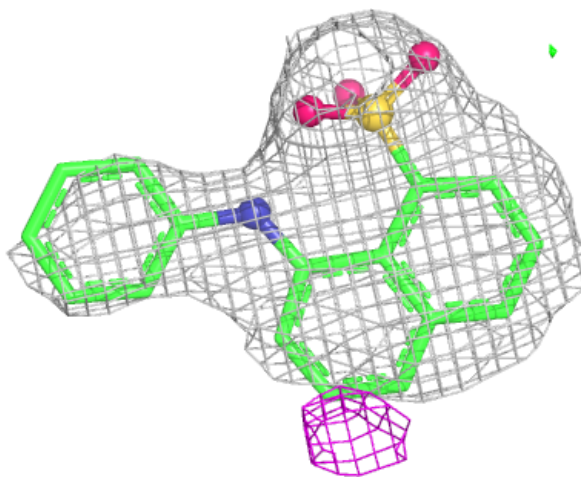
Electron density around 2AN O 203:

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



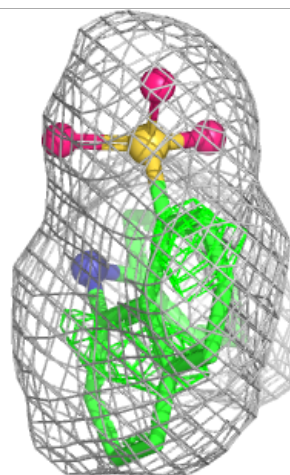
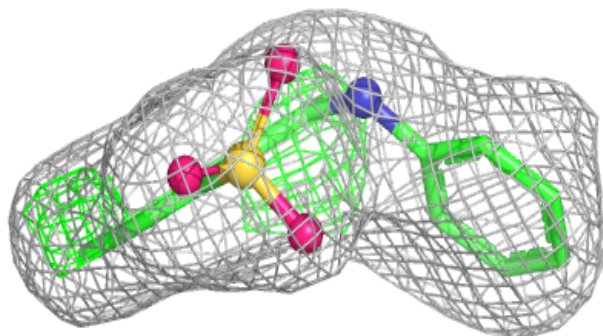
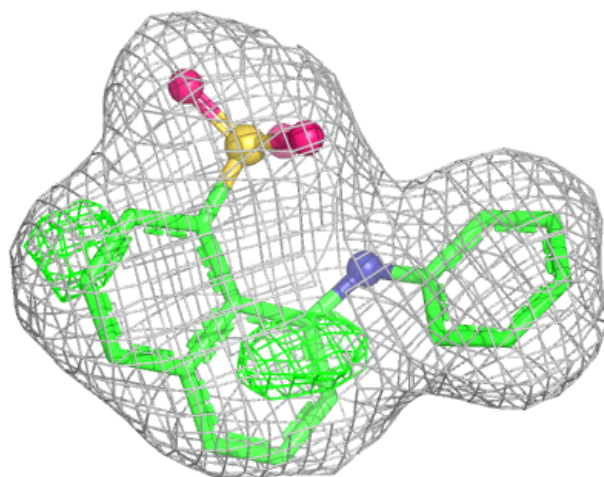
Electron density around 2AN g 201:

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



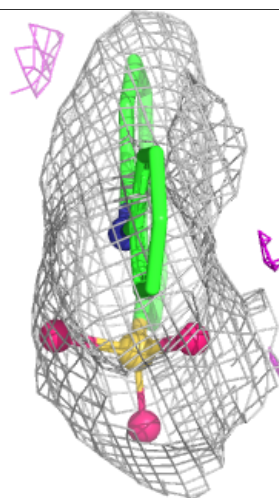
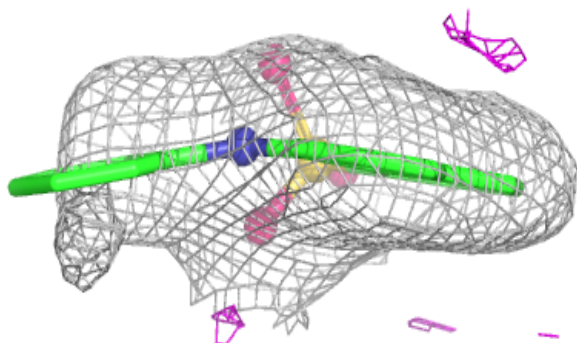
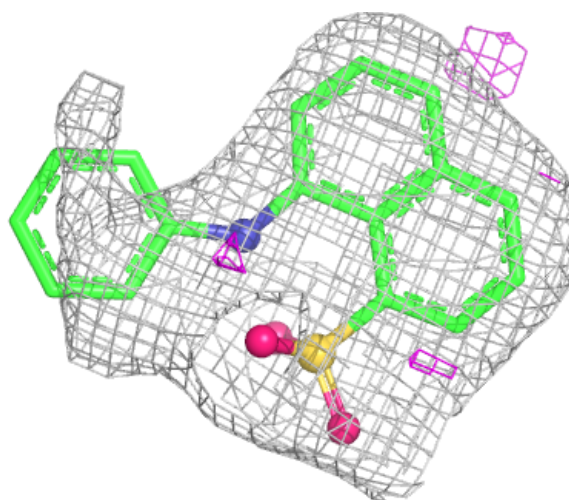
Electron density around 2AN g 203:

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



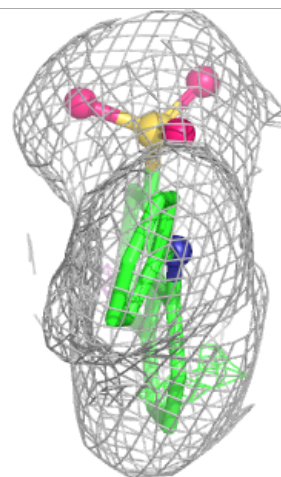
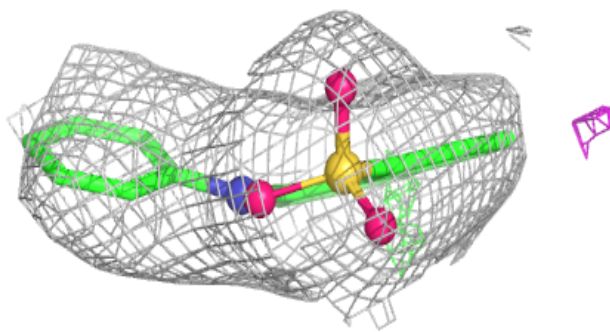
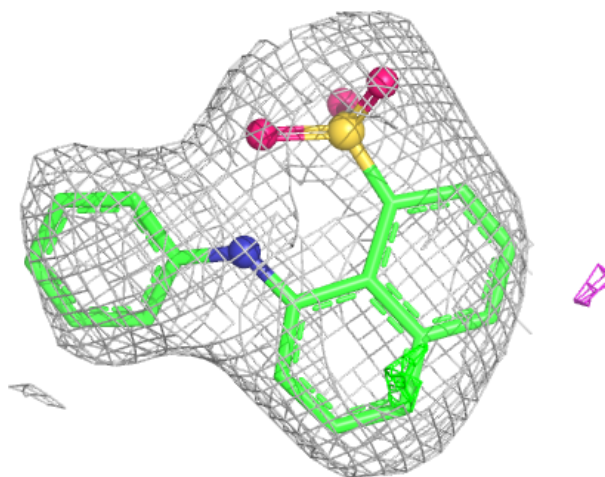
Electron density around 2AN Z 205:

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



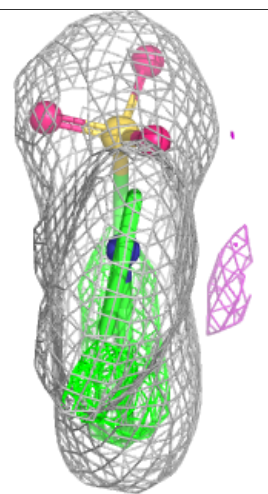
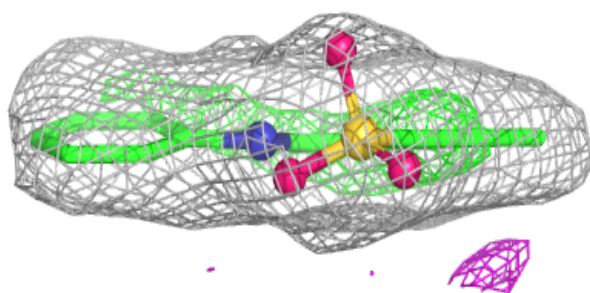
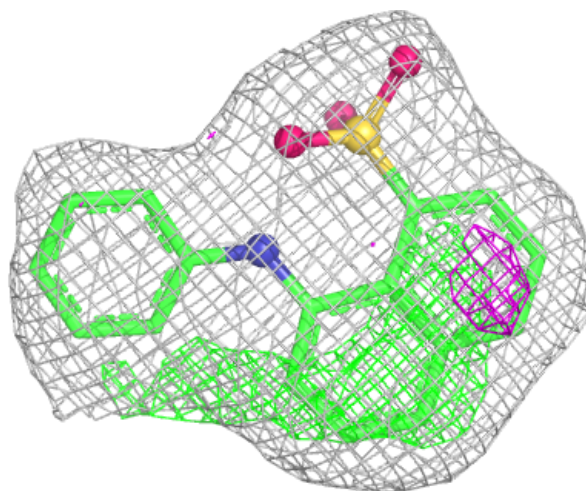
Electron density around 2AN D 203:

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



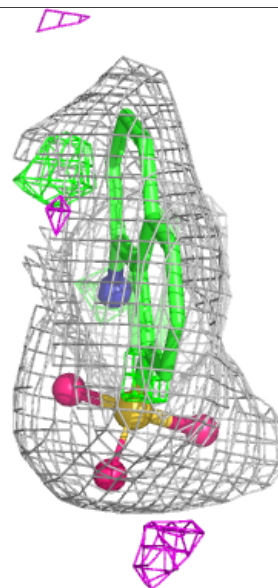
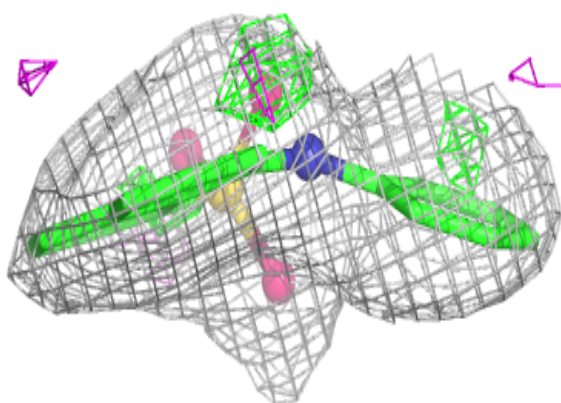
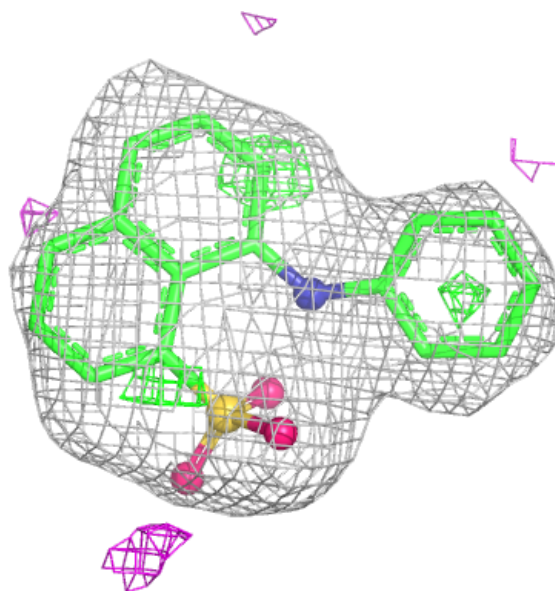
Electron density around 2AN P 203:

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



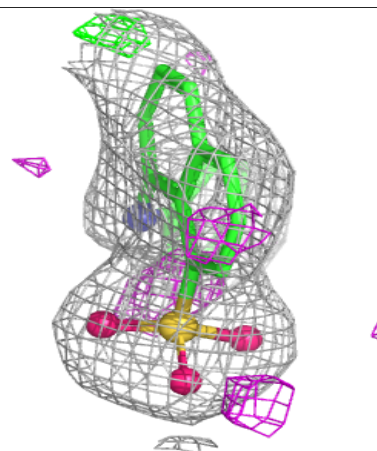
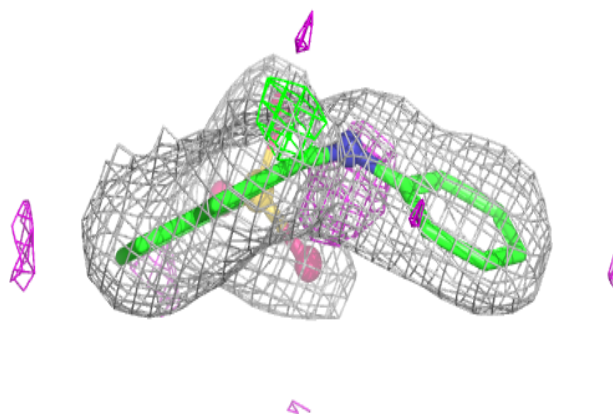
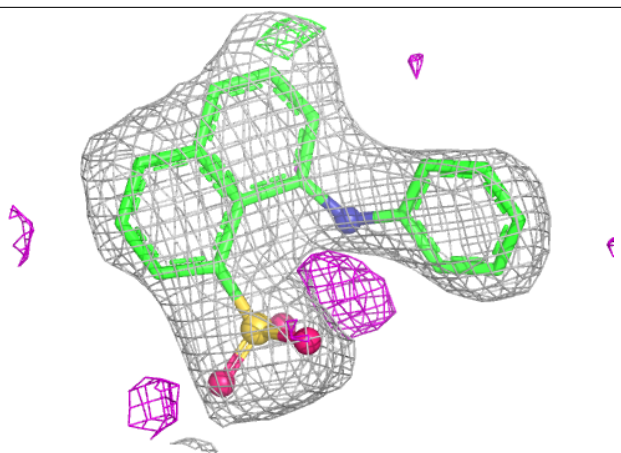
Electron density around 2AN F 205:

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



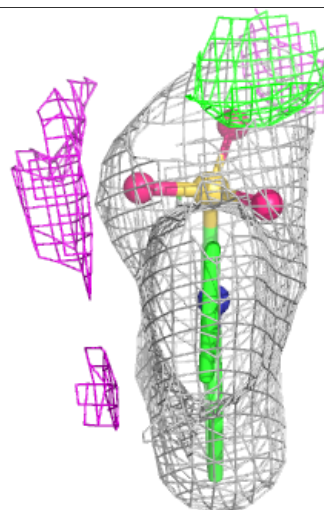
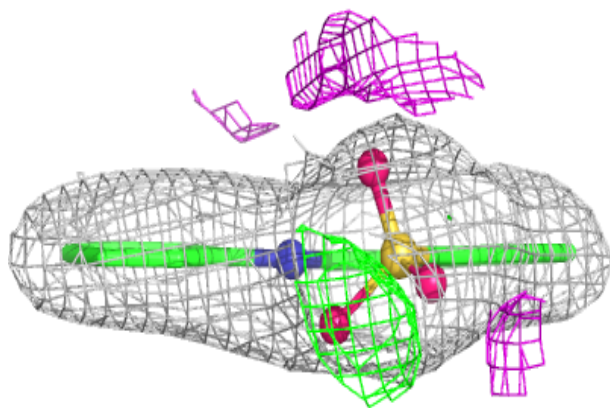
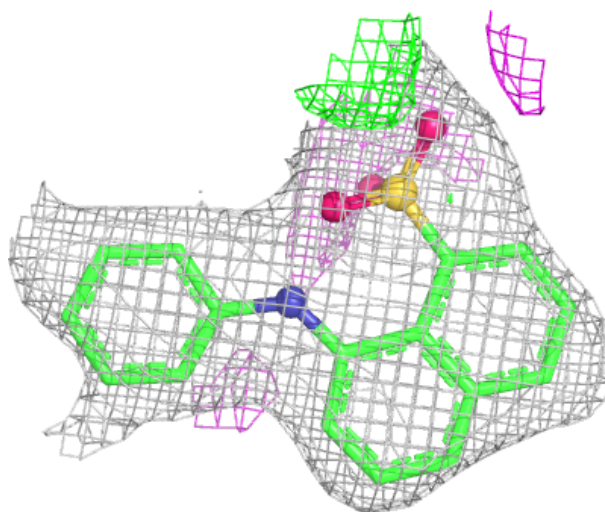
Electron density around 2AN Z 201:

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



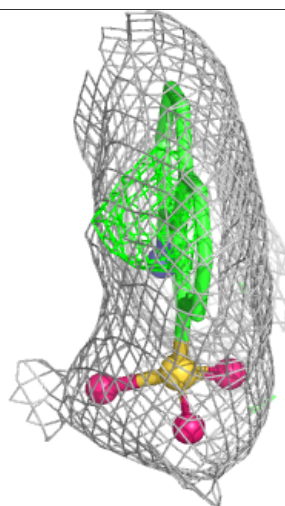
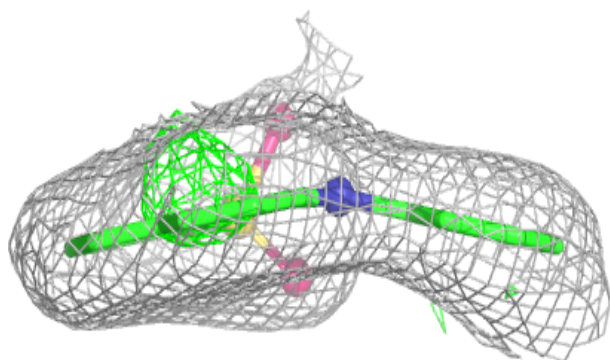
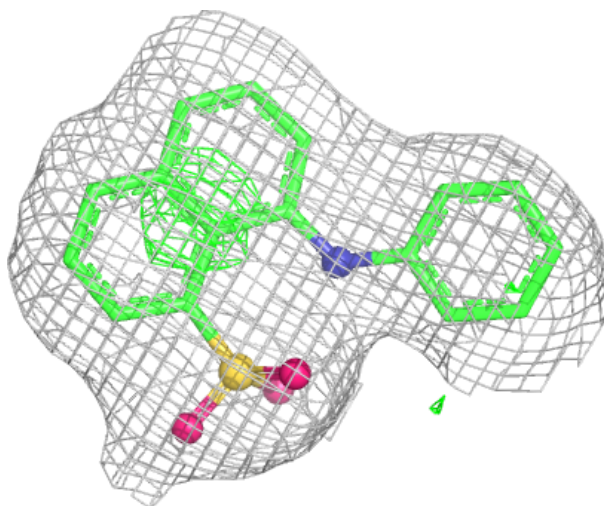
Electron density around 2AN X 204:

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



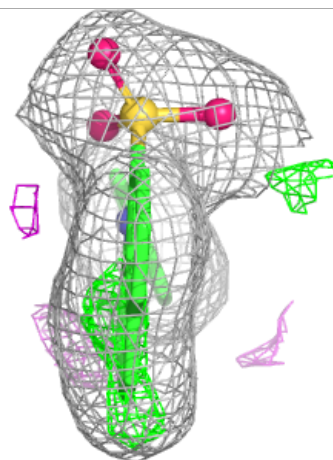
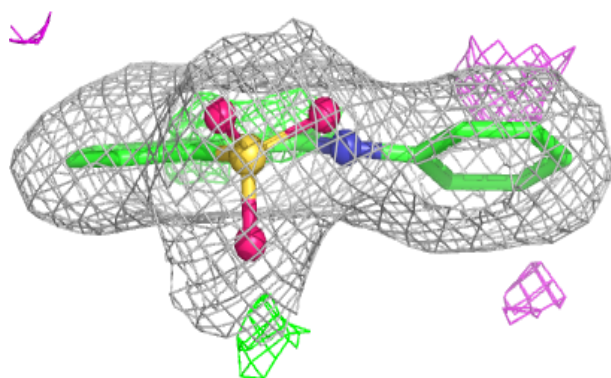
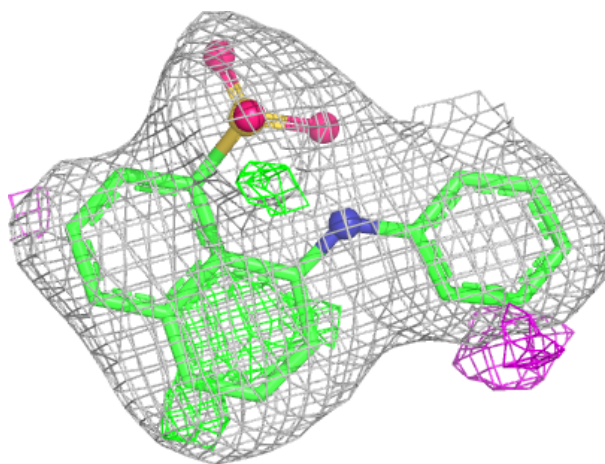
Electron density around 2AN d 201:

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



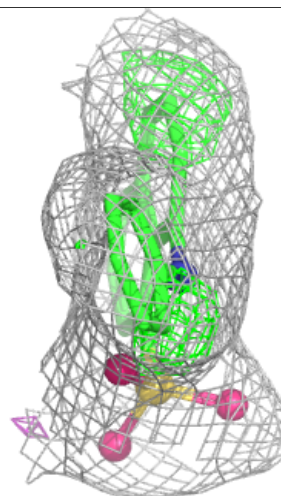
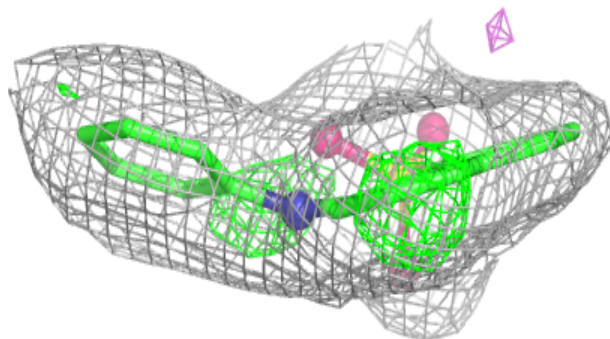
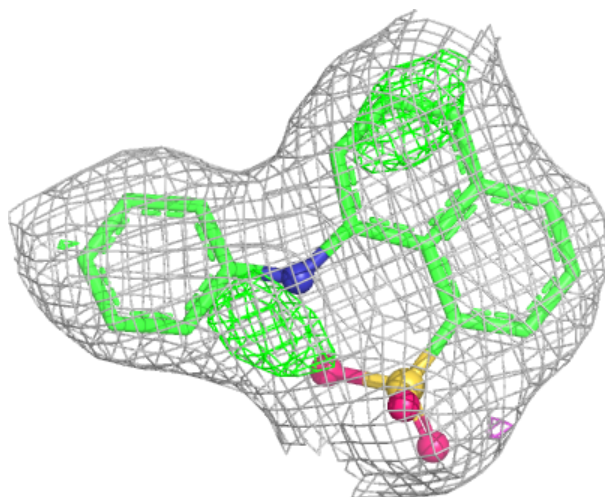
Electron density around 2AN j 201:

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



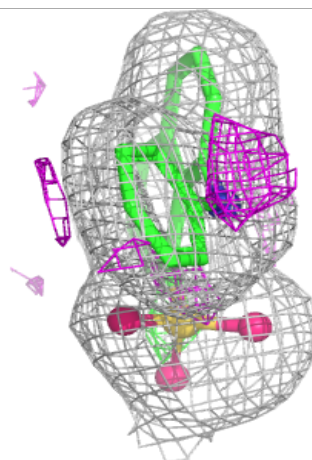
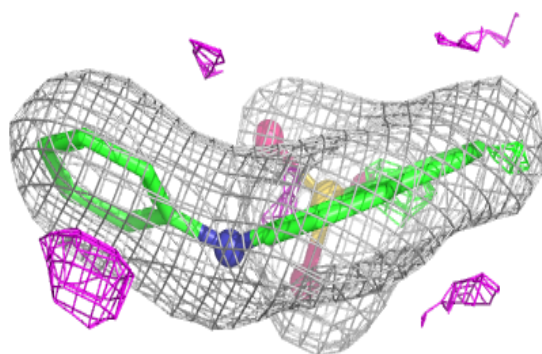
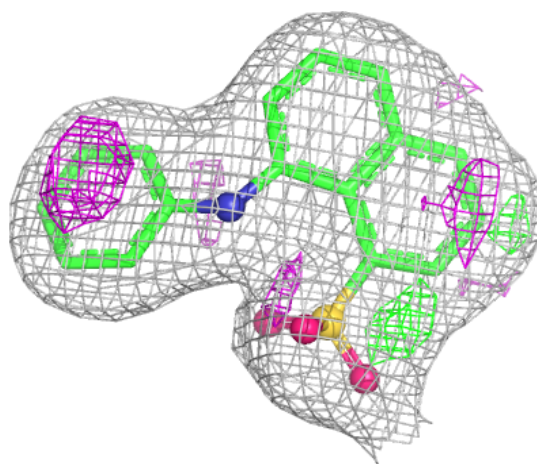
Electron density around 2AN d 202:

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



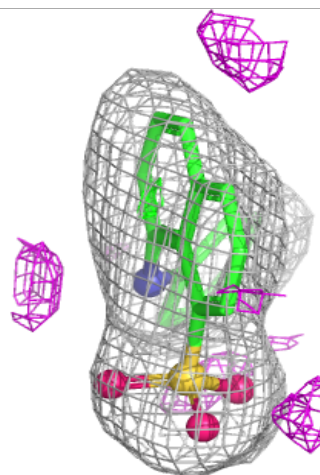
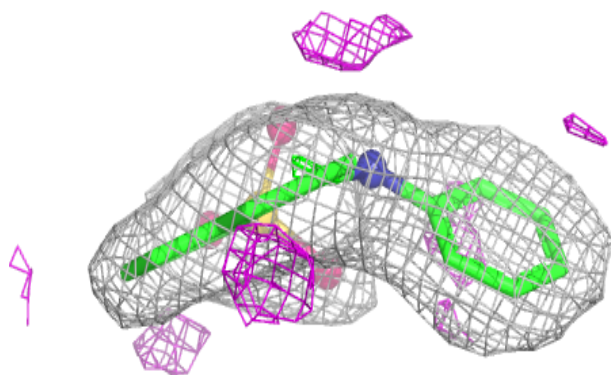
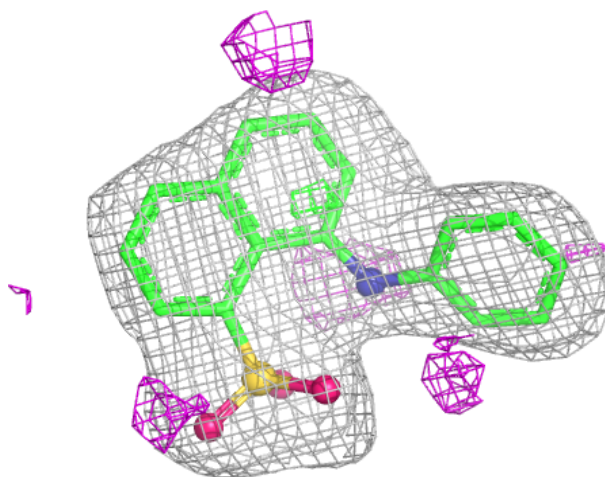
Electron density around 2AN R 202:

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



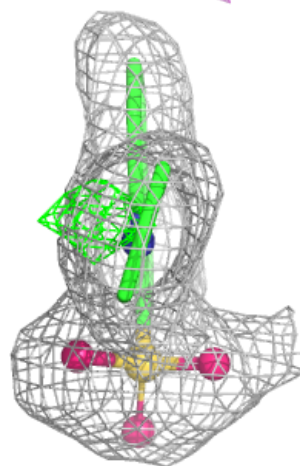
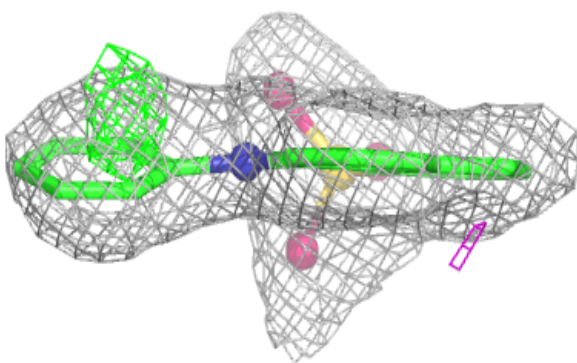
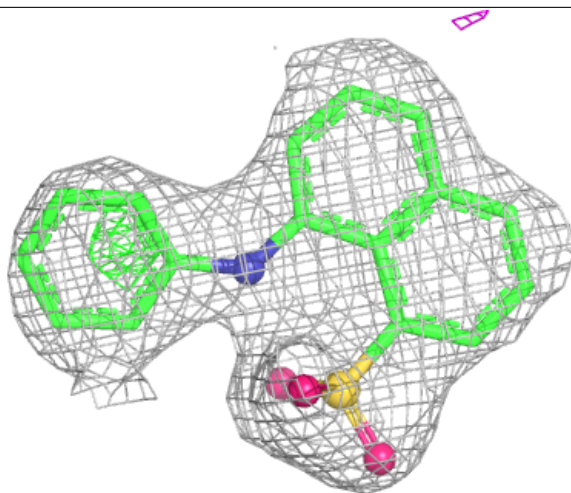
Electron density around 2AN C 201:

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



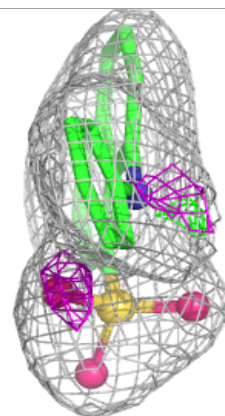
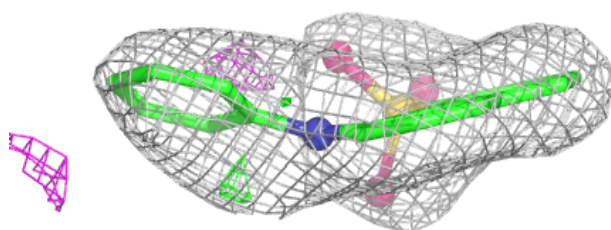
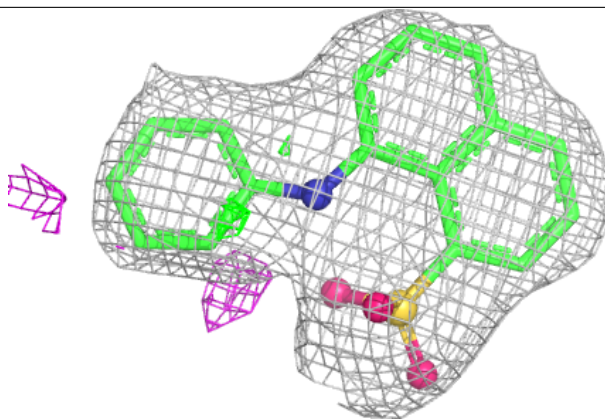
Electron density around 2AN B 204:

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



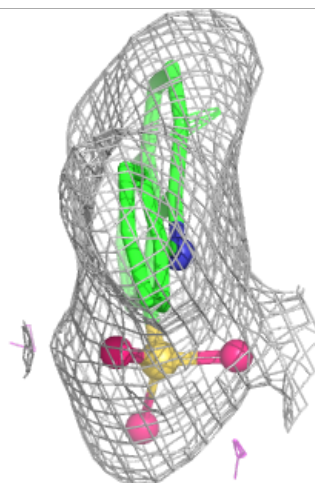
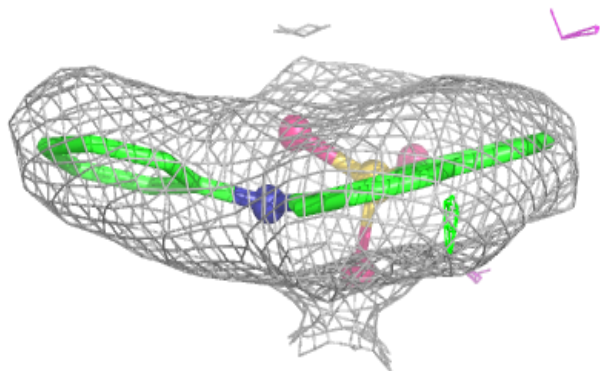
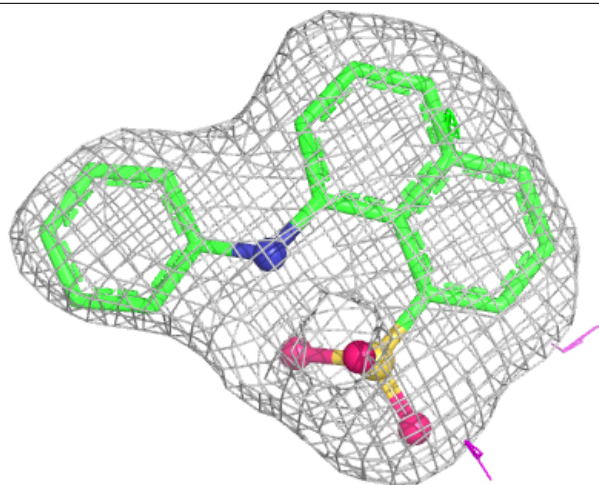
Electron density around 2AN b 202:

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



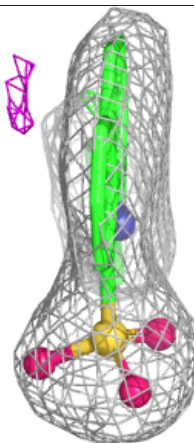
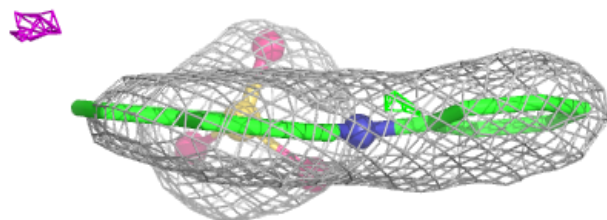
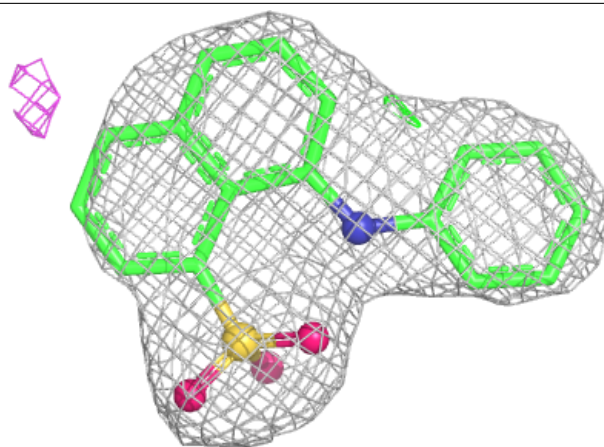
Electron density around 2AN b 204:

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



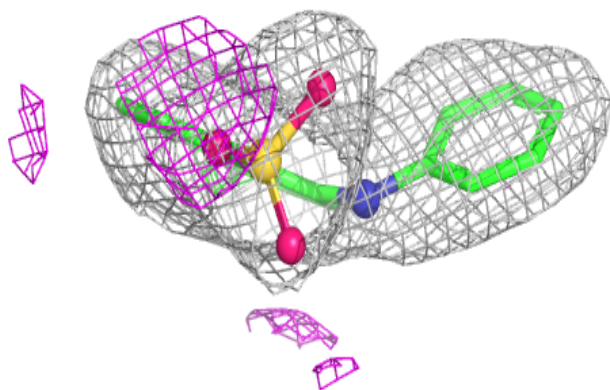
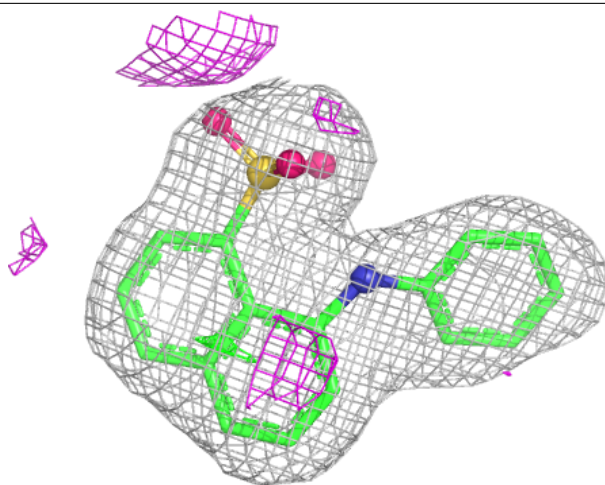
Electron density around 2AN Y 202:

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



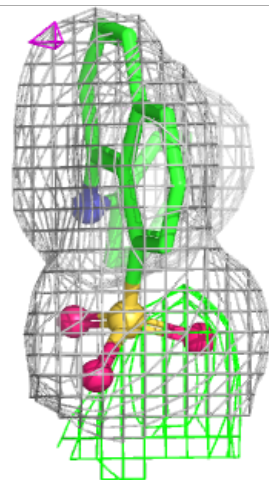
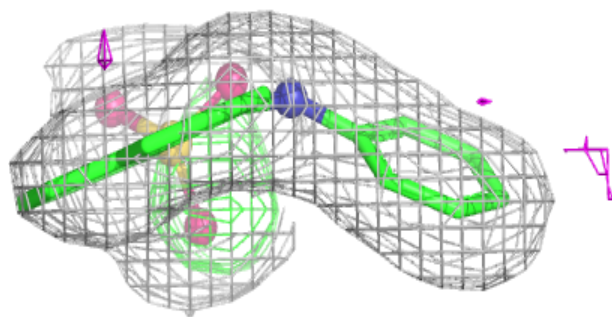
Electron density around 2AN G 201:

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



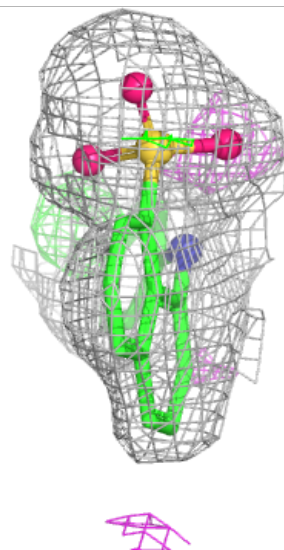
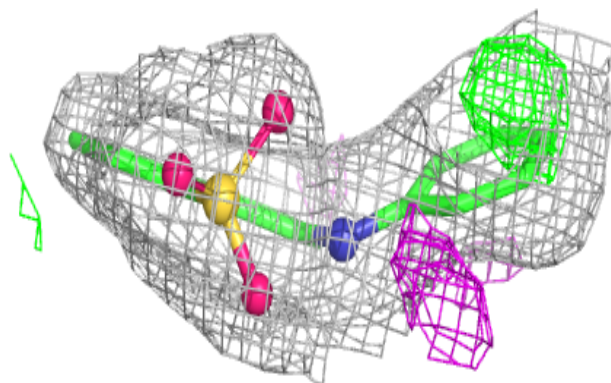
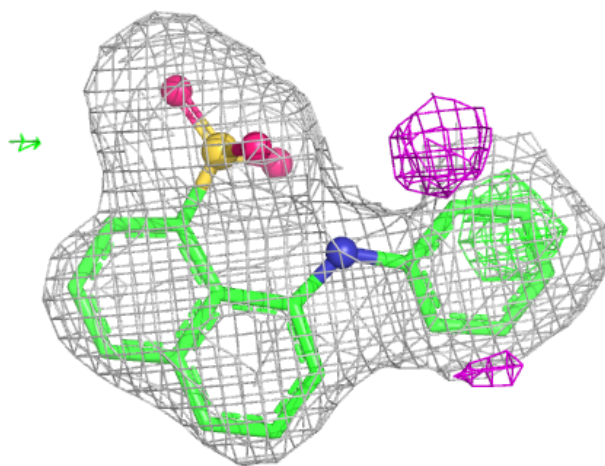
Electron density around 2AN B 205:

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



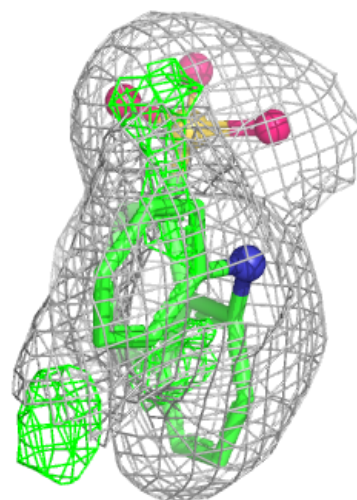
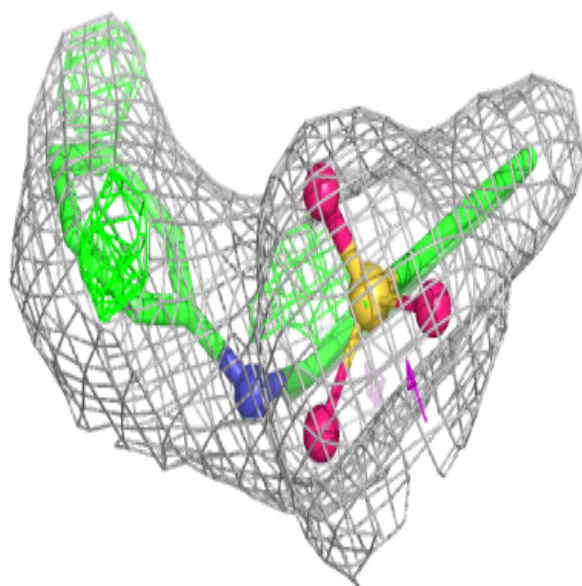
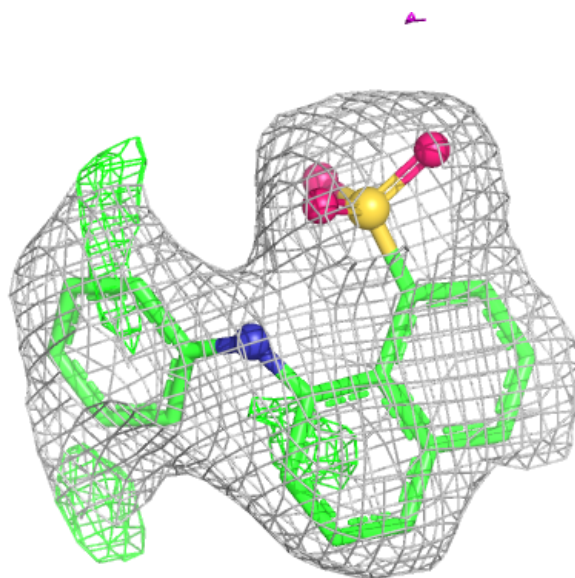
Electron density around 2AN h 206:

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



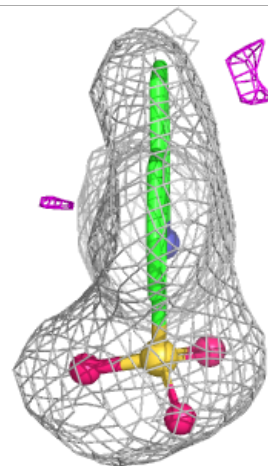
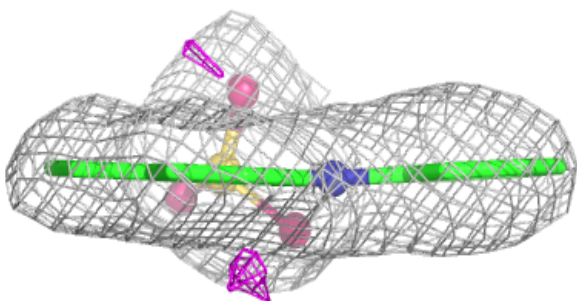
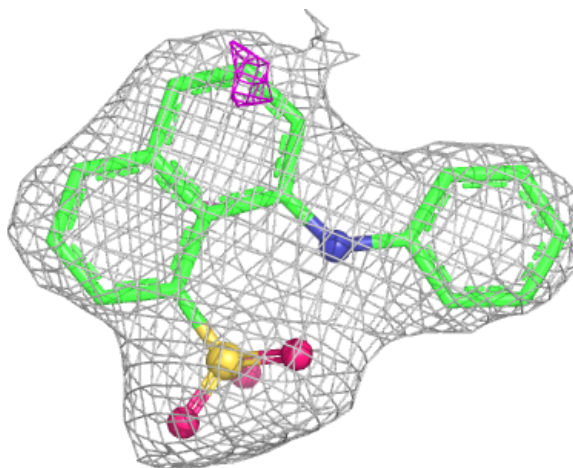
Electron density around 2AN M 203:

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



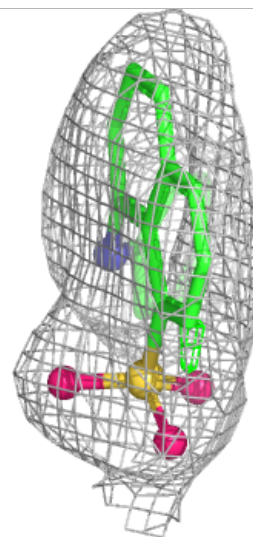
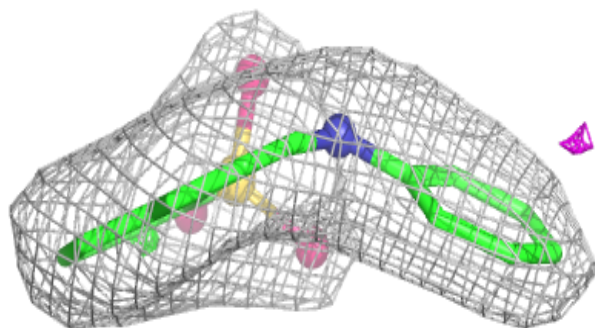
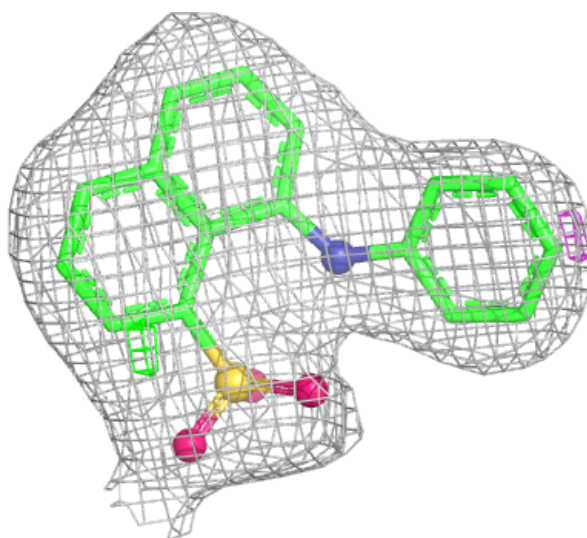
Electron density around 2AN L 204:

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



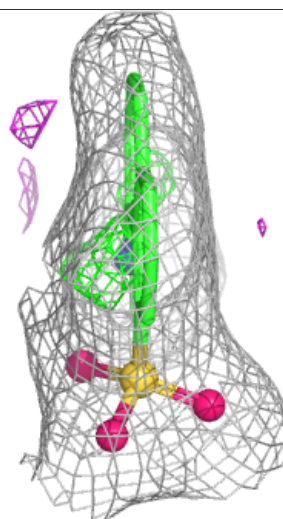
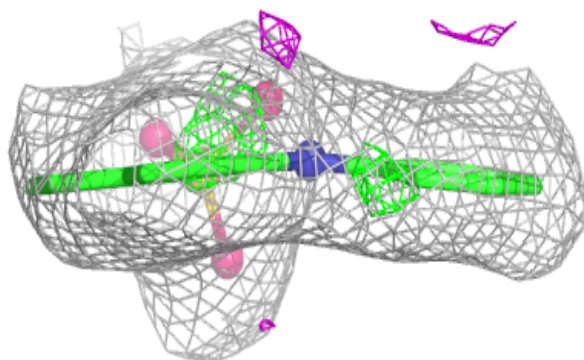
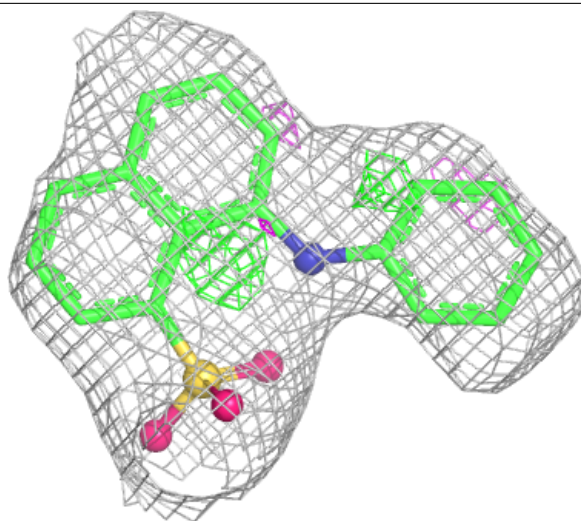
Electron density around 2AN D 202:

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



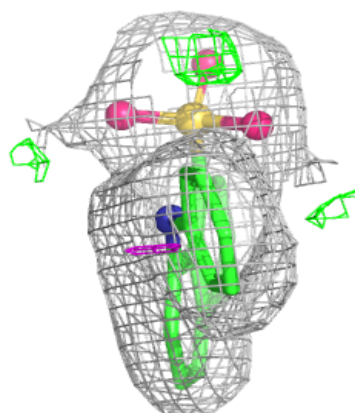
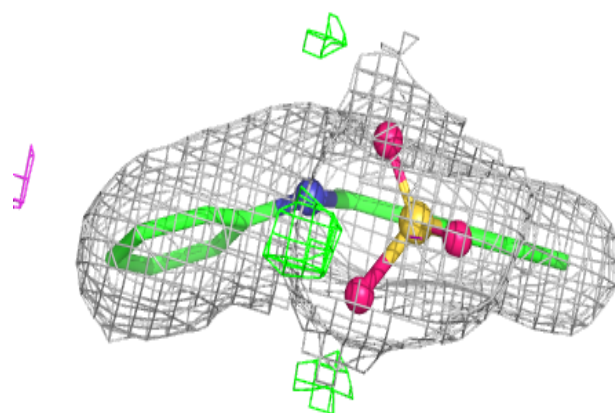
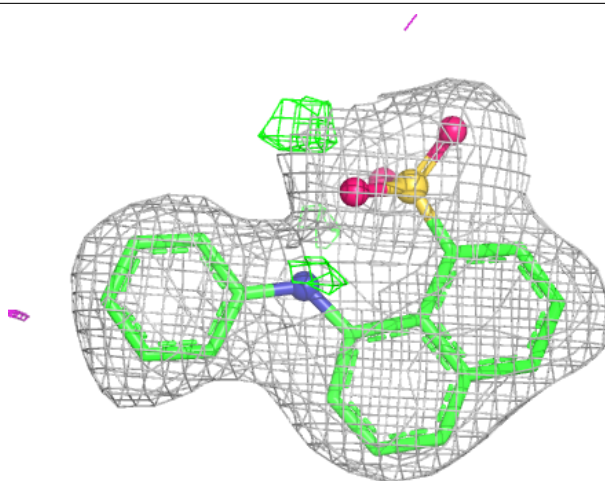
Electron density around 2AN F 201:

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



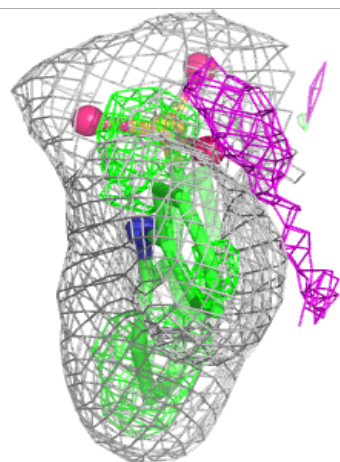
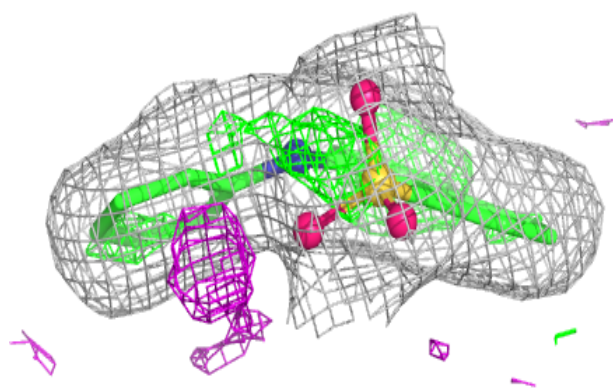
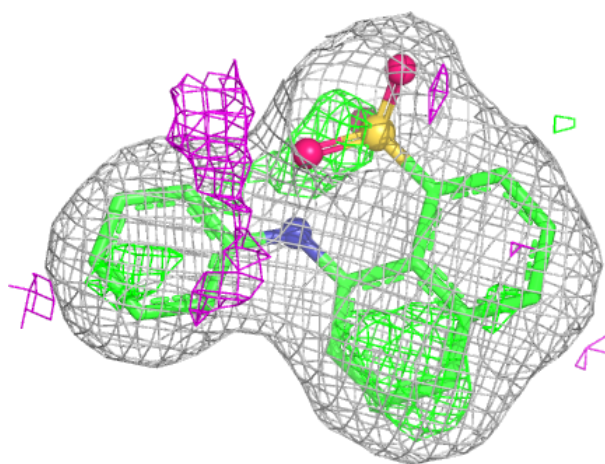
Electron density around 2AN X 205:

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



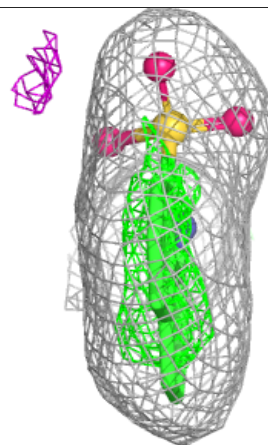
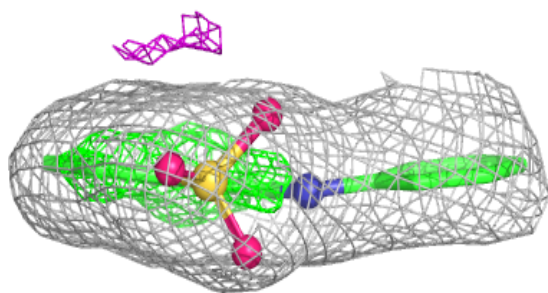
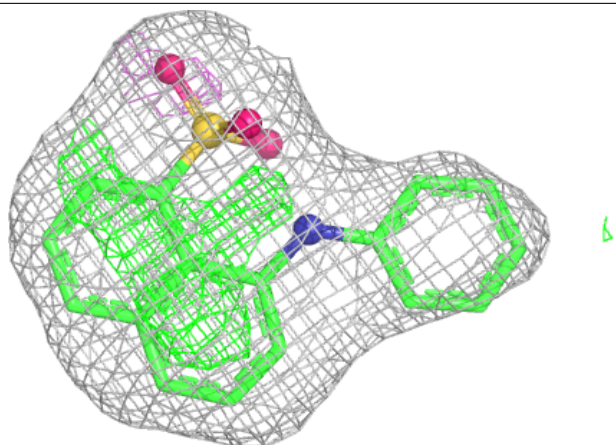
Electron density around 2AN f 204:

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



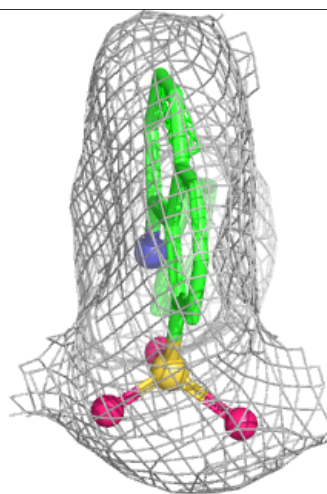
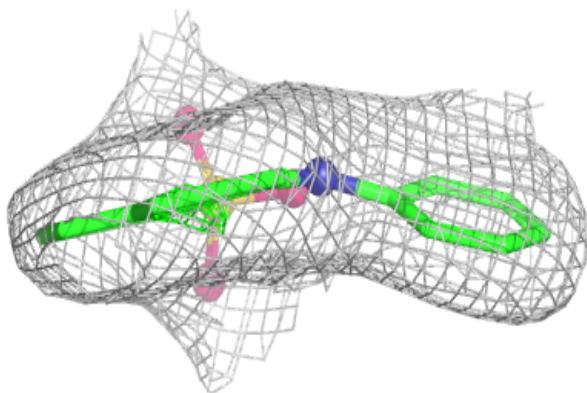
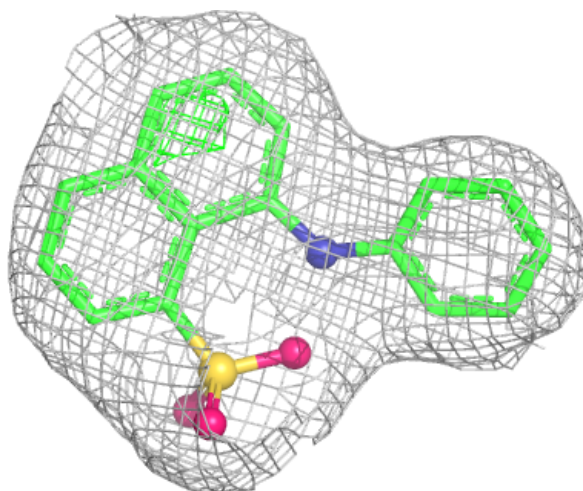
Electron density around 2AN J 201:

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



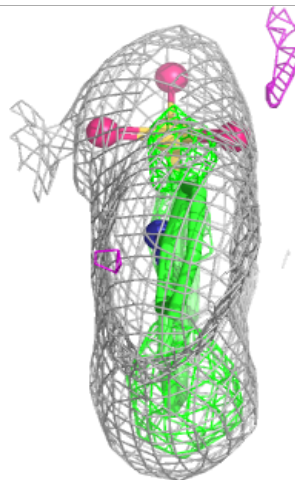
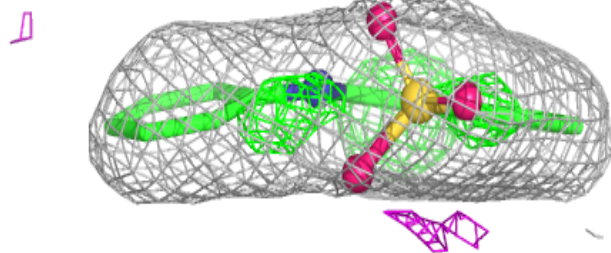
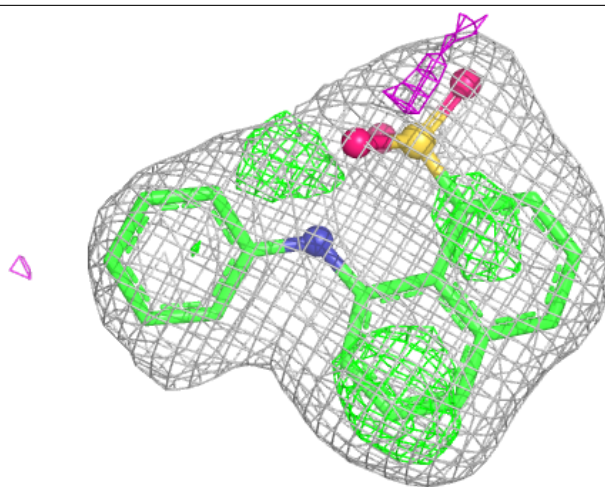
Electron density around 2AN b 203:

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



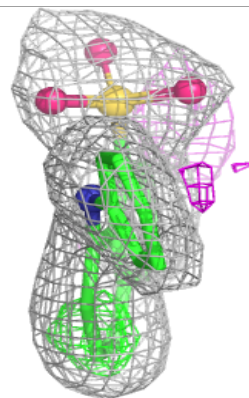
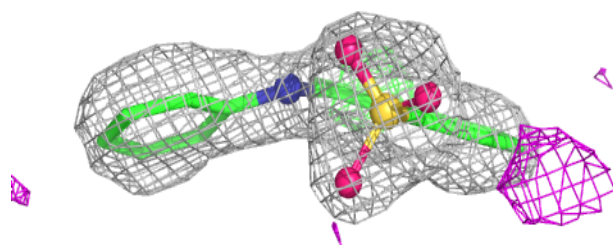
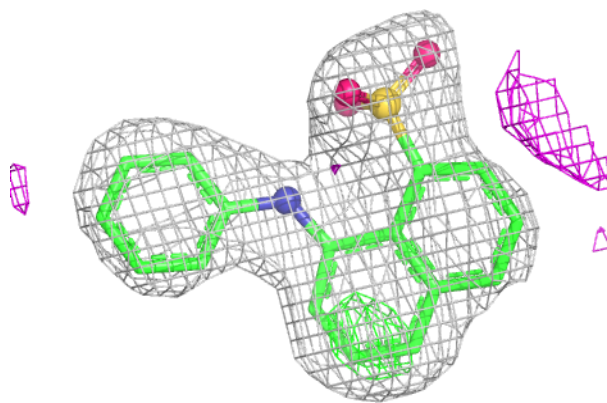
Electron density around 2AN B 203:

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

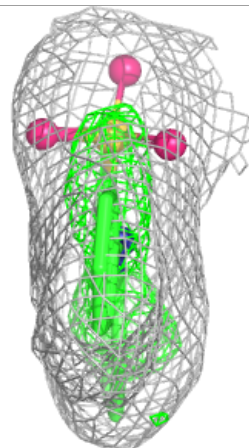
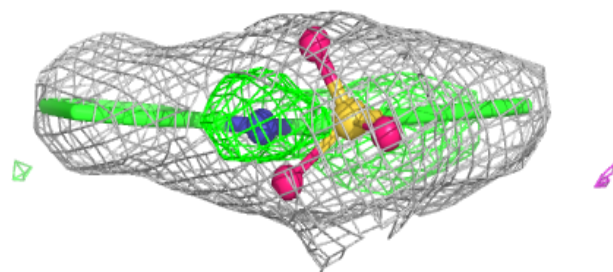
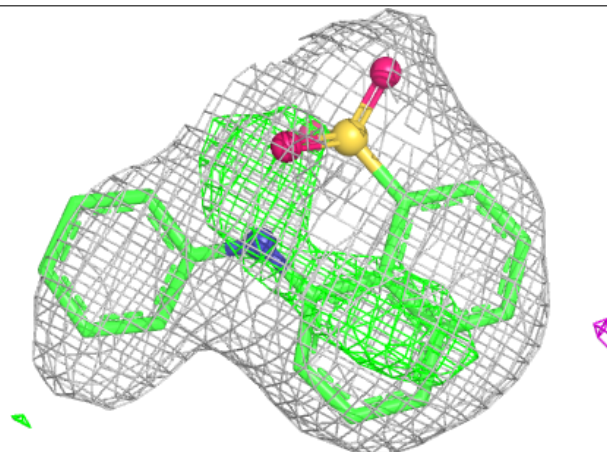


Electron density around 2AN i 201:

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

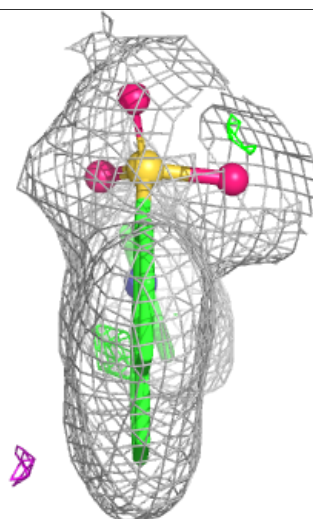
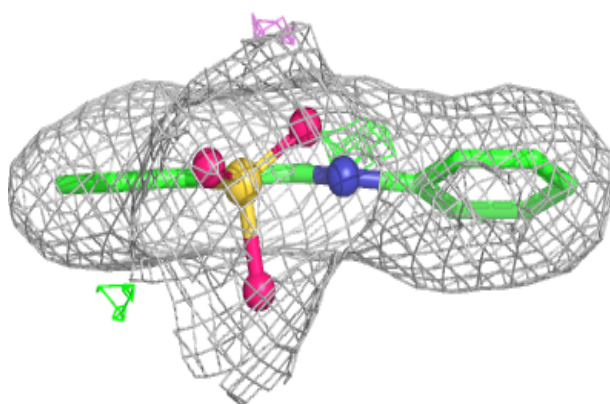
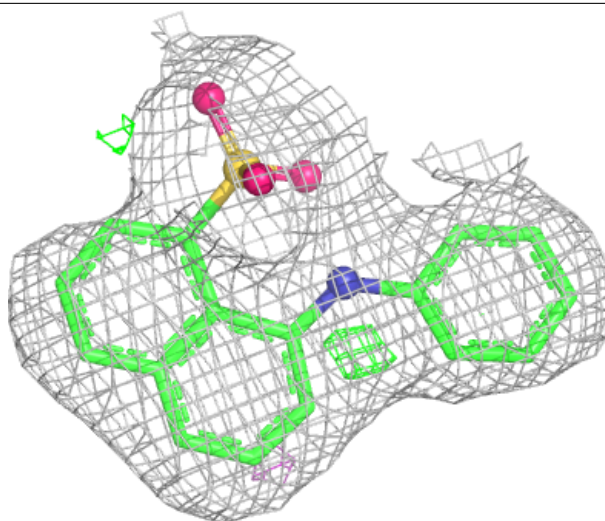
**Electron density around 2AN N 204:**

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



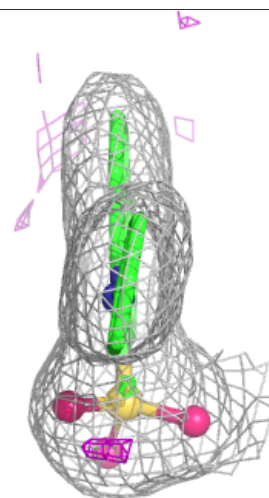
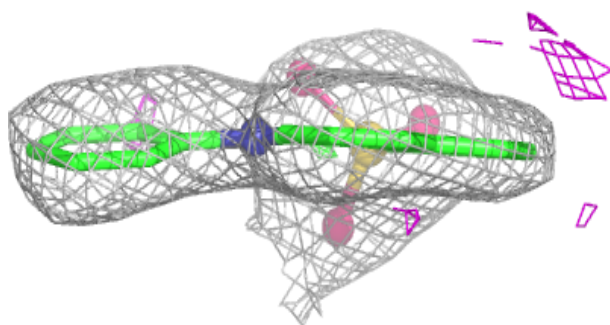
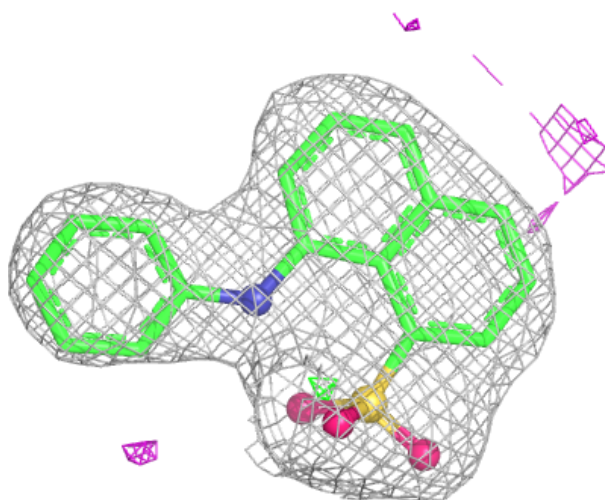
Electron density around 2AN V 201:

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



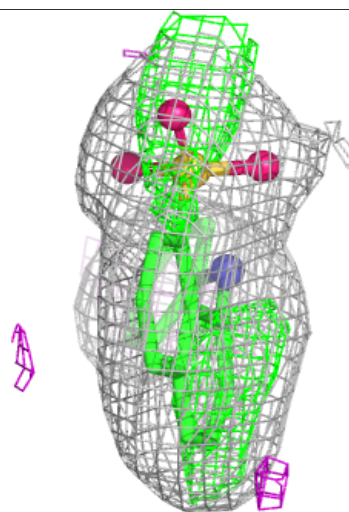
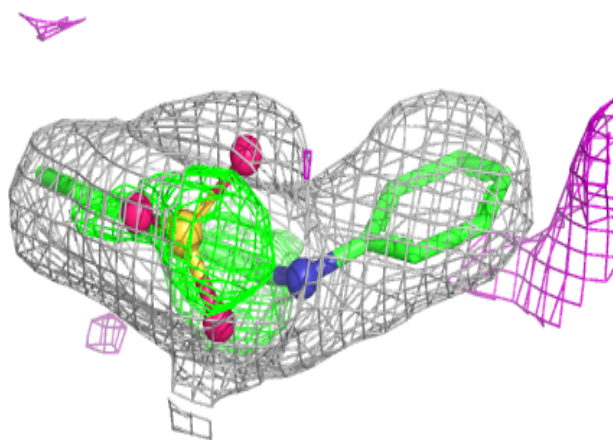
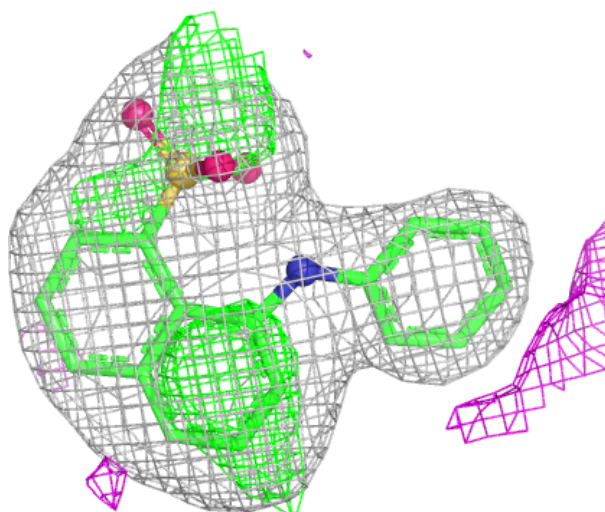
Electron density around 2AN c 204:

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



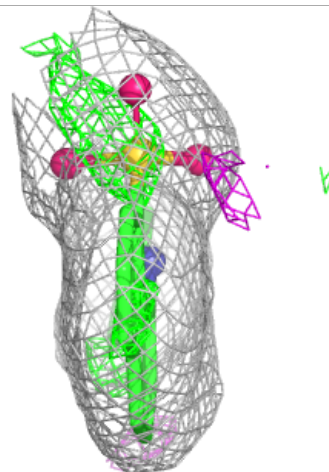
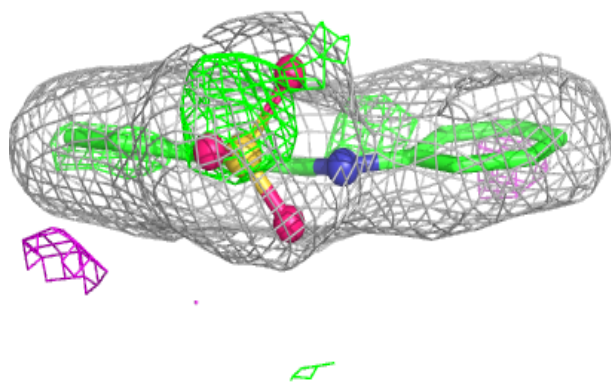
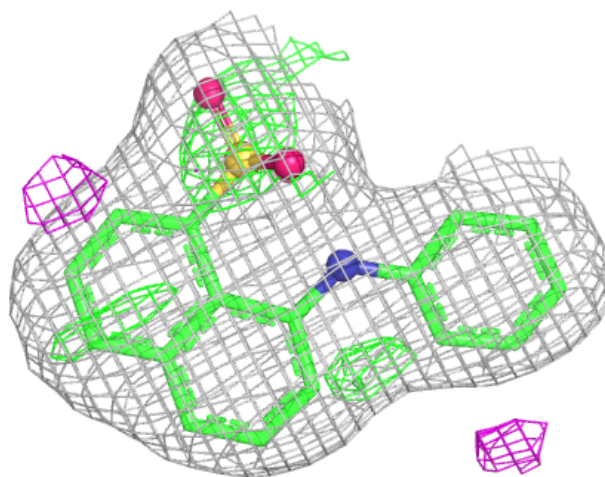
Electron density around 2AN P 204:

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



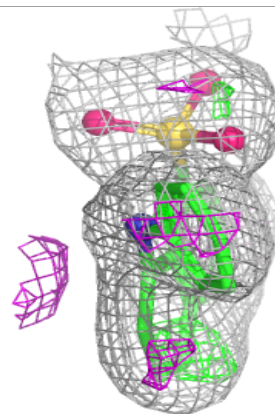
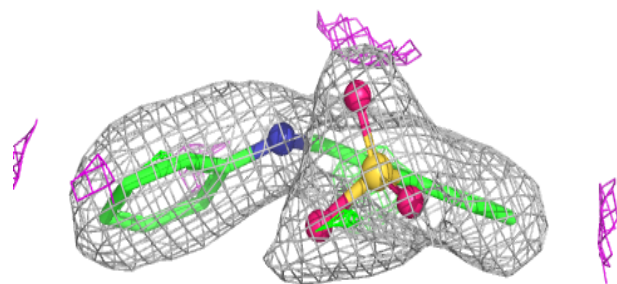
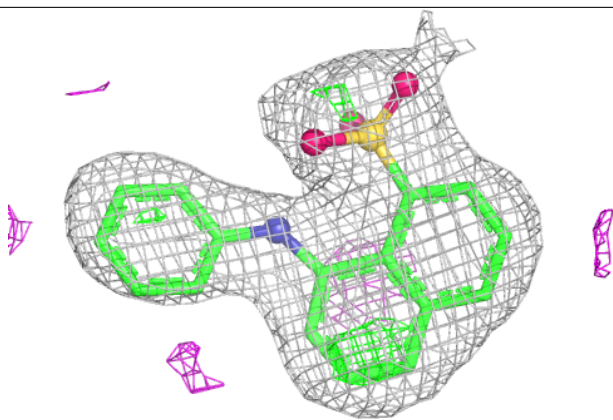
Electron density around 2AN b 201:

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



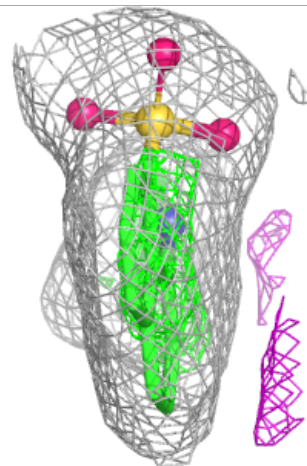
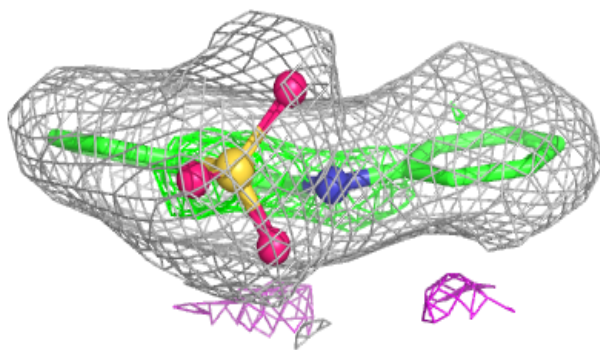
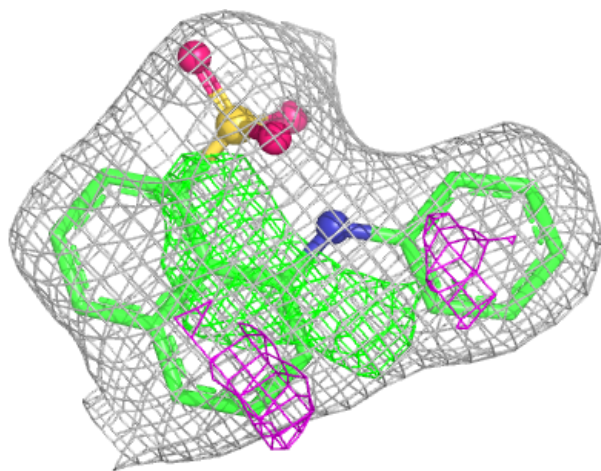
Electron density around 2AN T 202:

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



Electron density around 2AN J 202:

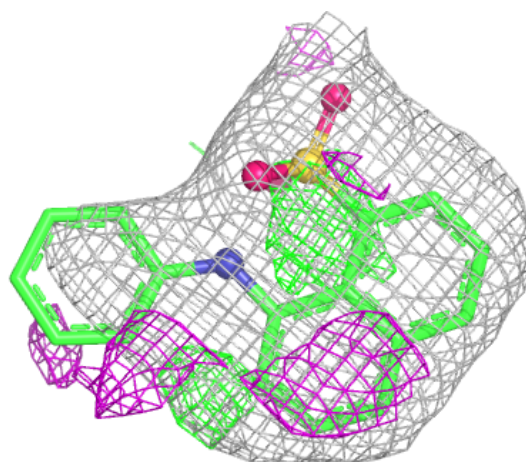
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



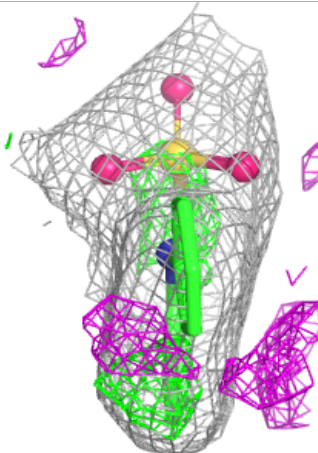
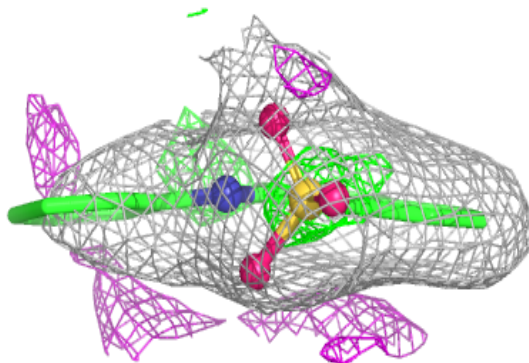
Electron density around 2AN G 203:

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

✓

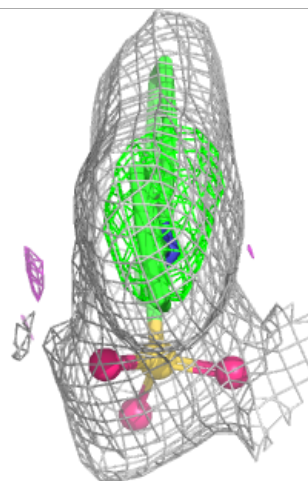
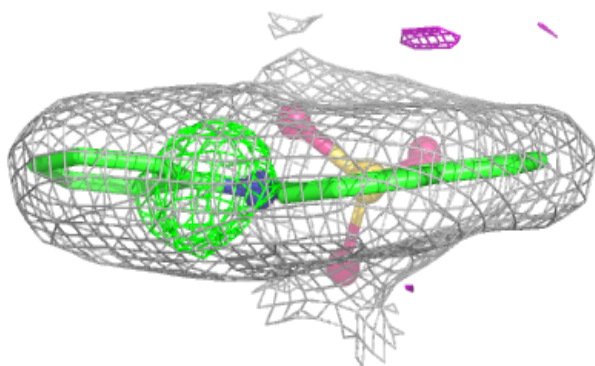
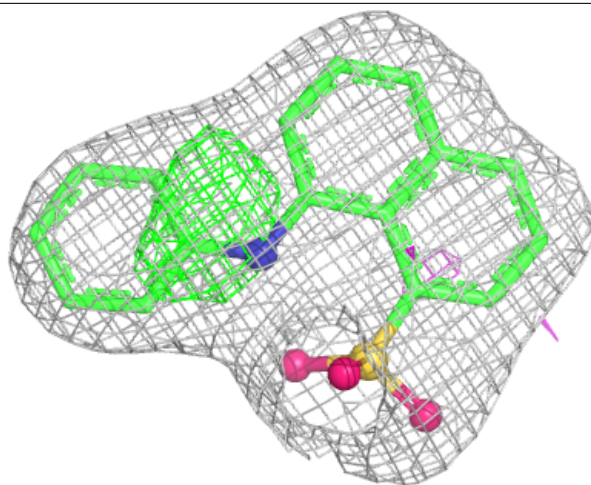


✓



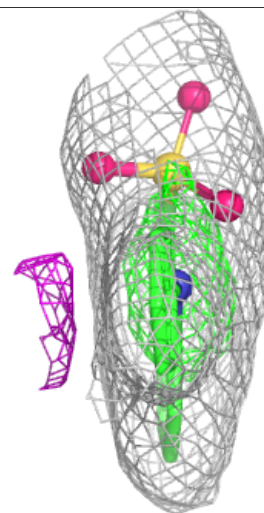
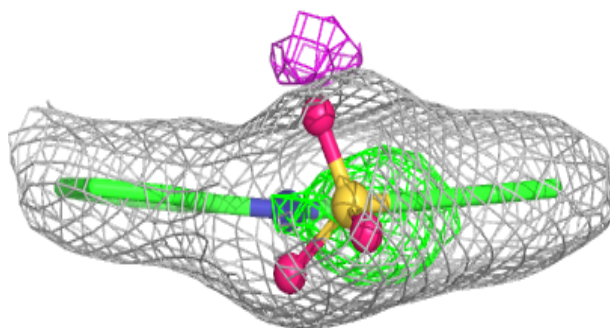
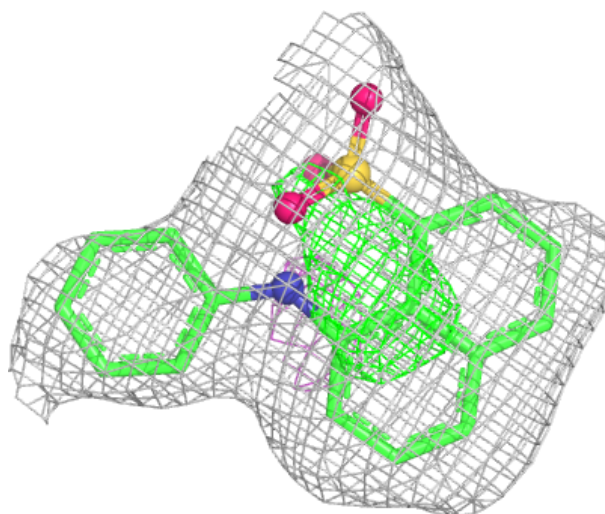
Electron density around 2AN f 205:

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



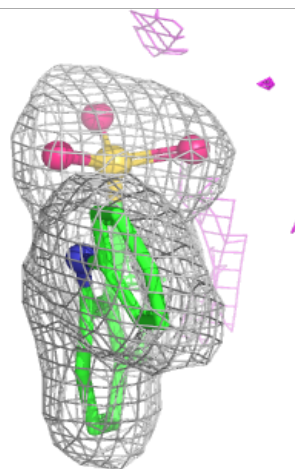
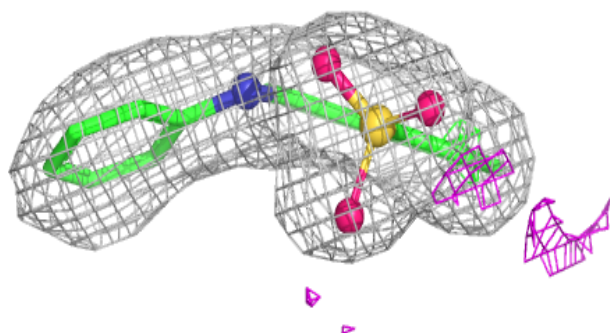
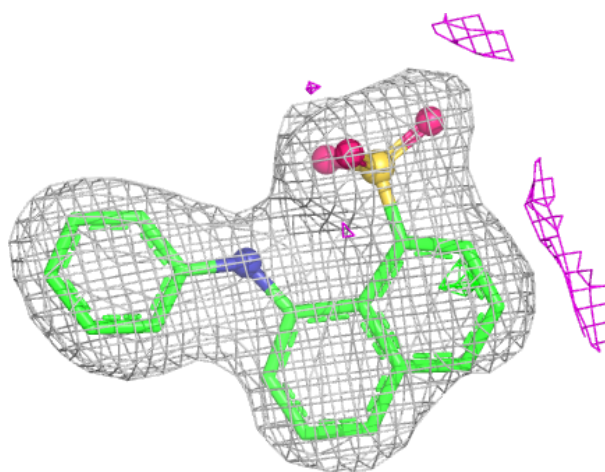
Electron density around 2AN O 201:

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



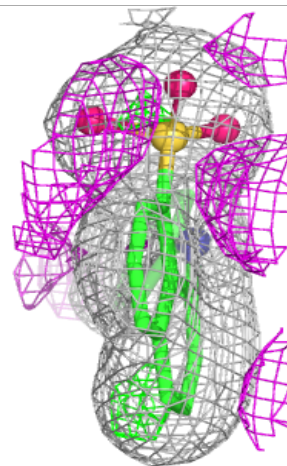
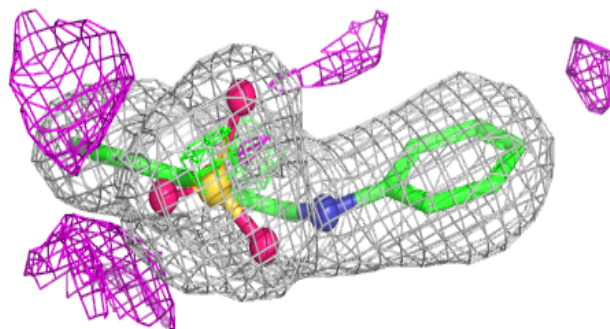
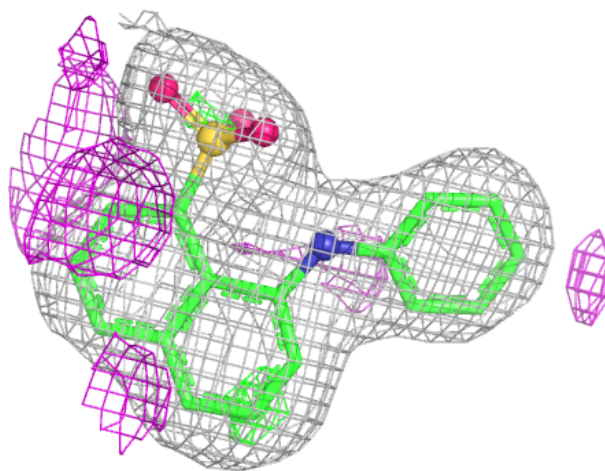
Electron density around 2AN S 202:

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



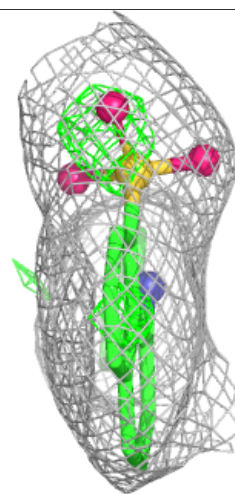
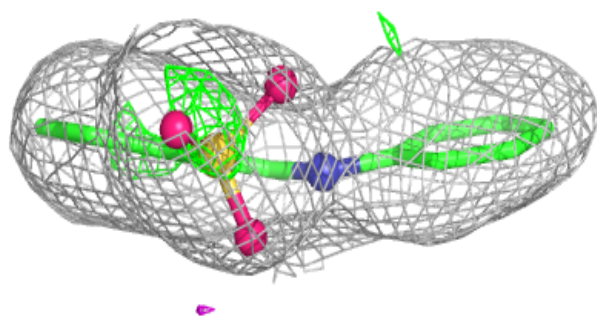
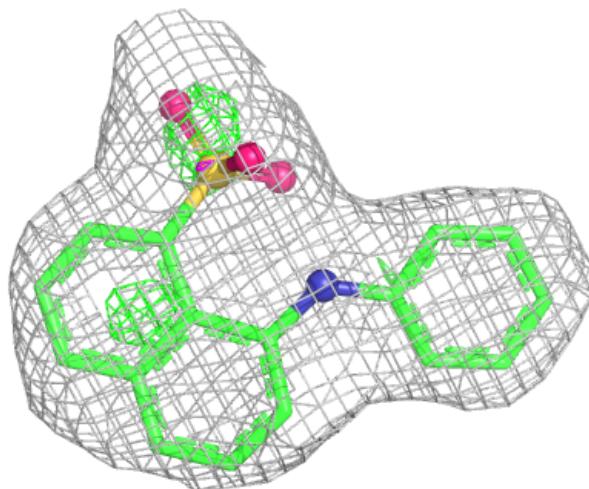
Electron density around 2AN e 201:

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



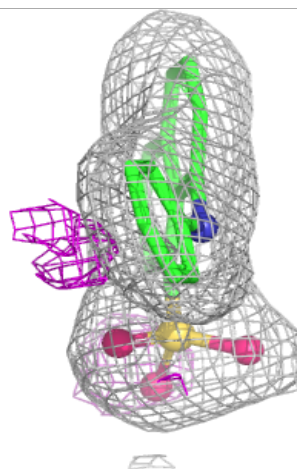
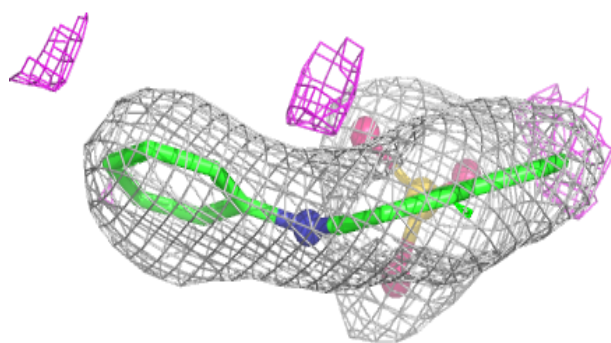
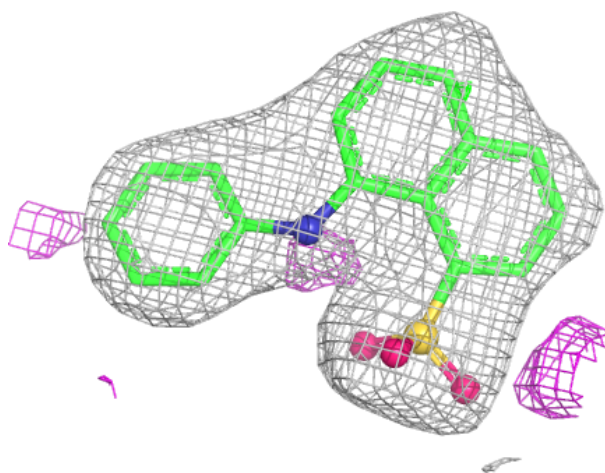
Electron density around 2AN Q 202:

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



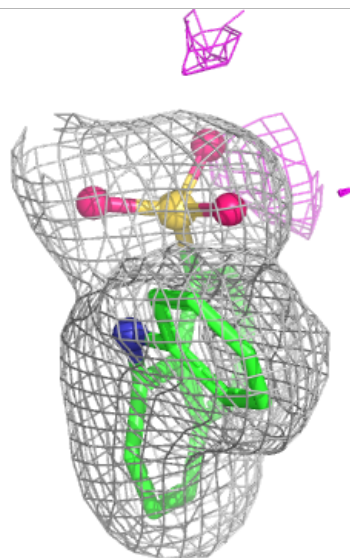
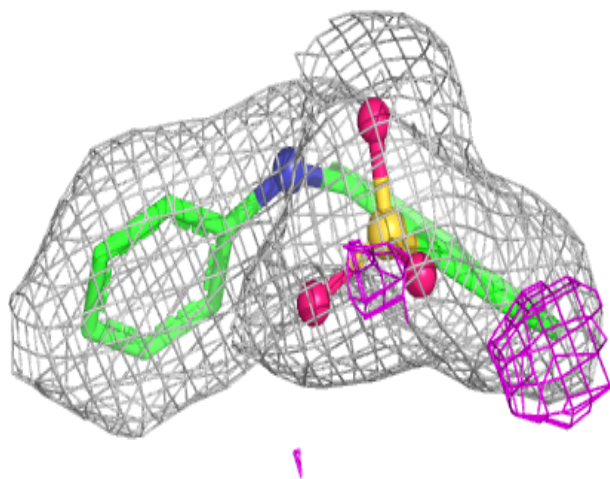
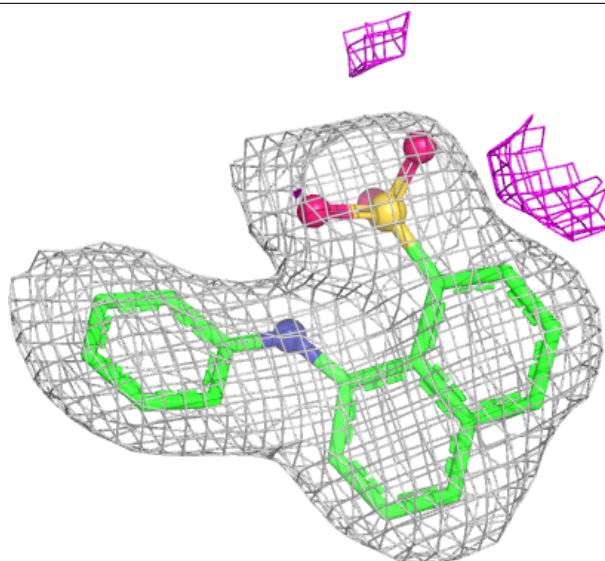
Electron density around 2AN a 202:

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



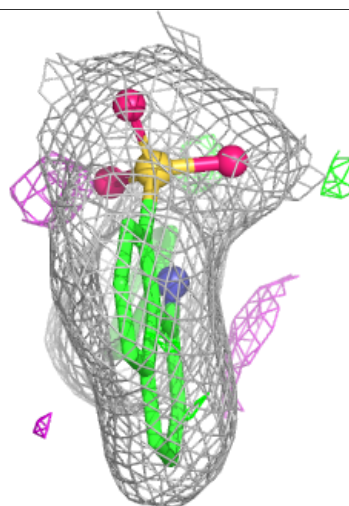
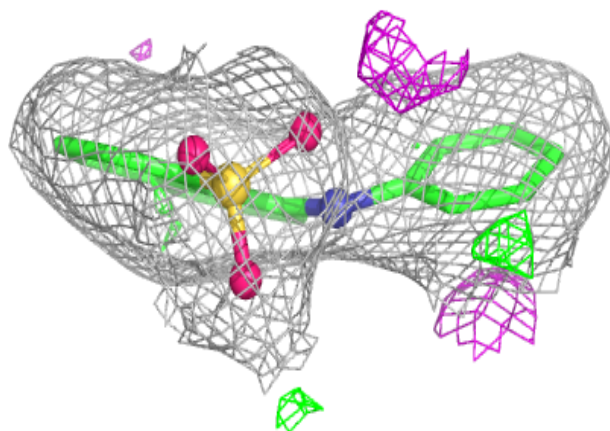
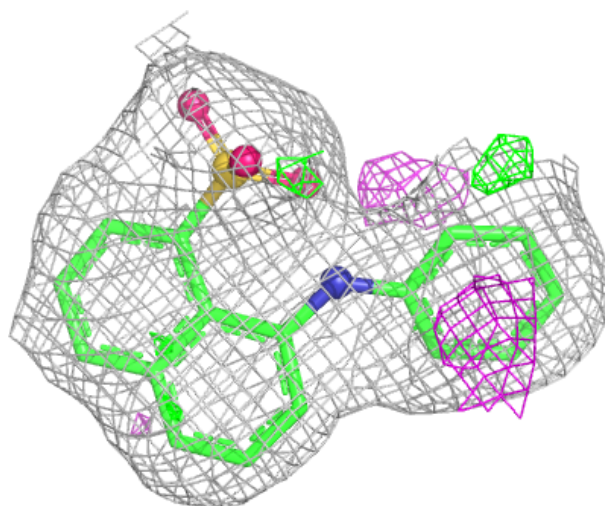
Electron density around 2AN L 203:

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



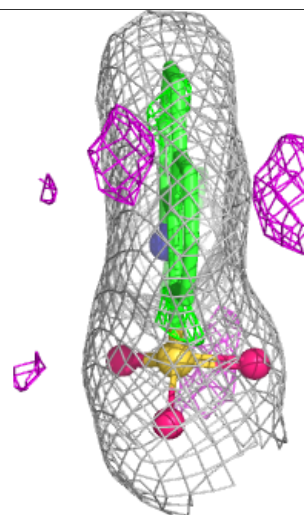
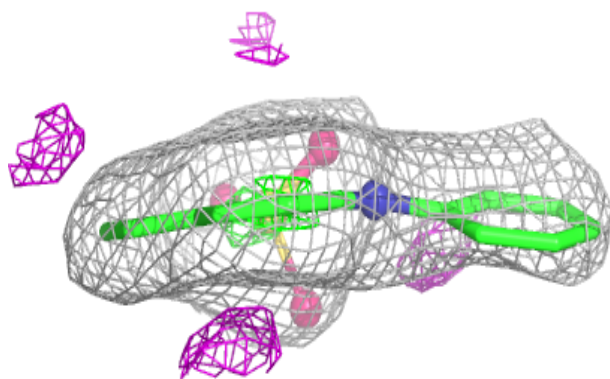
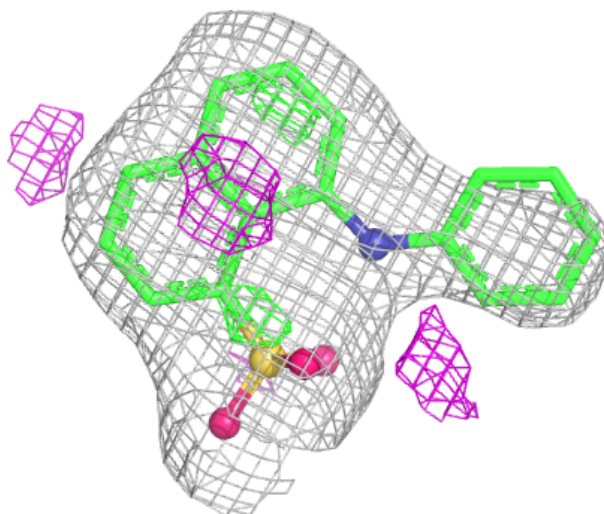
Electron density around 2AN B 202:

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



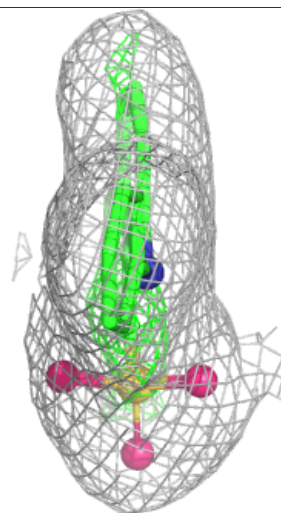
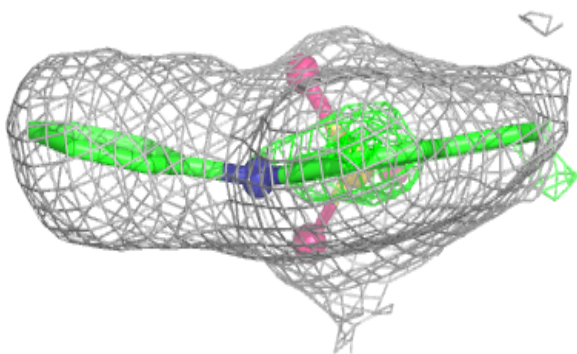
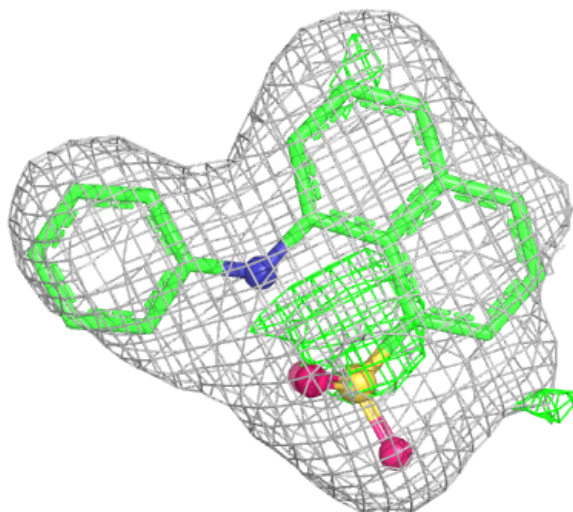
Electron density around 2AN A 201:

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



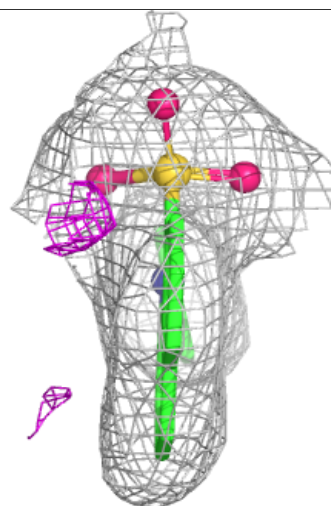
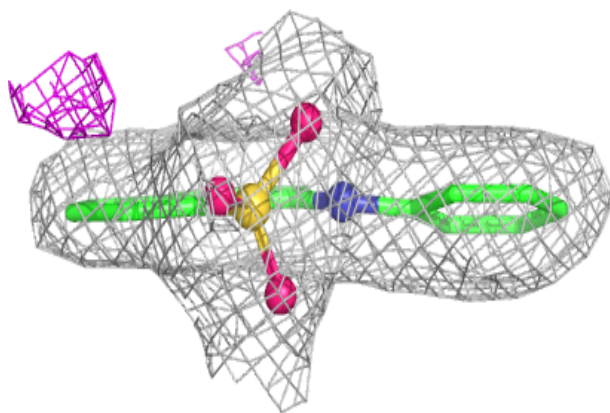
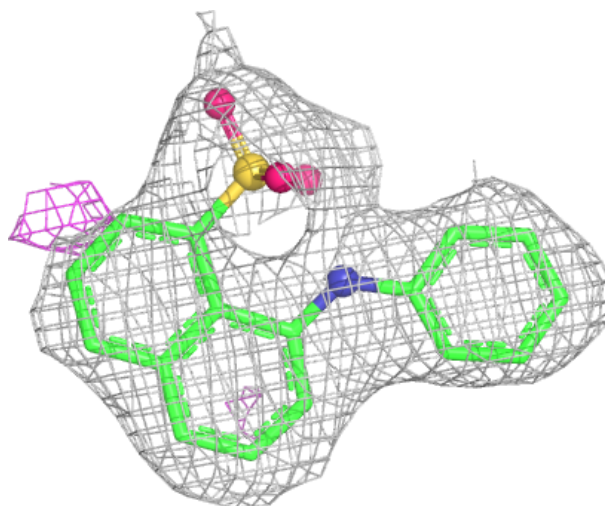
Electron density around 2AN F 203:

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



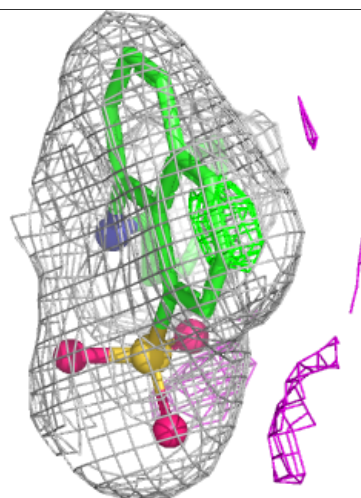
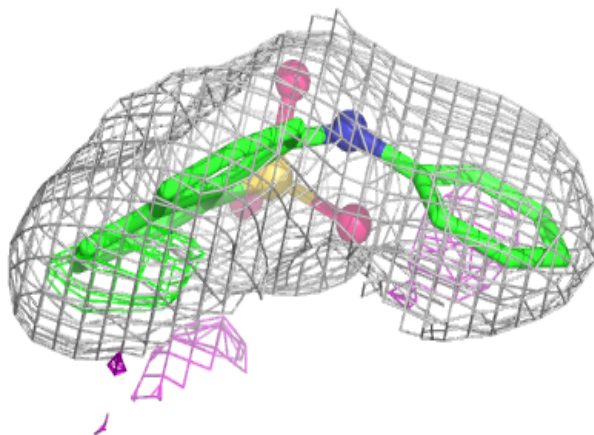
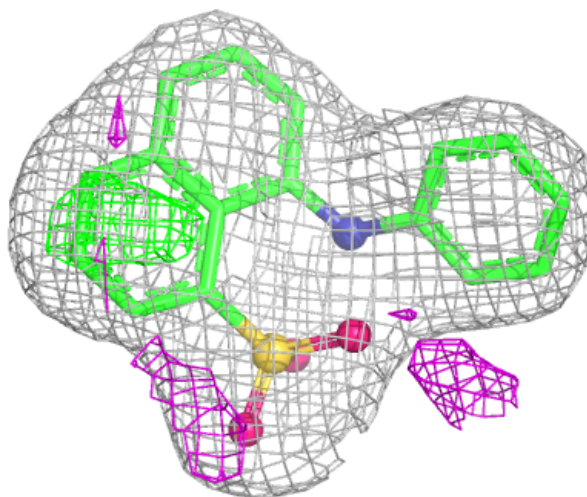
Electron density around 2AN V 204:

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



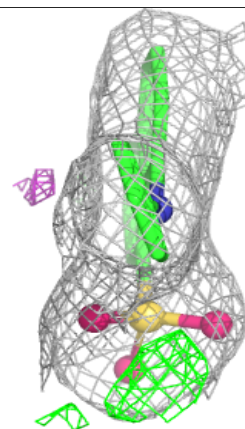
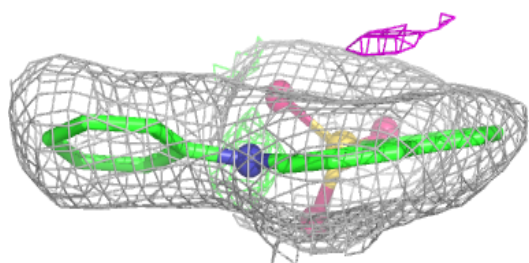
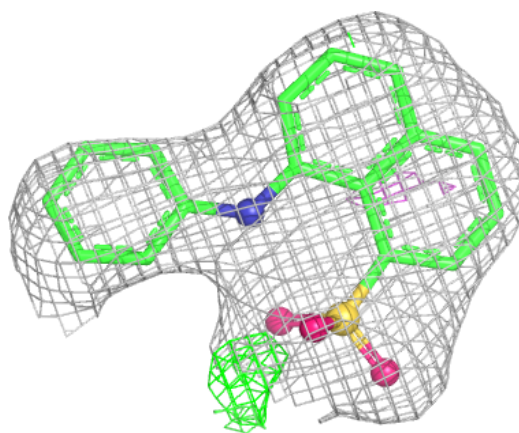
Electron density around 2AN V 205:

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



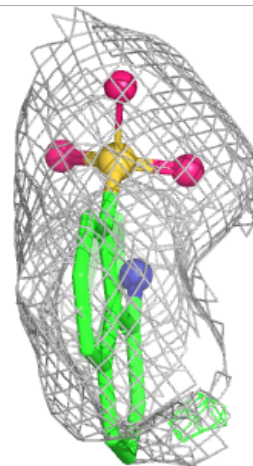
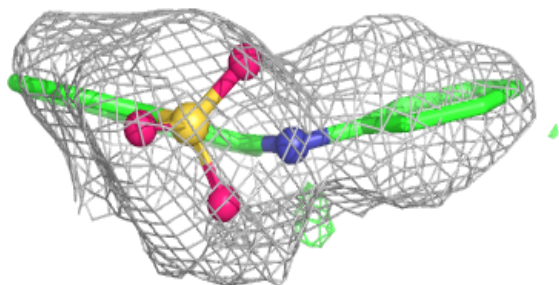
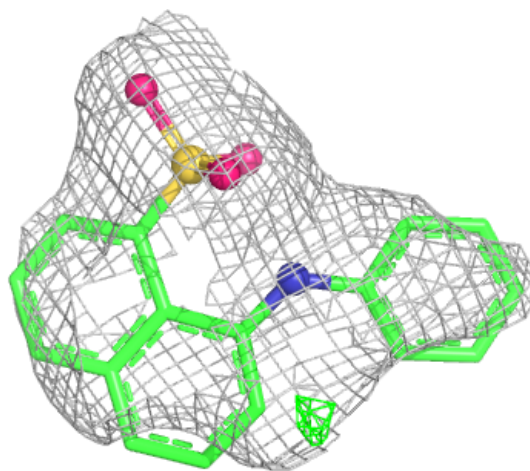
Electron density around 2AN Z 203:

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



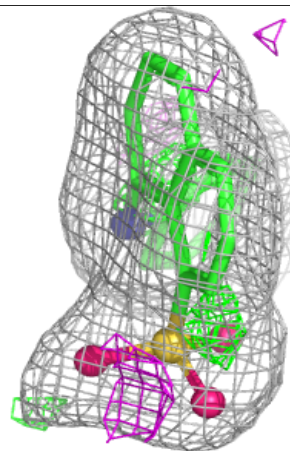
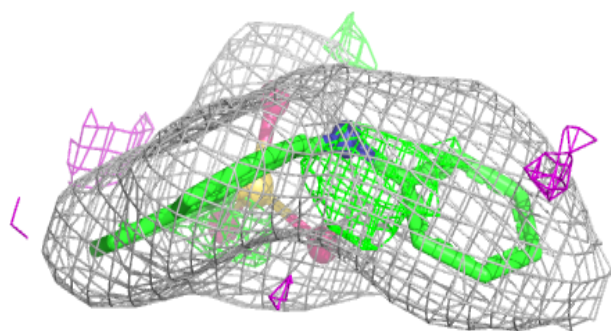
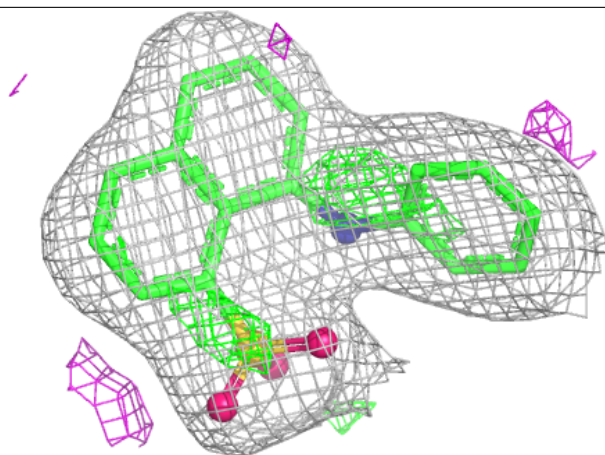
Electron density around 2AN C 202:

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



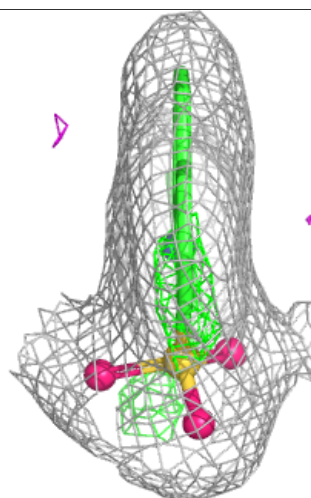
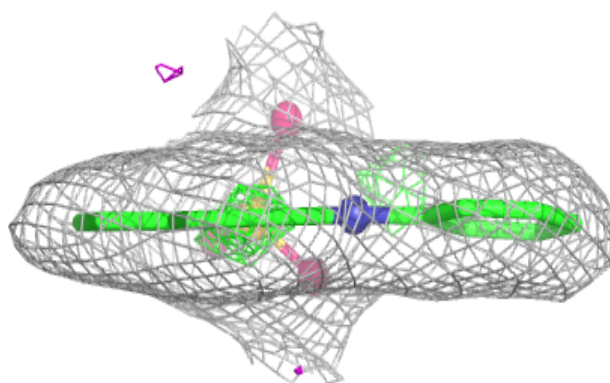
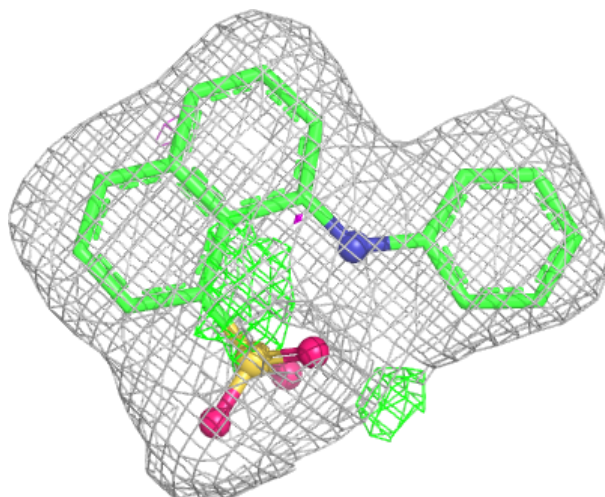
Electron density around 2AN P 202:

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



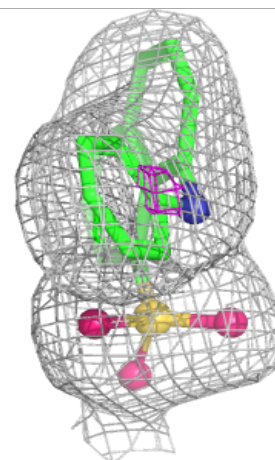
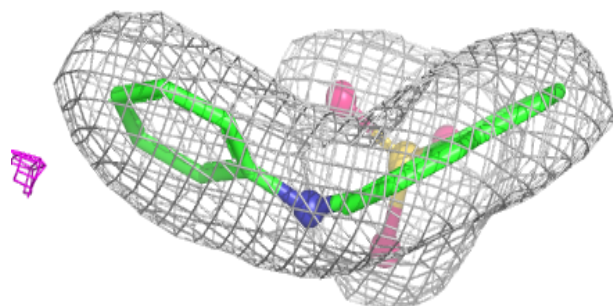
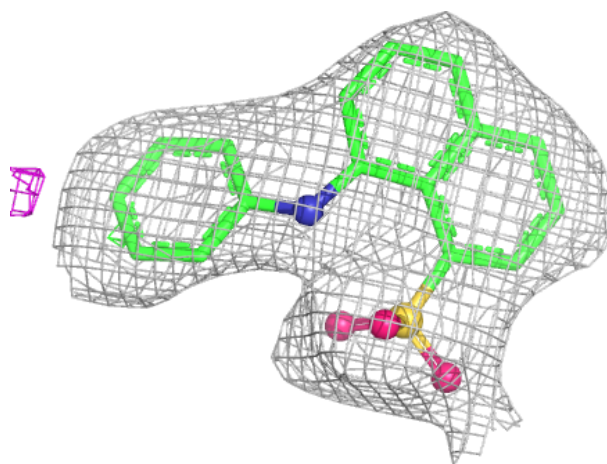
Electron density around 2AN L 202:

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



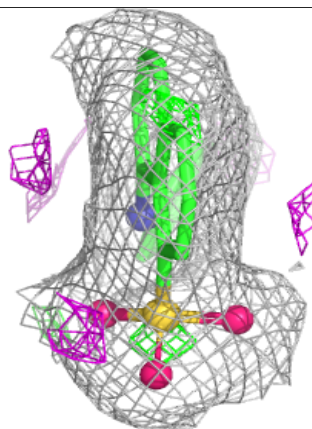
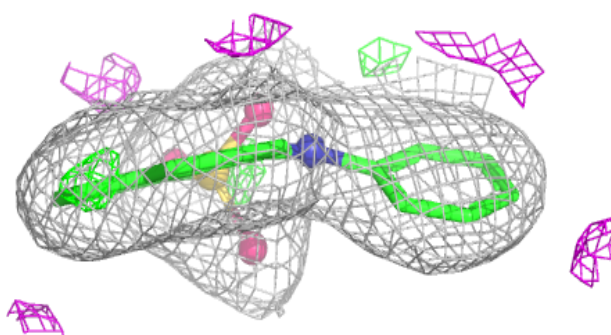
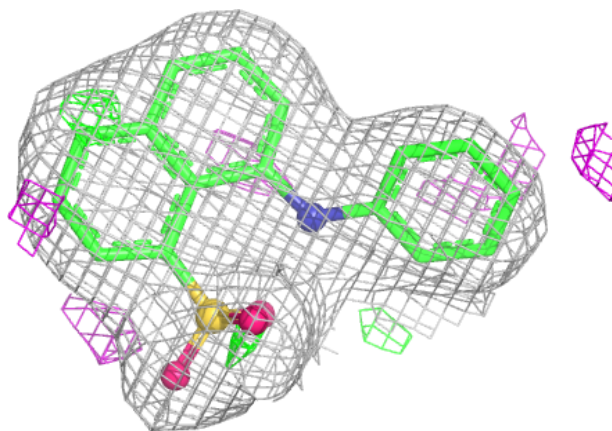
Electron density around 2AN H 202:

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



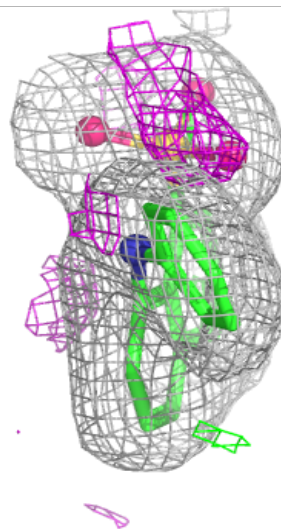
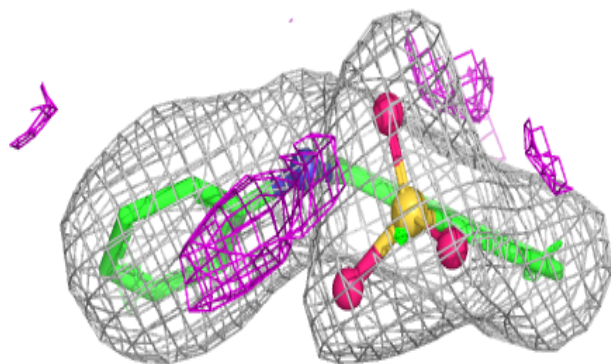
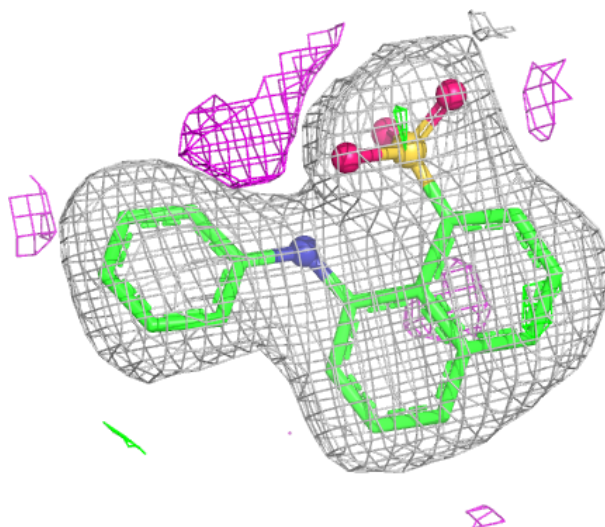
Electron density around 2AN V 203:

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



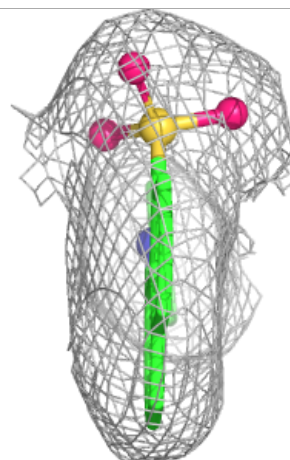
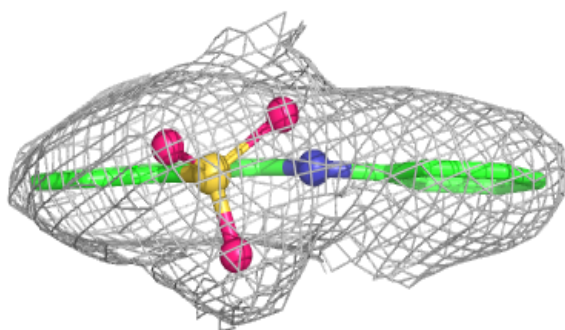
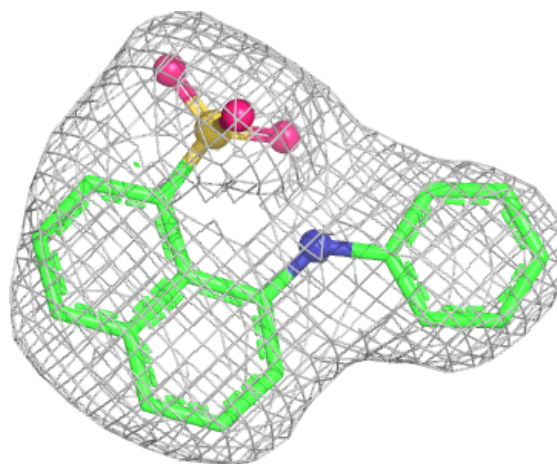
Electron density around 2AN f 202:

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



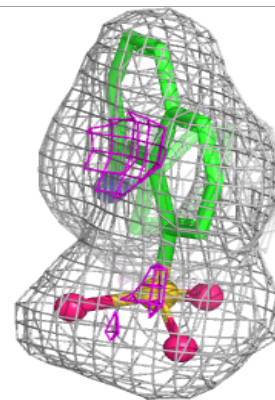
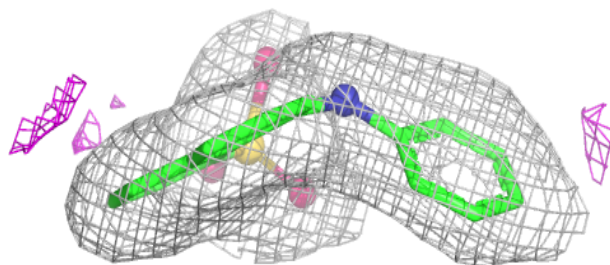
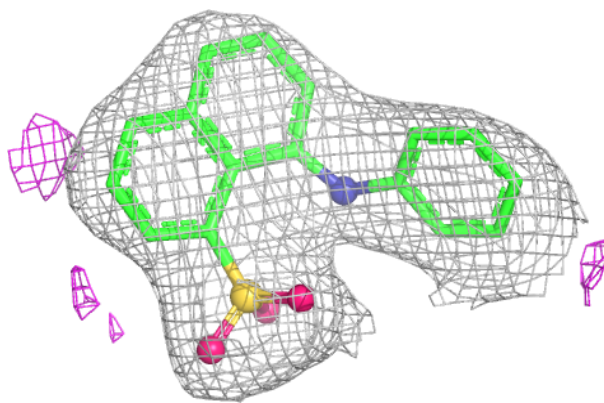
Electron density around 2AN H 203:

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



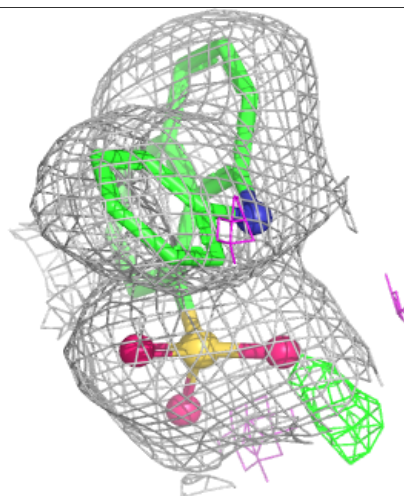
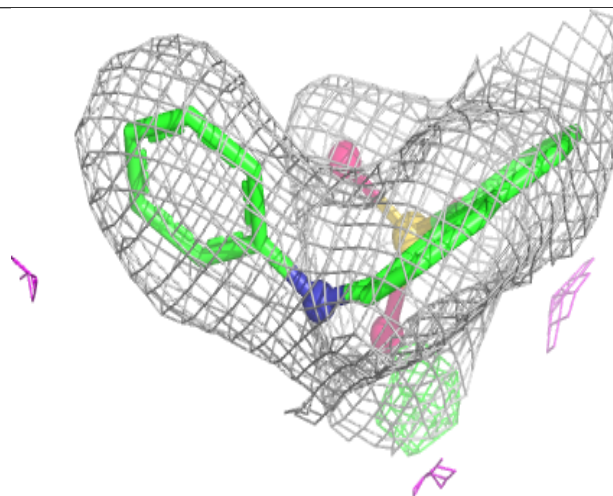
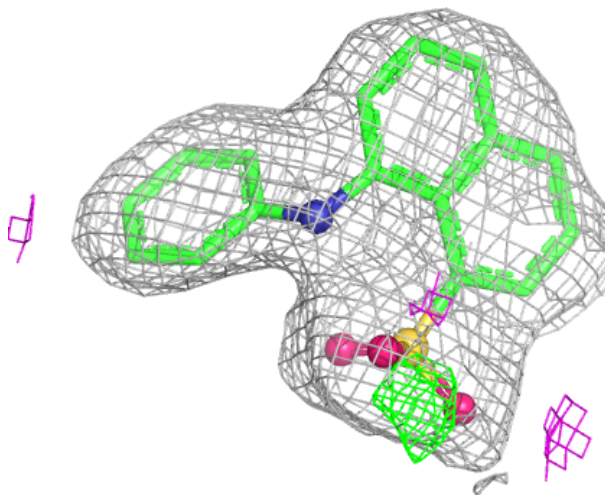
Electron density around 2AN B 201:

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



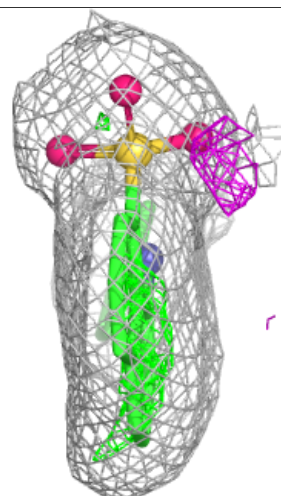
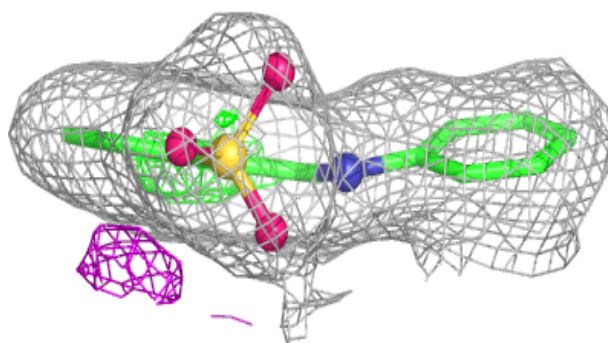
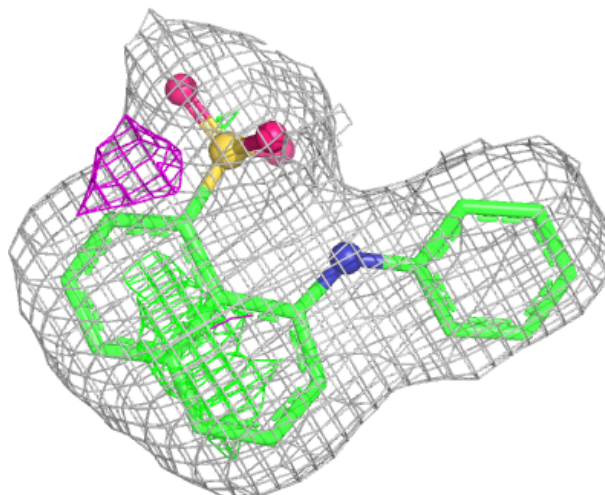
Electron density around 2AN J 203:

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



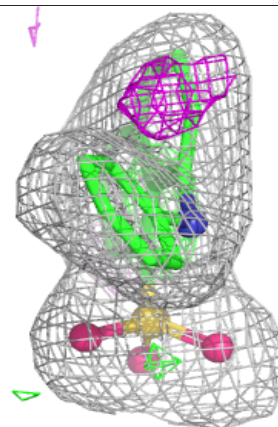
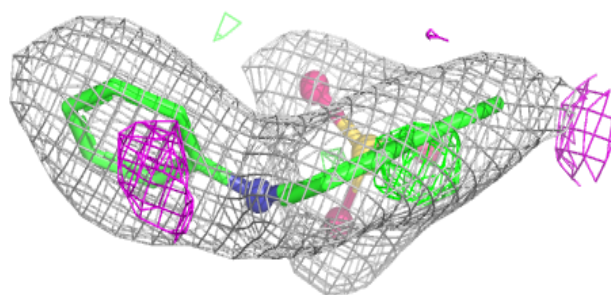
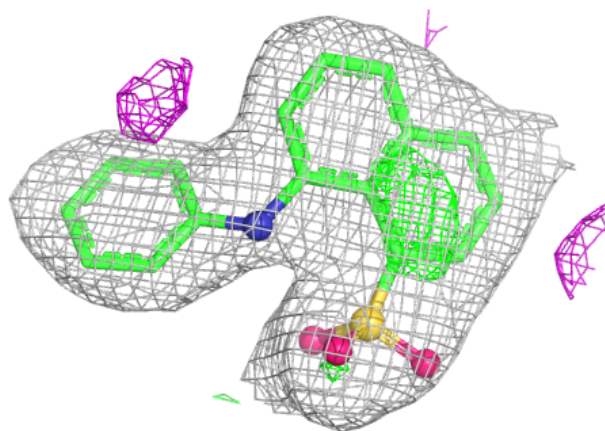
Electron density around 2AN E 201:

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



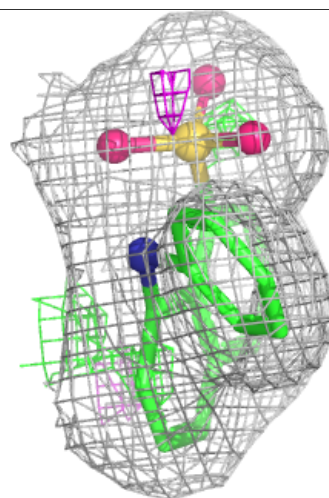
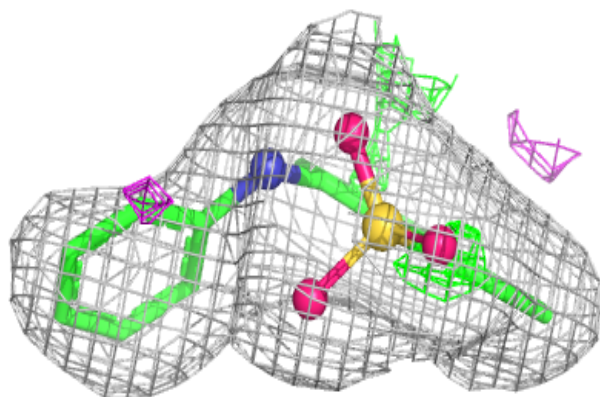
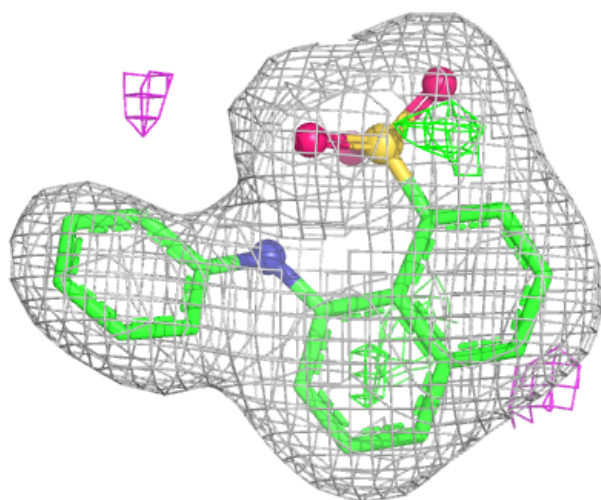
Electron density around 2AN E 202:

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



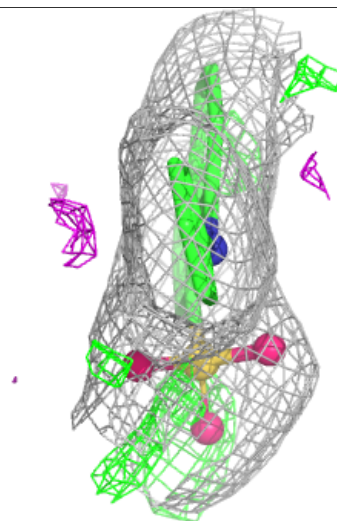
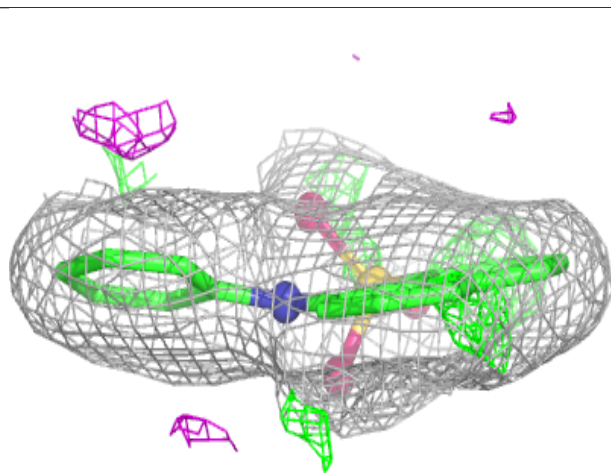
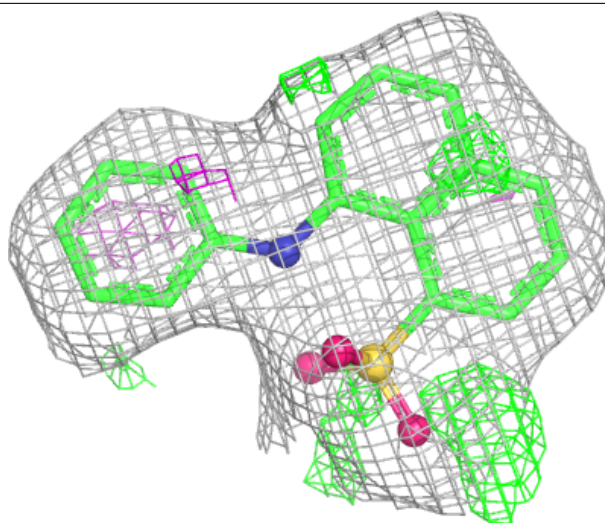
Electron density around 2AN G 202:

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



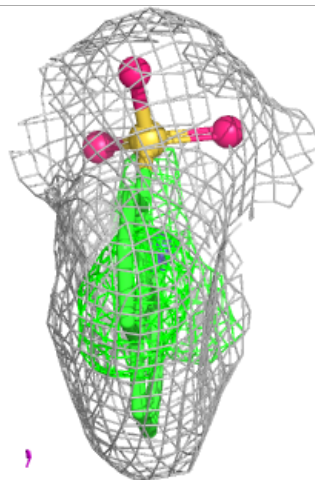
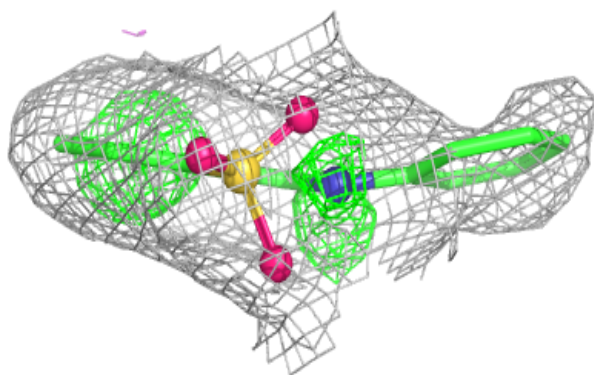
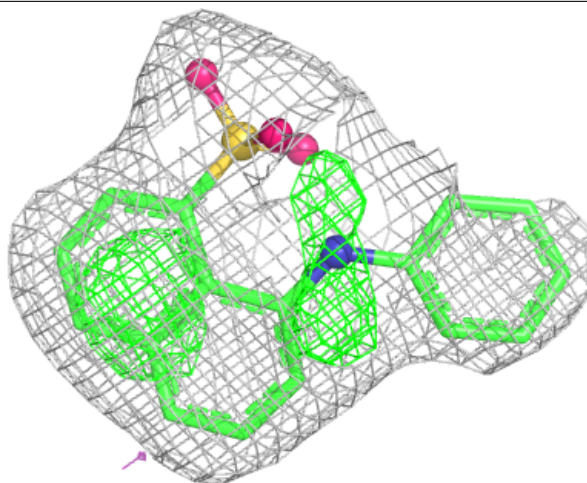
Electron density around 2AN T 201:

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



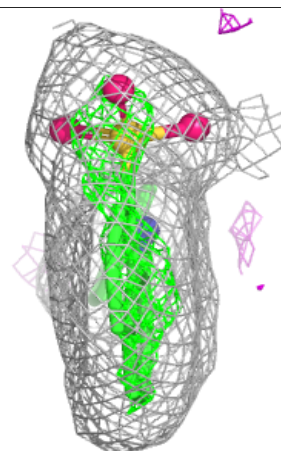
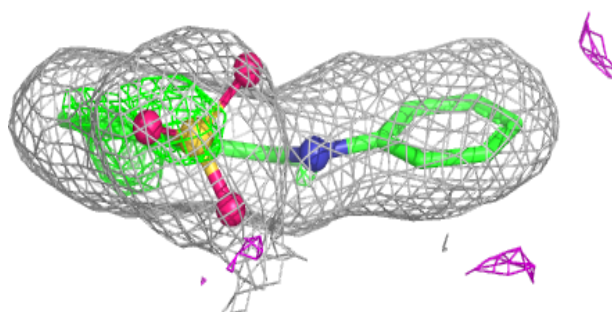
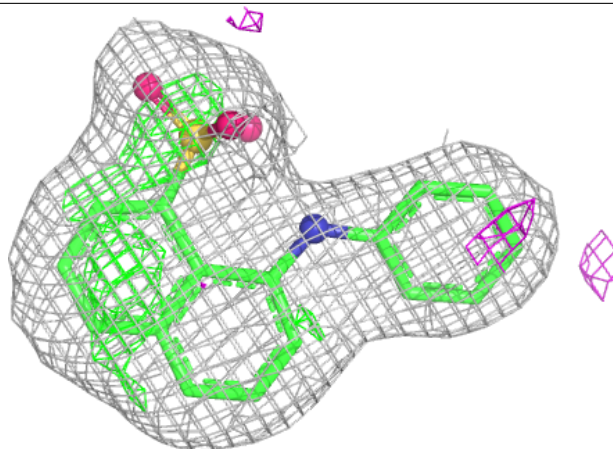
Electron density around 2AN h 204:

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



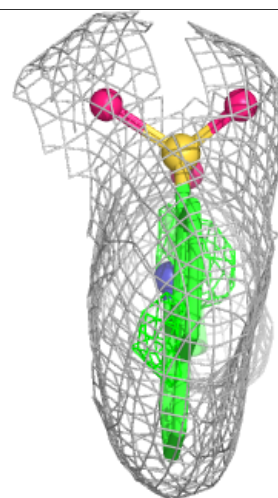
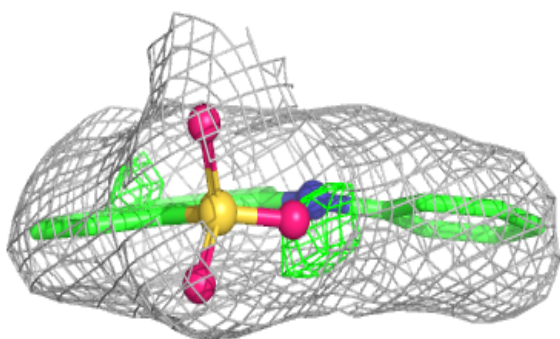
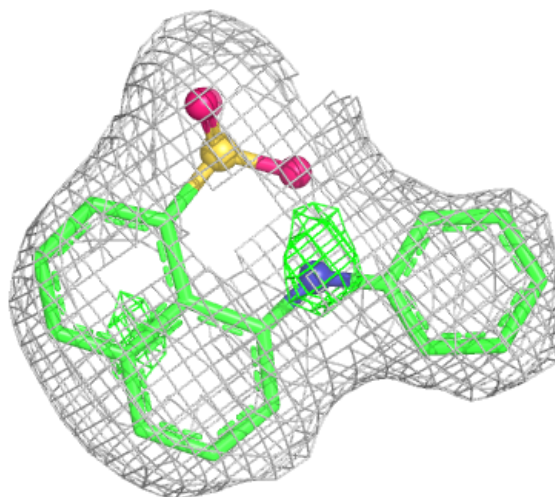
Electron density around 2AN I 202:

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



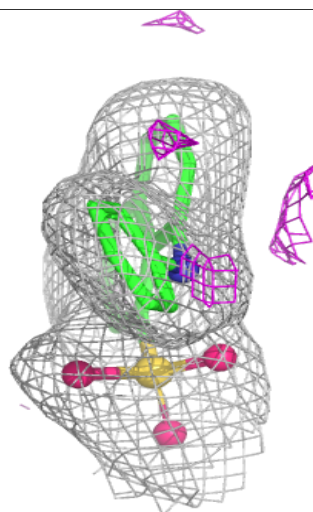
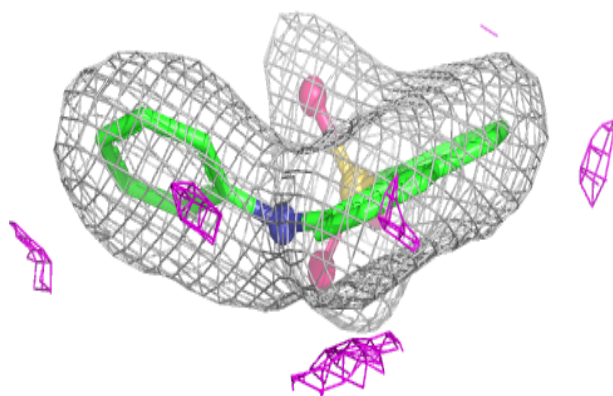
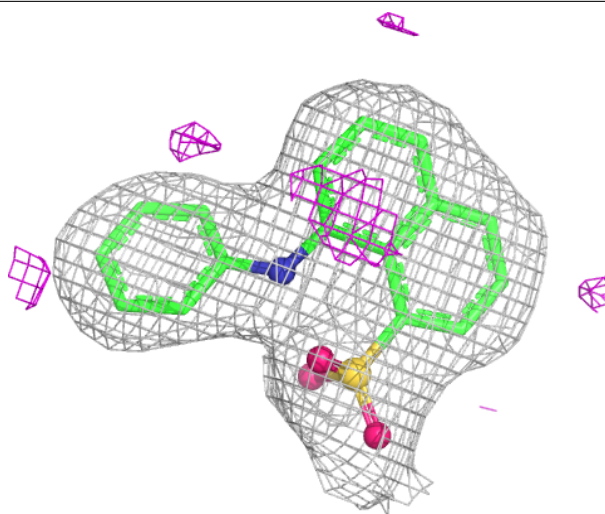
Electron density around 2AN R 203:

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



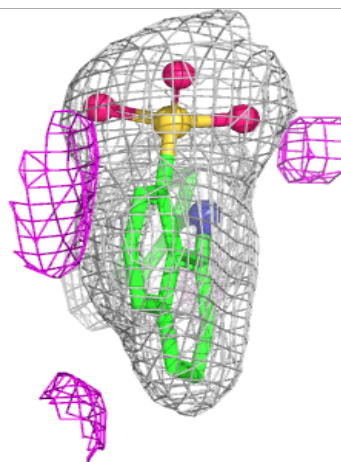
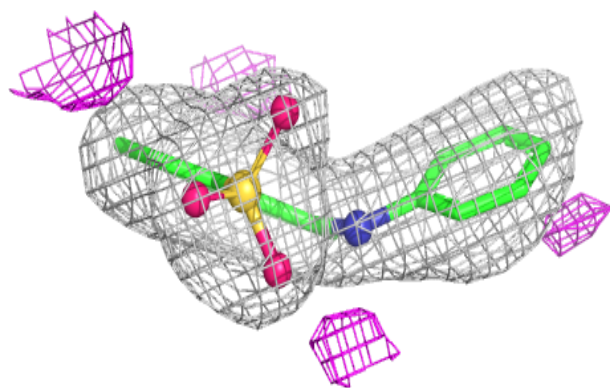
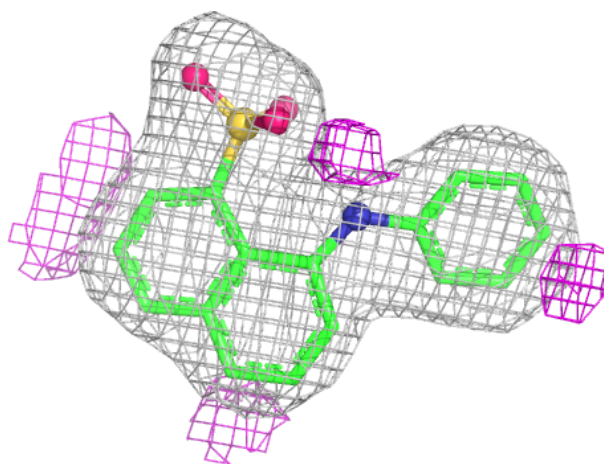
Electron density around 2AN K 201:

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



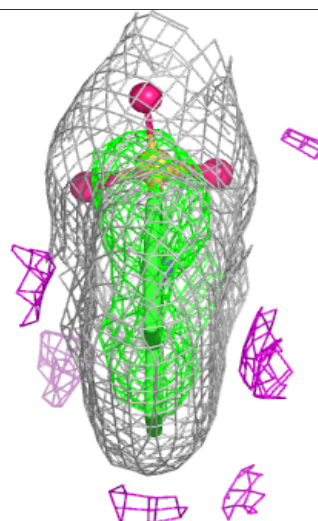
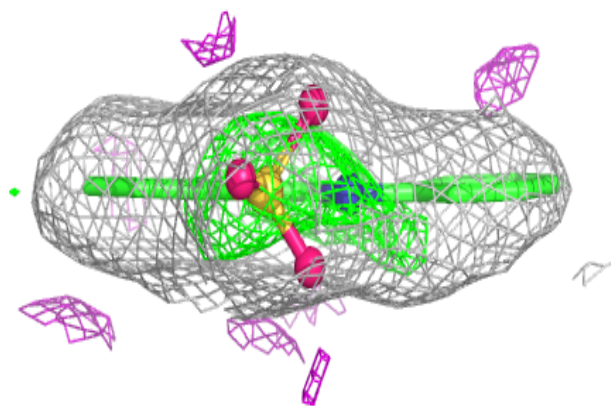
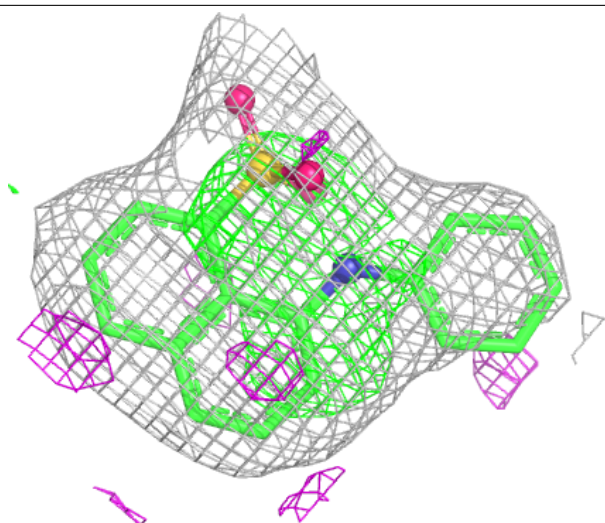
Electron density around 2AN g 202:

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



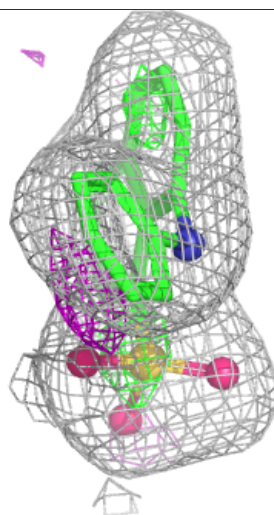
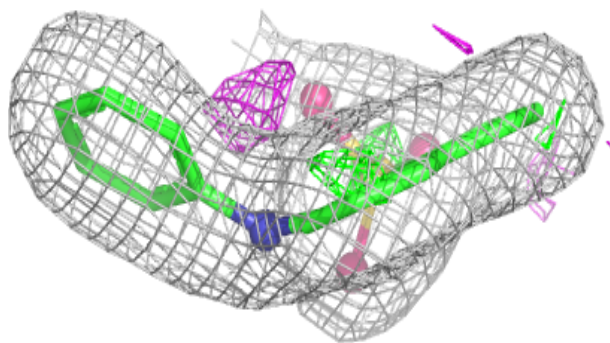
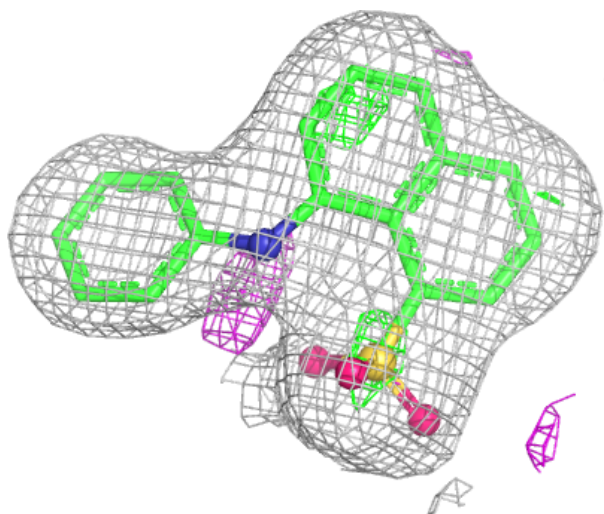
Electron density around 2AN K 202:

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



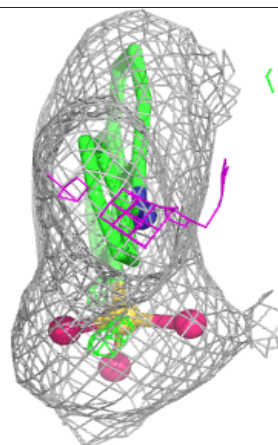
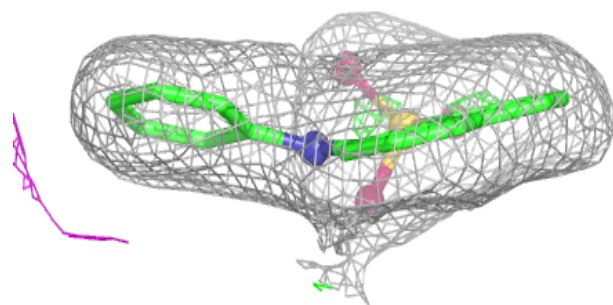
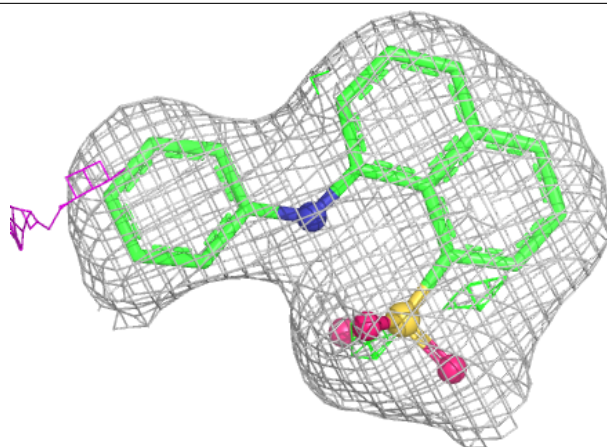
Electron density around 2AN V 202:

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



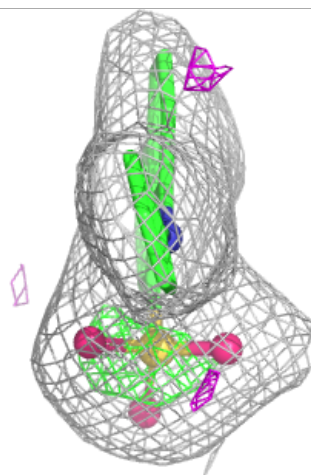
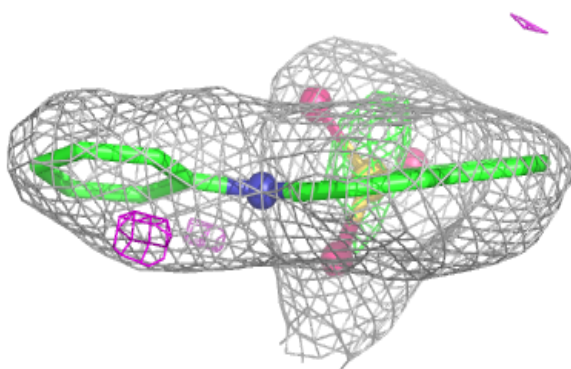
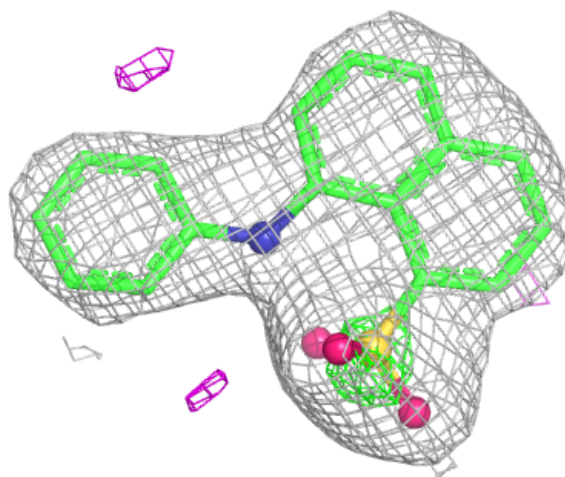
Electron density around 2AN h 202:

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



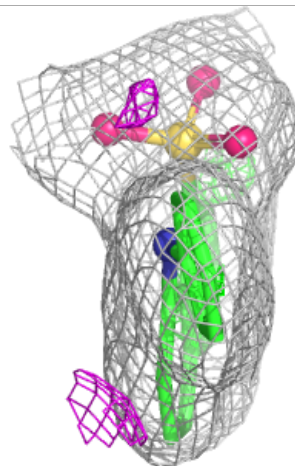
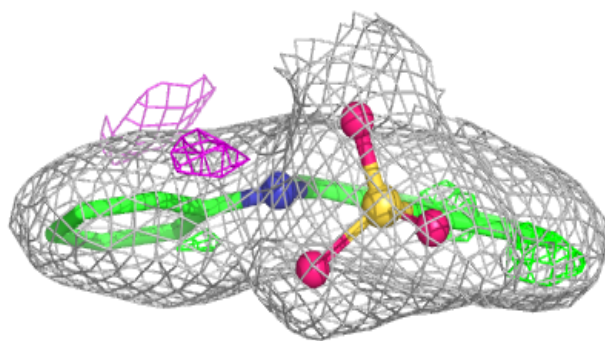
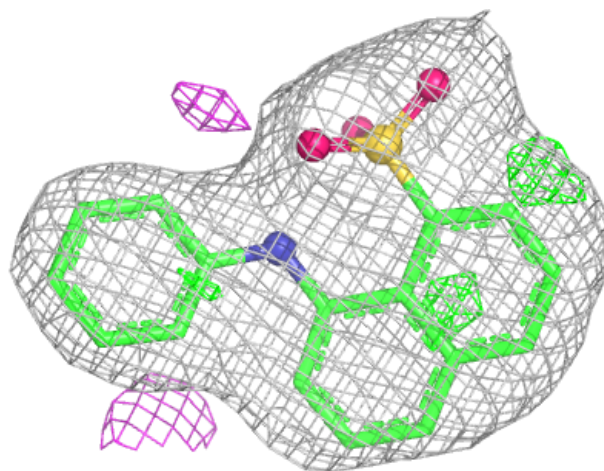
Electron density around 2AN D 201:

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



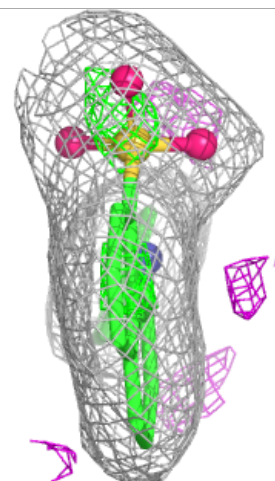
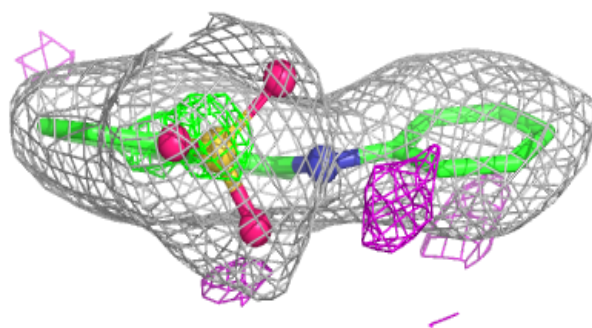
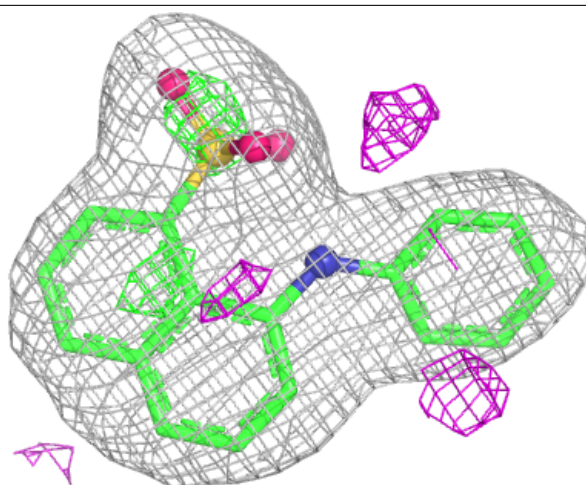
Electron density around 2AN N 201:

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



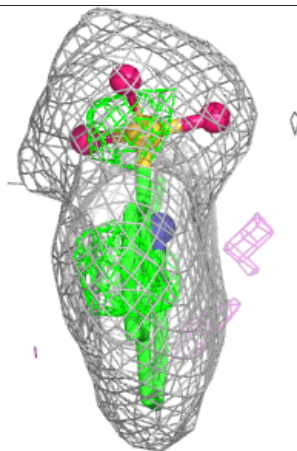
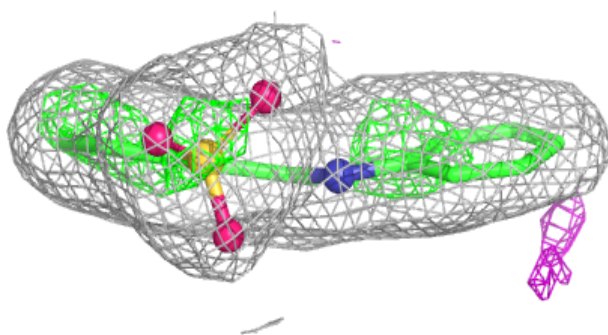
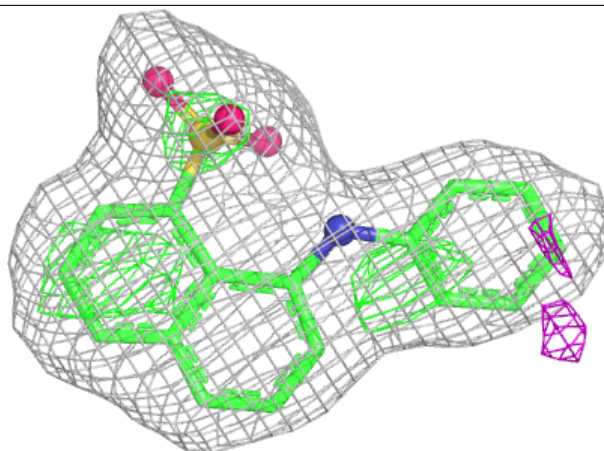
Electron density around 2AN H 201:

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



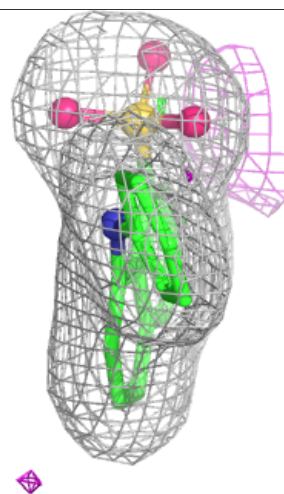
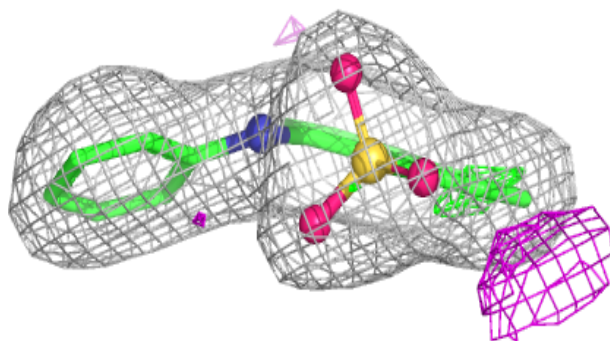
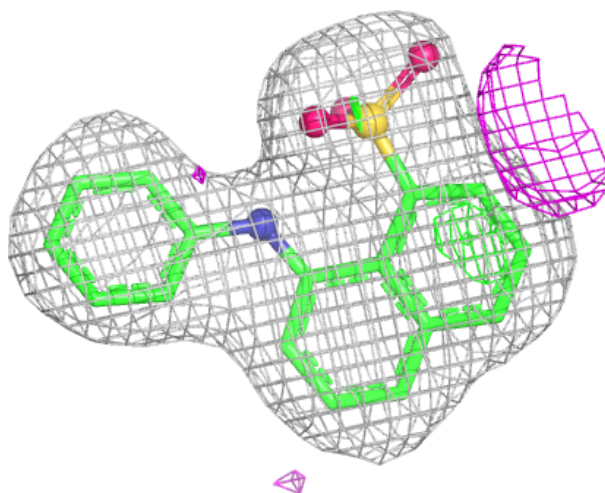
Electron density around 2AN M 201:

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



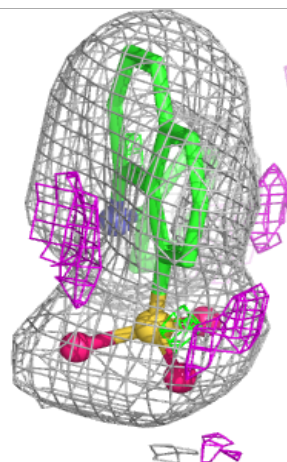
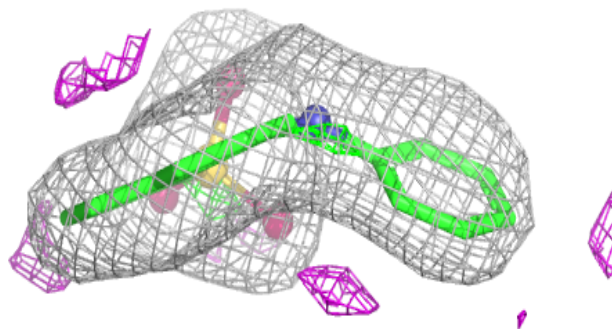
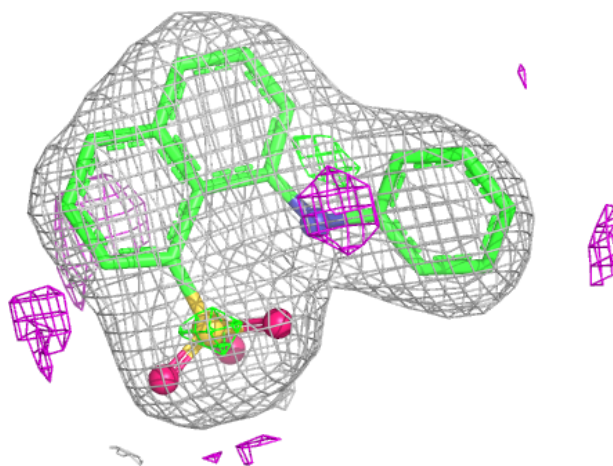
Electron density around 2AN c 206:

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



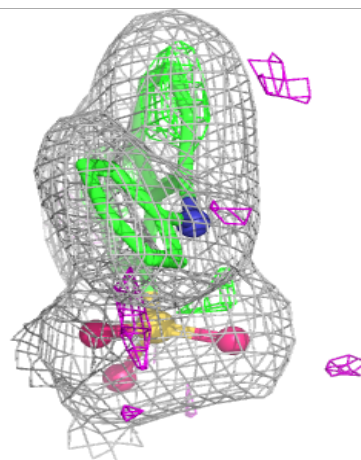
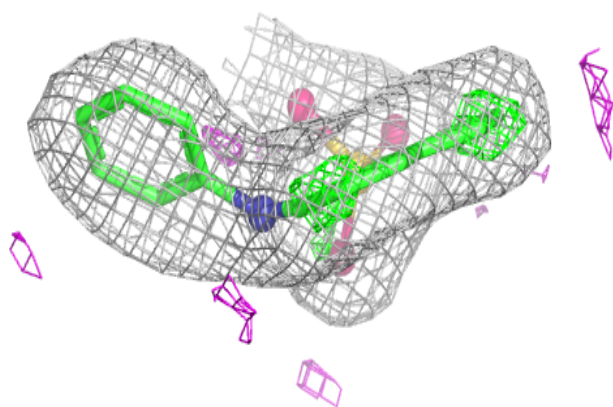
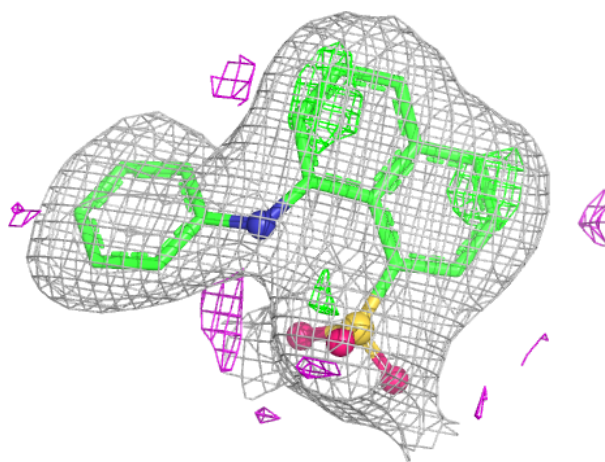
Electron density around 2AN N 202:

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



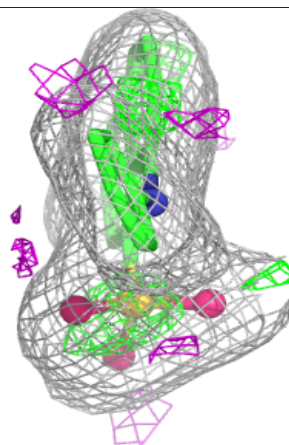
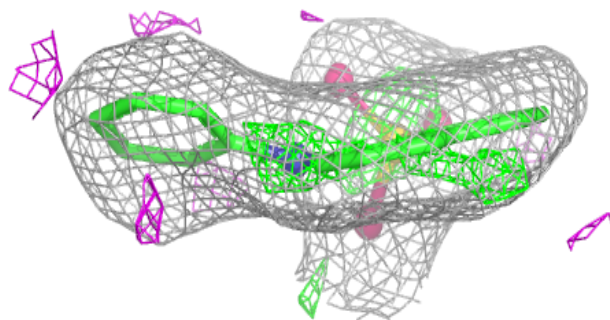
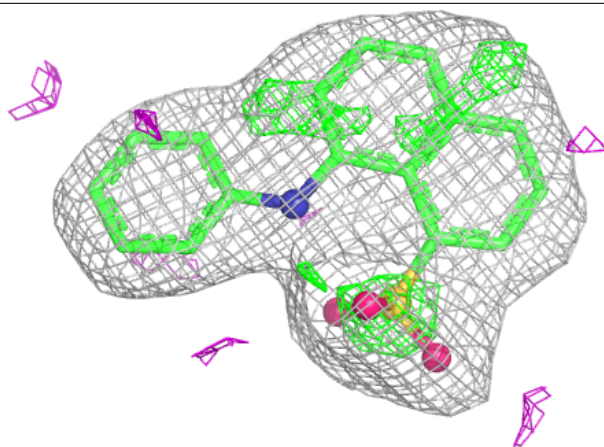
Electron density around 2AN j 202:

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



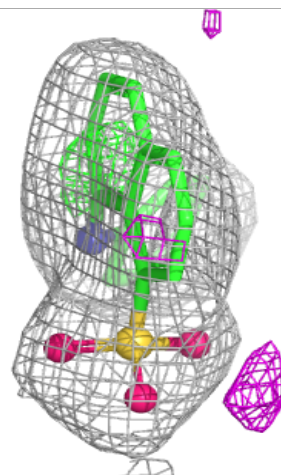
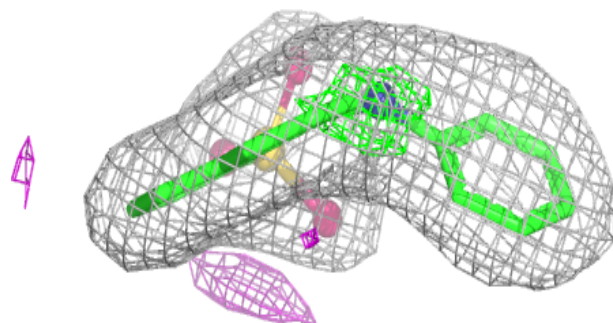
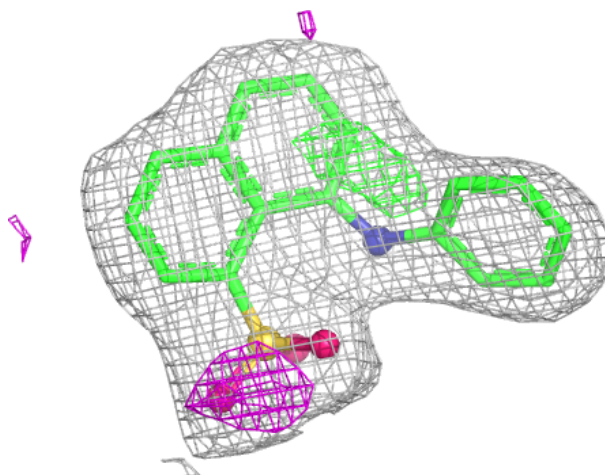
Electron density around 2AN L 201:

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



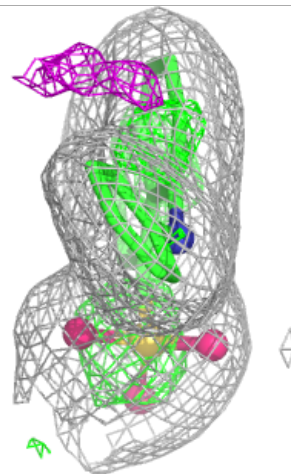
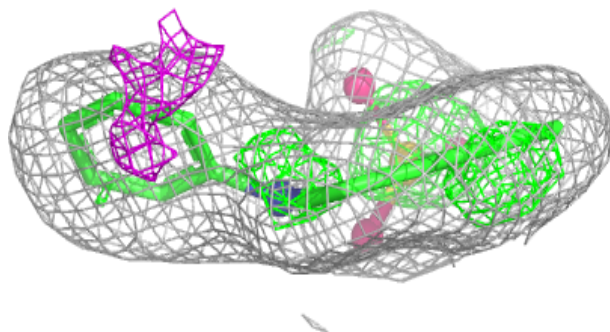
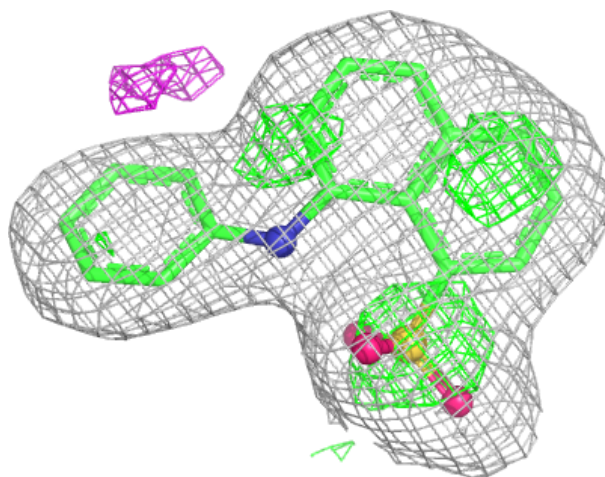
Electron density around 2AN Q 201:

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



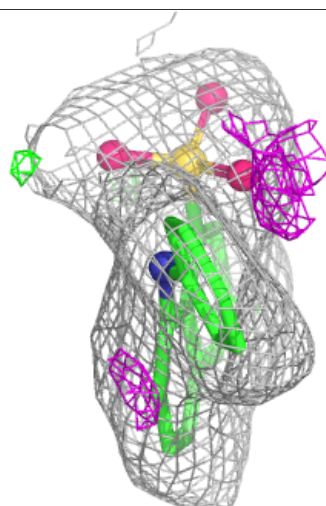
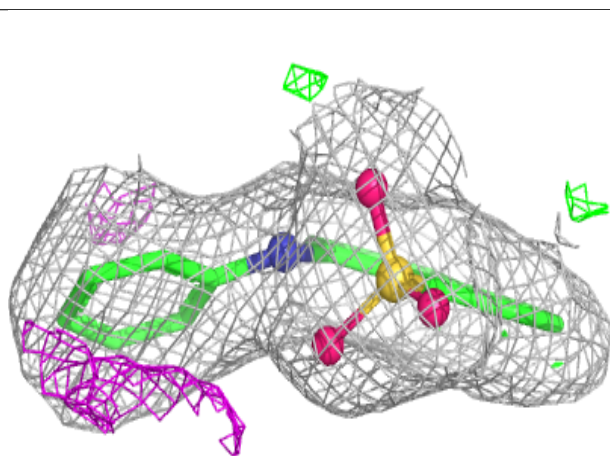
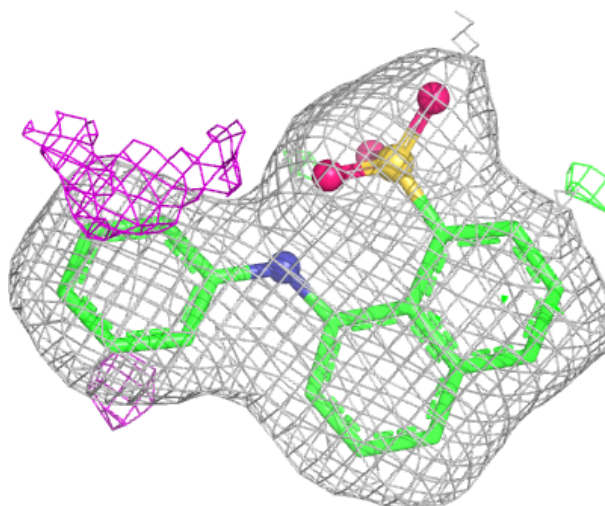
Electron density around 2AN f 201:

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



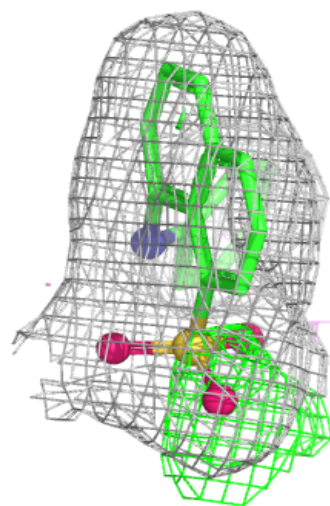
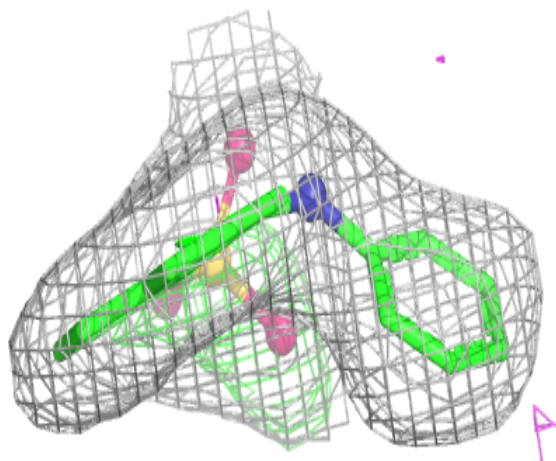
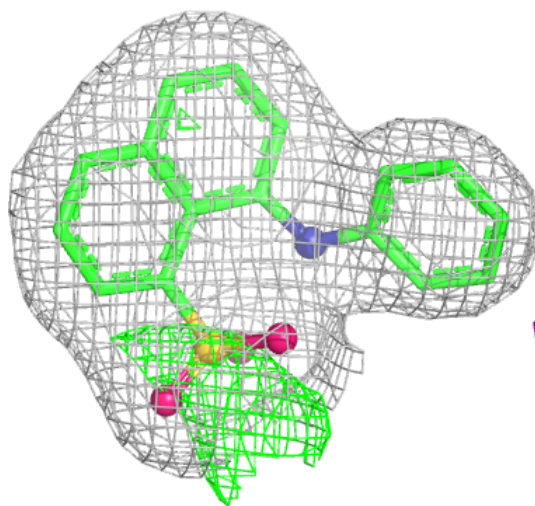
Electron density around 2AN P 201:

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



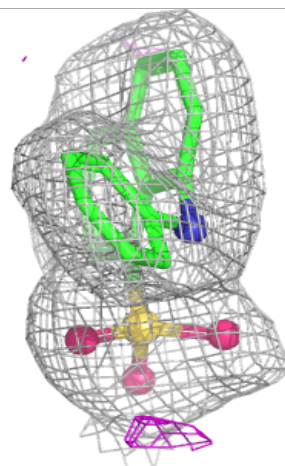
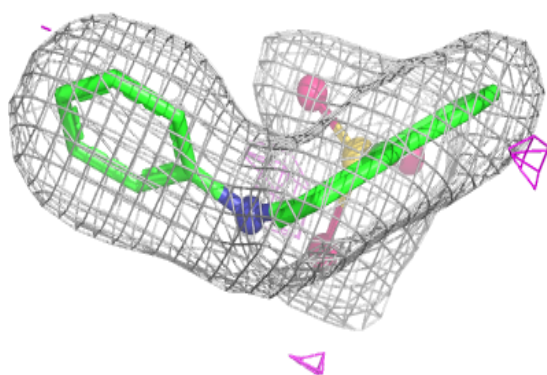
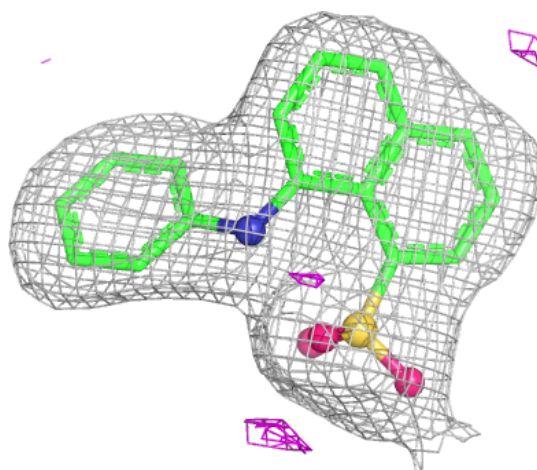
Electron density around 2AN c 201:

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



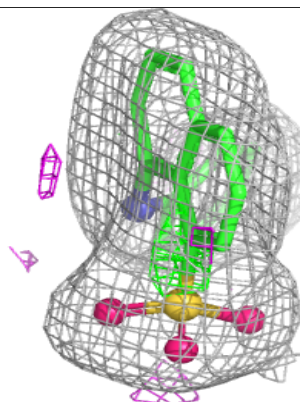
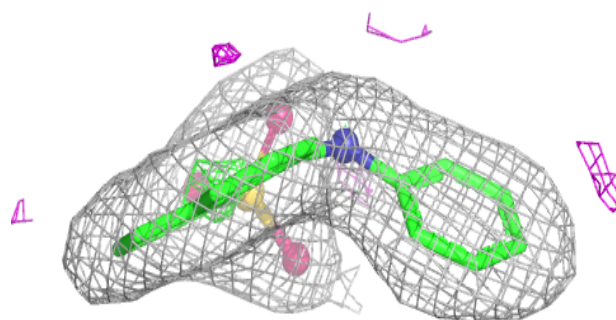
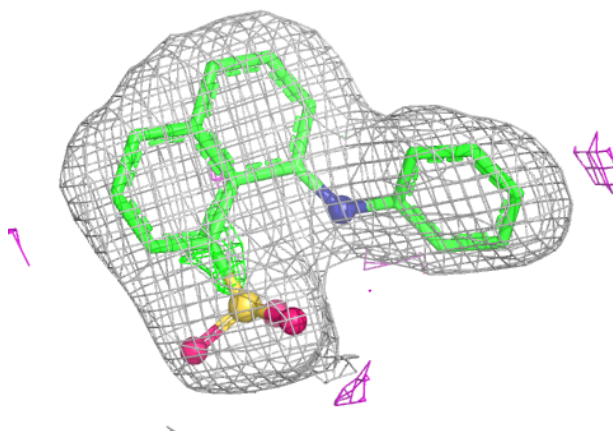
Electron density around 2AN M 202:

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



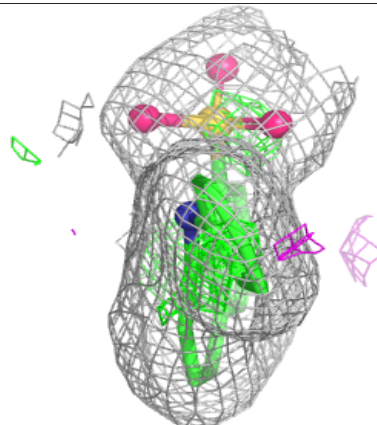
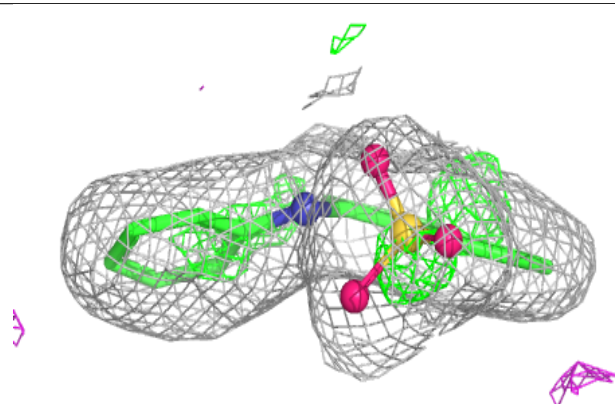
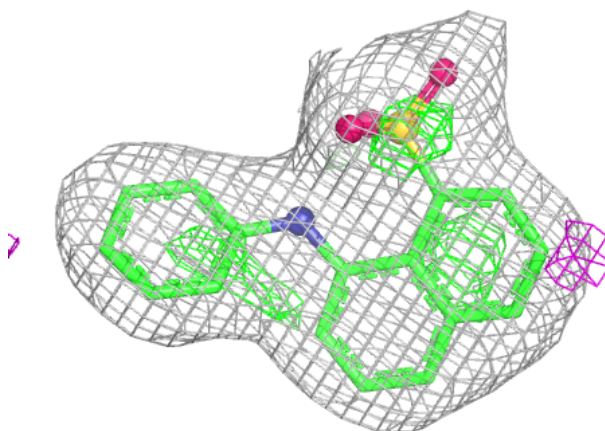
Electron density around 2AN I 201:

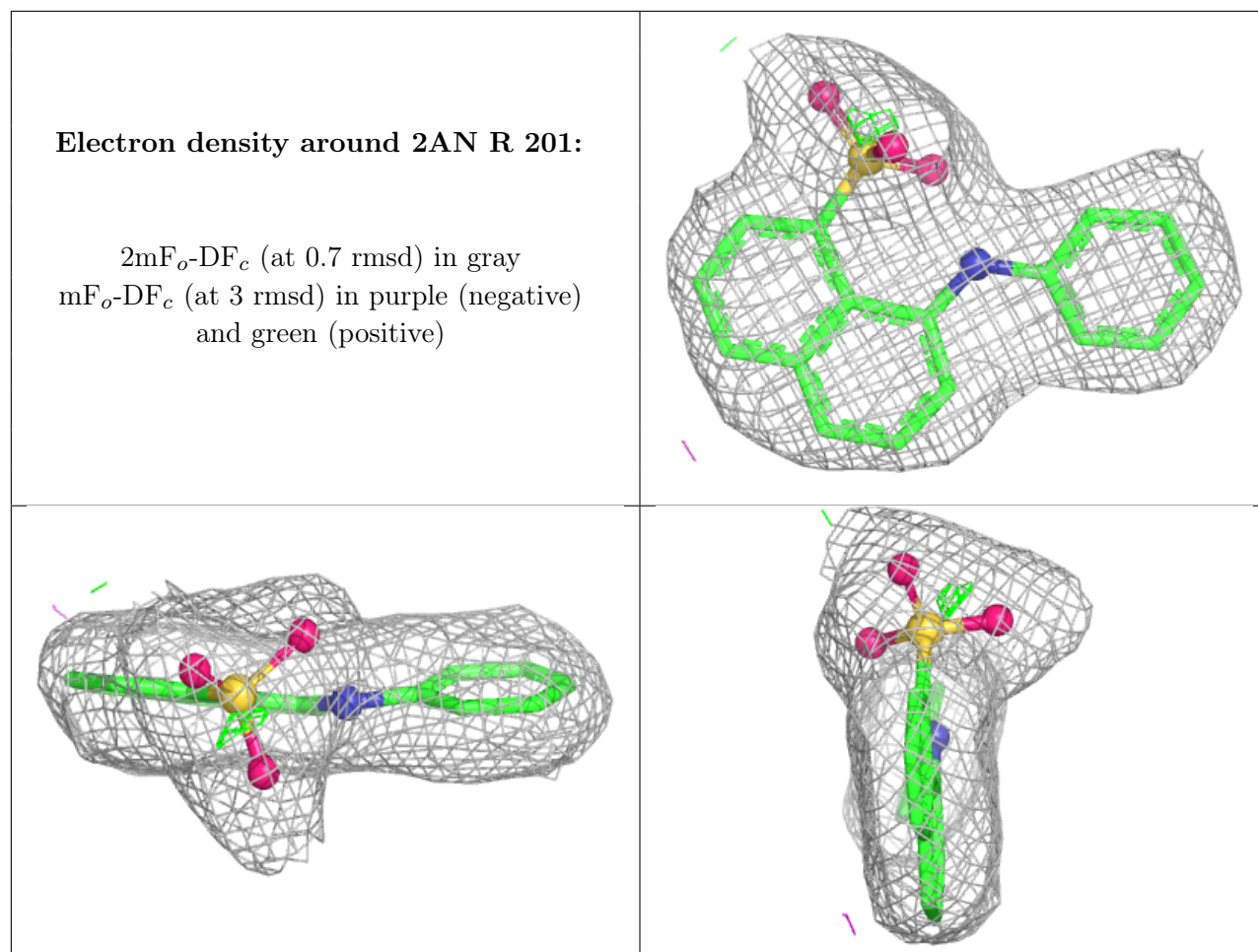
$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around 2AN j 203:

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





6.5 Other polymers [i](#)

There are no such residues in this entry.