



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 05:29 AM UTC

PDB ID : 4N3E / pdb_00004n3e
Title : Crystal structure of Hyp-1, a St John's wort PR-10 protein, in complex with 8-anilino-1-naphthalene sulfonate (ANS)
Authors : Sliwiak, J.; Dauter, Z.; McCoy, A.J.; Read, R.J.; Jaskolski, M.
Deposited on : 2013-10-07
Resolution : 2.43 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

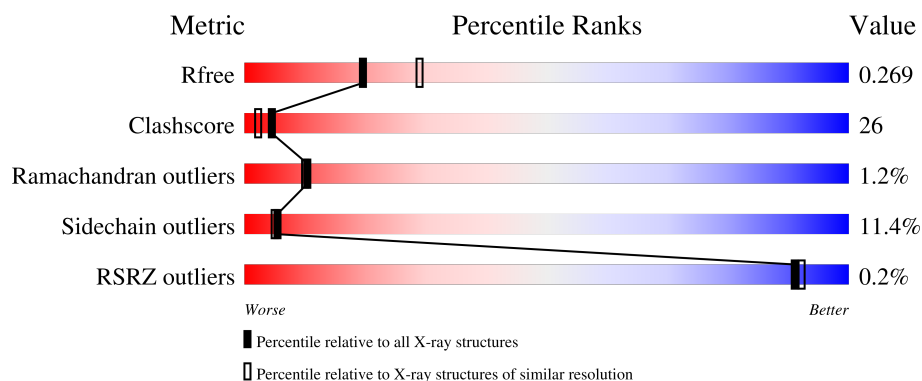
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.43 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.



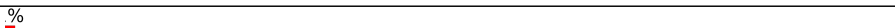
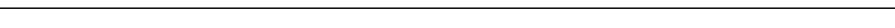
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	2340 (2.46-2.42)
Clashscore	190562	2400 (2.46-2.42)
Ramachandran outliers	187476	2379 (2.46-2.42)
Sidechain outliers	187428	2379 (2.46-2.42)
RSRZ outliers	180081	2340 (2.46-2.42)

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	165	43% 45% 7% . .
1	B	165	53% 36% 7% .
1	C	165	% 50% 37% 8% . .
1	D	165	% 61% 25% 8% . .
1	E	165	55% 35% 7% . .

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Mol	Chain	Length	Quality of chain
1	F	165	
1	G	165	
1	H	165	
1	I	165	
1	J	165	
1	K	165	
1	L	165	
1	M	165	
1	N	165	
1	O	165	
1	P	165	
1	Q	165	
1	R	165	
1	S	165	
1	T	165	
1	U	165	
1	V	165	
1	W	165	
1	X	165	
1	Y	165	
1	Z	165	
1	a	165	
1	b	165	

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	201	-	-	X	-
2	2AN	A	203	-	-	X	-
2	2AN	A	204	-	-	X	-
2	2AN	B	202	-	-	X	-
2	2AN	B	203	-	-	X	-
2	2AN	C	202	-	-	X	-
2	2AN	C	203	-	-	X	-
2	2AN	C	204	-	-	X	-
2	2AN	D	202	-	-	X	-
2	2AN	D	203	-	-	X	-
2	2AN	E	202	-	-	X	-
2	2AN	E	203	-	-	X	-
2	2AN	E	204	-	-	X	-
2	2AN	E	205	-	-	X	-
2	2AN	F	201	-	-	X	-
2	2AN	G	202	-	-	X	-
2	2AN	G	204	-	-	X	-
2	2AN	G	205	-	-	X	-
2	2AN	H	201	-	-	X	-
2	2AN	I	201	-	-	X	-
2	2AN	I	203	-	-	X	-
2	2AN	I	205	-	-	X	-
2	2AN	J	202	-	-	X	-
2	2AN	K	202	-	-	X	-
2	2AN	K	203	-	-	X	-
2	2AN	L	202	-	-	X	-
2	2AN	L	204	-	-	X	-
2	2AN	M	202	-	-	X	-
2	2AN	M	203	-	-	X	-
2	2AN	N	202	-	-	X	-
2	2AN	N	203	-	-	X	-
2	2AN	Q	201	-	-	X	-
2	2AN	Q	203	-	-	X	-
2	2AN	R	201	-	-	X	-
2	2AN	S	201	-	-	X	-
2	2AN	U	201	-	-	X	-
2	2AN	U	203	-	-	X	-
2	2AN	W	201	-	-	X	-
2	2AN	W	202	-	-	X	-
2	2AN	W	204	-	-	X	-
2	2AN	Y	202	-	-	X	-
2	2AN	Y	204	-	-	X	-
2	2AN	Z	203	-	-	X	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	2AN	a	201	-	-	X	-
2	2AN	b	201	-	-	X	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 37252 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 Phenolic oxidative coupling protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	159	Total	C	N	O	S	0	1	0
			1269	820	204	241	4			
1	B	159	Total	C	N	O	S	1	0	0
			1256	813	203	236	4			
1	C	159	Total	C	N	O	S	0	0	0
			1256	813	203	236	4			
1	D	159	Total	C	N	O	S	0	0	0
			1257	814	203	236	4			
1	E	159	Total	C	N	O	S	1	0	0
			1260	815	203	238	4			
1	F	159	Total	C	N	O	S	0	0	0
			1257	814	202	237	4			
1	G	159	Total	C	N	O	S	0	0	0
			1259	815	202	238	4			
1	H	159	Total	C	N	O	S	0	0	0
			1260	815	203	238	4			
1	I	159	Total	C	N	O	S	0	0	0
			1255	813	202	236	4			
1	J	159	Total	C	N	O	S	0	0	0
			1255	812	203	236	4			
1	K	159	Total	C	N	O	S	0	0	0
			1260	815	203	238	4			
1	L	159	Total	C	N	O	S	1	0	0
			1260	815	203	238	4			
1	M	159	Total	C	N	O	S	0	0	0
			1256	813	203	236	4			
1	N	159	Total	C	N	O	S	0	1	0
			1269	820	204	241	4			
1	O	159	Total	C	N	O	S	0	0	0
			1258	814	203	237	4			
1	P	159	Total	C	N	O	S	0	0	0
			1260	815	203	238	4			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	Q	159	Total	C	N	O	S	0	0	0
			1257	812	203	238	4			
1	R	159	Total	C	N	O	S	1	0	0
			1260	815	203	238	4			
1	S	159	Total	C	N	O	S	0	0	0
			1257	812	203	238	4			
1	T	159	Total	C	N	O	S	0	6	0
			1307	844	210	249	4			
1	U	159	Total	C	N	O	S	1	0	0
			1260	815	203	238	4			
1	V	159	Total	C	N	O	S	0	0	0
			1257	814	203	236	4			
1	W	159	Total	C	N	O	S	0	0	0
			1258	814	203	237	4			
1	X	159	Total	C	N	O	S	0	0	0
			1260	815	203	238	4			
1	Y	159	Total	C	N	O	S	1	0	0
			1260	815	203	238	4			
1	Z	159	Total	C	N	O	S	0	0	0
			1256	813	203	236	4			
1	a	159	Total	C	N	O	S	0	1	0
			1270	821	206	239	4			
1	b	159	Total	C	N	O	S	1	0	0
			1254	813	202	235	4			

There are 252 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-5	GLY	-	expression tag	UNP Q8H1L1
A	-4	ILE	-	expression tag	UNP Q8H1L1
A	-3	ASP	-	expression tag	UNP Q8H1L1
A	-2	PRO	-	expression tag	UNP Q8H1L1
A	-1	PHE	-	expression tag	UNP Q8H1L1
A	0	THR	-	expression tag	UNP Q8H1L1
A	14	ILE	THR	SEE REMARK 999	UNP Q8H1L1
A	86	LEU	ILE	SEE REMARK 999	UNP Q8H1L1
A	119	THR	SER	SEE REMARK 999	UNP Q8H1L1
B	-5	GLY	-	expression tag	UNP Q8H1L1
B	-4	ILE	-	expression tag	UNP Q8H1L1
B	-3	ASP	-	expression tag	UNP Q8H1L1
B	-2	PRO	-	expression tag	UNP Q8H1L1
B	-1	PHE	-	expression tag	UNP Q8H1L1
B	0	THR	-	expression tag	UNP Q8H1L1

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Chain	Residue	Modelled	Actual	Comment	Reference
B	14	ILE	THR	SEE REMARK 999	UNP Q8H1L1
B	86	LEU	ILE	SEE REMARK 999	UNP Q8H1L1
B	119	THR	SER	SEE REMARK 999	UNP Q8H1L1
C	-5	GLY	-	expression tag	UNP Q8H1L1
C	-4	ILE	-	expression tag	UNP Q8H1L1
C	-3	ASP	-	expression tag	UNP Q8H1L1
C	-2	PRO	-	expression tag	UNP Q8H1L1
C	-1	PHE	-	expression tag	UNP Q8H1L1
C	0	THR	-	expression tag	UNP Q8H1L1
C	14	ILE	THR	SEE REMARK 999	UNP Q8H1L1
C	86	LEU	ILE	SEE REMARK 999	UNP Q8H1L1
C	119	THR	SER	SEE REMARK 999	UNP Q8H1L1
D	-5	GLY	-	expression tag	UNP Q8H1L1
D	-4	ILE	-	expression tag	UNP Q8H1L1
D	-3	ASP	-	expression tag	UNP Q8H1L1
D	-2	PRO	-	expression tag	UNP Q8H1L1
D	-1	PHE	-	expression tag	UNP Q8H1L1
D	0	THR	-	expression tag	UNP Q8H1L1
D	14	ILE	THR	SEE REMARK 999	UNP Q8H1L1
D	86	LEU	ILE	SEE REMARK 999	UNP Q8H1L1
D	119	THR	SER	SEE REMARK 999	UNP Q8H1L1
E	-5	GLY	-	expression tag	UNP Q8H1L1
E	-4	ILE	-	expression tag	UNP Q8H1L1
E	-3	ASP	-	expression tag	UNP Q8H1L1
E	-2	PRO	-	expression tag	UNP Q8H1L1
E	-1	PHE	-	expression tag	UNP Q8H1L1
E	0	THR	-	expression tag	UNP Q8H1L1
E	14	ILE	THR	SEE REMARK 999	UNP Q8H1L1
E	86	LEU	ILE	SEE REMARK 999	UNP Q8H1L1
E	119	THR	SER	SEE REMARK 999	UNP Q8H1L1
F	-5	GLY	-	expression tag	UNP Q8H1L1
F	-4	ILE	-	expression tag	UNP Q8H1L1
F	-3	ASP	-	expression tag	UNP Q8H1L1
F	-2	PRO	-	expression tag	UNP Q8H1L1
F	-1	PHE	-	expression tag	UNP Q8H1L1
F	0	THR	-	expression tag	UNP Q8H1L1
F	14	ILE	THR	SEE REMARK 999	UNP Q8H1L1
F	86	LEU	ILE	SEE REMARK 999	UNP Q8H1L1
F	119	THR	SER	SEE REMARK 999	UNP Q8H1L1
G	-5	GLY	-	expression tag	UNP Q8H1L1
G	-4	ILE	-	expression tag	UNP Q8H1L1
G	-3	ASP	-	expression tag	UNP Q8H1L1

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Chain	Residue	Modelled	Actual	Comment	Reference
G	-2	PRO	-	expression tag	UNP Q8H1L1
G	-1	PHE	-	expression tag	UNP Q8H1L1
G	0	THR	-	expression tag	UNP Q8H1L1
G	14	ILE	THR	SEE REMARK 999	UNP Q8H1L1
G	86	LEU	ILE	SEE REMARK 999	UNP Q8H1L1
G	119	THR	SER	SEE REMARK 999	UNP Q8H1L1
H	-5	GLY	-	expression tag	UNP Q8H1L1
H	-4	ILE	-	expression tag	UNP Q8H1L1
H	-3	ASP	-	expression tag	UNP Q8H1L1
H	-2	PRO	-	expression tag	UNP Q8H1L1
H	-1	PHE	-	expression tag	UNP Q8H1L1
H	0	THR	-	expression tag	UNP Q8H1L1
H	14	ILE	THR	SEE REMARK 999	UNP Q8H1L1
H	86	LEU	ILE	SEE REMARK 999	UNP Q8H1L1
H	119	THR	SER	SEE REMARK 999	UNP Q8H1L1
I	-5	GLY	-	expression tag	UNP Q8H1L1
I	-4	ILE	-	expression tag	UNP Q8H1L1
I	-3	ASP	-	expression tag	UNP Q8H1L1
I	-2	PRO	-	expression tag	UNP Q8H1L1
I	-1	PHE	-	expression tag	UNP Q8H1L1
I	0	THR	-	expression tag	UNP Q8H1L1
I	14	ILE	THR	SEE REMARK 999	UNP Q8H1L1
I	86	LEU	ILE	SEE REMARK 999	UNP Q8H1L1
I	119	THR	SER	SEE REMARK 999	UNP Q8H1L1
J	-5	GLY	-	expression tag	UNP Q8H1L1
J	-4	ILE	-	expression tag	UNP Q8H1L1
J	-3	ASP	-	expression tag	UNP Q8H1L1
J	-2	PRO	-	expression tag	UNP Q8H1L1
J	-1	PHE	-	expression tag	UNP Q8H1L1
J	0	THR	-	expression tag	UNP Q8H1L1
J	14	ILE	THR	SEE REMARK 999	UNP Q8H1L1
J	86	LEU	ILE	SEE REMARK 999	UNP Q8H1L1
J	119	THR	SER	SEE REMARK 999	UNP Q8H1L1
K	-5	GLY	-	expression tag	UNP Q8H1L1
K	-4	ILE	-	expression tag	UNP Q8H1L1
K	-3	ASP	-	expression tag	UNP Q8H1L1
K	-2	PRO	-	expression tag	UNP Q8H1L1
K	-1	PHE	-	expression tag	UNP Q8H1L1
K	0	THR	-	expression tag	UNP Q8H1L1
K	14	ILE	THR	SEE REMARK 999	UNP Q8H1L1
K	86	LEU	ILE	SEE REMARK 999	UNP Q8H1L1
K	119	THR	SER	SEE REMARK 999	UNP Q8H1L1

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Chain	Residue	Modelled	Actual	Comment	Reference
L	-5	GLY	-	expression tag	UNP Q8H1L1
L	-4	ILE	-	expression tag	UNP Q8H1L1
L	-3	ASP	-	expression tag	UNP Q8H1L1
L	-2	PRO	-	expression tag	UNP Q8H1L1
L	-1	PHE	-	expression tag	UNP Q8H1L1
L	0	THR	-	expression tag	UNP Q8H1L1
L	14	ILE	THR	SEE REMARK 999	UNP Q8H1L1
L	86	LEU	ILE	SEE REMARK 999	UNP Q8H1L1
L	119	THR	SER	SEE REMARK 999	UNP Q8H1L1
M	-5	GLY	-	expression tag	UNP Q8H1L1
M	-4	ILE	-	expression tag	UNP Q8H1L1
M	-3	ASP	-	expression tag	UNP Q8H1L1
M	-2	PRO	-	expression tag	UNP Q8H1L1
M	-1	PHE	-	expression tag	UNP Q8H1L1
M	0	THR	-	expression tag	UNP Q8H1L1
M	14	ILE	THR	SEE REMARK 999	UNP Q8H1L1
M	86	LEU	ILE	SEE REMARK 999	UNP Q8H1L1
M	119	THR	SER	SEE REMARK 999	UNP Q8H1L1
N	-5	GLY	-	expression tag	UNP Q8H1L1
N	-4	ILE	-	expression tag	UNP Q8H1L1
N	-3	ASP	-	expression tag	UNP Q8H1L1
N	-2	PRO	-	expression tag	UNP Q8H1L1
N	-1	PHE	-	expression tag	UNP Q8H1L1
N	0	THR	-	expression tag	UNP Q8H1L1
N	14	ILE	THR	SEE REMARK 999	UNP Q8H1L1
N	86	LEU	ILE	SEE REMARK 999	UNP Q8H1L1
N	119	THR	SER	SEE REMARK 999	UNP Q8H1L1
O	-5	GLY	-	expression tag	UNP Q8H1L1
O	-4	ILE	-	expression tag	UNP Q8H1L1
O	-3	ASP	-	expression tag	UNP Q8H1L1
O	-2	PRO	-	expression tag	UNP Q8H1L1
O	-1	PHE	-	expression tag	UNP Q8H1L1
O	0	THR	-	expression tag	UNP Q8H1L1
O	14	ILE	THR	SEE REMARK 999	UNP Q8H1L1
O	86	LEU	ILE	SEE REMARK 999	UNP Q8H1L1
O	119	THR	SER	SEE REMARK 999	UNP Q8H1L1
P	-5	GLY	-	expression tag	UNP Q8H1L1
P	-4	ILE	-	expression tag	UNP Q8H1L1
P	-3	ASP	-	expression tag	UNP Q8H1L1
P	-2	PRO	-	expression tag	UNP Q8H1L1
P	-1	PHE	-	expression tag	UNP Q8H1L1
P	0	THR	-	expression tag	UNP Q8H1L1

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Chain	Residue	Modelled	Actual	Comment	Reference
P	14	ILE	THR	SEE REMARK 999	UNP Q8H1L1
P	86	LEU	ILE	SEE REMARK 999	UNP Q8H1L1
P	119	THR	SER	SEE REMARK 999	UNP Q8H1L1
Q	-5	GLY	-	expression tag	UNP Q8H1L1
Q	-4	ILE	-	expression tag	UNP Q8H1L1
Q	-3	ASP	-	expression tag	UNP Q8H1L1
Q	-2	PRO	-	expression tag	UNP Q8H1L1
Q	-1	PHE	-	expression tag	UNP Q8H1L1
Q	0	THR	-	expression tag	UNP Q8H1L1
Q	14	ILE	THR	SEE REMARK 999	UNP Q8H1L1
Q	86	LEU	ILE	SEE REMARK 999	UNP Q8H1L1
Q	119	THR	SER	SEE REMARK 999	UNP Q8H1L1
R	-5	GLY	-	expression tag	UNP Q8H1L1
R	-4	ILE	-	expression tag	UNP Q8H1L1
R	-3	ASP	-	expression tag	UNP Q8H1L1
R	-2	PRO	-	expression tag	UNP Q8H1L1
R	-1	PHE	-	expression tag	UNP Q8H1L1
R	0	THR	-	expression tag	UNP Q8H1L1
R	14	ILE	THR	SEE REMARK 999	UNP Q8H1L1
R	86	LEU	ILE	SEE REMARK 999	UNP Q8H1L1
R	119	THR	SER	SEE REMARK 999	UNP Q8H1L1
S	-5	GLY	-	expression tag	UNP Q8H1L1
S	-4	ILE	-	expression tag	UNP Q8H1L1
S	-3	ASP	-	expression tag	UNP Q8H1L1
S	-2	PRO	-	expression tag	UNP Q8H1L1
S	-1	PHE	-	expression tag	UNP Q8H1L1
S	0	THR	-	expression tag	UNP Q8H1L1
S	14	ILE	THR	SEE REMARK 999	UNP Q8H1L1
S	86	LEU	ILE	SEE REMARK 999	UNP Q8H1L1
S	119	THR	SER	SEE REMARK 999	UNP Q8H1L1
T	-5	GLY	-	expression tag	UNP Q8H1L1
T	-4	ILE	-	expression tag	UNP Q8H1L1
T	-3	ASP	-	expression tag	UNP Q8H1L1
T	-2	PRO	-	expression tag	UNP Q8H1L1
T	-1	PHE	-	expression tag	UNP Q8H1L1
T	0	THR	-	expression tag	UNP Q8H1L1
T	14	ILE	THR	SEE REMARK 999	UNP Q8H1L1
T	86	LEU	ILE	SEE REMARK 999	UNP Q8H1L1
T	119	THR	SER	SEE REMARK 999	UNP Q8H1L1
U	-5	GLY	-	expression tag	UNP Q8H1L1
U	-4	ILE	-	expression tag	UNP Q8H1L1
U	-3	ASP	-	expression tag	UNP Q8H1L1

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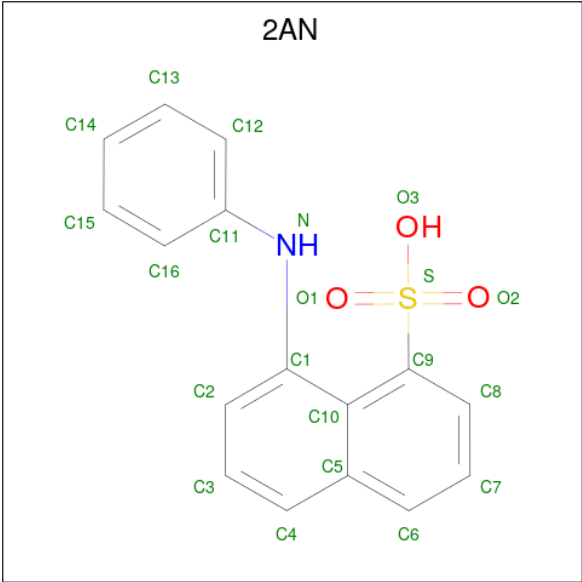
Chain	Residue	Modelled	Actual	Comment	Reference
U	-2	PRO	-	expression tag	UNP Q8H1L1
U	-1	PHE	-	expression tag	UNP Q8H1L1
U	0	THR	-	expression tag	UNP Q8H1L1
U	14	ILE	THR	SEE REMARK 999	UNP Q8H1L1
U	86	LEU	ILE	SEE REMARK 999	UNP Q8H1L1
U	119	THR	SER	SEE REMARK 999	UNP Q8H1L1
V	-5	GLY	-	expression tag	UNP Q8H1L1
V	-4	ILE	-	expression tag	UNP Q8H1L1
V	-3	ASP	-	expression tag	UNP Q8H1L1
V	-2	PRO	-	expression tag	UNP Q8H1L1
V	-1	PHE	-	expression tag	UNP Q8H1L1
V	0	THR	-	expression tag	UNP Q8H1L1
V	14	ILE	THR	SEE REMARK 999	UNP Q8H1L1
V	86	LEU	ILE	SEE REMARK 999	UNP Q8H1L1
V	119	THR	SER	SEE REMARK 999	UNP Q8H1L1
W	-5	GLY	-	expression tag	UNP Q8H1L1
W	-4	ILE	-	expression tag	UNP Q8H1L1
W	-3	ASP	-	expression tag	UNP Q8H1L1
W	-2	PRO	-	expression tag	UNP Q8H1L1
W	-1	PHE	-	expression tag	UNP Q8H1L1
W	0	THR	-	expression tag	UNP Q8H1L1
W	14	ILE	THR	SEE REMARK 999	UNP Q8H1L1
W	86	LEU	ILE	SEE REMARK 999	UNP Q8H1L1
W	119	THR	SER	SEE REMARK 999	UNP Q8H1L1
X	-5	GLY	-	expression tag	UNP Q8H1L1
X	-4	ILE	-	expression tag	UNP Q8H1L1
X	-3	ASP	-	expression tag	UNP Q8H1L1
X	-2	PRO	-	expression tag	UNP Q8H1L1
X	-1	PHE	-	expression tag	UNP Q8H1L1
X	0	THR	-	expression tag	UNP Q8H1L1
X	14	ILE	THR	SEE REMARK 999	UNP Q8H1L1
X	86	LEU	ILE	SEE REMARK 999	UNP Q8H1L1
X	119	THR	SER	SEE REMARK 999	UNP Q8H1L1
Y	-5	GLY	-	expression tag	UNP Q8H1L1
Y	-4	ILE	-	expression tag	UNP Q8H1L1
Y	-3	ASP	-	expression tag	UNP Q8H1L1
Y	-2	PRO	-	expression tag	UNP Q8H1L1
Y	-1	PHE	-	expression tag	UNP Q8H1L1
Y	0	THR	-	expression tag	UNP Q8H1L1
Y	14	ILE	THR	SEE REMARK 999	UNP Q8H1L1
Y	86	LEU	ILE	SEE REMARK 999	UNP Q8H1L1
Y	119	THR	SER	SEE REMARK 999	UNP Q8H1L1

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Chain	Residue	Modelled	Actual	Comment	Reference
Z	-5	GLY	-	expression tag	UNP Q8H1L1
Z	-4	ILE	-	expression tag	UNP Q8H1L1
Z	-3	ASP	-	expression tag	UNP Q8H1L1
Z	-2	PRO	-	expression tag	UNP Q8H1L1
Z	-1	PHE	-	expression tag	UNP Q8H1L1
Z	0	THR	-	expression tag	UNP Q8H1L1
Z	14	ILE	THR	SEE REMARK 999	UNP Q8H1L1
Z	86	LEU	ILE	SEE REMARK 999	UNP Q8H1L1
Z	119	THR	SER	SEE REMARK 999	UNP Q8H1L1
a	-5	GLY	-	expression tag	UNP Q8H1L1
a	-4	ILE	-	expression tag	UNP Q8H1L1
a	-3	ASP	-	expression tag	UNP Q8H1L1
a	-2	PRO	-	expression tag	UNP Q8H1L1
a	-1	PHE	-	expression tag	UNP Q8H1L1
a	0	THR	-	expression tag	UNP Q8H1L1
a	14	ILE	THR	SEE REMARK 999	UNP Q8H1L1
a	86	LEU	ILE	SEE REMARK 999	UNP Q8H1L1
a	119	THR	SER	SEE REMARK 999	UNP Q8H1L1
b	-5	GLY	-	expression tag	UNP Q8H1L1
b	-4	ILE	-	expression tag	UNP Q8H1L1
b	-3	ASP	-	expression tag	UNP Q8H1L1
b	-2	PRO	-	expression tag	UNP Q8H1L1
b	-1	PHE	-	expression tag	UNP Q8H1L1
b	0	THR	-	expression tag	UNP Q8H1L1
b	14	ILE	THR	SEE REMARK 999	UNP Q8H1L1
b	86	LEU	ILE	SEE REMARK 999	UNP Q8H1L1
b	119	THR	SER	SEE REMARK 999	UNP Q8H1L1

- Molecule 2 is 8-ANILINO-1-NAPHTHALENE SULFONATE (CCD ID: 2AN) (formula: $C_{16}H_{13}NO_3S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
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	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	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	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	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	F	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	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	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		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
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	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	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	L	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	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	O	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		
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		

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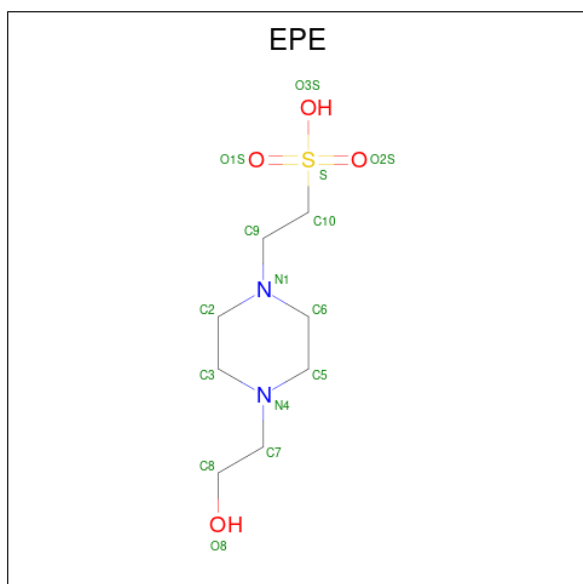
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	Q	1	Total	C	N	O	S	0	0
			21	16	1	3	1		
2	Q	1	Total	C	N	O	S	0	0
			21	16	1	3	1		
2	Q	1	Total	C	N	O	S	0	0
			21	16	1	3	1		
2	R	1	Total	C	N	O	S	0	0
			21	16	1	3	1		
2	R	1	Total	C	N	O	S	0	0
			21	16	1	3	1		
2	R	1	Total	C	N	O	S	0	0
			21	16	1	3	1		
2	R	1	Total	C	N	O	S	0	0
			21	16	1	3	1		
2	S	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	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	U	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	W	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	W	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	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		

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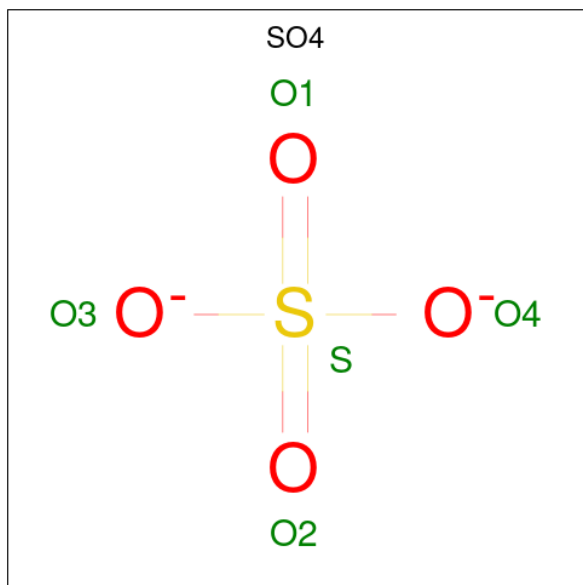
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	X	1	Total	C	N	O	S	0	0
			21	16	1	3	1		
2	Y	1	Total	C	N	O	S	0	0
			21	16	1	3	1		
2	Y	1	Total	C	N	O	S	0	0
			21	16	1	3	1		
2	Y	1	Total	C	N	O	S	0	0
			21	16	1	3	1		
2	Y	1	Total	C	N	O	S	0	0
			21	16	1	3	1		
2	Z	1	Total	C	N	O	S	0	0
			21	16	1	3	1		
2	Z	1	Total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

- Molecule 3 is 4-(2-HYDROXYETHYL)-1-PIPERAZINE ETHANESULFONIC ACID (CCD ID: EPE) (formula: $C_8H_{18}N_2O_4S$).



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

- Molecule 4 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	V	1	Total	O	S	0	0
			5	4	1		
4	X	1	Total	O	S	0	0
			5	4	1		
4	b	1	Total	O	S	0	0
			5	4	1		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	5	Total	O	0	0
			5	5		
5	C	2	Total	O	0	0
			2	2		
5	D	1	Total	O	0	0
			1	1		
5	E	2	Total	O	0	0
			2	2		
5	F	2	Total	O	0	0
			2	2		

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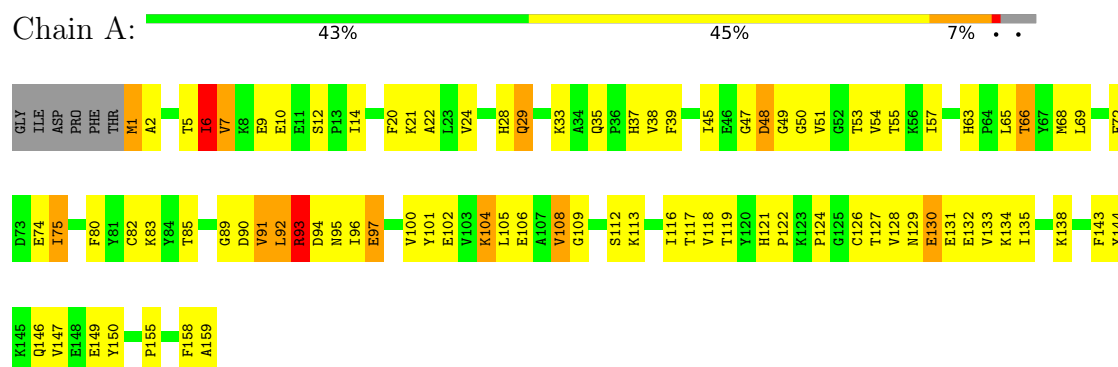
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	G	1	Total 1	O 1	0	0
5	H	4	Total 4	O 4	0	0
5	I	2	Total 2	O 2	0	0
5	L	2	Total 2	O 2	0	0
5	R	2	Total 2	O 2	0	0
5	T	1	Total 1	O 1	0	0
5	U	1	Total 1	O 1	0	0
5	W	2	Total 2	O 2	0	0
5	Y	2	Total 2	O 2	0	0
5	Z	3	Total 3	O 3	0	0
5	a	2	Total 2	O 2	0	0
5	b	1	Total 1	O 1	0	0

3 Residue-property plots

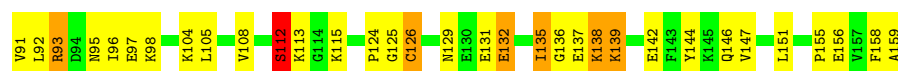
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Phenolic oxidative coupling protein

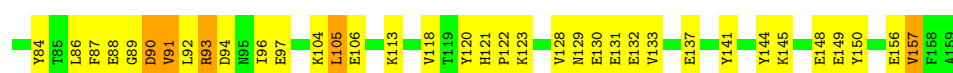




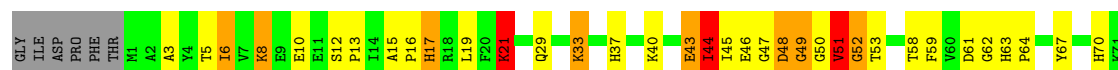
- Molecule 1: Phenolic oxidative coupling protein



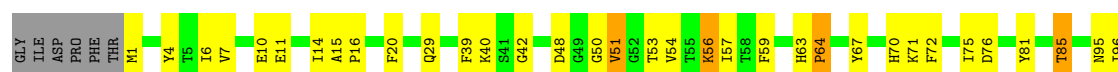
- Molecule 1: Phenolic oxidative coupling protein



- Molecule 1: Phenolic oxidative coupling protein

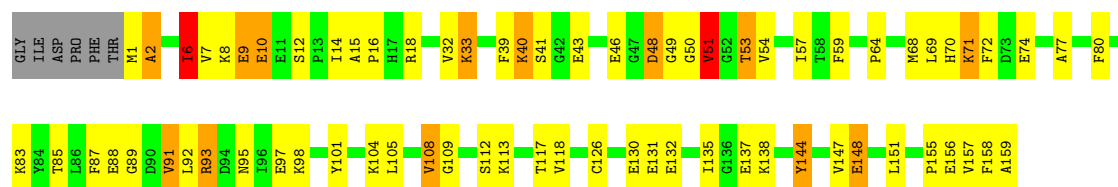


- Molecule 1: Phenolic oxidative coupling protein



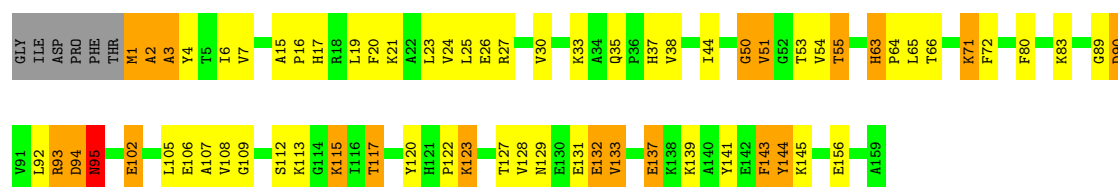
- Molecule 1: Phenolic oxidative coupling protein

Chain I: 



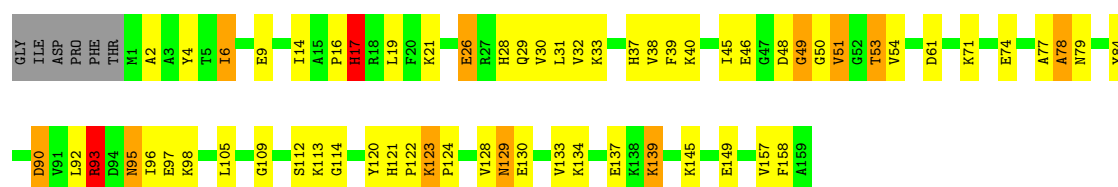
- Molecule 1: Phenolic oxidative coupling protein

Chain J: 



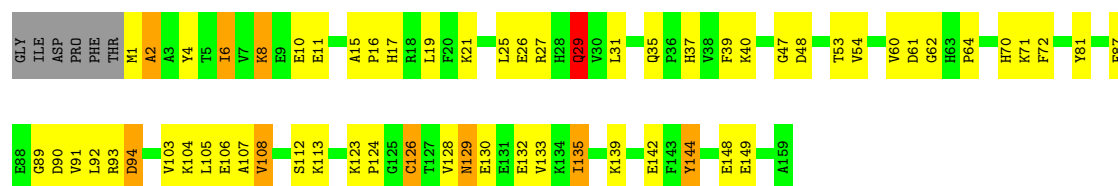
- Molecule 1: Phenolic oxidative coupling protein

Chain K: 



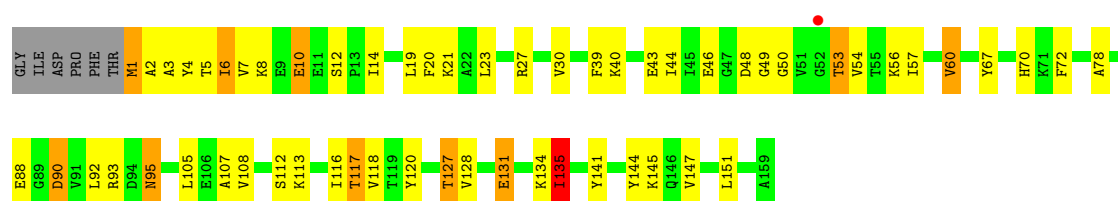
- Molecule 1: Phenolic oxidative coupling protein

Chain L: 



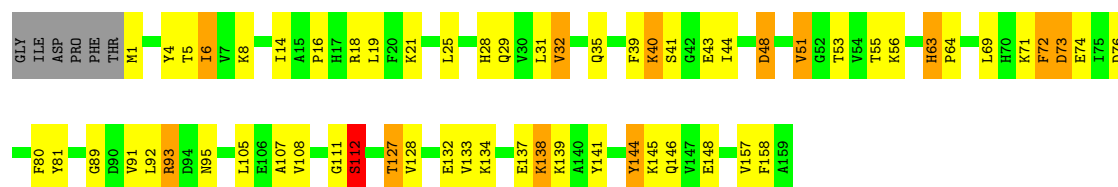
- Molecule 1: Phenolic oxidative coupling protein

Chain M: 



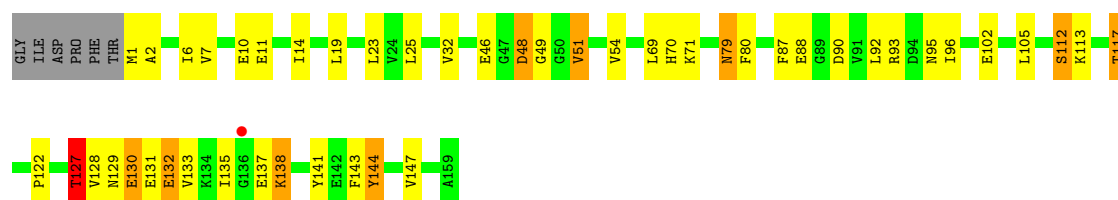
- Molecule 1: Phenolic oxidative coupling protein

Chain N: 



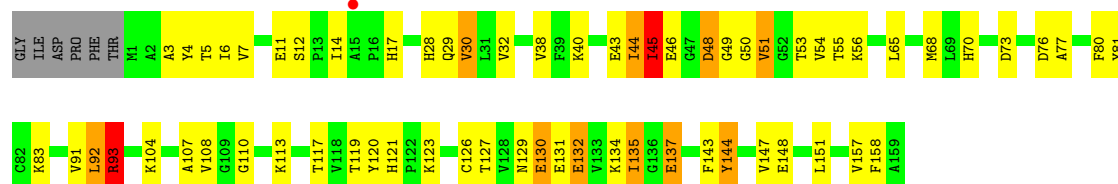
• Molecule 1: Phenolic oxidative coupling protein

Chain O: 



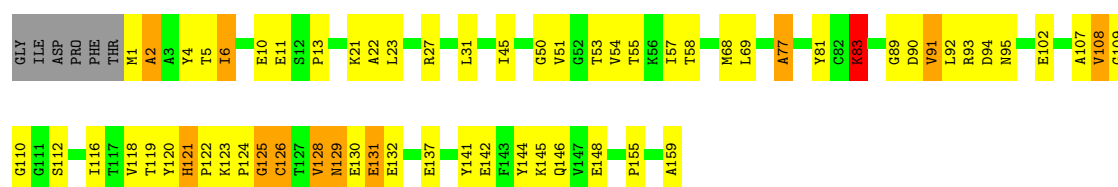
• Molecule 1: Phenolic oxidative coupling protein

Chain P: 



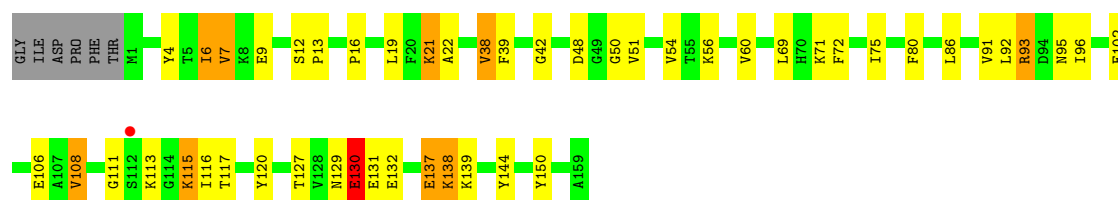
• Molecule 1: Phenolic oxidative coupling protein

Chain Q: 

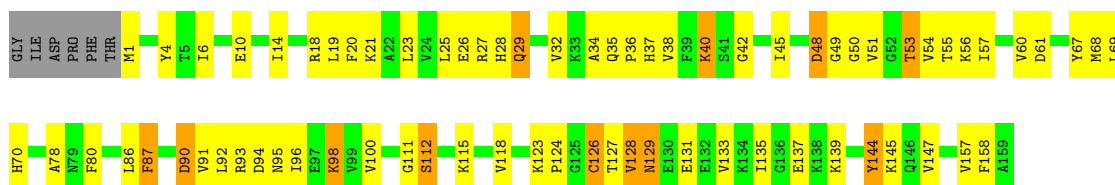


• Molecule 1: Phenolic oxidative coupling protein

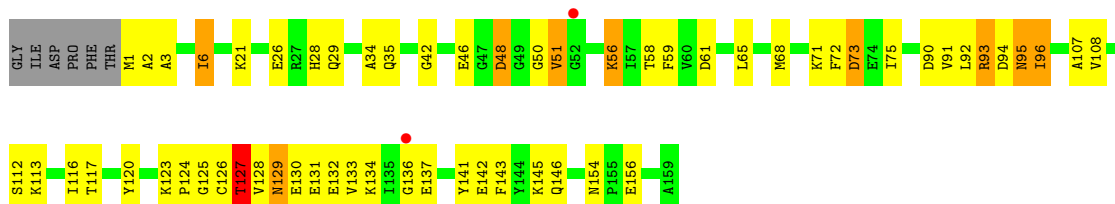
Chain R: 



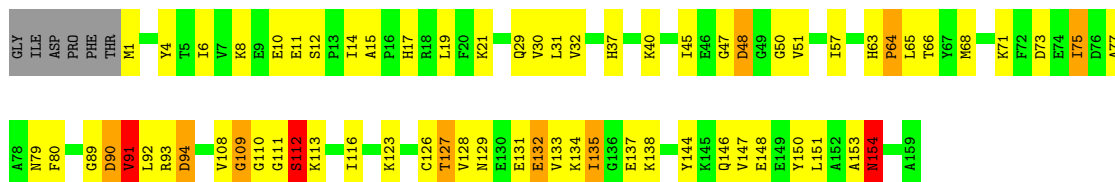
Chain S: 53% 36% 7% .



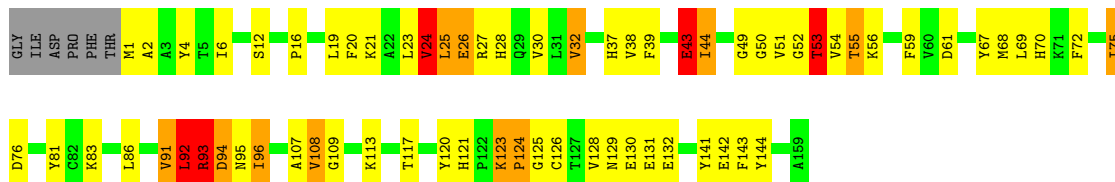
Chain T: %



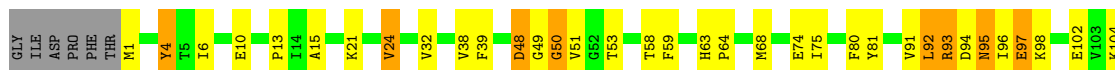
Chain U: 55% 34% 5% . .



Chain V: 55% 31% 7% . .

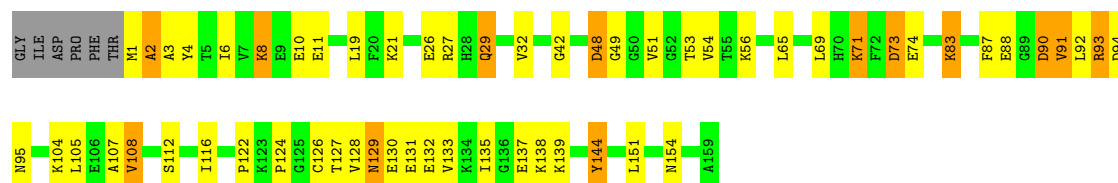


Chain W: %

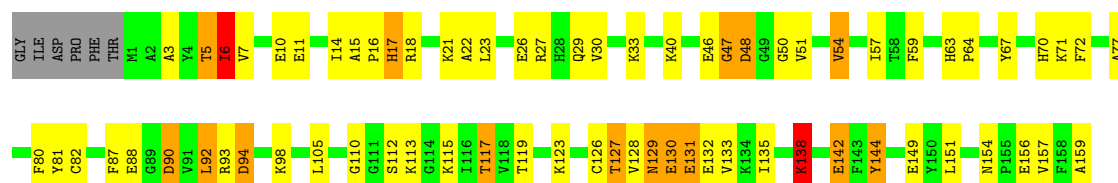




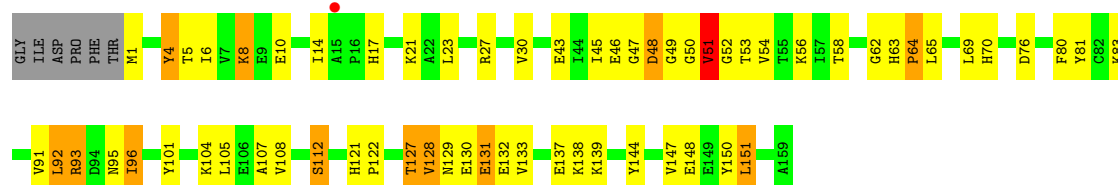
- Molecule 1: Phenolic oxidative coupling protein



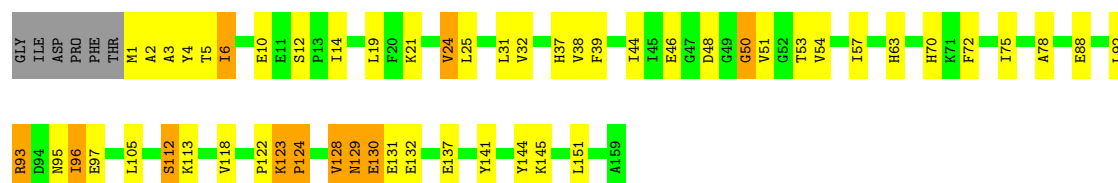
- Molecule 1: Phenolic oxidative coupling protein



- Molecule 1: Phenolic oxidative coupling protein

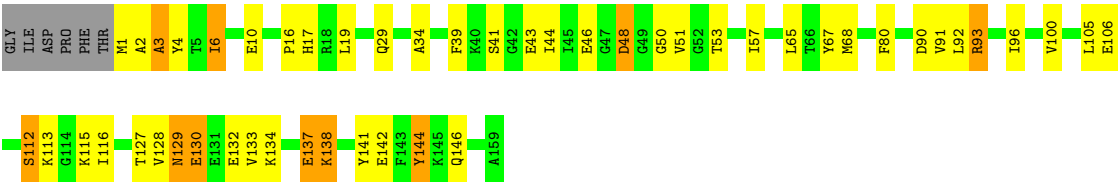


- Molecule 1: Phenolic oxidative coupling protein



- Molecule 1: Phenolic oxidative coupling protein





4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	146.29Å 146.29Å 298.56Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.87 – 2.43 48.87 – 2.43	Depositor EDS
% Data completeness (in resolution range)	99.7 (48.87-2.43) 99.7 (48.87-2.43)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.69 (at 2.42Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, R_{free}	0.223 , 0.278 0.225 , 0.269	Depositor DCC
R_{free} test set	3078 reflections (1.31%)	wwPDB-VP
Wilson B-factor (Å ²)	49.9	Xtriage
Anisotropy	0.143	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 37.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.489 for k,h,-l 0.489 for -k,-h,-l 0.489 for -h,-k,l	Xtriage
Reported twinning fraction	0.251 for H, K, L 0.292 for -K, -H, -L 0.249 for -h,-k,l 0.209 for K, H, -L	Depositor
Outliers	2 of 235350 reflections (0.001%)	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	37252	wwPDB-VP
Average B, all atoms (Å ²)	46.0	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 67.36 % 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 5.2079e-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: EPE, SO4, 2AN

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	0.96	0/1298	1.33	8/1753 (0.5%)
1	B	1.05	1/1285 (0.1%)	1.42	7/1736 (0.4%)
1	C	0.99	1/1285 (0.1%)	1.38	9/1736 (0.5%)
1	D	0.95	0/1286	1.34	8/1737 (0.5%)
1	E	1.24	3/1289 (0.2%)	1.55	16/1741 (0.9%)
1	F	0.84	1/1286 (0.1%)	1.22	3/1737 (0.2%)
1	G	1.32	4/1288 (0.3%)	1.56	23/1740 (1.3%)
1	H	1.02	0/1289	1.34	5/1741 (0.3%)
1	I	1.09	1/1284 (0.1%)	1.39	10/1735 (0.6%)
1	J	1.22	3/1284 (0.2%)	1.57	21/1734 (1.2%)
1	K	0.94	0/1289	1.35	10/1741 (0.6%)
1	L	1.18	1/1289 (0.1%)	1.51	16/1741 (0.9%)
1	M	1.02	1/1285 (0.1%)	1.39	4/1736 (0.2%)
1	N	1.02	2/1298 (0.2%)	1.39	14/1753 (0.8%)
1	O	0.96	0/1287	1.40	12/1738 (0.7%)
1	P	0.96	0/1289	1.34	9/1741 (0.5%)
1	Q	0.97	1/1286 (0.1%)	1.37	14/1737 (0.8%)
1	R	1.09	1/1289 (0.1%)	1.42	10/1741 (0.6%)
1	S	0.88	0/1286	1.29	9/1737 (0.5%)
1	T	0.85	0/1337	1.25	6/1806 (0.3%)
1	U	1.22	4/1289 (0.3%)	1.57	18/1741 (1.0%)
1	V	0.80	0/1286	1.28	10/1737 (0.6%)
1	W	1.13	1/1287 (0.1%)	1.47	9/1738 (0.5%)
1	X	1.07	1/1289 (0.1%)	1.39	14/1741 (0.8%)
1	Y	1.09	1/1289 (0.1%)	1.44	15/1741 (0.9%)
1	Z	1.09	1/1285 (0.1%)	1.40	12/1736 (0.7%)
1	a	1.03	1/1300 (0.1%)	1.45	12/1756 (0.7%)
1	b	1.23	5/1283 (0.4%)	1.47	11/1733 (0.6%)
All	All	1.05	34/36117 (0.1%)	1.41	315/48784 (0.6%)

All (34) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	b	41	SER	CA-C	-7.72	1.43	1.52
1	a	24	VAL	C-O	-7.45	1.15	1.24
1	C	13	PRO	N-CA	-7.11	1.41	1.47
1	L	60	VAL	CA-C	-7.08	1.44	1.53
1	E	15	ALA	CA-C	-6.84	1.44	1.52
1	U	148	GLU	C-O	-6.04	1.16	1.24
1	J	63	HIS	CA-C	-6.00	1.46	1.53
1	R	39	PHE	C-O	-5.92	1.16	1.23
1	Z	63	HIS	CA-C	-5.90	1.46	1.53
1	G	13	PRO	CA-C	-5.88	1.46	1.52
1	U	12	SER	N-CA	5.85	1.51	1.45
1	N	31	LEU	C-O	-5.68	1.16	1.24
1	b	146	GLN	CA-C	-5.66	1.45	1.52
1	M	78	ALA	CA-C	-5.50	1.45	1.52
1	U	66	THR	C-O	-5.39	1.16	1.24
1	F	69	LEU	CA-C	5.37	1.59	1.52
1	J	37	HIS	CA-C	-5.35	1.45	1.52
1	G	37	HIS	CA-C	-5.34	1.45	1.52
1	W	24	VAL	C-O	-5.31	1.17	1.24
1	b	67	TYR	CA-C	-5.31	1.46	1.52
1	B	32	VAL	C-O	-5.20	1.18	1.24
1	Y	3	ALA	CA-C	-5.19	1.45	1.53
1	Q	107	ALA	N-CA	5.17	1.52	1.45
1	G	51	VAL	CA-C	-5.12	1.46	1.52
1	N	41	SER	N-CA	-5.12	1.40	1.46
1	I	101	TYR	CA-C	-5.11	1.46	1.52
1	b	41	SER	C-O	-5.10	1.17	1.23
1	E	11	GLU	CA-C	-5.10	1.46	1.52
1	G	135	ILE	C-O	-5.08	1.18	1.24
1	b	34	ALA	N-CA	5.07	1.52	1.46
1	X	27	ARG	CA-C	-5.06	1.46	1.52
1	J	65	LEU	CA-C	-5.04	1.46	1.53
1	E	151	LEU	C-O	5.03	1.30	1.24
1	U	64	PRO	N-CA	-5.02	1.41	1.47

All (315) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	132	GLU	N-CA-C	-12.47	97.46	113.17
1	K	17	HIS	N-CA-C	-11.28	99.76	114.31
1	S	94	ASP	N-CA-C	-11.05	100.50	113.21
1	W	50	GLY	N-CA-C	-10.10	98.74	112.57
1	M	135	ILE	N-CA-C	-9.09	101.54	110.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	P	17	HIS	N-CA-C	-8.99	101.43	111.14
1	G	37	HIS	N-CA-C	-8.99	102.03	113.72
1	U	32	VAL	N-CA-C	-8.73	101.90	110.72
1	O	49	GLY	N-CA-C	-8.66	102.74	114.95
1	G	47	GLY	N-CA-C	8.55	124.04	110.87
1	M	49	GLY	N-CA-C	-8.52	102.04	116.01
1	D	93	ARG	N-CA-C	8.51	120.55	111.28
1	J	38	VAL	N-CA-C	-8.47	105.00	112.12
1	E	6	ILE	CB-CA-C	-8.28	99.87	111.21
1	J	112	SER	N-CA-C	8.24	120.48	108.86
1	G	51	VAL	CB-CA-C	-8.19	100.41	111.80
1	X	49	GLY	N-CA-C	-8.17	104.59	115.21
1	W	111	GLY	N-CA-C	8.09	122.45	111.20
1	G	12	SER	CA-C-N	-8.07	111.64	121.00
1	G	12	SER	C-N-CA	-8.07	111.64	121.00
1	Z	131	GLU	N-CA-C	-8.06	101.58	111.33
1	V	92	LEU	N-CA-C	-8.02	98.60	110.23
1	X	27	ARG	N-CA-C	-7.87	102.78	111.36
1	G	130	GLU	N-CA-C	-7.84	103.69	113.18
1	J	63	HIS	CA-C-N	-7.83	111.09	119.24
1	J	63	HIS	C-N-CA	-7.83	111.09	119.24
1	D	129	ASN	N-CA-C	7.83	120.90	111.82
1	Z	96	ILE	N-CA-C	7.83	119.13	108.17
1	S	49	GLY	N-CA-C	-7.81	103.70	114.64
1	Y	138	LYS	N-CA-C	7.77	122.52	112.89
1	I	40	LYS	N-CA-C	-7.76	102.61	112.93
1	R	150	TYR	N-CA-C	-7.73	102.79	111.14
1	I	6	ILE	CB-CA-C	-7.73	100.08	110.98
1	M	60	VAL	CB-CA-C	-7.70	101.35	111.13
1	Y	112	SER	N-CA-C	7.70	119.71	108.86
1	U	109	GLY	N-CA-C	-7.63	98.36	112.62
1	O	135	ILE	N-CA-C	-7.62	102.91	110.30
1	J	50	GLY	N-CA-C	-7.58	100.20	111.19
1	J	95	ASN	N-CA-C	7.54	120.38	111.71
1	V	61	ASP	N-CA-C	7.48	119.43	111.28
1	T	94	ASP	N-CA-C	7.44	119.03	111.07
1	Y	57	ILE	N-CA-C	-7.43	97.70	108.11
1	X	3	ALA	N-CA-C	-7.40	98.11	109.14
1	b	48	ASP	CB-CA-C	-7.39	100.99	111.85
1	U	113	LYS	N-CA-C	-7.34	97.91	109.07
1	D	19	LEU	N-CA-C	-7.33	102.90	111.03
1	N	139	LYS	N-CA-C	7.29	119.31	111.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	R	38	VAL	CB-CA-C	-7.25	104.68	111.06
1	L	21	LYS	N-CA-C	-7.25	102.78	111.69
1	H	112	SER	N-CA-C	7.23	118.72	108.74
1	J	17	HIS	N-CA-C	-7.19	103.37	111.14
1	H	138	LYS	N-CA-C	7.19	118.90	111.14
1	W	15	ALA	CA-C-N	7.14	126.98	119.05
1	W	15	ALA	C-N-CA	7.14	126.98	119.05
1	G	52	GLY	N-CA-C	-7.14	105.87	115.36
1	b	3	ALA	N-CA-C	-7.10	98.62	109.41
1	B	5	THR	N-CA-C	7.10	120.68	110.24
1	b	17	HIS	N-CA-C	-7.09	104.09	112.89
1	C	131	GLU	N-CA-C	-7.07	103.51	111.07
1	V	53	THR	N-CA-C	7.07	121.05	109.24
1	I	51	VAL	CB-CA-C	-7.04	100.58	111.71
1	P	12	SER	N-CA-C	7.01	114.53	108.22
1	Q	91	VAL	N-CA-C	-7.01	102.29	111.05
1	A	149	GLU	N-CA-C	-7.00	103.66	111.71
1	L	142	GLU	N-CA-C	6.95	119.45	111.11
1	a	50	GLY	N-CA-C	-6.95	101.99	112.41
1	E	37	HIS	N-CA-C	-6.93	104.83	113.28
1	K	61	ASP	N-CA-C	6.93	118.48	111.07
1	C	130	GLU	N-CA-C	-6.92	104.71	113.01
1	X	19	LEU	N-CA-C	-6.92	103.52	112.23
1	L	8	LYS	N-CA-C	6.91	118.27	108.74
1	U	135	ILE	N-CA-C	-6.90	103.94	110.42
1	D	90	ASP	N-CA-C	-6.89	102.93	111.75
1	D	92	LEU	N-CA-C	-6.89	98.71	109.25
1	C	52	GLY	N-CA-C	-6.86	105.76	115.30
1	b	137	GLU	N-CA-C	-6.84	103.05	111.40
1	I	33	LYS	N-CA-C	6.84	118.39	111.07
1	Z	121	HIS	CA-C-N	6.83	126.59	119.76
1	Z	121	HIS	C-N-CA	6.83	126.59	119.76
1	b	53	THR	N-CA-C	6.82	120.53	110.30
1	L	135	ILE	N-CA-C	-6.78	103.88	110.72
1	I	54	VAL	N-CA-C	-6.74	98.64	108.89
1	D	91	VAL	N-CA-C	6.74	120.55	112.80
1	G	61	ASP	N-CA-C	6.70	118.27	110.97
1	Y	131	GLU	N-CA-C	6.67	118.63	111.36
1	L	60	VAL	N-CA-C	-6.67	102.67	110.21
1	A	92	LEU	N-CA-C	6.66	118.53	111.28
1	C	51	VAL	N-CA-C	-6.62	99.62	107.70
1	S	51	VAL	N-CA-C	-6.61	100.06	109.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	T	61	ASP	N-CA-C	6.60	118.14	111.07
1	E	135	ILE	N-CA-C	-6.54	103.87	111.00
1	N	111	GLY	N-CA-C	6.54	121.16	110.77
1	U	128	VAL	CB-CA-C	-6.53	103.44	111.08
1	W	13	PRO	CB-CA-C	-6.53	101.85	110.27
1	M	21	LYS	N-CA-C	6.52	118.18	111.14
1	O	51	VAL	CB-CA-C	-6.52	100.69	111.32
1	K	49	GLY	N-CA-C	-6.50	103.70	114.76
1	D	130	GLU	N-CA-C	-6.50	103.85	113.72
1	P	45	ILE	CB-CA-C	-6.49	103.73	111.65
1	U	37	HIS	N-CA-C	-6.49	104.99	113.17
1	Z	45	ILE	CB-CA-C	-6.48	103.80	110.93
1	K	53	THR	N-CA-C	-6.46	100.27	109.96
1	a	141	TYR	N-CA-C	6.44	118.10	111.14
1	T	143	PHE	N-CA-C	-6.42	104.36	111.36
1	V	125	GLY	N-CA-C	6.41	123.55	115.21
1	U	40	LYS	N-CA-C	-6.40	104.42	112.93
1	Y	135	ILE	N-CA-C	-6.40	104.41	110.42
1	N	63	HIS	CA-C-N	-6.39	112.03	119.32
1	N	63	HIS	C-N-CA	-6.39	112.03	119.32
1	Q	146	GLN	N-CA-C	6.39	119.06	111.33
1	U	91	VAL	N-CA-C	-6.37	102.38	111.17
1	Q	131	GLU	N-CA-C	-6.36	105.52	113.28
1	O	127	THR	CB-CA-C	-6.36	99.34	111.48
1	R	137	GLU	N-CA-C	-6.34	105.37	113.23
1	Y	3	ALA	N-CA-C	-6.33	101.14	110.52
1	Q	94	ASP	N-CA-C	6.31	120.18	112.23
1	X	154	ASN	CA-C-N	6.31	126.00	119.82
1	X	154	ASN	C-N-CA	6.31	126.00	119.82
1	C	128	VAL	N-CA-C	6.29	117.86	108.23
1	E	135	ILE	CB-CA-C	-6.24	103.88	112.24
1	a	128	VAL	N-CA-C	6.24	117.46	108.48
1	J	139	LYS	CA-C-O	6.22	127.14	120.24
1	G	112	SER	CB-CA-C	-6.21	99.24	109.80
1	O	127	THR	CA-C-N	-6.21	115.49	123.19
1	O	127	THR	C-N-CA	-6.21	115.49	123.19
1	K	53	THR	CA-C-N	-6.20	115.02	123.14
1	K	53	THR	C-N-CA	-6.20	115.02	123.14
1	E	63	HIS	N-CA-C	-6.20	101.76	110.31
1	R	130	GLU	N-CA-C	-6.19	101.10	110.70
1	Z	47	GLY	N-CA-C	-6.19	105.31	111.56
1	B	22	ALA	N-CA-C	6.18	118.10	111.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	U	148	GLU	N-CA-C	-6.18	105.57	113.23
1	E	113	LYS	CA-C-N	-6.17	116.86	121.61
1	E	113	LYS	C-N-CA	-6.17	116.86	121.61
1	T	129	ASN	N-CA-C	-6.15	96.80	108.17
1	W	94	ASP	N-CA-C	-6.15	104.64	111.71
1	Q	121	HIS	CA-C-N	6.12	126.08	119.78
1	Q	121	HIS	C-N-CA	6.12	126.08	119.78
1	J	33	LYS	N-CA-C	6.11	118.02	111.36
1	E	2	ALA	N-CA-C	6.09	119.82	110.20
1	Y	92	LEU	N-CA-C	6.08	118.88	111.82
1	U	12	SER	CA-C-N	-6.08	114.63	120.83
1	U	12	SER	C-N-CA	-6.08	114.63	120.83
1	E	136	GLY	CA-C-N	6.05	128.89	120.29
1	E	136	GLY	C-N-CA	6.05	128.89	120.29
1	R	120	TYR	N-CA-C	6.05	119.01	107.75
1	A	12	SER	CA-C-N	-6.04	112.29	119.84
1	A	12	SER	C-N-CA	-6.04	112.29	119.84
1	Q	125	GLY	N-CA-C	-6.04	98.86	113.18
1	J	143	PHE	O-C-N	-6.04	115.62	122.08
1	Y	6	ILE	N-CA-CB	-6.04	104.14	111.21
1	L	112	SER	N-CA-C	6.02	117.04	108.74
1	C	44	ILE	N-CA-C	-6.00	99.76	108.71
1	P	38	VAL	CB-CA-C	-5.97	105.81	111.06
1	P	121	HIS	CA-C-N	5.97	125.88	119.85
1	P	121	HIS	C-N-CA	5.97	125.88	119.85
1	E	34	ALA	N-CA-C	5.96	117.78	111.28
1	Y	17	HIS	N-CA-C	-5.96	104.73	112.23
1	L	62	GLY	CA-C-N	5.94	128.93	120.49
1	L	62	GLY	C-N-CA	5.94	128.93	120.49
1	C	83	LYS	N-CA-C	-5.92	97.31	107.61
1	O	105	LEU	N-CA-C	5.91	119.15	110.59
1	F	38	VAL	N-CA-C	-5.90	107.12	111.90
1	U	154	ASN	CA-C-N	5.89	125.51	119.56
1	U	154	ASN	C-N-CA	5.89	125.51	119.56
1	K	95	ASN	N-CA-C	5.88	120.45	113.28
1	L	62	GLY	N-CA-C	5.87	121.13	114.67
1	N	40	LYS	N-CA-C	-5.87	104.29	112.45
1	X	137	GLU	N-CA-C	-5.86	104.48	111.69
1	G	21	LYS	N-CA-C	-5.85	103.70	111.24
1	H	117	THR	CB-CA-C	-5.84	97.83	109.33
1	R	22	ALA	N-CA-C	5.83	118.58	111.82
1	b	34	ALA	N-CA-C	5.83	118.58	111.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	112	SER	N-CA-C	5.83	117.93	109.07
1	Z	62	GLY	N-CA-C	5.83	121.45	113.99
1	Z	121	HIS	CB-CA-C	-5.83	104.40	110.17
1	D	75	ILE	CB-CA-C	-5.82	103.58	111.15
1	V	43	GLU	N-CA-C	5.82	117.63	108.96
1	H	85	THR	N-CA-C	5.80	118.56	108.76
1	X	29	GLN	CB-CA-C	-5.78	100.12	110.70
1	J	55	THR	N-CA-C	-5.76	100.74	109.85
1	a	112	SER	N-CA-C	5.76	117.72	109.14
1	O	95	ASN	N-CA-C	5.74	118.48	111.82
1	Y	117	THR	CB-CA-C	-5.73	100.64	110.16
1	O	25	LEU	N-CA-C	5.73	117.53	111.28
1	W	95	ASN	N-CA-C	5.73	120.11	113.18
1	b	6	ILE	CB-CA-C	-5.73	102.30	110.83
1	J	132	GLU	CA-C-N	-5.71	111.45	120.47
1	J	132	GLU	C-N-CA	-5.71	111.45	120.47
1	Q	83	LYS	CA-C-N	-5.70	113.23	122.36
1	Q	83	LYS	C-N-CA	-5.70	113.23	122.36
1	N	134	LYS	N-CA-C	5.68	117.47	111.28
1	G	91	VAL	N-CA-C	-5.67	104.10	112.04
1	U	112	SER	N-CA-C	5.65	116.83	108.86
1	Z	92	LEU	N-CA-C	5.65	117.13	110.97
1	P	51	VAL	CB-CA-C	-5.64	102.05	111.29
1	W	98	LYS	N-CA-C	5.63	116.82	108.60
1	N	148	GLU	N-CA-C	5.62	118.13	111.33
1	P	110	GLY	N-CA-C	-5.62	106.89	115.66
1	E	11	GLU	CA-C-N	-5.60	113.08	123.11
1	E	11	GLU	C-N-CA	-5.60	113.08	123.11
1	a	63	HIS	CA-C-N	5.59	126.83	119.84
1	a	63	HIS	C-N-CA	5.59	126.83	119.84
1	Y	142	GLU	CB-CA-C	-5.59	102.11	110.88
1	T	127	THR	CA-C-N	-5.58	115.17	122.37
1	T	127	THR	C-N-CA	-5.58	115.17	122.37
1	V	93	ARG	N-CA-C	5.57	120.07	113.16
1	Y	59	PHE	N-CA-C	5.57	118.07	110.55
1	G	13	PRO	N-CA-C	-5.56	108.30	114.92
1	X	53	THR	N-CA-C	5.56	118.39	110.10
1	E	35	GLN	CA-C-N	5.56	125.65	119.87
1	E	35	GLN	C-N-CA	5.56	125.65	119.87
1	a	12	SER	CA-C-N	-5.55	114.29	120.45
1	a	12	SER	C-N-CA	-5.55	114.29	120.45
1	a	24	VAL	CB-CA-C	-5.53	102.22	111.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	J	35	GLN	CA-C-N	5.53	126.26	120.12
1	J	35	GLN	C-N-CA	5.53	126.26	120.12
1	b	113	LYS	N-CA-C	-5.53	99.67	109.06
1	S	111	GLY	N-CA-C	5.51	118.86	111.20
1	G	134	LYS	N-CA-C	5.51	116.98	110.97
1	X	2	ALA	N-CA-C	5.51	117.95	110.35
1	N	112	SER	N-CA-C	5.51	118.05	109.52
1	G	44	ILE	CA-C-N	-5.50	112.61	120.42
1	G	44	ILE	C-N-CA	-5.50	112.61	120.42
1	L	81	TYR	N-CA-C	5.49	117.91	109.07
1	S	100	VAL	N-CA-C	5.49	115.69	107.51
1	V	32	VAL	N-CA-C	-5.47	107.02	113.42
1	G	49	GLY	N-CA-C	-5.44	107.76	115.43
1	J	115	LYS	N-CA-C	-5.44	100.04	108.90
1	J	94	ASP	N-CA-C	5.43	117.20	111.28
1	R	127	THR	N-CA-C	5.42	118.28	109.24
1	U	75	ILE	CB-CA-C	-5.41	102.42	110.33
1	I	53	THR	N-CA-C	5.41	117.86	110.24
1	K	6	ILE	CB-CA-C	5.41	118.23	110.33
1	G	137	GLU	N-CA-C	-5.40	104.95	112.45
1	L	94	ASP	N-CA-C	5.40	117.16	111.28
1	B	38	VAL	CB-CA-C	-5.38	105.64	110.91
1	X	94	ASP	N-CA-C	5.38	117.22	111.36
1	I	89	GLY	N-CA-C	-5.38	104.44	111.37
1	U	146	GLN	N-CA-C	-5.37	105.47	112.23
1	A	22	ALA	N-CA-C	5.36	117.20	111.36
1	K	26	GLU	N-CA-C	5.36	119.34	112.26
1	L	27	ARG	CB-CA-C	-5.36	101.90	110.79
1	G	90	ASP	CB-CA-C	-5.36	99.25	110.17
1	L	6	ILE	CB-CA-C	-5.35	104.48	110.96
1	S	23	LEU	N-CA-C	5.35	119.43	113.01
1	H	40	LYS	N-CA-C	-5.34	106.89	113.41
1	Y	6	ILE	CB-CA-C	5.34	118.30	110.98
1	U	29	GLN	CB-CA-C	-5.33	101.84	110.79
1	V	24	VAL	CB-CA-C	-5.33	102.55	111.29
1	S	112	SER	N-CA-C	5.33	116.90	108.96
1	R	111	GLY	N-CA-C	5.32	119.18	112.79
1	C	28	HIS	N-CA-C	5.32	117.76	111.33
1	B	94	ASP	N-CA-C	5.31	118.22	111.69
1	G	95	ASN	N-CA-C	5.31	119.62	113.20
1	N	93	ARG	CA-C-N	5.31	127.65	120.38
1	N	93	ARG	C-N-CA	5.31	127.65	120.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	93	ARG	N-CA-C	-5.30	99.51	110.80
1	S	40	LYS	N-CA-C	-5.30	104.41	112.04
1	N	32	VAL	N-CA-C	5.29	118.47	111.17
1	G	48	ASP	N-CA-C	-5.28	106.10	112.54
1	I	137	GLU	N-CA-C	-5.27	106.53	113.12
1	S	90	ASP	CB-CA-C	-5.27	101.28	110.09
1	R	7	VAL	N-CA-CB	-5.26	106.08	112.35
1	V	49	GLY	N-CA-C	5.26	122.87	115.30
1	Q	112	SER	CA-C-N	5.25	131.06	122.81
1	Q	112	SER	C-N-CA	5.25	131.06	122.81
1	Q	128	VAL	N-CA-C	5.25	115.46	108.11
1	L	17	HIS	N-CA-C	-5.25	105.62	112.23
1	L	29	GLN	CB-CA-C	-5.25	100.05	109.24
1	A	6	ILE	CB-CA-C	-5.24	103.87	111.68
1	F	50	GLY	N-CA-C	-5.21	104.02	112.31
1	K	113	LYS	N-CA-C	-5.21	100.91	109.40
1	V	130	GLU	N-CA-C	-5.21	105.72	111.71
1	P	77	ALA	N-CA-C	5.20	119.25	113.01
1	N	35	GLN	CA-C-N	5.19	125.27	119.87
1	N	35	GLN	C-N-CA	5.19	125.27	119.87
1	B	60	VAL	N-CA-C	-5.18	104.35	110.21
1	Z	51	VAL	CB-CA-C	-5.17	102.81	111.29
1	Q	77	ALA	N-CA-C	5.16	118.84	112.54
1	G	45	ILE	CA-C-N	-5.16	114.84	123.04
1	G	45	ILE	C-N-CA	-5.16	114.84	123.04
1	N	132	GLU	CB-CG-CD	5.15	121.36	112.60
1	X	151	LEU	N-CA-C	5.15	117.64	111.71
1	U	94	ASP	N-CA-C	5.15	117.79	111.82
1	b	100	VAL	CB-CA-C	-5.13	103.49	110.42
1	O	19	LEU	N-CA-C	-5.11	105.60	111.07
1	b	112	SER	N-CA-C	5.11	116.75	109.14
1	W	140	ALA	N-CA-C	-5.11	106.89	113.23
1	L	25	LEU	N-CA-C	-5.10	105.80	112.23
1	B	129	ASN	N-CA-C	-5.09	99.95	110.80
1	A	29	GLN	CA-CB-CG	-5.09	103.93	114.10
1	I	148	GLU	N-CA-C	-5.08	105.44	111.69
1	J	17	HIS	CB-CA-C	5.08	118.93	110.90
1	X	91	VAL	N-CA-C	-5.08	106.40	113.00
1	a	88	GLU	N-CA-C	5.08	117.69	109.06
1	b	53	THR	CB-CA-C	-5.07	103.01	110.06
1	E	112	SER	N-CA-C	5.07	116.70	109.14
1	Y	54	VAL	N-CA-C	-5.07	101.18	108.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	93	ARG	N-CA-C	-5.06	100.02	110.80
1	Z	4	TYR	CA-CB-CG	5.05	123.00	113.90
1	Q	22	ALA	N-CA-C	5.05	116.86	111.36
1	Z	133	VAL	N-CA-C	-5.05	106.23	111.58
1	C	20	PHE	N-CA-C	-5.04	106.64	112.89
1	F	91	VAL	CB-CA-C	-5.04	104.69	112.05
1	J	129	ASN	CB-CA-C	-5.04	102.90	110.16
1	J	137	GLU	N-CA-C	-5.03	107.22	113.55
1	Y	22	ALA	N-CA-C	5.03	117.65	111.82
1	G	78	ALA	N-CA-C	-5.02	106.41	112.54
1	O	79	ASN	N-CA-C	-5.02	106.85	113.17
1	a	130	GLU	N-CA-C	-5.02	106.26	112.38
1	R	42	GLY	N-CA-C	-5.01	101.31	113.18
1	a	145	LYS	N-CA-C	5.01	117.47	111.71
1	J	112	SER	CA-CB-OG	5.01	121.11	111.10
1	O	141	TYR	N-CA-C	5.01	116.55	111.14

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1269	0	1260	86	0
1	B	1256	0	1251	64	0
1	C	1256	0	1251	75	0
1	D	1257	0	1253	58	0
1	E	1260	0	1255	55	0
1	F	1257	0	1251	70	0
1	G	1259	0	1250	62	0
1	H	1260	0	1255	42	0
1	I	1255	0	1246	70	0
1	J	1255	0	1250	63	0
1	K	1260	0	1255	59	0
1	L	1260	0	1255	60	0
1	M	1256	0	1251	55	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	N	1269	0	1260	51	0
1	O	1258	0	1250	32	0
1	P	1260	0	1255	41	0
1	Q	1257	0	1246	48	0
1	R	1260	0	1255	39	0
1	S	1257	0	1246	60	0
1	T	1307	0	1286	41	0
1	U	1260	0	1255	50	0
1	V	1257	0	1253	54	0
1	W	1258	0	1250	53	0
1	X	1260	0	1255	46	0
1	Y	1260	0	1255	49	0
1	Z	1256	0	1251	58	0
1	a	1270	0	1261	52	0
1	b	1254	0	1249	37	0
2	A	84	0	49	30	0
2	B	105	0	63	30	0
2	C	84	0	49	28	0
2	D	63	0	36	22	0
2	E	105	0	62	46	0
2	F	21	0	13	8	0
2	G	105	0	60	36	0
2	H	63	0	39	18	0
2	I	105	0	62	36	0
2	J	42	0	25	13	0
2	K	63	0	36	30	0
2	L	105	0	63	31	0
2	M	63	0	37	24	0
2	N	84	0	51	32	0
2	O	42	0	24	10	0
2	P	42	0	24	10	0
2	Q	63	0	37	21	0
2	R	84	0	49	19	0
2	S	21	0	13	7	0
2	U	105	0	63	26	0
2	V	42	0	24	11	0
2	W	84	0	49	34	0
2	X	63	0	39	14	0
2	Y	84	0	49	24	0
2	Z	63	0	37	18	0
2	a	21	0	12	7	0
2	b	63	0	38	18	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	15	0	18	0	0
3	Z	15	0	18	0	0
4	V	5	0	0	0	0
4	X	5	0	0	0	0
4	b	5	0	0	0	0
5	A	5	0	0	1	0
5	C	2	0	0	0	0
5	D	1	0	0	0	0
5	E	2	0	0	0	0
5	F	2	0	0	0	0
5	G	1	0	0	1	0
5	H	4	0	0	0	0
5	I	2	0	0	0	0
5	L	2	0	0	0	0
5	R	2	0	0	0	0
5	T	1	0	0	0	0
5	U	1	0	0	0	0
5	W	2	0	0	0	0
5	Y	2	0	0	0	0
5	Z	3	0	0	0	0
5	a	2	0	0	0	0
5	b	1	0	0	0	0
All	All	37252	0	36249	1925	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 26.

All (1925) 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:L:128:VAL:CG1	1:L:129:ASN:HB3	1.48	1.40
1:a:123:LYS:HD2	1:a:124:PRO:CD	1.51	1.38
1:a:123:LYS:CD	1:a:124:PRO:HD2	1.51	1.37
1:A:37:HIS:CD2	1:A:38:VAL:HG23	1.62	1.34
1:A:96:ILE:CD1	1:A:128:VAL:HG22	1.68	1.22
1:I:14:ILE:CD1	1:I:148:GLU:HG3	1.72	1.19
1:W:49:GLY:HA2	1:W:53:THR:CB	1.73	1.18
1:L:128:VAL:HA	1:L:129:ASN:CB	1.75	1.16
2:A:204:2AN:H16	2:A:204:2AN:H2	1.27	1.14
1:D:4:TYR:CE1	1:D:128:VAL:HB	1.83	1.14
2:F:201:2AN:H2	2:F:201:2AN:C12	1.76	1.14

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:96:ILE:HD13	1:A:128:VAL:CG2	1.78	1.13
2:D:202:2AN:H16	2:D:202:2AN:C2	1.75	1.13
1:Z:95:ASN:HD21	1:Z:129:ASN:CB	1.62	1.12
2:K:202:2AN:H16	2:K:202:2AN:H2	1.13	1.12
2:I:203:2AN:H2	2:I:203:2AN:C16	1.74	1.12
2:D:202:2AN:H2	2:D:202:2AN:C16	1.76	1.11
1:V:68:MET:HG2	1:V:91:VAL:HG11	1.32	1.11
2:D:203:2AN:H2	2:D:203:2AN:C12	1.78	1.11
1:I:147:VAL:HG13	2:I:203:2AN:H6	1.13	1.11
2:Z:203:2AN:H16	2:Z:203:2AN:H2	1.30	1.11
1:I:147:VAL:HG13	2:I:203:2AN:C6	1.81	1.10
1:Z:95:ASN:ND2	1:Z:129:ASN:HB2	1.65	1.10
1:L:128:VAL:HA	1:L:129:ASN:HB2	1.28	1.10
2:D:203:2AN:C2	2:D:203:2AN:H12	1.75	1.09
2:I:203:2AN:H16	2:I:203:2AN:C2	1.77	1.09
1:I:14:ILE:HD11	1:I:148:GLU:HG3	1.34	1.09
2:K:203:2AN:C12	2:K:203:2AN:H2	1.80	1.08
1:S:37:HIS:CD2	1:S:38:VAL:HG23	1.88	1.07
1:E:8:LYS:HD3	1:E:10:GLU:OE1	1.54	1.07
2:F:201:2AN:H12	2:F:201:2AN:C2	1.82	1.06
2:K:203:2AN:H12	2:K:203:2AN:C2	1.83	1.06
2:M:203:2AN:C2	2:M:203:2AN:H16	1.85	1.06
1:B:4:TYR:CD2	1:B:128:VAL:HG11	1.91	1.05
2:E:205:2AN:H16	2:E:205:2AN:H2	1.37	1.05
2:E:203:2AN:C2	2:E:203:2AN:H12	1.82	1.05
1:L:128:VAL:HG13	1:L:129:ASN:HB3	1.13	1.05
1:V:93:ARG:O	1:V:94:ASP:HB3	1.53	1.04
1:a:122:PRO:HG3	1:a:128:VAL:CG2	1.88	1.04
2:H:203:2AN:H16	2:H:203:2AN:H2	1.39	1.04
2:G:202:2AN:H2	2:G:202:2AN:C16	1.87	1.04
2:K:203:2AN:H2	2:K:203:2AN:H12	1.07	1.03
2:E:203:2AN:H12	2:E:203:2AN:H2	1.04	1.03
2:L:203:2AN:H2	2:L:203:2AN:H12	1.41	1.03
1:a:95:ASN:HD21	1:a:129:ASN:ND2	1.54	1.03
1:A:66:THR:OG1	1:A:90:ASP:HB2	1.56	1.02
1:X:92:LEU:O	1:X:93:ARG:HB2	1.53	1.02
1:L:129:ASN:HD21	1:L:132:GLU:HB3	1.22	1.02
1:K:49:GLY:HA2	1:K:53:THR:OG1	1.58	1.01
1:R:130:GLU:O	1:R:130:GLU:HG2	1.54	1.01
2:Z:203:2AN:H16	2:Z:203:2AN:C2	1.88	1.01
2:G:202:2AN:H16	2:G:202:2AN:C2	1.91	1.01

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:33:LYS:HD3	2:E:203:2AN:O3	1.60	1.00
2:G:202:2AN:H2	2:G:202:2AN:H16	1.04	1.00
1:M:147:VAL:HG13	2:M:203:2AN:H6	1.38	1.00
1:X:93:ARG:HD2	1:X:132:GLU:OE1	1.62	1.00
1:D:86:LEU:HG	1:D:92:LEU:HD21	1.40	1.00
2:K:202:2AN:H2	2:K:202:2AN:C16	1.89	1.00
1:G:46:GLU:HG3	1:G:46:GLU:O	1.59	0.99
2:G:205:2AN:H12	2:G:205:2AN:C2	1.87	0.99
2:A:201:2AN:H16	2:A:201:2AN:H2	1.39	0.99
2:G:205:2AN:H2	2:G:205:2AN:C12	1.88	0.99
2:M:203:2AN:H16	2:M:203:2AN:H2	1.02	0.99
2:L:203:2AN:H2	2:L:203:2AN:C12	1.92	0.98
2:C:204:2AN:H12	2:C:204:2AN:O3	1.62	0.98
1:Z:95:ASN:HD21	1:Z:129:ASN:HB2	0.81	0.98
1:a:44:ILE:HG22	1:a:44:ILE:O	1.64	0.98
1:A:96:ILE:HD13	1:A:128:VAL:HG22	0.98	0.98
2:G:204:2AN:O1	2:G:204:2AN:H12	1.63	0.98
1:L:128:VAL:CG1	1:L:129:ASN:CB	2.42	0.98
1:I:33:LYS:HD3	2:I:203:2AN:O1	1.63	0.97
1:M:131:GLU:HG2	1:M:135:ILE:CD1	1.94	0.97
2:G:205:2AN:H12	2:G:205:2AN:H2	0.99	0.97
2:N:203:2AN:H12	2:N:203:2AN:O3	1.63	0.97
2:E:203:2AN:H2	2:E:203:2AN:C12	1.91	0.97
1:a:129:ASN:HD22	1:a:129:ASN:N	1.63	0.97
1:E:2:ALA:HB1	1:F:4:TYR:CE1	2.00	0.96
2:Z:201:2AN:H12	2:Z:201:2AN:H2	1.45	0.96
1:L:26:GLU:HG3	1:L:29:GLN:OE1	1.66	0.96
1:V:141:TYR:CD2	2:V:201:2AN:H12	2.00	0.96
1:N:133:VAL:O	1:N:137:GLU:HG2	1.64	0.96
2:H:203:2AN:H16	2:H:203:2AN:C2	1.93	0.95
1:M:131:GLU:O	1:M:135:ILE:HD12	1.65	0.95
2:A:201:2AN:H2	2:A:201:2AN:C16	1.92	0.95
2:Z:201:2AN:H12	2:Z:201:2AN:C2	1.94	0.95
1:V:141:TYR:HD2	2:V:201:2AN:H12	1.32	0.95
2:M:203:2AN:H2	2:M:203:2AN:C16	1.91	0.94
1:Y:129:ASN:HD22	1:Y:129:ASN:N	1.61	0.94
2:D:203:2AN:H2	2:D:203:2AN:H12	0.95	0.94
1:L:128:VAL:CA	1:L:129:ASN:CB	2.45	0.94
2:a:201:2AN:H2	2:a:201:2AN:H12	1.49	0.94
1:S:6:ILE:HD11	1:S:133:VAL:HG13	1.47	0.93
1:a:129:ASN:ND2	1:a:129:ASN:H	1.54	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:V:24:VAL:HG12	1:V:25:LEU:N	1.83	0.93
2:F:201:2AN:H2	2:F:201:2AN:H12	0.94	0.93
1:J:120:TYR:CE1	1:J:133:VAL:HG13	2.03	0.93
1:G:129:ASN:HD22	1:G:129:ASN:N	1.65	0.93
1:Z:93:ARG:HD2	1:Z:129:ASN:ND2	1.83	0.93
1:A:85:THR:CG2	1:A:100:VAL:HG23	1.99	0.92
1:X:8:LYS:HE3	1:X:10:GLU:OE1	1.70	0.92
1:O:96:ILE:HD11	1:O:128:VAL:HG13	1.52	0.92
1:D:129:ASN:O	1:D:129:ASN:ND2	2.02	0.92
1:b:92:LEU:O	1:b:93:ARG:HB2	1.69	0.92
1:N:73:ASP:O	1:N:74:GLU:HG2	1.70	0.91
2:R:202:2AN:H16	2:R:202:2AN:H2	1.51	0.91
1:G:49:GLY:HA2	1:G:53:THR:HG21	1.52	0.91
1:L:128:VAL:HG13	1:L:129:ASN:CB	1.99	0.90
1:B:4:TYR:HD2	1:B:128:VAL:HG11	1.32	0.90
1:J:95:ASN:HD22	1:J:95:ASN:N	1.68	0.90
2:S:201:2AN:H12	2:S:201:2AN:C2	2.00	0.90
1:X:6:ILE:HD11	1:X:133:VAL:HG13	1.53	0.90
1:Q:122:PRO:HG3	1:Q:128:VAL:HG23	1.52	0.90
2:H:203:2AN:H2	2:H:203:2AN:C16	1.97	0.89
2:Z:203:2AN:H2	2:Z:203:2AN:C16	1.99	0.89
1:A:1:MET:O	1:A:1:MET:HG2	1.70	0.89
1:X:129:ASN:HD22	1:X:129:ASN:H	0.91	0.89
2:a:201:2AN:H12	2:a:201:2AN:C2	2.00	0.89
1:Y:129:ASN:HD22	1:Y:129:ASN:H	1.14	0.89
1:a:92:LEU:O	1:a:93:ARG:HG3	1.72	0.89
1:D:4:TYR:CD1	1:D:128:VAL:HB	2.07	0.89
1:P:44:ILE:H	1:P:44:ILE:HD12	1.35	0.89
1:I:6:ILE:HG23	1:J:1:MET:HG2	1.53	0.89
1:W:6:ILE:HD11	1:W:133:VAL:HG13	1.52	0.89
2:G:204:2AN:H16	2:G:204:2AN:H2	1.54	0.89
2:I:204:2AN:H16	2:I:204:2AN:H2	1.55	0.88
1:O:7:VAL:HG22	1:O:117:THR:HG22	1.56	0.88
2:U:203:2AN:H2	2:U:203:2AN:C16	2.00	0.88
1:L:129:ASN:ND2	1:L:132:GLU:HB3	1.88	0.88
2:S:201:2AN:H12	2:S:201:2AN:H2	1.55	0.88
1:B:7:VAL:HG22	1:B:117:THR:HG22	1.53	0.88
1:E:33:LYS:CD	2:E:203:2AN:O3	2.22	0.88
1:V:21:LYS:O	1:V:26:GLU:HB2	1.73	0.88
1:A:96:ILE:HD11	1:A:128:VAL:HG13	1.55	0.88
2:a:201:2AN:H2	2:a:201:2AN:C12	2.00	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:147:VAL:CG1	2:I:203:2AN:H6	2.03	0.88
1:E:49:GLY:O	1:E:75:ILE:HD12	1.73	0.87
1:A:37:HIS:CD2	1:A:38:VAL:CG2	2.53	0.87
1:J:95:ASN:HD22	1:J:95:ASN:H	1.19	0.87
1:O:127:THR:OG1	1:O:128:VAL:N	2.01	0.87
1:B:95:ASN:HD21	1:B:129:ASN:CB	1.88	0.87
2:C:204:2AN:H16	2:C:204:2AN:H2	1.56	0.87
1:U:6:ILE:HD11	1:U:133:VAL:HG13	1.56	0.87
2:U:203:2AN:H2	2:U:203:2AN:H16	1.57	0.86
1:a:95:ASN:HD21	1:a:129:ASN:HD21	1.16	0.86
1:G:129:ASN:HD22	1:G:129:ASN:H	1.18	0.86
1:L:128:VAL:HG12	1:L:129:ASN:HB3	1.56	0.86
1:N:72:PHE:N	1:N:72:PHE:CD1	2.39	0.86
2:R:202:2AN:H16	2:R:202:2AN:C2	2.02	0.86
1:C:129:ASN:HD22	1:C:129:ASN:N	1.74	0.86
1:X:129:ASN:H	1:X:129:ASN:ND2	1.62	0.86
2:D:202:2AN:H16	2:D:202:2AN:H2	0.90	0.86
1:B:4:TYR:HD2	1:B:128:VAL:CG1	1.89	0.85
2:P:201:2AN:H16	2:P:201:2AN:C2	2.07	0.85
1:X:129:ASN:HD22	1:X:129:ASN:N	1.73	0.85
2:A:204:2AN:H2	2:A:204:2AN:C16	2.03	0.85
1:a:129:ASN:HD22	1:a:129:ASN:H	0.86	0.85
1:L:144:TYR:O	1:L:144:TYR:CD1	2.29	0.84
1:Z:10:GLU:HG2	2:Z:202:2AN:H12	1.58	0.84
1:G:49:GLY:HA2	1:G:53:THR:CG2	2.07	0.84
1:Z:127:THR:OG1	1:Z:128:VAL:N	2.09	0.84
1:B:4:TYR:CD2	1:B:128:VAL:CG1	2.61	0.84
1:b:144:TYR:O	1:b:144:TYR:CD1	2.31	0.84
2:N:203:2AN:H16	2:N:203:2AN:H2	1.58	0.84
1:P:44:ILE:HD12	1:P:44:ILE:N	1.92	0.84
1:A:14:ILE:O	1:A:112:SER:HB2	1.76	0.83
2:V:202:2AN:O1	2:V:202:2AN:H16	1.79	0.83
1:A:66:THR:OG1	1:A:90:ASP:CB	2.25	0.83
1:N:141:TYR:CD2	2:N:203:2AN:H3	2.13	0.83
1:F:96:ILE:HG13	1:F:132:GLU:OE1	1.78	0.83
1:K:158:PHE:CE2	2:K:203:2AN:H13	2.12	0.83
2:D:201:2AN:H16	2:D:201:2AN:C2	2.08	0.82
2:K:202:2AN:H16	2:K:202:2AN:C2	1.99	0.82
1:R:144:TYR:CZ	2:R:201:2AN:H13	2.14	0.82
2:O:201:2AN:H16	2:O:201:2AN:C2	2.08	0.82
2:O:201:2AN:H2	2:O:201:2AN:C16	2.10	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:204:2AN:H12	2:I:204:2AN:O1	1.79	0.82
1:A:108:VAL:O	1:A:108:VAL:HG12	1.79	0.82
1:N:72:PHE:N	1:N:72:PHE:HD1	1.77	0.82
1:M:44:ILE:HD12	1:M:53:THR:HG21	1.62	0.81
2:Z:201:2AN:H2	2:Z:201:2AN:C12	2.09	0.81
1:a:6:ILE:HD12	1:a:118:VAL:HB	1.62	0.81
1:L:128:VAL:CB	1:L:129:ASN:HB3	2.09	0.81
2:H:201:2AN:C12	2:H:201:2AN:H2	2.10	0.81
1:S:25:LEU:O	1:S:26:GLU:CG	2.29	0.81
1:T:6:ILE:HD11	1:T:133:VAL:CG1	2.11	0.81
1:B:95:ASN:HD21	1:B:129:ASN:HB2	1.44	0.81
2:W:202:2AN:H2	2:W:202:2AN:C16	2.11	0.81
2:A:201:2AN:H16	2:A:201:2AN:C2	2.10	0.80
1:C:2:ALA:O	1:C:122:PRO:CG	2.29	0.80
1:L:54:VAL:CG2	1:L:71:LYS:HD3	2.11	0.80
1:A:85:THR:HG22	1:A:100:VAL:HG23	1.62	0.80
1:L:128:VAL:HA	1:L:129:ASN:HB3	1.61	0.80
1:L:128:VAL:CA	1:L:129:ASN:HB3	2.07	0.80
1:M:131:GLU:HG2	1:M:135:ILE:HD11	1.61	0.80
1:b:93:ARG:HD2	1:b:132:GLU:CD	2.06	0.80
1:A:96:ILE:CD1	1:A:128:VAL:CG2	2.45	0.80
2:J:202:2AN:H2	2:J:202:2AN:C16	2.11	0.80
1:N:6:ILE:HD11	1:N:137:GLU:CD	2.07	0.80
1:B:85:THR:OG1	1:B:100:VAL:HG22	1.82	0.79
2:B:204:2AN:H16	2:B:204:2AN:C2	2.10	0.79
2:U:203:2AN:H16	2:U:203:2AN:C2	2.11	0.79
1:W:92:LEU:O	1:W:93:ARG:HB2	1.81	0.79
1:E:147:VAL:HG13	2:E:203:2AN:H6	1.64	0.79
1:a:4:TYR:CE1	1:b:2:ALA:HB2	2.16	0.79
1:D:129:ASN:HD22	1:D:129:ASN:C	1.85	0.79
1:M:4:TYR:CD2	1:M:128:VAL:HG11	2.17	0.79
1:G:92:LEU:O	1:G:93:ARG:HB2	1.81	0.79
2:B:205:2AN:H2	2:B:205:2AN:C16	2.12	0.79
1:I:14:ILE:HD11	1:I:148:GLU:CG	2.11	0.79
2:I:203:2AN:H2	2:I:203:2AN:H16	0.88	0.79
1:S:25:LEU:O	1:S:26:GLU:HG3	1.82	0.78
1:Y:54:VAL:HG22	1:Y:71:LYS:HG3	1.66	0.78
1:X:92:LEU:O	1:X:93:ARG:CB	2.31	0.78
1:Y:10:GLU:C	1:Y:11:GLU:HG3	2.09	0.78
1:B:104:LYS:C	1:B:105:LEU:HD23	2.08	0.78
2:E:205:2AN:H12	2:E:205:2AN:O3	1.84	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:51:VAL:HG23	1:F:75:ILE:HG13	1.64	0.78
1:U:6:ILE:HD11	1:U:133:VAL:CG1	2.13	0.78
2:C:203:2AN:S	2:C:203:2AN:N	2.57	0.77
2:L:203:2AN:H12	2:L:203:2AN:C2	2.07	0.77
1:G:92:LEU:O	1:G:93:ARG:CB	2.32	0.77
1:S:133:VAL:O	1:S:137:GLU:HG2	1.84	0.77
1:R:4:TYR:OH	1:R:130:GLU:HB2	1.85	0.77
1:J:122:PRO:HG3	1:J:128:VAL:HG23	1.65	0.77
2:C:204:2AN:S	2:C:204:2AN:N	2.58	0.77
1:J:2:ALA:O	1:J:3:ALA:HB2	1.84	0.77
1:Z:93:ARG:HD2	1:Z:129:ASN:HD21	1.51	0.76
1:E:144:TYR:CZ	2:E:202:2AN:H13	2.20	0.76
1:Y:129:ASN:H	1:Y:129:ASN:ND2	1.77	0.76
2:V:202:2AN:S	2:V:202:2AN:N	2.59	0.76
1:a:123:LYS:CE	1:a:124:PRO:HD2	2.16	0.76
1:X:6:ILE:HD11	1:X:133:VAL:CG1	2.15	0.76
1:G:129:ASN:H	1:G:129:ASN:ND2	1.83	0.76
1:K:133:VAL:O	1:K:137:GLU:HG2	1.86	0.76
2:W:204:2AN:O3	2:W:204:2AN:H16	1.84	0.76
2:b:202:2AN:H16	2:b:202:2AN:C2	2.14	0.76
1:J:133:VAL:O	1:J:137:GLU:HG2	1.86	0.76
1:C:138:LYS:HE3	2:C:204:2AN:O1	1.86	0.76
2:E:205:2AN:N	2:E:205:2AN:S	2.58	0.76
2:O:201:2AN:H16	2:O:201:2AN:H2	1.65	0.76
1:Y:90:ASP:OD1	1:Y:90:ASP:N	2.20	0.75
1:G:6:ILE:HG21	1:G:137:GLU:OE2	1.86	0.75
1:G:46:GLU:O	1:G:46:GLU:CG	2.32	0.75
1:D:91:VAL:CG2	1:D:91:VAL:O	2.33	0.75
1:D:91:VAL:O	1:D:91:VAL:HG23	1.85	0.75
1:L:128:VAL:HG12	1:L:129:ASN:O	1.86	0.75
1:I:92:LEU:O	1:I:93:ARG:HB2	1.85	0.75
1:a:92:LEU:O	1:a:93:ARG:CB	2.35	0.75
1:S:93:ARG:C	1:S:95:ASN:H	1.94	0.75
1:F:14:ILE:HD12	1:F:148:GLU:HG3	1.69	0.75
1:K:33:LYS:HD2	2:K:203:2AN:O1	1.86	0.75
2:G:204:2AN:O1	2:G:204:2AN:C12	2.34	0.75
1:G:133:VAL:O	1:G:137:GLU:HG2	1.87	0.75
1:a:92:LEU:O	1:a:93:ARG:CG	2.34	0.75
1:A:38:VAL:O	1:A:38:VAL:HG12	1.87	0.74
1:K:49:GLY:CA	1:K:53:THR:OG1	2.33	0.74
1:A:97:GLU:O	1:A:97:GLU:CD	2.30	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Q:203:2AN:S	2:Q:203:2AN:N	2.60	0.74
1:Q:92:LEU:O	1:Q:93:ARG:HB2	1.87	0.74
1:M:116:ILE:HD13	2:M:202:2AN:O3	1.88	0.74
1:C:92:LEU:O	1:C:96:ILE:HB	1.87	0.74
2:C:204:2AN:O3	2:C:204:2AN:C12	2.35	0.74
1:H:96:ILE:CD1	1:H:128:VAL:HG22	2.18	0.74
1:W:4:TYR:CE1	1:X:2:ALA:HB2	2.23	0.74
1:W:6:ILE:HD11	1:W:133:VAL:CG1	2.17	0.74
1:Z:129:ASN:OD1	1:Z:132:GLU:CB	2.36	0.74
1:b:10:GLU:HG2	2:b:201:2AN:C12	2.18	0.74
2:M:201:2AN:H16	2:M:201:2AN:C2	2.16	0.73
2:V:201:2AN:S	2:V:201:2AN:N	2.58	0.73
1:G:138:LYS:O	1:G:138:LYS:HD3	1.88	0.73
1:M:147:VAL:HG13	2:M:203:2AN:C6	2.15	0.73
2:U:203:2AN:C16	2:U:203:2AN:C2	2.64	0.73
2:W:204:2AN:S	2:W:204:2AN:N	2.61	0.73
1:Q:45:ILE:HD11	1:Q:54:VAL:HG12	1.69	0.73
1:G:138:LYS:CD	1:G:138:LYS:C	2.61	0.73
2:I:203:2AN:S	2:I:203:2AN:N	2.61	0.73
2:K:202:2AN:S	2:K:202:2AN:N	2.61	0.73
2:L:203:2AN:S	2:L:203:2AN:N	2.60	0.73
2:Z:203:2AN:N	2:Z:203:2AN:S	2.61	0.73
1:K:97:GLU:HB2	1:K:123:LYS:HG3	1.70	0.73
1:V:37:HIS:O	2:V:202:2AN:H7	1.88	0.73
2:G:203:2AN:S	2:G:203:2AN:N	2.61	0.73
2:N:203:2AN:S	2:N:203:2AN:N	2.62	0.73
1:Y:138:LYS:HG2	1:Y:138:LYS:O	1.85	0.73
2:Y:204:2AN:S	2:Y:204:2AN:N	2.61	0.73
1:D:92:LEU:HB3	1:D:96:ILE:HG22	1.70	0.73
1:I:156:GLU:HG2	1:I:157:VAL:N	2.04	0.73
2:D:202:2AN:S	2:D:202:2AN:N	2.62	0.73
1:I:1:MET:HG3	1:I:2:ALA:N	2.04	0.73
2:G:204:2AN:S	2:G:204:2AN:N	2.62	0.73
2:Y:202:2AN:H16	2:Y:202:2AN:C2	2.18	0.73
1:b:50:GLY:O	1:b:51:VAL:C	2.31	0.73
2:I:202:2AN:C15	2:I:205:2AN:H7	2.19	0.72
1:J:94:ASP:O	1:J:123:LYS:HD2	1.87	0.72
1:Q:83:LYS:HB2	1:Q:102:GLU:HG3	1.71	0.72
1:Z:92:LEU:O	1:Z:93:ARG:CB	2.36	0.72
2:D:201:2AN:S	2:D:201:2AN:N	2.62	0.72
1:L:144:TYR:CD1	1:L:144:TYR:C	2.68	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:b:129:ASN:ND2	1:b:132:GLU:CB	2.52	0.72
1:A:37:HIS:NE2	1:A:38:VAL:HG23	2.01	0.72
1:E:131:GLU:O	1:E:135:ILE:HG13	1.89	0.72
2:U:203:2AN:S	2:U:203:2AN:N	2.61	0.72
1:Z:8:LYS:HE3	1:Z:137:GLU:OE2	1.90	0.72
2:G:204:2AN:O1	2:G:204:2AN:N	2.23	0.72
2:W:201:2AN:N	2:W:201:2AN:S	2.63	0.72
1:b:129:ASN:ND2	1:b:132:GLU:HB3	2.04	0.72
1:A:38:VAL:HG13	1:A:63:HIS:CD2	2.25	0.72
1:A:65:LEU:HD22	1:A:91:VAL:HA	1.70	0.72
2:H:202:2AN:S	2:H:202:2AN:N	2.62	0.72
1:F:14:ILE:CD1	1:F:148:GLU:HG3	2.19	0.72
1:K:158:PHE:CZ	2:K:203:2AN:H13	2.24	0.72
2:Y:202:2AN:H2	2:Y:202:2AN:C16	2.20	0.72
2:F:201:2AN:S	2:F:201:2AN:N	2.59	0.71
1:O:46:GLU:HB2	1:O:54:VAL:HB	1.70	0.71
1:M:3:ALA:HB1	1:M:120:TYR:O	1.90	0.71
2:W:202:2AN:S	2:W:202:2AN:N	2.62	0.71
2:A:203:2AN:S	2:A:203:2AN:N	2.63	0.71
1:G:10:GLU:HB3	2:G:202:2AN:H13	1.71	0.71
2:I:204:2AN:H2	2:I:204:2AN:C16	2.20	0.71
1:K:92:LEU:O	1:K:93:ARG:CG	2.37	0.71
1:M:2:ALA:CB	1:N:4:TYR:CE1	2.74	0.71
2:L:202:2AN:H2	2:L:202:2AN:C16	2.21	0.71
2:E:203:2AN:S	2:E:203:2AN:N	2.58	0.71
2:E:204:2AN:H2	2:E:204:2AN:C12	2.19	0.71
2:H:201:2AN:S	2:H:201:2AN:N	2.60	0.71
1:Q:123:LYS:O	1:Q:126:CYS:CB	2.39	0.71
2:H:203:2AN:S	2:H:203:2AN:N	2.61	0.71
2:I:205:2AN:S	2:I:205:2AN:N	2.60	0.71
1:K:77:ALA:O	1:K:78:ALA:HB3	1.90	0.71
2:N:202:2AN:H2	2:N:202:2AN:C16	2.21	0.71
1:R:129:ASN:HB2	1:R:132:GLU:OE1	1.91	0.71
1:W:64:PRO:CG	2:W:201:2AN:O3	2.39	0.71
1:a:122:PRO:HG3	1:a:128:VAL:HG21	1.73	0.71
1:Z:92:LEU:O	1:Z:93:ARG:HB2	1.91	0.71
2:B:204:2AN:H16	2:B:204:2AN:H2	1.73	0.71
2:C:201:2AN:S	2:C:201:2AN:N	2.64	0.71
2:G:202:2AN:N	2:G:202:2AN:S	2.58	0.71
1:S:91:VAL:O	1:S:91:VAL:HG22	1.90	0.71
2:B:202:2AN:H2	2:B:202:2AN:C16	2.20	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:7:VAL:HG22	1:A:117:THR:HG22	1.72	0.70
2:E:205:2AN:H16	2:E:205:2AN:C2	2.18	0.70
2:K:201:2AN:S	2:K:201:2AN:N	2.64	0.70
1:M:90:ASP:OD1	1:M:90:ASP:N	2.18	0.70
2:N:204:2AN:S	2:N:204:2AN:N	2.64	0.70
2:N:203:2AN:O3	2:N:203:2AN:C12	2.39	0.70
1:V:96:ILE:HD11	1:V:132:GLU:OE2	1.92	0.70
2:B:203:2AN:N	2:B:203:2AN:S	2.62	0.70
1:K:92:LEU:C	1:K:93:ARG:HG2	2.17	0.70
1:R:116:ILE:HD11	2:R:201:2AN:H16	1.73	0.70
2:W:202:2AN:N	2:W:202:2AN:O3	2.25	0.70
2:b:203:2AN:S	2:b:203:2AN:N	2.64	0.70
1:C:120:TYR:CE1	1:C:133:VAL:HG13	2.26	0.70
2:G:204:2AN:H8	2:G:205:2AN:C15	2.22	0.70
1:I:1:MET:O	1:I:2:ALA:HB2	1.89	0.70
1:J:94:ASP:O	1:J:123:LYS:CD	2.39	0.70
2:W:203:2AN:S	2:W:203:2AN:N	2.65	0.70
1:a:93:ARG:HD2	1:a:129:ASN:OD1	1.92	0.70
1:I:68:MET:HG2	1:I:91:VAL:HG11	1.73	0.70
2:P:201:2AN:H16	2:P:201:2AN:H2	1.73	0.70
2:L:201:2AN:S	2:L:201:2AN:N	2.64	0.70
2:M:203:2AN:S	2:M:203:2AN:N	2.61	0.70
2:O:202:2AN:N	2:O:202:2AN:S	2.63	0.70
2:Q:202:2AN:S	2:Q:202:2AN:N	2.64	0.70
1:W:50:GLY:O	1:W:51:VAL:C	2.35	0.70
1:K:92:LEU:C	1:K:93:ARG:CG	2.65	0.70
1:S:86:LEU:CD2	1:S:92:LEU:HD21	2.20	0.70
1:B:106:GLU:OE2	1:B:113:LYS:HD3	1.92	0.70
2:C:202:2AN:H2	2:C:202:2AN:C16	2.22	0.70
1:H:139:LYS:HE2	2:H:202:2AN:C4	2.22	0.70
1:I:147:VAL:HG13	2:I:203:2AN:C7	2.21	0.70
1:S:37:HIS:NE2	1:S:38:VAL:HG23	2.05	0.70
1:U:116:ILE:HD11	2:U:201:2AN:H16	1.73	0.70
1:D:131:GLU:O	1:D:132:GLU:C	2.32	0.70
1:Q:124:PRO:O	1:Q:125:GLY:C	2.34	0.70
1:J:63:HIS:O	1:J:64:PRO:C	2.29	0.69
2:X:201:2AN:S	2:X:201:2AN:N	2.65	0.69
1:Z:48:ASP:OD1	1:Z:48:ASP:N	2.23	0.69
1:b:4:TYR:CD2	1:b:128:VAL:HB	2.27	0.69
2:B:204:2AN:N	2:B:204:2AN:S	2.60	0.69
2:E:205:2AN:O3	2:E:205:2AN:N	2.25	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:204:2AN:S	2:I:204:2AN:N	2.65	0.69
1:a:95:ASN:ND2	1:a:129:ASN:ND2	2.37	0.69
1:B:4:TYR:O	1:B:4:TYR:HD1	1.76	0.69
1:D:129:ASN:C	1:D:131:GLU:H	1.99	0.69
2:M:201:2AN:S	2:M:201:2AN:N	2.66	0.69
2:Q:201:2AN:S	2:Q:201:2AN:N	2.62	0.69
1:V:54:VAL:HA	1:V:70:HIS:O	1.92	0.69
2:b:201:2AN:S	2:b:201:2AN:N	2.65	0.69
1:C:2:ALA:O	1:C:122:PRO:HG2	1.93	0.69
2:C:202:2AN:O3	2:C:202:2AN:N	2.26	0.69
1:H:54:VAL:HG22	1:H:71:LYS:HB3	1.74	0.69
1:V:21:LYS:O	1:V:26:GLU:CB	2.40	0.69
2:W:202:2AN:H16	2:W:202:2AN:C2	2.21	0.69
2:Y:201:2AN:S	2:Y:201:2AN:N	2.66	0.69
2:A:204:2AN:S	2:A:204:2AN:N	2.60	0.69
2:L:205:2AN:S	2:L:205:2AN:N	2.62	0.69
1:a:44:ILE:O	1:a:44:ILE:CG2	2.37	0.69
2:a:201:2AN:S	2:a:201:2AN:N	2.62	0.69
1:J:27:ARG:NH1	2:J:201:2AN:O2	2.24	0.69
1:S:4:TYR:CE1	1:S:128:VAL:HB	2.27	0.69
1:V:143:PHE:O	1:V:143:PHE:CG	2.44	0.69
2:Z:201:2AN:S	2:Z:201:2AN:N	2.63	0.69
2:A:203:2AN:N	2:A:203:2AN:O3	2.26	0.69
1:E:92:LEU:O	1:E:93:ARG:CB	2.40	0.69
2:E:201:2AN:S	2:E:201:2AN:N	2.66	0.69
1:G:138:LYS:HG2	2:G:204:2AN:C1	2.23	0.69
2:R:202:2AN:N	2:R:202:2AN:S	2.66	0.69
2:S:201:2AN:S	2:S:201:2AN:N	2.66	0.69
2:U:204:2AN:N	2:U:204:2AN:O1	2.26	0.69
1:b:48:ASP:CG	1:b:48:ASP:O	2.32	0.69
2:E:204:2AN:O3	2:E:204:2AN:N	2.25	0.69
1:L:92:LEU:O	1:L:93:ARG:HB2	1.92	0.69
2:U:201:2AN:S	2:U:201:2AN:N	2.65	0.69
2:Y:202:2AN:S	2:Y:202:2AN:N	2.66	0.69
2:b:202:2AN:N	2:b:202:2AN:S	2.64	0.69
2:B:205:2AN:S	2:B:205:2AN:N	2.62	0.69
2:N:202:2AN:S	2:N:202:2AN:N	2.60	0.69
2:P:202:2AN:S	2:P:202:2AN:N	2.63	0.69
2:L:205:2AN:H2	2:L:205:2AN:C16	2.23	0.68
2:N:201:2AN:S	2:N:201:2AN:N	2.66	0.68
1:T:95:ASN:ND2	1:T:129:ASN:H	1.91	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:202:2AN:O3	2:M:202:2AN:N	2.26	0.68
1:A:33:LYS:HB3	2:A:201:2AN:O1	1.93	0.68
1:B:40:LYS:NZ	1:B:61:ASP:OD1	2.24	0.68
2:P:201:2AN:C2	2:P:201:2AN:C16	2.69	0.68
2:P:201:2AN:S	2:P:201:2AN:N	2.63	0.68
2:B:201:2AN:S	2:B:201:2AN:N	2.65	0.68
1:F:54:VAL:HG22	1:F:71:LYS:HG2	1.75	0.68
1:X:1:MET:HE1	1:X:124:PRO:HA	1.75	0.68
2:A:202:2AN:S	2:A:202:2AN:N	2.66	0.68
2:W:204:2AN:H2	2:W:204:2AN:H12	1.75	0.68
1:E:92:LEU:O	1:E:93:ARG:HB2	1.92	0.68
1:P:137:GLU:OE1	1:P:137:GLU:HA	1.92	0.68
2:A:201:2AN:O1	2:A:201:2AN:N	2.26	0.68
1:C:129:ASN:N	1:C:129:ASN:ND2	2.41	0.68
2:J:202:2AN:C16	2:J:202:2AN:C2	2.70	0.68
2:J:202:2AN:S	2:J:202:2AN:N	2.60	0.68
2:L:204:2AN:H2	2:L:204:2AN:C16	2.22	0.68
1:A:28:HIS:CD2	1:A:29:GLN:HG3	2.29	0.68
2:C:202:2AN:N	2:C:202:2AN:S	2.62	0.68
1:J:1:MET:O	1:J:2:ALA:HB3	1.93	0.68
2:Y:203:2AN:H2	2:Y:203:2AN:C16	2.23	0.68
2:D:201:2AN:H16	2:D:201:2AN:H2	1.75	0.68
1:Y:10:GLU:O	1:Y:11:GLU:HG3	1.94	0.68
2:B:204:2AN:H2	2:B:204:2AN:C16	2.24	0.68
2:M:203:2AN:N	2:M:203:2AN:O1	2.26	0.68
2:P:201:2AN:H2	2:P:201:2AN:C16	2.23	0.68
2:G:201:2AN:N	2:G:201:2AN:S	2.68	0.67
1:T:123:LYS:HB3	1:T:124:PRO:HD2	1.77	0.67
2:L:203:2AN:N	2:L:203:2AN:O3	2.27	0.67
1:B:7:VAL:HG22	1:B:117:THR:CG2	2.24	0.67
1:V:68:MET:HG2	1:V:91:VAL:CG1	2.19	0.67
1:V:96:ILE:CD1	1:V:132:GLU:OE2	2.42	0.67
1:a:123:LYS:HD2	1:a:124:PRO:HD2	0.71	0.67
1:A:47:GLY:HA3	1:A:53:THR:HA	1.76	0.67
2:A:201:2AN:N	2:A:201:2AN:S	2.63	0.67
2:H:201:2AN:H2	2:H:201:2AN:H12	1.75	0.67
1:O:10:GLU:C	1:O:11:GLU:HG3	2.19	0.67
1:P:48:ASP:OD1	1:P:48:ASP:N	2.26	0.67
2:G:205:2AN:S	2:G:205:2AN:N	2.63	0.67
2:J:201:2AN:S	2:J:201:2AN:N	2.63	0.67
2:J:202:2AN:C2	2:J:202:2AN:H16	2.22	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:123:LYS:O	1:Q:126:CYS:HB2	1.94	0.67
2:A:202:2AN:N	2:A:202:2AN:O3	2.27	0.67
2:I:203:2AN:N	2:I:203:2AN:O2	2.27	0.67
2:J:201:2AN:C2	2:J:201:2AN:H16	2.23	0.67
1:T:117[B]:THR:O	1:T:117[B]:THR:OG1	2.12	0.67
2:P:201:2AN:N	2:P:201:2AN:O3	2.27	0.67
2:b:203:2AN:N	2:b:203:2AN:O3	2.28	0.67
2:B:204:2AN:C2	2:B:204:2AN:C16	2.72	0.67
1:F:51:VAL:HG23	1:F:75:ILE:CG1	2.25	0.67
1:D:96:ILE:HG22	1:D:96:ILE:O	1.95	0.67
2:U:202:2AN:S	2:U:202:2AN:N	2.68	0.67
1:E:125:GLY:O	1:E:126:CYS:CB	2.42	0.66
1:M:131:GLU:HG2	1:M:135:ILE:HD12	1.76	0.66
2:N:202:2AN:H16	2:N:202:2AN:C2	2.25	0.66
1:C:138:LYS:HD2	1:C:138:LYS:C	2.19	0.66
1:M:116:ILE:HD11	2:M:202:2AN:H16	1.76	0.66
1:U:6:ILE:CD1	1:U:133:VAL:HG13	2.25	0.66
2:I:202:2AN:S	2:I:202:2AN:N	2.68	0.66
2:F:201:2AN:N	2:F:201:2AN:O1	2.28	0.66
1:G:19:LEU:HD13	2:G:202:2AN:C15	2.26	0.66
1:I:92:LEU:O	1:I:93:ARG:CB	2.41	0.66
1:J:95:ASN:H	1:J:95:ASN:ND2	1.85	0.66
1:K:96:ILE:CD1	1:K:128:VAL:HG22	2.26	0.66
1:V:76:ASP:HB3	1:V:81:TYR:HB3	1.76	0.66
2:W:202:2AN:C16	2:W:202:2AN:C2	2.70	0.66
2:D:201:2AN:C2	2:D:201:2AN:C16	2.72	0.66
2:X:202:2AN:O3	2:X:202:2AN:N	2.28	0.66
1:Y:23:LEU:O	1:Y:27:ARG:HD2	1.96	0.66
2:Q:201:2AN:H2	2:Q:201:2AN:C16	2.24	0.66
1:V:86:LEU:HG	1:V:92:LEU:HD11	1.77	0.66
1:L:15:ALA:HB1	1:L:16:PRO:HD2	1.78	0.66
1:C:2:ALA:O	1:C:122:PRO:HG3	1.95	0.66
1:E:142:GLU:O	1:E:146:GLN:HG3	1.96	0.66
2:R:204:2AN:N	2:R:204:2AN:O3	2.29	0.66
1:E:104:LYS:NZ	1:E:105:LEU:O	2.28	0.66
1:G:138:LYS:O	1:G:138:LYS:CD	2.44	0.66
1:O:96:ILE:CD1	1:O:128:VAL:HG13	2.26	0.66
1:P:144:TYR:CD1	1:P:144:TYR:O	2.49	0.66
2:S:201:2AN:H2	2:S:201:2AN:C12	2.26	0.66
2:W:202:2AN:H2	2:W:202:2AN:H16	1.77	0.66
2:Y:202:2AN:C2	2:Y:202:2AN:C16	2.69	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:93:ARG:NH1	1:a:131:GLU:OE2	2.22	0.66
1:K:158:PHE:CD2	2:K:203:2AN:H13	2.30	0.66
2:L:204:2AN:H16	2:L:204:2AN:C2	2.26	0.66
1:S:93:ARG:C	1:S:95:ASN:N	2.52	0.66
1:A:135:ILE:HG22	2:A:202:2AN:H15	1.77	0.65
1:N:63:HIS:O	1:N:64:PRO:C	2.36	0.65
1:Q:123:LYS:C	1:Q:126:CYS:HB2	2.21	0.65
1:W:144:TYR:CZ	2:W:202:2AN:H13	2.31	0.65
1:X:129:ASN:OD1	1:X:132:GLU:HB2	1.96	0.65
2:D:203:2AN:S	2:D:203:2AN:N	2.63	0.65
1:S:4:TYR:CD1	1:S:128:VAL:HB	2.31	0.65
2:U:204:2AN:N	2:U:204:2AN:S	2.63	0.65
1:D:94:ASP:C	1:D:94:ASP:OD1	2.37	0.65
1:H:53:THR:HB	1:H:72:PHE:CD2	2.32	0.65
1:H:129:ASN:OD1	1:H:130:GLU:N	2.29	0.65
2:H:201:2AN:N	2:H:201:2AN:O1	2.29	0.65
1:I:77:ALA:HB1	2:Q:203:2AN:H3	1.77	0.65
1:N:51:VAL:CG2	1:N:51:VAL:O	2.45	0.65
1:C:49:GLY:HA2	1:C:53:THR:CG2	2.26	0.65
1:F:71:LYS:O	1:F:84:TYR:HB2	1.95	0.65
2:K:203:2AN:S	2:K:203:2AN:N	2.60	0.65
2:U:203:2AN:N	2:U:203:2AN:O3	2.29	0.65
1:X:93:ARG:CD	1:X:132:GLU:OE1	2.40	0.65
1:b:129:ASN:HD21	1:b:132:GLU:HB3	1.60	0.65
2:A:203:2AN:H2	2:A:203:2AN:C16	2.26	0.65
1:W:63:HIS:HA	2:W:201:2AN:C16	2.27	0.65
1:a:122:PRO:HG3	1:a:128:VAL:HG23	1.77	0.65
2:E:202:2AN:H2	2:E:202:2AN:C16	2.25	0.65
2:I:204:2AN:O1	2:I:204:2AN:N	2.30	0.65
1:Z:10:GLU:HG2	2:Z:202:2AN:C12	2.27	0.65
1:J:106:GLU:OE2	1:J:113:LYS:HE3	1.95	0.65
2:O:201:2AN:N	2:O:201:2AN:S	2.63	0.65
1:S:48:ASP:CG	1:S:50:GLY:H	2.05	0.65
1:X:90:ASP:OD2	1:X:90:ASP:N	2.29	0.65
1:Z:129:ASN:OD1	1:Z:132:GLU:N	2.29	0.65
1:G:138:LYS:C	1:G:138:LYS:HD2	2.21	0.65
1:I:68:MET:HG2	1:I:91:VAL:CG1	2.26	0.65
1:M:4:TYR:CD2	1:M:128:VAL:CG1	2.79	0.65
2:Y:203:2AN:O3	2:Y:203:2AN:N	2.29	0.65
1:C:138:LYS:C	1:C:138:LYS:CD	2.70	0.65
1:A:74:GLU:OE2	1:A:83:LYS:NZ	2.21	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:R:201:2AN:O3	2:R:201:2AN:N	2.29	0.64
2:Z:201:2AN:N	2:Z:201:2AN:O2	2.30	0.64
2:L:204:2AN:C16	2:L:204:2AN:C2	2.73	0.64
2:X:203:2AN:S	2:X:203:2AN:N	2.64	0.64
2:b:201:2AN:N	2:b:201:2AN:O3	2.30	0.64
1:C:129:ASN:ND2	1:C:129:ASN:O	2.30	0.64
2:E:202:2AN:S	2:E:202:2AN:N	2.66	0.64
1:G:90:ASP:OD1	1:G:90:ASP:N	2.30	0.64
2:E:201:2AN:N	2:E:201:2AN:O3	2.31	0.64
2:G:201:2AN:H16	2:G:201:2AN:C2	2.27	0.64
1:A:150:TYR:CG	2:A:201:2AN:O3	2.50	0.64
2:B:205:2AN:N	2:B:205:2AN:O3	2.30	0.64
1:J:90:ASP:OD1	1:J:90:ASP:N	2.31	0.64
1:R:144:TYR:O	1:R:144:TYR:CD1	2.50	0.64
1:H:63:HIS:CD2	1:H:64:PRO:HD2	2.32	0.64
1:W:48:ASP:OD1	1:W:48:ASP:N	2.31	0.64
1:A:96:ILE:HD11	1:A:128:VAL:CG1	2.28	0.64
1:H:53:THR:HB	1:H:72:PHE:HD2	1.61	0.64
1:I:144:TYR:O	1:I:144:TYR:CD1	2.51	0.64
1:Y:127:THR:OG1	1:Y:128:VAL:N	2.29	0.64
2:B:202:2AN:C16	2:B:202:2AN:C2	2.76	0.64
1:b:144:TYR:CE2	2:b:201:2AN:H12	2.33	0.64
1:O:129:ASN:HB3	1:O:132:GLU:OE1	1.98	0.64
2:O:201:2AN:N	2:O:201:2AN:O3	2.30	0.64
1:U:144:TYR:O	1:U:144:TYR:CD1	2.49	0.64
2:V:201:2AN:N	2:V:201:2AN:O3	2.30	0.64
1:N:141:TYR:CD2	2:N:203:2AN:C3	2.81	0.64
1:X:95:ASN:HD21	1:X:129:ASN:ND2	1.96	0.64
1:D:4:TYR:CD1	1:D:128:VAL:CB	2.81	0.63
2:I:202:2AN:H16	2:I:202:2AN:C2	2.28	0.63
1:U:108:VAL:O	1:U:108:VAL:HG12	1.99	0.63
2:Y:203:2AN:N	2:Y:203:2AN:S	2.62	0.63
1:B:105:LEU:HD23	1:B:105:LEU:N	2.13	0.63
1:F:48:ASP:OD1	1:F:49:GLY:N	2.32	0.63
1:K:139:LYS:HA	1:K:139:LYS:HE3	1.79	0.63
1:T:58:THR:HG22	1:T:59:PHE:O	1.98	0.63
2:U:205:2AN:S	2:U:205:2AN:N	2.61	0.63
2:H:203:2AN:N	2:H:203:2AN:O1	2.28	0.63
2:O:202:2AN:N	2:O:202:2AN:O3	2.31	0.63
1:Q:6:ILE:HD12	1:Q:137:GLU:CD	2.24	0.63
1:T:92:LEU:O	1:T:93:ARG:HB2	1.98	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:W:68:MET:HG2	1:W:91:VAL:HG11	1.80	0.63
1:W:133:VAL:O	1:W:137:GLU:HG2	1.98	0.63
1:X:95:ASN:OD1	1:X:95:ASN:N	2.30	0.63
2:Y:202:2AN:N	2:Y:202:2AN:O3	2.31	0.63
1:Z:14:ILE:HG21	1:Z:151:LEU:HD12	1.81	0.63
1:a:96:ILE:HD11	1:a:128:VAL:HG13	1.81	0.63
1:A:97:GLU:N	1:A:121:HIS:O	2.27	0.63
1:P:44:ILE:H	1:P:44:ILE:CD1	2.10	0.63
2:P:202:2AN:H2	2:P:202:2AN:C16	2.28	0.63
1:Q:83:LYS:HG3	1:Q:83:LYS:O	1.98	0.63
1:T:96:ILE:HD11	1:T:128:VAL:HG22	1.80	0.63
2:B:202:2AN:S	2:B:202:2AN:N	2.65	0.63
2:D:203:2AN:N	2:D:203:2AN:O1	2.29	0.63
1:V:44:ILE:HA	1:V:55:THR:HG22	1.81	0.63
1:W:139:LYS:NZ	2:W:204:2AN:O2	2.32	0.63
1:b:6:ILE:HD11	1:b:133:VAL:HG13	1.79	0.63
1:D:17:HIS:NE2	1:D:159:ALA:O	2.32	0.63
2:C:202:2AN:C16	2:C:202:2AN:C2	2.75	0.63
2:D:201:2AN:H2	2:D:201:2AN:C16	2.28	0.63
1:I:46:GLU:HG2	1:I:46:GLU:O	1.99	0.63
1:L:128:VAL:HG12	1:L:129:ASN:C	2.23	0.63
2:L:202:2AN:S	2:L:202:2AN:N	2.65	0.63
1:T:68:MET:HG2	1:T:91:VAL:HG11	1.79	0.63
1:a:93:ARG:HG3	1:a:132:GLU:OE2	1.99	0.63
1:D:48:ASP:OD1	1:D:48:ASP:N	2.32	0.62
2:G:202:2AN:N	2:G:202:2AN:O3	2.31	0.62
2:Y:204:2AN:N	2:Y:204:2AN:O1	2.31	0.62
2:B:205:2AN:H2	2:B:205:2AN:H16	1.81	0.62
1:W:93:ARG:HB3	1:W:95:ASN:OD1	2.00	0.62
1:A:80:PHE:HB3	1:A:105:LEU:HB2	1.81	0.62
1:F:19:LEU:HD13	2:F:201:2AN:C13	2.30	0.62
1:J:2:ALA:O	1:J:3:ALA:CB	2.47	0.62
1:L:31:LEU:HD22	1:L:39:PHE:CE2	2.34	0.62
1:J:106:GLU:OE2	1:J:113:LYS:HG3	1.99	0.62
2:K:201:2AN:H16	2:K:201:2AN:C2	2.30	0.62
2:Q:201:2AN:H16	2:Q:201:2AN:C2	2.29	0.62
1:B:21:LYS:HE3	1:B:158:PHE:CD1	2.34	0.62
2:D:202:2AN:N	2:D:202:2AN:O1	2.32	0.62
1:Q:2:ALA:HB1	1:R:4:TYR:CE1	2.35	0.62
1:A:97:GLU:CD	1:A:97:GLU:C	2.67	0.62
1:I:50:GLY:N	1:I:53:THR:OG1	2.32	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:13:PRO:HD2	1:Q:148:GLU:OE2	2.00	0.62
1:S:93:ARG:O	1:S:96:ILE:N	2.29	0.62
1:A:97:GLU:HA	1:A:97:GLU:OE1	2.00	0.62
1:A:155:PRO:O	1:A:159:ALA:HB2	1.99	0.62
1:K:77:ALA:O	1:K:78:ALA:CB	2.48	0.62
1:K:92:LEU:O	1:K:93:ARG:CB	2.47	0.62
1:P:68:MET:HG2	1:P:91:VAL:HG11	1.80	0.62
1:S:35:GLN:OE1	2:S:201:2AN:H6	2.00	0.62
2:I:205:2AN:N	2:I:205:2AN:O3	2.31	0.62
1:J:89:GLY:O	1:J:92:LEU:HB2	2.00	0.62
2:N:204:2AN:N	2:N:204:2AN:O3	2.33	0.62
2:A:203:2AN:C16	2:A:203:2AN:C2	2.78	0.62
1:I:18:ARG:NH1	1:I:151:LEU:O	2.32	0.62
1:L:128:VAL:HG13	1:L:129:ASN:HD22	1.62	0.62
1:A:48:ASP:N	1:A:48:ASP:OD1	2.32	0.61
2:C:204:2AN:O3	2:C:204:2AN:N	2.33	0.61
1:E:125:GLY:O	1:E:126:CYS:SG	2.58	0.61
1:M:27:ARG:O	1:M:30:VAL:N	2.33	0.61
2:Q:201:2AN:C16	2:Q:201:2AN:C2	2.76	0.61
2:W:203:2AN:C2	2:W:203:2AN:H12	2.28	0.61
1:N:71:LYS:C	1:N:72:PHE:HD1	2.07	0.61
1:U:116:ILE:HD11	2:U:201:2AN:C16	2.29	0.61
1:O:1:MET:HE2	1:O:122:PRO:HG2	1.82	0.61
1:R:102:GLU:OE1	1:R:115:LYS:NZ	2.30	0.61
1:E:95:ASN:CB	1:E:126:CYS:HB3	2.31	0.61
1:K:130:GLU:O	1:K:134:LYS:HG3	2.00	0.61
1:L:104:LYS:C	1:L:105:LEU:HD12	2.24	0.61
1:V:93:ARG:O	1:V:94:ASP:CB	2.33	0.61
1:b:92:LEU:O	1:b:93:ARG:CB	2.41	0.61
2:E:202:2AN:N	2:E:202:2AN:O1	2.33	0.61
2:L:204:2AN:S	2:L:204:2AN:N	2.62	0.61
2:J:202:2AN:H2	2:J:202:2AN:H16	1.79	0.61
1:M:2:ALA:HB2	1:N:4:TYR:HE1	1.66	0.61
1:Q:92:LEU:O	1:Q:93:ARG:CB	2.48	0.61
1:C:33:LYS:HD2	2:C:203:2AN:C12	2.30	0.61
1:D:131:GLU:OE2	1:D:135:ILE:HD11	2.01	0.61
1:C:129:ASN:HD22	1:C:129:ASN:H	1.49	0.61
2:N:202:2AN:C16	2:N:202:2AN:C2	2.74	0.61
2:Q:203:2AN:H16	2:Q:203:2AN:C2	2.30	0.61
1:a:10:GLU:HB3	2:a:201:2AN:C15	2.30	0.61
1:P:76:ASP:HB3	1:P:81:TYR:HB3	1.83	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:204:2AN:C12	2:E:204:2AN:C2	2.76	0.61
1:N:89:GLY:O	1:N:92:LEU:HB2	2.01	0.61
1:S:48:ASP:OD1	1:S:48:ASP:N	2.30	0.61
2:Z:203:2AN:C2	2:Z:203:2AN:C16	2.59	0.61
1:C:129:ASN:OD1	1:C:132:GLU:CB	2.49	0.60
1:E:3:ALA:O	1:F:5:THR:N	2.30	0.60
2:E:204:2AN:C2	2:E:204:2AN:H12	2.31	0.60
1:O:71:LYS:HB2	1:O:87:PHE:CE2	2.35	0.60
1:S:57:ILE:O	1:S:67:TYR:HA	2.01	0.60
1:X:8:LYS:CE	1:X:10:GLU:OE1	2.46	0.60
1:B:129:ASN:OD1	1:B:132:GLU:HB2	2.00	0.60
2:C:201:2AN:H12	2:C:201:2AN:C2	2.31	0.60
1:X:129:ASN:OD1	1:X:132:GLU:CB	2.49	0.60
2:Z:203:2AN:N	2:Z:203:2AN:O3	2.34	0.60
2:E:201:2AN:H16	2:E:201:2AN:C2	2.31	0.60
2:E:201:2AN:C15	2:E:204:2AN:H7	2.32	0.60
1:F:44:ILE:HG23	1:F:53:THR:CG2	2.31	0.60
2:M:203:2AN:C2	2:M:203:2AN:C16	2.59	0.60
1:P:92:LEU:O	1:P:93:ARG:HB2	2.01	0.60
1:U:92:LEU:O	1:U:93:ARG:HB2	2.01	0.60
1:B:89:GLY:O	1:B:91:VAL:N	2.34	0.60
2:L:202:2AN:N	2:L:202:2AN:O1	2.31	0.60
1:O:1:MET:HE1	1:O:122:PRO:O	2.01	0.60
1:Q:81:TYR:CD1	1:Q:81:TYR:C	2.79	0.60
2:R:202:2AN:H2	2:R:202:2AN:C16	2.27	0.60
2:W:201:2AN:C16	2:W:201:2AN:H2	2.30	0.60
1:Y:149:GLU:C	1:Y:149:GLU:OE1	2.44	0.60
2:I:201:2AN:S	2:I:201:2AN:N	2.66	0.60
1:V:50:GLY:O	1:V:53:THR:HB	2.02	0.60
1:W:64:PRO:HG3	2:W:201:2AN:O3	2.02	0.60
1:a:48:ASP:OD1	1:a:48:ASP:N	2.34	0.60
1:F:6:ILE:HD13	1:F:133:VAL:HG11	1.84	0.60
2:I:205:2AN:C12	2:I:205:2AN:H2	2.30	0.60
2:J:201:2AN:C2	2:J:201:2AN:C16	2.77	0.60
1:O:10:GLU:C	1:O:11:GLU:CG	2.75	0.60
1:A:45:ILE:CG1	1:A:54:VAL:HG12	2.31	0.60
1:B:130:GLU:O	1:B:131:GLU:CB	2.49	0.60
1:S:45:ILE:HG21	1:S:56:LYS:HD3	1.83	0.60
1:T:26[A]:GLU:OE1	1:T:29:GLN:NE2	2.35	0.60
1:U:144:TYR:CZ	2:U:201:2AN:H12	2.36	0.60
2:W:201:2AN:N	2:W:201:2AN:O1	2.35	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:138:LYS:HD2	1:C:138:LYS:O	2.02	0.60
1:G:97:GLU:HB2	1:G:123:LYS:HG3	1.84	0.60
2:K:203:2AN:N	2:K:203:2AN:O3	2.34	0.60
1:O:131:GLU:C	1:O:133:VAL:H	2.10	0.60
2:W:204:2AN:H2	2:W:204:2AN:C12	2.32	0.60
2:M:201:2AN:N	2:M:201:2AN:O3	2.35	0.60
2:b:203:2AN:H2	2:b:203:2AN:C16	2.32	0.60
2:L:202:2AN:H16	2:L:202:2AN:C2	2.32	0.59
1:P:28:HIS:CD2	1:P:55:THR:HG21	2.37	0.59
1:T:3:ALA:HB1	1:T:120:TYR:O	2.02	0.59
1:U:90:ASP:OD1	1:U:90:ASP:N	2.28	0.59
1:D:87:PHE:C	1:D:92:LEU:HD11	2.27	0.59
2:E:203:2AN:N	2:E:203:2AN:O1	2.34	0.59
1:F:51:VAL:HG21	1:F:74:GLU:CA	2.32	0.59
1:J:108:VAL:O	1:J:109:GLY:C	2.42	0.59
1:K:97:GLU:CB	1:K:123:LYS:HG3	2.31	0.59
1:S:95:ASN:N	1:S:95:ASN:OD1	2.35	0.59
1:T:6:ILE:HD11	1:T:133:VAL:HG12	1.83	0.59
1:X:116:ILE:HD11	2:X:202:2AN:H16	1.84	0.59
1:B:54:VAL:HA	1:B:70:HIS:O	2.02	0.59
1:b:4:TYR:HD2	1:b:128:VAL:HB	1.66	0.59
1:C:144:TYR:CE1	2:C:202:2AN:H13	2.37	0.59
1:L:90:ASP:N	1:L:90:ASP:OD1	2.34	0.59
1:A:68:MET:HG2	1:A:91:VAL:HG21	1.84	0.59
1:G:53:THR:HB	1:G:72:PHE:CD2	2.38	0.59
1:I:15:ALA:HB1	1:I:16:PRO:HD2	1.84	0.59
1:M:50:GLY:N	1:M:53:THR:OG1	2.35	0.59
1:M:147:VAL:CG1	2:M:203:2AN:H6	2.23	0.59
1:B:95:ASN:ND2	1:B:129:ASN:HB2	2.16	0.59
1:L:128:VAL:HG12	1:L:129:ASN:CB	2.26	0.59
1:A:38:VAL:O	1:A:38:VAL:CG1	2.50	0.59
1:B:4:TYR:O	1:B:4:TYR:CD1	2.54	0.59
1:B:100:VAL:HB	1:B:119:THR:HG23	1.85	0.59
1:H:144:TYR:CD1	1:H:144:TYR:O	2.56	0.59
1:L:54:VAL:HG22	1:L:71:LYS:HD3	1.83	0.59
1:Y:16:PRO:HB2	1:Y:80:PHE:CE2	2.37	0.59
1:a:46:GLU:O	1:a:53:THR:HG23	2.02	0.59
1:I:144:TYR:CD1	1:I:144:TYR:C	2.80	0.59
1:Q:45:ILE:HD11	1:Q:54:VAL:CG1	2.32	0.59
1:S:37:HIS:CD2	1:S:38:VAL:CG2	2.78	0.59
1:Y:11:GLU:HG2	1:Y:113:LYS:HG3	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:7:VAL:HG22	1:R:117:THR:HG22	1.85	0.59
1:a:129:ASN:OD1	1:a:132:GLU:HB2	2.03	0.59
1:A:65:LEU:HD13	1:A:91:VAL:HG13	1.84	0.58
1:C:129:ASN:ND2	1:C:129:ASN:H	1.98	0.58
2:C:202:2AN:C2	2:C:202:2AN:H16	2.33	0.58
2:L:204:2AN:N	2:L:204:2AN:O3	2.30	0.58
1:M:108:VAL:HG21	1:M:113:LYS:HG3	1.84	0.58
1:D:80:PHE:HB2	1:D:105:LEU:O	2.02	0.58
1:J:92:LEU:O	1:J:93:ARG:CB	2.51	0.58
1:U:90:ASP:C	1:U:92:LEU:N	2.58	0.58
2:X:202:2AN:H2	2:X:202:2AN:C16	2.33	0.58
1:E:32:VAL:HG21	1:E:41:SER:HA	1.86	0.58
1:H:129:ASN:CG	1:H:130:GLU:N	2.61	0.58
1:V:67:TYR:C	1:V:67:TYR:CD1	2.80	0.58
1:X:129:ASN:ND2	1:X:129:ASN:N	2.33	0.58
1:a:6:ILE:HD13	1:a:137:GLU:HG3	1.84	0.58
1:N:28:HIS:CD2	1:N:29:GLN:HG3	2.38	0.58
1:C:127:THR:CG2	1:C:128:VAL:N	2.66	0.58
1:C:130:GLU:HG2	1:C:130:GLU:O	2.03	0.58
1:S:129:ASN:ND2	1:S:129:ASN:H	2.02	0.58
1:K:19:LEU:HD13	2:K:202:2AN:C15	2.33	0.58
1:K:92:LEU:O	1:K:93:ARG:HG3	2.02	0.58
1:N:141:TYR:HD2	2:N:203:2AN:C3	2.17	0.58
1:Z:93:ARG:NH1	1:Z:131:GLU:OE2	2.29	0.58
2:E:205:2AN:O3	2:E:205:2AN:C12	2.52	0.58
1:N:73:ASP:C	1:N:74:GLU:CG	2.76	0.58
1:R:48:ASP:OD1	1:R:48:ASP:N	2.35	0.58
1:U:147:VAL:O	1:U:147:VAL:HG12	2.03	0.58
1:A:7:VAL:CG2	1:A:117:THR:HG22	2.33	0.58
1:B:21:LYS:HE3	1:B:158:PHE:CE1	2.38	0.58
1:E:2:ALA:CB	1:F:4:TYR:CE1	2.82	0.58
2:L:202:2AN:C16	2:L:202:2AN:C2	2.74	0.58
1:U:1:MET:O	1:V:6:ILE:HD13	2.04	0.58
2:V:202:2AN:O1	2:V:202:2AN:C16	2.51	0.58
1:b:65:LEU:HD22	1:b:91:VAL:HA	1.86	0.58
1:C:157:VAL:O	1:C:158:PHE:HB2	2.03	0.58
2:C:203:2AN:N	2:C:203:2AN:O3	2.37	0.58
1:E:95:ASN:HB3	1:E:126:CYS:HB3	1.86	0.58
1:E:125:GLY:O	1:E:126:CYS:HB2	2.03	0.58
1:G:10:GLU:HB3	2:G:202:2AN:C13	2.34	0.58
2:L:204:2AN:H6	1:R:21:LYS:HG3	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:32:VAL:O	1:O:32:VAL:HG12	2.03	0.57
1:W:4:TYR:HE1	1:X:2:ALA:HB2	1.69	0.57
1:X:1:MET:CE	1:X:124:PRO:HA	2.34	0.57
1:Z:46:GLU:HB2	1:Z:54:VAL:HB	1.86	0.57
1:A:35:GLN:HB3	1:A:37:HIS:CE1	2.39	0.57
1:A:144:TYR:CZ	2:A:203:2AN:H13	2.39	0.57
1:B:15:ALA:HB1	1:B:16:PRO:HD2	1.86	0.57
1:D:76:ASP:HB3	1:D:81:TYR:HB3	1.86	0.57
1:F:4:TYR:CD2	1:F:128:VAL:HG11	2.39	0.57
1:F:20:PHE:HB2	1:F:105:LEU:HD12	1.86	0.57
1:H:72:PHE:CD2	1:H:75:ILE:HD11	2.39	0.57
1:J:1:MET:O	1:J:2:ALA:CB	2.51	0.57
2:Q:203:2AN:C2	2:Q:203:2AN:C16	2.81	0.57
1:B:89:GLY:O	1:B:92:LEU:N	2.32	0.57
2:E:205:2AN:H2	2:E:205:2AN:C16	2.20	0.57
1:L:89:GLY:O	1:L:90:ASP:C	2.46	0.57
2:I:204:2AN:O1	2:I:204:2AN:C12	2.52	0.57
1:X:104:LYS:NZ	1:X:105:LEU:O	2.37	0.57
2:X:203:2AN:C16	2:X:203:2AN:H2	2.34	0.57
1:B:123:LYS:HD3	1:B:124:PRO:HD2	1.86	0.57
1:I:48:ASP:OD1	1:I:50:GLY:N	2.30	0.57
2:U:201:2AN:C16	2:U:201:2AN:H2	2.34	0.57
1:C:86:LEU:HG	1:C:92:LEU:HD21	1.87	0.57
1:F:129:ASN:C	1:F:131:GLU:N	2.60	0.57
1:I:144:TYR:CD1	2:I:201:2AN:H12	2.39	0.57
1:V:37:HIS:CD2	1:V:38:VAL:HG23	2.40	0.57
1:W:68:MET:HG2	1:W:91:VAL:CG1	2.35	0.57
1:A:28:HIS:CD2	1:A:29:GLN:CG	2.88	0.57
1:Z:92:LEU:O	1:Z:93:ARG:CG	2.52	0.57
1:G:50:GLY:O	1:G:75:ILE:HD12	2.04	0.57
1:M:92:LEU:O	1:M:93:ARG:HB2	2.05	0.57
1:a:92:LEU:O	1:a:93:ARG:HB2	2.04	0.57
1:A:158:PHE:CE2	2:A:201:2AN:H6	2.39	0.57
1:H:53:THR:O	1:H:71:LYS:HA	2.05	0.57
1:R:130:GLU:O	1:R:130:GLU:CG	2.35	0.57
1:Z:14:ILE:O	1:Z:112:SER:OG	2.22	0.57
2:B:202:2AN:N	2:B:202:2AN:O1	2.35	0.56
2:I:201:2AN:N	2:I:201:2AN:O3	2.38	0.56
2:J:202:2AN:N	2:J:202:2AN:O3	2.38	0.56
1:N:51:VAL:O	1:N:51:VAL:HG22	2.05	0.56
1:U:48:ASP:OD1	1:U:48:ASP:N	2.34	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:131:GLU:O	1:U:135:ILE:HG13	2.04	0.56
1:Z:129:ASN:O	1:Z:132:GLU:CB	2.53	0.56
2:B:203:2AN:H2	2:B:203:2AN:C16	2.34	0.56
2:G:204:2AN:H2	2:G:204:2AN:C16	2.32	0.56
2:K:202:2AN:N	2:K:202:2AN:O1	2.31	0.56
1:L:144:TYR:CD2	2:L:202:2AN:H12	2.40	0.56
1:D:10:GLU:HG2	2:D:202:2AN:H12	1.87	0.56
1:D:14:ILE:O	1:D:112:SER:OG	2.23	0.56
1:I:1:MET:HG3	1:I:2:ALA:H	1.70	0.56
1:J:54:VAL:CG2	1:J:71:LYS:HE2	2.34	0.56
1:B:8:LYS:HE2	1:B:116:ILE:HB	1.86	0.56
2:B:202:2AN:C2	2:B:202:2AN:H16	2.35	0.56
2:L:205:2AN:N	2:L:205:2AN:O3	2.33	0.56
1:S:21:LYS:HA	1:S:25:LEU:HB2	1.88	0.56
1:a:32:VAL:HG22	1:a:39:PHE:HB3	1.88	0.56
1:A:45:ILE:HG12	1:A:54:VAL:HG12	1.86	0.56
1:K:48:ASP:OD1	1:K:48:ASP:C	2.49	0.56
2:K:203:2AN:C12	2:K:203:2AN:C2	2.52	0.56
1:M:44:ILE:HG23	1:M:53:THR:CG2	2.35	0.56
2:X:202:2AN:N	2:X:202:2AN:S	2.65	0.56
1:D:42:GLY:HA2	1:D:56:LYS:O	2.06	0.56
1:E:158:PHE:CE2	2:E:203:2AN:H8	2.40	0.56
1:G:92:LEU:O	1:G:93:ARG:HG3	2.06	0.56
1:J:92:LEU:O	1:J:93:ARG:HB2	2.05	0.56
1:J:106:GLU:OE2	1:J:113:LYS:CG	2.54	0.56
2:K:202:2AN:C16	2:K:202:2AN:C2	2.63	0.56
1:N:95:ASN:OD1	1:N:95:ASN:N	2.32	0.56
2:Q:203:2AN:N	2:Q:203:2AN:O1	2.38	0.56
1:X:54:VAL:HG22	1:X:71:LYS:HG3	1.86	0.56
1:Y:67:TYR:OH	1:Y:88:GLU:OE2	2.21	0.56
2:N:201:2AN:C2	2:N:201:2AN:H12	2.35	0.56
2:O:202:2AN:H16	2:O:202:2AN:C2	2.35	0.56
2:A:203:2AN:C2	2:A:203:2AN:H16	2.36	0.56
1:B:51:VAL:CG1	1:B:73:ASP:O	2.53	0.56
1:I:77:ALA:HB1	2:Q:203:2AN:C3	2.36	0.56
1:J:55:THR:HG23	1:J:72:PHE:HE2	1.69	0.56
1:K:17:HIS:HB3	1:Q:110:GLY:HA2	1.88	0.56
1:M:2:ALA:HB2	1:N:4:TYR:CE1	2.39	0.56
2:M:201:2AN:C2	2:M:201:2AN:C16	2.81	0.56
2:b:202:2AN:C2	2:b:202:2AN:C16	2.76	0.56
1:G:157:VAL:O	1:G:158:PHE:HB2	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:65:LEU:HD22	1:E:91:VAL:HA	1.87	0.55
1:Y:92:LEU:O	1:Y:93:ARG:HB2	2.06	0.55
2:C:204:2AN:H2	2:C:204:2AN:C16	2.34	0.55
1:D:54:VAL:HA	1:D:70:HIS:O	2.06	0.55
1:D:129:ASN:C	1:D:131:GLU:N	2.61	0.55
1:S:42:GLY:HA2	1:S:56:LYS:O	2.06	0.55
1:A:150:TYR:CD2	2:A:201:2AN:O3	2.59	0.55
1:D:129:ASN:CG	1:D:131:GLU:HB2	2.31	0.55
1:D:144:TYR:C	1:D:144:TYR:CD1	2.85	0.55
2:G:202:2AN:C16	2:G:202:2AN:C2	2.59	0.55
1:K:158:PHE:CZ	2:K:203:2AN:C13	2.88	0.55
2:N:201:2AN:N	2:N:201:2AN:O3	2.39	0.55
1:S:28:HIS:CD2	1:S:29:GLN:N	2.75	0.55
2:b:203:2AN:C16	2:b:203:2AN:C2	2.82	0.55
1:K:97:GLU:HB2	1:K:123:LYS:CG	2.37	0.55
1:C:49:GLY:HA2	1:C:53:THR:HG21	1.88	0.55
1:E:137:GLU:OE2	1:F:1:MET:HG2	2.06	0.55
1:H:95:ASN:OD1	1:H:95:ASN:N	2.39	0.55
2:J:201:2AN:C16	2:J:201:2AN:H2	2.36	0.55
2:Q:201:2AN:N	2:Q:201:2AN:O1	2.34	0.55
1:S:86:LEU:HD23	1:S:92:LEU:HD21	1.88	0.55
1:F:68:MET:HB2	1:F:86:LEU:HD11	1.89	0.55
1:M:1:MET:SD	1:M:1:MET:N	2.78	0.55
1:M:134:LYS:HA	1:M:134:LYS:CE	2.37	0.55
1:N:14:ILE:HG22	1:N:18:ARG:HB2	1.88	0.55
1:A:96:ILE:HG13	1:A:132:GLU:OE2	2.07	0.55
1:W:157:VAL:O	1:W:158:PHE:HB2	2.06	0.55
2:Y:203:2AN:C16	2:Y:203:2AN:C2	2.83	0.55
1:D:6:ILE:HD11	1:D:133:VAL:HG13	1.88	0.55
2:G:201:2AN:N	2:G:201:2AN:O1	2.31	0.55
1:O:48:ASP:N	1:O:48:ASP:OD1	2.37	0.55
1:C:1:MET:O	1:C:2:ALA:HB3	2.06	0.55
1:E:71:LYS:HB3	1:E:87:PHE:CE2	2.42	0.55
1:G:19:LEU:HD13	2:G:202:2AN:H15	1.88	0.55
2:N:202:2AN:N	2:N:202:2AN:O3	2.40	0.55
1:R:54:VAL:HG22	1:R:71:LYS:HG3	1.89	0.55
1:R:144:TYR:CZ	2:R:201:2AN:C13	2.89	0.55
2:S:201:2AN:N	2:S:201:2AN:O3	2.40	0.55
1:V:143:PHE:O	1:V:143:PHE:CD1	2.60	0.55
1:W:129:ASN:HB3	1:W:132:GLU:OE2	2.07	0.55
1:Y:94:ASP:OD1	1:Y:94:ASP:N	2.39	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:204:2AN:H2	2:E:204:2AN:H12	1.89	0.55
1:K:21:LYS:HD3	1:K:158:PHE:CD1	2.42	0.55
1:S:25:LEU:O	1:S:26:GLU:HG2	2.07	0.55
1:H:105:LEU:HD22	2:H:203:2AN:H15	1.87	0.54
2:I:202:2AN:N	2:I:202:2AN:O1	2.36	0.54
2:N:203:2AN:H2	2:N:203:2AN:C16	2.35	0.54
1:O:138:LYS:HD2	1:O:138:LYS:O	2.07	0.54
1:a:4:TYR:OH	1:a:130:GLU:HG3	2.07	0.54
1:E:129:ASN:O	1:E:132:GLU:HG3	2.06	0.54
1:I:157:VAL:O	1:I:158:PHE:HB2	2.07	0.54
1:O:2:ALA:HB2	1:P:4:TYR:CZ	2.43	0.54
1:Q:23:LEU:O	1:Q:27:ARG:HD2	2.07	0.54
2:A:204:2AN:H16	2:A:204:2AN:C2	2.13	0.54
1:F:51:VAL:HG21	1:F:74:GLU:HA	1.89	0.54
2:I:205:2AN:C12	2:I:205:2AN:C2	2.85	0.54
1:Z:4:TYR:CE2	1:Z:130:GLU:HG3	2.43	0.54
1:Z:122:PRO:HB3	1:Z:128:VAL:HG23	1.89	0.54
1:C:14:ILE:O	1:C:112:SER:OG	2.24	0.54
1:G:49:GLY:C	1:G:53:THR:OG1	2.51	0.54
2:G:205:2AN:C2	2:G:205:2AN:C12	2.59	0.54
1:I:14:ILE:HD12	1:I:148:GLU:HG3	1.79	0.54
1:L:148:GLU:O	1:L:149:GLU:C	2.50	0.54
1:C:144:TYR:CE1	2:C:202:2AN:C13	2.91	0.54
1:L:128:VAL:HG13	1:L:129:ASN:ND2	2.23	0.54
1:S:135:ILE:HG23	1:S:139:LYS:HE2	1.90	0.54
1:U:14:ILE:O	1:U:112:SER:OG	2.20	0.54
1:U:154:ASN:N	1:U:154:ASN:ND2	2.55	0.54
2:E:202:2AN:C16	2:E:202:2AN:C2	2.81	0.54
2:H:202:2AN:N	2:H:202:2AN:O3	2.40	0.54
1:Z:8:LYS:NZ	2:Z:202:2AN:H8	2.23	0.54
1:b:48:ASP:OD1	1:b:48:ASP:N	2.33	0.54
1:A:97:GLU:OE1	1:A:97:GLU:CA	2.55	0.54
1:H:57:ILE:O	1:H:67:TYR:HA	2.08	0.54
1:N:73:ASP:C	1:N:74:GLU:HG2	2.33	0.54
2:O:202:2AN:C2	2:O:202:2AN:C16	2.85	0.54
2:b:202:2AN:H16	2:b:202:2AN:H2	1.90	0.54
1:M:151:LEU:HD21	2:M:203:2AN:H7	1.89	0.54
1:N:91:VAL:O	1:N:91:VAL:HG22	2.07	0.54
1:A:96:ILE:HD11	1:A:128:VAL:HG22	1.77	0.54
1:G:17:HIS:CB	1:U:110:GLY:HA2	2.38	0.54
1:G:21:LYS:HD3	1:G:158:PHE:CD1	2.43	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:95:ASN:HB2	1:I:126:CYS:HB3	1.90	0.54
1:J:16:PRO:HB2	1:J:80:PHE:CE2	2.42	0.54
1:L:26:GLU:CG	1:L:29:GLN:OE1	2.50	0.54
2:M:201:2AN:H16	2:M:201:2AN:H2	1.90	0.54
1:N:32:VAL:HG22	1:N:39:PHE:HB3	1.90	0.54
2:N:204:2AN:H16	2:N:204:2AN:C2	2.38	0.54
1:R:144:TYR:CD2	2:R:201:2AN:H12	2.43	0.54
2:R:201:2AN:N	2:R:201:2AN:S	2.65	0.54
2:U:205:2AN:N	2:U:205:2AN:O3	2.39	0.54
1:X:69:LEU:HD12	1:X:88:GLU:HB3	1.89	0.54
1:Z:8:LYS:CE	1:Z:137:GLU:OE2	2.56	0.54
1:a:93:ARG:HB3	1:a:95:ASN:OD1	2.08	0.54
1:B:120:TYR:CE2	1:B:132:GLU:HG2	2.43	0.54
1:I:50:GLY:O	1:I:51:VAL:C	2.51	0.54
1:P:46:GLU:HB2	1:P:54:VAL:HB	1.90	0.54
2:Q:202:2AN:N	2:Q:202:2AN:O1	2.41	0.54
2:B:203:2AN:C16	2:B:203:2AN:C2	2.85	0.53
2:D:203:2AN:C12	2:D:203:2AN:C2	2.50	0.53
1:F:28:HIS:CD2	1:F:29:GLN:HG3	2.43	0.53
1:A:33:LYS:HD3	2:A:201:2AN:C1	2.38	0.53
1:Z:27:ARG:CG	1:Z:27:ARG:O	2.56	0.53
2:C:204:2AN:H16	2:C:204:2AN:C2	2.35	0.53
1:R:144:TYR:CE1	2:R:201:2AN:H13	2.42	0.53
2:Y:202:2AN:H16	2:Y:202:2AN:H2	1.87	0.53
2:b:202:2AN:C16	2:b:202:2AN:H2	2.37	0.53
1:a:24:VAL:HG12	1:a:25:LEU:N	2.21	0.53
1:A:108:VAL:HG21	1:A:113:LYS:HB2	1.91	0.53
1:B:144:TYR:CZ	2:B:202:2AN:H12	2.43	0.53
1:H:20:PHE:CZ	1:H:81:TYR:O	2.62	0.53
1:M:127:THR:OG1	1:M:128:VAL:N	2.38	0.53
2:P:202:2AN:N	2:P:202:2AN:O3	2.41	0.53
1:S:129:ASN:H	1:S:129:ASN:HD22	1.56	0.53
1:T:95:ASN:OD1	1:T:95:ASN:N	2.30	0.53
1:U:129:ASN:N	1:U:129:ASN:OD1	2.41	0.53
1:U:147:VAL:O	1:U:151:LEU:HG	2.09	0.53
1:V:123:LYS:CG	1:V:124:PRO:HD2	2.38	0.53
1:F:4:TYR:HD2	1:F:128:VAL:HG11	1.72	0.53
2:G:205:2AN:N	2:G:205:2AN:O3	2.32	0.53
1:K:90:ASP:OD1	1:K:90:ASP:N	2.38	0.53
1:R:92:LEU:O	1:R:93:ARG:HB2	2.09	0.53
1:X:107:ALA:C	1:X:108:VAL:HG23	2.33	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:95:ASN:O	1:H:123:LYS:N	2.38	0.53
1:J:50:GLY:O	1:J:51:VAL:C	2.50	0.53
1:M:6:ILE:HD12	1:M:118:VAL:HB	1.89	0.53
1:M:48:ASP:OD1	1:M:48:ASP:O	2.27	0.53
1:F:133:VAL:O	1:F:137:GLU:HG2	2.08	0.53
1:W:97:GLU:HB2	1:W:123:LYS:HG3	1.90	0.53
1:a:96:ILE:CD1	1:a:128:VAL:HG13	2.39	0.53
1:b:16:PRO:HB2	1:b:80:PHE:CE2	2.44	0.53
1:C:72:PHE:CD2	1:C:75:ILE:HD11	2.43	0.53
1:D:20:PHE:HB2	1:D:105:LEU:HD12	1.90	0.53
1:H:50:GLY:O	1:H:51:VAL:C	2.52	0.53
1:L:89:GLY:C	1:L:91:VAL:N	2.65	0.53
1:M:131:GLU:CG	1:M:135:ILE:HD11	2.36	0.53
1:B:54:VAL:HG11	1:B:87:PHE:HZ	1.74	0.53
2:B:203:2AN:N	2:B:203:2AN:O3	2.36	0.53
1:E:8:LYS:C	1:E:9:GLU:HG3	2.33	0.53
2:N:204:2AN:H2	2:N:204:2AN:C16	2.38	0.53
1:O:92:LEU:O	1:O:93:ARG:CB	2.56	0.53
1:C:72:PHE:HD2	1:C:75:ILE:HD11	1.74	0.52
2:E:203:2AN:C2	2:E:203:2AN:C12	2.57	0.52
2:G:201:2AN:C2	2:G:201:2AN:C16	2.84	0.52
2:L:204:2AN:C6	1:R:21:LYS:HG3	2.39	0.52
2:L:205:2AN:C16	2:L:205:2AN:C2	2.80	0.52
1:O:2:ALA:HB2	1:P:4:TYR:CE1	2.44	0.52
1:R:92:LEU:O	1:R:93:ARG:CB	2.56	0.52
2:N:204:2AN:C2	2:N:204:2AN:C16	2.83	0.52
1:X:127:THR:OG1	1:X:128:VAL:N	2.39	0.52
2:X:201:2AN:H16	2:X:201:2AN:C2	2.39	0.52
2:X:203:2AN:C16	2:X:203:2AN:C2	2.85	0.52
1:B:77:ALA:HB3	2:B:203:2AN:H15	1.92	0.52
2:G:204:2AN:H16	2:G:204:2AN:C2	2.34	0.52
1:M:144:TYR:CE1	2:M:202:2AN:H12	2.43	0.52
2:U:201:2AN:C16	2:U:201:2AN:C2	2.83	0.52
2:C:201:2AN:C2	2:C:201:2AN:C12	2.86	0.52
1:I:1:MET:O	1:I:2:ALA:CB	2.55	0.52
1:I:144:TYR:CG	2:I:201:2AN:H12	2.44	0.52
1:K:31:LEU:HD22	1:K:39:PHE:CE2	2.44	0.52
1:K:49:GLY:HA2	1:K:53:THR:CG2	2.40	0.52
1:M:10:GLU:OE1	1:M:10:GLU:HA	2.08	0.52
1:N:16:PRO:CG	1:N:107:ALA:HB2	2.40	0.52
1:S:93:ARG:O	1:S:95:ASN:N	2.42	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:95:ASN:HB2	1:A:127:THR:O	2.10	0.52
1:C:63:HIS:HD2	1:C:65:LEU:H	1.56	0.52
1:L:108:VAL:O	1:L:108:VAL:HG12	2.08	0.52
1:Z:64:PRO:O	1:Z:65:LEU:HD23	2.10	0.52
1:F:43:GLU:HG3	1:F:56:LYS:HB3	1.90	0.52
1:F:94:ASP:O	1:F:123:LYS:HD2	2.09	0.52
1:J:83:LYS:HG3	1:J:102:GLU:HG3	1.91	0.52
1:P:14:ILE:HG21	1:P:151:LEU:HD12	1.92	0.52
1:T:65:LEU:HD22	1:T:91:VAL:HA	1.92	0.52
1:Y:129:ASN:OD1	1:Y:132:GLU:HB2	2.10	0.52
1:A:66:THR:CB	1:A:90:ASP:HB2	2.40	0.52
1:C:17:HIS:CB	1:Y:110:GLY:HA2	2.39	0.52
1:C:33:LYS:HD2	2:C:203:2AN:H12	1.92	0.52
1:J:7:VAL:HG22	1:J:117:THR:HB	1.91	0.52
2:K:201:2AN:C2	2:K:201:2AN:C16	2.86	0.52
1:Q:119:THR:HG22	1:Q:121:HIS:CD2	2.44	0.52
1:V:39:PHE:CE1	1:V:59:PHE:CE1	2.98	0.52
1:B:95:ASN:ND2	1:B:129:ASN:H	2.08	0.52
1:C:63:HIS:CD2	1:C:65:LEU:H	2.28	0.52
1:F:54:VAL:HG23	1:F:71:LYS:HD3	1.92	0.52
1:I:2:ALA:HB1	1:J:4:TYR:CE1	2.45	0.52
1:J:127:THR:OG1	1:J:128:VAL:N	2.42	0.52
1:X:71:LYS:HD2	1:X:87:PHE:CE2	2.45	0.52
2:Y:201:2AN:H16	2:Y:201:2AN:C2	2.40	0.52
1:P:50:GLY:O	1:P:53:THR:OG1	2.26	0.52
1:P:144:TYR:CD1	1:P:144:TYR:C	2.88	0.52
1:S:135:ILE:HG23	1:S:139:LYS:CE	2.40	0.52
1:Q:108:VAL:O	1:Q:108:VAL:HG12	2.10	0.52
1:Q:116:ILE:HD11	2:Q:201:2AN:H16	1.92	0.52
1:R:56:LYS:HG3	1:R:69:LEU:CD2	2.40	0.52
1:U:129:ASN:O	1:U:129:ASN:CG	2.51	0.52
1:F:19:LEU:HD13	2:F:201:2AN:C14	2.41	0.51
1:L:47:GLY:HA2	2:L:204:2AN:C11	2.39	0.51
1:L:144:TYR:O	1:L:144:TYR:HD1	1.87	0.51
1:V:128:VAL:CG1	1:V:129:ASN:N	2.73	0.51
1:C:66:THR:HG22	1:C:67:TYR:HD2	1.75	0.51
1:I:156:GLU:HG2	1:I:157:VAL:HG23	1.91	0.51
1:J:122:PRO:HG3	1:J:128:VAL:CG2	2.38	0.51
1:M:48:ASP:OD1	1:M:48:ASP:C	2.53	0.51
1:V:16:PRO:HG3	1:V:107:ALA:HB2	1.92	0.51
1:a:54:VAL:HA	1:a:70:HIS:O	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:104:LYS:O	1:C:105:LEU:HD12	2.10	0.51
1:G:8:LYS:NZ	2:G:202:2AN:O2	2.31	0.51
1:N:55:THR:HG23	1:N:72:PHE:CZ	2.45	0.51
1:S:93:ARG:CB	1:S:95:ASN:OD1	2.59	0.51
2:X:203:2AN:N	2:X:203:2AN:O3	2.43	0.51
1:H:6:ILE:HD11	1:H:133:VAL:CG1	2.41	0.51
1:S:93:ARG:HB3	1:S:95:ASN:OD1	2.10	0.51
1:Z:76:ASP:HB3	1:Z:81:TYR:HB3	1.91	0.51
1:C:83:LYS:HE2	1:C:100:VAL:HG11	1.92	0.51
1:C:92:LEU:O	1:C:96:ILE:CB	2.58	0.51
1:H:15:ALA:HB1	1:H:16:PRO:HD2	1.91	0.51
1:T:96:ILE:HD13	1:T:96:ILE:N	2.25	0.51
1:U:154:ASN:N	1:U:154:ASN:HD22	2.08	0.51
1:W:135:ILE:HG22	2:W:203:2AN:H13	1.91	0.51
1:X:48:ASP:OD1	1:X:48:ASP:N	2.36	0.51
1:a:5:THR:HB	1:b:3:ALA:HB3	1.92	0.51
1:B:71:LYS:HB2	1:B:87:PHE:CE1	2.46	0.51
1:D:94:ASP:OD1	1:D:94:ASP:O	2.29	0.51
1:D:144:TYR:CD1	1:D:144:TYR:O	2.64	0.51
1:F:78:ALA:HA	1:V:109:GLY:H	1.74	0.51
1:G:92:LEU:C	1:G:93:ARG:HG3	2.36	0.51
1:M:67:TYR:OH	1:M:88:GLU:OE2	2.25	0.51
1:U:31:LEU:CD1	1:U:57:ILE:HD13	2.40	0.51
2:U:201:2AN:N	2:U:201:2AN:O3	2.44	0.51
1:Z:150:TYR:CD2	2:Z:203:2AN:O3	2.63	0.51
1:b:138:LYS:HD3	1:b:142:GLU:OE2	2.11	0.51
1:F:43:GLU:CG	1:F:56:LYS:HB3	2.41	0.51
1:I:104:LYS:NZ	1:I:105:LEU:O	2.44	0.51
1:N:16:PRO:HG3	1:N:107:ALA:CA	2.40	0.51
1:W:107:ALA:O	1:W:108:VAL:CG2	2.58	0.51
1:I:95:ASN:CB	1:I:126:CYS:HB3	2.40	0.51
1:J:23:LEU:O	1:J:27:ARG:HD2	2.11	0.51
1:P:137:GLU:OE1	1:P:137:GLU:CA	2.57	0.51
1:S:27:ARG:NH1	2:S:201:2AN:O2	2.36	0.51
1:S:60:VAL:HG12	1:S:61:ASP:H	1.76	0.51
1:V:142:GLU:HG3	2:V:201:2AN:O3	2.11	0.51
1:b:129:ASN:ND2	1:b:132:GLU:HB2	2.25	0.51
1:A:10[A]:GLU:HA	1:A:10[A]:GLU:OE2	2.11	0.51
1:D:130:GLU:O	1:D:134:LYS:HG3	2.11	0.51
1:G:6:ILE:CG2	1:G:137:GLU:OE2	2.57	0.51
1:U:63:HIS:O	1:U:64:PRO:C	2.53	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:90:ASP:C	1:U:92:LEU:H	2.19	0.51
2:a:201:2AN:N	2:a:201:2AN:O1	2.34	0.51
1:b:65:LEU:CD2	1:b:91:VAL:HA	2.41	0.51
1:A:37:HIS:NE2	1:A:38:VAL:CG2	2.71	0.50
1:C:127:THR:HG22	1:C:128:VAL:N	2.25	0.50
1:G:92:LEU:O	1:G:93:ARG:CG	2.59	0.50
1:Q:5:THR:HA	1:Q:118:VAL:O	2.12	0.50
1:B:51:VAL:HG13	1:B:73:ASP:O	2.11	0.50
1:I:71:LYS:HB3	1:I:87:PHE:CD2	2.46	0.50
1:P:45:ILE:HG12	1:P:56:LYS:HB2	1.92	0.50
1:E:96:ILE:HD11	1:E:132:GLU:OE1	2.10	0.50
2:I:202:2AN:H15	2:I:205:2AN:H7	1.93	0.50
1:J:44:ILE:HG23	1:J:53:THR:CG2	2.40	0.50
1:J:44:ILE:HG23	1:J:53:THR:HG23	1.93	0.50
1:Q:89:GLY:O	1:Q:92:LEU:HB2	2.11	0.50
1:W:122:PRO:HG3	1:W:128:VAL:HG23	1.93	0.50
1:X:95:ASN:ND2	1:X:127:THR:O	2.37	0.50
1:Y:7:VAL:HG22	1:Y:117:THR:HG23	1.92	0.50
1:C:83:LYS:HE2	1:C:100:VAL:CG1	2.40	0.50
2:E:205:2AN:C2	2:E:205:2AN:C16	2.81	0.50
1:G:17:HIS:CE1	1:U:15:ALA:HB1	2.47	0.50
1:H:48:ASP:OD1	1:H:48:ASP:N	2.38	0.50
1:L:1:MET:HE1	1:L:124:PRO:HA	1.92	0.50
1:L:89:GLY:O	1:L:91:VAL:N	2.44	0.50
1:X:4:TYR:CD2	1:X:128:VAL:HB	2.46	0.50
1:I:6:ILE:CG2	1:J:1:MET:HG2	2.31	0.50
1:I:14:ILE:CD1	1:I:148:GLU:CG	2.65	0.50
1:I:32:VAL:HG21	1:I:41:SER:HA	1.93	0.50
1:N:141:TYR:CG	2:N:203:2AN:H3	2.46	0.50
1:R:50:GLY:O	1:R:51:VAL:C	2.51	0.50
1:Z:27:ARG:O	1:Z:27:ARG:HG2	2.12	0.50
1:D:132:GLU:O	1:D:133:VAL:C	2.53	0.50
1:N:141:TYR:HB3	2:N:203:2AN:H3	1.92	0.50
1:S:34:ALA:O	1:S:36:PRO:HD3	2.11	0.50
1:A:85:THR:HG23	1:A:100:VAL:HG23	1.89	0.50
1:A:131:GLU:O	1:A:135:ILE:HG13	2.11	0.50
1:B:95:ASN:HD21	1:B:129:ASN:HB3	1.70	0.50
1:C:42:GLY:O	1:C:43:GLU:HG3	2.11	0.50
2:C:203:2AN:O3	2:C:203:2AN:H12	2.10	0.50
1:D:129:ASN:ND2	1:D:129:ASN:C	2.53	0.50
1:F:11:GLU:HA	1:F:113:LYS:HA	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:70:HIS:HA	1:I:85:THR:O	2.12	0.50
1:K:50:GLY:O	1:K:51:VAL:O	2.30	0.50
2:X:201:2AN:C2	2:X:201:2AN:C16	2.88	0.50
1:b:144:TYR:CZ	2:b:201:2AN:H12	2.45	0.50
1:E:90:ASP:OD1	1:E:90:ASP:N	2.41	0.50
1:S:60:VAL:HG12	1:S:61:ASP:N	2.26	0.50
1:V:20:PHE:O	1:V:25:LEU:HB2	2.11	0.50
1:X:91:VAL:O	1:X:91:VAL:HG22	2.11	0.50
1:b:130:GLU:OE2	1:b:134:LYS:NZ	2.30	0.50
1:H:70:HIS:HA	1:H:85:THR:O	2.11	0.50
1:K:96:ILE:HD11	1:K:128:VAL:HG22	1.94	0.50
2:N:201:2AN:C2	2:N:201:2AN:C12	2.87	0.50
2:N:203:2AN:H16	2:N:203:2AN:C2	2.36	0.50
1:P:46:GLU:CB	1:P:54:VAL:HB	2.42	0.50
1:W:49:GLY:CA	1:W:53:THR:CB	2.67	0.50
1:W:144:TYR:CZ	2:W:202:2AN:C13	2.95	0.50
2:W:203:2AN:N	2:W:203:2AN:O1	2.34	0.50
1:Y:92:LEU:O	1:Y:93:ARG:CB	2.60	0.50
1:F:129:ASN:O	1:F:131:GLU:N	2.45	0.49
1:K:48:ASP:OD1	1:K:48:ASP:O	2.30	0.49
1:Q:90:ASP:C	1:Q:92:LEU:N	2.61	0.49
1:R:16:PRO:HB2	1:R:80:PHE:CE2	2.47	0.49
1:T:130:GLU:OE1	1:T:130:GLU:O	2.30	0.49
1:A:95:ASN:O	1:A:122:PRO:HA	2.12	0.49
1:D:32:VAL:HG12	1:D:32:VAL:O	2.12	0.49
1:E:69:LEU:HD12	1:E:88:GLU:HB3	1.93	0.49
1:F:74:GLU:O	1:F:75:ILE:HG12	2.11	0.49
1:H:54:VAL:HA	1:H:70:HIS:O	2.12	0.49
2:L:205:2AN:C2	2:L:205:2AN:H16	2.42	0.49
1:D:23:LEU:O	1:D:27:ARG:HD2	2.12	0.49
1:G:129:ASN:N	1:G:129:ASN:ND2	2.35	0.49
1:J:15:ALA:HB1	1:J:16:PRO:HD2	1.94	0.49
1:L:10:GLU:C	1:L:11:GLU:HG3	2.37	0.49
1:V:123:LYS:HG2	1:V:124:PRO:HD2	1.94	0.49
1:A:48:ASP:N	1:A:53:THR:OG1	2.46	0.49
1:H:72:PHE:CG	1:H:75:ILE:HD11	2.48	0.49
1:L:71:LYS:HB2	1:L:87:PHE:CE2	2.47	0.49
1:Q:123:LYS:HG2	1:Q:124:PRO:HD2	1.94	0.49
1:R:129:ASN:C	1:R:131:GLU:H	2.21	0.49
1:T:6:ILE:HD13	1:T:137:GLU:CG	2.41	0.49
1:W:81:TYR:OH	1:W:102:GLU:OE1	2.28	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:W:92:LEU:O	1:W:93:ARG:CB	2.57	0.49
1:Z:144:TYR:O	1:Z:144:TYR:CD1	2.64	0.49
1:A:130:GLU:O	1:A:134:LYS:HG3	2.12	0.49
1:B:31:LEU:HD12	1:B:57:ILE:HD13	1.94	0.49
1:N:55:THR:CG2	1:N:72:PHE:HZ	2.25	0.49
1:Y:46:GLU:O	1:Y:47:GLY:O	2.30	0.49
1:E:144:TYR:CE1	2:E:202:2AN:H13	2.46	0.49
1:E:144:TYR:CE1	2:E:202:2AN:C13	2.96	0.49
1:H:6:ILE:HD11	1:H:133:VAL:HG13	1.95	0.49
1:J:16:PRO:HG3	1:J:107:ALA:CA	2.42	0.49
1:T:73:ASP:OD1	1:T:73:ASP:N	2.46	0.49
1:V:21:LYS:O	1:V:26:GLU:N	2.45	0.49
2:Y:204:2AN:H2	2:Y:204:2AN:C16	2.43	0.49
1:Z:4:TYR:HE2	1:Z:130:GLU:HG3	1.76	0.49
1:C:90:ASP:O	1:C:91:VAL:C	2.55	0.49
1:D:142:GLU:O	1:D:146:GLN:HG3	2.13	0.49
1:P:130:GLU:O	1:P:131:GLU:C	2.56	0.49
1:S:69:LEU:HB3	1:S:87:PHE:CE1	2.48	0.49
1:X:116:ILE:HD12	1:X:116:ILE:N	2.28	0.49
2:Y:201:2AN:C2	2:Y:201:2AN:C16	2.89	0.49
1:Z:107:ALA:C	1:Z:108:VAL:HG23	2.38	0.49
2:A:204:2AN:N	2:A:204:2AN:O1	2.30	0.49
1:C:4:TYR:CD2	1:C:128:VAL:HG11	2.48	0.49
1:C:63:HIS:HD2	1:C:65:LEU:N	2.10	0.49
1:N:16:PRO:HG3	1:N:107:ALA:HA	1.94	0.49
1:U:50:GLY:O	1:U:75:ILE:HD12	2.13	0.49
1:W:10:GLU:HG3	2:W:202:2AN:C13	2.42	0.49
1:W:107:ALA:C	1:W:108:VAL:HG23	2.38	0.49
1:X:71:LYS:CD	1:X:87:PHE:CE2	2.96	0.49
2:X:202:2AN:C16	2:X:202:2AN:C2	2.91	0.49
1:A:102:GLU:HB3	1:A:117:THR:OG1	2.13	0.49
2:C:204:2AN:C16	2:C:204:2AN:C2	2.90	0.49
1:D:138:LYS:HD2	2:D:203:2AN:O2	2.12	0.49
1:I:92:LEU:C	1:I:93:ARG:O	2.54	0.49
1:M:7:VAL:HG22	1:M:117:THR:HB	1.95	0.49
1:R:72:PHE:CD2	1:R:75:ILE:HD11	2.48	0.49
1:S:144:TYR:O	1:S:147:VAL:N	2.44	0.49
2:Y:204:2AN:C16	2:Y:204:2AN:C2	2.89	0.49
1:b:10:GLU:OE2	1:b:141:TYR:HE1	1.96	0.49
2:A:204:2AN:C16	2:A:204:2AN:C2	2.74	0.49
1:B:4:TYR:HD2	1:B:128:VAL:CB	2.26	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:129:ASN:C	1:F:131:GLU:H	2.18	0.49
1:L:123:LYS:O	1:L:126:CYS:HB2	2.12	0.49
1:N:48:ASP:OD1	1:N:48:ASP:N	2.29	0.49
1:P:65:LEU:HD22	1:P:91:VAL:HA	1.95	0.49
1:T:35:GLN:NE2	1:T:146[B]:GLN:OE1	2.44	0.49
2:U:205:2AN:N	2:U:205:2AN:O1	2.45	0.49
1:W:96:ILE:CG1	1:W:132:GLU:OE1	2.61	0.49
2:B:205:2AN:C16	2:B:205:2AN:C2	2.81	0.48
1:D:39:PHE:HA	1:D:59:PHE:HA	1.95	0.48
1:G:141:TYR:O	1:G:145:LYS:HG2	2.13	0.48
2:H:201:2AN:C12	2:H:201:2AN:C2	2.81	0.48
1:I:7:VAL:HG22	1:I:117:THR:HG23	1.94	0.48
1:M:141:TYR:O	1:M:145:LYS:HG2	2.13	0.48
1:N:141:TYR:HD2	2:N:203:2AN:C2	2.25	0.48
1:P:3:ALA:HB1	1:P:120:TYR:O	2.13	0.48
1:P:107:ALA:O	1:P:108:VAL:CG2	2.61	0.48
2:Q:203:2AN:C16	2:Q:203:2AN:H2	2.43	0.48
1:T:48:ASP:OD1	1:T:48:ASP:N	2.33	0.48
1:G:40:LYS:HE2	1:G:58:THR:CG2	2.43	0.48
1:J:141:TYR:O	1:J:145:LYS:HG2	2.14	0.48
1:L:1:MET:O	1:L:2:ALA:CB	2.60	0.48
1:M:134:LYS:HA	1:M:134:LYS:HE2	1.96	0.48
1:N:107:ALA:C	1:N:108:VAL:HG23	2.38	0.48
1:S:129:ASN:HD22	1:S:129:ASN:N	2.11	0.48
1:a:31:LEU:CD1	1:a:57:ILE:HD13	2.44	0.48
1:b:127:THR:OG1	1:b:128:VAL:N	2.46	0.48
2:b:203:2AN:C2	2:b:203:2AN:H16	2.44	0.48
1:D:131:GLU:O	1:D:133:VAL:N	2.46	0.48
1:E:3:ALA:HB3	1:F:5:THR:HB	1.96	0.48
1:F:51:VAL:CG2	1:F:74:GLU:C	2.86	0.48
1:G:89:GLY:O	1:G:92:LEU:HB2	2.13	0.48
1:I:40:LYS:HB2	1:I:59:PHE:O	2.12	0.48
1:N:14:ILE:O	1:N:112:SER:OG	2.28	0.48
1:P:134:LYS:O	1:P:135:ILE:C	2.56	0.48
1:A:109:GLY:CA	1:a:78:ALA:HA	2.42	0.48
1:C:4:TYR:HD2	1:C:128:VAL:CG1	2.27	0.48
1:O:129:ASN:O	1:O:130:GLU:C	2.56	0.48
1:S:14:ILE:HG22	1:S:18:ARG:HB2	1.94	0.48
1:S:144:TYR:CE2	1:S:145:LYS:HD2	2.48	0.48
1:T:50:GLY:O	1:T:51:VAL:C	2.56	0.48
1:Z:105:LEU:HD22	2:Z:202:2AN:H15	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:b:201:2AN:H2	2:b:201:2AN:C16	2.44	0.48
1:C:80:PHE:HB3	1:C:105:LEU:HB2	1.95	0.48
1:L:144:TYR:CE2	2:L:202:2AN:H12	2.49	0.48
2:N:202:2AN:H2	2:N:202:2AN:H16	1.90	0.48
1:O:138:LYS:O	1:O:138:LYS:CD	2.62	0.48
1:Q:1:MET:O	1:Q:2:ALA:HB3	2.13	0.48
1:Q:155:PRO:O	1:Q:159:ALA:HB2	2.14	0.48
1:T:129:ASN:O	1:T:132:GLU:N	2.43	0.48
1:X:26:GLU:OE1	1:X:29:GLN:NE2	2.47	0.48
1:D:122:PRO:HG3	1:D:128:VAL:HG23	1.95	0.48
1:G:70:HIS:CE1	1:G:86:LEU:HD13	2.48	0.48
1:H:150:TYR:HH	2:H:201:2AN:HO3	1.61	0.48
2:J:202:2AN:N	2:J:202:2AN:O1	2.41	0.48
1:O:92:LEU:O	1:O:93:ARG:HB2	2.14	0.48
1:P:32:VAL:O	1:P:32:VAL:HG12	2.14	0.48
1:P:68:MET:HG2	1:P:91:VAL:CG1	2.43	0.48
2:B:201:2AN:C16	2:B:201:2AN:C2	2.91	0.48
2:G:203:2AN:N	2:G:203:2AN:O1	2.47	0.48
1:L:11:GLU:HG2	1:L:113:LYS:HG3	1.94	0.48
1:N:80:PHE:HB2	1:N:105:LEU:O	2.14	0.48
1:R:108:VAL:HG12	1:R:108:VAL:O	2.13	0.48
1:V:21:LYS:HA	1:V:25:LEU:HB2	1.94	0.48
1:Y:129:ASN:O	1:Y:130:GLU:C	2.56	0.48
1:C:4:TYR:HD2	1:C:128:VAL:HG11	1.79	0.48
1:D:129:ASN:O	1:D:130:GLU:HB2	2.12	0.48
1:S:14:ILE:HG23	1:S:18:ARG:HD3	1.95	0.48
1:a:123:LYS:HD2	1:a:124:PRO:N	2.22	0.48
1:A:116:ILE:HD11	2:A:203:2AN:H16	1.95	0.48
1:B:23:LEU:O	1:B:27:ARG:HD2	2.14	0.48
1:K:158:PHE:CE2	2:K:203:2AN:C13	2.91	0.48
1:Q:90:ASP:O	1:Q:91:VAL:C	2.57	0.48
2:Y:201:2AN:N	2:Y:201:2AN:O3	2.47	0.48
1:B:14:ILE:O	1:B:112:SER:OG	2.28	0.48
1:B:144:TYR:CE1	2:B:202:2AN:H12	2.49	0.48
1:a:14:ILE:HG21	1:a:151:LEU:CD1	2.44	0.48
1:C:15:ALA:HB1	1:C:17:HIS:CE1	2.48	0.47
1:K:49:GLY:HA2	1:K:53:THR:CB	2.43	0.47
1:L:54:VAL:HA	1:L:70:HIS:O	2.13	0.47
2:M:202:2AN:N	2:M:202:2AN:S	2.65	0.47
1:V:95:ASN:OD1	1:V:95:ASN:N	2.46	0.47
1:A:80:PHE:O	1:A:104:LYS:HA	2.13	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:89:GLY:C	1:A:91:VAL:HG23	2.39	0.47
1:C:54:VAL:HA	1:C:70:HIS:O	2.14	0.47
1:D:50:GLY:O	1:D:51:VAL:C	2.57	0.47
1:D:95:ASN:O	1:D:122:PRO:HA	2.14	0.47
1:D:132:GLU:O	1:D:134:LYS:N	2.47	0.47
1:I:72:PHE:N	1:I:72:PHE:CD1	2.81	0.47
1:U:31:LEU:HD12	1:U:57:ILE:HD13	1.94	0.47
2:D:201:2AN:N	2:D:201:2AN:O3	2.47	0.47
1:F:106:GLU:OE2	1:F:113:LYS:HB3	2.15	0.47
1:G:138:LYS:HG2	2:G:204:2AN:C10	2.45	0.47
1:L:132:GLU:HG3	1:L:132:GLU:O	2.13	0.47
1:P:107:ALA:C	1:P:108:VAL:HG23	2.38	0.47
1:B:144:TYR:O	1:B:144:TYR:CD1	2.67	0.47
1:N:157:VAL:O	1:N:158:PHE:HB2	2.13	0.47
1:Q:77:ALA:HB3	2:Q:202:2AN:C15	2.45	0.47
1:Q:129:ASN:HB3	1:Q:132:GLU:HB3	1.97	0.47
1:V:108:VAL:HG21	1:V:113:LYS:NZ	2.30	0.47
1:V:141:TYR:CD2	2:V:201:2AN:C12	2.88	0.47
1:Y:77:ALA:O	2:Y:204:2AN:H3	2.14	0.47
1:C:92:LEU:O	1:C:93:ARG:CB	2.61	0.47
1:E:144:TYR:CZ	2:E:202:2AN:C13	2.95	0.47
1:T:42:GLY:HA2	1:T:56:LYS:O	2.15	0.47
1:U:144:TYR:CE2	2:U:201:2AN:H12	2.49	0.47
1:Z:30:VAL:HG13	2:Z:203:2AN:O1	2.15	0.47
1:C:97:GLU:HA	1:C:123:LYS:HE2	1.96	0.47
1:E:68:MET:HG2	1:E:91:VAL:CG1	2.45	0.47
1:F:89:GLY:O	1:F:92:LEU:HB2	2.14	0.47
1:I:2:ALA:CB	1:J:4:TYR:HE1	2.26	0.47
1:Q:119:THR:CG2	1:Q:121:HIS:CD2	2.97	0.47
1:T:65:LEU:HD13	1:T:91:VAL:HG23	1.97	0.47
1:W:4:TYR:CE1	1:X:2:ALA:CB	2.97	0.47
1:F:63:HIS:O	1:F:64:PRO:C	2.58	0.47
1:H:50:GLY:N	1:H:53:THR:OG1	2.47	0.47
1:I:10:GLU:O	1:I:113:LYS:HB2	2.15	0.47
1:L:53:THR:O	1:L:72:PHE:HD1	1.98	0.47
1:L:128:VAL:HG12	1:L:129:ASN:CA	2.45	0.47
1:M:108:VAL:HG21	1:M:113:LYS:CG	2.45	0.47
1:O:131:GLU:C	1:O:133:VAL:N	2.73	0.47
1:S:50:GLY:O	1:S:53:THR:OG1	2.30	0.47
1:T:95:ASN:HB2	1:T:96:ILE:HD13	1.96	0.47
1:V:53:THR:HG21	1:V:72:PHE:CD2	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:14:ILE:HG21	1:a:151:LEU:HD13	1.97	0.47
1:a:31:LEU:HD13	1:a:57:ILE:HD13	1.96	0.47
1:b:130:GLU:HG2	1:b:134:LYS:HE2	1.97	0.47
1:A:2:ALA:HB3	1:B:4:TYR:HE1	1.80	0.47
1:C:142:GLU:O	1:C:146:GLN:HG3	2.14	0.47
1:I:144:TYR:CE1	2:I:201:2AN:H12	2.50	0.47
1:M:131:GLU:C	1:M:135:ILE:HD12	2.38	0.47
1:C:16:PRO:HB2	1:C:80:PHE:CE2	2.50	0.47
1:E:12:SER:HB2	2:E:202:2AN:H14	1.96	0.47
1:U:129:ASN:HD21	1:U:132:GLU:HB2	1.80	0.47
1:C:51:VAL:CG2	1:C:52:GLY:N	2.76	0.47
1:H:39:PHE:HA	1:H:59:PHE:HA	1.97	0.47
1:Q:124:PRO:C	1:Q:126:CYS:N	2.65	0.47
2:Q:201:2AN:H2	2:Q:201:2AN:H16	1.96	0.47
1:Z:93:ARG:CD	1:Z:129:ASN:HD21	2.25	0.47
1:Z:95:ASN:ND2	1:Z:129:ASN:CB	2.46	0.47
1:B:12:SER:HB2	2:B:202:2AN:H13	1.96	0.46
2:B:204:2AN:N	2:B:204:2AN:O1	2.48	0.46
2:C:203:2AN:C12	2:C:203:2AN:O3	2.63	0.46
1:E:14:ILE:O	1:E:112:SER:OG	2.23	0.46
1:F:54:VAL:HA	1:F:70:HIS:O	2.14	0.46
1:J:54:VAL:HG22	1:J:71:LYS:HD2	1.96	0.46
1:K:37:HIS:CD2	1:K:38:VAL:HG23	2.50	0.46
1:O:23:LEU:HD13	2:O:201:2AN:C2	2.45	0.46
1:C:86:LEU:CD2	1:C:92:LEU:HD21	2.46	0.46
1:E:28:HIS:CD2	1:E:29:GLN:NE2	2.83	0.46
1:I:10:GLU:HB3	2:I:201:2AN:C15	2.45	0.46
1:N:76:ASP:HB3	1:N:81:TYR:HB3	1.97	0.46
1:W:63:HIS:NE2	2:W:204:2AN:H15	2.31	0.46
1:Z:129:ASN:CG	1:Z:132:GLU:CB	2.88	0.46
1:a:129:ASN:ND2	1:a:129:ASN:N	2.31	0.46
1:H:144:TYR:CD1	1:H:144:TYR:C	2.93	0.46
1:V:94:ASP:O	1:V:94:ASP:CG	2.59	0.46
2:b:201:2AN:C16	2:b:201:2AN:C2	2.90	0.46
1:A:6:ILE:HG13	1:A:118:VAL:HB	1.97	0.46
1:F:14:ILE:HD13	1:F:148:GLU:HA	1.97	0.46
2:I:203:2AN:C16	2:I:203:2AN:C2	2.50	0.46
1:U:144:TYR:CE1	2:U:201:2AN:H12	2.50	0.46
1:X:144:TYR:CD1	1:X:144:TYR:O	2.68	0.46
1:Y:5:THR:HG23	1:Y:119:THR:OG1	2.15	0.46
1:K:122:PRO:HG3	1:K:128:VAL:HG23	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:138:LYS:HD2	2:N:203:2AN:O1	2.16	0.46
2:N:202:2AN:N	2:N:202:2AN:O1	2.40	0.46
1:O:102:GLU:HB3	1:O:117:THR:OG1	2.16	0.46
1:O:143:PHE:O	1:O:147:VAL:HG23	2.16	0.46
1:P:5:THR:OG1	1:P:119:THR:HG23	2.15	0.46
2:V:202:2AN:O1	2:V:202:2AN:N	2.49	0.46
1:W:38:VAL:HG22	2:W:204:2AN:H14	1.96	0.46
1:B:89:GLY:C	1:B:91:VAL:N	2.74	0.46
1:F:97:GLU:HB3	1:F:121:HIS:O	2.15	0.46
1:P:80:PHE:O	1:P:104:LYS:HA	2.15	0.46
1:T:108:VAL:HG21	1:T:113:LYS:HG3	1.97	0.46
1:U:153:ALA:C	1:U:154:ASN:ND2	2.74	0.46
1:F:92:LEU:O	1:F:93:ARG:CB	2.64	0.46
2:H:202:2AN:C2	2:H:202:2AN:C16	2.93	0.46
1:M:44:ILE:HD12	1:M:53:THR:CG2	2.40	0.46
1:O:138:LYS:HD3	1:O:138:LYS:HA	1.58	0.46
1:P:65:LEU:HD13	1:P:91:VAL:HG23	1.96	0.46
1:P:157:VAL:O	1:P:158:PHE:HB2	2.16	0.46
1:Q:10:GLU:C	1:Q:11:GLU:HG2	2.40	0.46
1:X:138:LYS:O	1:X:139:LYS:C	2.57	0.46
1:Y:144:TYR:CD1	1:Y:144:TYR:O	2.69	0.46
1:C:1:MET:O	1:C:2:ALA:CB	2.64	0.46
1:C:83:LYS:HG2	1:C:102:GLU:HG3	1.97	0.46
1:D:19:LEU:HD13	2:D:202:2AN:C15	2.46	0.46
1:E:79:ASN:O	1:E:104:LYS:NZ	2.34	0.46
1:H:20:PHE:HZ	1:H:81:TYR:O	1.97	0.46
1:T:141:TYR:O	1:T:145:LYS:HG2	2.16	0.46
1:Z:50:GLY:O	1:Z:53:THR:OG1	2.30	0.46
1:a:3:ALA:O	1:b:4:TYR:HA	2.15	0.46
1:F:49:GLY:CA	1:F:53:THR:OG1	2.64	0.46
1:F:54:VAL:CG2	1:F:71:LYS:HD3	2.45	0.46
1:H:10:GLU:C	1:H:11:GLU:HG3	2.41	0.46
1:Q:50:GLY:O	1:Q:53:THR:OG1	2.26	0.46
1:V:51:VAL:HG12	1:V:52:GLY:H	1.81	0.46
1:Z:129:ASN:OD1	1:Z:129:ASN:C	2.58	0.46
1:A:101:TYR:HE2	5:A:305:HOH:O	1.99	0.46
1:B:51:VAL:HG11	1:B:73:ASP:O	2.17	0.46
1:D:104:LYS:O	1:D:104:LYS:HG3	2.15	0.46
2:J:201:2AN:N	2:J:201:2AN:O3	2.49	0.46
1:Q:129:ASN:HB3	1:Q:132:GLU:CB	2.46	0.46
1:Q:144:TYR:O	1:Q:144:TYR:CD1	2.69	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:V:1:MET:N	1:V:2:ALA:HA	2.31	0.46
1:V:4:TYR:HB3	1:V:120:TYR:HB2	1.97	0.46
1:A:50:GLY:CA	1:A:75:ILE:HD11	2.45	0.45
1:E:68:MET:HG2	1:E:91:VAL:HG11	1.98	0.45
1:J:95:ASN:N	1:J:95:ASN:ND2	2.39	0.45
1:K:4:TYR:HB3	1:K:120:TYR:HB2	1.98	0.45
1:P:53:THR:HG22	1:P:54:VAL:N	2.30	0.45
1:P:123:LYS:O	1:P:126:CYS:SG	2.74	0.45
1:T:116:ILE:HD12	1:T:116:ILE:N	2.31	0.45
1:C:144:TYR:CD1	1:C:144:TYR:O	2.70	0.45
1:E:33:LYS:NZ	2:E:203:2AN:O3	2.46	0.45
1:I:2:ALA:CB	1:J:4:TYR:CE1	2.99	0.45
1:I:72:PHE:N	1:I:72:PHE:HD1	2.14	0.45
1:M:20:PHE:HB2	1:M:105:LEU:HD12	1.97	0.45
1:Q:95:ASN:HD21	1:Q:129:ASN:HB2	1.81	0.45
1:S:68:MET:HG2	1:S:91:VAL:HG11	1.98	0.45
1:X:122:PRO:HG3	1:X:128:VAL:HG23	1.98	0.45
1:A:50:GLY:HA2	1:A:75:ILE:HD11	1.99	0.45
1:I:49:GLY:HA2	1:I:53:THR:HG21	1.99	0.45
1:I:69:LEU:HD12	1:I:88:GLU:HB3	1.97	0.45
1:W:96:ILE:HD11	1:W:132:GLU:OE1	2.15	0.45
1:W:144:TYR:CD1	1:W:144:TYR:C	2.95	0.45
1:b:92:LEU:HD22	1:b:96:ILE:HG22	1.98	0.45
1:A:5:THR:HG22	1:A:119:THR:OG1	2.16	0.45
1:H:131:GLU:HG3	1:H:135:ILE:HD12	1.98	0.45
1:I:8:LYS:C	1:I:9:GLU:HG2	2.40	0.45
1:J:143:PHE:O	1:J:144:TYR:C	2.59	0.45
1:K:158:PHE:CE1	2:K:203:2AN:H13	2.52	0.45
1:V:23:LEU:HA	1:V:23:LEU:HD23	1.72	0.45
1:W:144:TYR:OH	2:W:202:2AN:H13	2.15	0.45
1:Y:63:HIS:O	1:Y:64:PRO:C	2.58	0.45
1:Z:65:LEU:HD22	1:Z:91:VAL:HA	1.99	0.45
1:b:115:LYS:C	1:b:116:ILE:HD12	2.41	0.45
1:C:98:LYS:HE3	1:C:121:HIS:ND1	2.30	0.45
1:T:6:ILE:HD13	1:T:137:GLU:HG2	1.99	0.45
1:C:42:GLY:HA2	1:C:56:LYS:O	2.16	0.45
1:D:131:GLU:OE2	1:D:135:ILE:CD1	2.63	0.45
1:G:92:LEU:C	1:G:93:ARG:CG	2.85	0.45
1:J:26:GLU:O	1:J:30:VAL:HG23	2.17	0.45
1:L:10:GLU:O	1:L:11:GLU:CG	2.64	0.45
1:U:17:HIS:O	2:U:204:2AN:H6	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:75:ILE:HG23	1:A:82:CYS:SG	2.57	0.45
1:C:86:LEU:CG	1:C:92:LEU:HD21	2.47	0.45
1:E:139:LYS:HZ3	2:E:205:2AN:H12	1.80	0.45
1:G:51:VAL:O	1:G:51:VAL:CG2	2.54	0.45
1:H:42:GLY:HA2	1:H:56:LYS:O	2.17	0.45
1:L:16:PRO:HG3	1:L:107:ALA:HB2	1.99	0.45
1:N:21:LYS:HG3	1:N:25:LEU:HD12	1.99	0.45
1:Q:90:ASP:C	1:Q:92:LEU:H	2.23	0.45
1:T:92:LEU:HD22	1:T:96:ILE:HG22	1.97	0.45
1:T:131:GLU:O	1:T:134:LYS:HB2	2.16	0.45
2:U:201:2AN:H16	2:U:201:2AN:C2	2.45	0.45
1:Y:17:HIS:O	2:Y:204:2AN:H6	2.17	0.45
1:B:83:LYS:HE2	1:B:100:VAL:CG1	2.46	0.45
1:D:89:GLY:C	1:D:91:VAL:N	2.69	0.45
1:F:120:TYR:CE1	1:F:133:VAL:HG13	2.52	0.45
1:G:33:LYS:N	1:G:33:LYS:HD2	2.32	0.45
1:G:40:LYS:HE2	1:G:58:THR:HG21	1.97	0.45
2:M:201:2AN:C16	2:M:201:2AN:H2	2.46	0.45
1:T:6:ILE:HD11	1:T:133:VAL:HG13	1.94	0.45
1:U:147:VAL:O	1:U:147:VAL:CG1	2.64	0.45
1:Y:6:ILE:CD1	1:Y:133:VAL:HG12	2.47	0.45
1:b:137:GLU:O	1:b:138:LYS:C	2.58	0.45
1:A:158:PHE:CZ	2:A:201:2AN:H6	2.52	0.45
1:V:32:VAL:HG22	1:V:39:PHE:HB3	1.98	0.45
1:W:58:THR:HG22	1:W:59:PHE:O	2.16	0.45
1:W:145:LYS:HD2	1:W:145:LYS:HA	1.81	0.45
1:B:5:THR:HG22	1:B:6:ILE:O	2.17	0.45
1:F:14:ILE:HD11	1:F:148:GLU:O	2.17	0.45
1:K:28:HIS:CD2	1:K:29:GLN:HG3	2.52	0.45
1:N:44:ILE:HG23	1:N:53:THR:CG2	2.47	0.45
1:N:145:LYS:HA	1:N:145:LYS:HD2	1.68	0.45
1:R:129:ASN:C	1:R:131:GLU:N	2.71	0.45
1:S:20:PHE:CE1	1:S:80:PHE:C	2.95	0.45
1:Y:129:ASN:O	1:Y:129:ASN:CG	2.55	0.45
1:Y:156:GLU:O	1:Y:159:ALA:HB2	2.16	0.45
1:A:51:VAL:HA	1:A:72:PHE:O	2.16	0.44
1:C:6:ILE:CD1	1:C:137:GLU:CG	2.95	0.44
1:C:129:ASN:CG	1:C:132:GLU:CB	2.90	0.44
1:E:144:TYR:CG	2:E:202:2AN:H12	2.53	0.44
1:H:4:TYR:N	1:H:4:TYR:CD1	2.85	0.44
1:H:117:THR:O	1:H:117:THR:OG1	2.26	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:139:LYS:HE2	2:H:202:2AN:C5	2.47	0.44
1:K:9:GLU:HA	1:K:114:GLY:O	2.17	0.44
1:P:30:VAL:HG23	1:P:143:PHE:HZ	1.82	0.44
1:Q:128:VAL:HG12	1:Q:129:ASN:O	2.17	0.44
1:S:69:LEU:HB3	1:S:87:PHE:HE1	1.81	0.44
2:W:201:2AN:C16	2:W:201:2AN:C2	2.95	0.44
2:W:204:2AN:O3	2:W:204:2AN:N	2.50	0.44
1:Y:72:PHE:HD2	1:Y:82:CYS:SG	2.40	0.44
1:Y:81:TYR:CD1	1:Y:81:TYR:C	2.94	0.44
1:D:53:THR:HB	1:D:72:PHE:CD2	2.52	0.44
1:N:16:PRO:HG2	1:N:107:ALA:HB2	2.00	0.44
1:T:132:GLU:O	1:T:136:GLY:N	2.48	0.44
1:W:6:ILE:HD12	1:W:118:VAL:HB	1.98	0.44
1:W:96:ILE:HG13	1:W:132:GLU:OE1	2.18	0.44
1:W:144:TYR:CE1	2:W:202:2AN:C13	3.01	0.44
1:Y:46:GLU:C	1:Y:47:GLY:O	2.60	0.44
1:Y:138:LYS:O	1:Y:142:GLU:HG3	2.17	0.44
1:Z:92:LEU:O	1:Z:93:ARG:HG3	2.17	0.44
1:D:17:HIS:CD2	1:D:159:ALA:O	2.71	0.44
1:D:19:LEU:HD23	1:D:19:LEU:HA	1.91	0.44
1:D:57:ILE:O	1:D:67:TYR:HA	2.17	0.44
2:E:201:2AN:C2	2:E:201:2AN:C16	2.88	0.44
1:S:144:TYR:O	1:S:145:LYS:C	2.60	0.44
1:U:109:GLY:C	1:U:111:GLY:H	2.25	0.44
1:Y:48:ASP:OD1	1:Y:50:GLY:N	2.45	0.44
1:Y:105:LEU:HD22	2:Y:202:2AN:H15	2.00	0.44
1:a:131:GLU:O	1:a:132:GLU:C	2.60	0.44
1:A:1:MET:HA	1:A:2:ALA:HA	1.70	0.44
1:E:27:ARG:O	1:E:28:HIS:C	2.60	0.44
2:E:202:2AN:C2	2:E:202:2AN:H16	2.47	0.44
1:G:51:VAL:O	1:G:51:VAL:HG22	2.15	0.44
1:J:144:TYR:C	1:J:144:TYR:CD1	2.96	0.44
1:L:15:ALA:HB1	1:L:16:PRO:CD	2.46	0.44
2:L:201:2AN:N	2:L:201:2AN:O1	2.34	0.44
1:N:92:LEU:O	1:N:93:ARG:HB2	2.16	0.44
1:N:141:TYR:CB	2:N:203:2AN:H3	2.48	0.44
1:R:144:TYR:CG	2:R:201:2AN:H12	2.52	0.44
2:R:201:2AN:C16	2:R:201:2AN:H2	2.47	0.44
1:X:32:VAL:O	1:X:32:VAL:HG12	2.16	0.44
1:A:39:PHE:CD1	1:A:57:ILE:CG2	3.01	0.44
1:A:150:TYR:CD1	2:A:201:2AN:O3	2.70	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:5:THR:HG23	1:B:118:VAL:O	2.17	0.44
1:E:155:PRO:O	1:E:159:ALA:HB2	2.16	0.44
1:F:49:GLY:N	1:F:53:THR:OG1	2.49	0.44
1:F:94:ASP:C	1:F:96:ILE:H	2.26	0.44
1:G:93:ARG:HG3	1:G:132:GLU:OE1	2.18	0.44
2:H:201:2AN:H12	2:H:201:2AN:C2	2.44	0.44
1:I:16:PRO:HB2	1:I:80:PHE:CE2	2.53	0.44
1:T:72[A]:PHE:CD2	1:T:75:ILE:HD11	2.53	0.44
1:T:123:LYS:O	1:T:124:PRO:C	2.59	0.44
1:Z:147:VAL:O	1:Z:148:GLU:C	2.59	0.44
2:F:201:2AN:C12	2:F:201:2AN:C2	2.52	0.44
1:G:96:ILE:CD1	1:G:128:VAL:HG22	2.48	0.44
1:J:20:PHE:CE1	1:J:24:VAL:HG21	2.52	0.44
1:L:135:ILE:O	1:L:139:LYS:HG2	2.18	0.44
1:Q:144:TYR:CE2	2:Q:201:2AN:H12	2.52	0.44
1:B:119:THR:HG1	1:B:121:HIS:CE1	2.31	0.44
1:G:119:THR:HG22	1:G:121:HIS:CE1	2.52	0.44
1:K:149:GLU:C	1:K:149:GLU:OE1	2.60	0.44
1:M:23:LEU:O	1:M:27:ARG:HD2	2.18	0.44
1:O:14:ILE:O	1:O:112:SER:OG	2.36	0.44
1:T:95:ASN:HB3	1:T:127:THR:O	2.18	0.44
1:U:45:ILE:HD13	1:U:45:ILE:HG21	1.70	0.44
1:Y:14:ILE:HG21	1:Y:151:LEU:HD13	1.99	0.44
1:O:79:ASN:O	1:O:80:PHE:HB2	2.17	0.44
1:R:116:ILE:HD13	2:R:201:2AN:O3	2.18	0.44
1:U:77:ALA:O	2:U:204:2AN:H3	2.18	0.44
2:U:202:2AN:C16	2:U:202:2AN:C2	2.94	0.44
1:Z:93:ARG:CD	1:Z:129:ASN:ND2	2.70	0.44
1:F:90:ASP:C	1:F:92:LEU:N	2.71	0.44
1:G:15:ALA:HB1	1:G:16:PRO:HD2	1.99	0.44
1:G:17:HIS:CE1	1:U:15:ALA:CB	3.01	0.44
1:K:33:LYS:HE3	2:K:203:2AN:N	2.33	0.44
1:R:91:VAL:O	1:R:91:VAL:HG22	2.17	0.44
1:X:129:ASN:OD1	1:X:132:GLU:HB3	2.17	0.44
1:Z:23:LEU:O	1:Z:27:ARG:HD2	2.17	0.44
1:B:54:VAL:HG11	1:B:87:PHE:CZ	2.51	0.43
1:B:89:GLY:O	1:B:90:ASP:C	2.61	0.43
2:B:205:2AN:H16	2:B:205:2AN:C2	2.44	0.43
1:F:118:VAL:HG21	1:F:137:GLU:OE2	2.17	0.43
1:G:63:HIS:O	1:G:64:PRO:C	2.61	0.43
1:K:17:HIS:CB	1:Q:110:GLY:HA2	2.47	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:109:GLY:HA2	2:Q:202:2AN:C2	2.47	0.43
1:M:151:LEU:HD21	2:M:203:2AN:C7	2.47	0.43
1:N:144:TYR:CD1	1:N:144:TYR:C	2.92	0.43
1:b:4:TYR:CE2	1:b:128:VAL:HB	2.53	0.43
1:C:134:LYS:O	1:C:135:ILE:C	2.61	0.43
1:E:97:GLU:HG3	1:E:98:LYS:HG2	1.99	0.43
1:I:6:ILE:CG2	1:J:1:MET:CG	2.96	0.43
1:K:33:LYS:HE3	2:K:203:2AN:C1	2.47	0.43
1:K:145:LYS:HA	1:K:145:LYS:HD2	1.86	0.43
1:M:72:PHE:N	1:M:72:PHE:CD1	2.86	0.43
1:M:144:TYR:CD1	2:M:202:2AN:H12	2.54	0.43
1:Q:130:GLU:O	1:Q:130:GLU:HG2	2.17	0.43
1:a:50:GLY:HA2	1:a:75:ILE:HD12	1.99	0.43
1:B:4:TYR:CG	1:B:128:VAL:HG11	2.50	0.43
2:B:203:2AN:N	2:B:203:2AN:O1	2.51	0.43
1:F:8:LYS:HD3	1:F:9:GLU:H	1.83	0.43
1:G:134:LYS:O	1:G:135:ILE:C	2.61	0.43
1:S:87:PHE:HA	1:S:98:LYS:HB3	1.99	0.43
1:W:51:VAL:HG12	1:W:74:GLU:HA	1.99	0.43
1:Z:51:VAL:HG13	1:Z:52:GLY:N	2.31	0.43
1:a:123:LYS:CD	1:a:124:PRO:CD	2.42	0.43
2:C:201:2AN:N	2:C:201:2AN:O3	2.52	0.43
1:F:51:VAL:HG13	1:F:72:PHE:O	2.18	0.43
1:H:39:PHE:CE1	1:H:59:PHE:CE2	3.06	0.43
1:I:6:ILE:HG23	1:J:1:MET:CG	2.36	0.43
1:Z:8:LYS:HZ2	2:Z:202:2AN:H8	1.84	0.43
1:A:35:GLN:NE2	1:A:146:GLN:HE22	2.17	0.43
1:B:51:VAL:HG13	1:B:73:ASP:C	2.44	0.43
1:D:72:PHE:CD2	1:D:75:ILE:HD11	2.53	0.43
1:G:51:VAL:HG23	1:G:52:GLY:N	2.27	0.43
2:G:204:2AN:O1	2:G:204:2AN:C11	2.66	0.43
1:H:85:THR:HG21	1:H:98:LYS:HD2	2.01	0.43
1:L:6:ILE:HD11	1:L:133:VAL:CG1	2.48	0.43
1:P:30:VAL:HB	2:P:202:2AN:O3	2.18	0.43
1:W:50:GLY:HA2	1:W:75:ILE:HD12	1.99	0.43
1:Y:14:ILE:HG22	1:Y:15:ALA:N	2.33	0.43
1:B:31:LEU:CD1	1:B:57:ILE:HD13	2.48	0.43
1:F:91:VAL:CG1	1:F:92:LEU:N	2.77	0.43
1:L:10:GLU:C	1:L:11:GLU:CG	2.90	0.43
1:M:5:THR:OG1	1:N:5:THR:OG1	2.27	0.43
1:O:71:LYS:HB2	1:O:87:PHE:HE2	1.82	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:106:GLU:HG2	1:A:113:LYS:HB3	2.01	0.43
1:C:21:LYS:O	1:C:26:GLU:HB2	2.18	0.43
1:C:74:GLU:O	1:C:75:ILE:CG1	2.67	0.43
1:C:145:LYS:HA	1:C:145:LYS:HD2	1.76	0.43
1:F:86:LEU:HD21	1:F:91:VAL:HG11	2.00	0.43
1:I:6:ILE:HD12	1:I:118:VAL:HB	2.01	0.43
1:J:24:VAL:O	1:J:25:LEU:C	2.62	0.43
1:K:157:VAL:CG1	2:K:203:2AN:C12	2.96	0.43
2:K:203:2AN:O1	2:K:203:2AN:N	2.50	0.43
1:P:28:HIS:CD2	1:P:28:HIS:H	2.36	0.43
1:E:73:ASP:O	1:E:74:GLU:HG3	2.19	0.43
1:I:155:PRO:O	1:I:159:ALA:HB2	2.18	0.43
1:L:47:GLY:HA2	2:L:204:2AN:C16	2.48	0.43
1:L:106:GLU:OE2	1:L:113:LYS:CE	2.66	0.43
1:R:56:LYS:HG3	1:R:69:LEU:HD23	2.00	0.43
1:S:54:VAL:HA	1:S:70:HIS:O	2.18	0.43
1:B:110:GLY:HA2	1:Z:17:HIS:CB	2.49	0.43
1:C:14:ILE:HG22	1:C:18:ARG:HB2	1.99	0.43
2:D:202:2AN:C2	2:D:202:2AN:C16	2.50	0.43
1:F:32:VAL:O	1:F:32:VAL:HG12	2.19	0.43
1:R:144:TYR:CE2	2:R:201:2AN:H12	2.54	0.43
1:S:123:LYS:HG2	1:S:124:PRO:HD2	2.00	0.43
1:W:138:LYS:HE2	1:W:139:LYS:HD2	2.01	0.43
1:Y:71:LYS:HE3	1:Y:87:PHE:CE2	2.54	0.43
1:B:48:ASP:OD1	1:B:48:ASP:N	2.45	0.43
1:G:3:ALA:HB2	1:G:121:HIS:CD2	2.54	0.43
1:I:131:GLU:O	1:I:135:ILE:HG13	2.19	0.43
1:K:96:ILE:HD13	1:K:128:VAL:HG22	1.97	0.43
2:K:201:2AN:N	2:K:201:2AN:O1	2.52	0.43
1:U:65:LEU:HD22	1:U:91:VAL:HA	2.01	0.43
1:W:93:ARG:HD2	1:W:132:GLU:OE2	2.18	0.43
1:A:55:THR:O	1:A:69:LEU:HA	2.19	0.42
1:L:93:ARG:HH12	1:L:132:GLU:HB2	1.84	0.42
1:N:6:ILE:CD1	1:N:137:GLU:HG3	2.49	0.42
1:U:30:VAL:O	1:U:31:LEU:C	2.62	0.42
1:Y:7:VAL:O	1:Y:7:VAL:HG12	2.19	0.42
1:A:143:PHE:O	1:A:147:VAL:HG23	2.19	0.42
1:E:72:PHE:N	1:E:72:PHE:CD1	2.85	0.42
1:P:30:VAL:HG23	1:P:143:PHE:CZ	2.54	0.42
1:R:138:LYS:HE3	1:R:139:LYS:HD2	2.02	0.42
1:S:90:ASP:C	1:S:92:LEU:H	2.26	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:89:GLY:O	1:U:92:LEU:HB2	2.18	0.42
1:Y:10:GLU:O	1:Y:11:GLU:CG	2.66	0.42
1:A:47:GLY:HA2	2:Y:204:2AN:C13	2.49	0.42
1:D:140:ALA:HB1	2:D:202:2AN:C8	2.49	0.42
1:E:147:VAL:HA	2:E:203:2AN:H4	2.01	0.42
2:G:204:2AN:C16	2:G:204:2AN:C2	2.91	0.42
1:H:76:ASP:HB3	1:H:81:TYR:HB3	2.01	0.42
1:J:24:VAL:O	1:J:26:GLU:N	2.52	0.42
1:K:16:PRO:HD3	1:K:112:SER:HB3	2.01	0.42
1:M:39:PHE:CD1	1:M:57:ILE:CG2	3.03	0.42
1:T:107:ALA:C	1:T:108:VAL:HG23	2.44	0.42
1:T:124:PRO:HG2	1:T:124:PRO:O	2.18	0.42
1:Z:80:PHE:O	1:Z:104:LYS:HA	2.19	0.42
1:C:91:VAL:HG13	1:C:92:LEU:N	2.34	0.42
1:G:144:TYR:O	1:G:144:TYR:CD1	2.72	0.42
2:I:202:2AN:H16	2:I:205:2AN:H6	2.01	0.42
1:S:55:THR:O	1:S:69:LEU:HA	2.19	0.42
1:T:34:ALA:O	1:T:146[A]:GLN:NE2	2.46	0.42
1:W:10:GLU:CG	2:W:202:2AN:C13	2.98	0.42
1:Y:18:ARG:NH2	1:Y:154:ASN:O	2.52	0.42
1:Y:123:LYS:O	1:Y:126:CYS:HB2	2.18	0.42
2:A:201:2AN:C16	2:A:201:2AN:C2	2.63	0.42
2:A:204:2AN:N	2:A:204:2AN:O3	2.53	0.42
1:E:138:LYS:NZ	1:E:139:LYS:HD3	2.34	0.42
1:K:30:VAL:HG13	2:K:203:2AN:C3	2.49	0.42
1:N:144:TYR:CD1	1:N:144:TYR:O	2.72	0.42
1:R:144:TYR:CE1	2:R:201:2AN:C13	3.02	0.42
2:R:204:2AN:N	2:R:204:2AN:S	2.62	0.42
1:S:91:VAL:O	1:S:91:VAL:CG2	2.62	0.42
1:S:129:ASN:ND2	1:S:129:ASN:O	2.51	0.42
1:V:19:LEU:O	1:V:23:LEU:HB2	2.20	0.42
1:W:141:TYR:O	1:W:145:LYS:HG2	2.19	0.42
1:W:142:GLU:O	1:W:146:GLN:HG3	2.20	0.42
1:C:121:HIS:HA	1:C:122:PRO:HD2	1.97	0.42
2:E:201:2AN:O3	2:E:201:2AN:C11	2.68	0.42
1:F:44:ILE:HG12	1:F:55:THR:HG22	2.02	0.42
1:H:123:LYS:O	1:H:124:PRO:C	2.59	0.42
1:L:35:GLN:C	1:L:37:HIS:H	2.28	0.42
1:M:44:ILE:CD1	1:M:53:THR:HG21	2.41	0.42
1:V:21:LYS:HA	1:V:25:LEU:CB	2.50	0.42
1:W:107:ALA:O	1:W:108:VAL:HG23	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:6:ILE:CD1	1:C:137:GLU:HG2	2.50	0.42
1:C:9:GLU:HA	1:C:114:GLY:O	2.19	0.42
1:F:71:LYS:HG2	1:F:87:PHE:CE2	2.54	0.42
1:I:1:MET:CG	1:I:2:ALA:H	2.29	0.42
1:J:54:VAL:HG22	1:J:71:LYS:CD	2.50	0.42
1:S:56:LYS:HB3	1:S:56:LYS:HE2	1.84	0.42
1:V:43:GLU:HG2	1:V:44:ILE:H	1.85	0.42
1:V:55:THR:O	1:V:69:LEU:HA	2.18	0.42
1:W:32:VAL:HG22	1:W:39:PHE:HB3	2.01	0.42
1:b:48:ASP:OD1	1:b:48:ASP:C	2.62	0.42
2:E:203:2AN:O3	2:E:203:2AN:N	2.44	0.42
1:I:80:PHE:O	1:I:104:LYS:HA	2.20	0.42
1:K:98:LYS:HE3	1:K:121:HIS:CD2	2.54	0.42
2:R:201:2AN:C16	2:R:201:2AN:C2	2.96	0.42
1:U:127:THR:O	1:U:127:THR:CG2	2.66	0.42
1:V:75:ILE:O	1:V:75:ILE:HG22	2.20	0.42
1:Z:54:VAL:HA	1:Z:70:HIS:O	2.19	0.42
1:A:92:LEU:O	1:A:93:ARG:CB	2.68	0.42
1:D:93:ARG:O	1:D:94:ASP:CB	2.66	0.42
1:F:51:VAL:CG2	1:F:75:ILE:N	2.82	0.42
1:F:150:TYR:HE1	1:F:157:VAL:HG11	1.84	0.42
1:H:14:ILE:HG21	1:H:151:LEU:HD13	2.01	0.42
1:K:71:LYS:O	1:K:84:TYR:HB2	2.20	0.42
1:L:103:VAL:HG21	2:L:202:2AN:H4	2.02	0.42
1:R:129:ASN:N	1:R:129:ASN:HD22	2.18	0.42
1:Z:129:ASN:OD1	1:Z:129:ASN:O	2.38	0.42
2:a:201:2AN:N	2:a:201:2AN:O3	2.53	0.42
1:A:97:GLU:O	1:A:97:GLU:OE1	2.37	0.42
1:K:29:GLN:O	1:K:32:VAL:N	2.51	0.42
1:M:14:ILE:HB	1:M:19:LEU:HG	2.02	0.42
1:R:86:LEU:HG	1:R:92:LEU:HD21	2.01	0.42
1:V:56:LYS:HD3	1:V:69:LEU:HD21	2.02	0.42
1:W:144:TYR:CD1	1:W:144:TYR:O	2.73	0.42
1:B:144:TYR:CE1	2:B:202:2AN:C12	3.03	0.41
1:E:20:PHE:O	1:E:24:VAL:HB	2.20	0.41
1:F:3:ALA:HA	1:F:122:PRO:HD3	2.01	0.41
1:F:80:PHE:HB2	1:F:105:LEU:O	2.20	0.41
1:I:144:TYR:CE1	2:I:201:2AN:H13	2.56	0.41
1:J:66:THR:CB	1:J:90:ASP:OD2	2.68	0.41
1:K:78:ALA:HA	1:Q:109:GLY:N	2.35	0.41
2:L:201:2AN:C16	2:L:201:2AN:C2	2.95	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:54:VAL:HA	1:M:70:HIS:O	2.20	0.41
1:O:54:VAL:HA	1:O:70:HIS:O	2.20	0.41
1:P:11:GLU:HG2	1:P:113:LYS:HG2	2.02	0.41
1:P:129:ASN:O	1:P:132:GLU:HG2	2.20	0.41
2:E:204:2AN:N	2:E:204:2AN:S	2.63	0.41
1:I:39:PHE:CE1	1:I:57:ILE:HG21	2.55	0.41
1:J:4:TYR:CD2	1:J:128:VAL:HG11	2.54	0.41
1:K:129:ASN:HD22	1:K:129:ASN:N	2.17	0.41
1:N:127:THR:CG2	1:N:128:VAL:N	2.82	0.41
2:N:203:2AN:O3	2:N:203:2AN:N	2.53	0.41
2:Q:201:2AN:N	2:Q:201:2AN:O3	2.52	0.41
1:U:10:GLU:C	1:U:11:GLU:CG	2.92	0.41
1:U:71:LYS:HE2	1:U:73:ASP:OD1	2.20	0.41
2:U:203:2AN:HN	2:U:203:2AN:HO3	1.62	0.41
1:W:80:PHE:O	1:W:104:LYS:HA	2.20	0.41
1:Y:6:ILE:HD12	1:Y:133:VAL:HG12	2.02	0.41
1:Z:95:ASN:OD1	1:Z:95:ASN:N	2.46	0.41
1:a:95:ASN:ND2	1:a:129:ASN:HD21	1.99	0.41
1:B:54:VAL:HG13	1:B:70:HIS:O	2.20	0.41
1:B:70:HIS:CE1	1:B:86:LEU:HD13	2.54	0.41
1:E:2:ALA:CB	1:F:4:TYR:CZ	3.02	0.41
1:E:96:ILE:HG23	1:E:96:ILE:HD12	1.84	0.41
1:M:107:ALA:O	1:M:108:VAL:HG23	2.21	0.41
1:O:144:TYR:O	1:O:144:TYR:CD1	2.72	0.41
1:P:147:VAL:O	1:P:148:GLU:C	2.60	0.41
1:Q:141:TYR:O	1:Q:145:LYS:HG2	2.20	0.41
1:T:95:ASN:C	1:T:96:ILE:HD13	2.45	0.41
1:X:144:TYR:CD1	1:X:144:TYR:C	2.97	0.41
2:Y:203:2AN:C2	2:Y:203:2AN:H16	2.49	0.41
1:b:10:GLU:CG	2:b:201:2AN:C12	2.93	0.41
1:D:87:PHE:C	1:D:92:LEU:CD1	2.94	0.41
1:F:88:GLU:C	1:F:92:LEU:HD12	2.46	0.41
1:H:1:MET:CG	1:H:1:MET:O	2.68	0.41
1:I:109:GLY:CA	1:S:78:ALA:HA	2.50	0.41
1:K:78:ALA:HA	1:Q:109:GLY:H	1.85	0.41
1:K:92:LEU:HD22	1:K:96:ILE:HG22	2.02	0.41
1:N:43[A]:GLU:HG3	1:N:56:LYS:HB3	2.03	0.41
1:R:6:ILE:O	1:R:117:THR:HA	2.21	0.41
1:S:157:VAL:O	1:S:158:PHE:HB2	2.20	0.41
1:U:90:ASP:O	1:U:91:VAL:C	2.63	0.41
1:Z:130:GLU:O	1:Z:131:GLU:C	2.64	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:46:GLU:HB2	1:a:54:VAL:HB	2.02	0.41
1:C:33:LYS:HD2	2:C:203:2AN:C13	2.50	0.41
1:C:144:TYR:CZ	2:C:202:2AN:H13	2.55	0.41
1:E:155:PRO:O	1:E:159:ALA:CB	2.68	0.41
1:J:16:PRO:HG3	1:J:107:ALA:HA	2.02	0.41
1:J:66:THR:HB	1:J:90:ASP:OD2	2.20	0.41
1:R:38:VAL:O	1:R:38:VAL:HG12	2.18	0.41
1:A:20:PHE:O	1:A:24:VAL:HB	2.21	0.41
1:A:80:PHE:CB	1:A:105:LEU:HB2	2.48	0.41
1:B:157:VAL:O	1:B:158:PHE:HB2	2.20	0.41
1:C:6:ILE:HD12	1:C:137:GLU:HG2	2.02	0.41
1:E:33:LYS:CE	2:E:203:2AN:O3	2.67	0.41
1:H:6:ILE:O	1:H:117:THR:HA	2.19	0.41
1:I:97:GLU:HG3	1:I:98:LYS:HG2	2.01	0.41
1:Q:120:TYR:O	1:Q:122:PRO:HD3	2.21	0.41
1:T:124:PRO:O	1:T:125:GLY:C	2.62	0.41
1:V:53:THR:CG2	1:V:72:PHE:CD2	3.02	0.41
2:W:203:2AN:C2	2:W:203:2AN:C12	2.88	0.41
1:X:65:LEU:HD12	2:X:201:2AN:H3	2.03	0.41
1:C:95:ASN:OD1	1:C:95:ASN:N	2.32	0.41
1:F:16:PRO:HB2	1:F:80:PHE:CD2	2.55	0.41
1:G:8:LYS:NZ	5:G:301:HOH:O	2.53	0.41
1:L:71:LYS:HB2	1:L:87:PHE:HE2	1.86	0.41
2:L:204:2AN:H2	2:L:204:2AN:H16	1.93	0.41
2:N:203:2AN:C16	2:N:203:2AN:C2	2.92	0.41
1:P:54:VAL:HA	1:P:70:HIS:O	2.20	0.41
1:S:32:VAL:O	1:S:32:VAL:HG12	2.20	0.41
1:Y:26:GLU:O	1:Y:30:VAL:HG23	2.21	0.41
1:Z:107:ALA:O	1:Z:108:VAL:CG2	2.69	0.41
1:b:92:LEU:O	1:b:96:ILE:HB	2.21	0.41
1:I:147:VAL:HG13	2:I:203:2AN:H7	1.99	0.41
1:K:45:ILE:HG12	1:K:54:VAL:O	2.21	0.41
1:U:10:GLU:C	1:U:11:GLU:HG2	2.45	0.41
1:X:42:GLY:HA2	1:X:56:LYS:O	2.21	0.41
1:Y:6:ILE:HD12	1:Y:133:VAL:CG1	2.51	0.41
1:Z:144:TYR:CD1	1:Z:144:TYR:C	2.97	0.41
1:A:45:ILE:HD11	1:A:54:VAL:CG1	2.50	0.41
1:B:155:PRO:O	1:B:159:ALA:CB	2.68	0.41
2:B:203:2AN:C2	2:B:203:2AN:H16	2.50	0.41
1:D:53:THR:O	1:D:71:LYS:HA	2.21	0.41
1:F:92:LEU:C	1:F:93:ARG:CG	2.91	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:141:TYR:O	1:F:145:LYS:HG2	2.20	0.41
1:G:5:THR:HA	1:G:118:VAL:O	2.20	0.41
1:G:17:HIS:HB3	1:U:110:GLY:HA2	2.02	0.41
1:G:59:PHE:CD1	1:G:59:PHE:N	2.89	0.41
1:J:120:TYR:OH	1:J:137:GLU:OE1	2.30	0.41
1:K:29:GLN:O	1:K:30:VAL:C	2.62	0.41
1:K:95:ASN:HD21	1:K:129:ASN:ND2	2.19	0.41
1:M:4:TYR:CE2	1:M:128:VAL:HG12	2.55	0.41
1:S:124:PRO:O	1:S:126:CYS:SG	2.78	0.41
1:T:129:ASN:OD1	1:T:131:GLU:HB3	2.21	0.41
1:U:79:ASN:O	1:U:80:PHE:HB2	2.20	0.41
1:V:86:LEU:HG	1:V:92:LEU:CD1	2.46	0.41
1:W:64:PRO:CD	2:W:201:2AN:O3	2.69	0.41
1:Y:54:VAL:HA	1:Y:70:HIS:O	2.21	0.41
1:a:72:PHE:N	1:a:72:PHE:CD1	2.89	0.41
1:C:21:LYS:HD3	1:C:158:PHE:CD1	2.56	0.41
1:D:132:GLU:O	1:D:135:ILE:N	2.54	0.41
1:J:15:ALA:HB1	1:J:16:PRO:CD	2.51	0.41
1:M:12:SER:HB2	2:M:202:2AN:H13	2.02	0.41
1:M:50:GLY:O	1:M:53:THR:OG1	2.32	0.41
1:V:27:ARG:O	1:V:28:HIS:C	2.63	0.41
1:V:50:GLY:HA2	1:V:75:ILE:HD12	2.03	0.41
1:X:74:GLU:HB2	1:X:83:LYS:HB2	2.03	0.41
1:E:76:ASP:C	1:E:76:ASP:OD1	2.63	0.40
1:F:73:ASP:C	1:F:74:GLU:HG3	2.46	0.40
1:J:90:ASP:C	1:J:92:LEU:N	2.79	0.40
1:J:106:GLU:CD	1:J:113:LYS:HE3	2.46	0.40
2:K:202:2AN:N	2:K:202:2AN:O3	2.54	0.40
1:M:95:ASN:OD1	1:M:95:ASN:N	2.31	0.40
1:Z:83:LYS:HA	1:Z:101:TYR:O	2.21	0.40
1:Z:139:LYS:HD3	1:Z:139:LYS:HA	1.79	0.40
1:b:90:ASP:C	1:b:92:LEU:N	2.80	0.40
1:B:72:PHE:CD2	1:B:75:ILE:HD11	2.56	0.40
1:G:62:GLY:O	1:G:63:HIS:C	2.64	0.40
1:G:97:GLU:HG3	1:G:123:LYS:HE3	2.04	0.40
1:I:12:SER:HB2	2:I:201:2AN:H14	2.02	0.40
1:Q:123:LYS:C	1:Q:126:CYS:CB	2.90	0.40
1:S:28:HIS:CG	1:S:29:GLN:N	2.88	0.40
1:U:150:TYR:O	1:U:154:ASN:ND2	2.51	0.40
1:Y:157:VAL:C	1:Y:159:ALA:H	2.28	0.40
1:A:45:ILE:HD11	1:A:54:VAL:HG11	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:108:VAL:HG21	1:I:113:LYS:HD2	2.02	0.40
1:J:132:GLU:O	1:J:133:VAL:C	2.63	0.40
1:J:133:VAL:H	1:J:133:VAL:HG23	1.43	0.40
1:N:56:LYS:HG3	1:N:69:LEU:HD23	2.03	0.40
1:O:69:LEU:HD12	1:O:88:GLU:HB3	2.02	0.40
2:Q:202:2AN:O1	2:Q:202:2AN:C11	2.69	0.40
1:V:30:VAL:HG12	1:V:30:VAL:O	2.22	0.40
1:V:37:HIS:NE2	1:V:38:VAL:HG23	2.35	0.40
1:X:73:ASP:O	1:X:74:GLU:HG3	2.21	0.40
1:Y:47:GLY:HA2	2:Y:203:2AN:C11	2.51	0.40
1:B:21:LYS:CE	1:B:158:PHE:CD1	3.03	0.40
1:G:43:GLU:HG2	1:G:44:ILE:N	2.36	0.40
1:M:40:LYS:HB2	1:M:60:VAL:HA	2.02	0.40
1:Z:56:LYS:HD2	1:Z:69:LEU:HD21	2.03	0.40
1:a:37:HIS:CD2	1:a:38:VAL:HG23	2.56	0.40
1:b:39:PHE:CD1	1:b:57:ILE:CG2	3.05	0.40
1:F:51:VAL:CG2	1:F:75:ILE:HG13	2.44	0.40
1:F:54:VAL:CG2	1:F:71:LYS:CD	2.99	0.40
2:G:201:2AN:C16	2:G:201:2AN:H2	2.51	0.40
1:J:108:VAL:C	1:J:109:GLY:O	2.63	0.40
1:Q:31:LEU:CD1	1:Q:57:ILE:HD13	2.52	0.40
1:Q:55:THR:O	1:Q:69:LEU:HA	2.20	0.40
1:R:12:SER:HA	1:R:13:PRO:HD2	1.97	0.40
1:R:115:LYS:HG3	1:R:115:LYS:O	2.20	0.40
1:U:109:GLY:C	1:U:111:GLY:N	2.78	0.40
2:W:203:2AN:N	2:W:203:2AN:O3	2.55	0.40
2:X:203:2AN:C2	2:X:203:2AN:H16	2.51	0.40
1:Z:92:LEU:HD22	1:Z:96:ILE:HG22	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	158/165 (96%)	148 (94%)	7 (4%)	3 (2%)	6	4
1	B	157/165 (95%)	143 (91%)	12 (8%)	2 (1%)	9	9
1	C	157/165 (95%)	139 (88%)	16 (10%)	2 (1%)	9	9
1	D	157/165 (95%)	140 (89%)	14 (9%)	3 (2%)	6	4
1	E	157/165 (95%)	142 (90%)	12 (8%)	3 (2%)	6	4
1	F	157/165 (95%)	145 (92%)	11 (7%)	1 (1%)	21	25
1	G	157/165 (95%)	145 (92%)	9 (6%)	3 (2%)	6	4
1	H	157/165 (95%)	150 (96%)	7 (4%)	0	100	100
1	I	157/165 (95%)	145 (92%)	10 (6%)	2 (1%)	9	9
1	J	157/165 (95%)	143 (91%)	12 (8%)	2 (1%)	9	9
1	K	157/165 (95%)	143 (91%)	10 (6%)	4 (2%)	4	2
1	L	157/165 (95%)	149 (95%)	6 (4%)	2 (1%)	9	9
1	M	157/165 (95%)	147 (94%)	10 (6%)	0	100	100
1	N	158/165 (96%)	145 (92%)	13 (8%)	0	100	100
1	O	157/165 (95%)	147 (94%)	10 (6%)	0	100	100
1	P	157/165 (95%)	139 (88%)	14 (9%)	4 (2%)	4	2
1	Q	157/165 (95%)	142 (90%)	13 (8%)	2 (1%)	9	9
1	R	157/165 (95%)	146 (93%)	9 (6%)	2 (1%)	9	9
1	S	157/165 (95%)	141 (90%)	15 (10%)	1 (1%)	21	25
1	T	163/165 (99%)	151 (93%)	11 (7%)	1 (1%)	21	25
1	U	157/165 (95%)	145 (92%)	11 (7%)	1 (1%)	21	25
1	V	157/165 (95%)	139 (88%)	16 (10%)	2 (1%)	9	9
1	W	157/165 (95%)	151 (96%)	4 (2%)	2 (1%)	9	9
1	X	157/165 (95%)	148 (94%)	7 (4%)	2 (1%)	9	9
1	Y	157/165 (95%)	145 (92%)	11 (7%)	1 (1%)	21	25
1	Z	157/165 (95%)	142 (90%)	12 (8%)	3 (2%)	6	4
1	a	158/165 (96%)	143 (90%)	13 (8%)	2 (1%)	9	9
1	b	157/165 (95%)	141 (90%)	15 (10%)	1 (1%)	21	25
All	All	4405/4620 (95%)	4044 (92%)	310 (7%)	51 (1%)	10	10

All (51) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	94	ASP
1	D	131	GLU
1	E	126	CYS
1	I	2	ALA
1	J	3	ALA
1	L	2	ALA
1	L	129	ASN
1	P	93	ARG
1	Q	2	ALA
1	W	93	ARG
1	Z	93	ARG
1	a	93	ARG
1	A	108	VAL
1	B	108	VAL
1	D	133	VAL
1	F	130	GLU
1	G	93	ARG
1	J	2	ALA
1	K	2	ALA
1	K	51	VAL
1	T	2	ALA
1	V	24	VAL
1	X	93	ARG
1	K	78	ALA
1	R	93	ARG
1	a	2	ALA
1	A	124	PRO
1	B	90	ASP
1	C	2	ALA
1	K	93	ARG
1	Q	108	VAL
1	P	92	LEU
1	R	108	VAL
1	S	144	TYR
1	V	124	PRO
1	b	46	GLU
1	C	75	ILE
1	P	130	GLU
1	U	47	GLY
1	Z	49	GLY
1	Z	64	PRO
1	E	49	GLY
1	I	108	VAL

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Mol	Chain	Res	Type
1	W	24	VAL
1	Y	47	GLY
1	G	124	PRO
1	X	108	VAL
1	A	49	GLY
1	P	49	GLY
1	E	108	VAL
1	G	108	VAL

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	135/139 (97%)	117 (87%)	18 (13%)	4	3
1	B	133/139 (96%)	118 (89%)	15 (11%)	5	5
1	C	133/139 (96%)	116 (87%)	17 (13%)	4	3
1	D	133/139 (96%)	119 (90%)	14 (10%)	6	6
1	E	134/139 (96%)	123 (92%)	11 (8%)	10	12
1	F	133/139 (96%)	119 (90%)	14 (10%)	6	6
1	G	133/139 (96%)	113 (85%)	20 (15%)	3	2
1	H	134/139 (96%)	125 (93%)	9 (7%)	15	19
1	I	132/139 (95%)	116 (88%)	16 (12%)	5	4
1	J	133/139 (96%)	115 (86%)	18 (14%)	4	3
1	K	134/139 (96%)	119 (89%)	15 (11%)	6	5
1	L	134/139 (96%)	121 (90%)	13 (10%)	8	8
1	M	133/139 (96%)	118 (89%)	15 (11%)	5	5
1	N	135/139 (97%)	121 (90%)	14 (10%)	7	6
1	O	133/139 (96%)	120 (90%)	13 (10%)	7	7
1	P	134/139 (96%)	115 (86%)	19 (14%)	3	2
1	Q	133/139 (96%)	122 (92%)	11 (8%)	10	12

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	R	134/139 (96%)	121 (90%)	13 (10%)	8	8
1	S	133/139 (96%)	116 (87%)	17 (13%)	4	3
1	T	139/139 (100%)	118 (85%)	21 (15%)	3	2
1	U	134/139 (96%)	115 (86%)	19 (14%)	3	2
1	V	133/139 (96%)	111 (84%)	22 (16%)	2	1
1	W	133/139 (96%)	125 (94%)	8 (6%)	17	23
1	X	134/139 (96%)	119 (89%)	15 (11%)	6	5
1	Y	134/139 (96%)	116 (87%)	18 (13%)	4	3
1	Z	133/139 (96%)	119 (90%)	14 (10%)	6	6
1	a	135/139 (97%)	121 (90%)	14 (10%)	7	6
1	b	132/139 (95%)	118 (89%)	14 (11%)	6	6
All	All	3743/3892 (96%)	3316 (89%)	427 (11%)	5	5

All (427) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	6	ILE
1	A	7	VAL
1	A	9	GLU
1	A	21	LYS
1	A	48	ASP
1	A	66	THR
1	A	75	ILE
1	A	91	VAL
1	A	93	ARG
1	A	94	ASP
1	A	97	GLU
1	A	104	LYS
1	A	126	CYS
1	A	129	ASN
1	A	130	GLU
1	A	133	VAL
1	A	138	LYS
1	B	6	ILE
1	B	8	LYS
1	B	40	LYS
1	B	68	MET

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Mol	Chain	Res	Type
1	B	69	LEU
1	B	82	CYS
1	B	97	GLU
1	B	104	LYS
1	B	105	LEU
1	B	112	SER
1	B	115	LYS
1	B	119	THR
1	B	123	LYS
1	B	134	LYS
1	B	156	GLU
1	C	6	ILE
1	C	8	LYS
1	C	17	HIS
1	C	44	ILE
1	C	46	GLU
1	C	48	ASP
1	C	51	VAL
1	C	83	LYS
1	C	90	ASP
1	C	93	ARG
1	C	94	ASP
1	C	112	SER
1	C	116	ILE
1	C	129	ASN
1	C	137	GLU
1	C	138	LYS
1	C	139	LYS
1	D	1	MET
1	D	43	GLU
1	D	44	ILE
1	D	48	ASP
1	D	91	VAL
1	D	93	ARG
1	D	94	ASP
1	D	96	ILE
1	D	104	LYS
1	D	112	SER
1	D	131	GLU
1	D	132	GLU
1	D	138	LYS
1	D	144	TYR

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Mol	Chain	Res	Type
1	E	8	LYS
1	E	74	GLU
1	E	90	ASP
1	E	93	ARG
1	E	112	SER
1	E	115	LYS
1	E	124	PRO
1	E	132	GLU
1	E	138	LYS
1	E	139	LYS
1	E	156	GLU
1	F	1	MET
1	F	4	TYR
1	F	6	ILE
1	F	8	LYS
1	F	75	ILE
1	F	79	ASN
1	F	90	ASP
1	F	93	ARG
1	F	104	LYS
1	F	105	LEU
1	F	144	TYR
1	F	149	GLU
1	F	156	GLU
1	F	157	VAL
1	G	6	ILE
1	G	8	LYS
1	G	17	HIS
1	G	21	LYS
1	G	29	GLN
1	G	33	LYS
1	G	43	GLU
1	G	44	ILE
1	G	48	ASP
1	G	51	VAL
1	G	67	TYR
1	G	90	ASP
1	G	105	LEU
1	G	116	ILE
1	G	124	PRO
1	G	127	THR
1	G	129	ASN

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Mol	Chain	Res	Type
1	G	138	LYS
1	G	146	GLN
1	G	156	GLU
1	H	7	VAL
1	H	29	GLN
1	H	51	VAL
1	H	56	LYS
1	H	64	PRO
1	H	105	LEU
1	H	112	SER
1	H	130	GLU
1	H	135	ILE
1	I	6	ILE
1	I	9	GLU
1	I	10	GLU
1	I	43	GLU
1	I	48	ASP
1	I	51	VAL
1	I	64	PRO
1	I	71	LYS
1	I	74	GLU
1	I	83	LYS
1	I	91	VAL
1	I	112	SER
1	I	130	GLU
1	I	132	GLU
1	I	138	LYS
1	I	144	TYR
1	J	1	MET
1	J	6	ILE
1	J	19	LEU
1	J	21	LYS
1	J	51	VAL
1	J	71	LYS
1	J	90	ASP
1	J	93	ARG
1	J	95	ASN
1	J	102	GLU
1	J	105	LEU
1	J	115	LYS
1	J	117	THR
1	J	123	LYS

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Mol	Chain	Res	Type
1	J	131	GLU
1	J	133	VAL
1	J	144	TYR
1	J	156	GLU
1	K	6	ILE
1	K	14	ILE
1	K	17	HIS
1	K	26	GLU
1	K	40	LYS
1	K	46	GLU
1	K	74	GLU
1	K	79	ASN
1	K	90	ASP
1	K	93	ARG
1	K	105	LEU
1	K	123	LYS
1	K	124	PRO
1	K	129	ASN
1	K	139	LYS
1	L	4	TYR
1	L	8	LYS
1	L	19	LEU
1	L	29	GLN
1	L	40	LYS
1	L	48	ASP
1	L	61	ASP
1	L	64	PRO
1	L	94	ASP
1	L	108	VAL
1	L	126	CYS
1	L	130	GLU
1	L	144	TYR
1	M	1	MET
1	M	6	ILE
1	M	8	LYS
1	M	10	GLU
1	M	43	GLU
1	M	46	GLU
1	M	53	THR
1	M	56	LYS
1	M	90	ASP
1	M	95	ASN

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Mol	Chain	Res	Type
1	M	112	SER
1	M	117	THR
1	M	127	THR
1	M	131	GLU
1	M	135	ILE
1	N	1	MET
1	N	6	ILE
1	N	8	LYS
1	N	19	LEU
1	N	40	LYS
1	N	48	ASP
1	N	51	VAL
1	N	72	PHE
1	N	73	ASP
1	N	112	SER
1	N	127	THR
1	N	138	LYS
1	N	144	TYR
1	N	146	GLN
1	O	6	ILE
1	O	48	ASP
1	O	51	VAL
1	O	90	ASP
1	O	112	SER
1	O	113	LYS
1	O	117	THR
1	O	127	THR
1	O	130	GLU
1	O	132	GLU
1	O	137	GLU
1	O	138	LYS
1	O	144	TYR
1	P	6	ILE
1	P	7	VAL
1	P	29	GLN
1	P	30	VAL
1	P	40	LYS
1	P	43	GLU
1	P	44	ILE
1	P	45	ILE
1	P	48	ASP
1	P	51	VAL

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Mol	Chain	Res	Type
1	P	73	ASP
1	P	83	LYS
1	P	93	ARG
1	P	117	THR
1	P	127	THR
1	P	132	GLU
1	P	135	ILE
1	P	137	GLU
1	P	144	TYR
1	Q	4	TYR
1	Q	6	ILE
1	Q	21	LYS
1	Q	51	VAL
1	Q	58	THR
1	Q	68	MET
1	Q	83	LYS
1	Q	126	CYS
1	Q	129	ASN
1	Q	131	GLU
1	Q	142	GLU
1	R	6	ILE
1	R	9	GLU
1	R	19	LEU
1	R	21	LYS
1	R	60	VAL
1	R	95	ASN
1	R	96	ILE
1	R	106	GLU
1	R	113	LYS
1	R	115	LYS
1	R	130	GLU
1	R	137	GLU
1	R	138	LYS
1	S	1	MET
1	S	10	GLU
1	S	19	LEU
1	S	29	GLN
1	S	40	LYS
1	S	48	ASP
1	S	53	THR
1	S	87	PHE
1	S	98	LYS

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Mol	Chain	Res	Type
1	S	112	SER
1	S	115	LYS
1	S	118	VAL
1	S	126	CYS
1	S	127	THR
1	S	128	VAL
1	S	129	ASN
1	S	131	GLU
1	T	1	MET
1	T	6	ILE
1	T	21	LYS
1	T	28	HIS
1	T	46	GLU
1	T	48	ASP
1	T	51	VAL
1	T	56	LYS
1	T	71	LYS
1	T	73	ASP
1	T	90	ASP
1	T	93	ARG
1	T	95	ASN
1	T	96	ILE
1	T	112[A]	SER
1	T	112[B]	SER
1	T	126	CYS
1	T	127	THR
1	T	142	GLU
1	T	154	ASN
1	T	156	GLU
1	U	4	TYR
1	U	8	LYS
1	U	19	LEU
1	U	21	LYS
1	U	48	ASP
1	U	51	VAL
1	U	68	MET
1	U	90	ASP
1	U	91	VAL
1	U	94	ASP
1	U	112	SER
1	U	123	LYS
1	U	126	CYS

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Mol	Chain	Res	Type
1	U	127	THR
1	U	132	GLU
1	U	134	LYS
1	U	137	GLU
1	U	138	LYS
1	U	154	ASN
1	V	12	SER
1	V	24	VAL
1	V	25	LEU
1	V	26	GLU
1	V	43	GLU
1	V	44	ILE
1	V	53	THR
1	V	55	THR
1	V	75	ILE
1	V	83	LYS
1	V	91	VAL
1	V	92	LEU
1	V	93	ARG
1	V	94	ASP
1	V	96	ILE
1	V	108	VAL
1	V	117	THR
1	V	121	HIS
1	V	123	LYS
1	V	126	CYS
1	V	131	GLU
1	V	144	TYR
1	W	1	MET
1	W	4	TYR
1	W	21	LYS
1	W	48	ASP
1	W	92	LEU
1	W	97	GLU
1	W	132	GLU
1	W	144	TYR
1	X	8	LYS
1	X	11	GLU
1	X	21	LYS
1	X	48	ASP
1	X	51	VAL
1	X	71	LYS

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Mol	Chain	Res	Type
1	X	73	ASP
1	X	83	LYS
1	X	90	ASP
1	X	126	CYS
1	X	129	ASN
1	X	130	GLU
1	X	131	GLU
1	X	135	ILE
1	X	144	TYR
1	Y	5	THR
1	Y	6	ILE
1	Y	21	LYS
1	Y	29	GLN
1	Y	33	LYS
1	Y	40	LYS
1	Y	48	ASP
1	Y	51	VAL
1	Y	90	ASP
1	Y	94	ASP
1	Y	98	LYS
1	Y	115	LYS
1	Y	127	THR
1	Y	129	ASN
1	Y	130	GLU
1	Y	131	GLU
1	Y	138	LYS
1	Y	144	TYR
1	Z	1	MET
1	Z	5	THR
1	Z	6	ILE
1	Z	8	LYS
1	Z	21	LYS
1	Z	43	GLU
1	Z	48	ASP
1	Z	51	VAL
1	Z	58	THR
1	Z	112	SER
1	Z	127	THR
1	Z	128	VAL
1	Z	138	LYS
1	Z	151	LEU
1	a	1	MET

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Mol	Chain	Res	Type
1	a	6	ILE
1	a	19	LEU
1	a	21	LYS
1	a	51	VAL
1	a	96	ILE
1	a	97	GLU
1	a	105	LEU
1	a	112	SER
1	a	113	LYS
1	a	123	LYS
1	a	124	PRO
1	a	129	ASN
1	a	144	TYR
1	b	1	MET
1	b	19	LEU
1	b	29	GLN
1	b	43	GLU
1	b	44	ILE
1	b	68	MET
1	b	93	ARG
1	b	105	LEU
1	b	106	GLU
1	b	112	SER
1	b	129	ASN
1	b	130	GLU
1	b	138	LYS
1	b	144	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (57) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	28	HIS
1	A	35	GLN
1	A	37	HIS
1	B	29	GLN
1	B	95	ASN
1	C	17	HIS
1	C	63	HIS
1	C	129	ASN
1	D	35	GLN
1	E	29	GLN
1	E	35	GLN

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Mol	Chain	Res	Type
1	F	79	ASN
1	G	29	GLN
1	G	129	ASN
1	G	154	ASN
1	H	70	HIS
1	I	29	GLN
1	J	95	ASN
1	J	121	HIS
1	J	129	ASN
1	K	79	ASN
1	K	129	ASN
1	L	28	HIS
1	L	35	GLN
1	L	70	HIS
1	L	79	ASN
1	L	129	ASN
1	N	129	ASN
1	N	154	ASN
1	P	28	HIS
1	Q	35	GLN
1	R	129	ASN
1	R	154	ASN
1	S	28	HIS
1	S	37	HIS
1	S	129	ASN
1	S	154	ASN
1	T	29	GLN
1	T	79	ASN
1	T	154	ASN
1	U	154	ASN
1	V	70	HIS
1	V	121	HIS
1	V	129	ASN
1	X	17	HIS
1	X	70	HIS
1	X	129	ASN
1	Y	28	HIS
1	Y	129	ASN
1	Z	35	GLN
1	Z	146	GLN
1	Z	154	ASN
1	a	28	HIS

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Mol	Chain	Res	Type
1	a	35	GLN
1	a	121	HIS
1	a	129	ASN
1	b	129	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

94 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	a	201	-	22,23,23	0.55	0	29,33,33	0.71	1 (3%)
2	2AN	B	203	-	22,23,23	0.61	0	29,33,33	0.78	0
2	2AN	R	204	-	22,23,23	0.80	0	29,33,33	0.80	1 (3%)
2	2AN	C	202	-	22,23,23	0.73	0	29,33,33	0.91	2 (6%)
2	2AN	J	201	-	22,23,23	0.81	0	29,33,33	0.72	1 (3%)
2	2AN	S	201	-	22,23,23	0.87	1 (4%)	29,33,33	0.77	0
2	2AN	G	203	-	22,23,23	0.74	0	29,33,33	0.75	0
2	2AN	D	202	-	22,23,23	0.64	0	29,33,33	0.87	1 (3%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	2AN	H	201	-	22,23,23	0.84	0	29,33,33	1.02	2 (6%)
2	2AN	X	202	-	22,23,23	0.56	0	29,33,33	1.00	2 (6%)
2	2AN	b	202	-	22,23,23	0.86	0	29,33,33	0.87	0
2	2AN	Y	202	-	22,23,23	0.74	0	29,33,33	0.85	1 (3%)
2	2AN	Q	203	-	22,23,23	0.67	0	29,33,33	0.77	0
2	2AN	Q	202	-	22,23,23	0.65	0	29,33,33	0.88	0
2	2AN	X	203	-	22,23,23	0.56	0	29,33,33	0.91	1 (3%)
2	2AN	X	201	-	22,23,23	0.71	0	29,33,33	0.76	1 (3%)
2	2AN	G	202	-	22,23,23	0.85	1 (4%)	29,33,33	0.94	1 (3%)
2	2AN	U	201	-	22,23,23	0.73	1 (4%)	29,33,33	0.79	0
2	2AN	I	203	-	22,23,23	0.60	0	29,33,33	0.91	1 (3%)
2	2AN	A	201	-	22,23,23	0.83	0	29,33,33	1.04	1 (3%)
2	2AN	B	201	-	22,23,23	0.63	0	29,33,33	0.75	0
2	2AN	D	201	-	22,23,23	0.71	0	29,33,33	0.68	0
2	2AN	N	202	-	22,23,23	0.79	0	29,33,33	0.83	1 (3%)
2	2AN	Q	201	-	22,23,23	0.68	0	29,33,33	0.87	1 (3%)
2	2AN	W	204	-	22,23,23	0.93	1 (4%)	29,33,33	1.05	2 (6%)
2	2AN	L	201	-	22,23,23	0.60	0	29,33,33	0.76	0
2	2AN	G	204	-	22,23,23	1.13	1 (4%)	29,33,33	1.12	2 (6%)
2	2AN	C	201	-	22,23,23	0.86	0	29,33,33	0.81	0
2	2AN	W	201	-	22,23,23	0.96	1 (4%)	29,33,33	1.07	3 (10%)
2	2AN	R	203	-	22,23,23	0.64	0	29,33,33	0.98	2 (6%)
2	2AN	V	201	-	22,23,23	0.72	0	29,33,33	0.89	1 (3%)
2	2AN	B	204	-	22,23,23	0.84	0	29,33,33	0.87	1 (3%)
4	SO4	X	204	-	4,4,4	0.60	0	6,6,6	0.66	0
2	2AN	B	202	-	22,23,23	0.61	0	29,33,33	0.93	2 (6%)
2	2AN	E	205	-	22,23,23	0.89	2 (9%)	29,33,33	0.97	1 (3%)
2	2AN	C	203	-	22,23,23	0.67	0	29,33,33	0.95	1 (3%)
2	2AN	P	202	-	22,23,23	0.70	0	29,33,33	1.06	3 (10%)
2	2AN	J	202	-	22,23,23	0.80	1 (4%)	29,33,33	0.98	2 (6%)
2	2AN	V	202	-	22,23,23	0.67	0	29,33,33	1.08	3 (10%)
2	2AN	L	202	-	22,23,23	0.86	0	29,33,33	0.86	1 (3%)
2	2AN	K	203	-	22,23,23	0.54	0	29,33,33	0.87	2 (6%)
2	2AN	B	205	-	22,23,23	0.61	0	29,33,33	0.89	1 (3%)
2	2AN	Y	201	-	22,23,23	0.94	2 (9%)	29,33,33	0.79	0
2	2AN	L	205	-	22,23,23	0.69	0	29,33,33	0.75	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	EPE	Z	204	-	15,15,15	2.25	1 (6%)	19,20,20	3.70	11 (57%)
2	2AN	K	202	-	22,23,23	0.55	0	29,33,33	0.88	1 (3%)
2	2AN	A	204	-	22,23,23	1.01	1 (4%)	29,33,33	0.97	1 (3%)
2	2AN	I	202	-	22,23,23	0.98	0	29,33,33	0.80	0
2	2AN	A	203	-	22,23,23	0.72	0	29,33,33	0.80	2 (6%)
2	2AN	W	203	-	22,23,23	0.90	0	29,33,33	0.84	1 (3%)
2	2AN	Z	203	-	22,23,23	0.49	0	29,33,33	0.96	2 (6%)
2	2AN	Z	202	-	22,23,23	0.85	0	29,33,33	1.05	3 (10%)
2	2AN	U	202	-	22,23,23	0.93	0	29,33,33	0.89	1 (3%)
2	2AN	E	204	-	22,23,23	0.85	1 (4%)	29,33,33	0.93	2 (6%)
2	2AN	M	202	-	22,23,23	0.85	1 (4%)	29,33,33	0.84	1 (3%)
2	2AN	I	201	-	22,23,23	0.69	0	29,33,33	0.94	2 (6%)
2	2AN	O	202	-	22,23,23	0.90	1 (4%)	29,33,33	0.81	0
2	2AN	b	203	-	22,23,23	0.70	0	29,33,33	0.89	2 (6%)
2	2AN	L	204	-	22,23,23	0.63	0	29,33,33	0.95	1 (3%)
2	2AN	E	203	-	22,23,23	0.82	1 (4%)	29,33,33	0.93	1 (3%)
2	2AN	M	203	-	22,23,23	0.54	0	29,33,33	0.85	1 (3%)
2	2AN	Y	204	-	22,23,23	0.60	0	29,33,33	0.79	0
2	2AN	W	202	-	22,23,23	0.73	1 (4%)	29,33,33	0.83	1 (3%)
2	2AN	L	203	-	22,23,23	0.86	1 (4%)	29,33,33	1.01	1 (3%)
2	2AN	A	202	-	22,23,23	0.86	0	29,33,33	0.80	0
2	2AN	G	205	-	22,23,23	0.57	0	29,33,33	0.87	1 (3%)
2	2AN	R	202	-	22,23,23	0.77	0	29,33,33	0.91	1 (3%)
2	2AN	I	204	-	22,23,23	0.77	0	29,33,33	1.34	4 (13%)
2	2AN	R	201	-	22,23,23	0.75	1 (4%)	29,33,33	1.00	2 (6%)
2	2AN	H	203	-	22,23,23	0.87	1 (4%)	29,33,33	1.03	1 (3%)
2	2AN	F	201	-	22,23,23	0.76	0	29,33,33	0.90	1 (3%)
2	2AN	U	204	-	22,23,23	0.77	0	29,33,33	0.76	0
4	SO4	V	203	-	4,4,4	0.53	0	6,6,6	1.19	0
2	2AN	Y	203	-	22,23,23	0.56	0	29,33,33	0.85	1 (3%)
2	2AN	M	201	-	22,23,23	0.89	1 (4%)	29,33,33	0.76	0
2	2AN	N	203	-	22,23,23	0.87	0	29,33,33	1.02	2 (6%)
2	2AN	I	205	-	22,23,23	0.60	0	29,33,33	0.90	2 (6%)
2	2AN	P	201	-	22,23,23	0.76	0	29,33,33	0.78	1 (3%)
2	2AN	N	201	-	22,23,23	0.77	0	29,33,33	0.91	1 (3%)
2	2AN	U	203	-	22,23,23	0.80	0	29,33,33	0.91	2 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	2AN	C	204	-	22,23,23	0.91	1 (4%)	29,33,33	0.84	1 (3%)
2	2AN	G	201	-	22,23,23	1.31	3 (13%)	29,33,33	1.03	2 (6%)
2	2AN	Z	201	-	22,23,23	0.75	0	29,33,33	0.84	1 (3%)
2	2AN	E	202	-	22,23,23	0.61	0	29,33,33	1.06	3 (10%)
2	2AN	D	203	-	22,23,23	0.63	0	29,33,33	0.84	1 (3%)
2	2AN	N	204	-	22,23,23	1.16	2 (9%)	29,33,33	1.01	2 (6%)
2	2AN	K	201	-	22,23,23	0.88	0	29,33,33	0.86	0
2	2AN	U	205	-	22,23,23	0.58	0	29,33,33	0.70	0
2	2AN	O	201	-	22,23,23	0.89	1 (4%)	29,33,33	0.86	1 (3%)
3	EPE	C	205	-	15,15,15	1.89	2 (13%)	19,20,20	3.42	12 (63%)
2	2AN	b	201	-	22,23,23	0.62	0	29,33,33	1.07	2 (6%)
2	2AN	E	201	-	22,23,23	1.22	2 (9%)	29,33,33	1.14	3 (10%)
2	2AN	H	202	-	22,23,23	0.70	0	29,33,33	0.70	0
4	SO4	b	204	-	4,4,4	0.44	0	6,6,6	1.21	0

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	a	201	-	-	0/10/10/10	0/3/3/3
2	2AN	B	203	-	-	0/10/10/10	0/3/3/3
2	2AN	R	204	-	-	2/10/10/10	0/3/3/3
2	2AN	C	202	-	-	0/10/10/10	0/3/3/3
2	2AN	J	201	-	-	0/10/10/10	0/3/3/3
2	2AN	S	201	-	-	0/10/10/10	0/3/3/3
2	2AN	G	203	-	-	1/10/10/10	0/3/3/3
2	2AN	D	202	-	-	0/10/10/10	0/3/3/3
2	2AN	H	201	-	-	0/10/10/10	0/3/3/3
2	2AN	X	202	-	-	1/10/10/10	0/3/3/3
2	2AN	b	202	-	-	0/10/10/10	0/3/3/3
2	2AN	Y	202	-	-	0/10/10/10	0/3/3/3
2	2AN	Q	203	-	-	0/10/10/10	0/3/3/3
2	2AN	Q	202	-	-	2/10/10/10	0/3/3/3
2	2AN	X	203	-	-	0/10/10/10	0/3/3/3
2	2AN	X	201	-	-	1/10/10/10	0/3/3/3
2	2AN	G	202	-	-	0/10/10/10	0/3/3/3
2	2AN	U	201	-	-	0/10/10/10	0/3/3/3
2	2AN	I	203	-	-	0/10/10/10	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	2AN	A	201	-	-	0/10/10/10	0/3/3/3
2	2AN	B	201	-	-	0/10/10/10	0/3/3/3
2	2AN	D	201	-	-	0/10/10/10	0/3/3/3
2	2AN	N	202	-	-	0/10/10/10	0/3/3/3
2	2AN	Q	201	-	-	0/10/10/10	0/3/3/3
2	2AN	W	204	-	-	1/10/10/10	0/3/3/3
2	2AN	L	201	-	-	0/10/10/10	0/3/3/3
2	2AN	G	204	-	-	1/10/10/10	0/3/3/3
2	2AN	C	201	-	-	0/10/10/10	0/3/3/3
2	2AN	W	201	-	-	1/10/10/10	0/3/3/3
2	2AN	R	203	-	-	0/10/10/10	0/3/3/3
2	2AN	V	201	-	-	2/10/10/10	0/3/3/3
2	2AN	B	204	-	-	0/10/10/10	0/3/3/3
2	2AN	B	202	-	-	0/10/10/10	0/3/3/3
2	2AN	E	205	-	-	0/10/10/10	0/3/3/3
2	2AN	C	203	-	-	2/10/10/10	0/3/3/3
2	2AN	P	202	-	-	1/10/10/10	0/3/3/3
2	2AN	J	202	-	-	0/10/10/10	0/3/3/3
2	2AN	V	202	-	-	2/10/10/10	0/3/3/3
2	2AN	L	202	-	-	0/10/10/10	0/3/3/3
2	2AN	K	203	-	-	0/10/10/10	0/3/3/3
2	2AN	B	205	-	-	0/10/10/10	0/3/3/3
2	2AN	Y	201	-	-	0/10/10/10	0/3/3/3
2	2AN	L	205	-	-	0/10/10/10	0/3/3/3
3	EPE	Z	204	-	-	6/9/19/19	0/1/1/1
2	2AN	K	202	-	-	0/10/10/10	0/3/3/3
2	2AN	A	204	-	-	0/10/10/10	0/3/3/3
2	2AN	I	202	-	-	2/10/10/10	0/3/3/3
2	2AN	A	203	-	-	0/10/10/10	0/3/3/3
2	2AN	W	203	-	-	2/10/10/10	0/3/3/3
2	2AN	Z	203	-	-	0/10/10/10	0/3/3/3
2	2AN	Z	202	-	-	0/10/10/10	0/3/3/3
2	2AN	U	202	-	-	1/10/10/10	0/3/3/3
2	2AN	E	204	-	-	0/10/10/10	0/3/3/3
2	2AN	M	202	-	-	1/10/10/10	0/3/3/3
2	2AN	I	201	-	-	1/10/10/10	0/3/3/3
2	2AN	O	202	-	-	0/10/10/10	0/3/3/3
2	2AN	b	203	-	-	0/10/10/10	0/3/3/3
2	2AN	L	204	-	-	0/10/10/10	0/3/3/3
2	2AN	E	203	-	-	0/10/10/10	0/3/3/3
2	2AN	M	203	-	-	0/10/10/10	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	2AN	Y	204	-	-	0/10/10/10	0/3/3/3
2	2AN	W	202	-	-	0/10/10/10	0/3/3/3
2	2AN	L	203	-	-	0/10/10/10	0/3/3/3
2	2AN	A	202	-	-	0/10/10/10	0/3/3/3
2	2AN	G	205	-	-	0/10/10/10	0/3/3/3
2	2AN	R	202	-	-	0/10/10/10	0/3/3/3
2	2AN	I	204	-	-	0/10/10/10	0/3/3/3
2	2AN	R	201	-	-	1/10/10/10	0/3/3/3
2	2AN	H	203	-	-	0/10/10/10	0/3/3/3
2	2AN	F	201	-	-	0/10/10/10	0/3/3/3
2	2AN	U	204	-	-	0/10/10/10	0/3/3/3
2	2AN	Y	203	-	-	0/10/10/10	0/3/3/3
2	2AN	M	201	-	-	1/10/10/10	0/3/3/3
2	2AN	N	203	-	-	1/10/10/10	0/3/3/3
2	2AN	I	205	-	-	0/10/10/10	0/3/3/3
2	2AN	P	201	-	-	0/10/10/10	0/3/3/3
2	2AN	N	201	-	-	0/10/10/10	0/3/3/3
2	2AN	U	203	-	-	0/10/10/10	0/3/3/3
2	2AN	C	204	-	-	1/10/10/10	0/3/3/3
2	2AN	G	201	-	-	0/10/10/10	0/3/3/3
2	2AN	Z	201	-	-	0/10/10/10	0/3/3/3
2	2AN	E	202	-	-	0/10/10/10	0/3/3/3
2	2AN	D	203	-	-	0/10/10/10	0/3/3/3
2	2AN	N	204	-	-	0/10/10/10	0/3/3/3
2	2AN	K	201	-	-	1/10/10/10	0/3/3/3
2	2AN	U	205	-	-	2/10/10/10	0/3/3/3
2	2AN	O	201	-	-	0/10/10/10	0/3/3/3
3	EPE	C	205	-	-	3/9/19/19	0/1/1/1
2	2AN	b	201	-	-	0/10/10/10	0/3/3/3
2	2AN	E	201	-	-	1/10/10/10	0/3/3/3
2	2AN	H	202	-	-	0/10/10/10	0/3/3/3

All (33) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	Z	204	EPE	C10-S	-8.06	1.66	1.77
3	C	205	EPE	C10-S	-6.09	1.69	1.77
2	G	204	2AN	C13-C12	-3.89	1.32	1.38
2	N	204	2AN	C16-C11	-3.23	1.33	1.39
2	W	201	2AN	C7-C8	2.81	1.43	1.38
2	O	201	2AN	C16-C11	-2.71	1.34	1.39
2	G	201	2AN	C3-C4	-2.66	1.31	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	201	2AN	C16-C11	-2.57	1.34	1.39
2	M	201	2AN	C16-C11	-2.57	1.34	1.39
2	E	203	2AN	C3-C4	-2.55	1.31	1.36
2	Y	201	2AN	C7-C6	-2.48	1.31	1.36
2	W	204	2AN	C15-C16	-2.43	1.34	1.38
2	R	201	2AN	C7-C8	2.40	1.43	1.38
2	O	202	2AN	C1-C10	2.39	1.46	1.43
2	U	201	2AN	C16-C11	-2.35	1.35	1.39
2	A	204	2AN	C7-C8	2.35	1.42	1.38
2	H	203	2AN	C12-C11	-2.34	1.35	1.39
2	M	202	2AN	C1-C10	2.34	1.46	1.43
2	G	201	2AN	C9-C10	2.29	1.48	1.44
2	G	201	2AN	C13-C12	-2.29	1.35	1.38
2	E	201	2AN	C8-C9	-2.26	1.34	1.37
2	G	202	2AN	C7-C6	-2.23	1.32	1.36
2	C	204	2AN	C13-C12	-2.22	1.35	1.38
2	S	201	2AN	C12-C11	-2.20	1.35	1.39
2	Y	201	2AN	C16-C11	-2.20	1.35	1.39
2	J	202	2AN	C7-C6	-2.17	1.32	1.36
2	E	204	2AN	C12-C11	-2.13	1.35	1.39
2	E	205	2AN	C13-C12	-2.12	1.35	1.38
2	L	203	2AN	C1-C10	2.10	1.45	1.43
3	C	205	EPE	C3-N4	-2.06	1.41	1.46
2	W	202	2AN	C16-C11	-2.06	1.35	1.39
2	N	204	2AN	C12-C11	-2.04	1.35	1.39
2	E	205	2AN	C7-C8	2.00	1.42	1.38

All (126) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	Z	204	EPE	O3S-S-C10	7.99	121.63	106.00
3	C	205	EPE	C7-N4-C3	7.11	130.19	111.24
3	Z	204	EPE	C6-N1-C2	7.08	124.09	108.84
3	Z	204	EPE	O2S-S-C10	-5.96	97.72	106.73
3	C	205	EPE	C2-C3-N4	-4.68	101.22	110.65
3	C	205	EPE	O1S-S-C10	4.62	113.71	106.73
3	C	205	EPE	C9-N1-C6	4.39	122.92	111.24
2	I	204	2AN	C2-C1-C10	-4.15	116.37	120.21
3	C	205	EPE	C5-C6-N1	4.14	119.00	110.65
3	C	205	EPE	O3S-S-O2S	4.13	121.73	111.40
3	Z	204	EPE	C7-N4-C5	4.13	122.24	111.24
3	Z	204	EPE	C9-N1-C6	3.98	121.84	111.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	205	EPE	O2S-S-O1S	-3.86	101.28	113.82
3	Z	204	EPE	C7-N4-C3	3.80	121.36	111.24
3	Z	204	EPE	O3S-S-O2S	-3.76	101.99	111.40
3	C	205	EPE	C9-N1-C2	3.57	120.75	111.24
3	C	205	EPE	O3S-S-O1S	-3.47	102.71	111.40
3	Z	204	EPE	O2S-S-O1S	3.46	125.09	113.82
3	Z	204	EPE	C5-N4-C3	3.44	116.26	108.84
3	C	205	EPE	C6-N1-C2	3.42	116.21	108.84
2	H	203	2AN	C11-N-C1	-3.17	119.45	126.36
2	F	201	2AN	C11-N-C1	-3.16	119.47	126.36
2	G	202	2AN	C11-N-C1	-3.14	119.51	126.36
3	C	205	EPE	C7-N4-C5	3.09	119.47	111.24
2	L	203	2AN	C11-N-C1	-3.07	119.66	126.36
3	Z	204	EPE	C2-C3-N4	3.07	116.84	110.65
2	Z	202	2AN	C11-N-C1	-2.99	119.83	126.36
2	A	201	2AN	C11-N-C1	-2.98	119.86	126.36
2	C	203	2AN	C10-C1-N	-2.97	116.06	120.39
2	E	201	2AN	C7-C8-C9	2.93	123.63	120.37
2	G	204	2AN	C11-N-C1	-2.90	120.03	126.36
2	I	203	2AN	C11-N-C1	-2.89	120.05	126.36
2	D	202	2AN	C11-N-C1	-2.89	120.07	126.36
2	I	201	2AN	C11-N-C1	-2.83	120.20	126.36
2	D	203	2AN	C11-N-C1	-2.83	120.20	126.36
2	Z	203	2AN	C2-C1-C10	-2.81	117.61	120.21
2	H	201	2AN	C11-N-C1	-2.78	120.31	126.36
2	b	201	2AN	C11-N-C1	-2.75	120.36	126.36
2	N	204	2AN	C11-N-C1	-2.73	120.40	126.36
2	R	203	2AN	C11-N-C1	-2.73	120.41	126.36
2	Z	203	2AN	C11-N-C1	-2.72	120.44	126.36
2	J	202	2AN	C11-N-C1	-2.70	120.47	126.36
3	Z	204	EPE	C6-C5-N4	-2.70	105.21	110.65
2	E	202	2AN	C15-C16-C11	2.68	122.81	119.73
2	H	201	2AN	C2-C1-C10	-2.67	117.74	120.21
2	E	205	2AN	C11-N-C1	-2.66	120.55	126.36
2	G	205	2AN	C11-N-C1	-2.65	120.57	126.36
2	R	203	2AN	C16-C11-C12	2.61	122.51	119.04
2	I	204	2AN	C11-N-C1	-2.53	120.84	126.36
2	E	203	2AN	C11-N-C1	-2.50	120.91	126.36
2	L	202	2AN	C11-N-C1	-2.49	120.94	126.36
2	X	202	2AN	C11-N-C1	-2.47	120.97	126.36
2	V	202	2AN	C2-C1-C10	-2.46	117.93	120.21
2	N	204	2AN	C2-C1-C10	-2.45	117.94	120.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	I	204	2AN	C15-C16-C11	2.44	122.54	119.73
2	Y	202	2AN	C11-N-C1	-2.44	121.04	126.36
3	C	205	EPE	C8-C7-N4	2.44	121.99	113.44
2	K	202	2AN	C11-N-C1	-2.43	121.06	126.36
2	U	203	2AN	C11-N-C1	-2.42	121.08	126.36
2	M	203	2AN	C11-N-C1	-2.42	121.08	126.36
2	A	204	2AN	C11-N-C1	-2.40	121.12	126.36
2	K	203	2AN	C11-N-C1	-2.40	121.12	126.36
2	X	203	2AN	C2-C1-C10	-2.40	117.99	120.21
2	R	201	2AN	C11-N-C1	-2.39	121.14	126.36
2	C	202	2AN	C2-C1-C10	-2.39	118.00	120.21
2	I	205	2AN	C2-C1-C10	-2.38	118.01	120.21
2	M	202	2AN	C11-N-C1	-2.36	121.21	126.36
2	W	201	2AN	C13-C12-C11	2.36	122.45	119.73
2	b	203	2AN	C2-C1-C10	-2.35	118.03	120.21
2	B	205	2AN	C11-N-C1	-2.34	121.26	126.36
2	C	202	2AN	C11-N-C1	-2.34	121.27	126.36
2	Z	202	2AN	C13-C12-C11	2.32	122.40	119.73
2	P	202	2AN	C13-C12-C11	2.31	122.39	119.73
2	Z	201	2AN	C11-N-C1	-2.31	121.32	126.36
2	G	204	2AN	C15-C16-C11	2.31	122.39	119.73
2	P	202	2AN	C11-N-C1	-2.30	121.35	126.36
2	E	201	2AN	C8-C9-C10	-2.29	116.69	120.18
2	P	202	2AN	C2-C1-C10	-2.28	118.10	120.21
2	U	202	2AN	C2-C1-C10	-2.25	118.12	120.21
2	G	201	2AN	C11-N-C1	-2.25	121.45	126.36
2	L	204	2AN	C11-N-C1	-2.25	121.45	126.36
2	a	201	2AN	C11-N-C1	-2.25	121.45	126.36
2	V	202	2AN	C10-C1-N	-2.23	117.14	120.39
2	E	202	2AN	C11-N-C1	-2.22	121.51	126.36
2	W	201	2AN	C2-C1-C10	-2.22	118.15	120.21
2	J	201	2AN	C11-N-C1	-2.22	121.53	126.36
2	X	201	2AN	C11-N-C1	-2.20	121.55	126.36
2	J	202	2AN	C13-C12-C11	2.20	122.27	119.73
2	Z	202	2AN	C2-C1-C10	-2.20	118.17	120.21
2	B	202	2AN	C11-N-C1	-2.20	121.57	126.36
2	C	204	2AN	C11-N-C1	-2.20	121.57	126.36
2	X	202	2AN	C15-C16-C11	2.19	122.26	119.73
2	b	203	2AN	C11-N-C1	-2.19	121.58	126.36
2	W	203	2AN	C11-N-C1	-2.19	121.59	126.36
2	B	202	2AN	C15-C16-C11	2.18	122.25	119.73
2	N	203	2AN	C11-N-C1	-2.18	121.60	126.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	I	201	2AN	C15-C16-C11	2.18	122.24	119.73
2	W	204	2AN	C11-N-C1	-2.17	121.62	126.36
2	N	201	2AN	C11-N-C1	-2.16	121.66	126.36
2	W	201	2AN	C11-N-C1	-2.15	121.67	126.36
2	O	201	2AN	C11-N-C1	-2.13	121.72	126.36
2	P	201	2AN	C11-N-C1	-2.13	121.72	126.36
2	R	202	2AN	C2-C1-C10	-2.13	118.24	120.21
2	R	201	2AN	C15-C16-C11	2.12	122.17	119.73
2	A	203	2AN	C11-N-C1	-2.11	121.75	126.36
2	E	202	2AN	C14-C15-C16	-2.11	117.64	120.24
2	E	204	2AN	C11-N-C1	-2.10	121.77	126.36
2	R	204	2AN	C11-N-C1	-2.09	121.81	126.36
2	V	202	2AN	C11-N-C1	-2.08	121.82	126.36
2	W	204	2AN	C15-C16-C11	2.07	122.12	119.73
2	K	203	2AN	C2-C1-C10	-2.07	118.30	120.21
2	E	204	2AN	C15-C16-C11	2.07	122.11	119.73
2	G	201	2AN	C13-C12-C11	2.06	122.10	119.73
2	A	203	2AN	C15-C16-C11	2.06	122.10	119.73
2	W	202	2AN	C11-N-C1	-2.06	121.88	126.36
2	E	201	2AN	C11-N-C1	-2.05	121.88	126.36
2	B	204	2AN	C2-C1-C10	-2.05	118.31	120.21
2	Y	203	2AN	C11-N-C1	-2.04	121.90	126.36
2	N	203	2AN	C13-C12-C11	2.03	122.07	119.73
2	U	203	2AN	C4-C3-C2	2.02	124.10	121.00
2	Q	201	2AN	C11-N-C1	-2.02	121.95	126.36
2	b	201	2AN	C13-C12-C11	2.02	122.06	119.73
2	I	205	2AN	C11-N-C1	-2.01	121.97	126.36
2	N	202	2AN	C11-N-C1	-2.01	121.97	126.36
2	I	204	2AN	C3-C2-C1	2.00	123.22	120.05
2	V	201	2AN	C13-C12-C11	2.00	122.04	119.73

There are no chirality outliers.

All (41) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	205	EPE	C8-C7-N4-C3
3	Z	204	EPE	C10-C9-N1-C6
3	Z	204	EPE	N4-C7-C8-O8
3	Z	204	EPE	C9-C10-S-O3S
2	R	204	2AN	C16-C11-N-C1
2	C	203	2AN	C16-C11-N-C1
2	V	202	2AN	C16-C11-N-C1

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Mol	Chain	Res	Type	Atoms
2	U	205	2AN	C12-C11-N-C1
2	V	201	2AN	C16-C11-N-C1
3	C	205	EPE	C10-C9-N1-C2
2	C	203	2AN	C12-C11-N-C1
2	R	204	2AN	C12-C11-N-C1
2	U	205	2AN	C16-C11-N-C1
2	V	202	2AN	C12-C11-N-C1
3	Z	204	EPE	C9-C10-S-O1S
3	Z	204	EPE	C9-C10-S-O2S
3	C	205	EPE	S-C10-C9-N1
3	Z	204	EPE	S-C10-C9-N1
2	M	202	2AN	C12-C11-N-C1
2	V	201	2AN	C12-C11-N-C1
2	I	202	2AN	C2-C1-N-C11
2	I	201	2AN	C12-C11-N-C1
2	P	202	2AN	C12-C11-N-C1
2	W	201	2AN	C12-C11-N-C1
2	W	203	2AN	C2-C1-N-C11
2	I	202	2AN	C10-C1-N-C11
2	Q	202	2AN	C10-C1-N-C11
2	W	203	2AN	C10-C1-N-C11
2	W	204	2AN	C16-C11-N-C1
2	R	201	2AN	C12-C11-N-C1
2	X	202	2AN	C12-C11-N-C1
2	Q	202	2AN	C2-C1-N-C11
2	C	204	2AN	C10-C1-N-C11
2	E	201	2AN	C10-C1-N-C11
2	G	203	2AN	C10-C1-N-C11
2	G	204	2AN	C10-C1-N-C11
2	K	201	2AN	C10-C1-N-C11
2	M	201	2AN	C10-C1-N-C11
2	N	203	2AN	C10-C1-N-C11
2	U	202	2AN	C10-C1-N-C11
2	X	201	2AN	C10-C1-N-C11

There are no ring outliers.

88 monomers are involved in 603 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	a	201	2AN	7	0
2	B	203	2AN	7	0
2	R	204	2AN	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	202	2AN	8	0
2	J	201	2AN	6	0
2	S	201	2AN	7	0
2	G	203	2AN	2	0
2	D	202	2AN	9	0
2	H	201	2AN	7	0
2	X	202	2AN	5	0
2	b	202	2AN	5	0
2	Y	202	2AN	7	0
2	Q	203	2AN	7	0
2	Q	202	2AN	5	0
2	X	203	2AN	5	0
2	X	201	2AN	4	0
2	G	202	2AN	11	0
2	U	201	2AN	10	0
2	I	203	2AN	12	0
2	A	201	2AN	13	0
2	B	201	2AN	2	0
2	D	201	2AN	6	0
2	N	202	2AN	7	0
2	Q	201	2AN	9	0
2	W	204	2AN	8	0
2	L	201	2AN	3	0
2	G	204	2AN	12	0
2	C	201	2AN	4	0
2	W	201	2AN	8	0
2	V	201	2AN	6	0
2	B	204	2AN	6	0
2	B	202	2AN	9	0
2	E	205	2AN	9	0
2	C	203	2AN	7	0
2	P	202	2AN	4	0
2	J	202	2AN	7	0
2	V	202	2AN	5	0
2	L	202	2AN	8	0
2	K	203	2AN	18	0
2	B	205	2AN	6	0
2	Y	201	2AN	4	0
2	L	205	2AN	5	0
2	K	202	2AN	8	0
2	A	204	2AN	7	0
2	I	202	2AN	6	0

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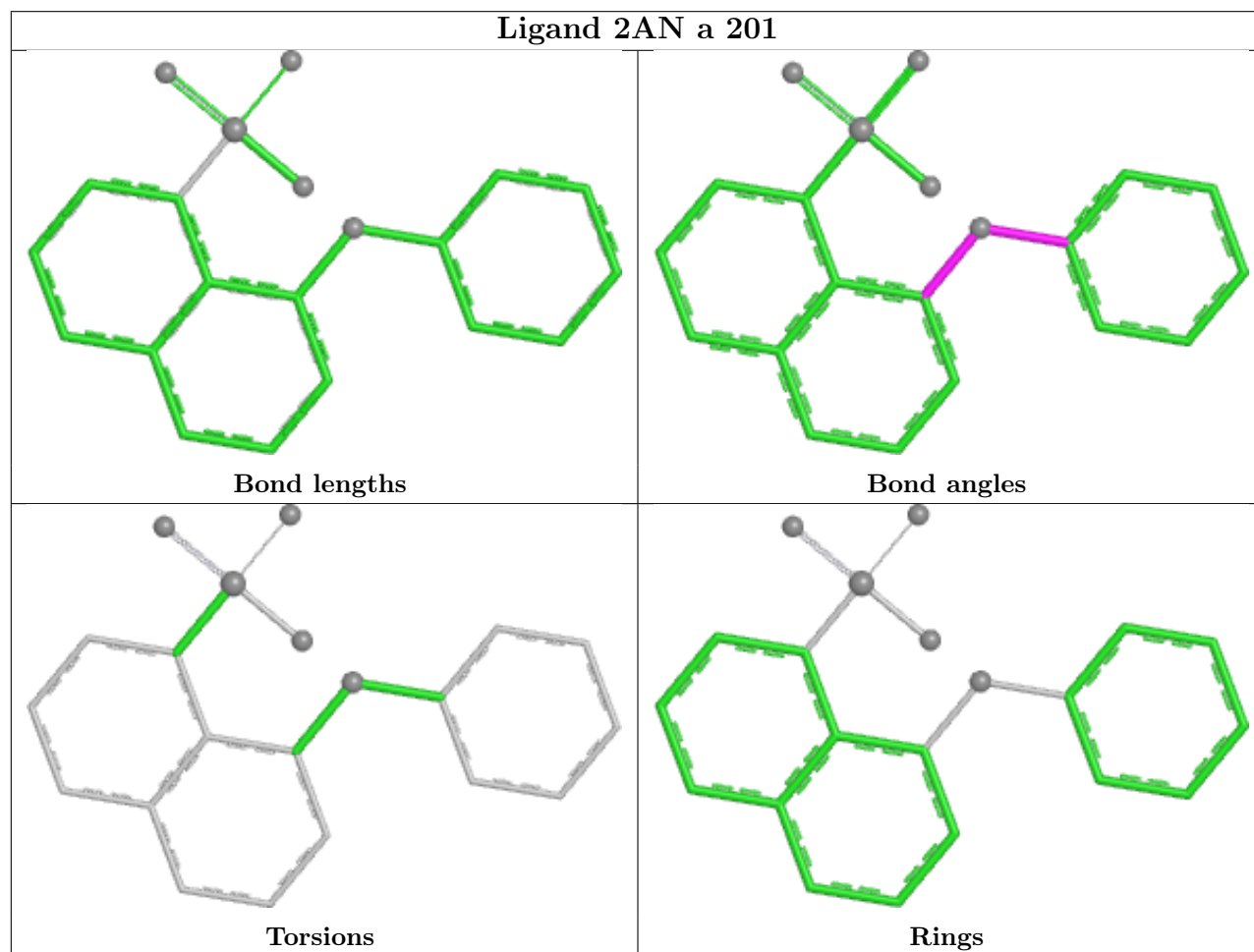
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	203	2AN	7	0
2	W	203	2AN	6	0
2	Z	203	2AN	8	0
2	Z	202	2AN	5	0
2	U	202	2AN	2	0
2	E	204	2AN	7	0
2	M	202	2AN	7	0
2	I	201	2AN	8	0
2	O	202	2AN	4	0
2	b	203	2AN	5	0
2	L	204	2AN	10	0
2	E	203	2AN	14	0
2	M	203	2AN	11	0
2	Y	204	2AN	7	0
2	W	202	2AN	12	0
2	L	203	2AN	5	0
2	A	202	2AN	3	0
2	G	205	2AN	7	0
2	R	202	2AN	4	0
2	I	204	2AN	6	0
2	R	201	2AN	13	0
2	H	203	2AN	6	0
2	F	201	2AN	8	0
2	U	204	2AN	4	0
2	Y	203	2AN	6	0
2	M	201	2AN	6	0
2	N	203	2AN	16	0
2	I	205	2AN	7	0
2	P	201	2AN	6	0
2	N	201	2AN	4	0
2	U	203	2AN	7	0
2	C	204	2AN	9	0
2	G	201	2AN	5	0
2	Z	201	2AN	5	0
2	E	202	2AN	11	0
2	D	203	2AN	7	0
2	N	204	2AN	5	0
2	K	201	2AN	4	0
2	U	205	2AN	3	0
2	O	201	2AN	6	0
2	b	201	2AN	8	0
2	E	201	2AN	6	0

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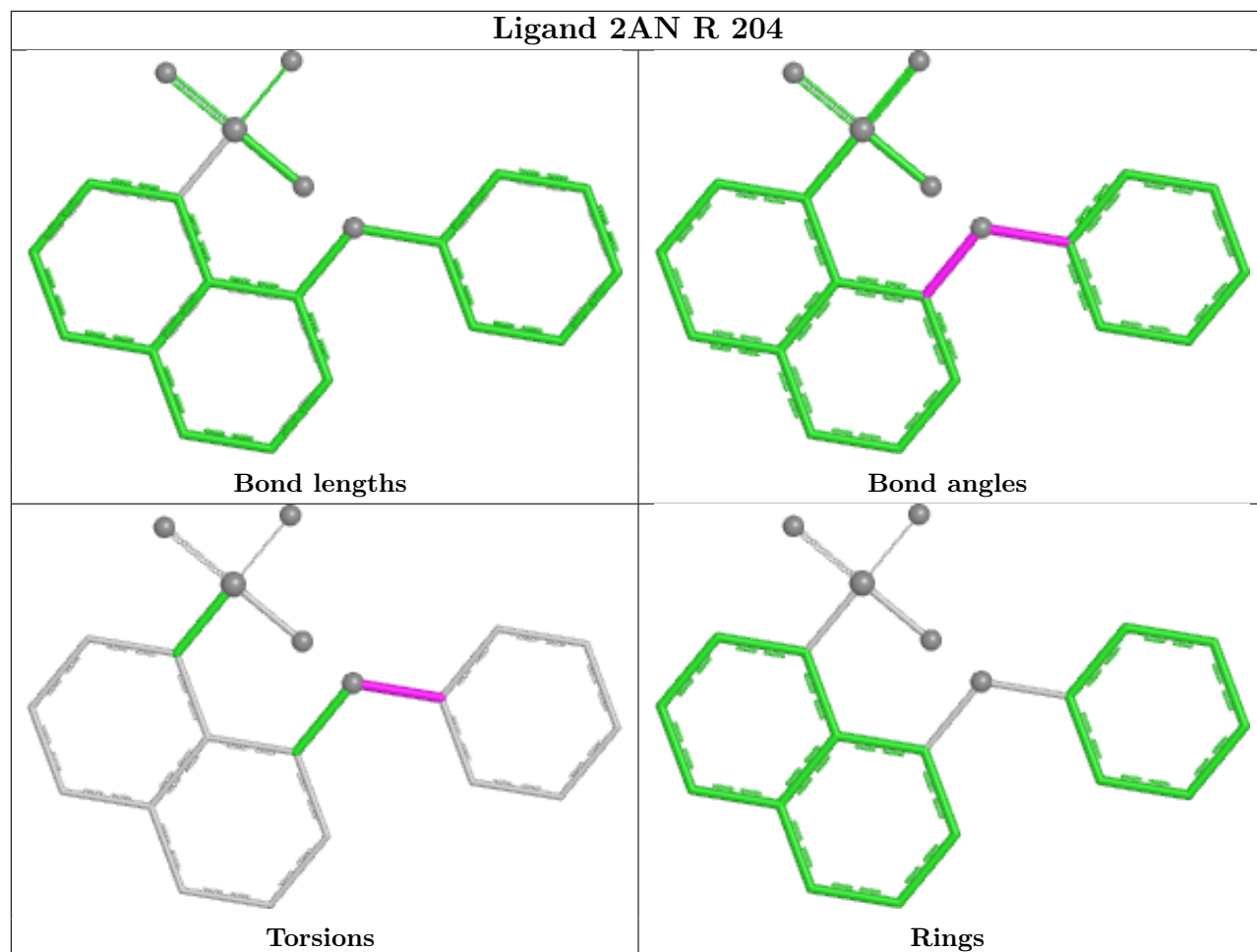
Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	H	202	2AN	5	0

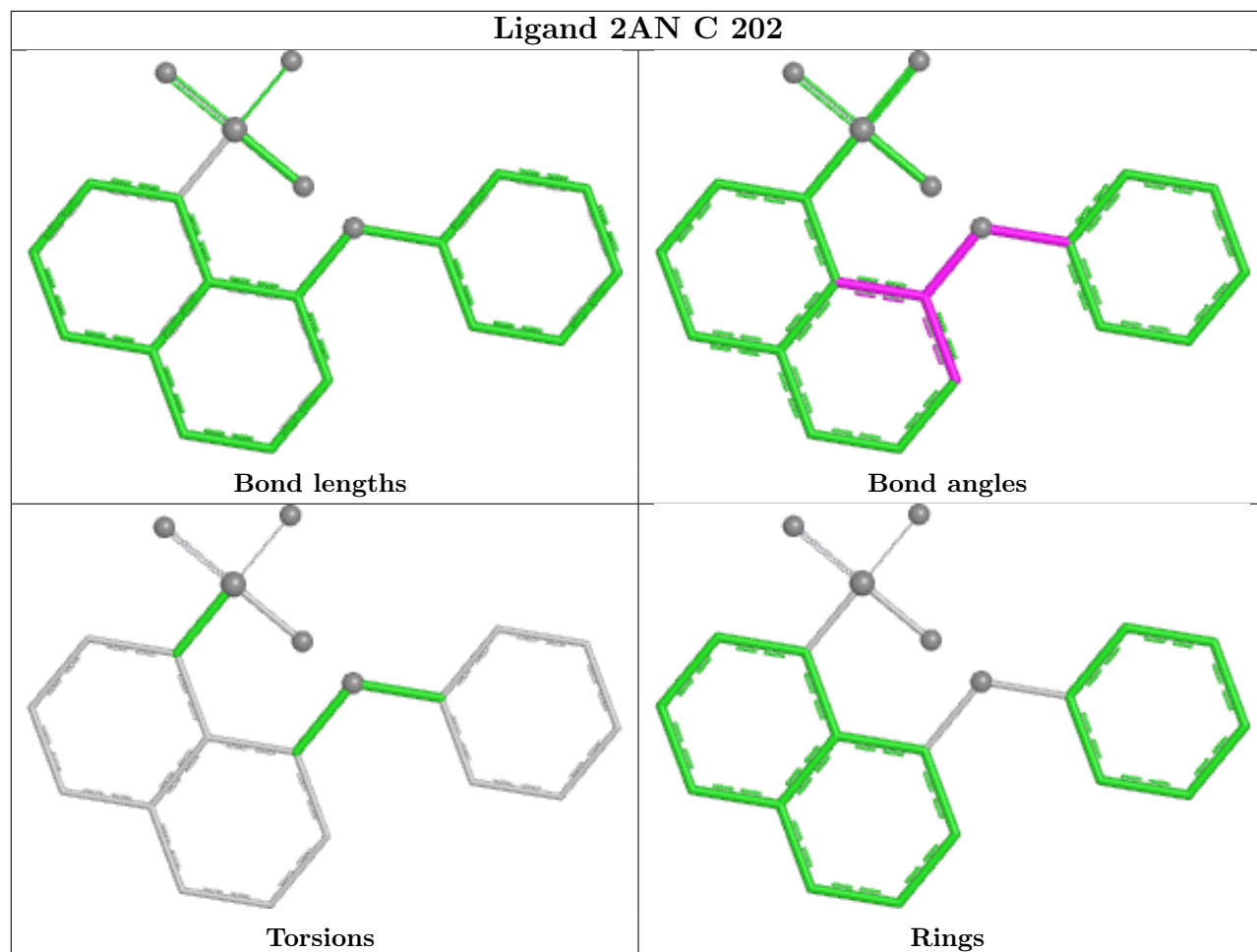
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



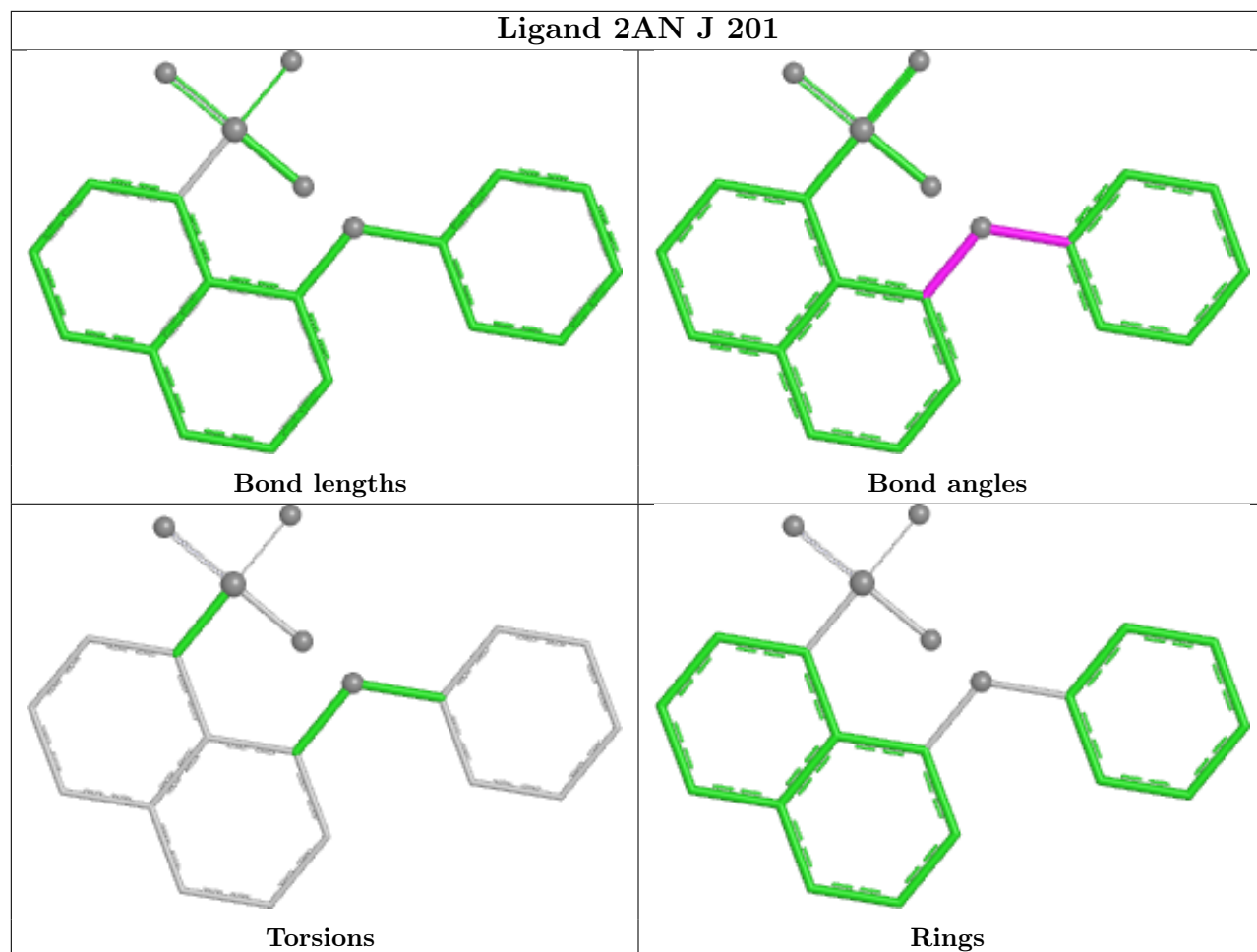
Ligand 2AN R 204



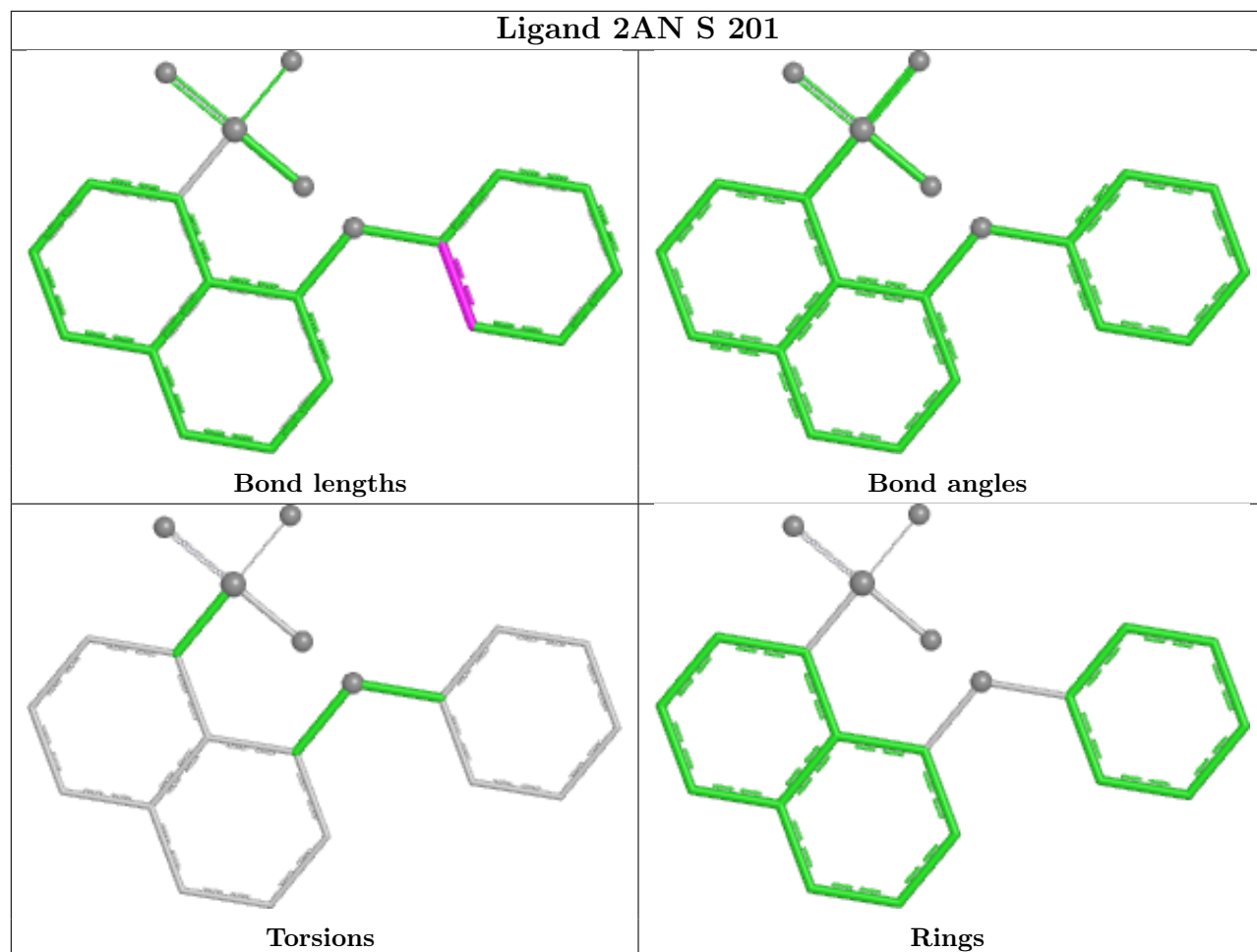
Ligand 2AN C 202



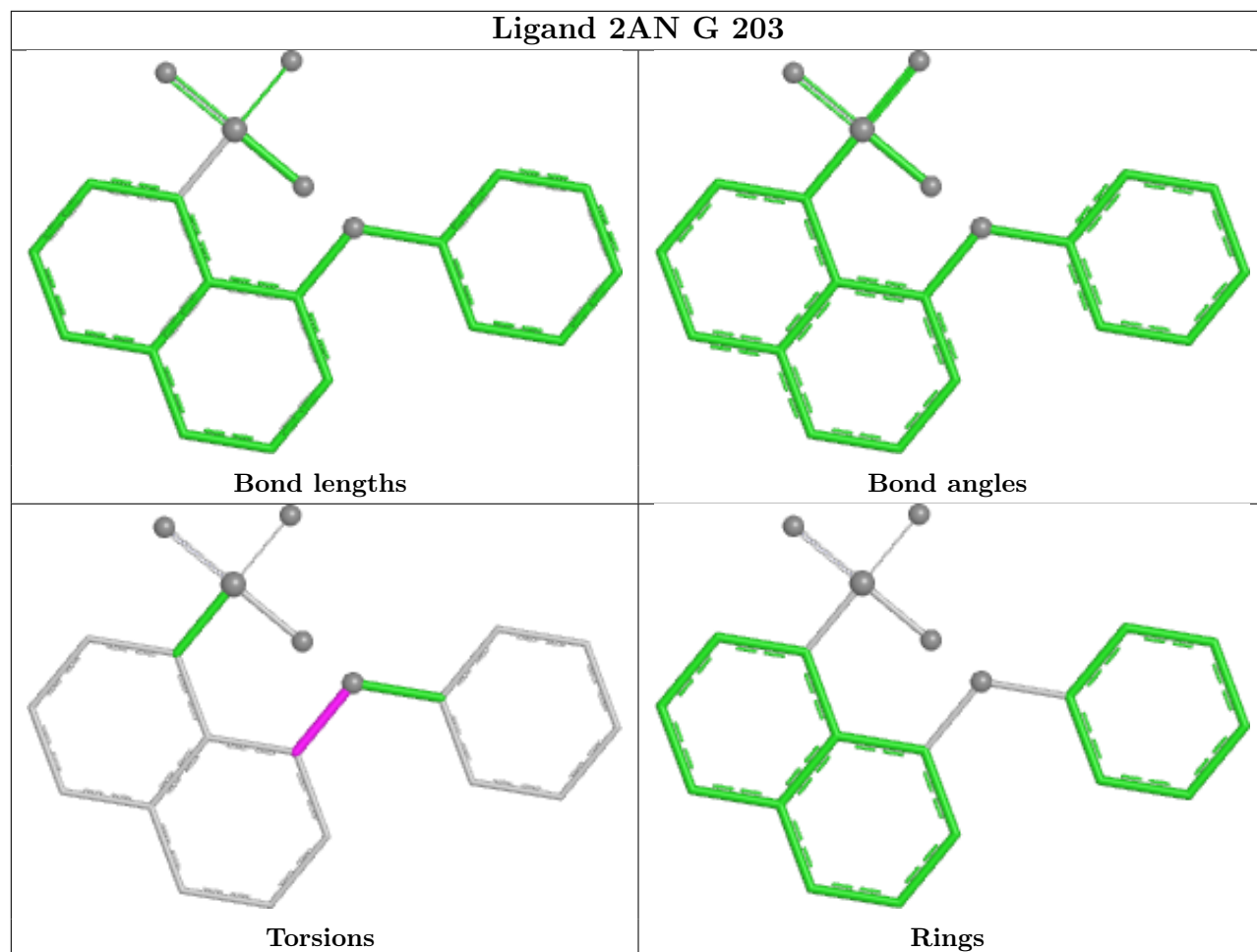
Ligand 2AN J 201



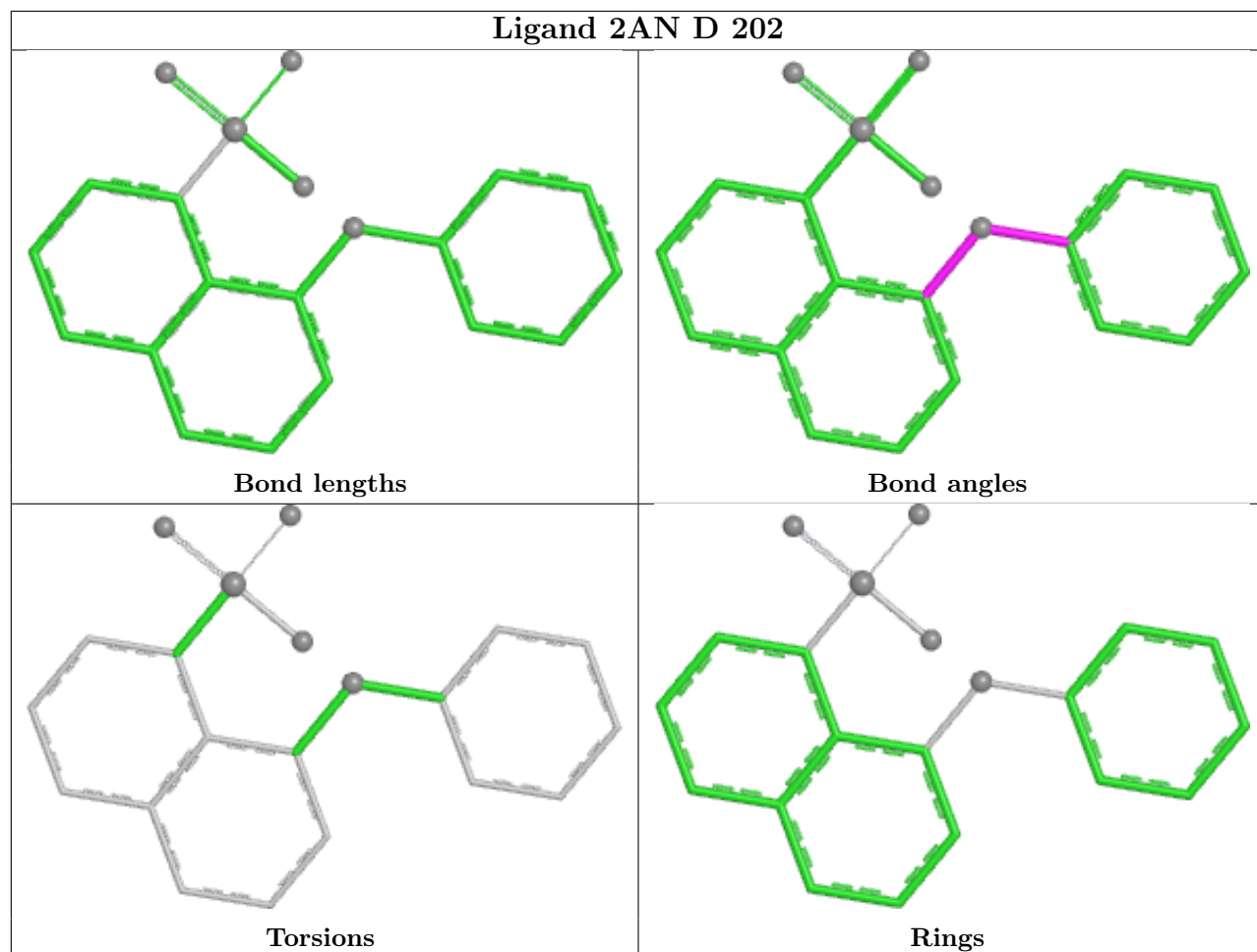
Ligand 2AN S 201

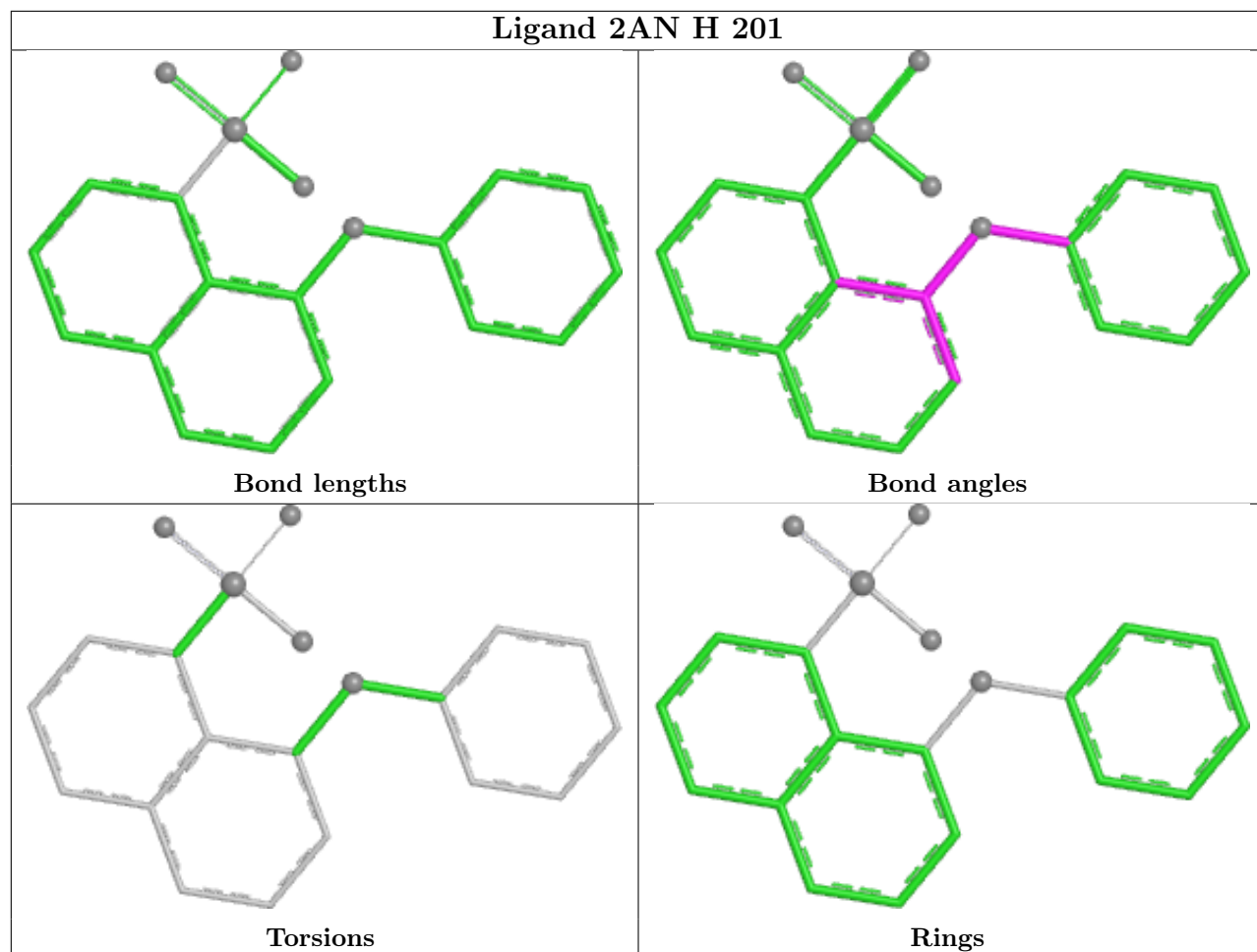


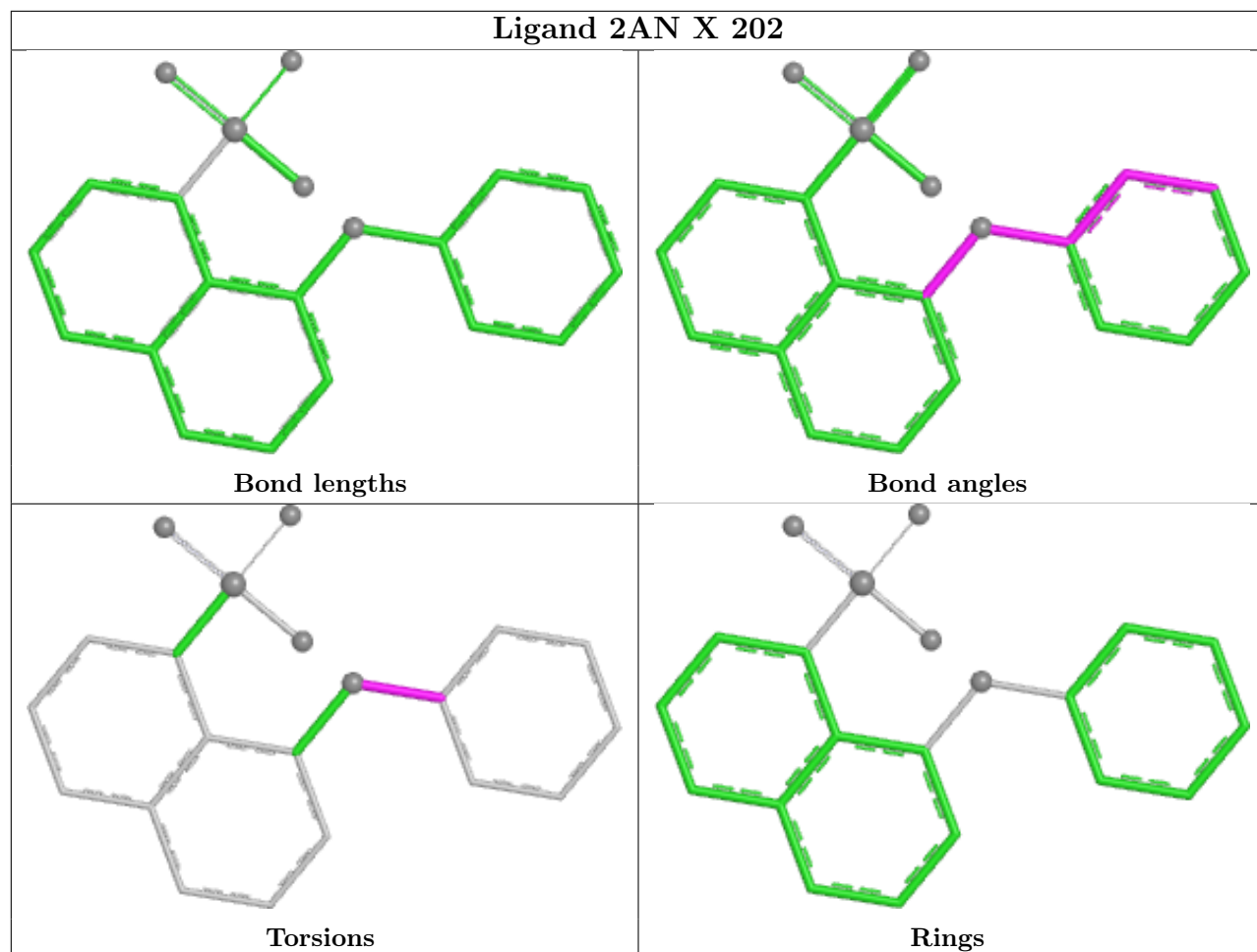
Ligand 2AN G 203



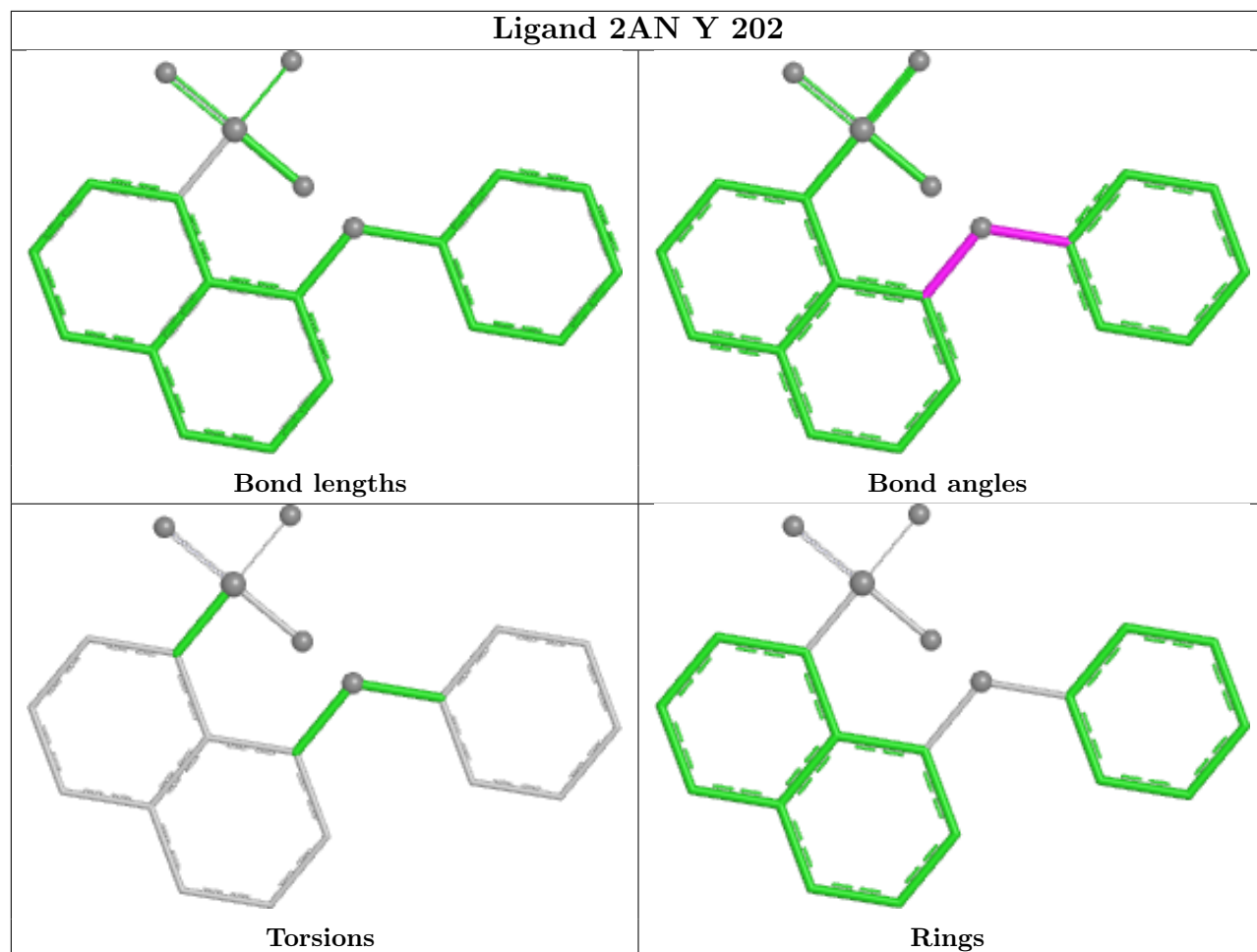
Ligand 2AN D 202

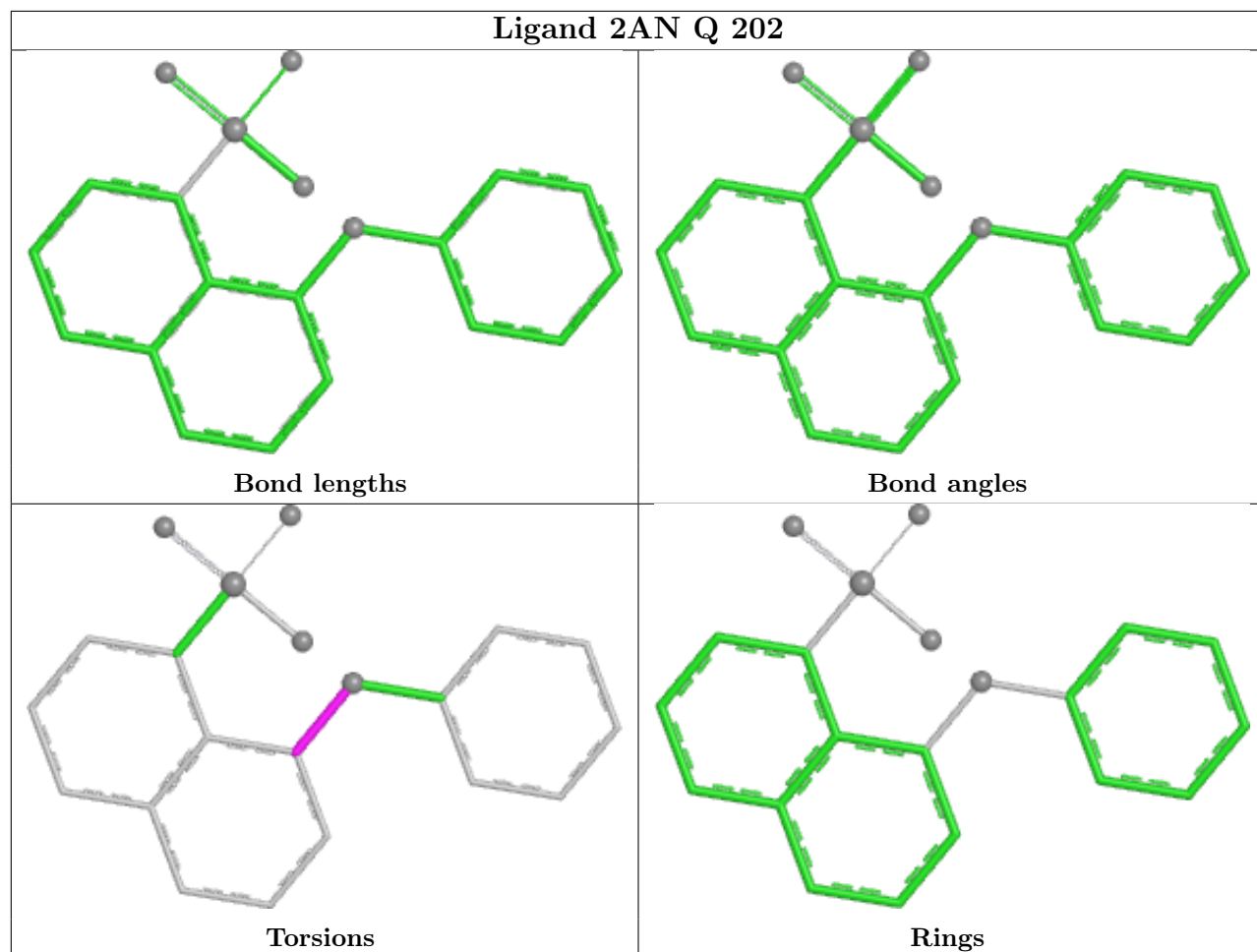


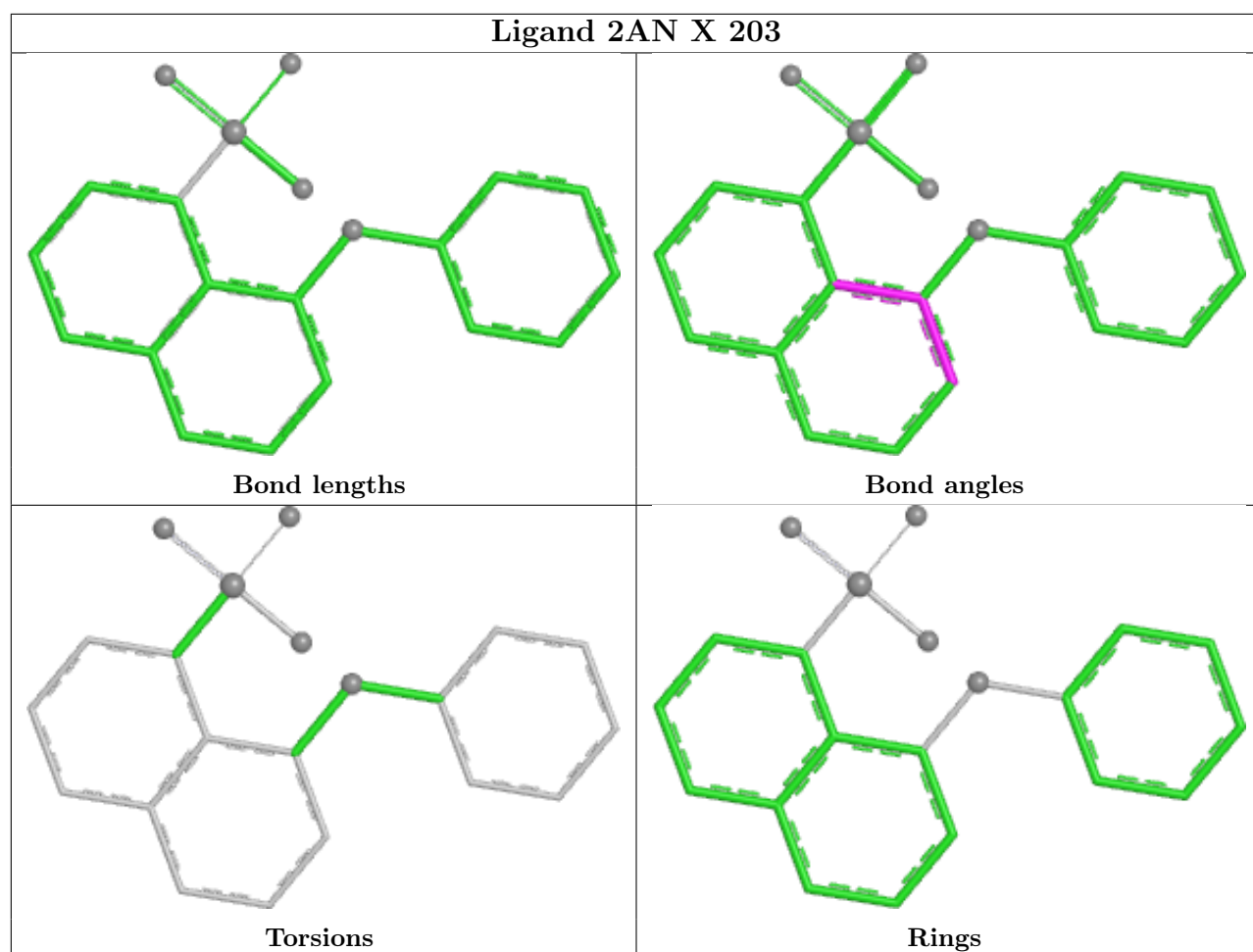


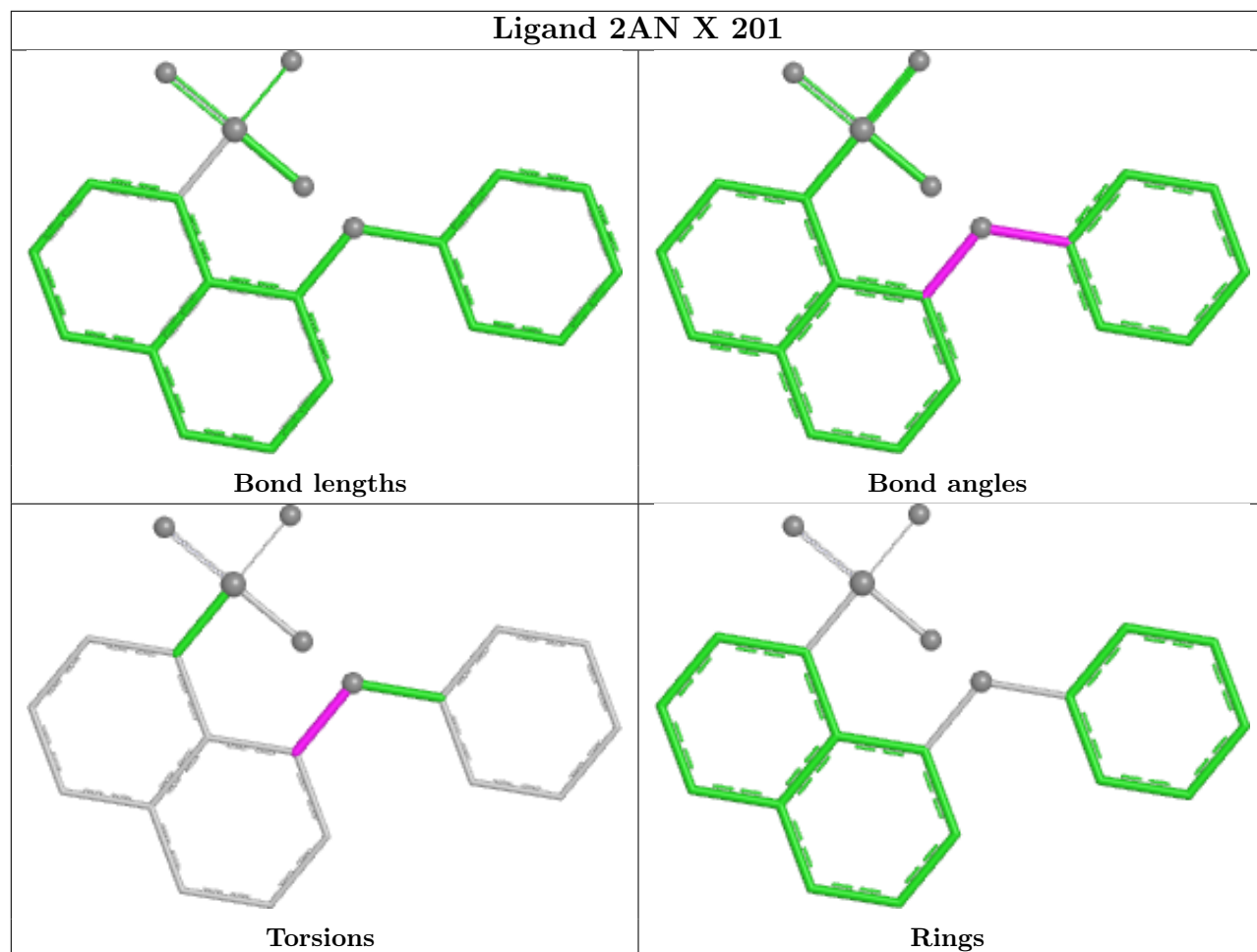


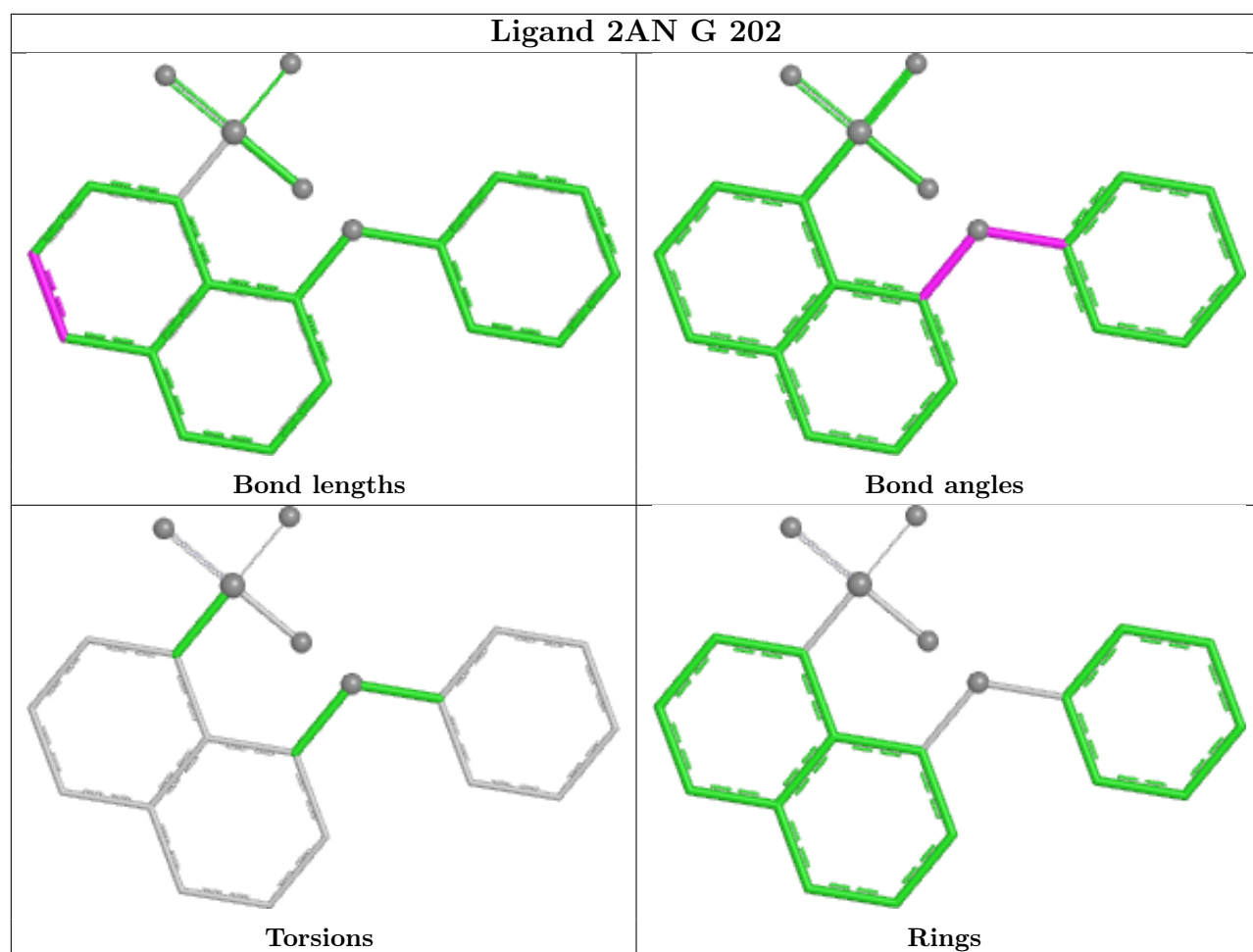
Ligand 2AN Y 202

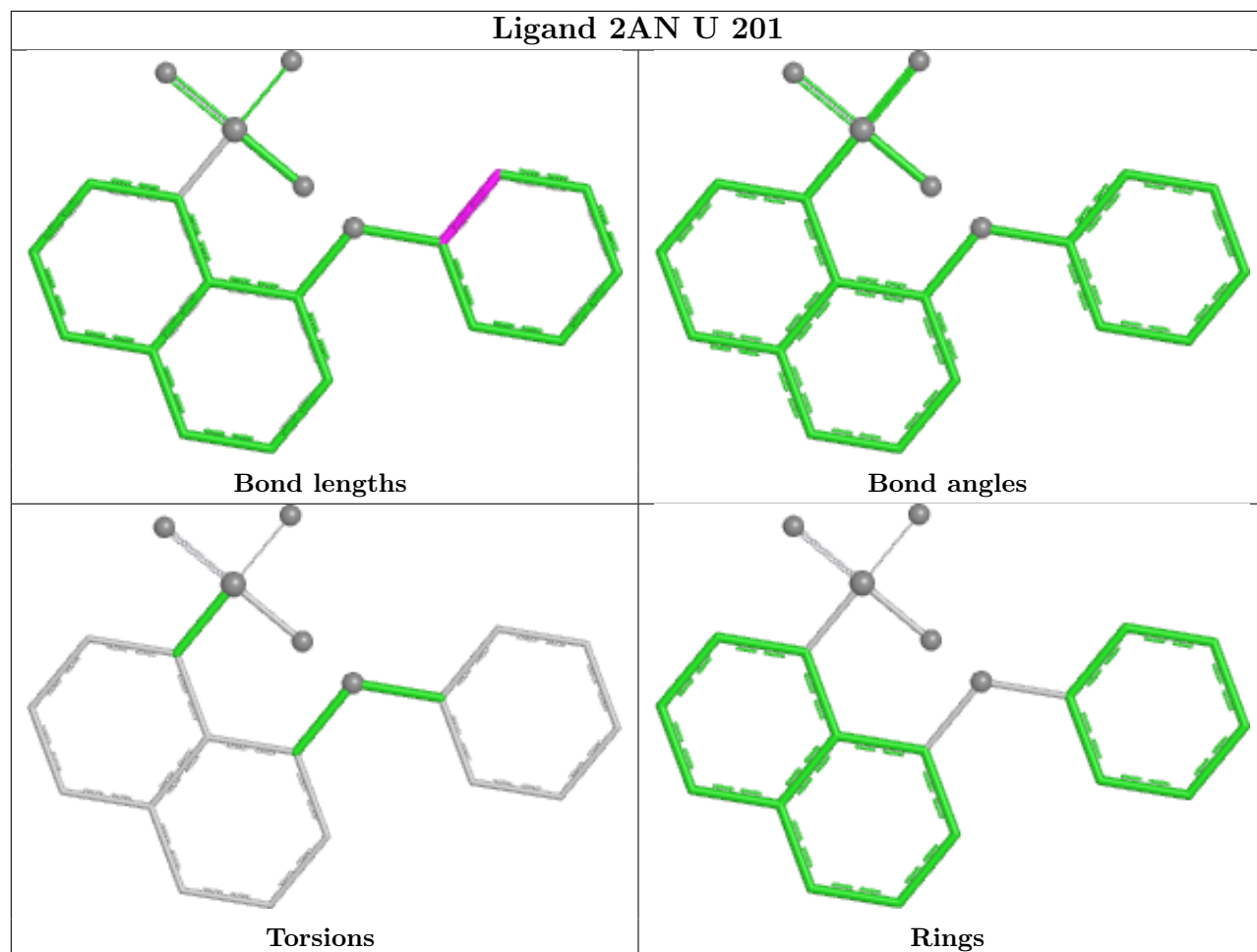




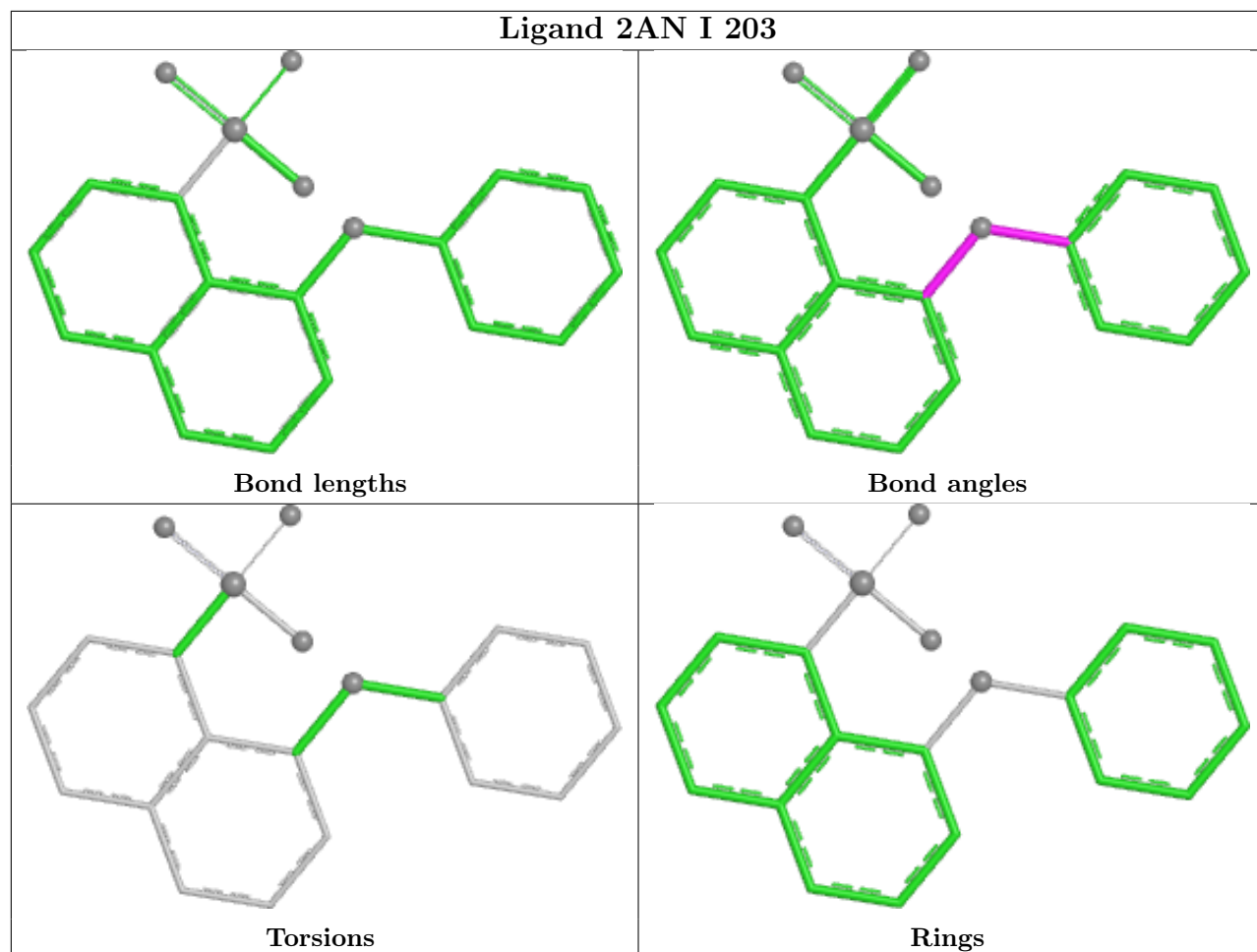




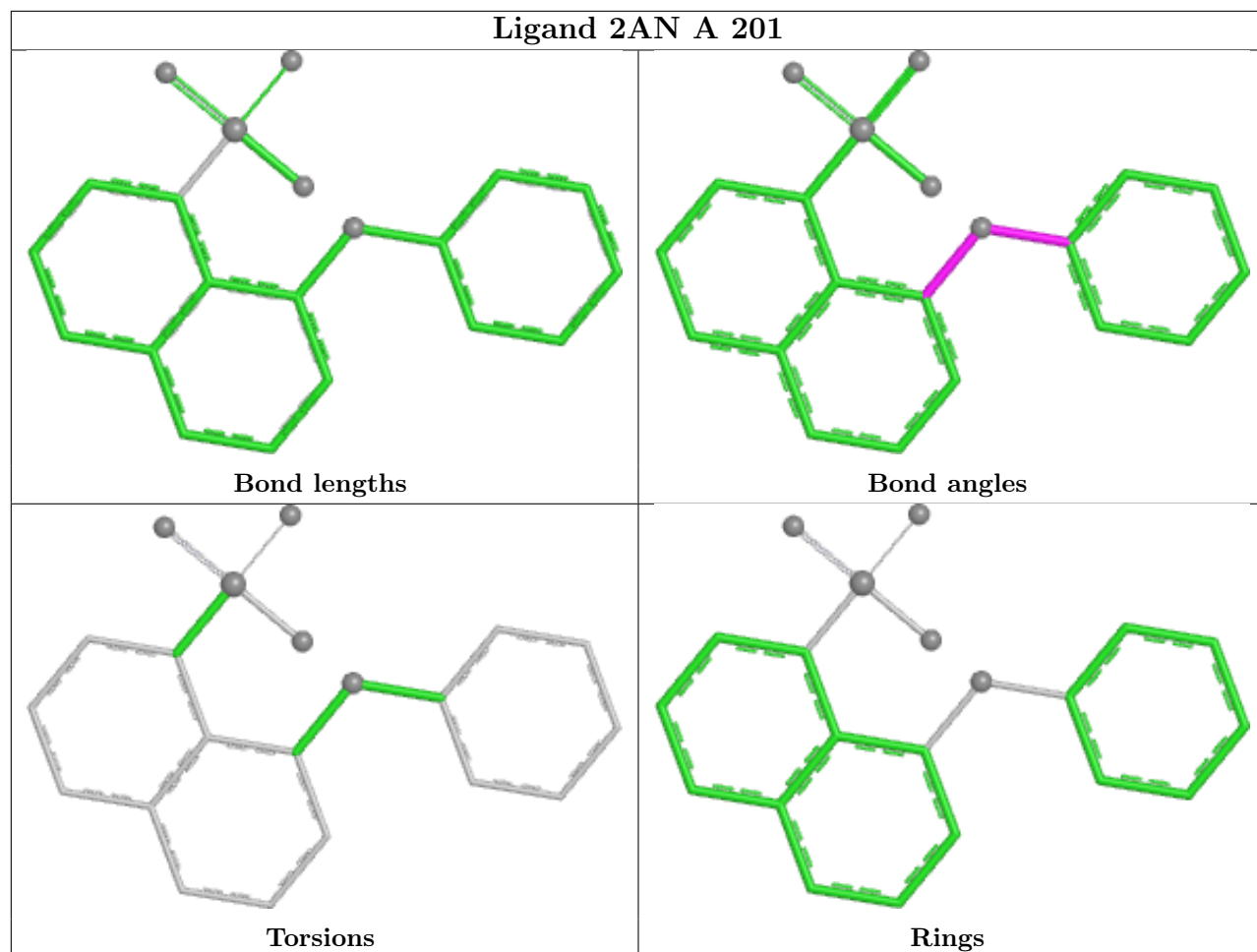


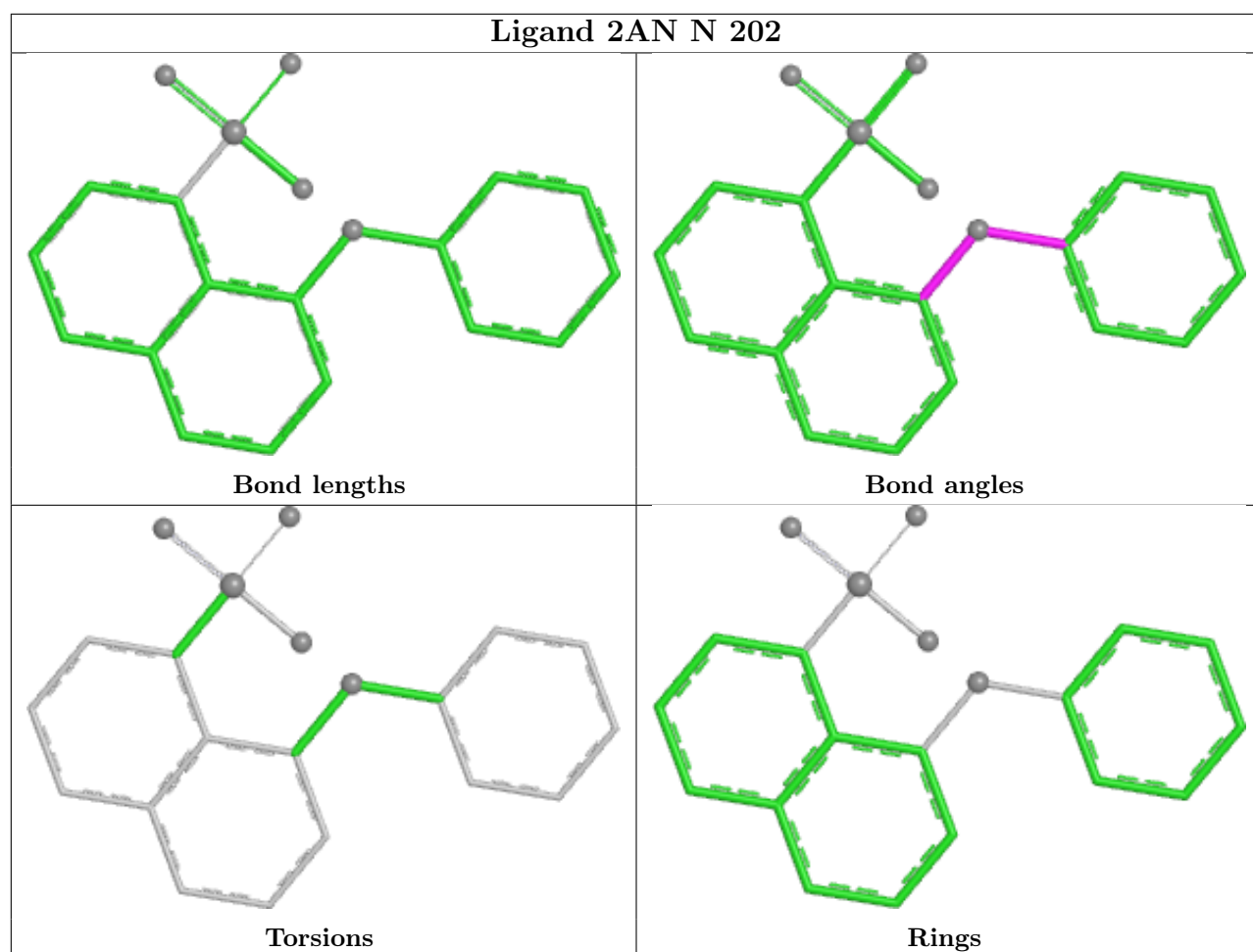


Ligand 2AN I 203

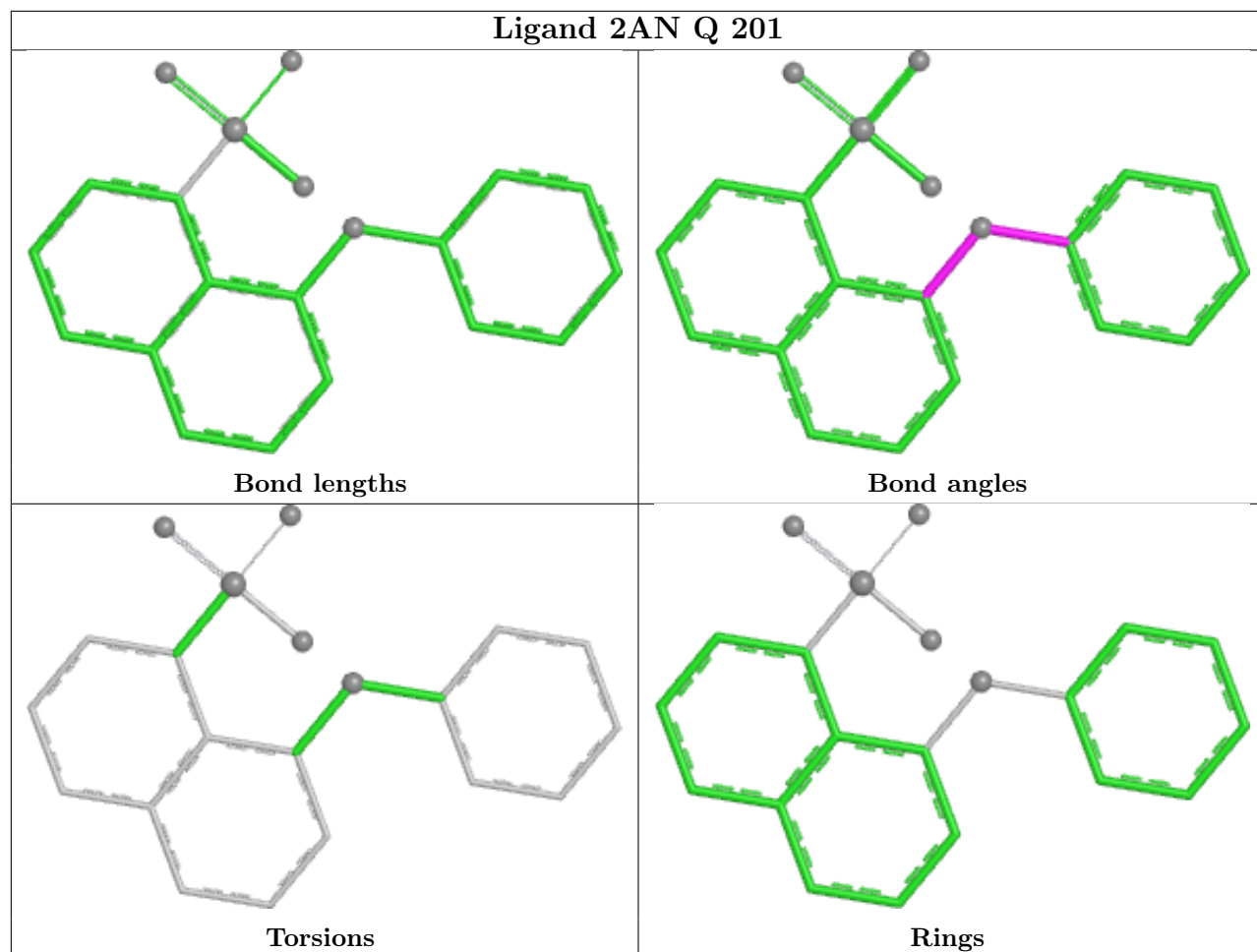


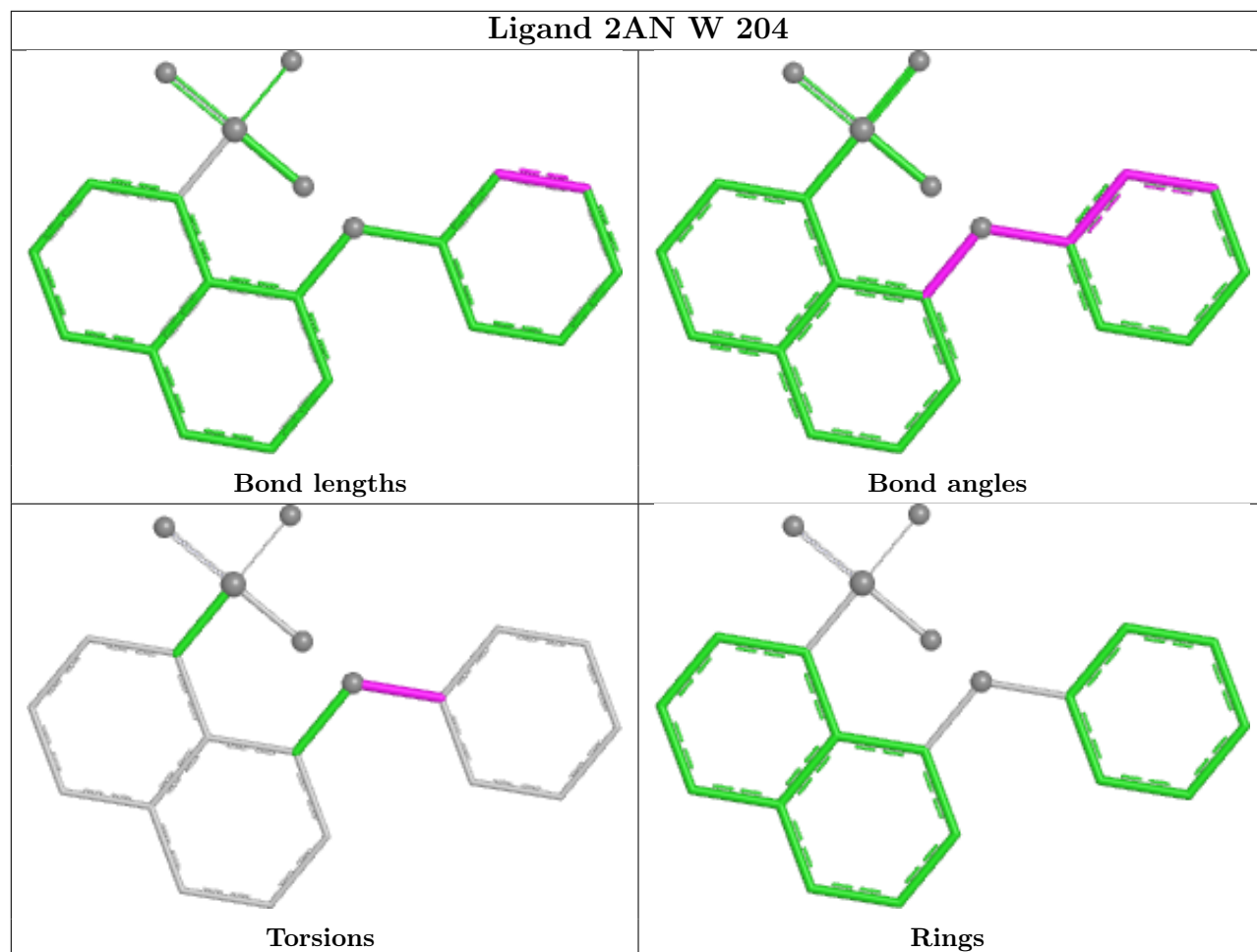
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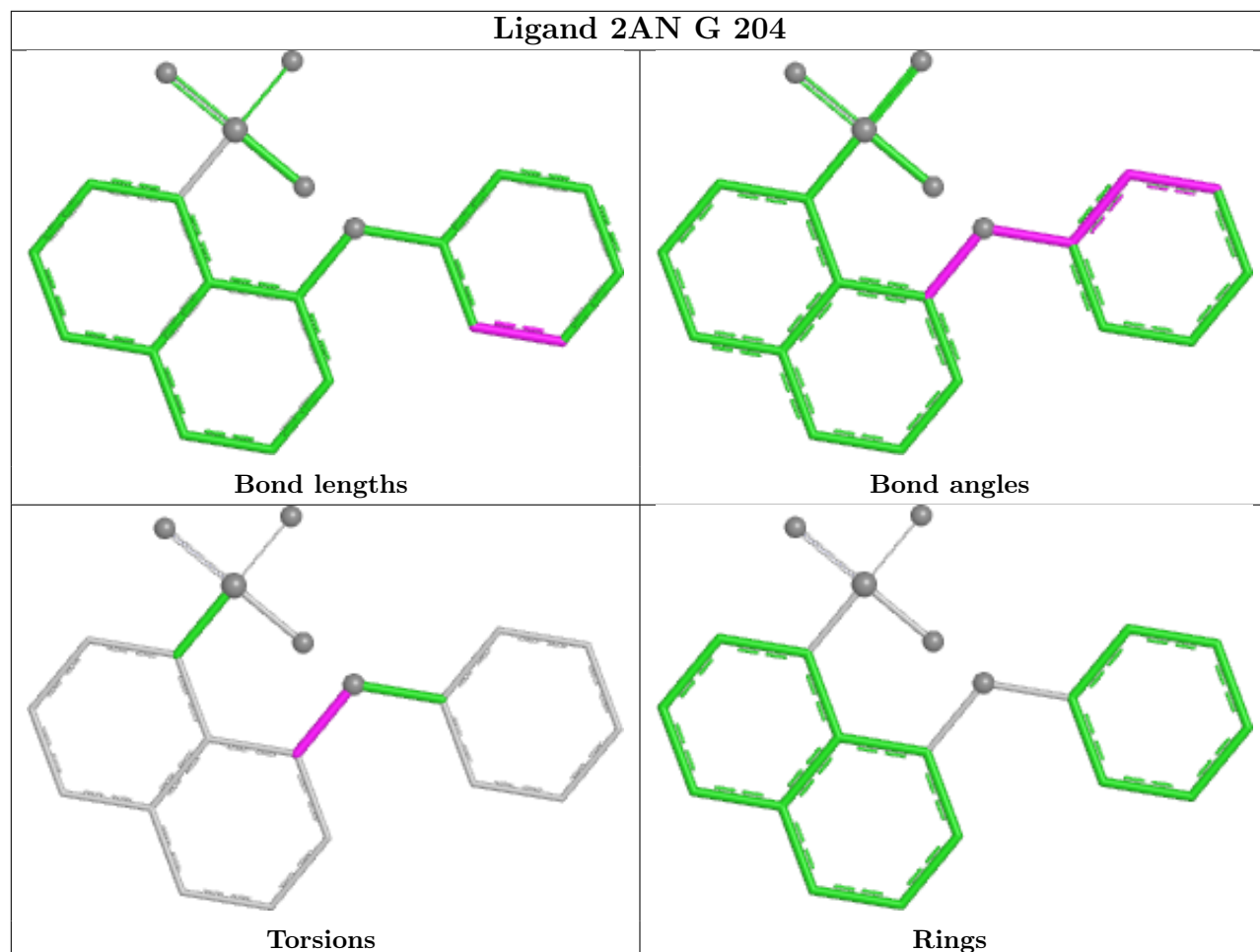


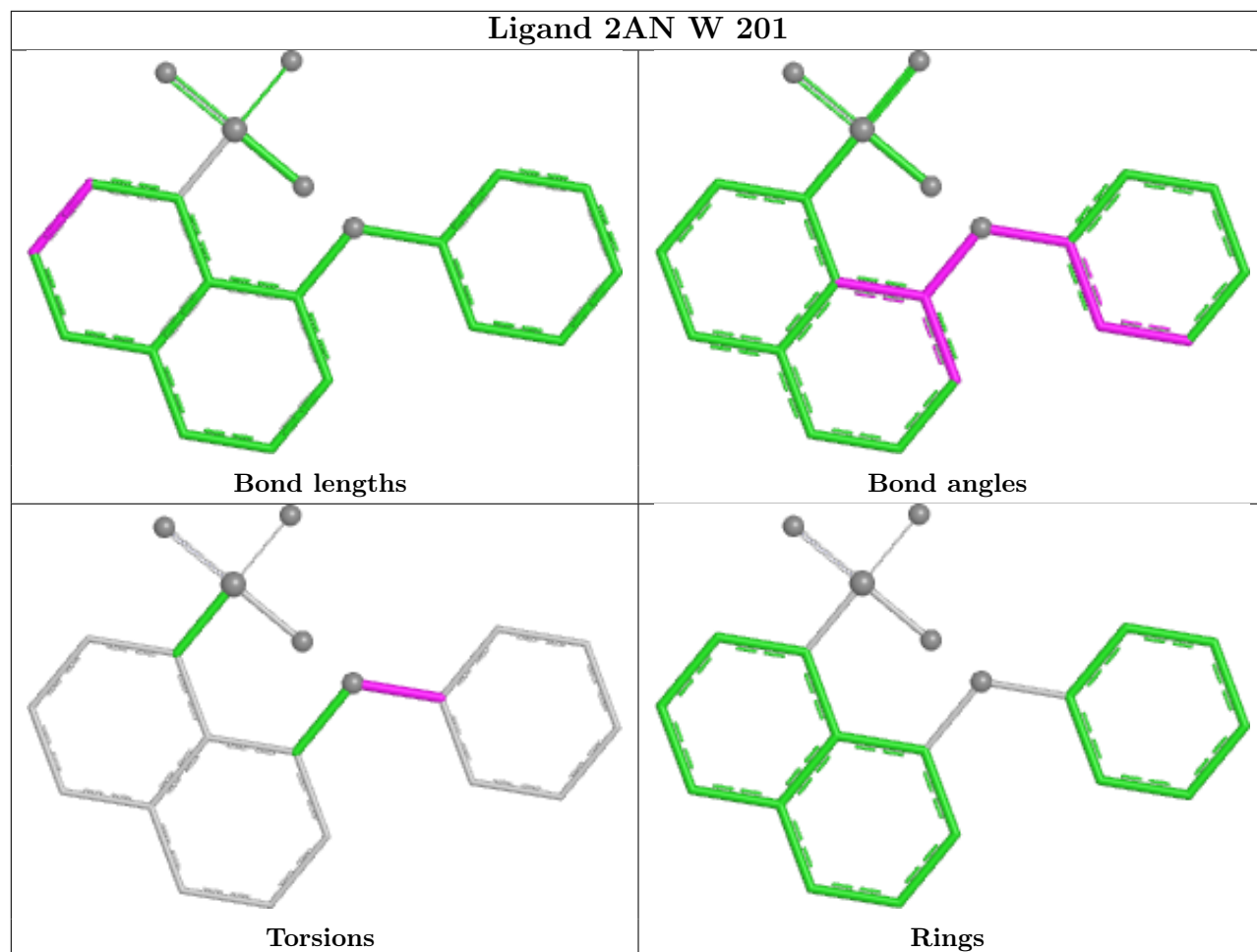
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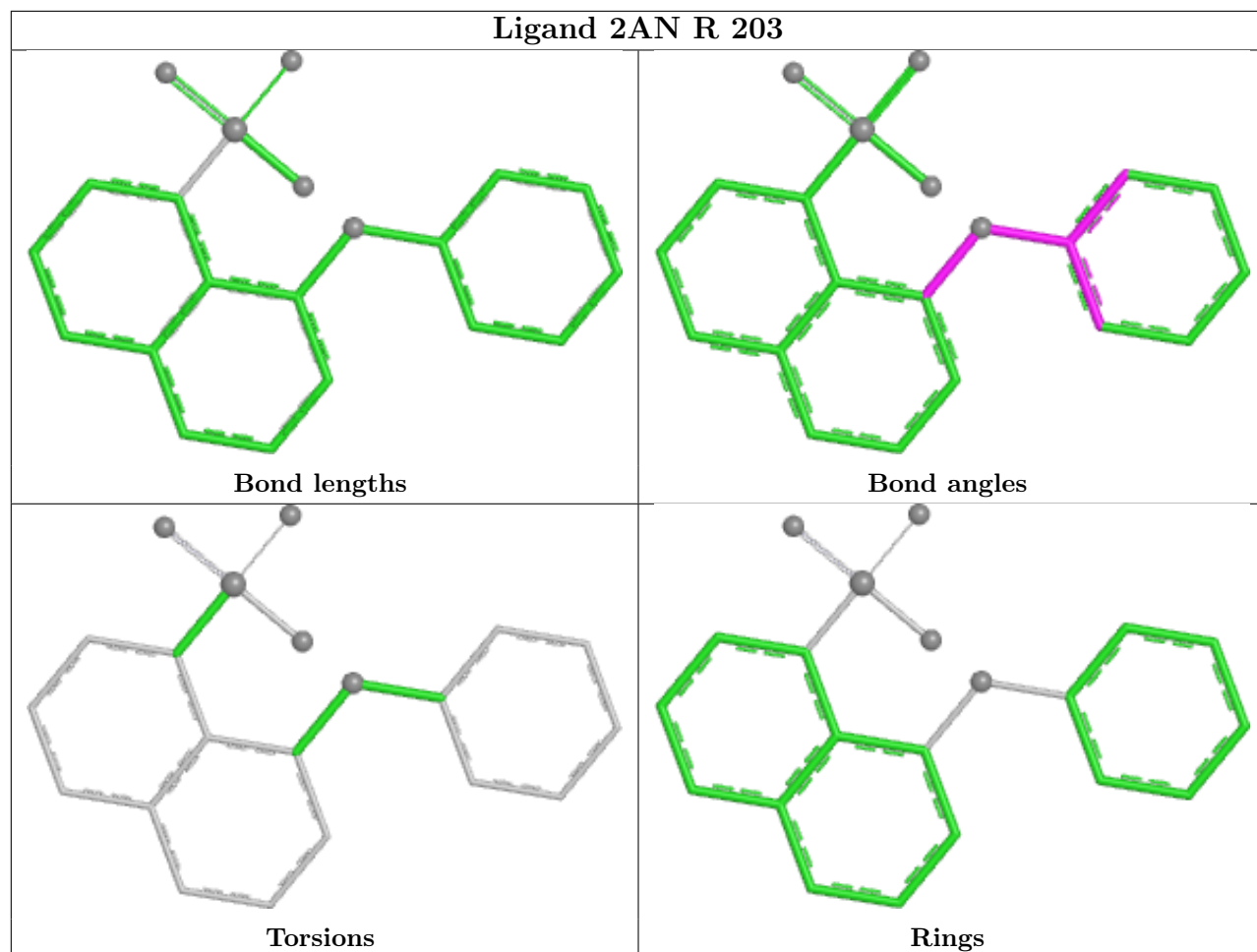


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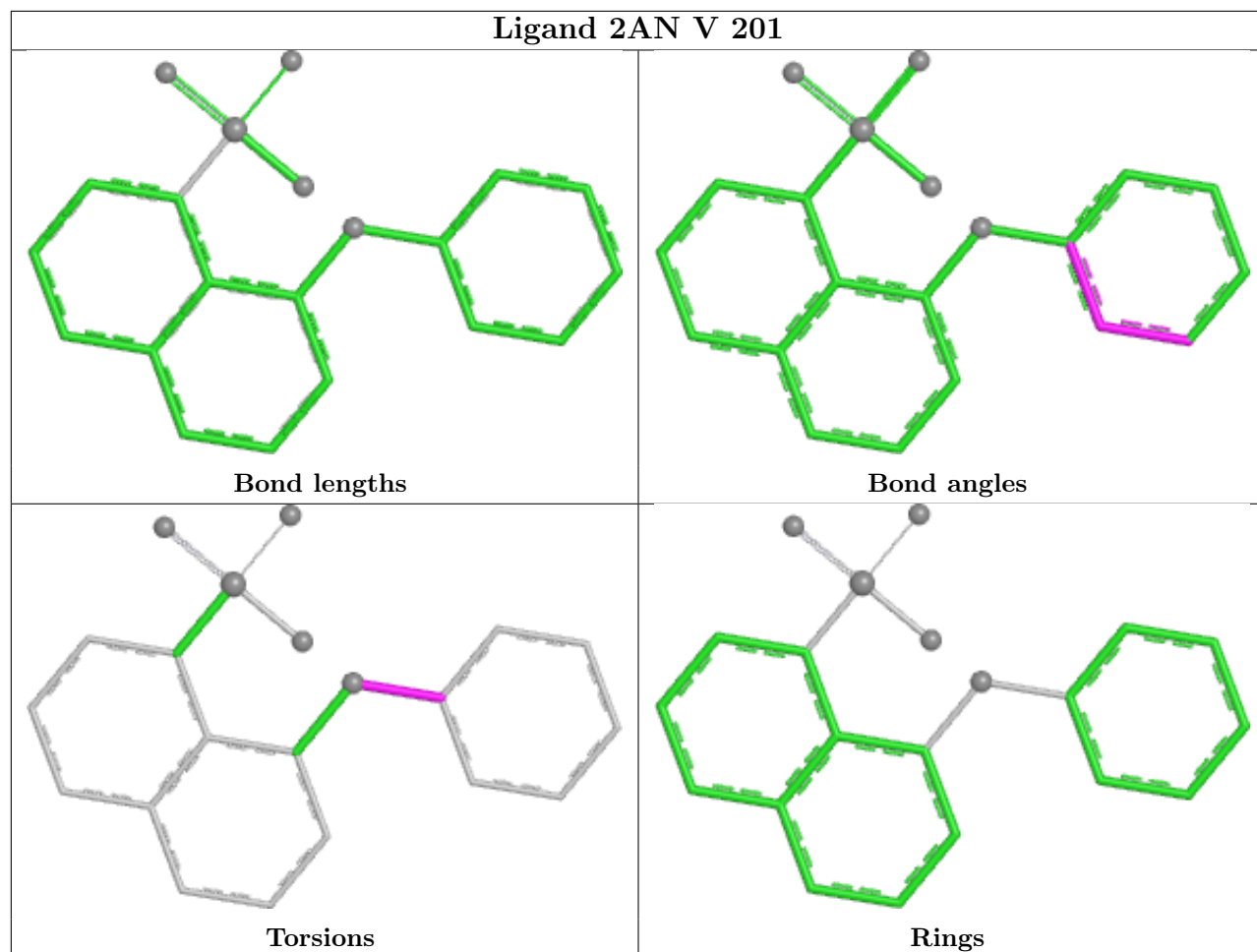




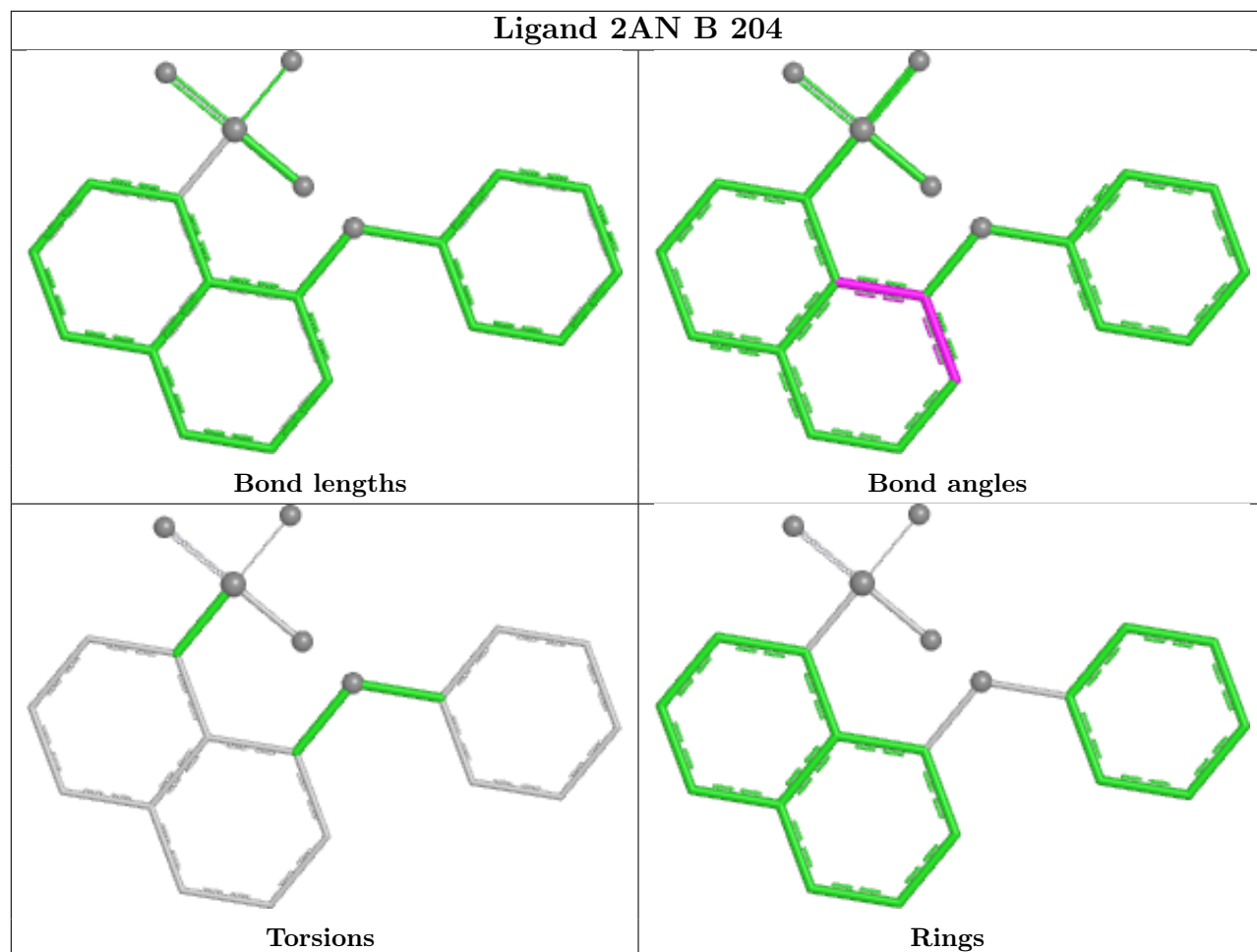
Ligand 2AN R 203



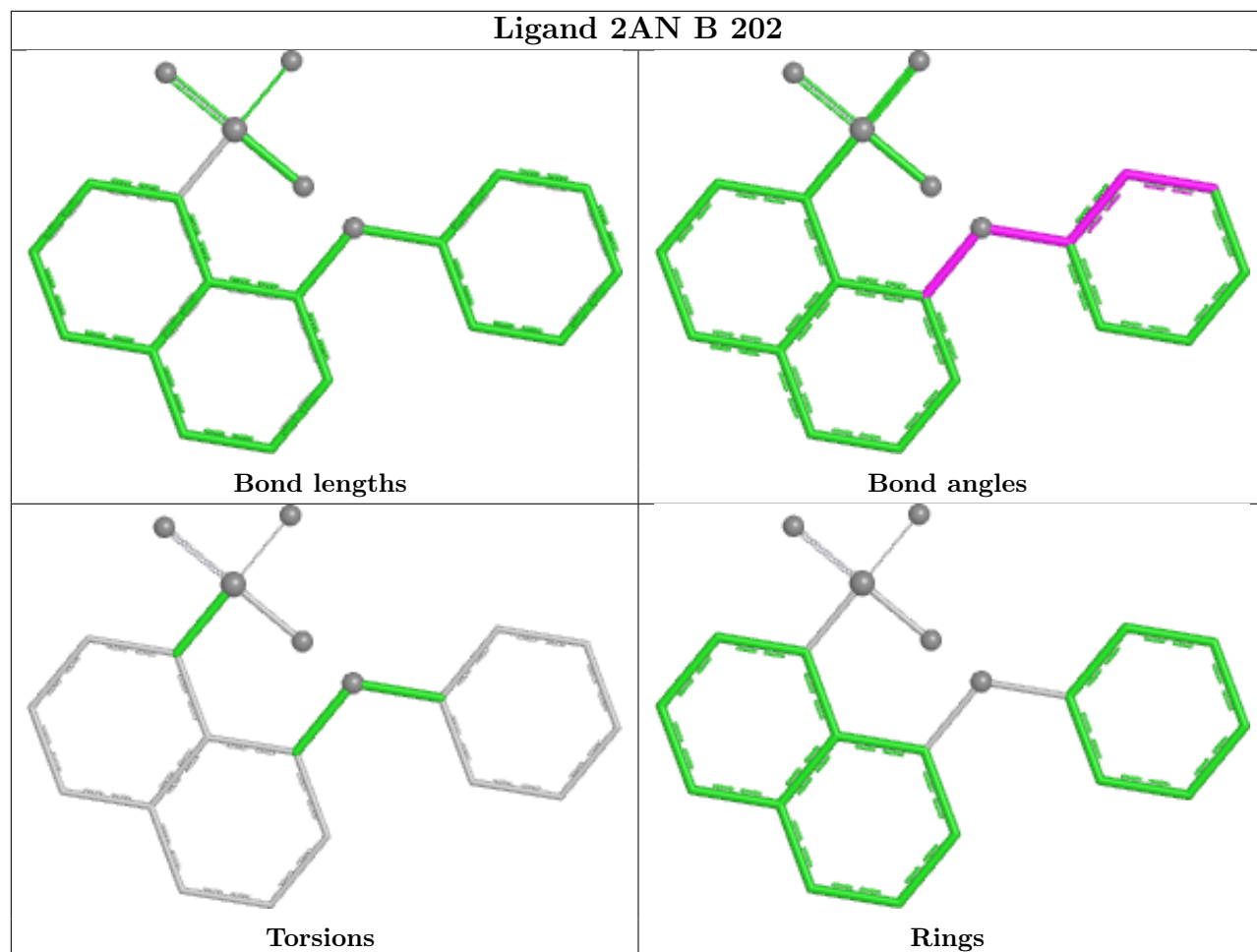
Ligand 2AN V 201



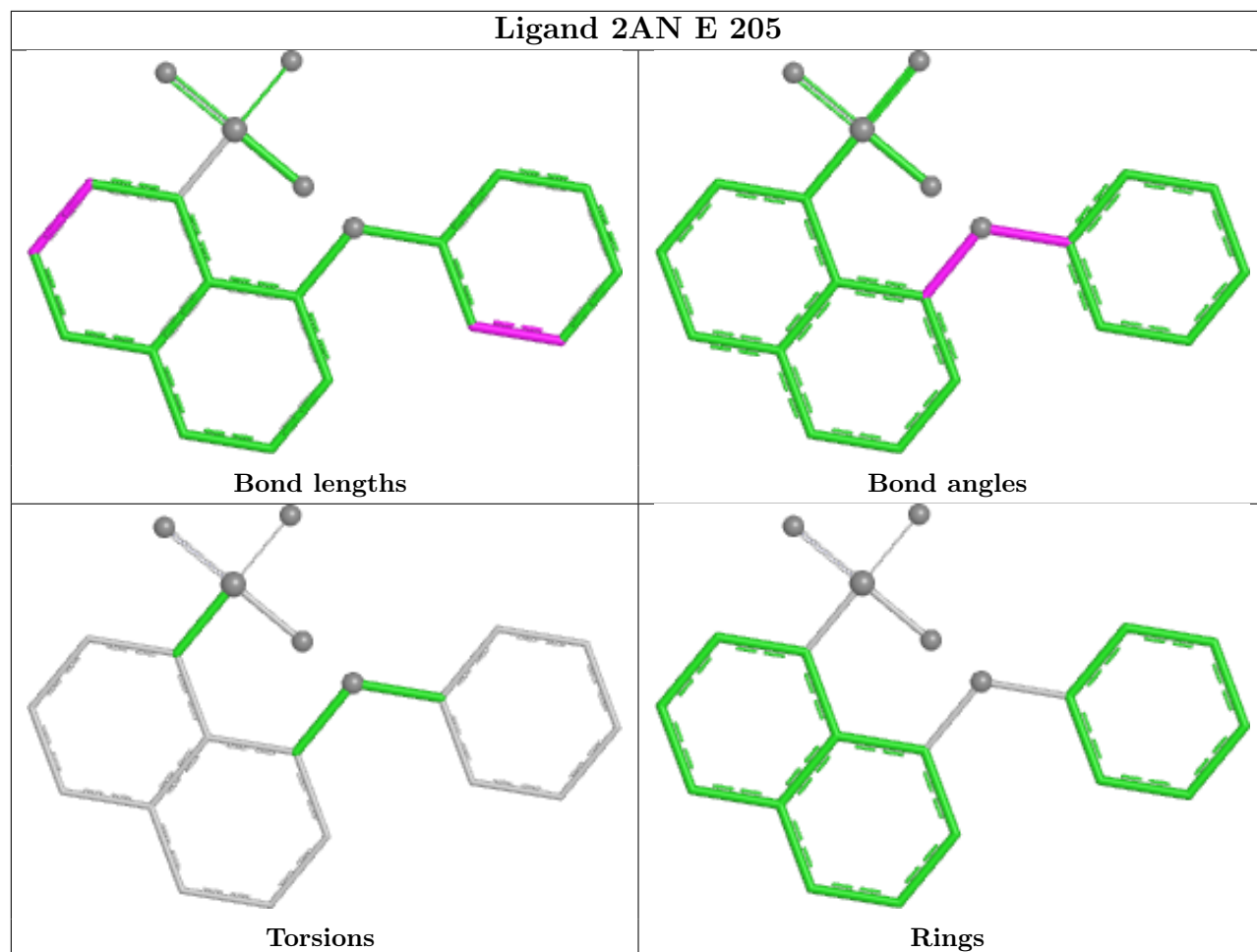
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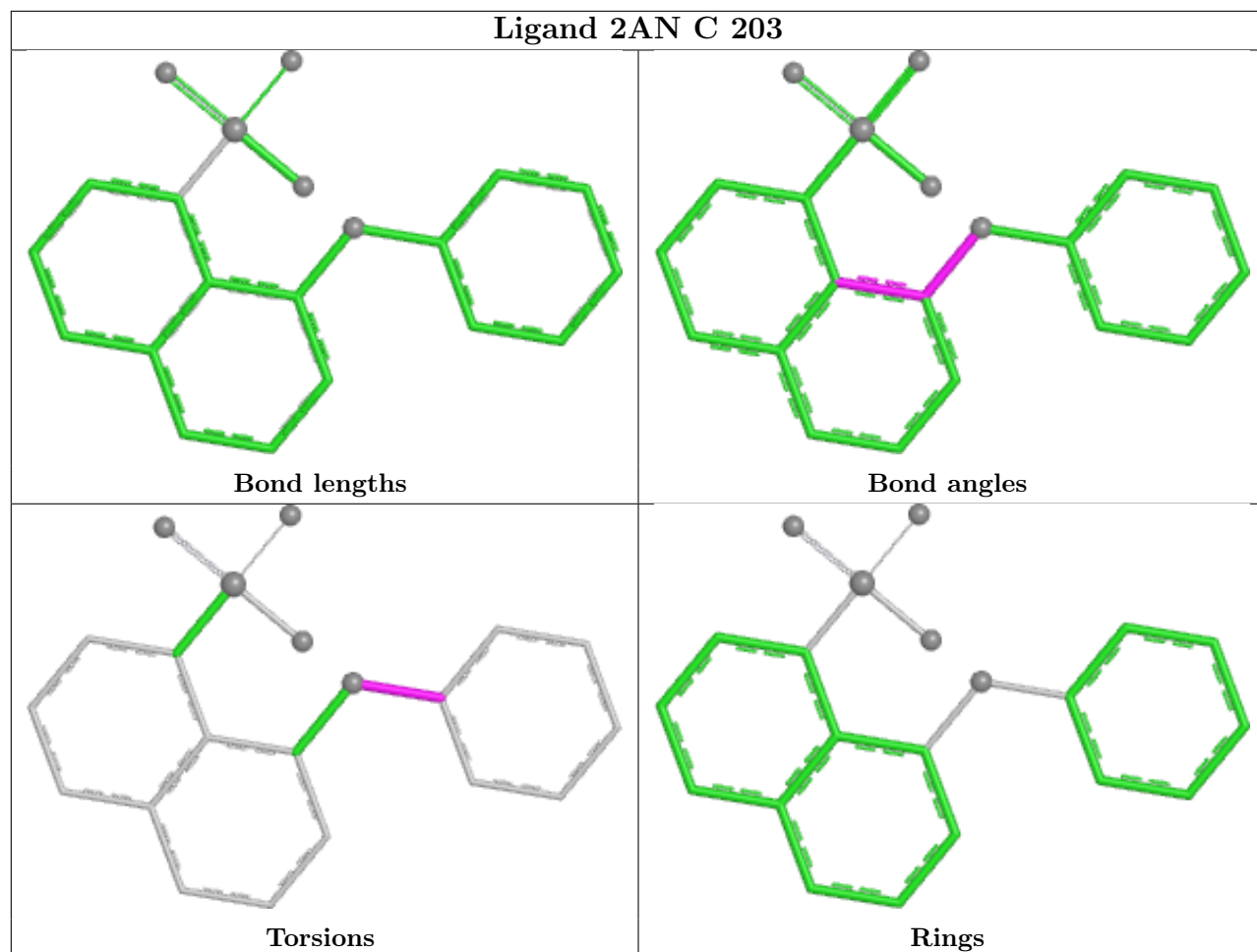


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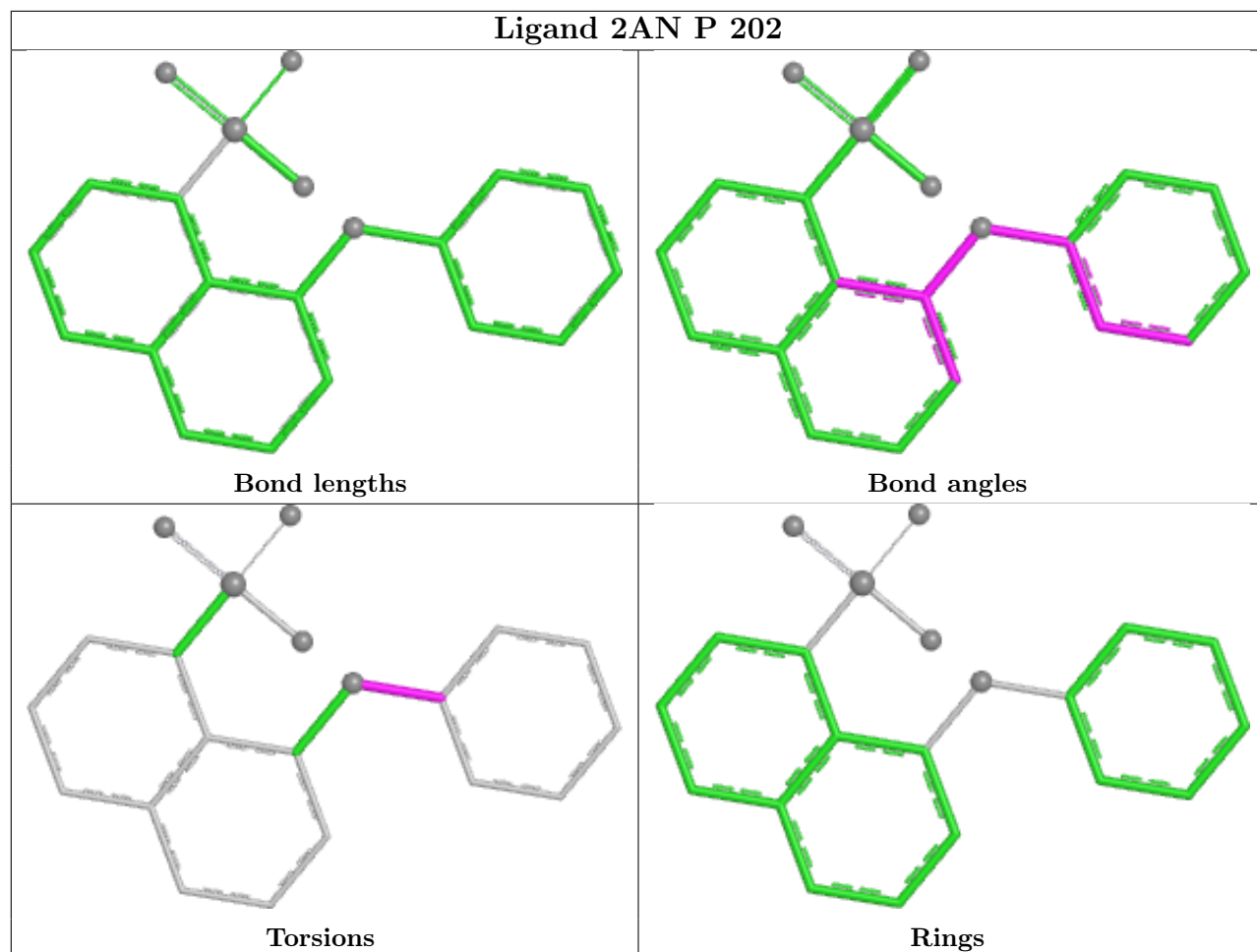


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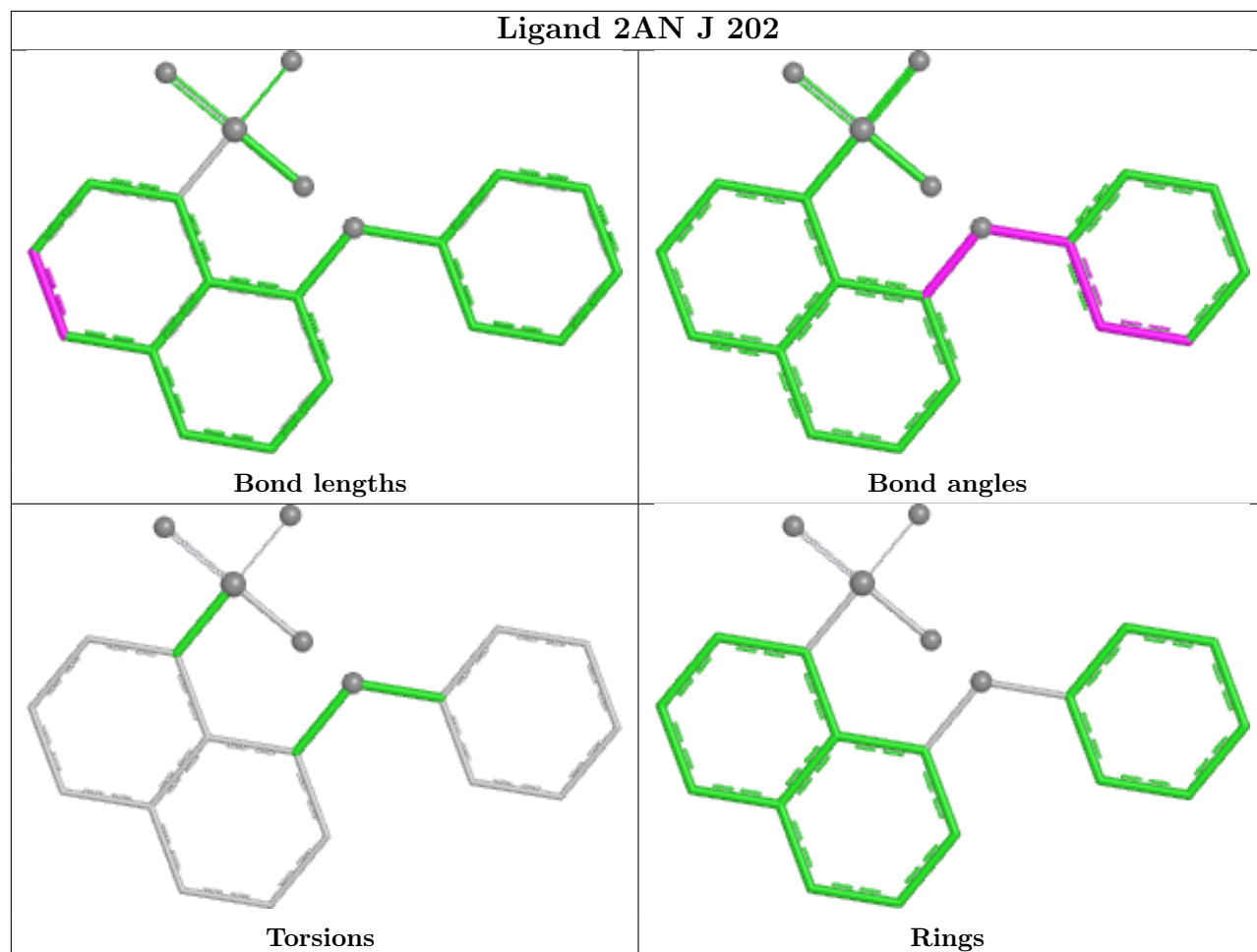


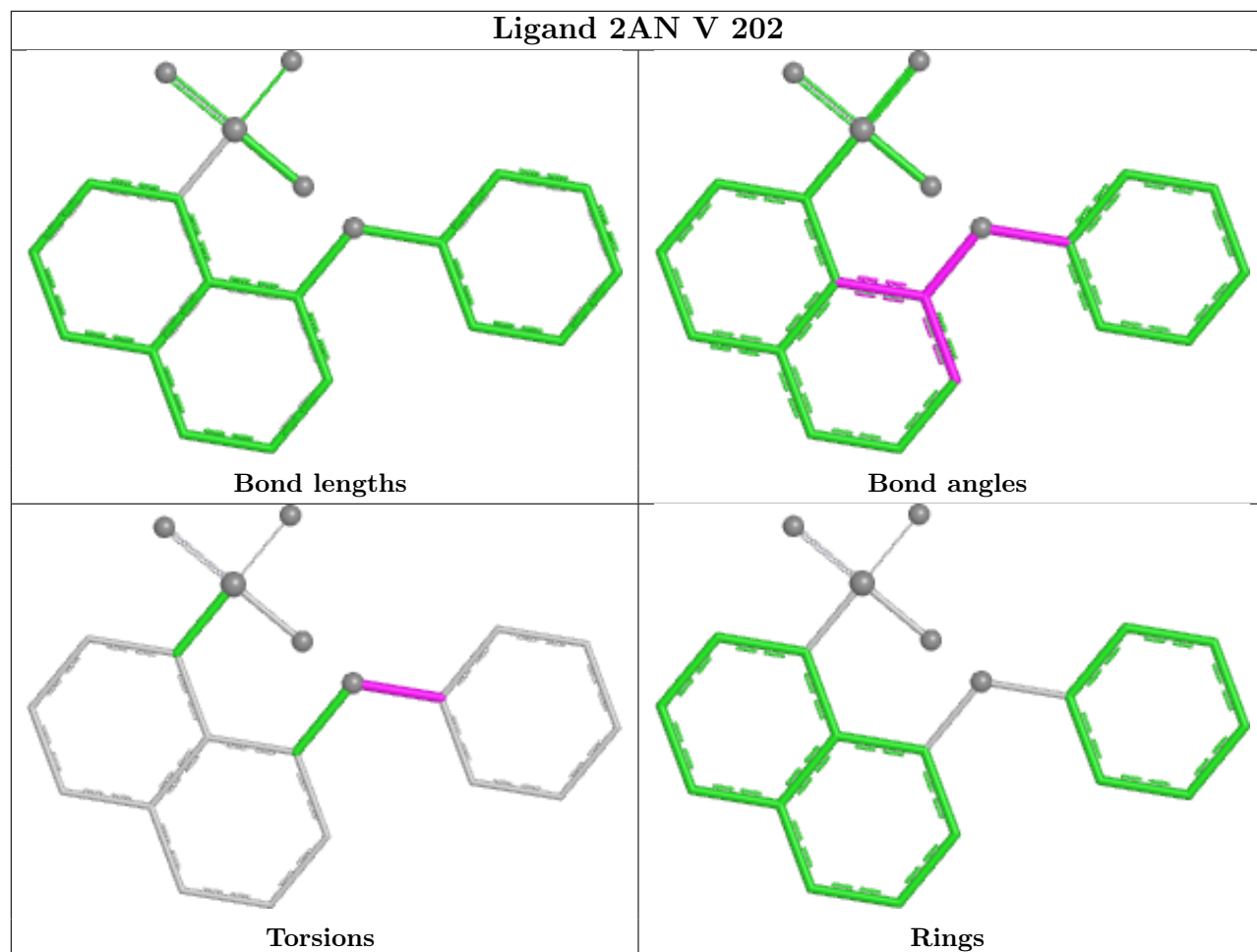


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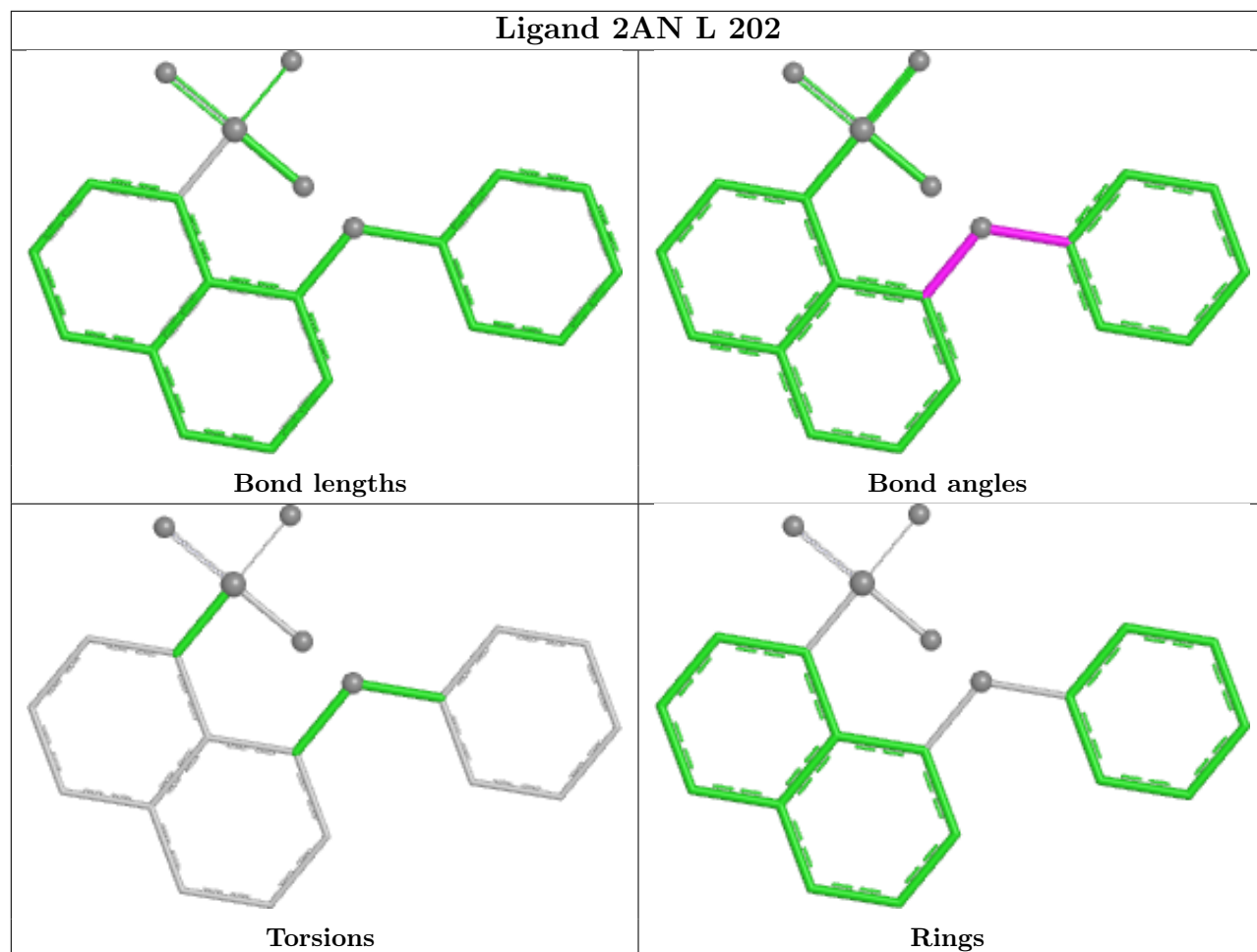


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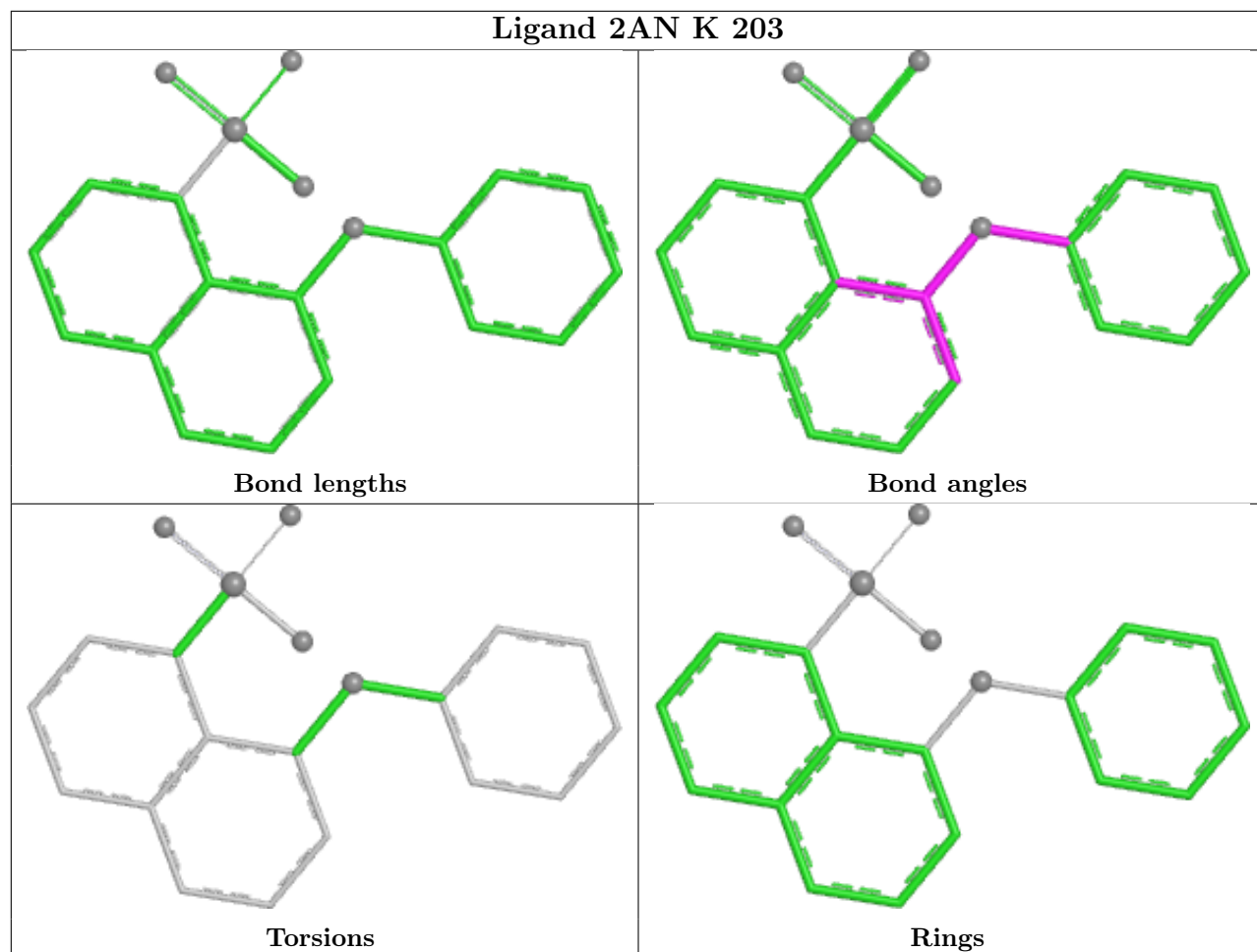




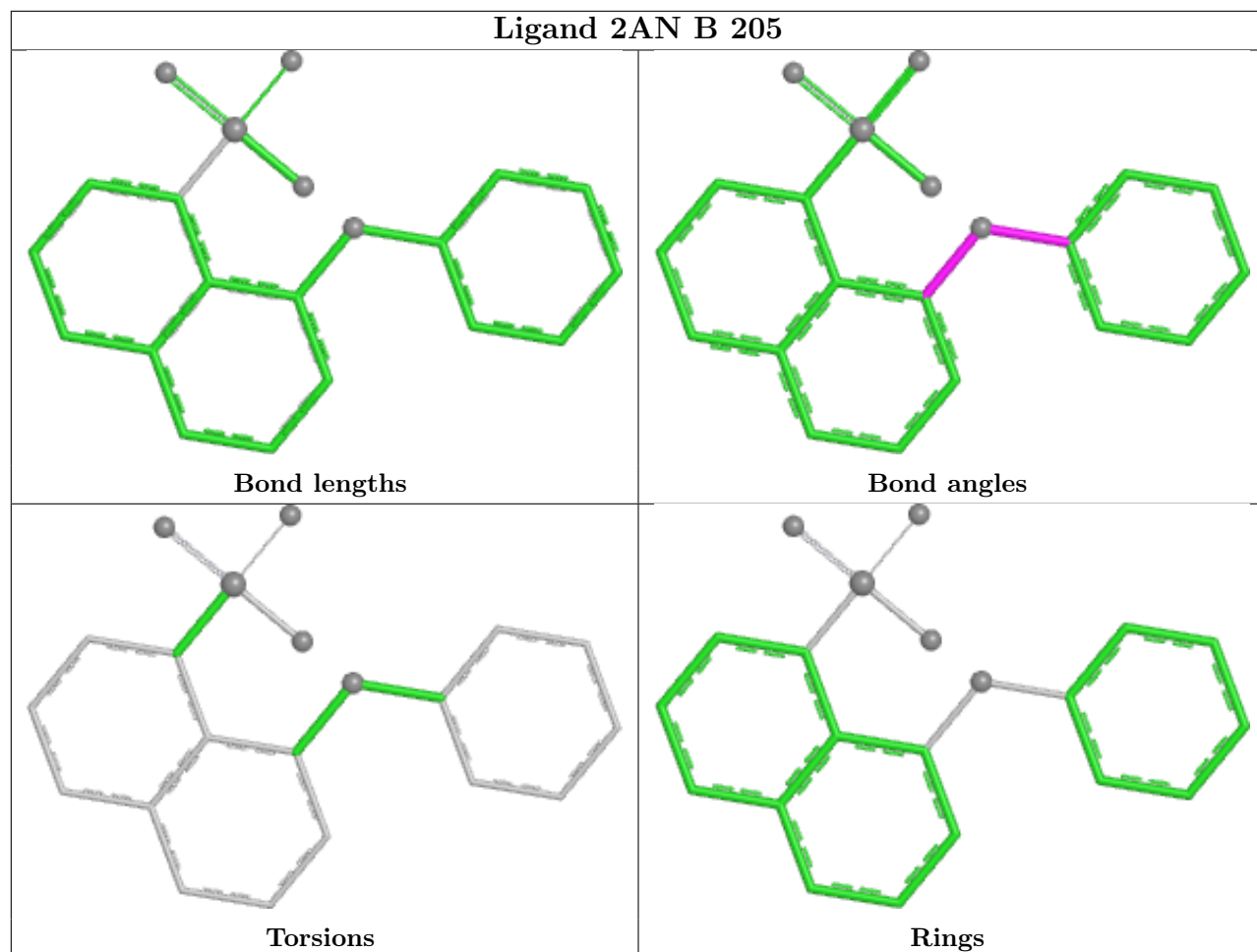
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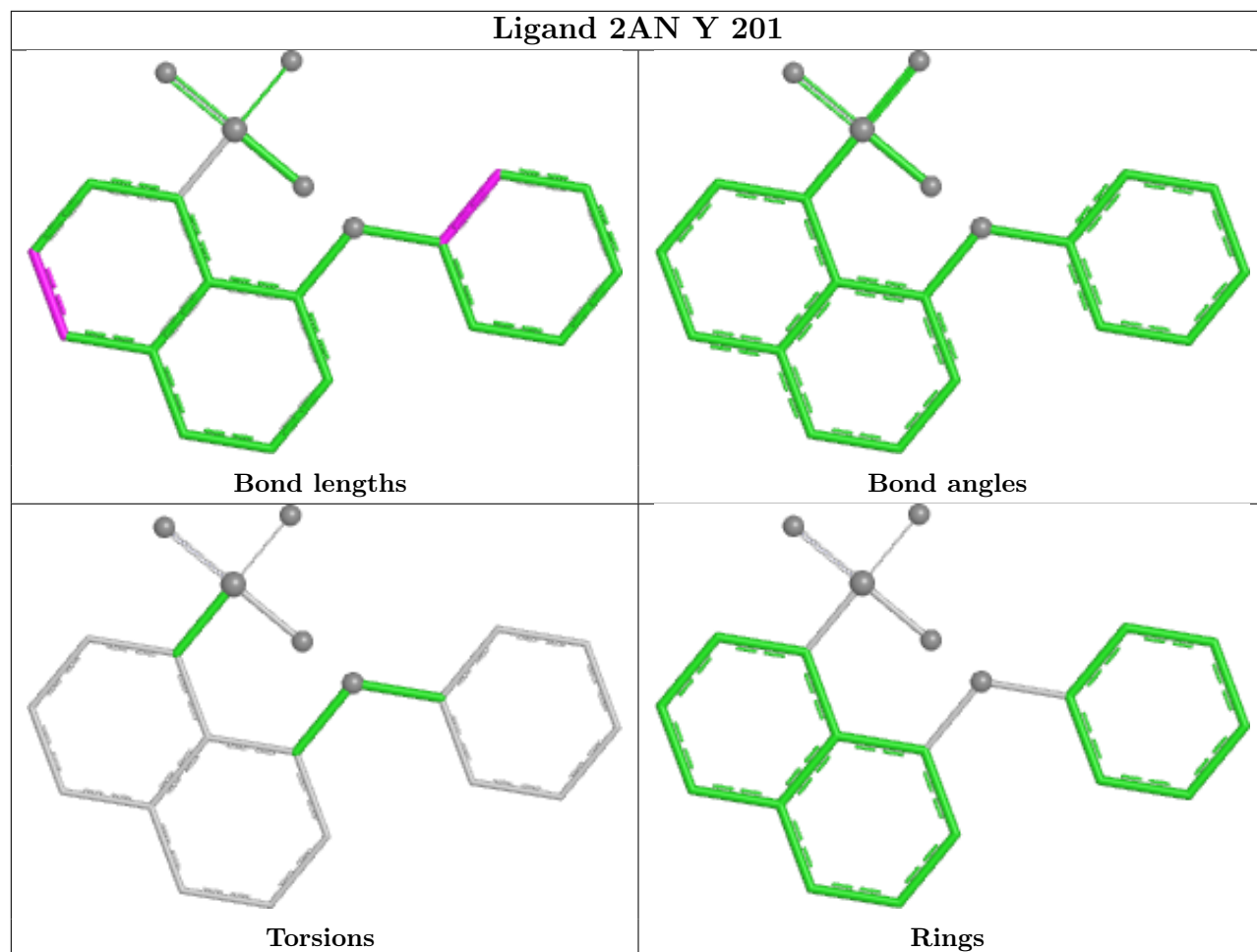


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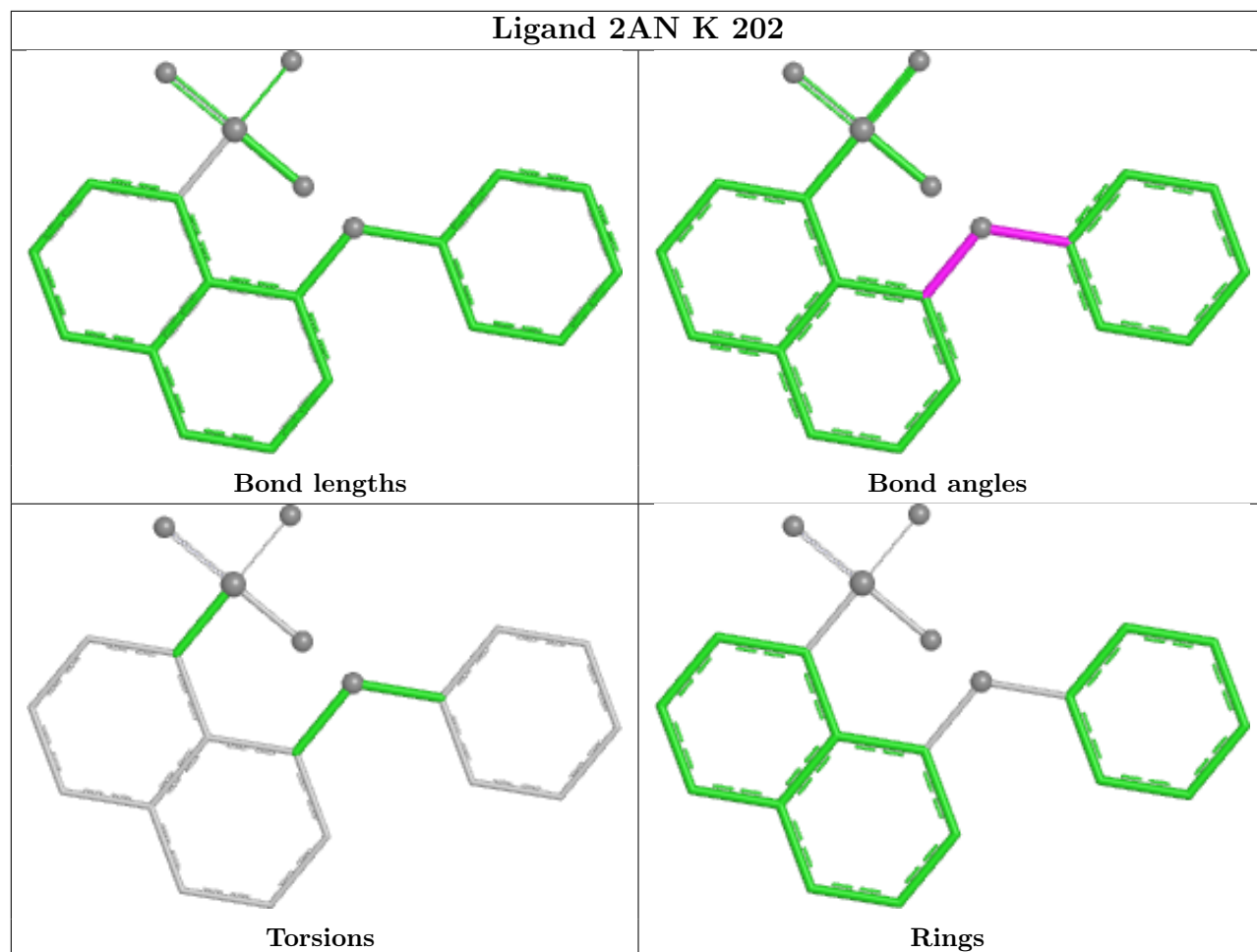


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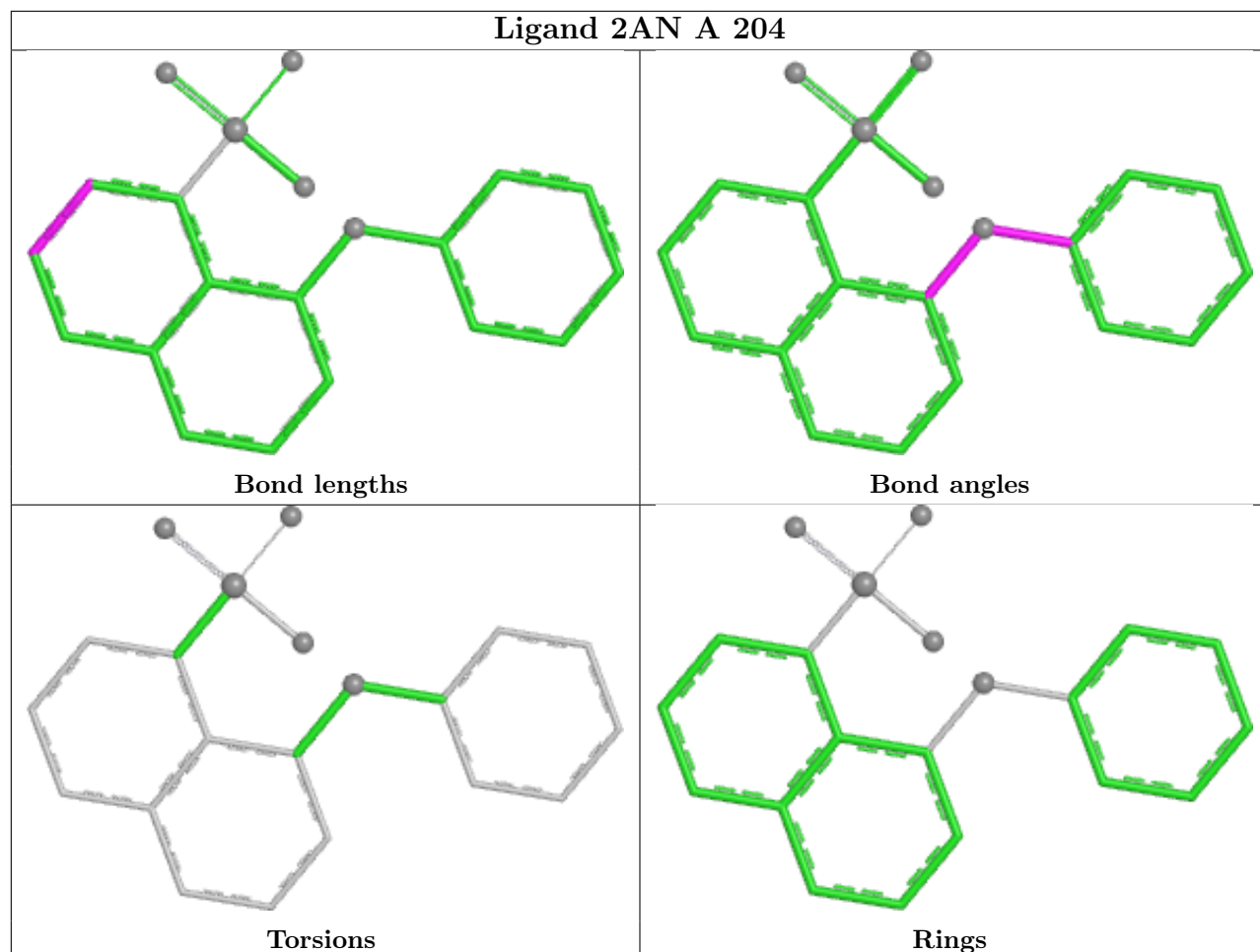




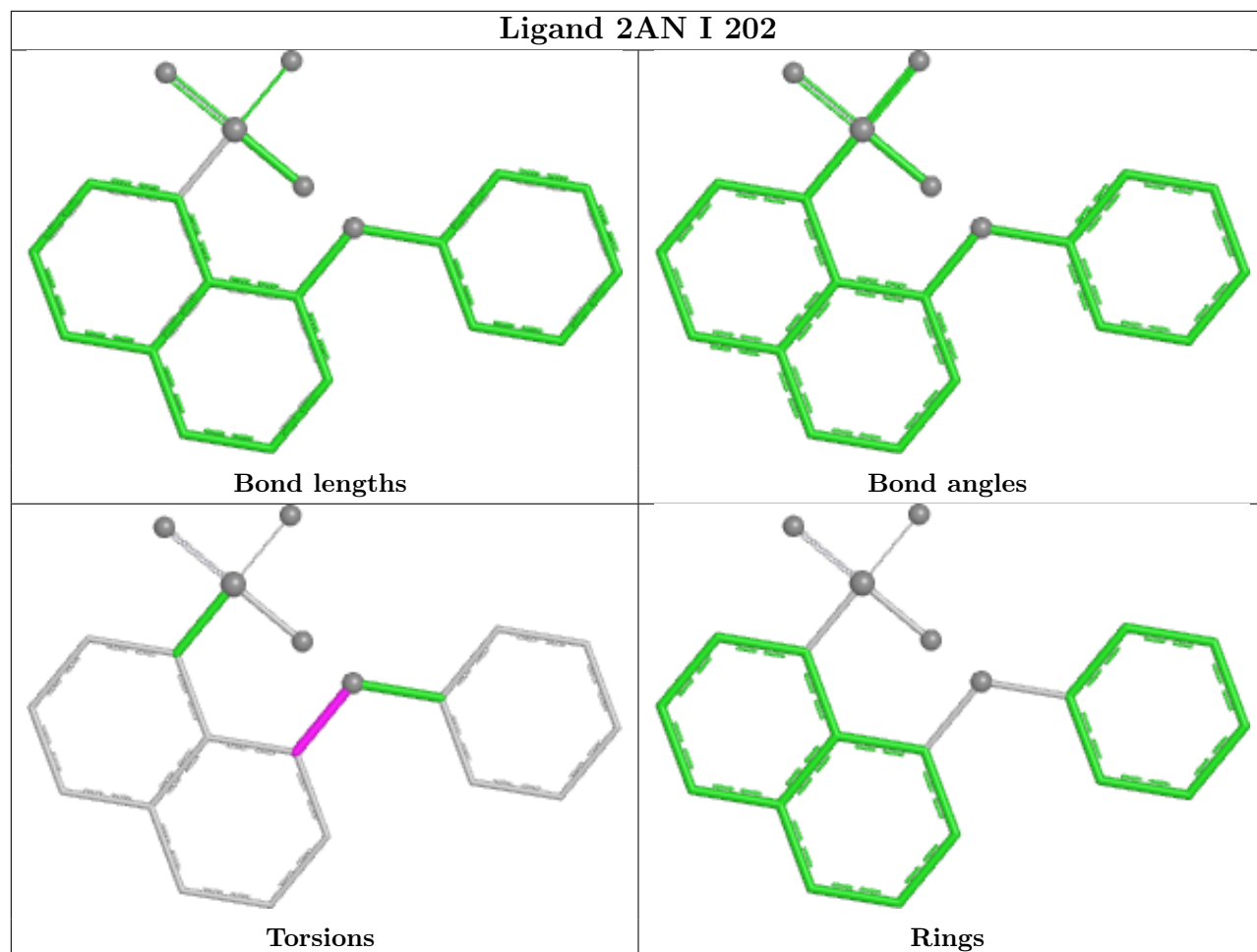
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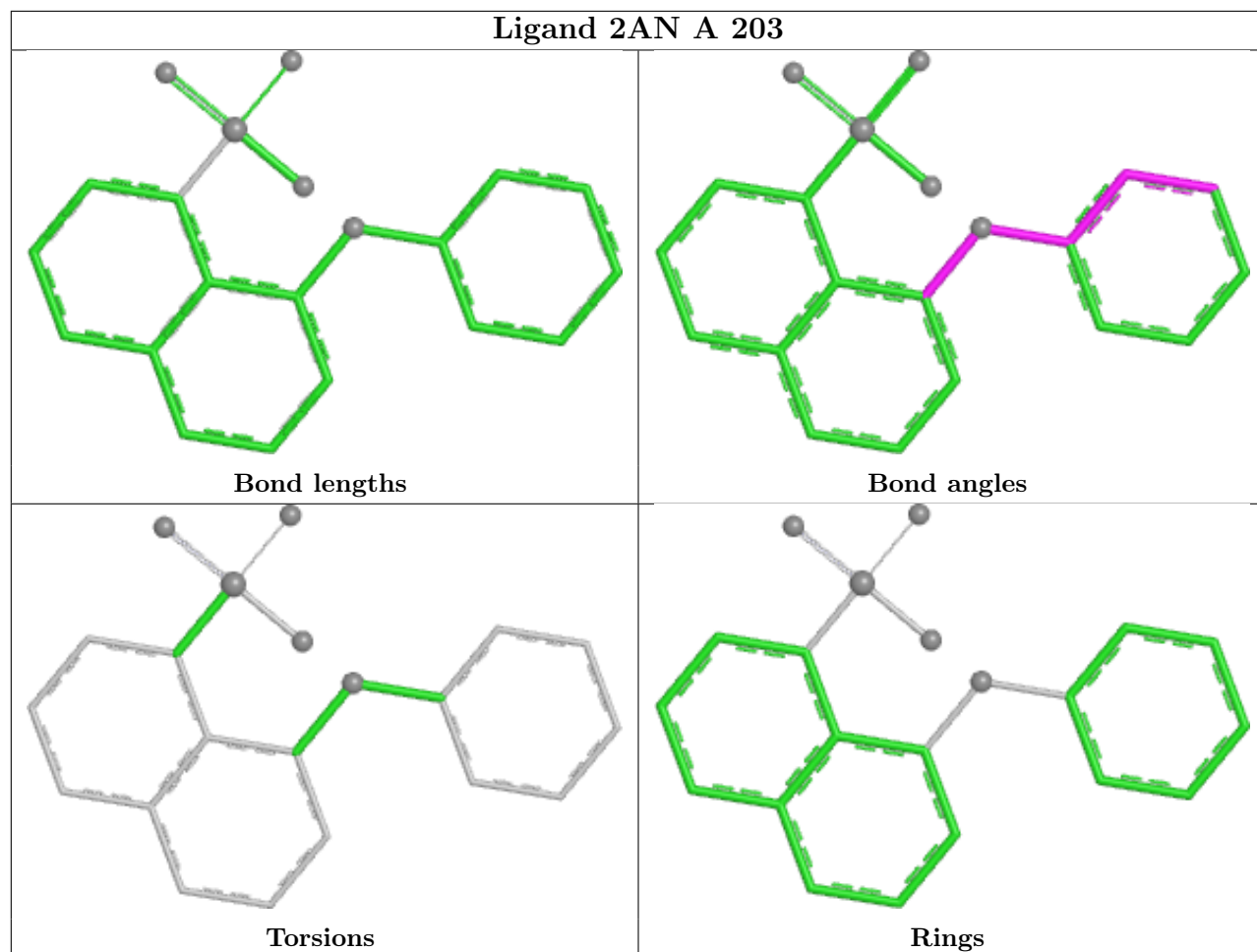
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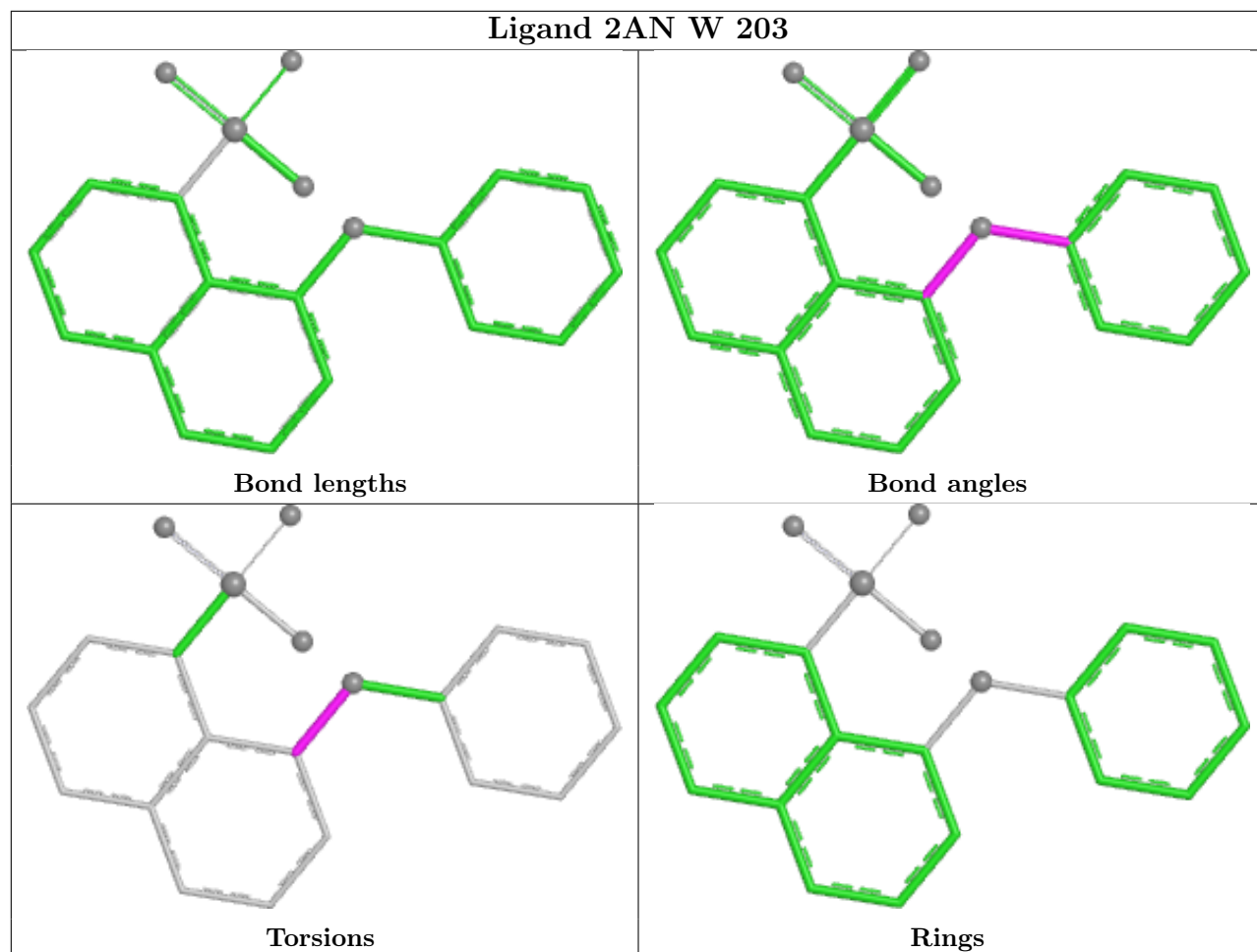


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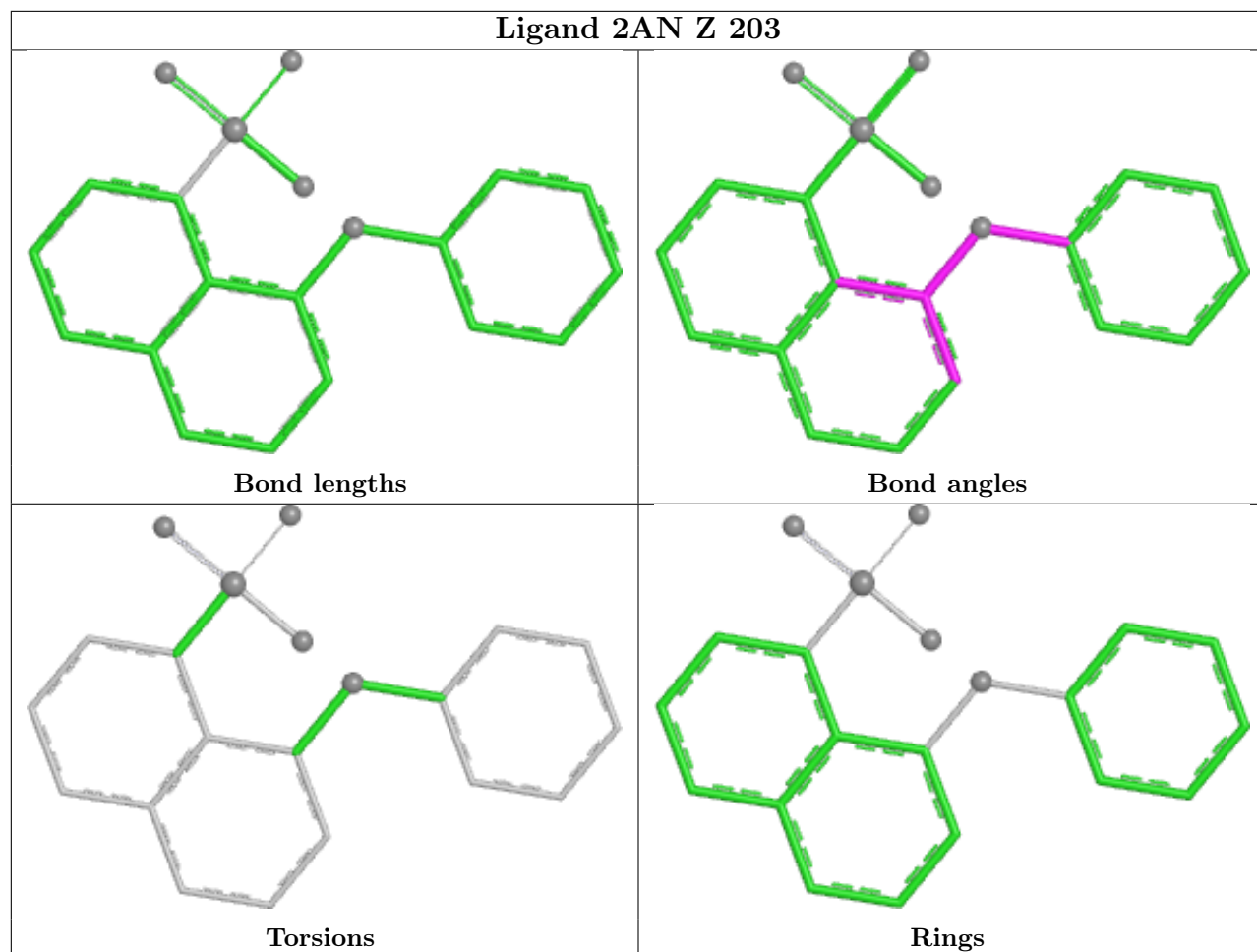


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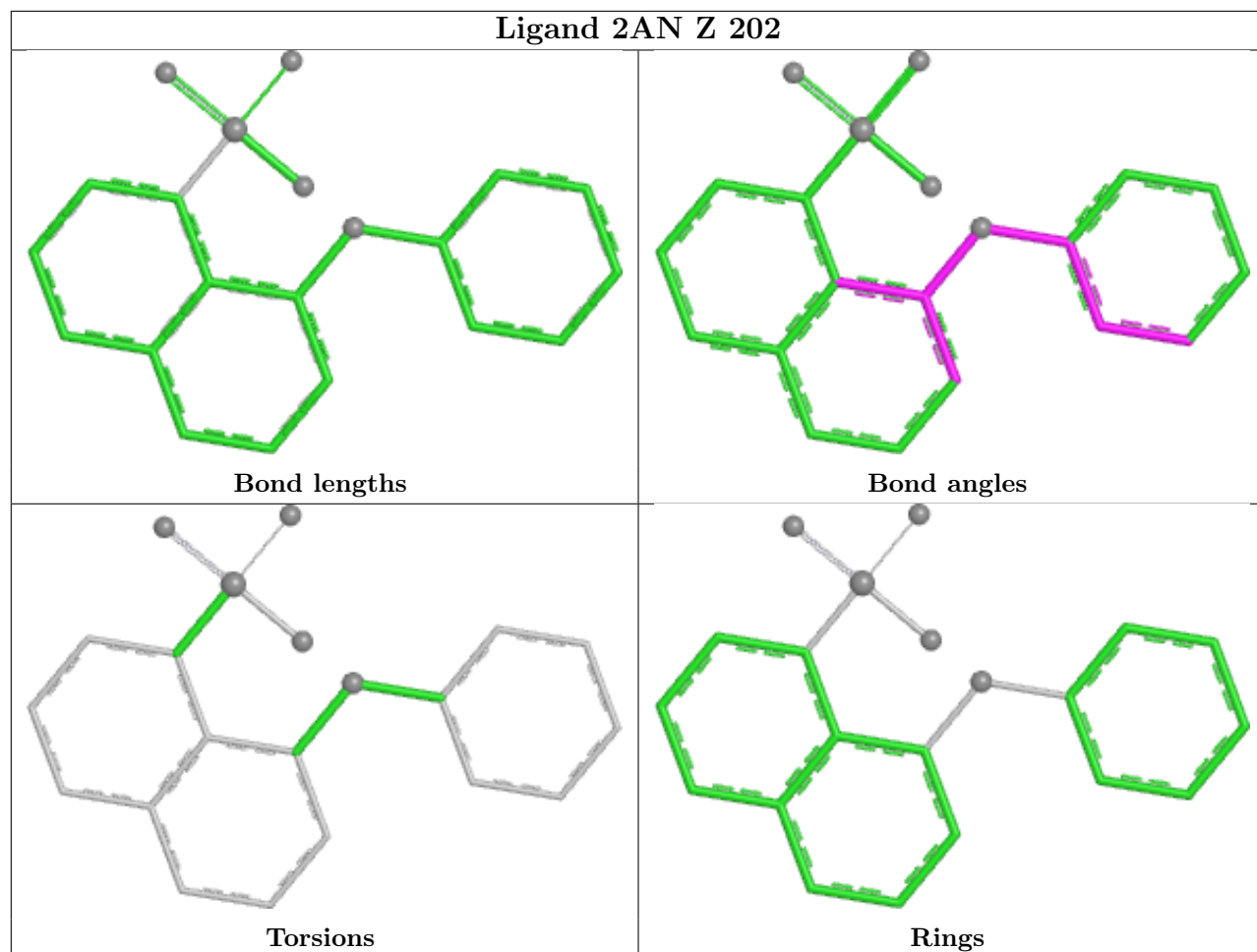




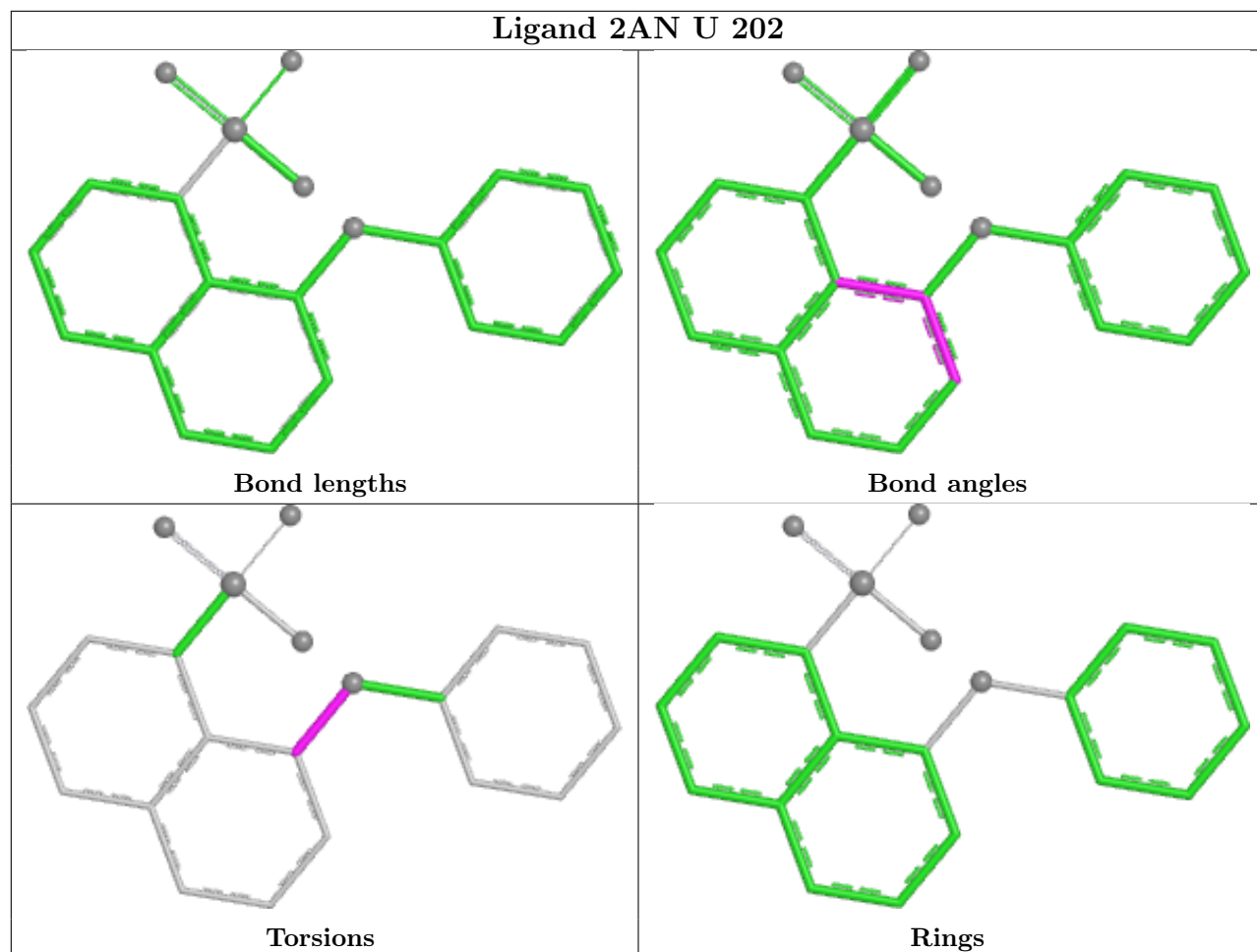
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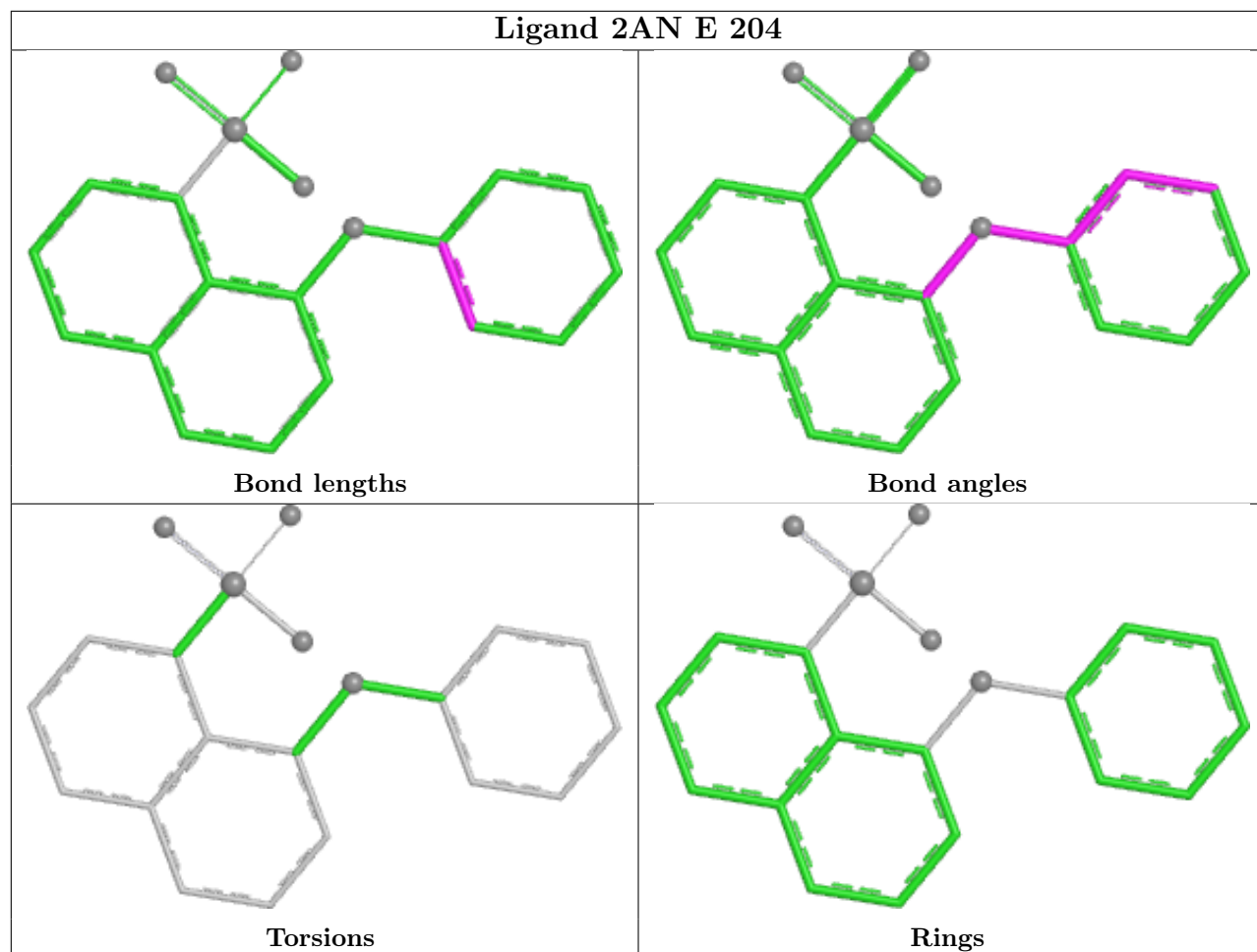
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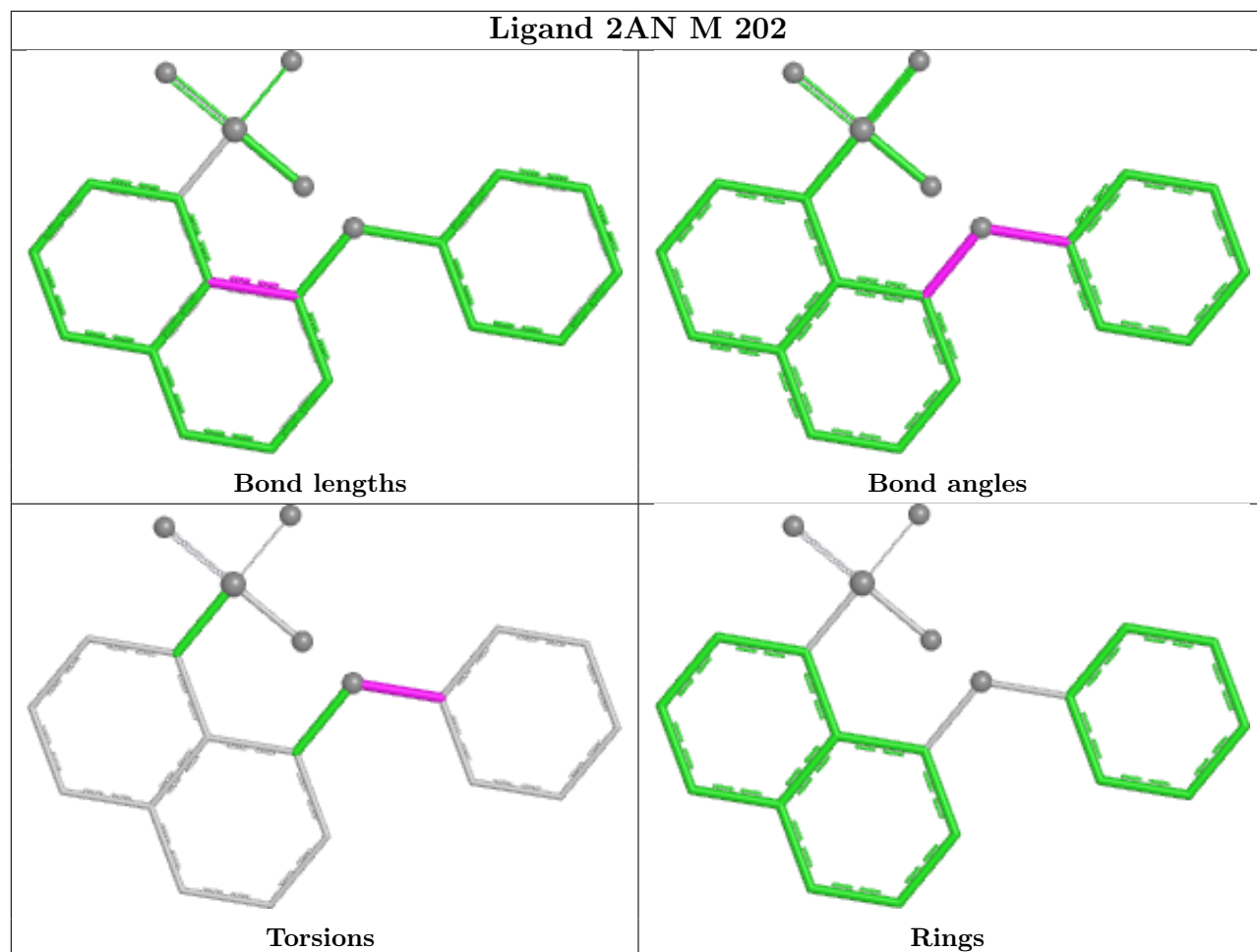


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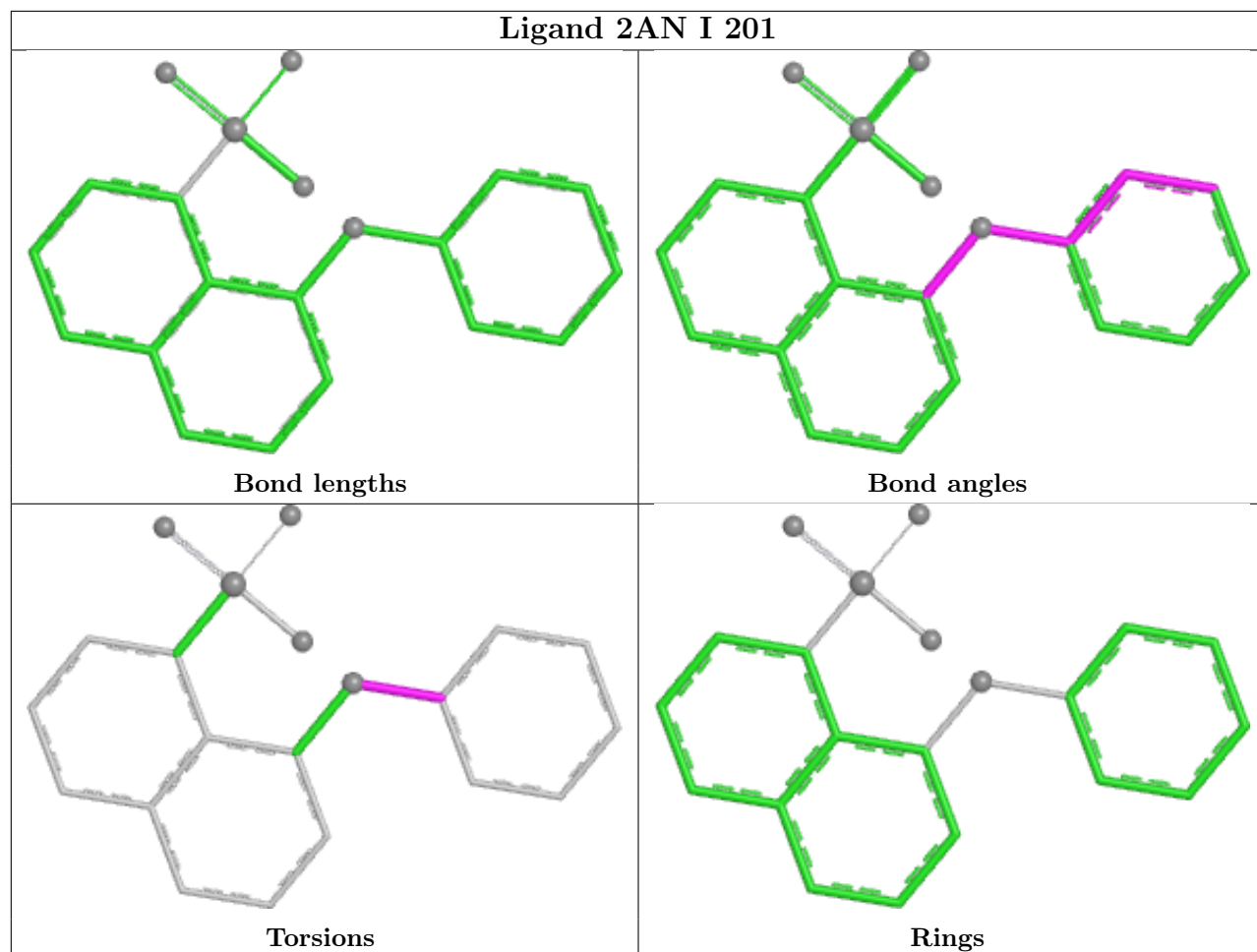


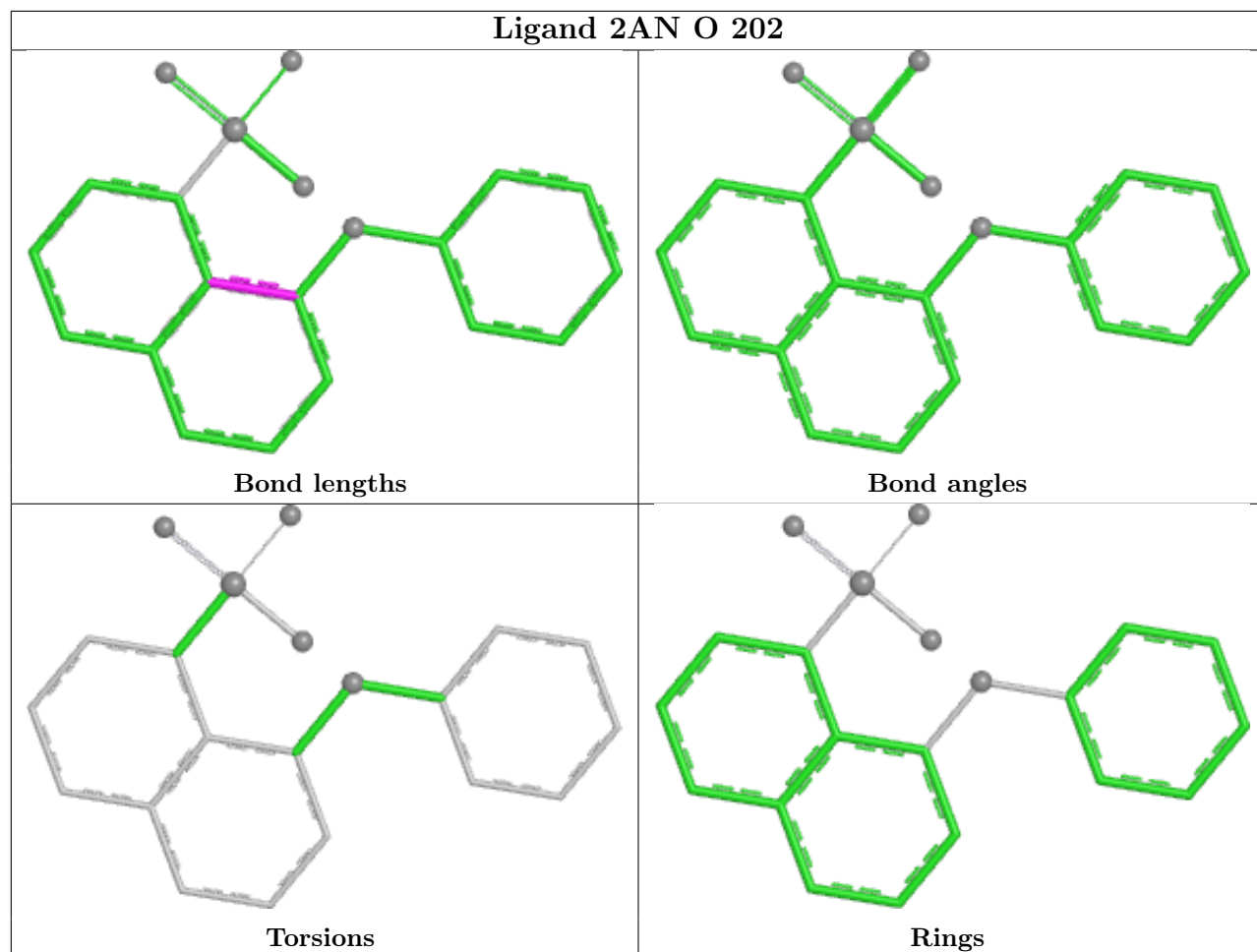
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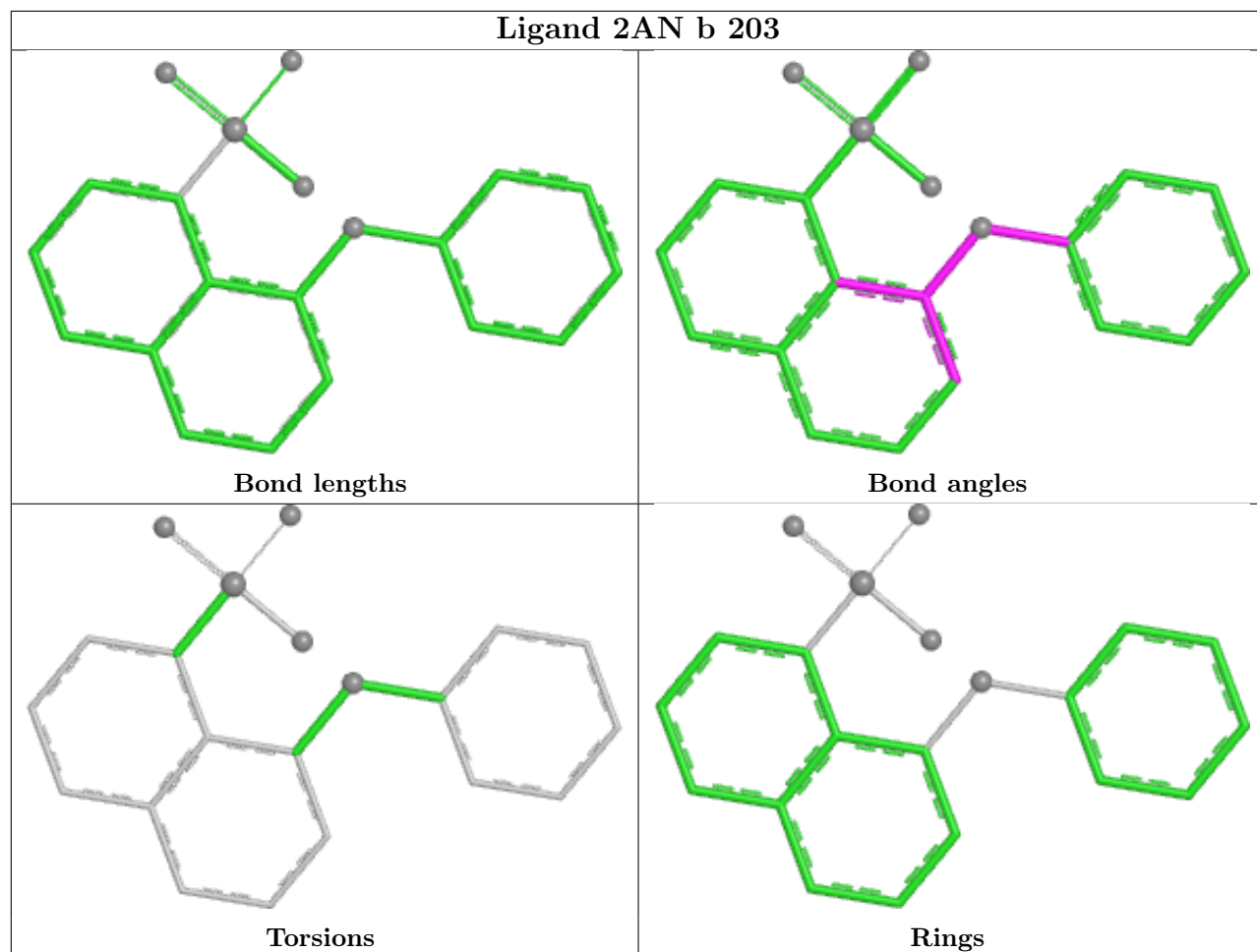


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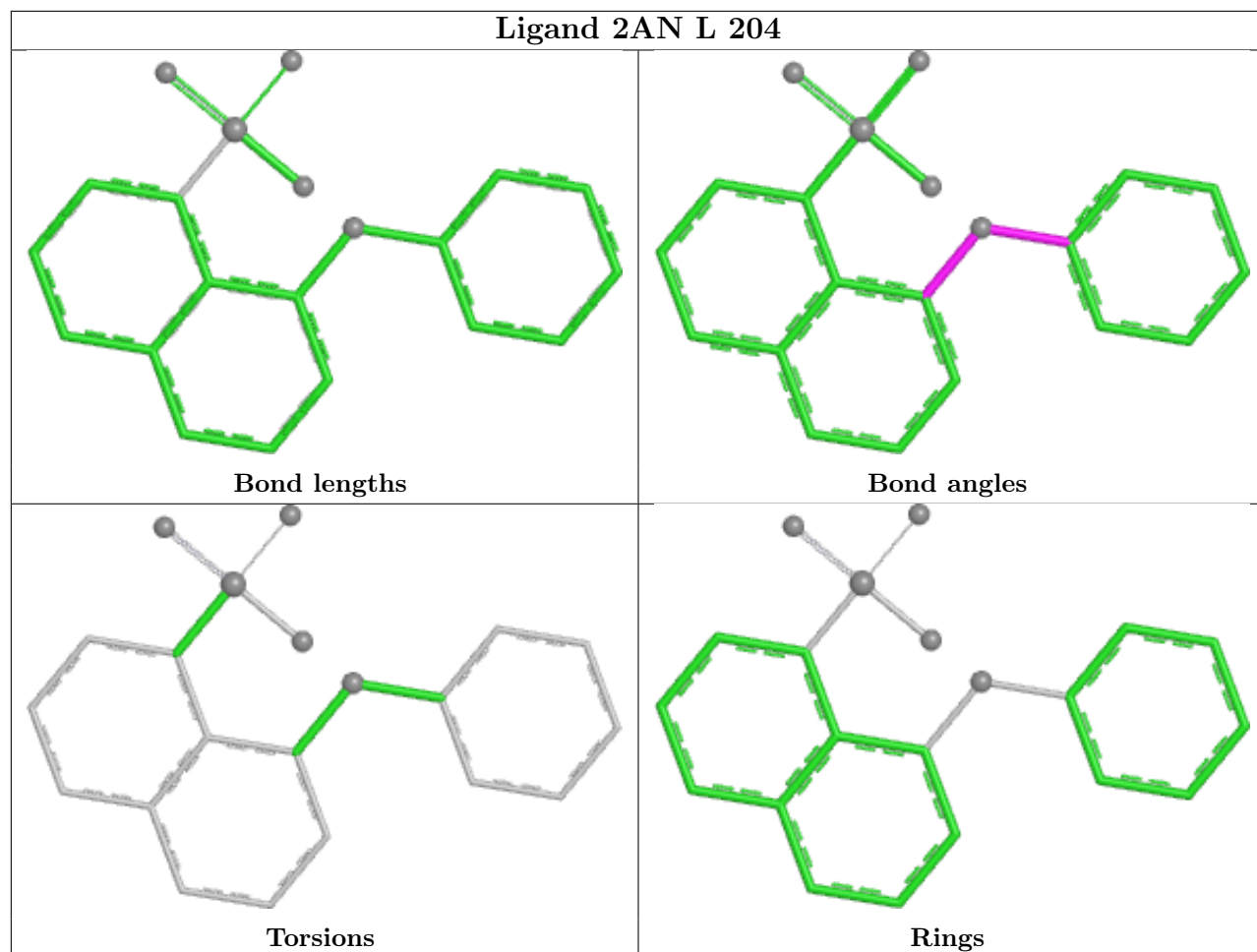




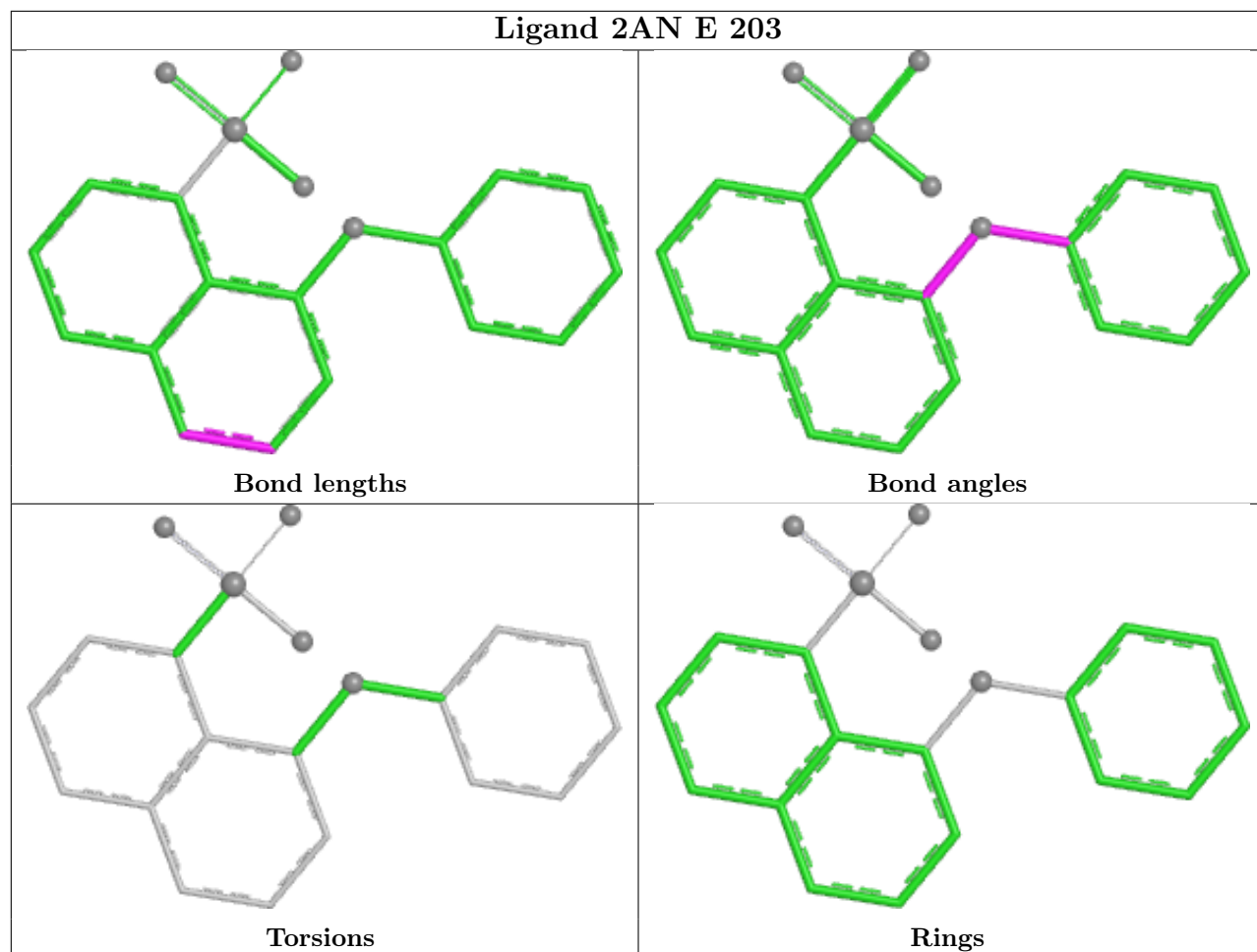
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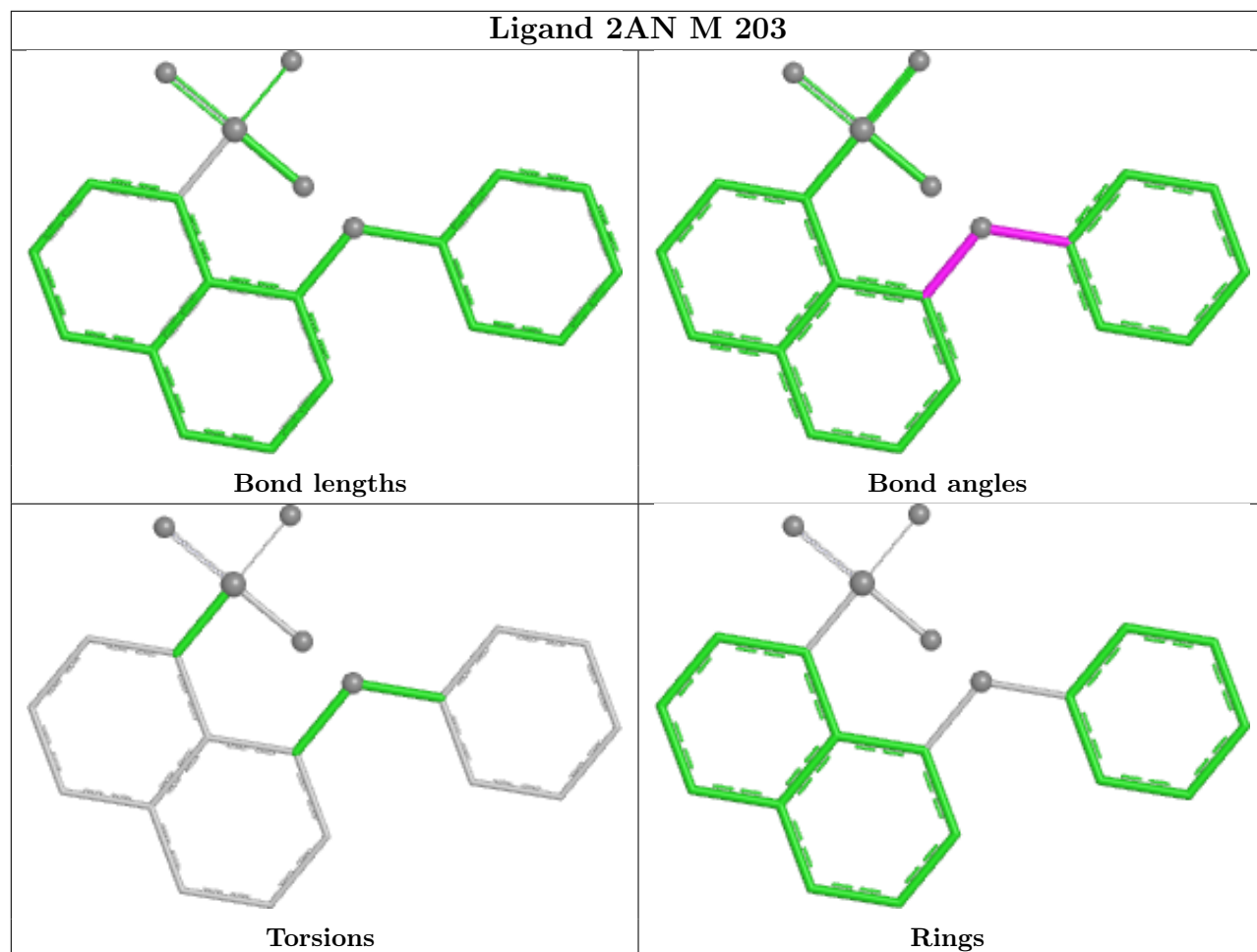


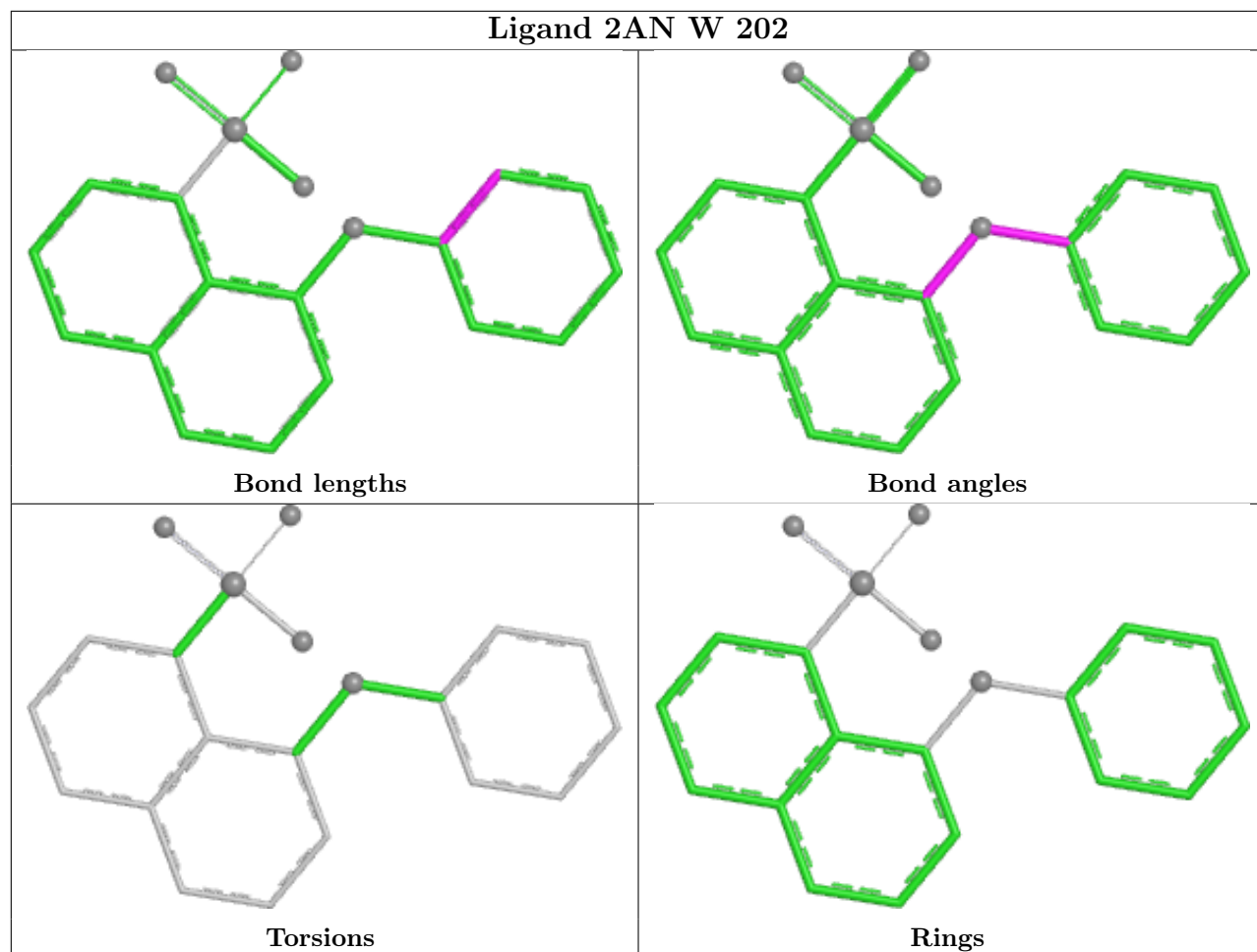
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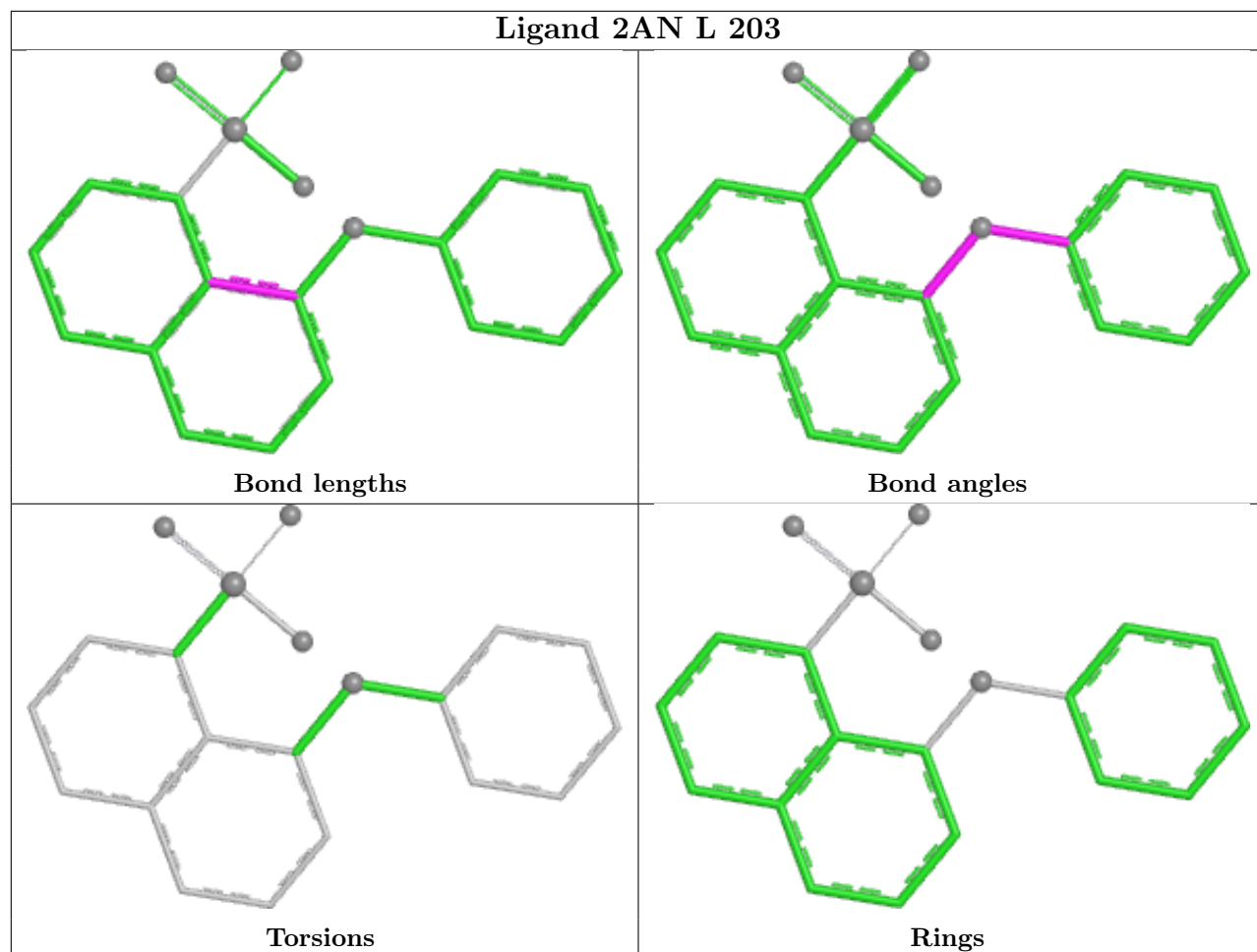
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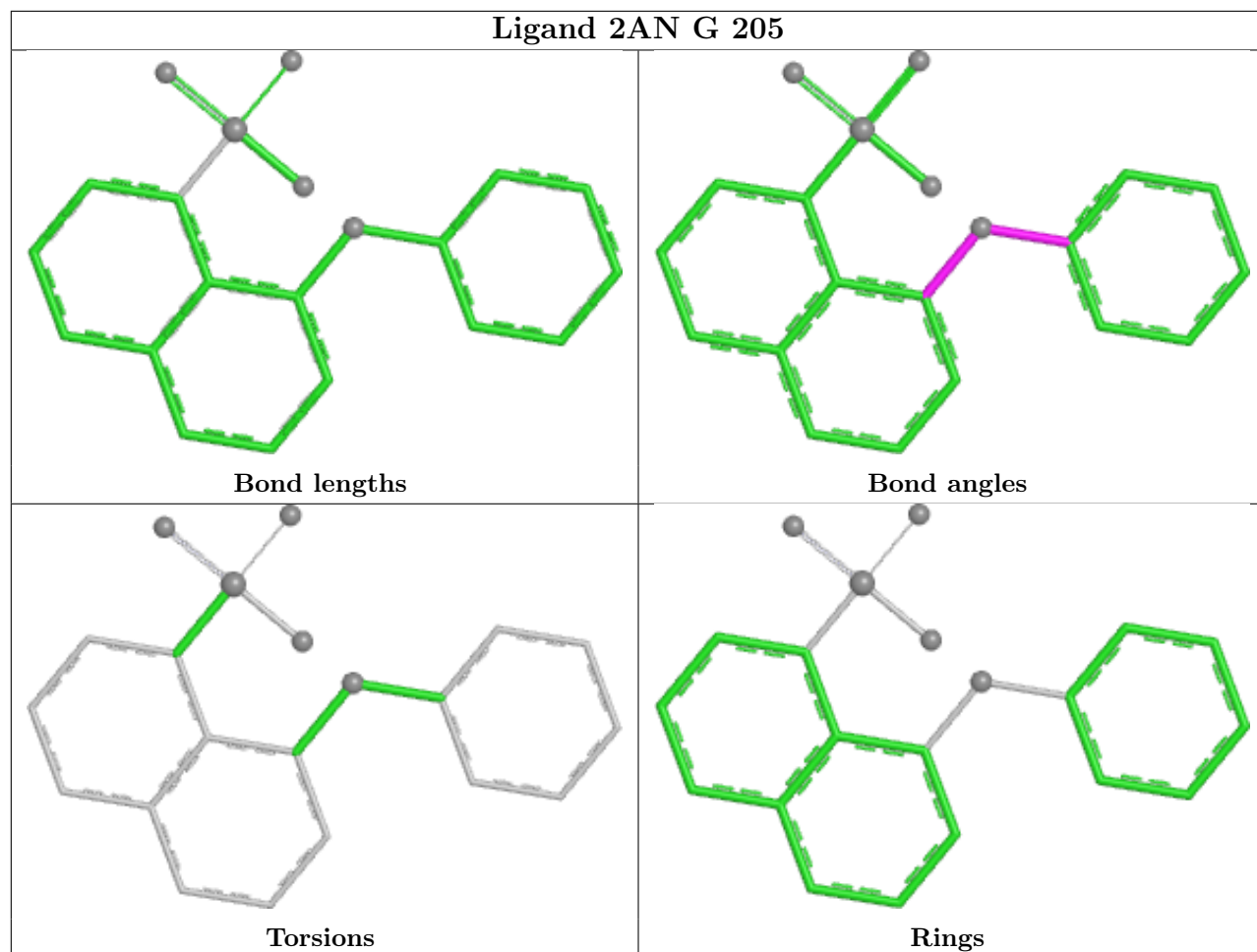


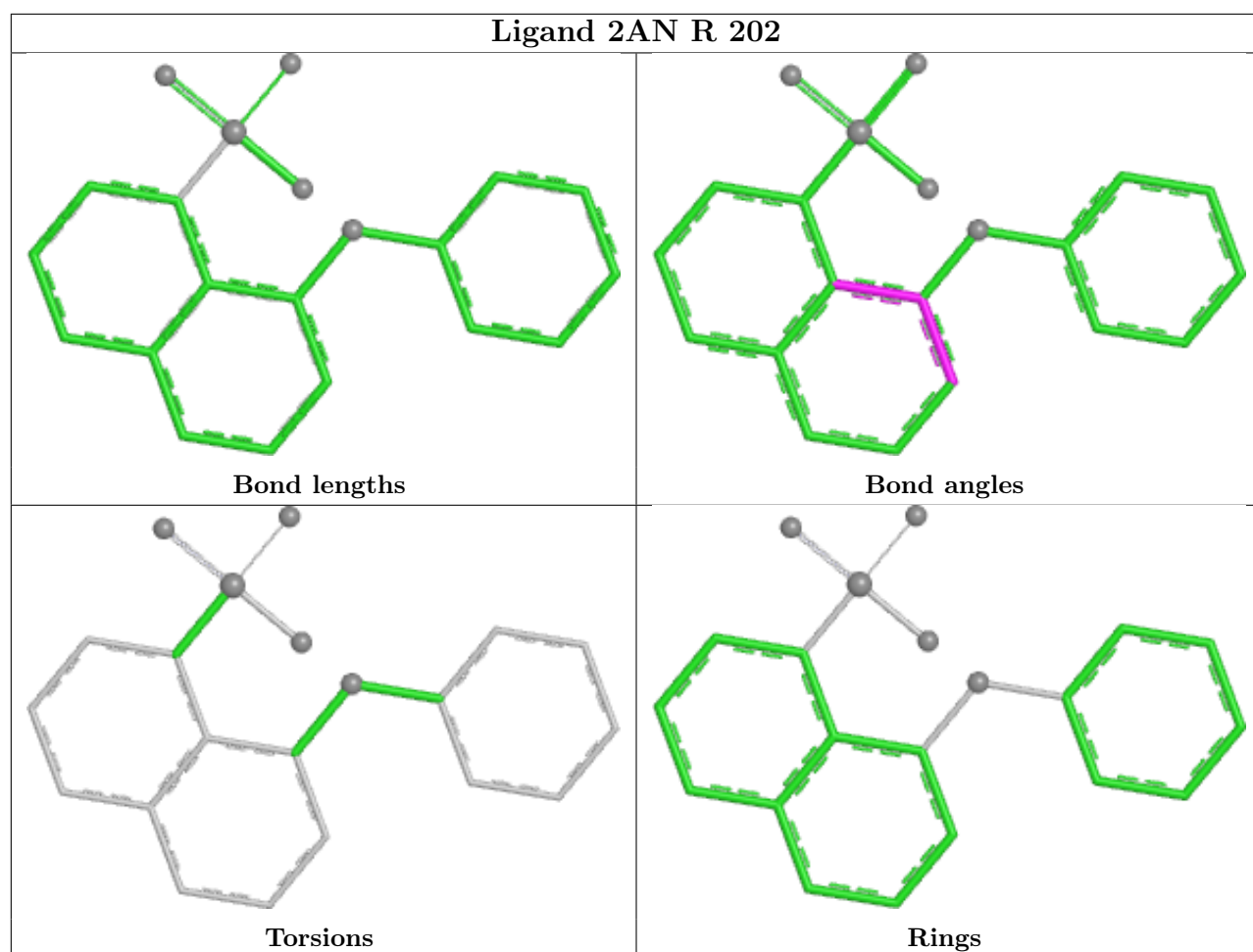




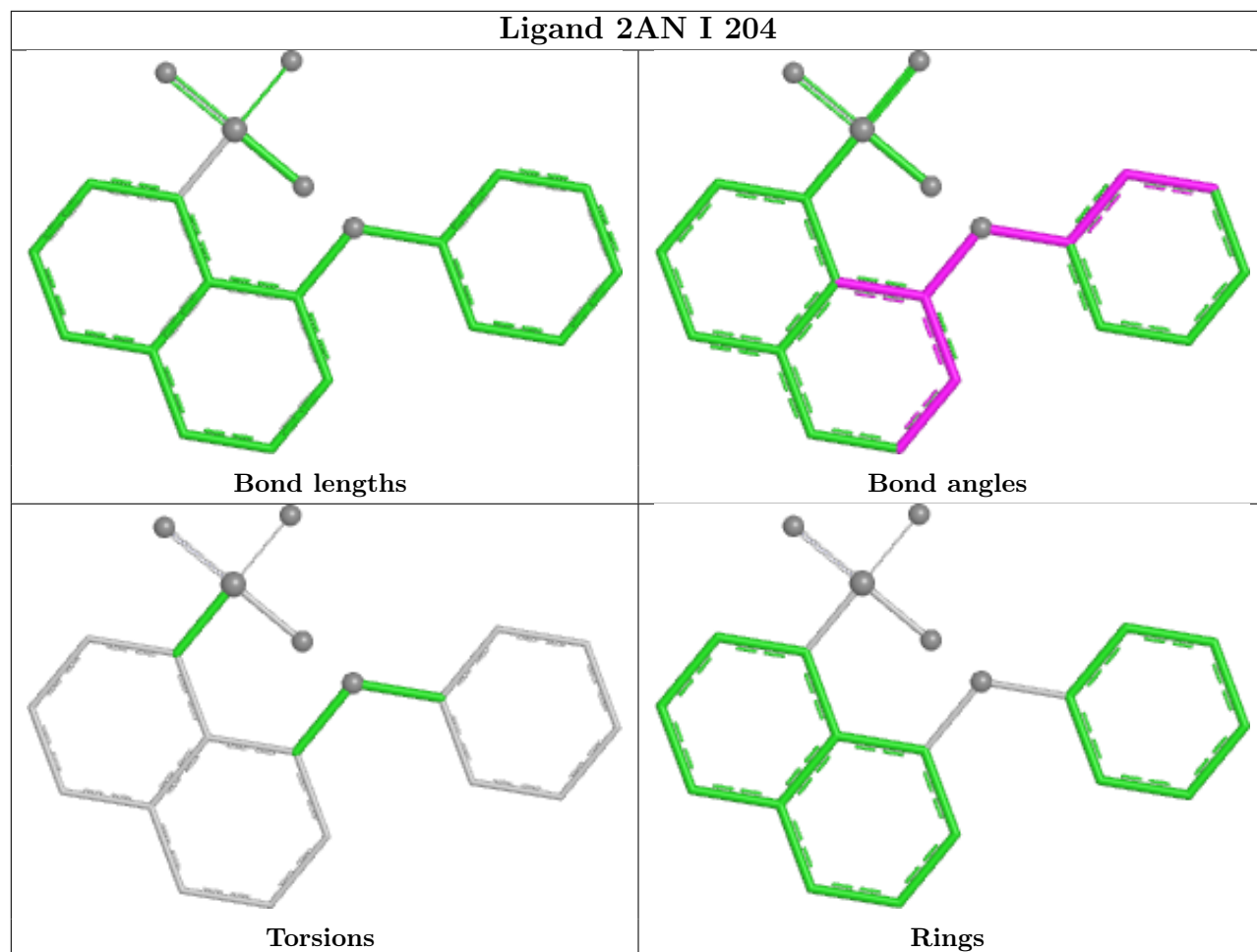
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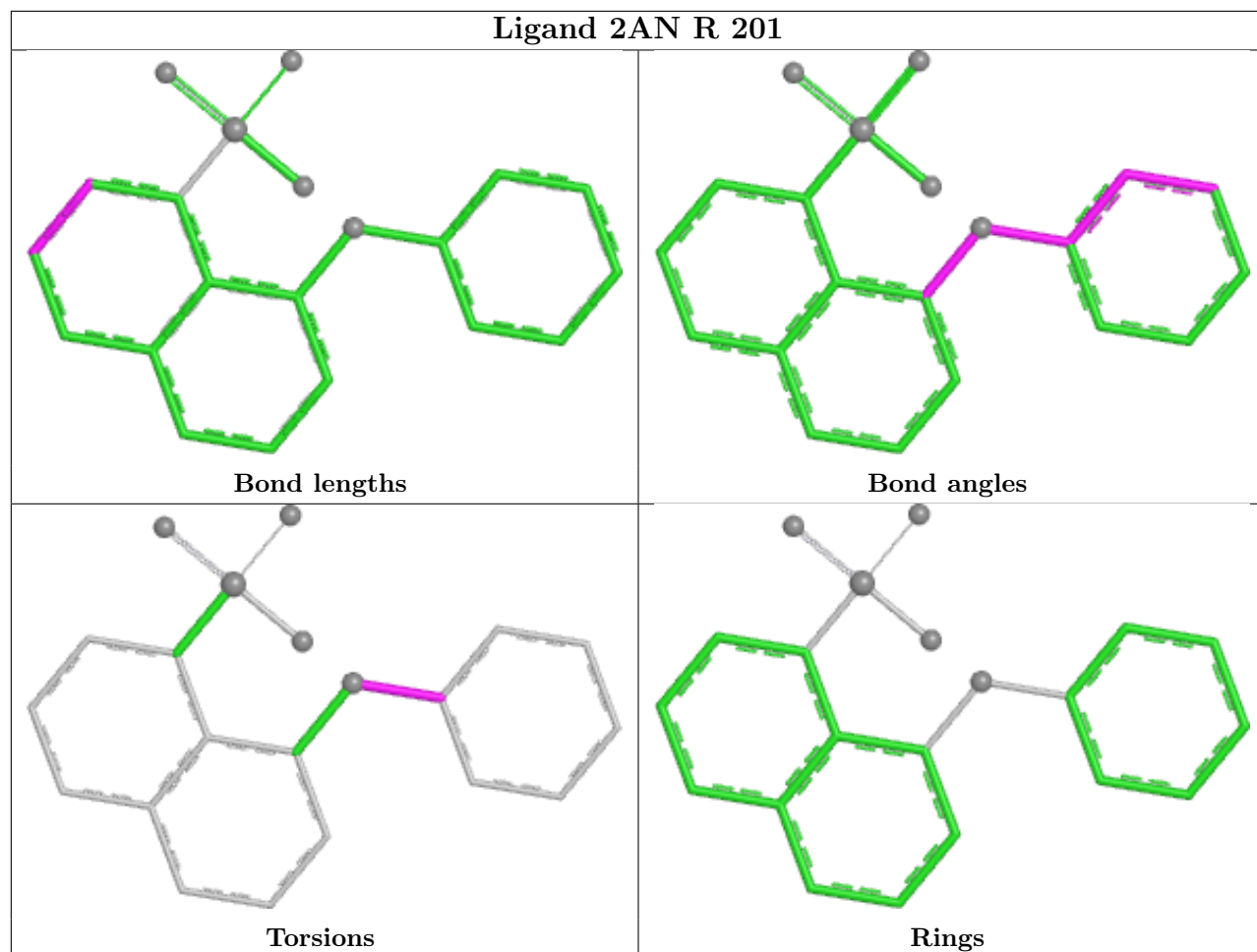




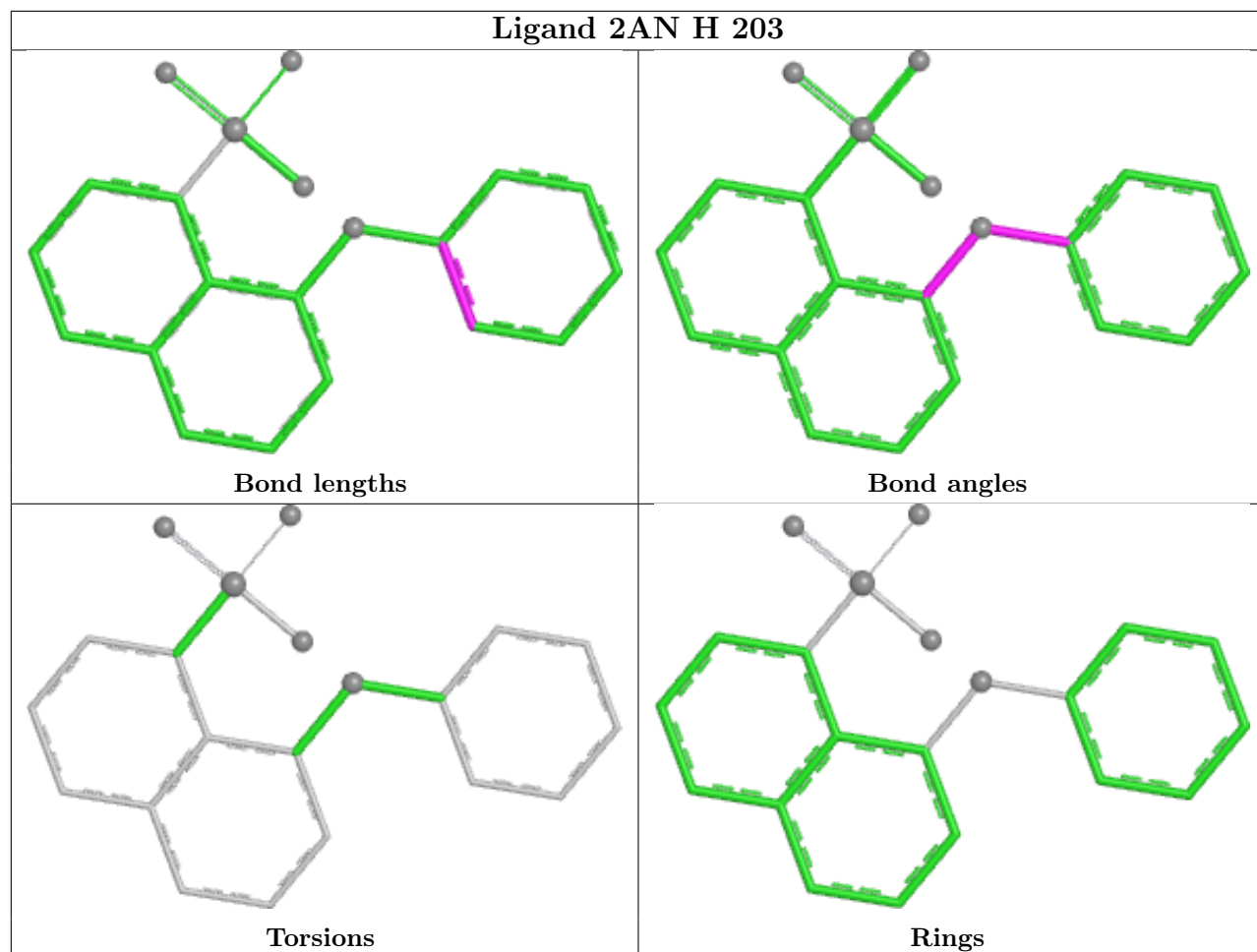
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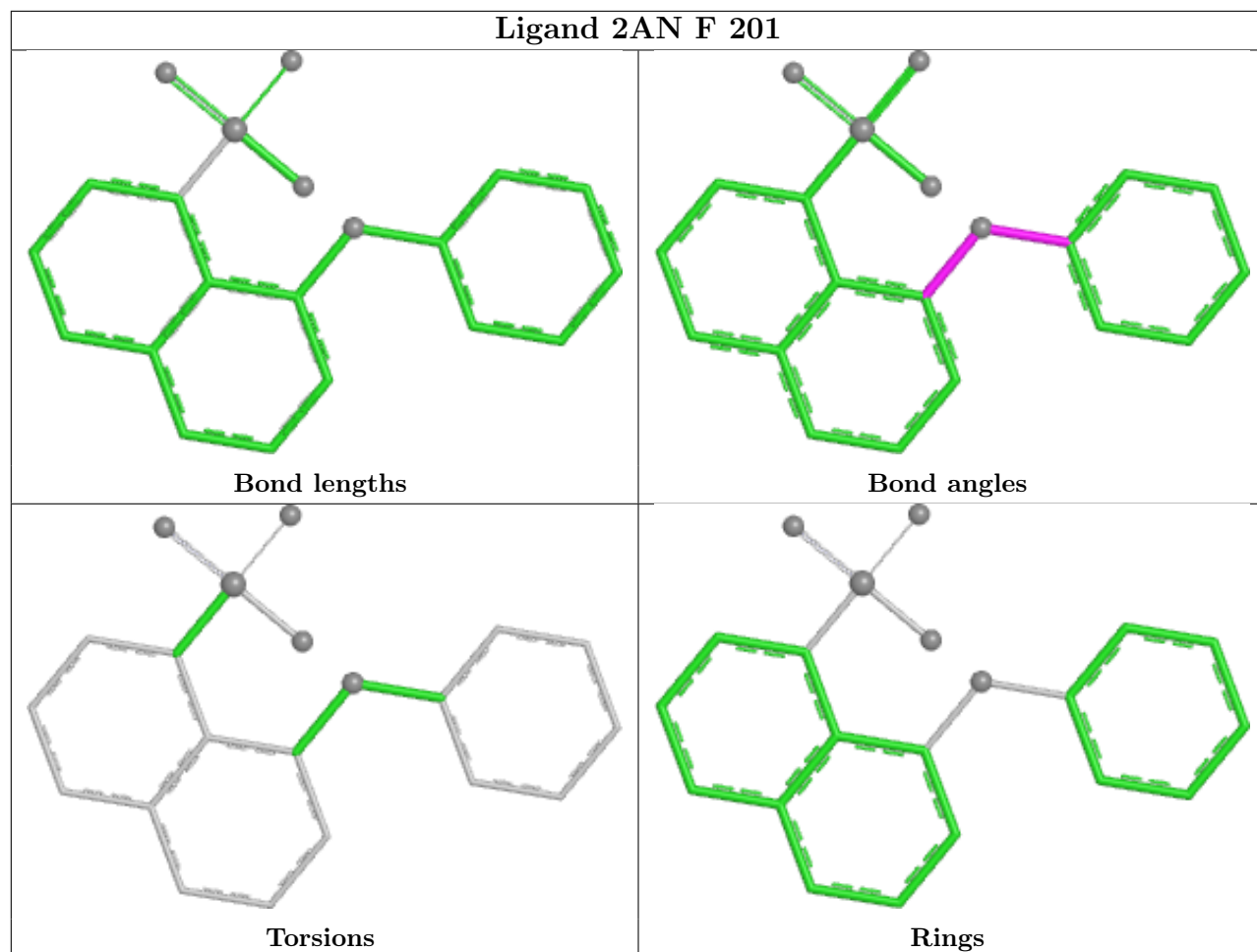
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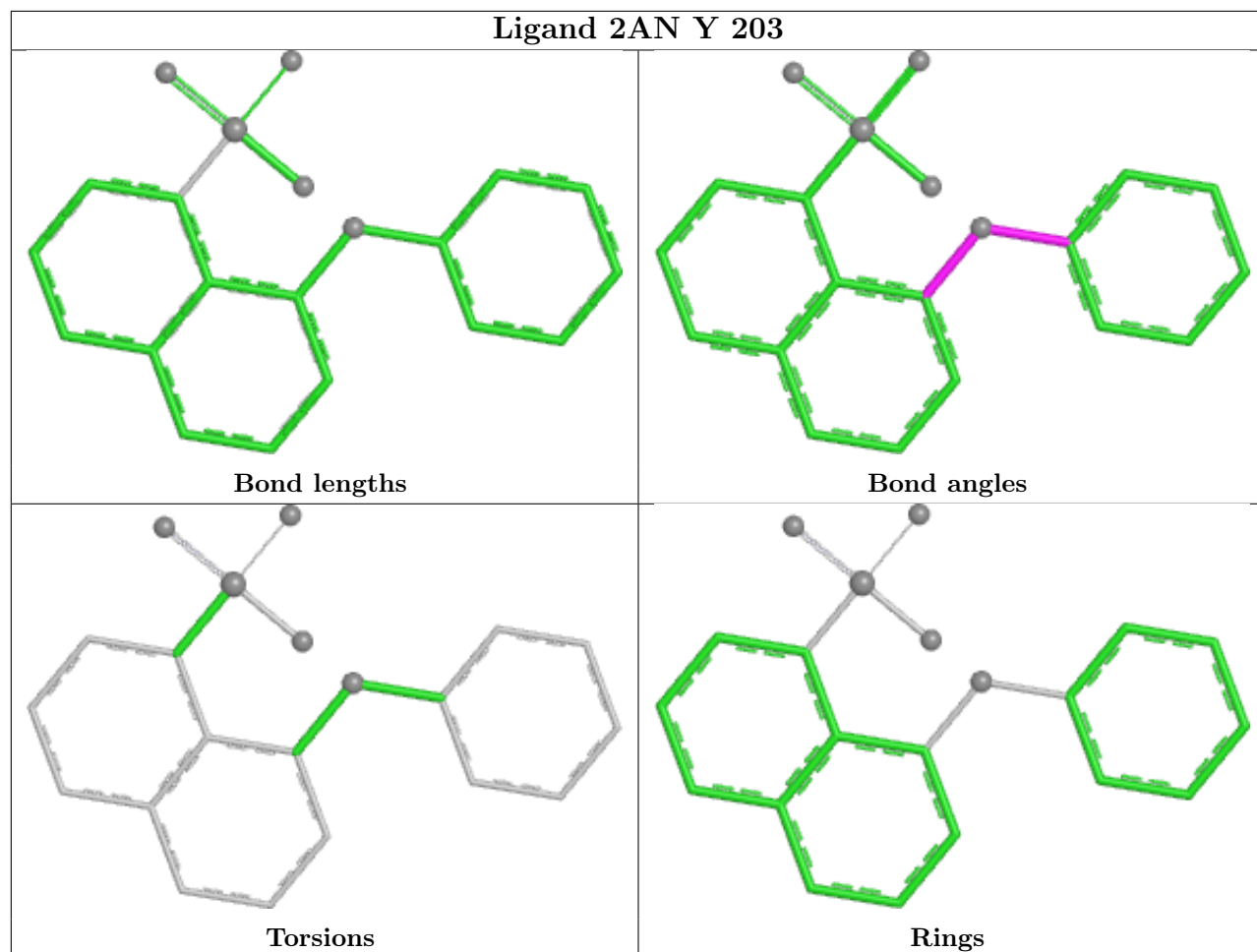
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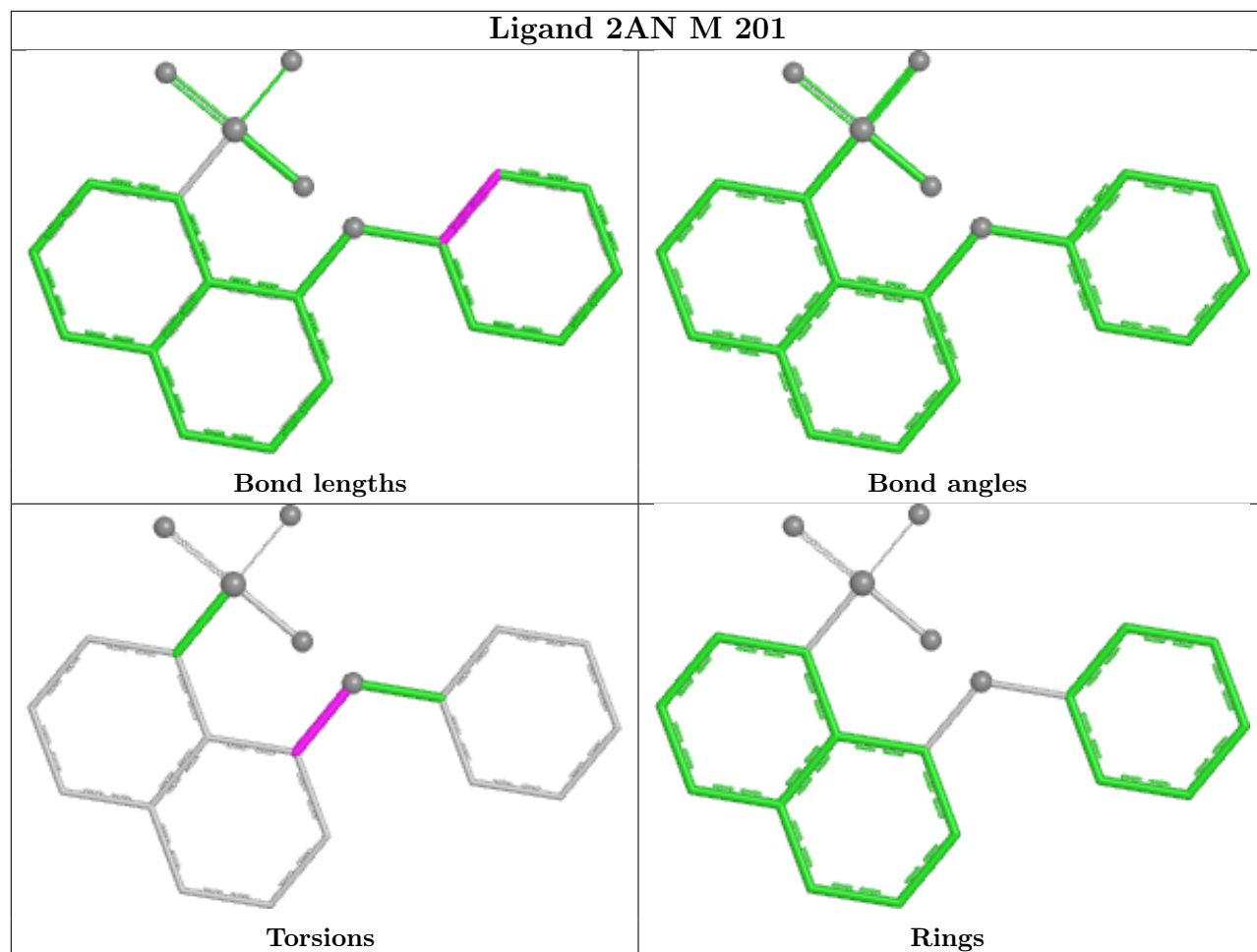


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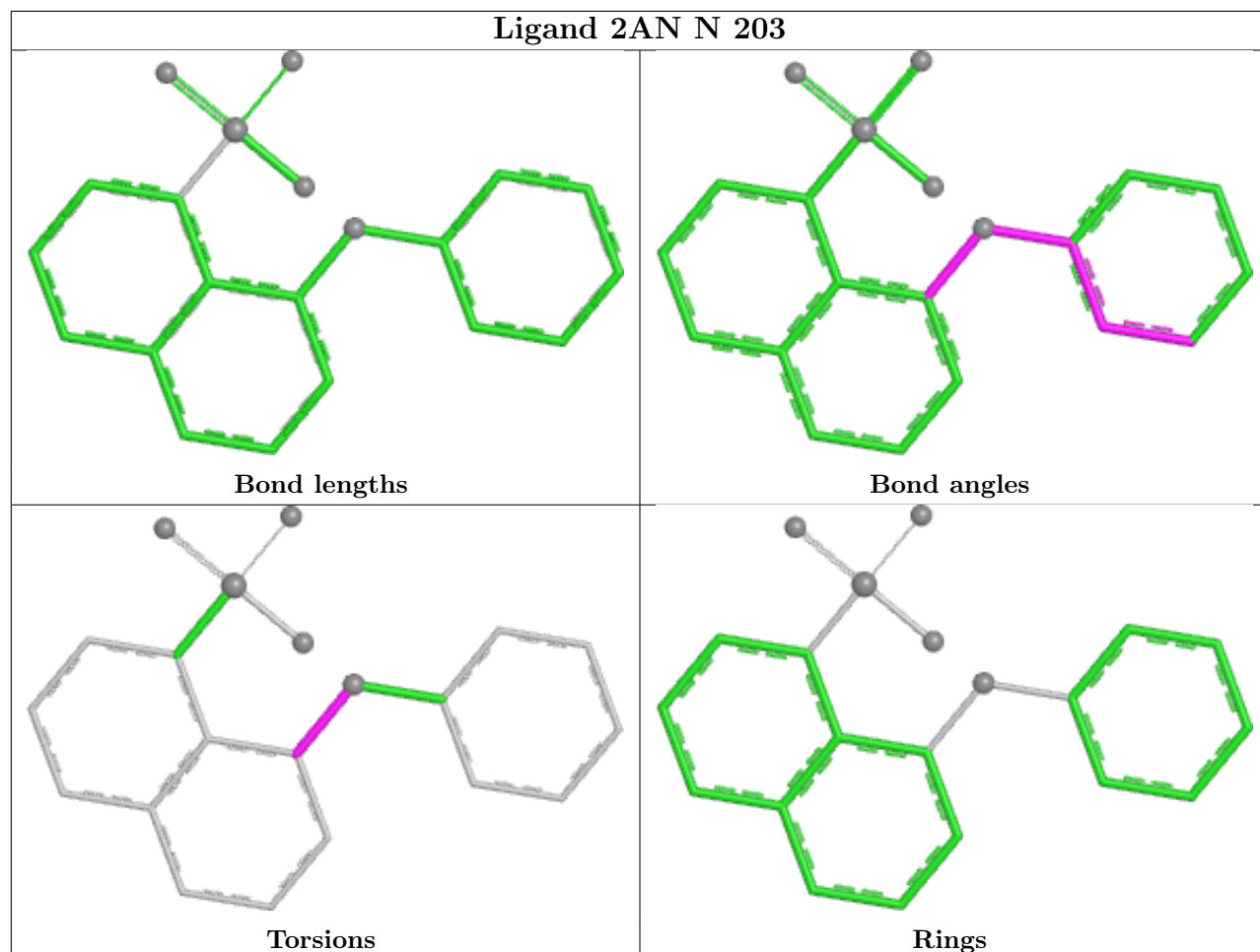


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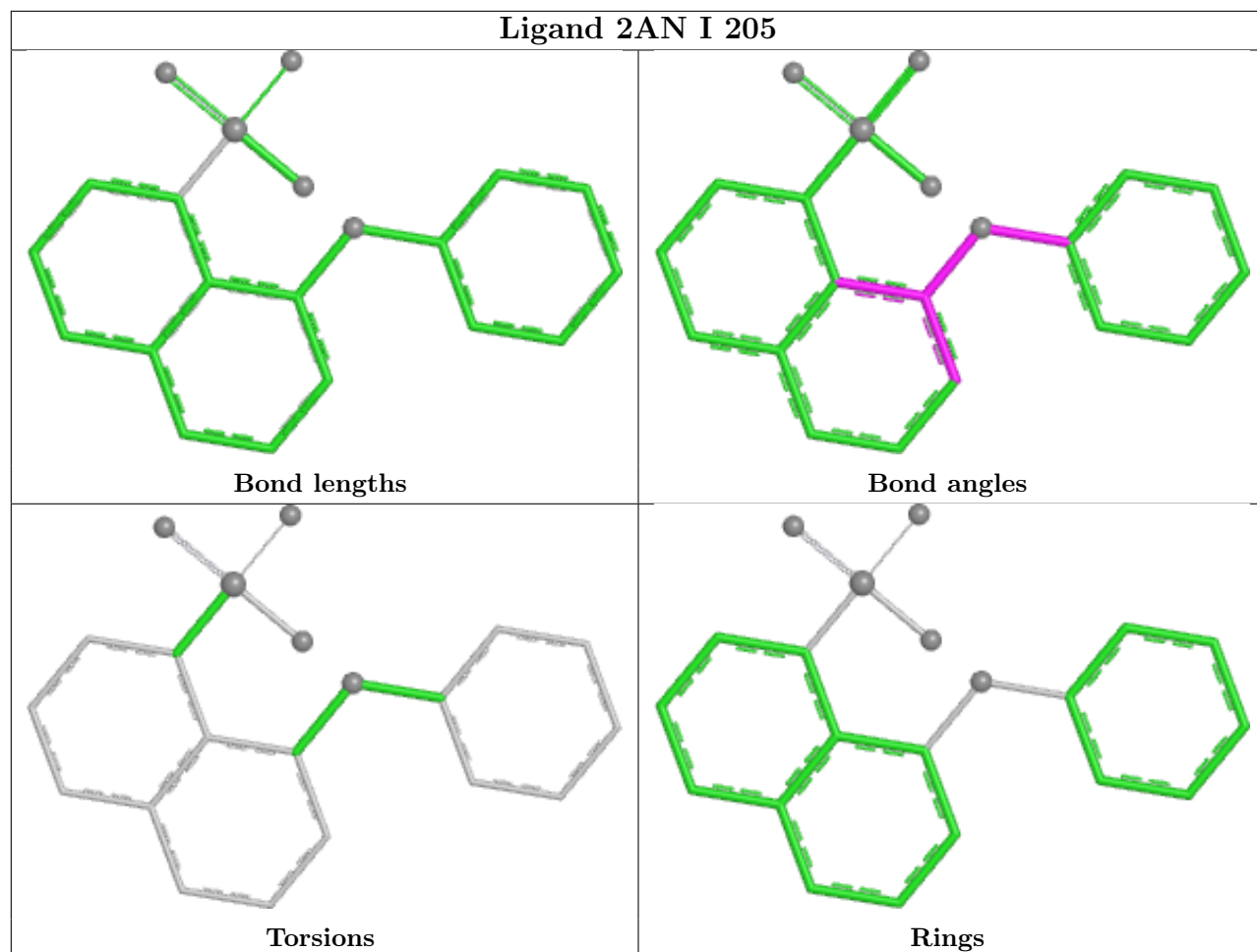




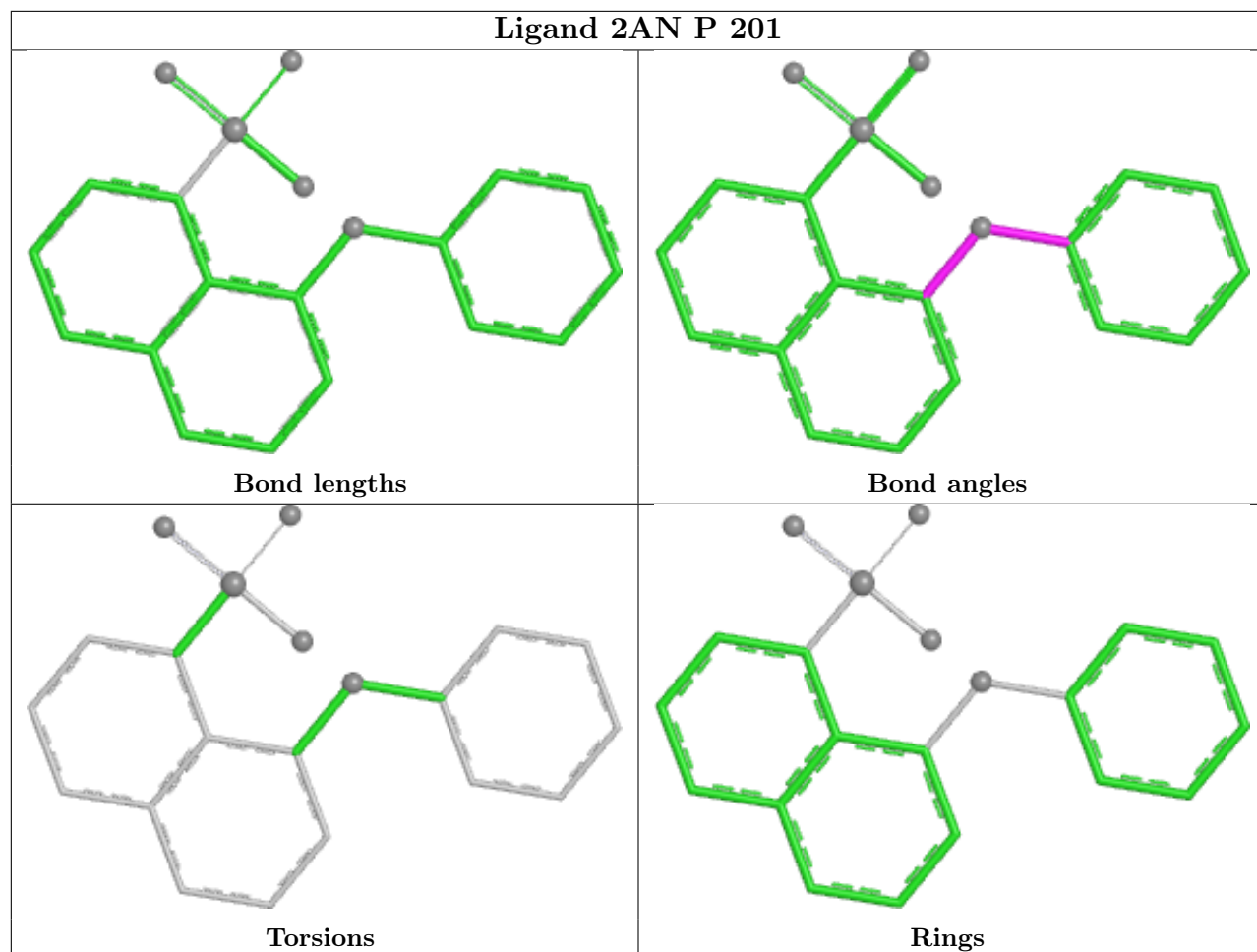
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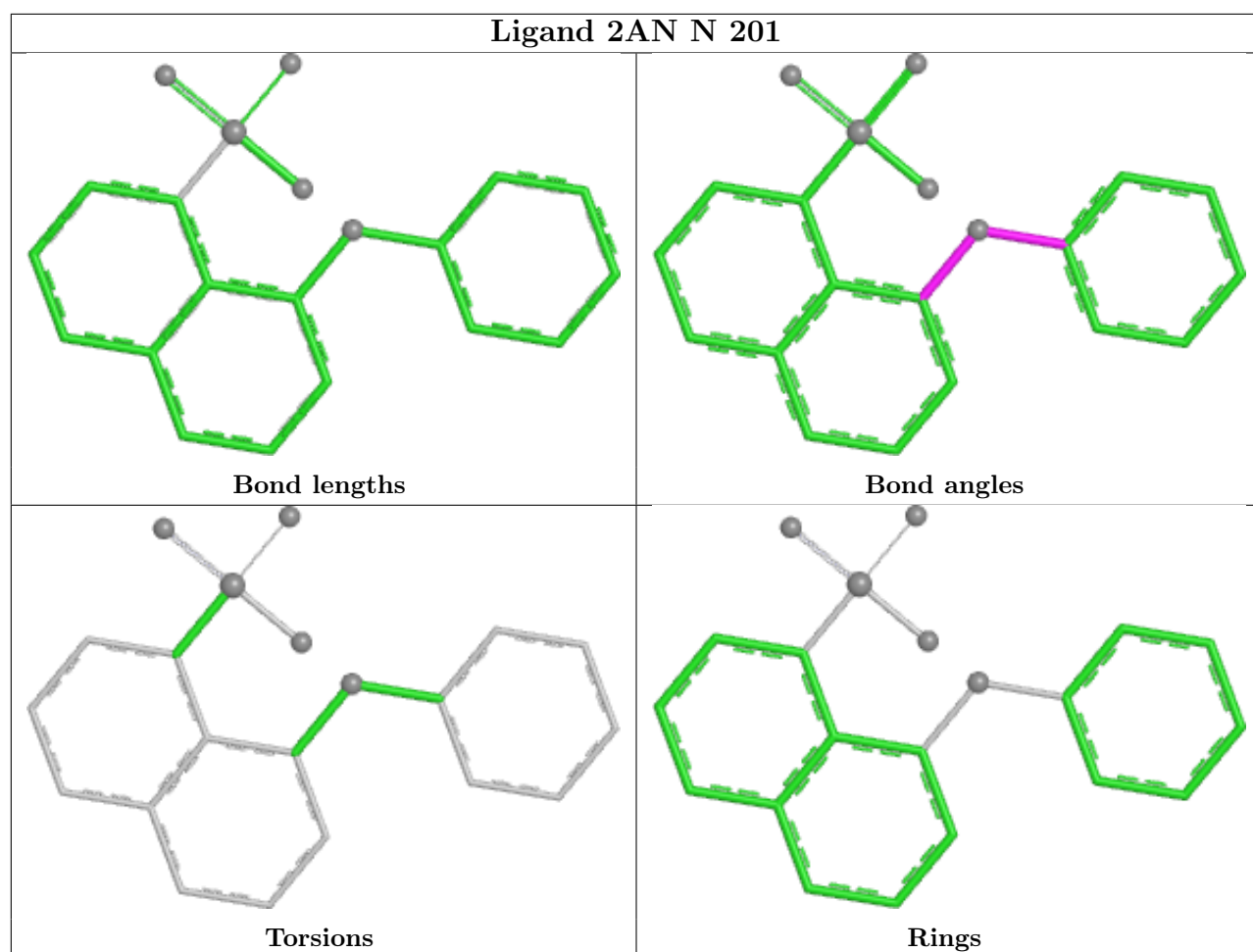


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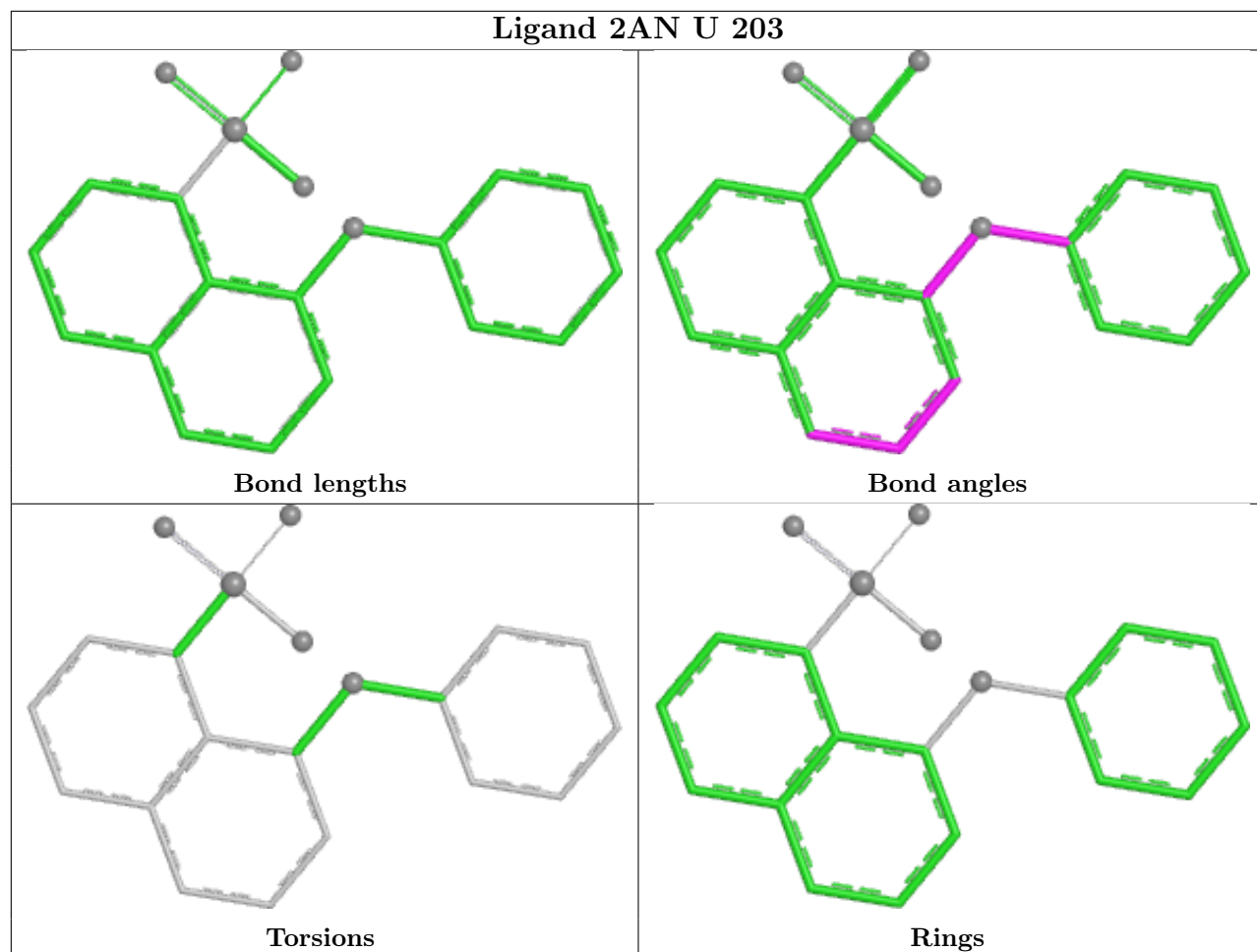


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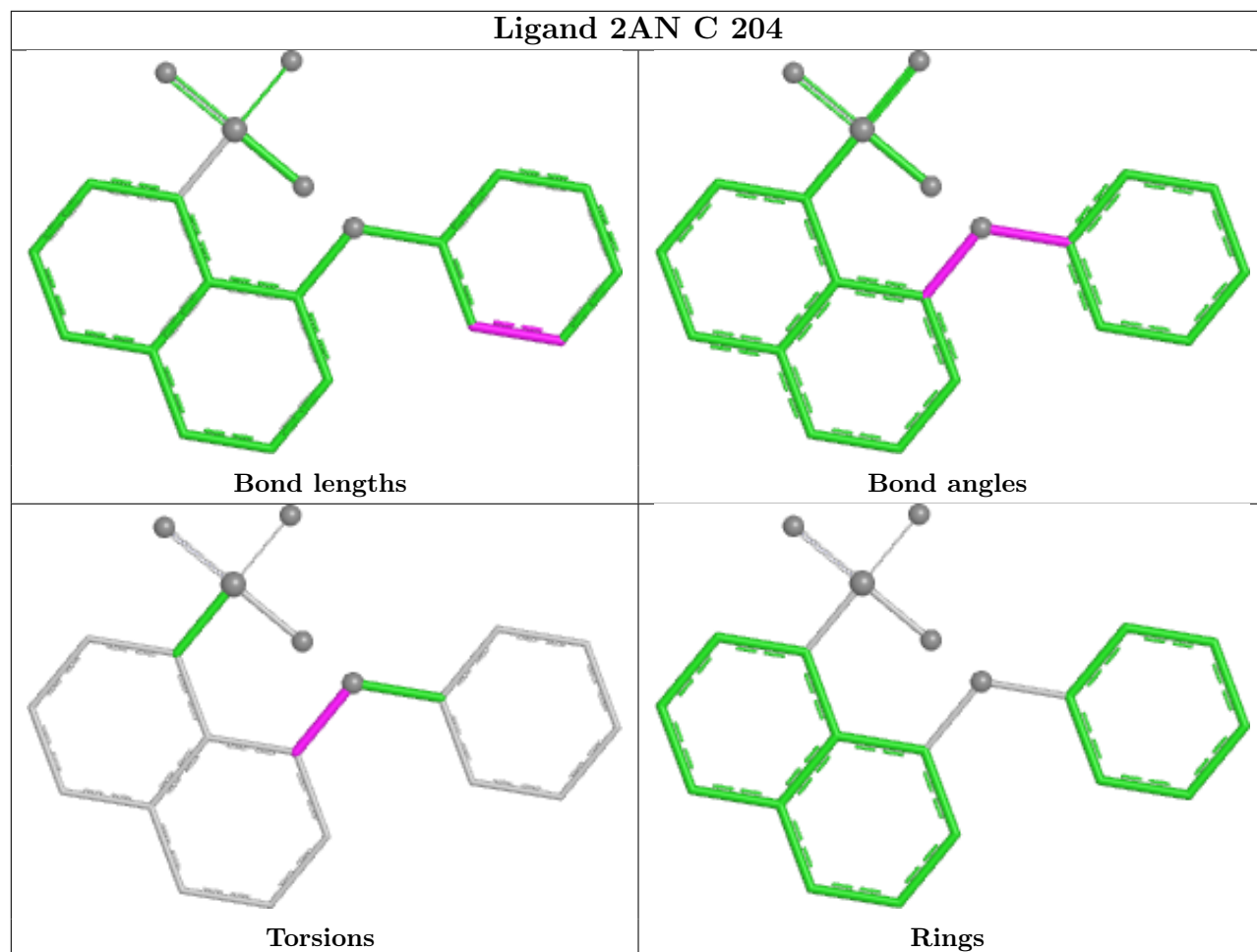




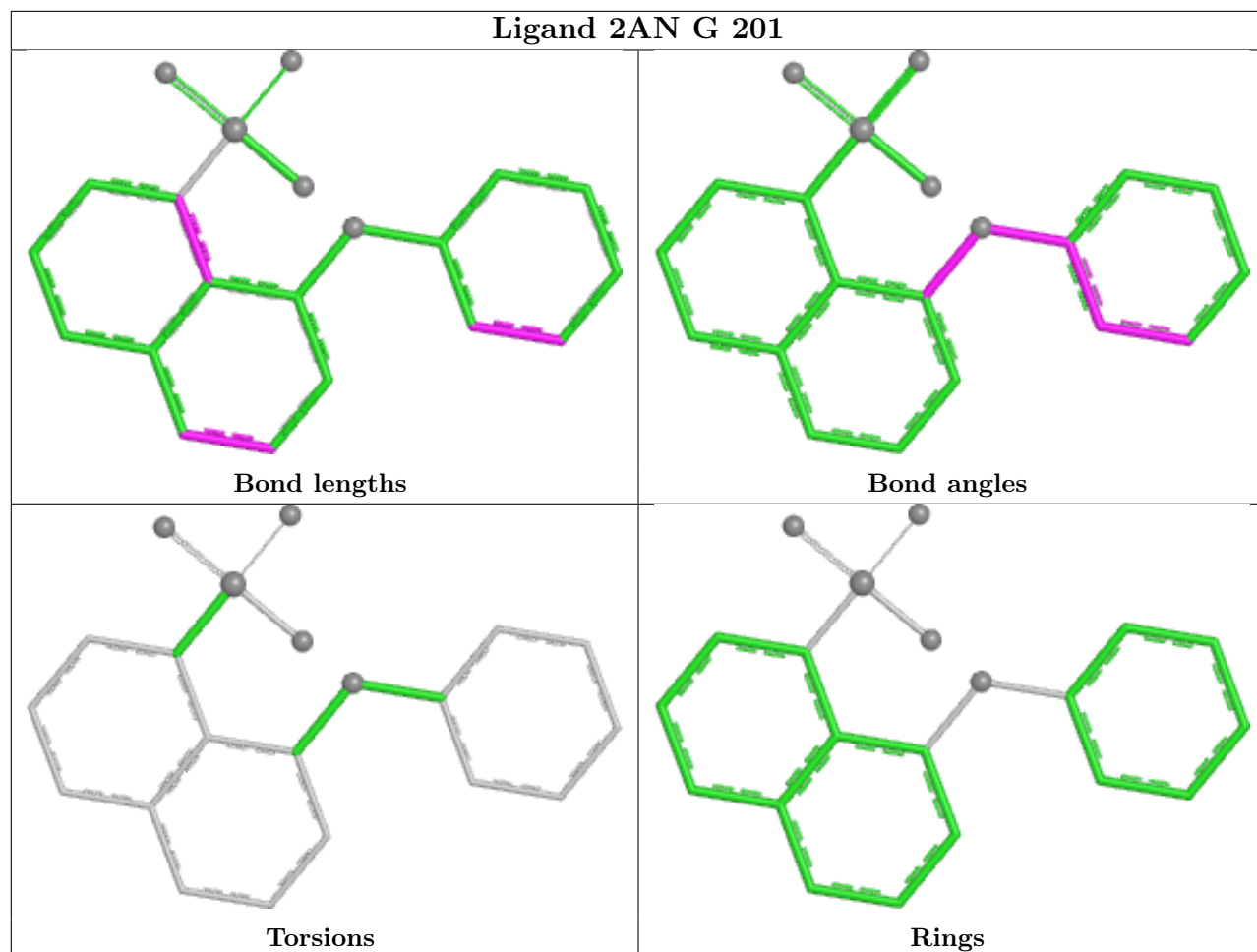
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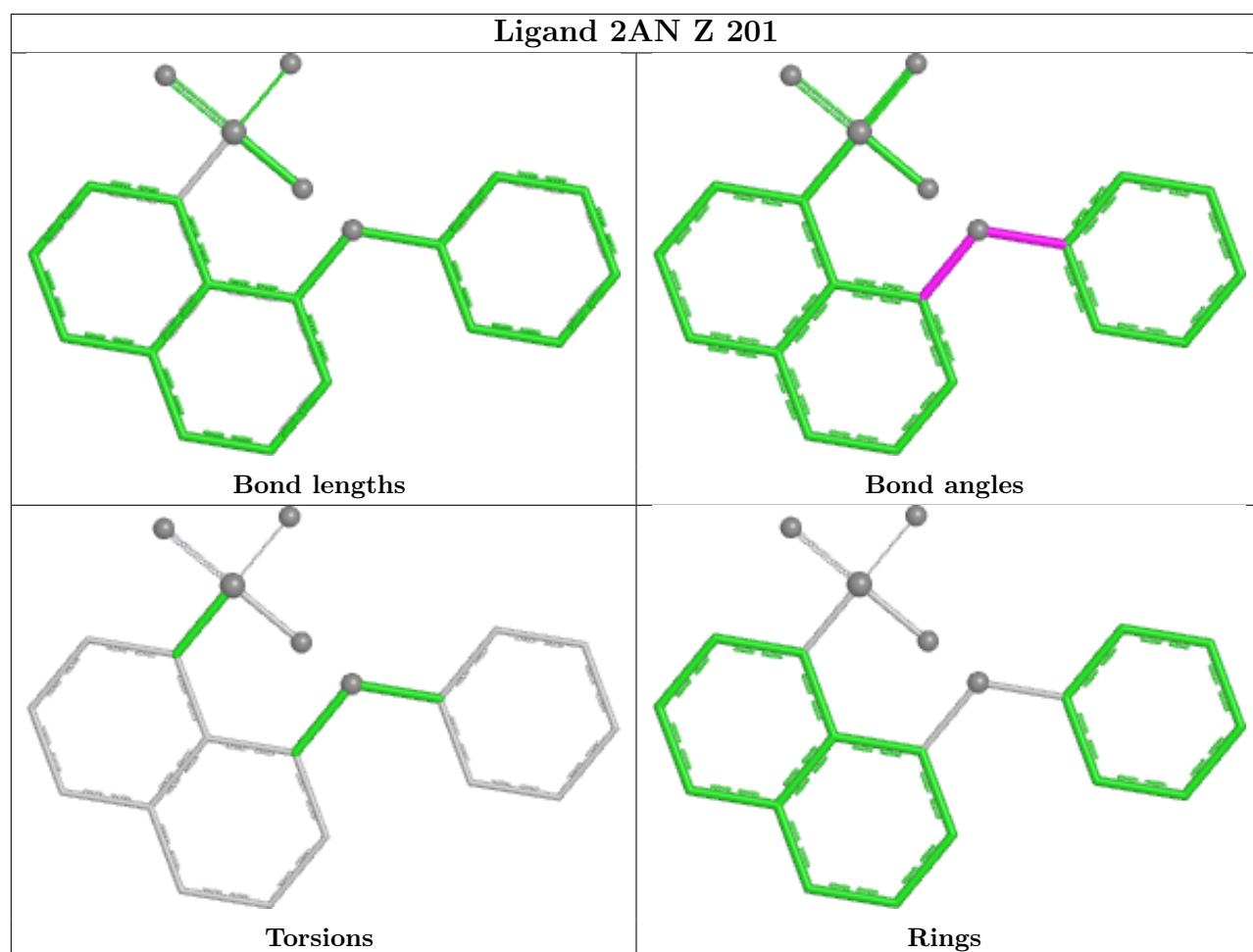


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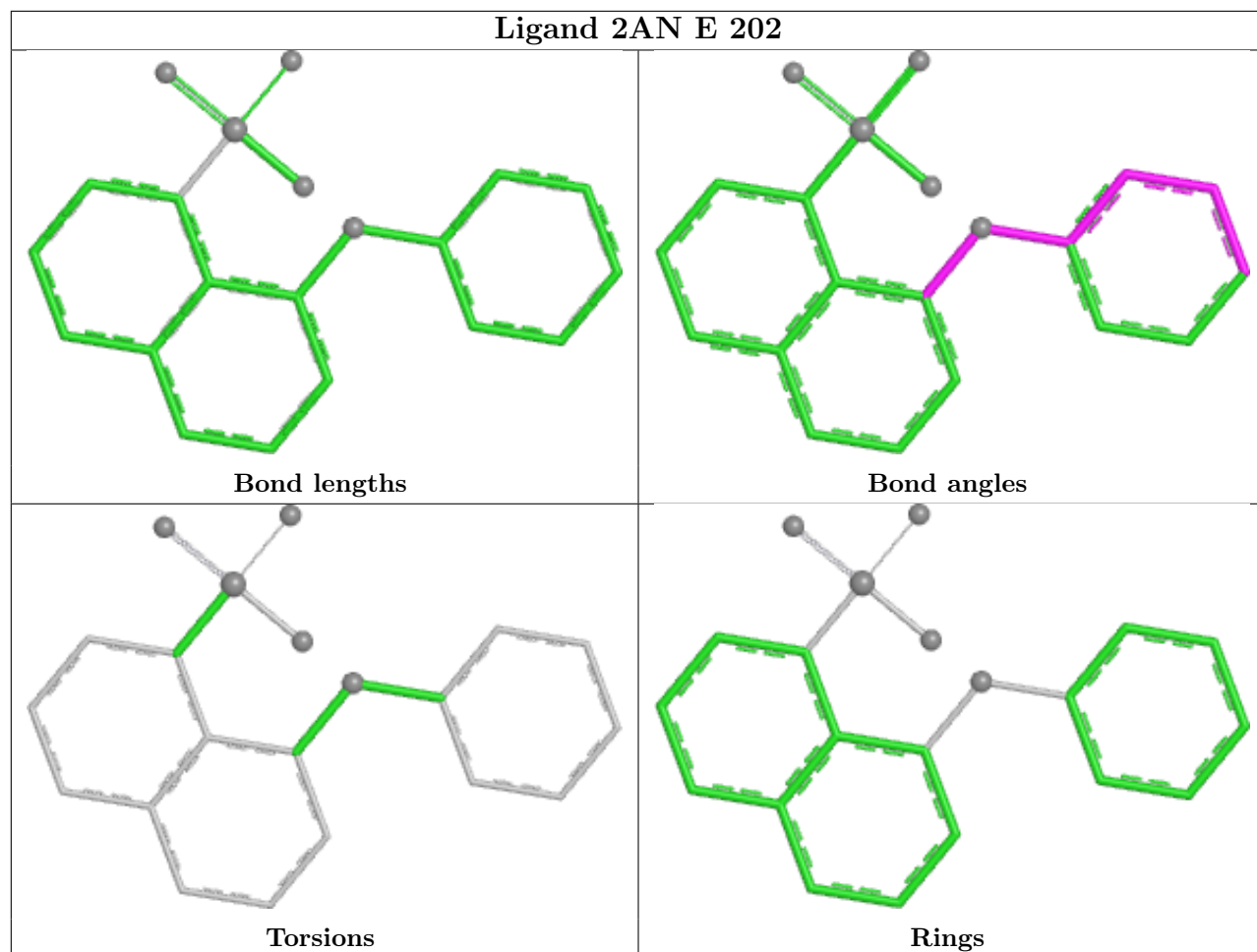


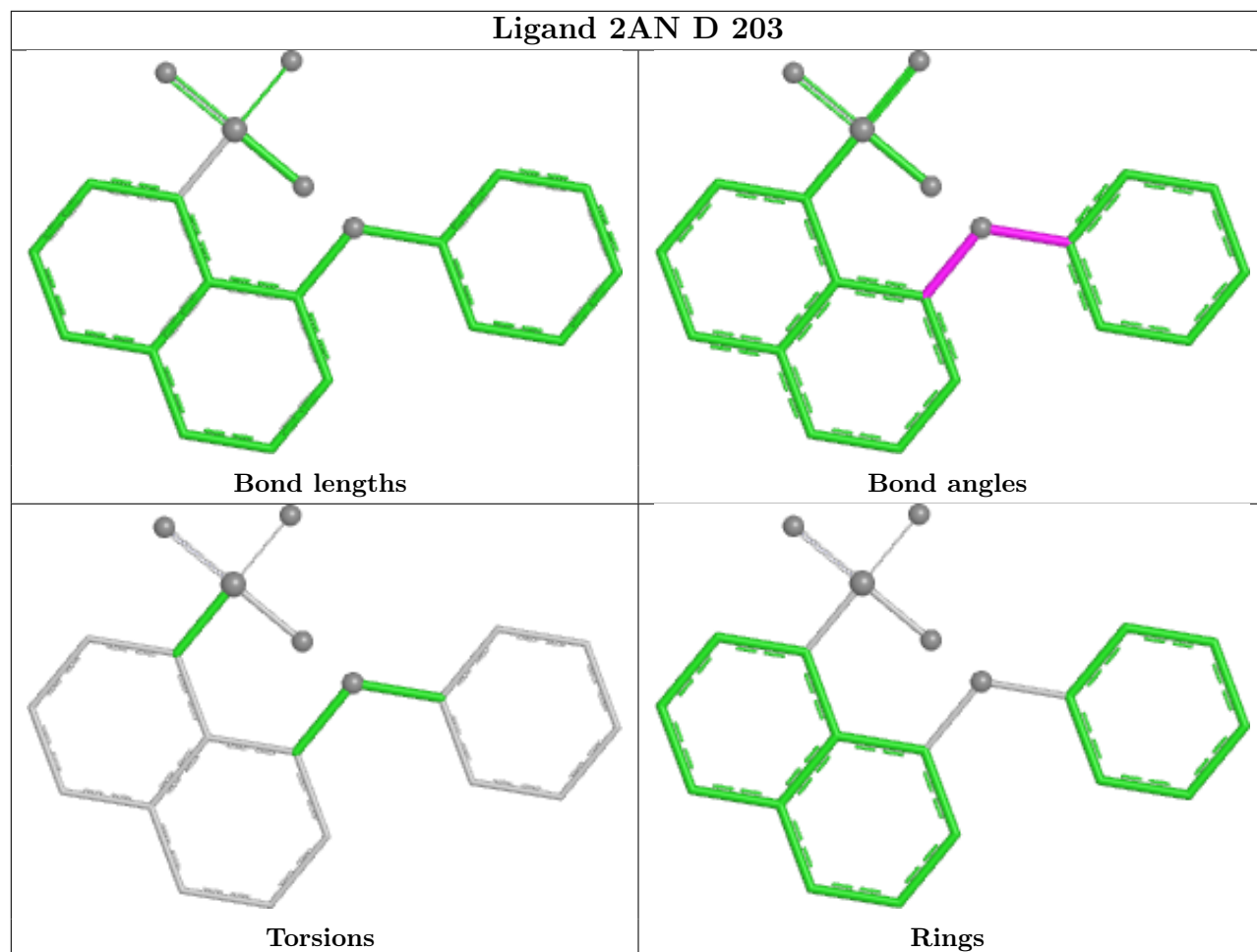
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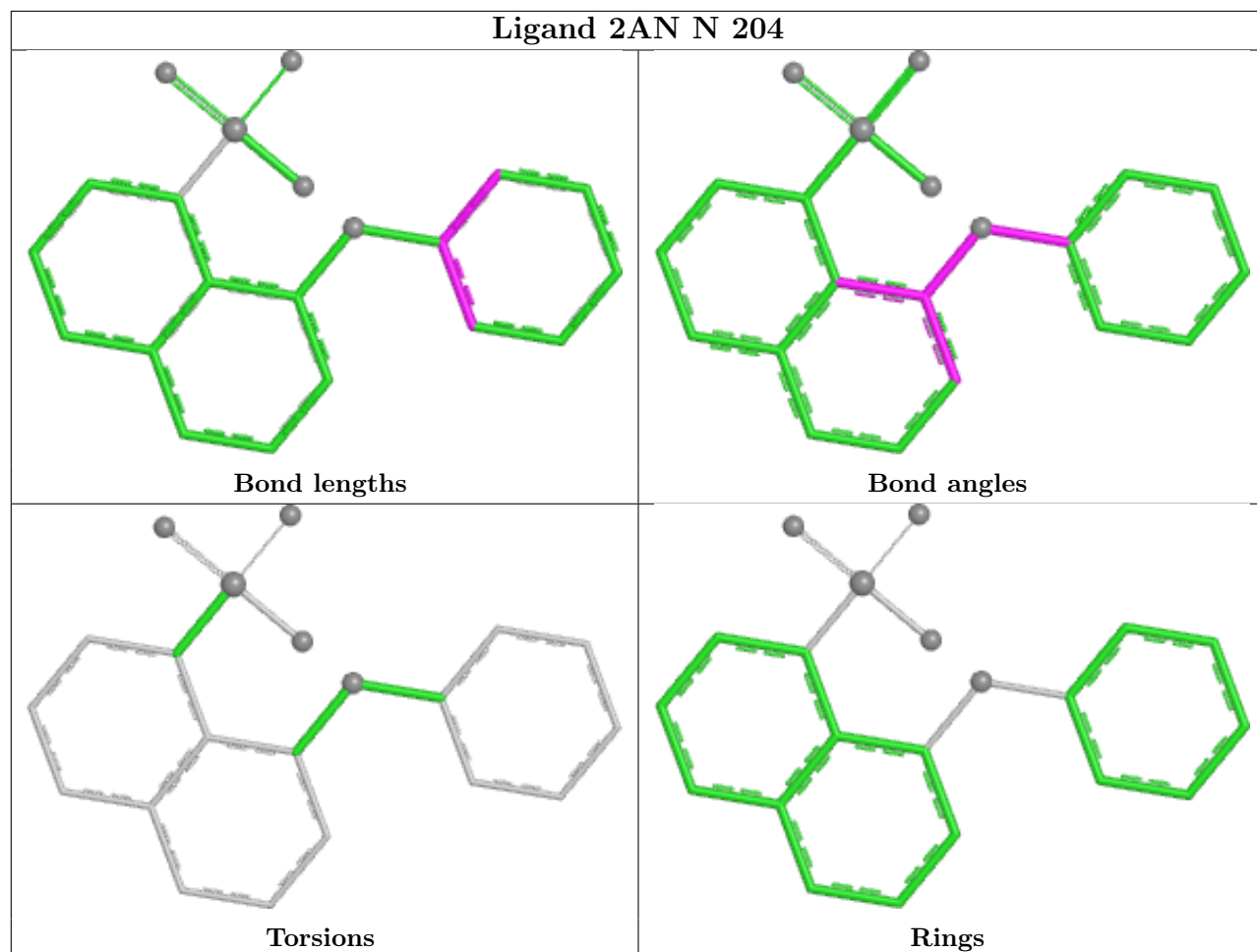


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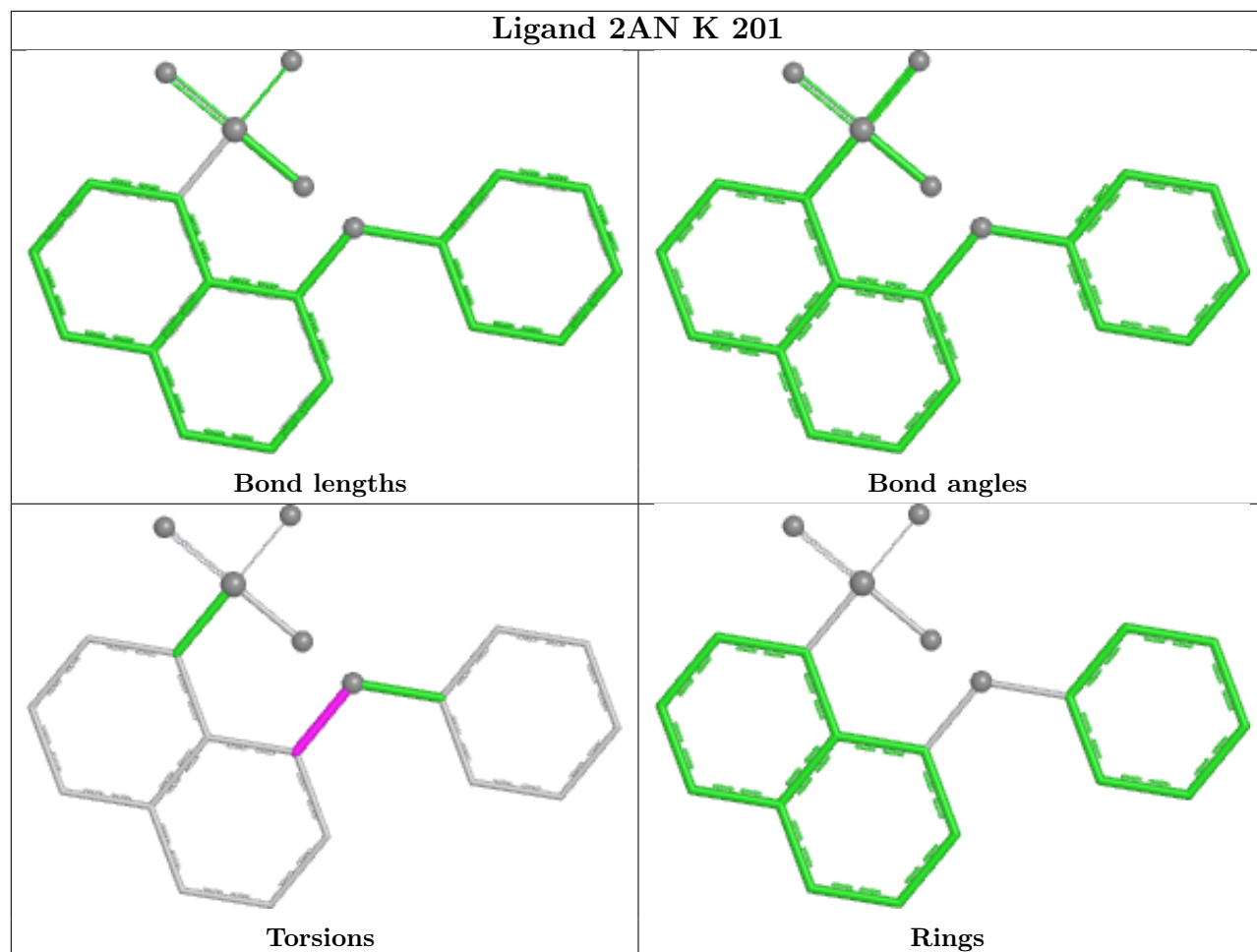




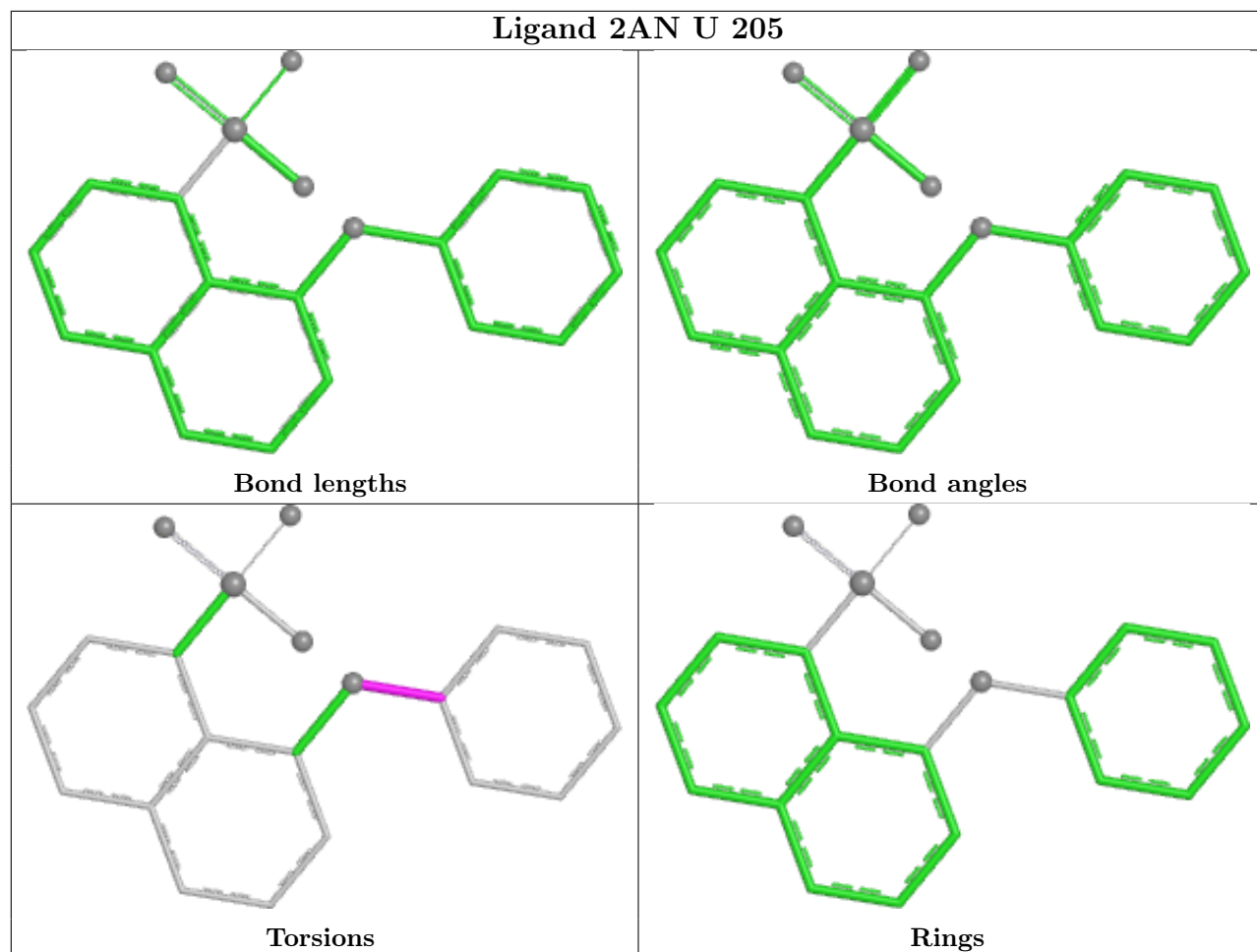
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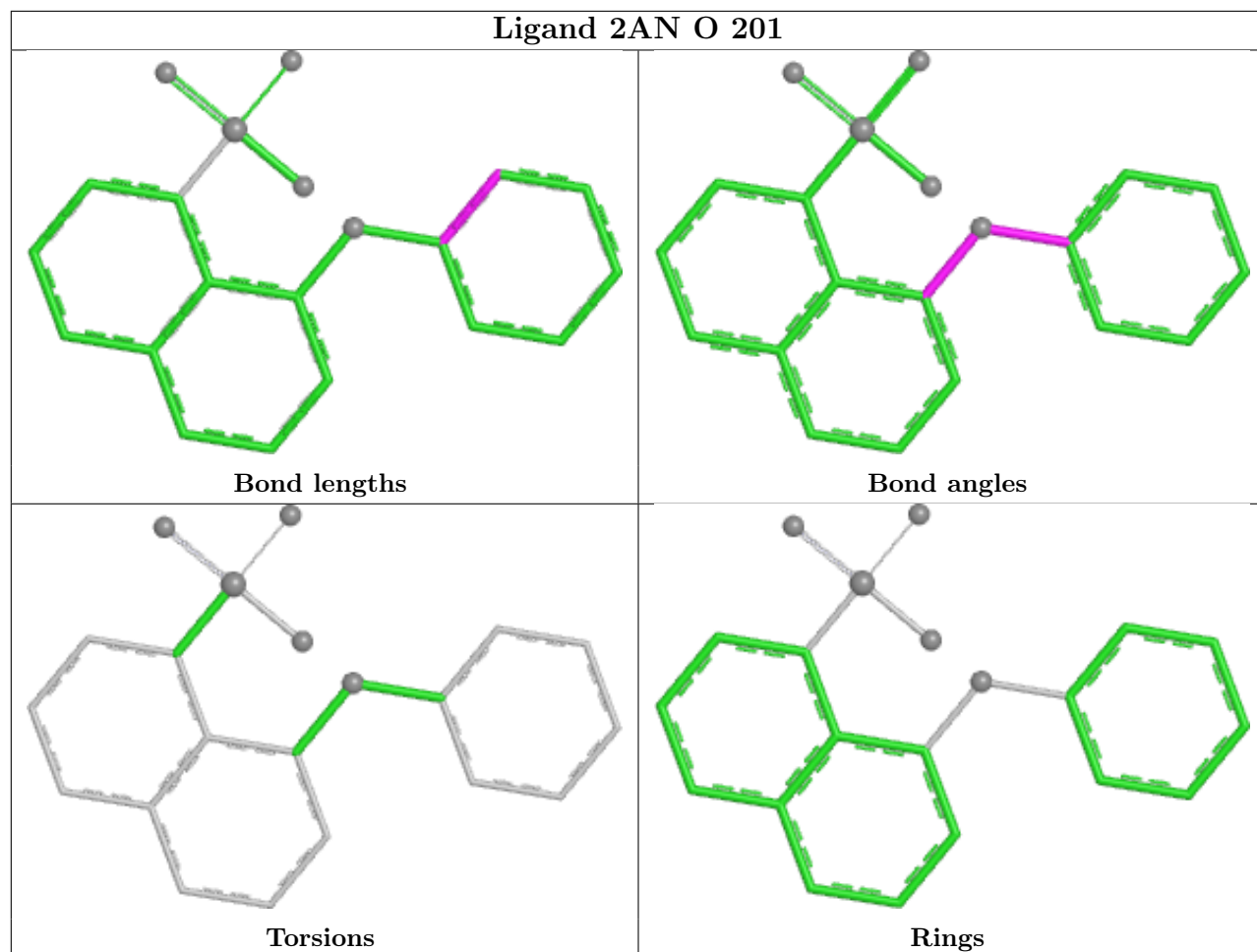
Ligand 2AN K 201



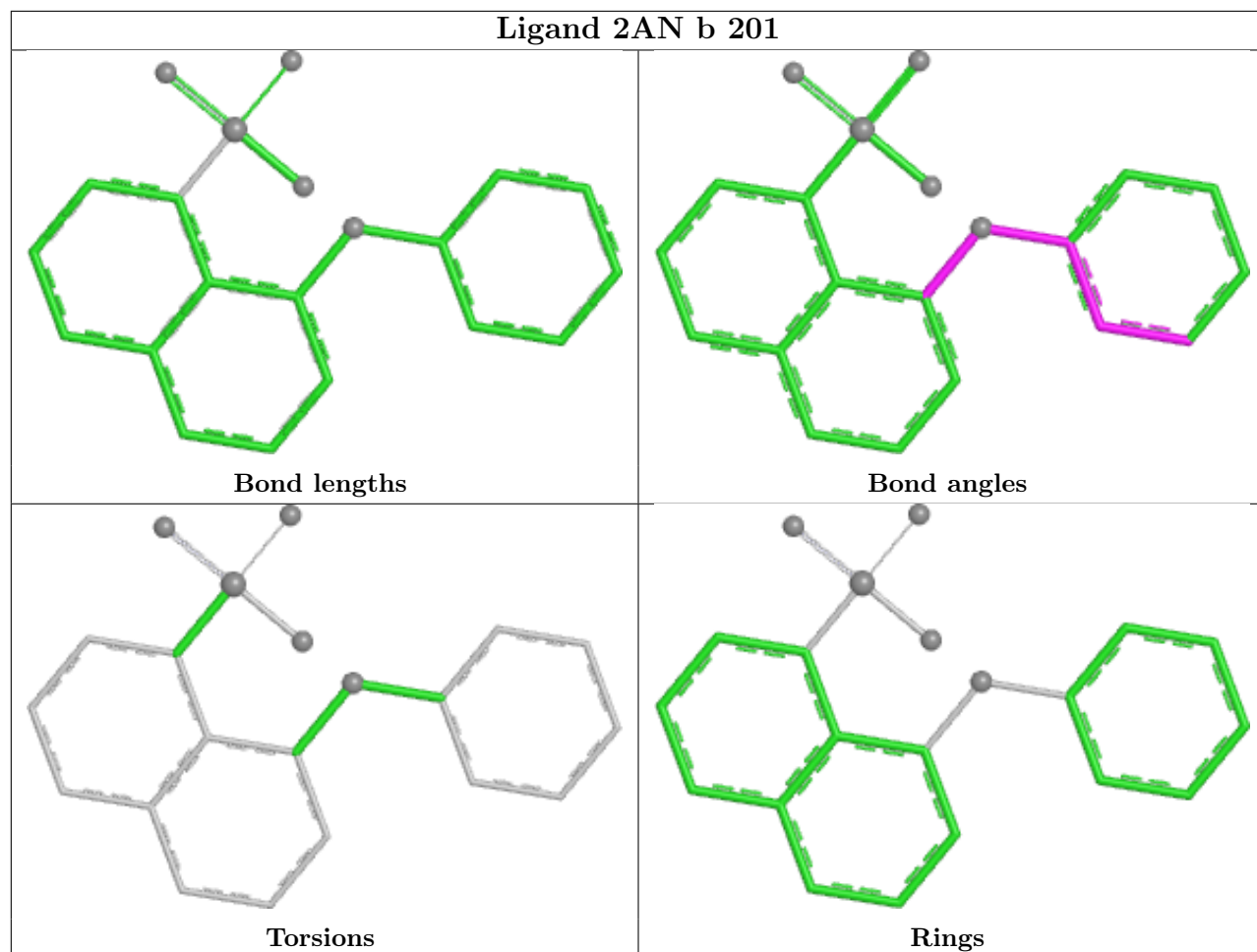
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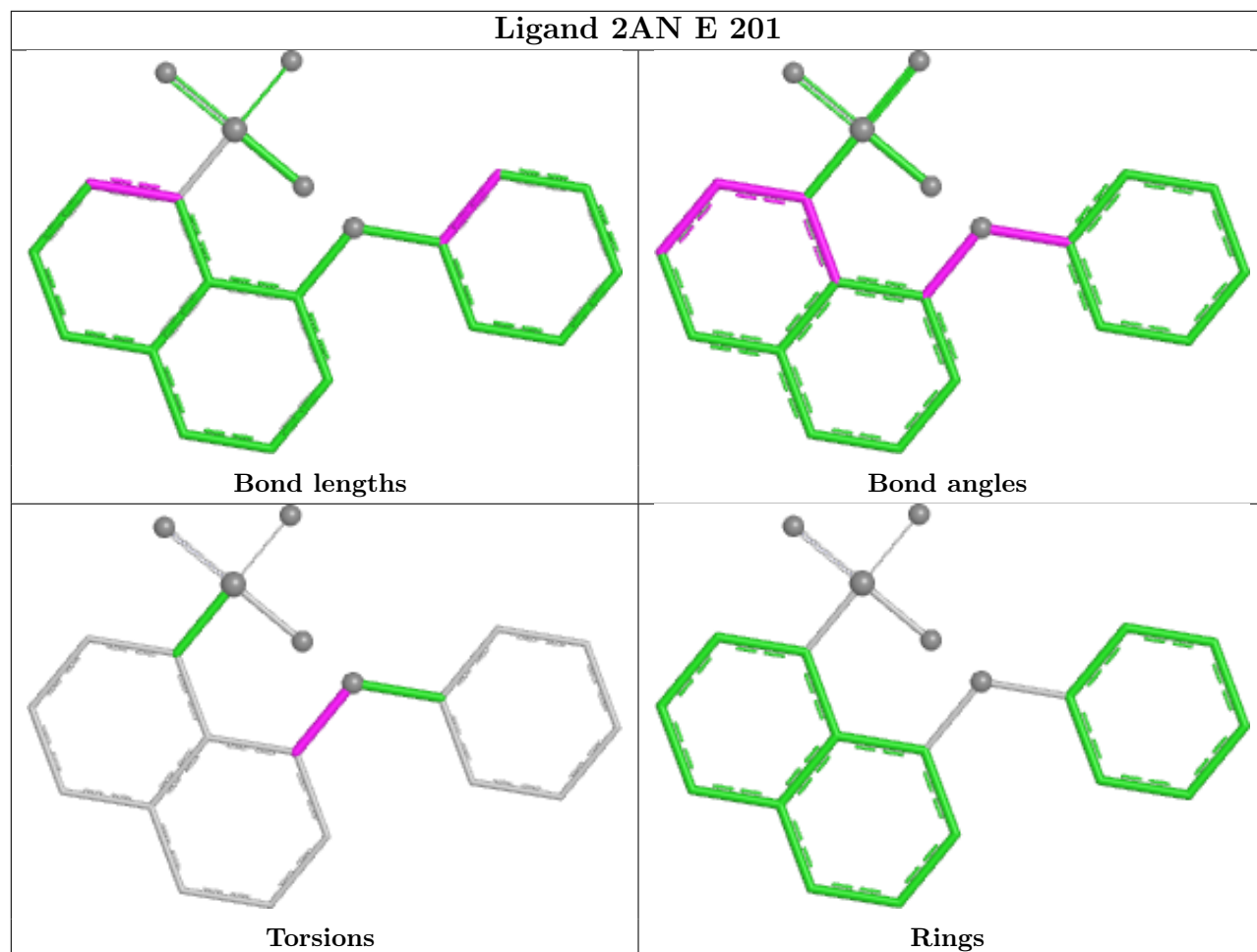


Ligand 2AN O 201



Ligand 2AN b 201





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	159/165 (96%)	-0.64	0 100 100	22, 48, 69, 87	2 (1%)
1	B	159/165 (96%)	-0.67	0 100 100	25, 45, 77, 108	1 (0%)
1	C	159/165 (96%)	-0.63	1 (0%) 85 87	29, 50, 73, 84	0
1	D	159/165 (96%)	-0.58	1 (0%) 85 87	29, 50, 83, 123	0
1	E	159/165 (96%)	-0.90	0 100 100	20, 35, 57, 76	2 (1%)
1	F	159/165 (96%)	-0.58	0 100 100	34, 56, 82, 98	2 (1%)
1	G	159/165 (96%)	-0.79	0 100 100	20, 39, 64, 83	2 (1%)
1	H	159/165 (96%)	-0.79	0 100 100	24, 44, 64, 77	2 (1%)
1	I	159/165 (96%)	-0.79	0 100 100	21, 40, 66, 83	4 (2%)
1	J	159/165 (96%)	-0.81	0 100 100	17, 40, 63, 72	1 (0%)
1	K	159/165 (96%)	-0.64	0 100 100	31, 48, 71, 77	3 (1%)
1	L	159/165 (96%)	-0.78	0 100 100	19, 37, 62, 83	2 (1%)
1	M	159/165 (96%)	-0.69	1 (0%) 85 87	25, 46, 79, 91	1 (0%)
1	N	159/165 (96%)	-0.63	0 100 100	23, 47, 72, 96	3 (1%)
1	O	159/165 (96%)	-0.65	1 (0%) 85 87	28, 47, 76, 92	2 (1%)
1	P	159/165 (96%)	-0.69	1 (0%) 85 87	29, 46, 70, 83	1 (0%)
1	Q	159/165 (96%)	-0.59	0 100 100	26, 50, 75, 86	2 (1%)
1	R	159/165 (96%)	-0.72	1 (0%) 85 87	23, 44, 65, 107	2 (1%)
1	S	159/165 (96%)	-0.50	0 100 100	31, 57, 86, 99	1 (0%)
1	T	159/165 (96%)	-0.54	2 (1%) 75 77	18, 54, 88, 115	7 (4%)
1	U	159/165 (96%)	-0.91	0 100 100	17, 36, 55, 103	2 (1%)
1	V	159/165 (96%)	-0.52	0 100 100	35, 61, 85, 102	0
1	W	159/165 (96%)	-0.73	1 (0%) 85 87	23, 40, 67, 74	2 (1%)
1	X	159/165 (96%)	-0.73	0 100 100	25, 44, 67, 80	1 (0%)

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	Y	159/165 (96%)	-0.85	0 100 100	20, 39, 58, 78	3 (1%)
1	Z	159/165 (96%)	-0.72	1 (0%) 85 87	27, 44, 63, 75	2 (1%)
1	a	159/165 (96%)	-0.77	0 100 100	17, 43, 65, 76	3 (1%)
1	b	159/165 (96%)	-0.82	0 100 100	20, 38, 59, 65	1 (0%)
All	All	4452/4620 (96%)	-0.70	10 (0%) 91 92	17, 45, 73, 123	54 (1%)

All (10) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	M	52	GLY	4.1
1	R	112	SER	4.0
1	P	15	ALA	3.4
1	C	15	ALA	2.5
1	W	156	GLU	2.3
1	T	52	GLY	2.2
1	T	136	GLY	2.2
1	O	136	GLY	2.1
1	Z	15	ALA	2.0
1	D	127	THR	2.0

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

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

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

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	R	203	21/21	0.96	0.11	21,26,39,41	21
2	2AN	Q	203	21/21	0.97	0.08	70,81,96,100	0

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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	0.97	0.08	52,66,74,85	0
2	2AN	Z	202	21/21	0.97	0.09	21,29,35,38	21
2	2AN	F	201	21/21	0.98	0.06	31,37,47,56	0
2	2AN	G	203	21/21	0.98	0.06	25,34,56,60	0
2	2AN	G	204	21/21	0.98	0.08	22,32,42,45	0
2	2AN	A	203	21/21	0.98	0.06	31,43,46,54	0
2	2AN	H	201	21/21	0.98	0.05	26,31,43,45	0
2	2AN	I	201	21/21	0.98	0.06	21,28,35,42	0
2	2AN	I	204	21/21	0.98	0.07	42,57,68,81	0
2	2AN	I	205	21/21	0.98	0.07	46,60,65,70	0
2	2AN	K	202	21/21	0.98	0.05	43,46,53,59	0
2	2AN	K	203	21/21	0.98	0.05	33,42,66,74	0
2	2AN	L	202	21/21	0.98	0.05	23,28,32,33	0
2	2AN	L	204	21/21	0.98	0.06	31,40,46,52	0
2	2AN	L	205	21/21	0.98	0.06	37,44,50,54	0
2	2AN	M	202	21/21	0.98	0.06	26,30,37,43	0
2	2AN	N	203	21/21	0.98	0.07	41,48,58,62	0
2	2AN	N	204	21/21	0.98	0.07	25,32,44,52	0
2	2AN	O	201	21/21	0.98	0.07	28,35,40,43	0
2	2AN	Q	202	21/21	0.98	0.05	35,50,64,68	0
2	2AN	B	203	21/21	0.98	0.04	38,44,50,56	0
2	2AN	B	205	21/21	0.98	0.06	39,54,64,68	0
2	2AN	U	205	21/21	0.98	0.05	37,47,60,78	0
2	2AN	V	201	21/21	0.98	0.05	44,51,56,61	0
2	2AN	W	201	21/21	0.98	0.07	35,44,54,63	0
2	2AN	W	202	21/21	0.98	0.05	24,30,35,40	0
2	2AN	W	203	21/21	0.98	0.07	16,21,29,33	21
2	2AN	W	204	21/21	0.98	0.07	41,53,68,75	0
2	2AN	X	202	21/21	0.98	0.08	27,32,37,44	21
2	2AN	Y	203	21/21	0.98	0.06	32,38,47,48	0
2	2AN	Y	204	21/21	0.98	0.05	30,47,51,57	0
2	2AN	E	202	21/21	0.98	0.06	23,31,39,53	0
2	2AN	Z	203	21/21	0.98	0.05	35,43,56,64	0
2	2AN	a	201	21/21	0.98	0.06	25,36,46,49	0
2	2AN	b	201	21/21	0.98	0.08	34,44,49,52	0
3	EPE	C	205	15/15	0.98	0.07	29,34,52,57	0
3	EPE	Z	204	15/15	0.98	0.06	36,44,54,54	0
4	SO4	V	203	5/5	0.98	0.05	35,48,55,57	0
4	SO4	X	204	5/5	0.98	0.04	39,42,44,49	0
2	2AN	D	202	21/21	0.99	0.06	32,39,44,48	0
2	2AN	L	203	21/21	0.99	0.04	18,31,40,48	0
2	2AN	D	203	21/21	0.99	0.08	40,48,58,62	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	2AN	E	201	21/21	0.99	0.05	15,21,28,38	0
2	2AN	M	201	21/21	0.99	0.04	30,35,38,45	0
2	2AN	A	204	21/21	0.99	0.04	35,43,51,54	0
2	2AN	M	203	21/21	0.99	0.06	42,53,70,74	0
2	2AN	N	201	21/21	0.99	0.05	24,29,34,37	0
2	2AN	N	202	21/21	0.99	0.04	25,30,46,54	0
2	2AN	E	203	21/21	0.99	0.06	23,32,48,61	0
2	2AN	E	204	21/21	0.99	0.06	35,46,58,73	0
2	2AN	E	205	21/21	0.99	0.06	31,42,54,63	0
2	2AN	O	202	21/21	0.99	0.04	23,28,33,37	0
2	2AN	P	201	21/21	0.99	0.06	25,30,38,41	21
2	2AN	P	202	21/21	0.99	0.06	40,51,66,71	0
2	2AN	Q	201	21/21	0.99	0.05	30,37,45,51	0
2	2AN	B	201	21/21	0.99	0.04	27,34,44,47	0
2	2AN	G	201	21/21	0.99	0.04	15,23,26,34	0
2	2AN	R	201	21/21	0.99	0.06	35,45,68,70	0
2	2AN	R	202	21/21	0.99	0.05	21,29,48,53	0
2	2AN	G	202	21/21	0.99	0.04	18,27,34,41	0
2	2AN	R	204	21/21	0.99	0.05	30,39,58,61	0
2	2AN	S	201	21/21	0.99	0.05	27,33,38,52	0
2	2AN	U	201	21/21	0.99	0.04	28,34,43,47	0
2	2AN	U	202	21/21	0.99	0.05	24,31,42,48	0
2	2AN	U	203	21/21	0.99	0.05	24,38,46,50	0
2	2AN	U	204	21/21	0.99	0.04	24,26,34,45	0
2	2AN	B	202	21/21	0.99	0.05	28,34,53,63	0
2	2AN	A	202	21/21	0.99	0.05	23,35,40,41	0
2	2AN	V	202	21/21	0.99	0.06	34,46,79,82	0
2	2AN	B	204	21/21	0.99	0.05	29,40,59,67	0
2	2AN	A	201	21/21	0.99	0.05	25,34,46,71	0
2	2AN	H	202	21/21	0.99	0.05	25,36,40,43	0
2	2AN	H	203	21/21	0.99	0.05	22,28,34,38	0
2	2AN	X	201	21/21	0.99	0.05	37,41,48,50	0
2	2AN	C	201	21/21	0.99	0.06	28,39,47,61	0
2	2AN	X	203	21/21	0.99	0.06	22,31,53,61	0
2	2AN	Y	201	21/21	0.99	0.04	22,24,30,36	0
2	2AN	Y	202	21/21	0.99	0.05	27,32,35,38	0
2	2AN	I	202	21/21	0.99	0.04	19,23,30,38	0
2	2AN	I	203	21/21	0.99	0.06	23,32,55,59	0
2	2AN	Z	201	21/21	0.99	0.05	26,36,46,48	0
2	2AN	C	202	21/21	0.99	0.05	24,39,49,53	0
2	2AN	C	203	21/21	0.99	0.05	41,51,70,81	0
2	2AN	J	201	21/21	0.99	0.06	20,23,29,33	21

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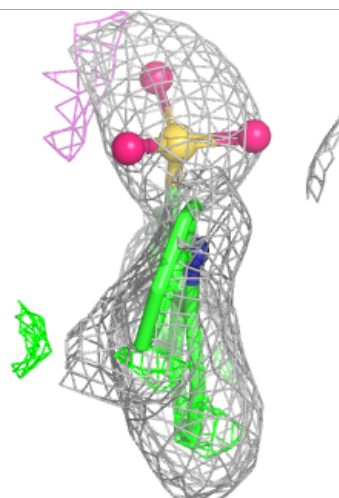
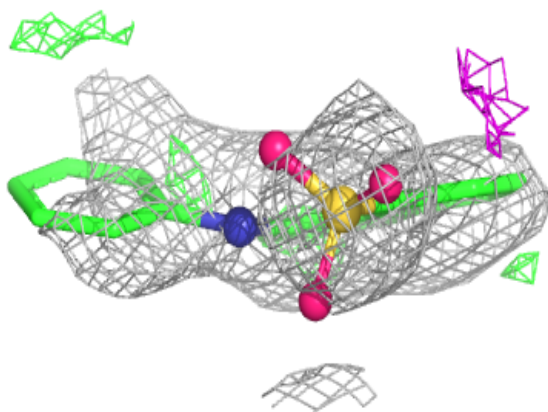
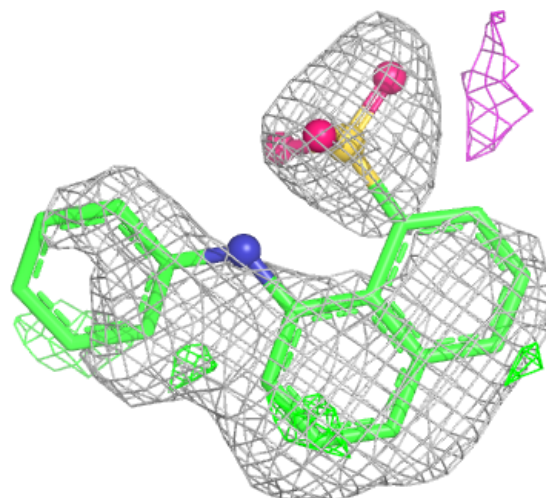
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	2AN	J	202	21/21	0.99	0.06	22,27,39,44	0
2	2AN	b	202	21/21	0.99	0.05	19,23,34,40	0
2	2AN	b	203	21/21	0.99	0.08	29,43,52,55	0
2	2AN	K	201	21/21	0.99	0.05	28,33,36,42	0
2	2AN	C	204	21/21	0.99	0.06	33,39,48,56	0
2	2AN	D	201	21/21	0.99	0.05	37,45,53,56	0
2	2AN	L	201	21/21	0.99	0.05	19,26,30,37	0
4	SO4	b	204	5/5	0.99	0.04	32,36,40,41	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.

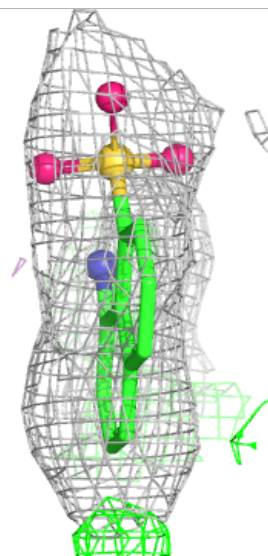
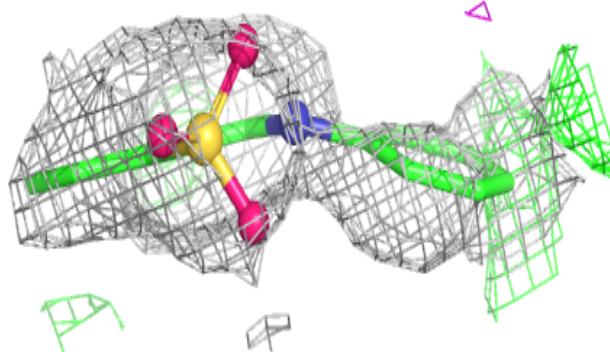
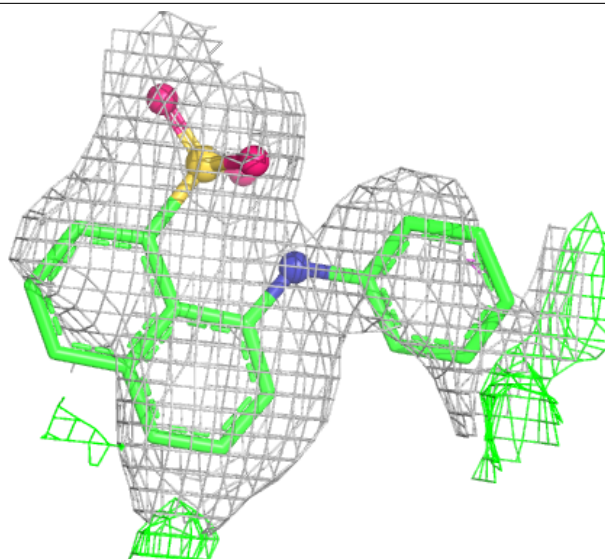
Electron density around 2AN R 203:

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



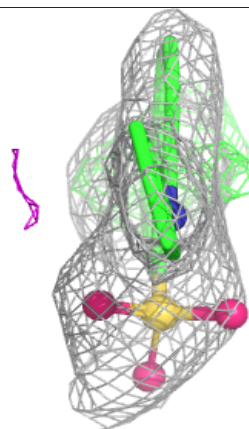
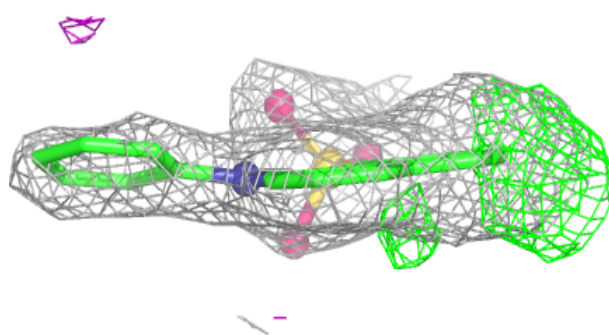
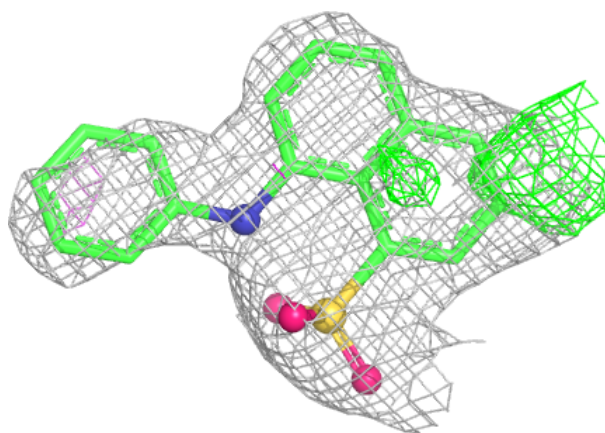
Electron density around 2AN G 205:

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



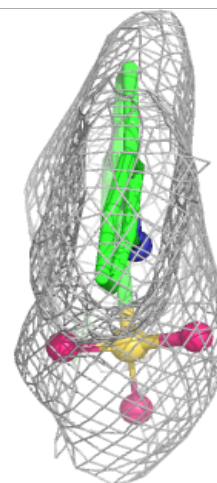
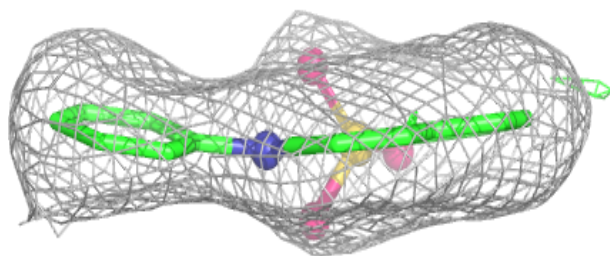
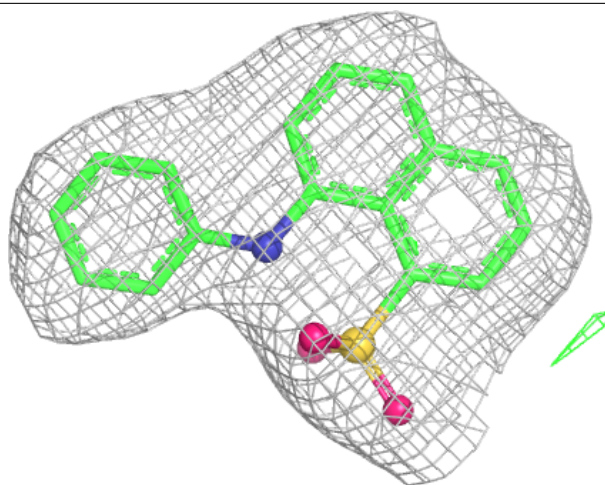
Electron density around 2AN Z 202:

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and green (positive)



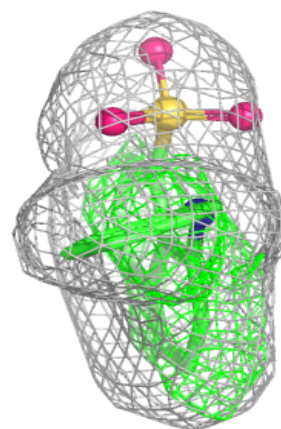
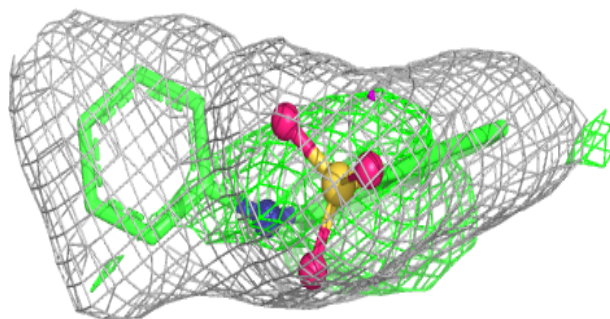
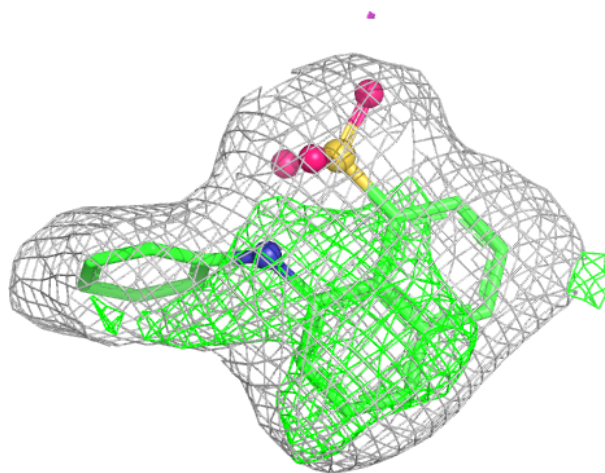
Electron density around 2AN F 201:

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



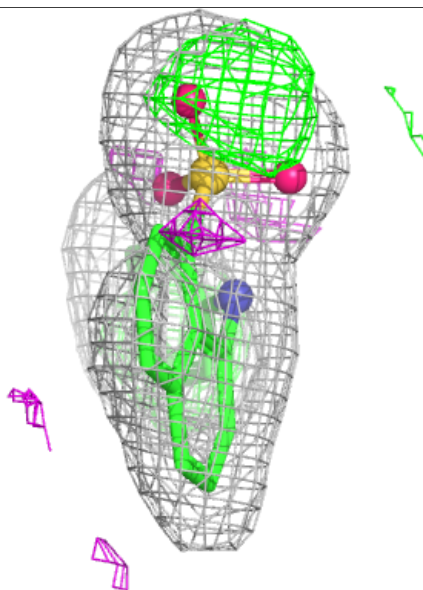
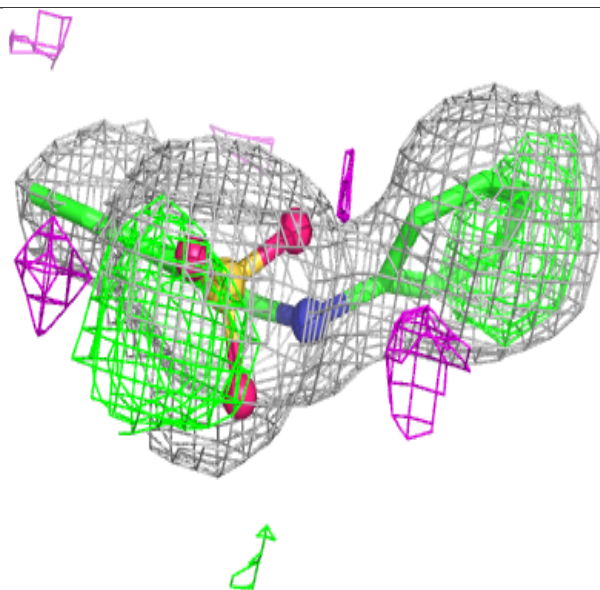
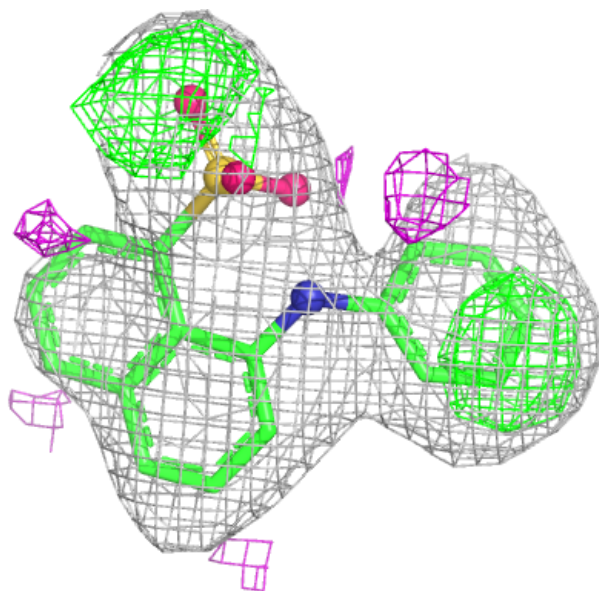
Electron density around 2AN G 203:

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and green (positive)



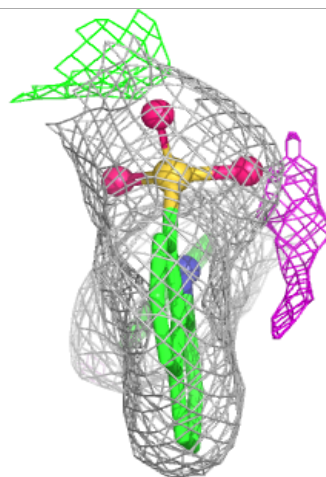
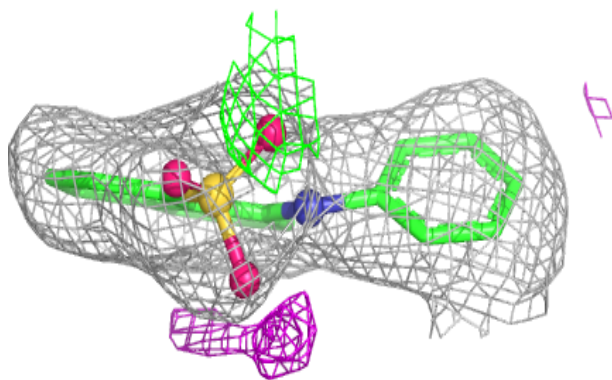
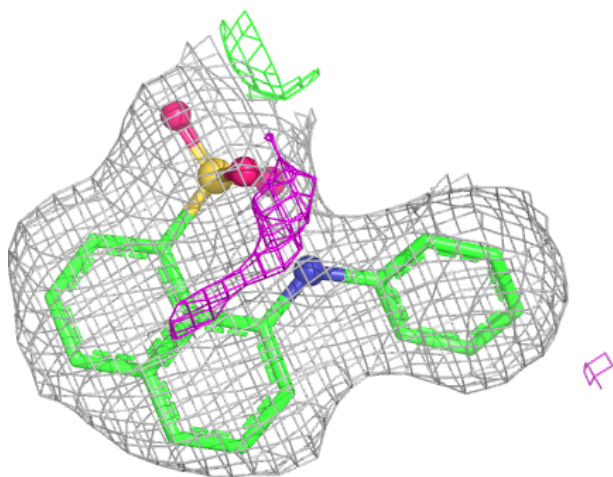
Electron density around 2AN G 204:

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and green (positive)



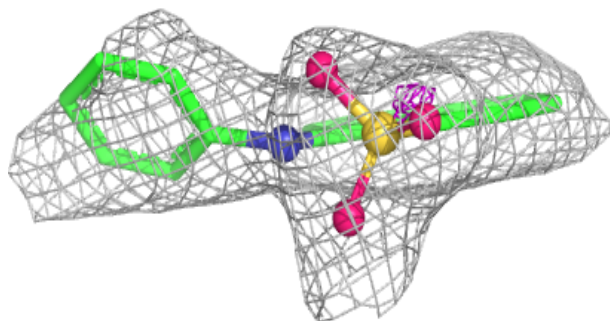
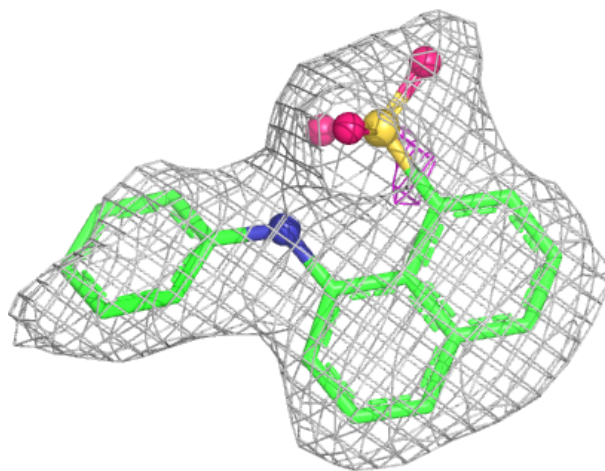
Electron density around 2AN A 203:

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and green (positive)



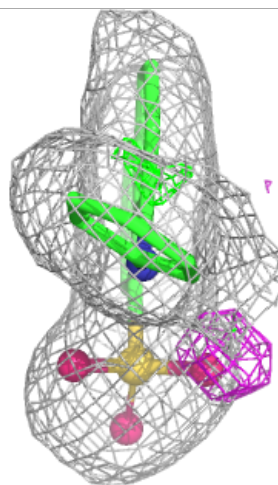
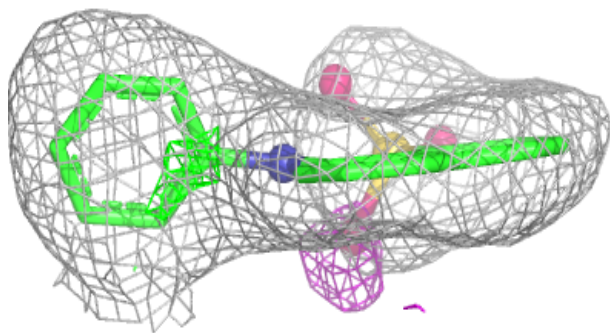
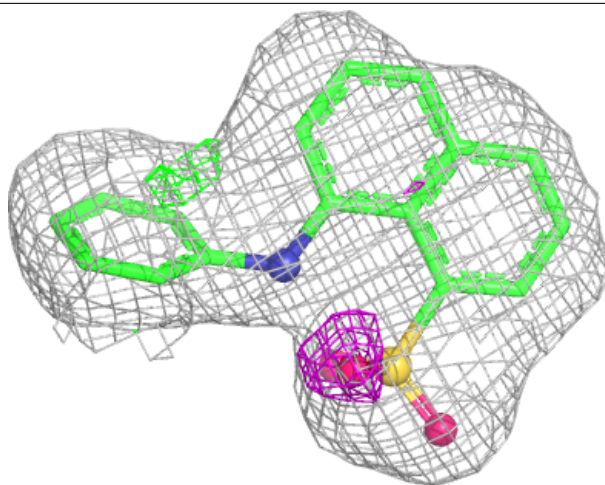
Electron density around 2AN H 201:

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and green (positive)



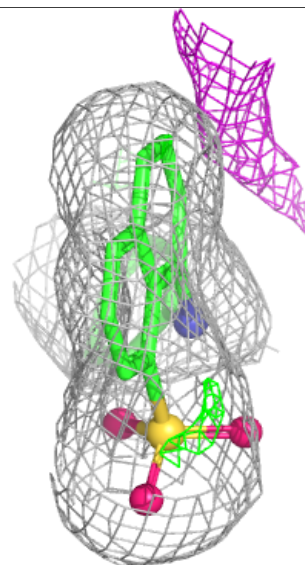
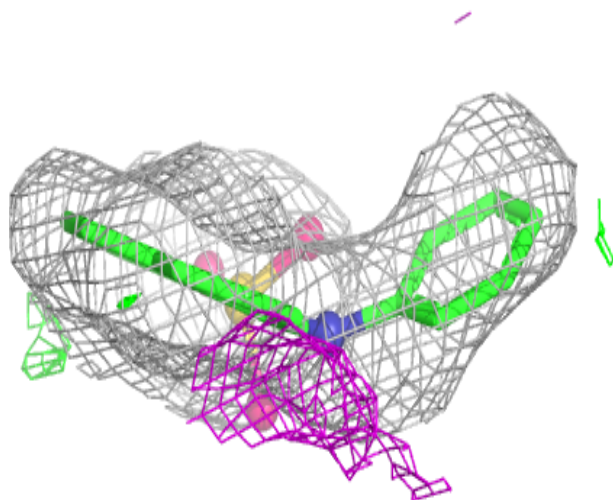
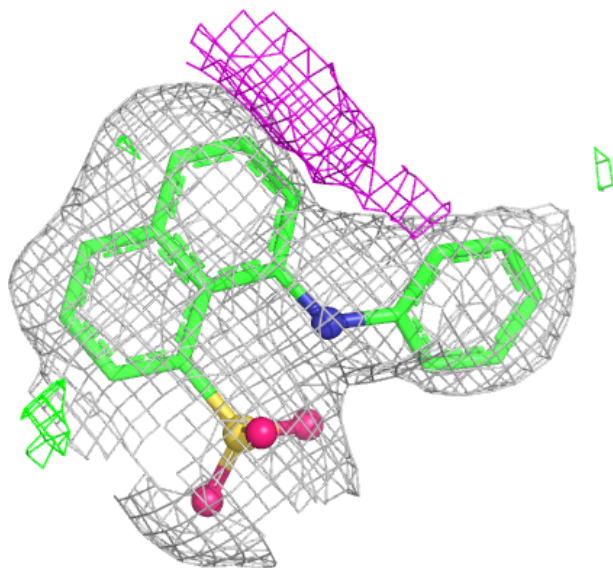
Electron density around 2AN I 201:

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and green (positive)



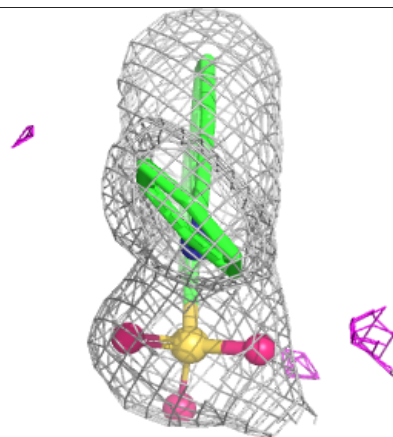
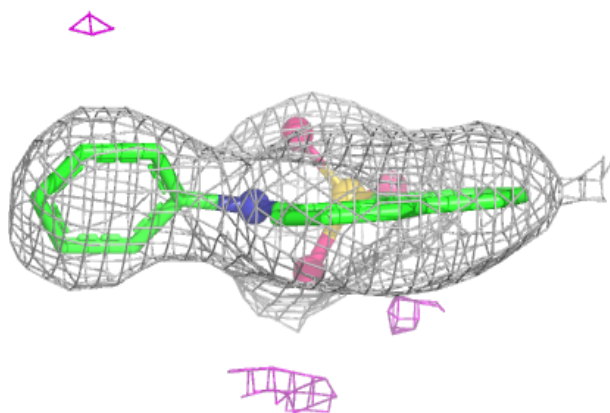
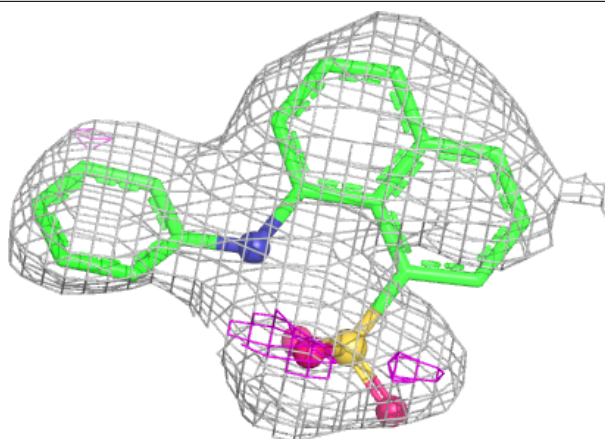
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and green (positive)



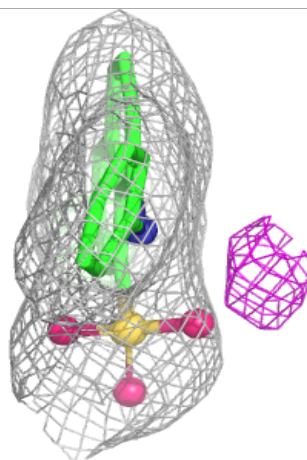
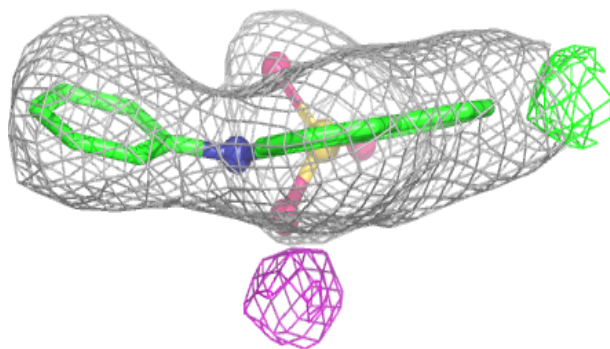
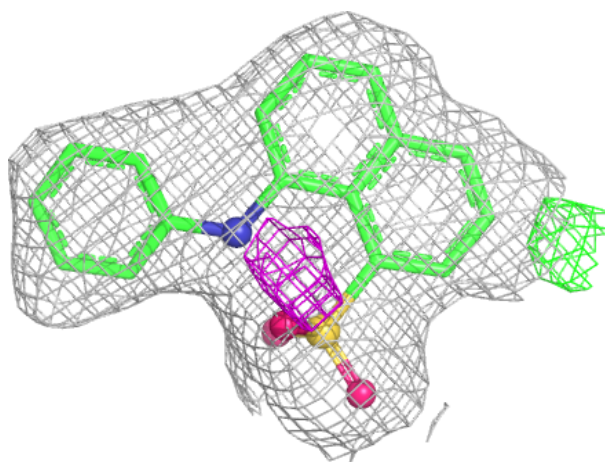
Electron density around 2AN I 205:

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



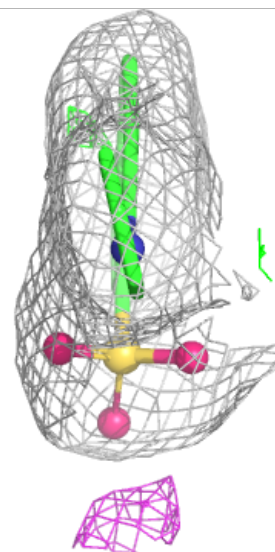
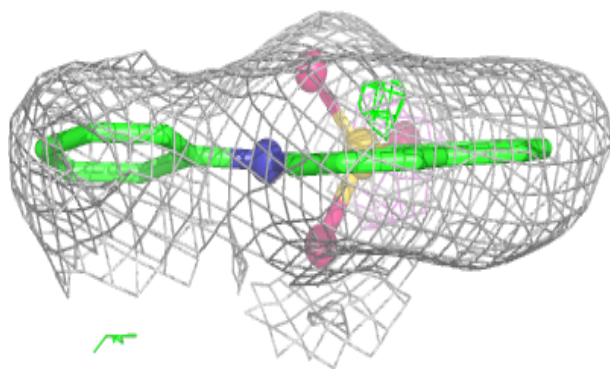
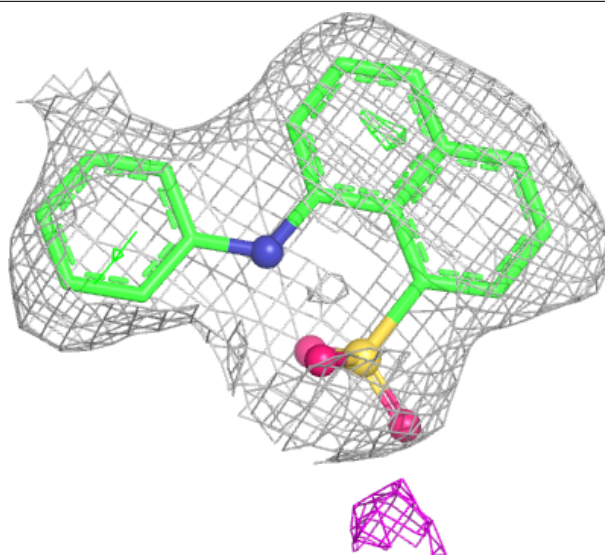
Electron density around 2AN K 202:

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



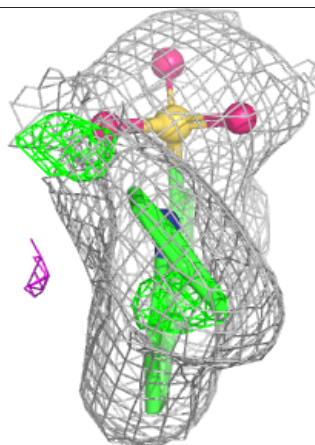
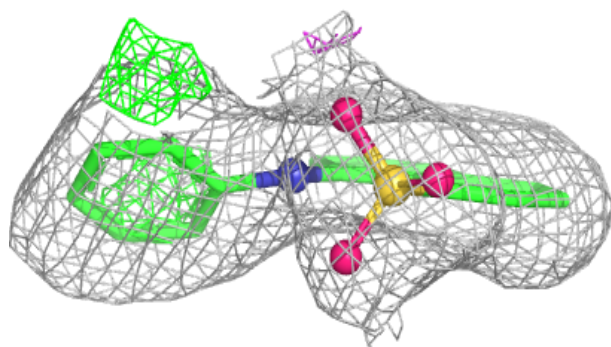
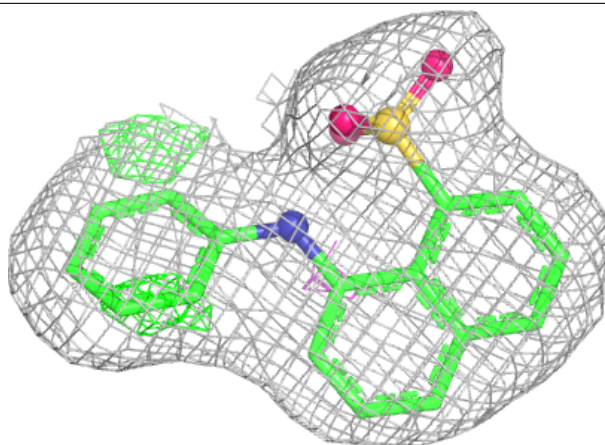
Electron density around 2AN K 203:

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



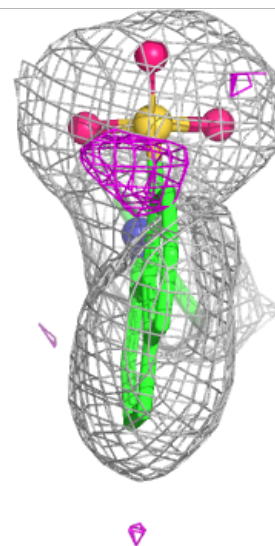
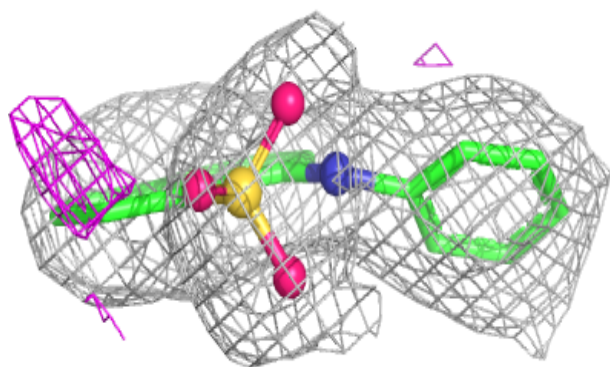
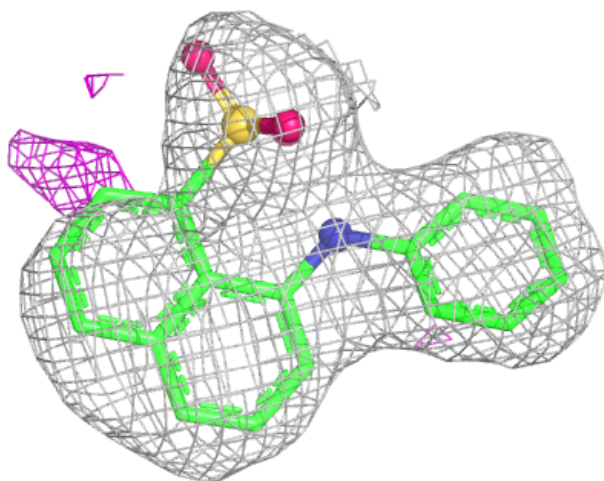
Electron density around 2AN L 202:

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



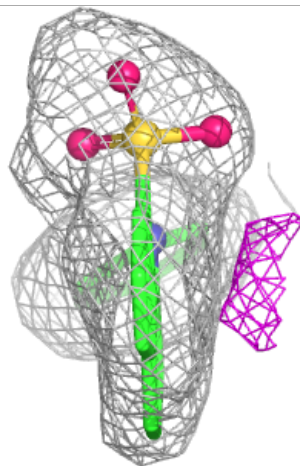
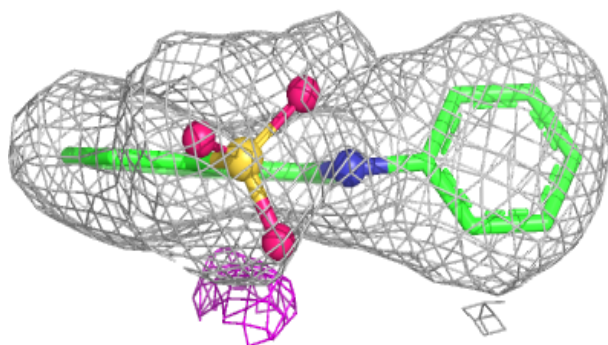
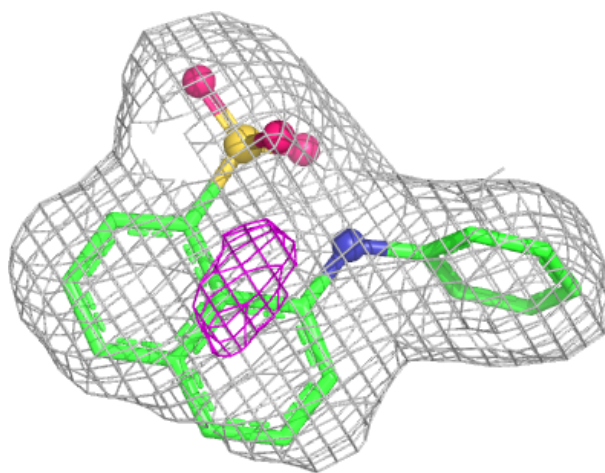
Electron density around 2AN L 204:

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



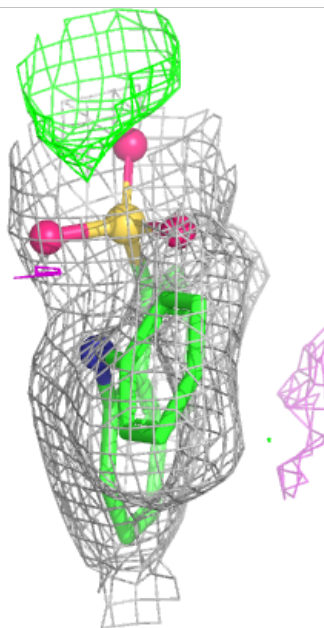
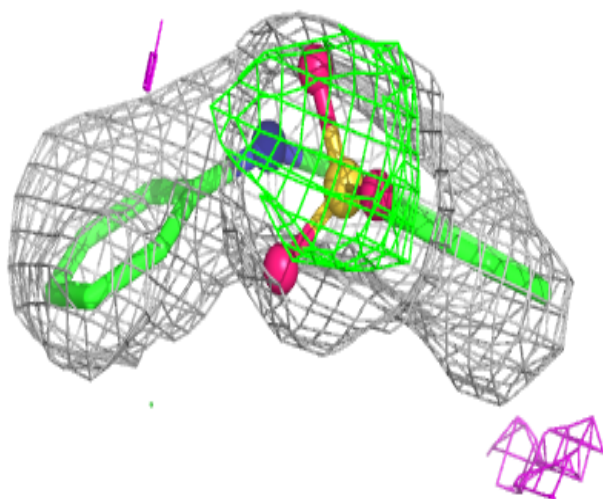
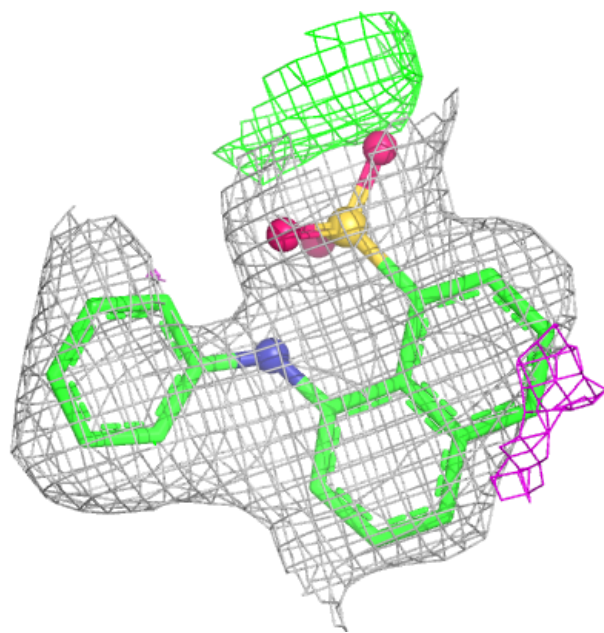
Electron density around 2AN M 202:

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



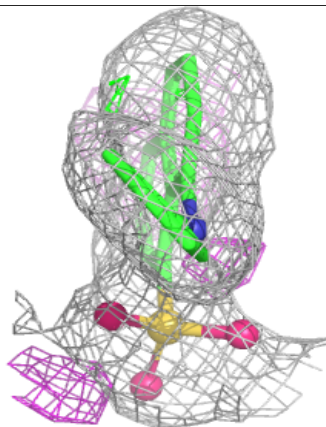
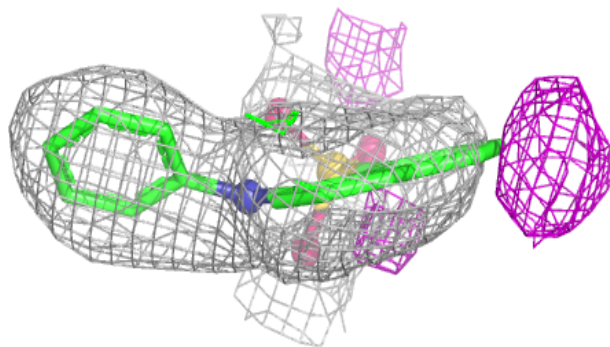
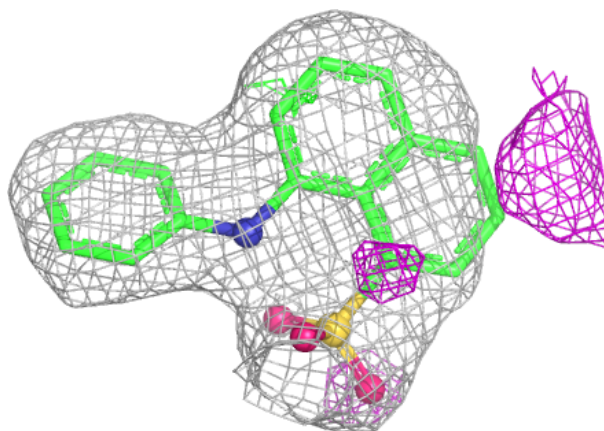
Electron density around 2AN N 203:

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



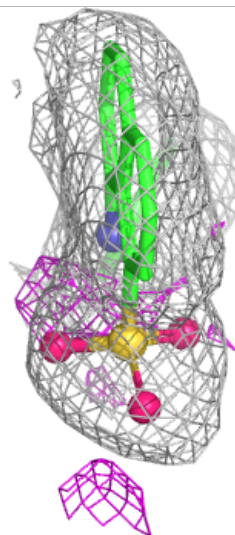
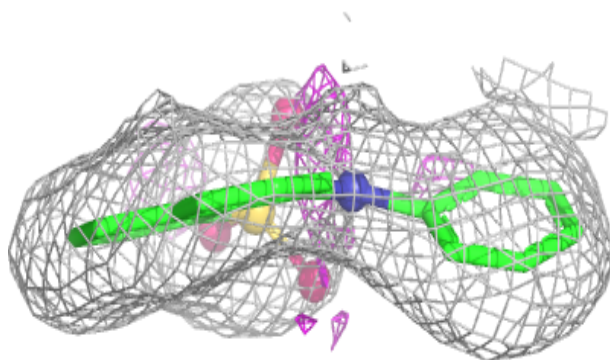
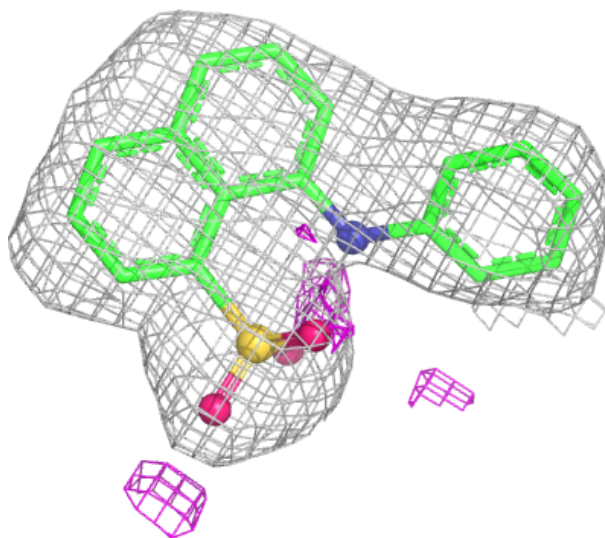
Electron density around 2AN N 204:

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



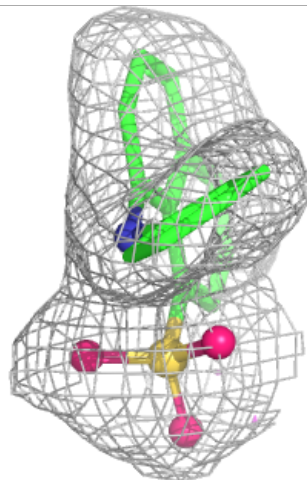
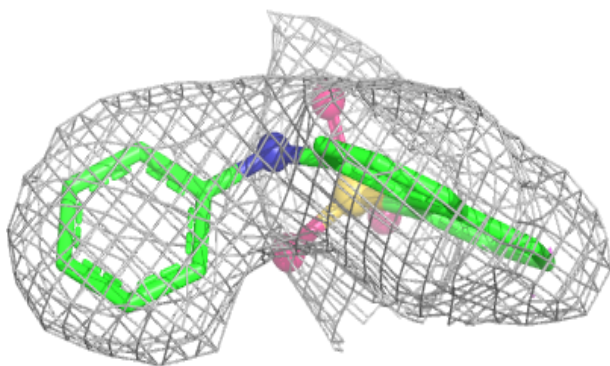
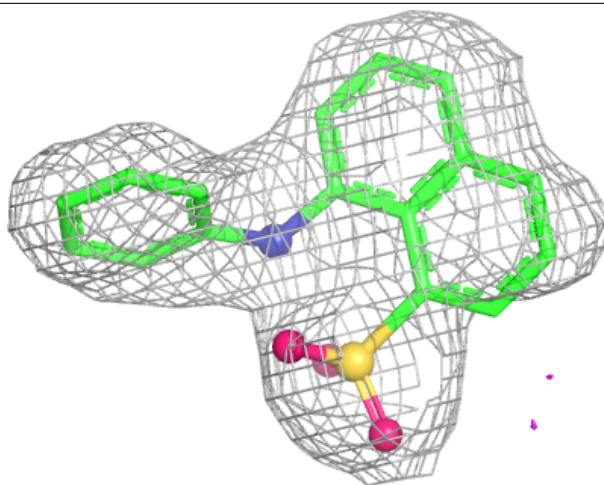
Electron density around 2AN O 201:

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



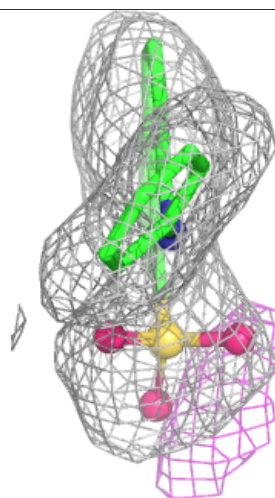
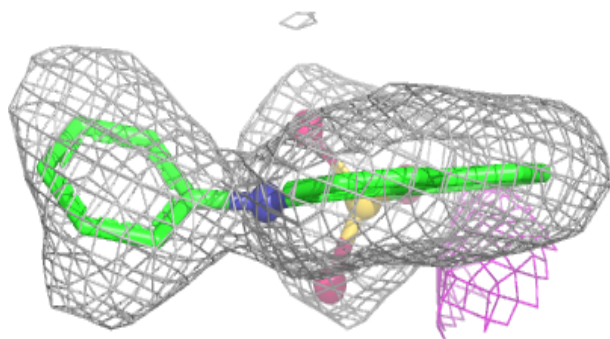
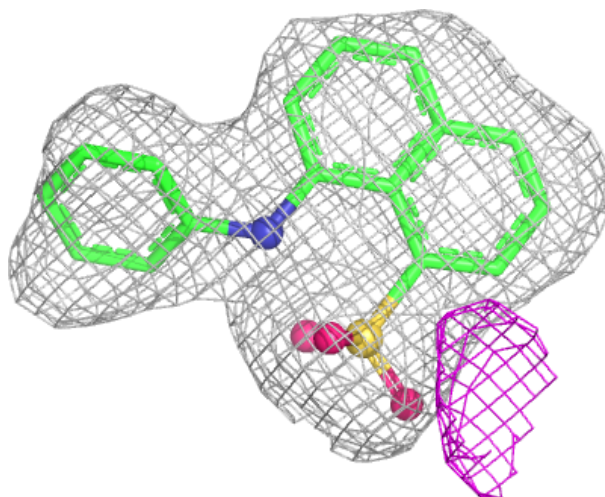
Electron density around 2AN Q 202:

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



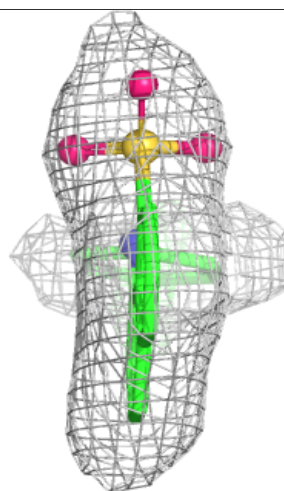
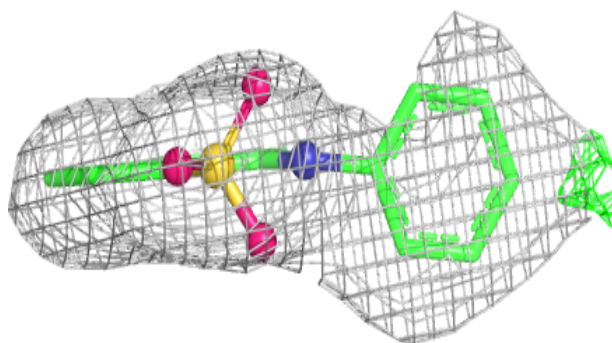
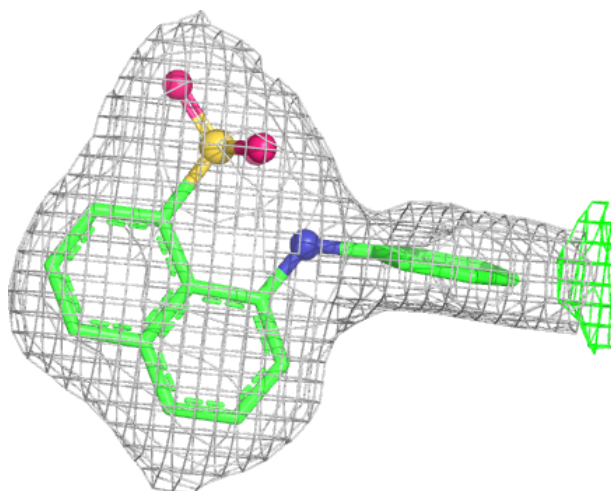
Electron density around 2AN B 205:

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



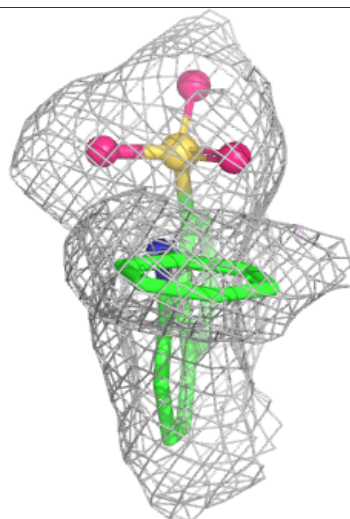
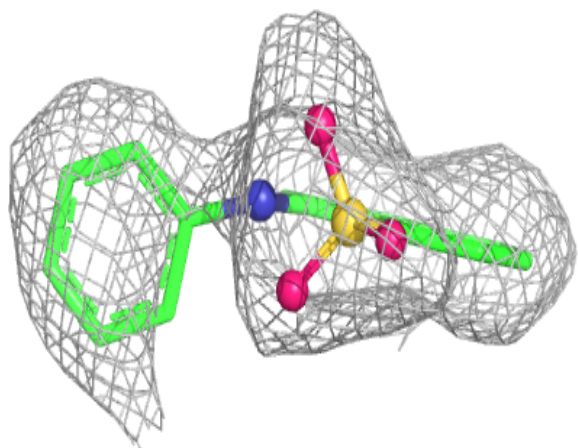
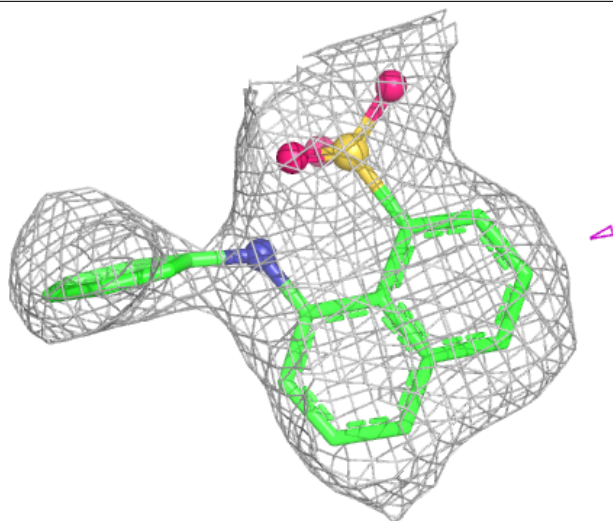
Electron density around 2AN U 205:

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



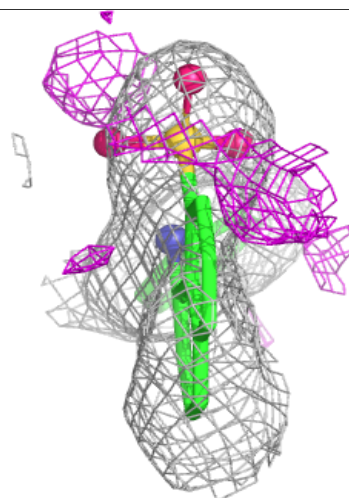
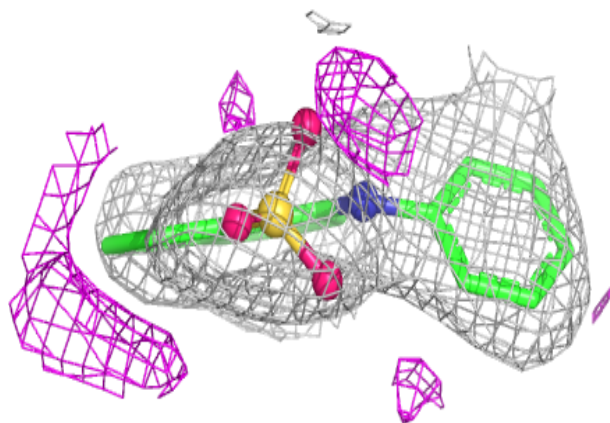
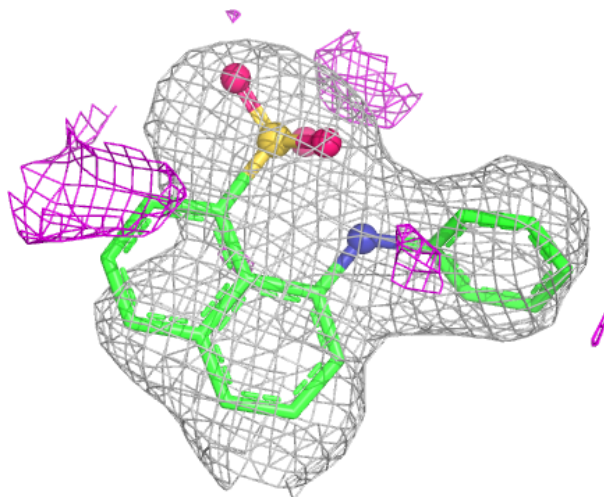
Electron density around 2AN V 201:

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



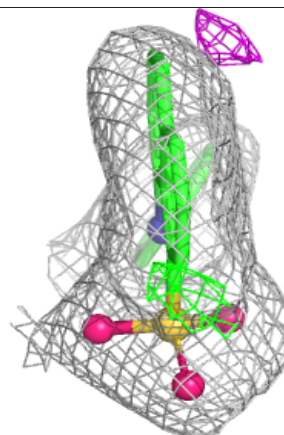
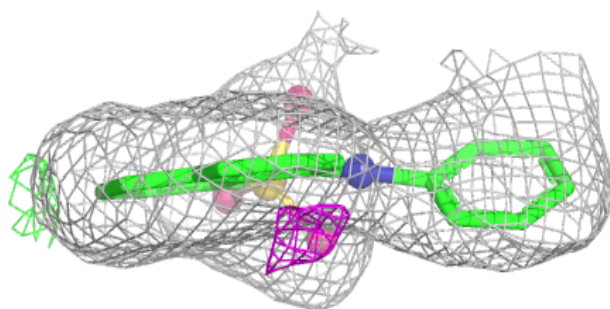
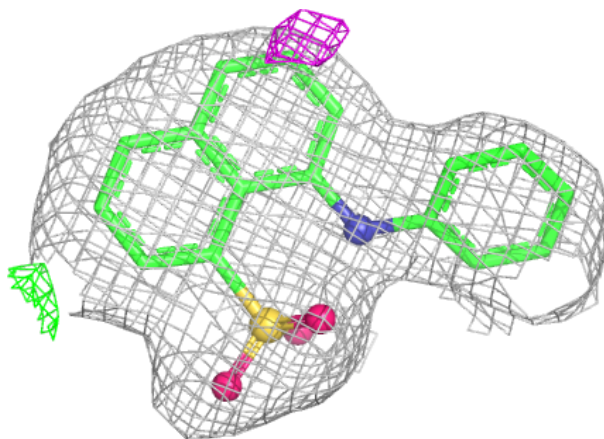
Electron density around 2AN W 201:

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



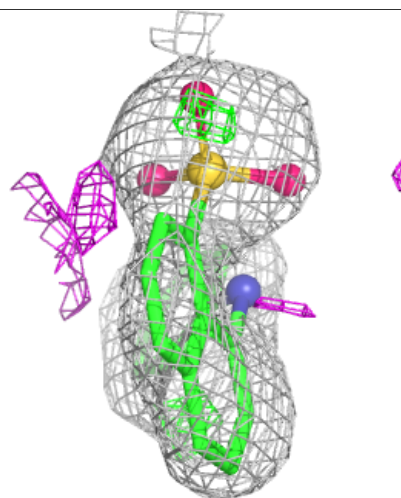
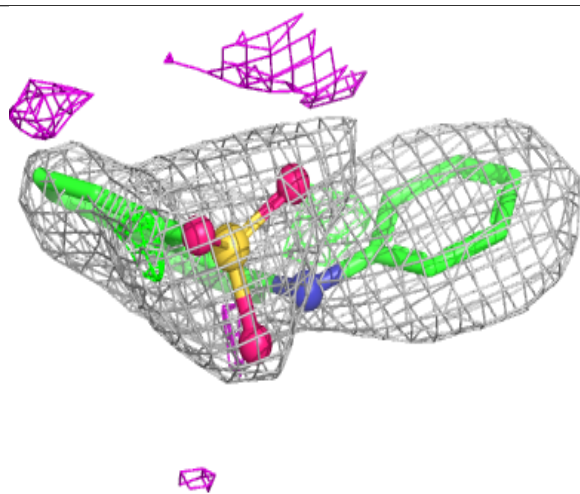
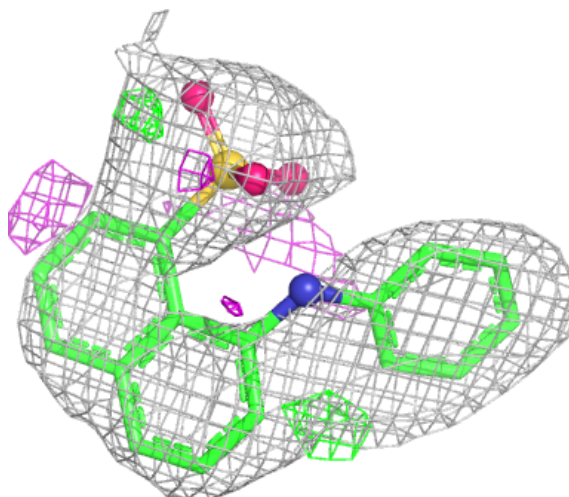
Electron density around 2AN W 202:

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



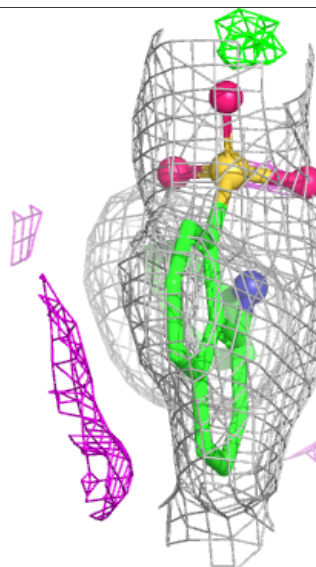
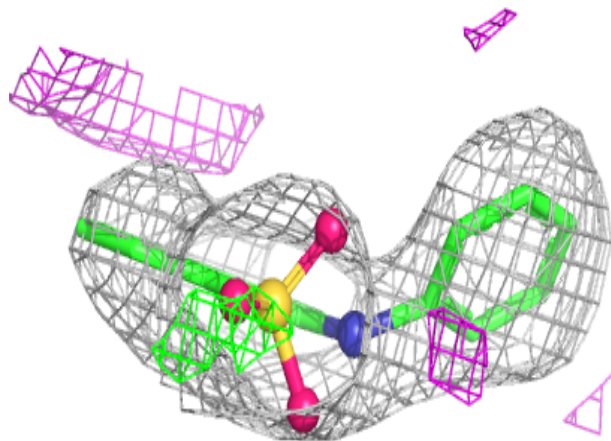
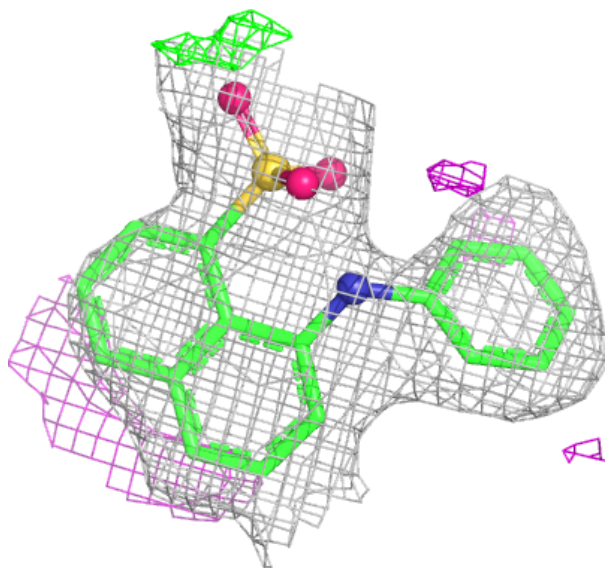
Electron density around 2AN W 203:

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



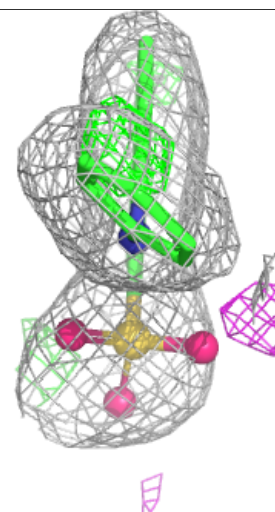
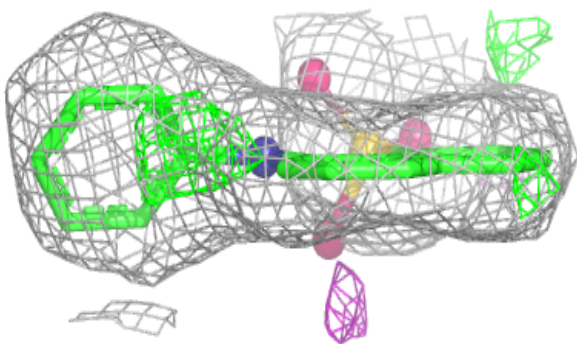
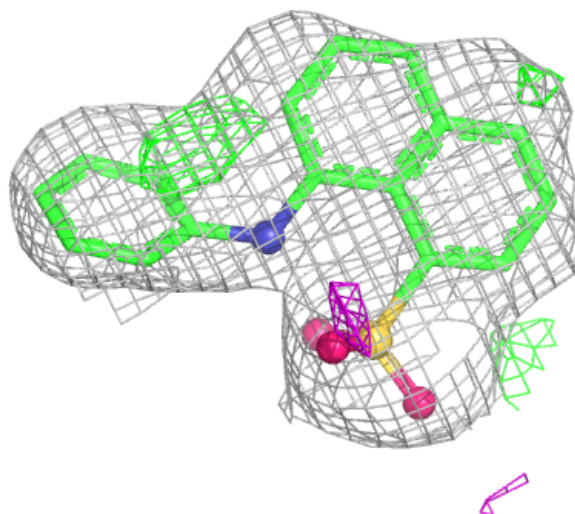
Electron density around 2AN W 204:

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



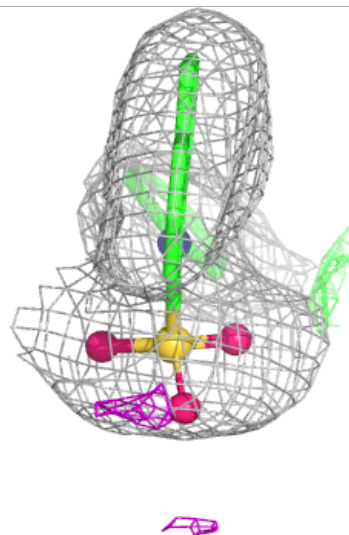
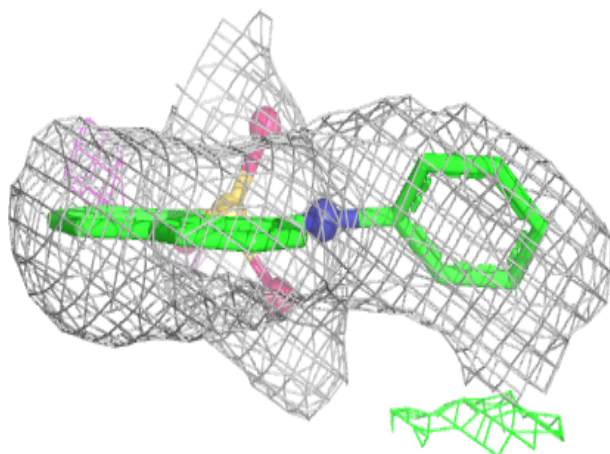
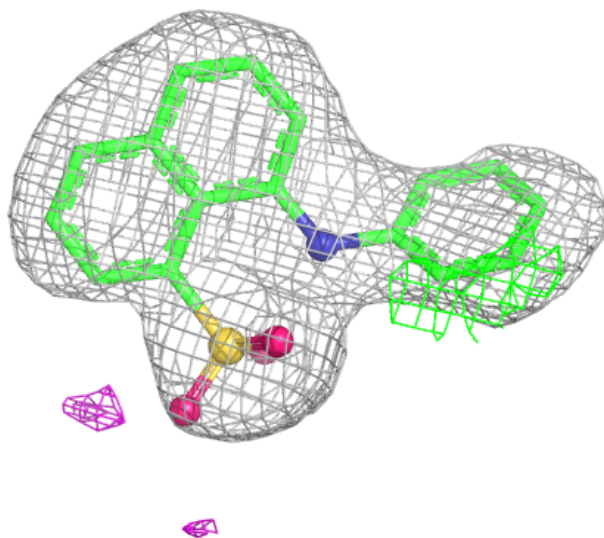
Electron density around 2AN X 202:

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



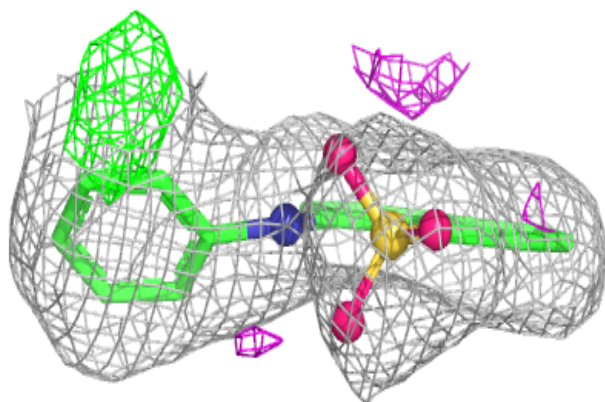
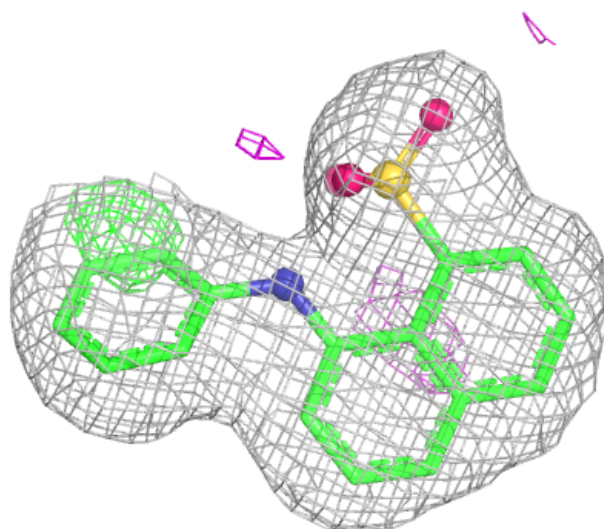
Electron density around 2AN Y 203:

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



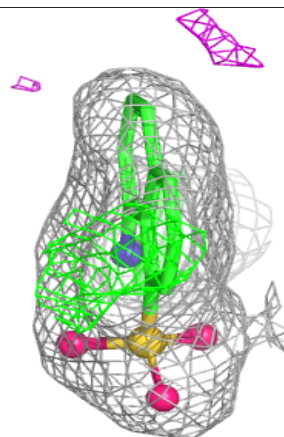
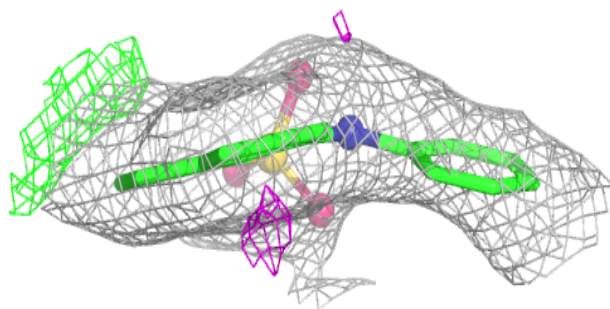
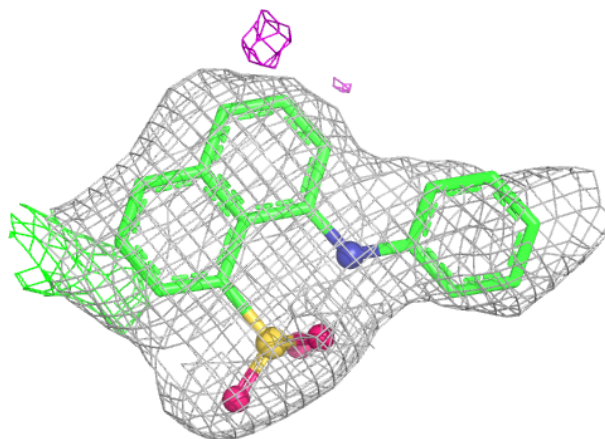
Electron density around 2AN E 202:

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



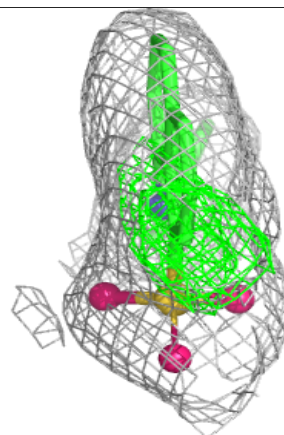
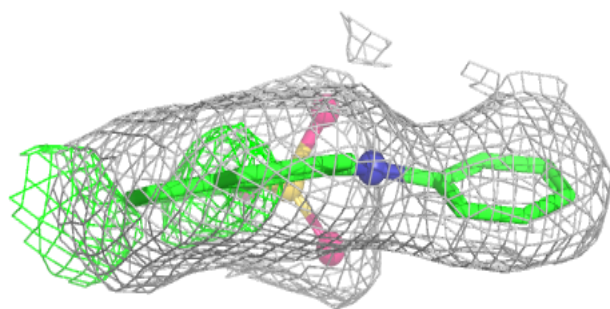
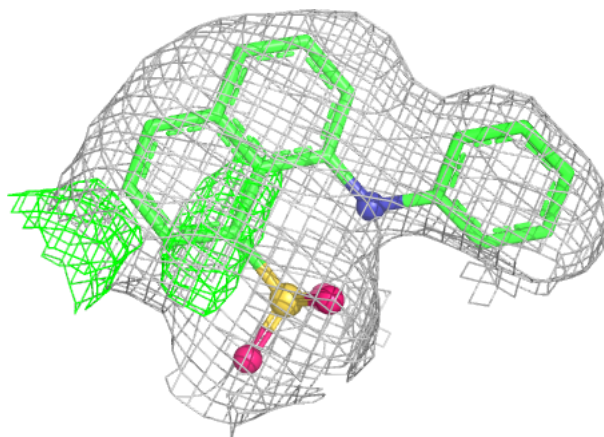
Electron density around 2AN Z 203:

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



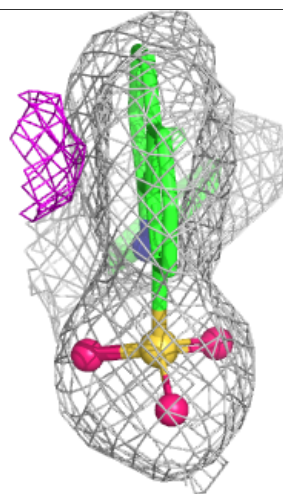
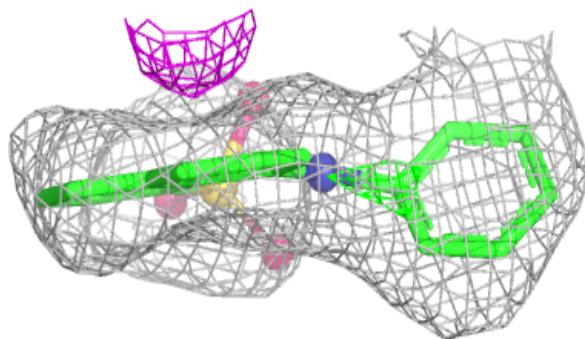
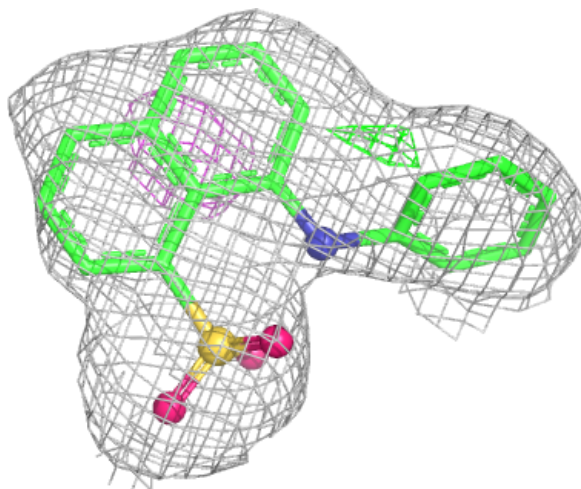
Electron density around 2AN a 201:

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



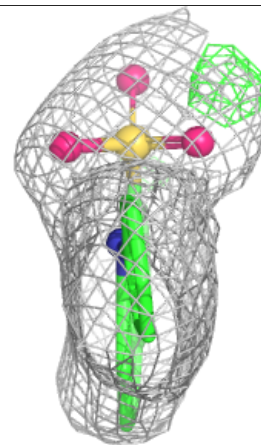
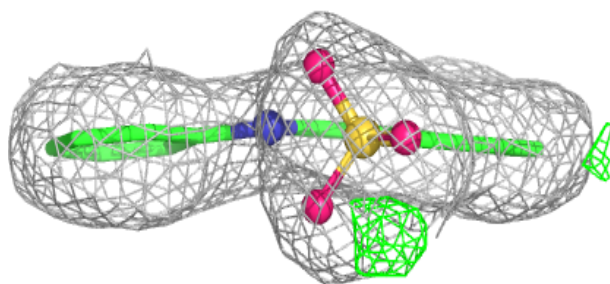
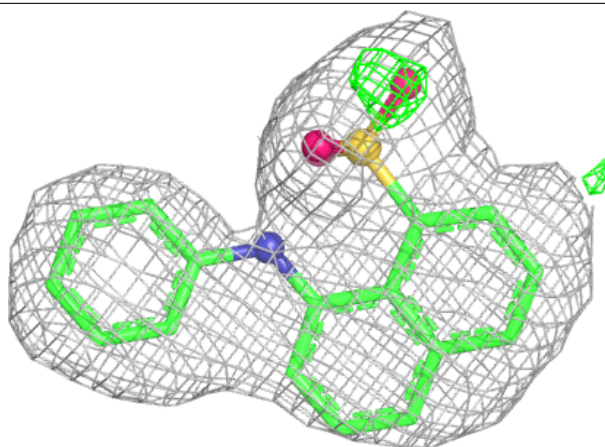
Electron density around 2AN b 201:

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



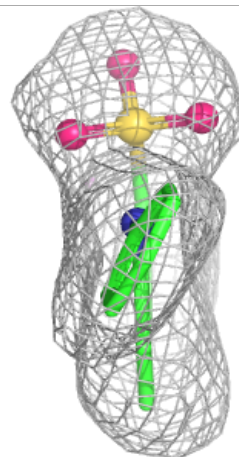
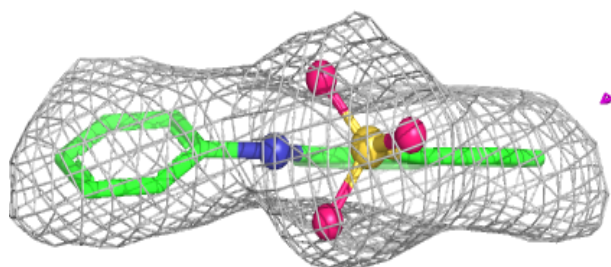
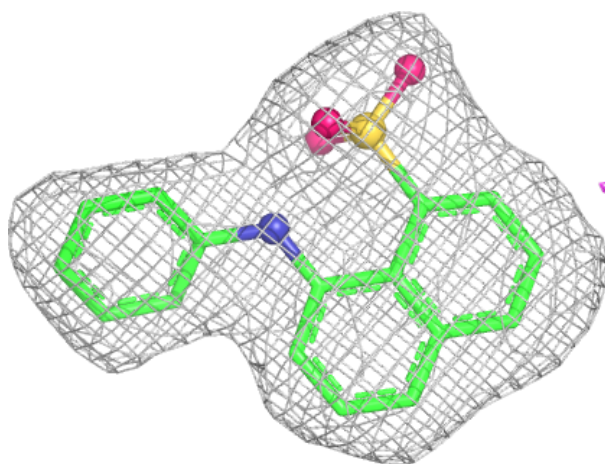
Electron density around 2AN D 202:

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



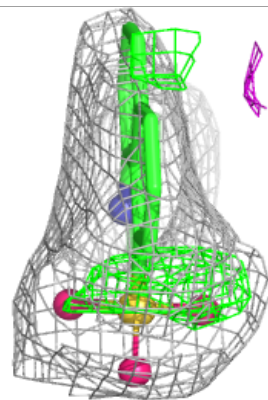
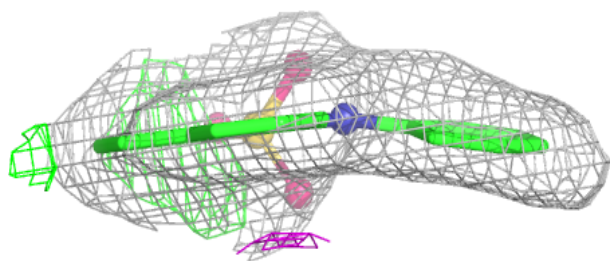
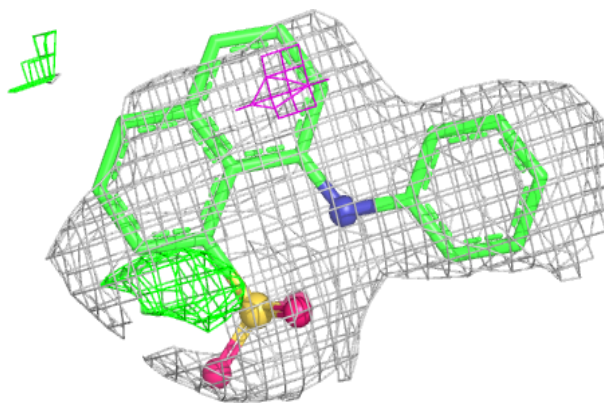
Electron density around 2AN L 203:

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



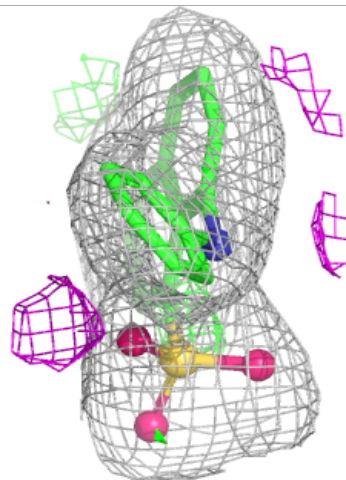
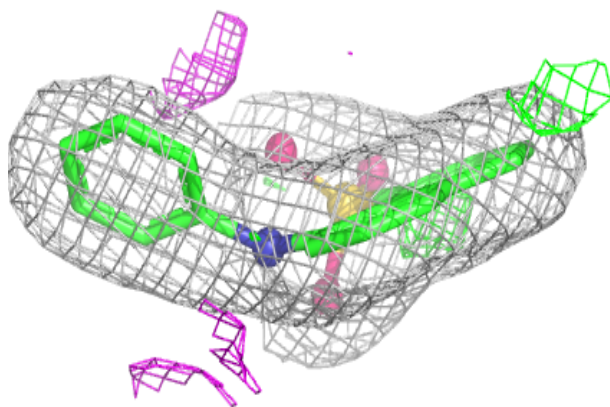
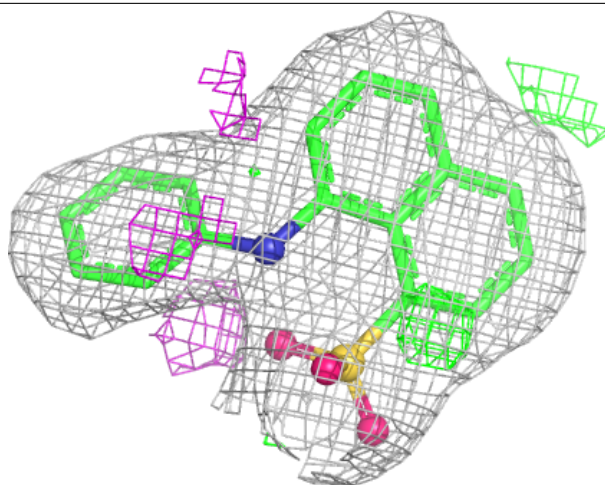
Electron density around 2AN D 203:

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



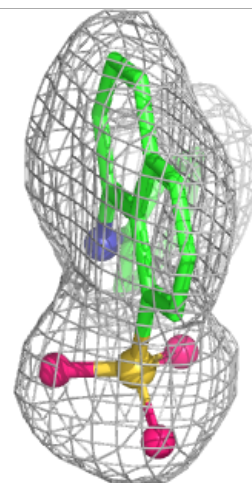
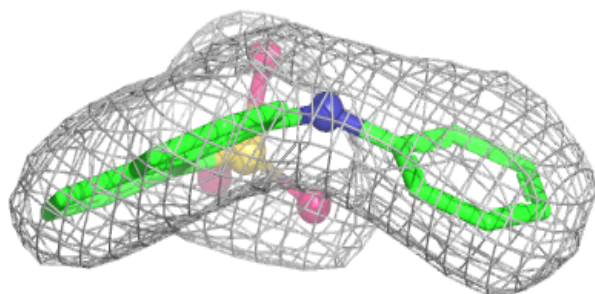
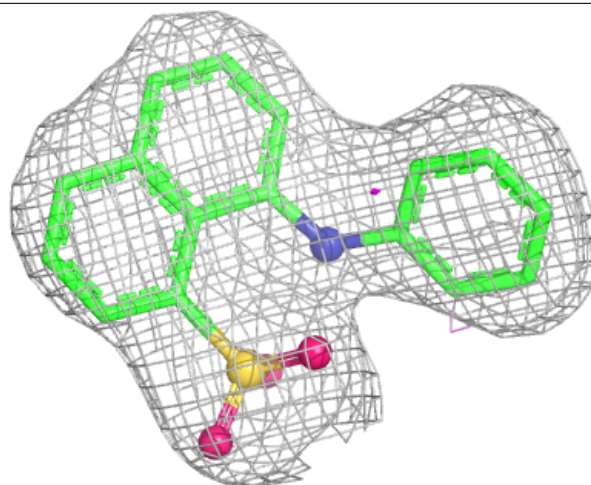
Electron density around 2AN E 201:

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



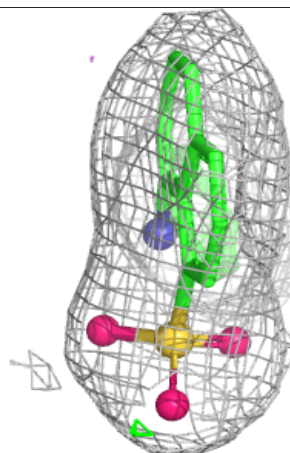
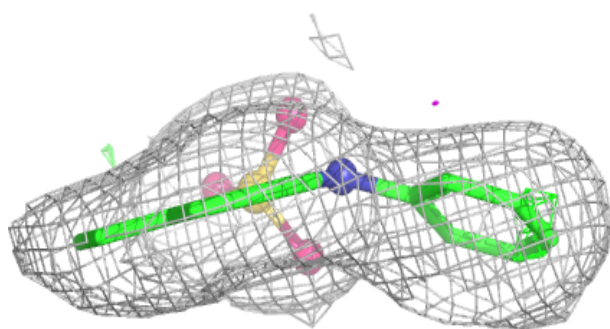
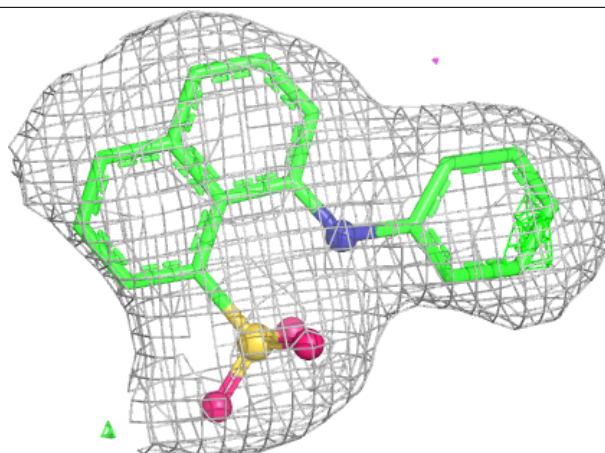
Electron density around 2AN M 201:

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



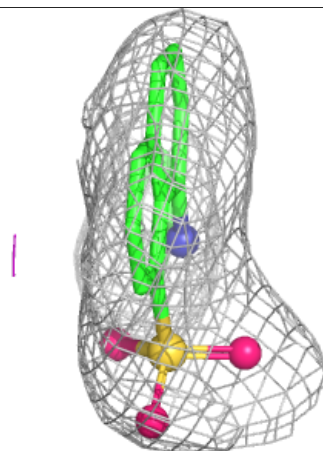
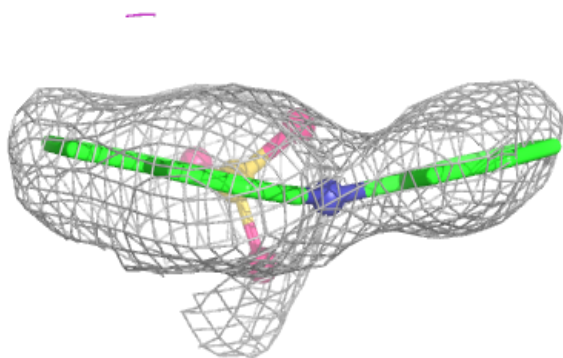
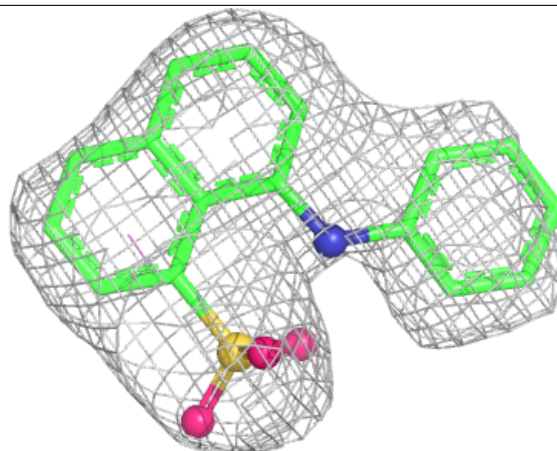
Electron density around 2AN A 204:

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



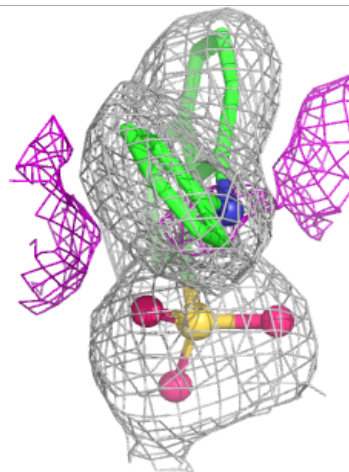
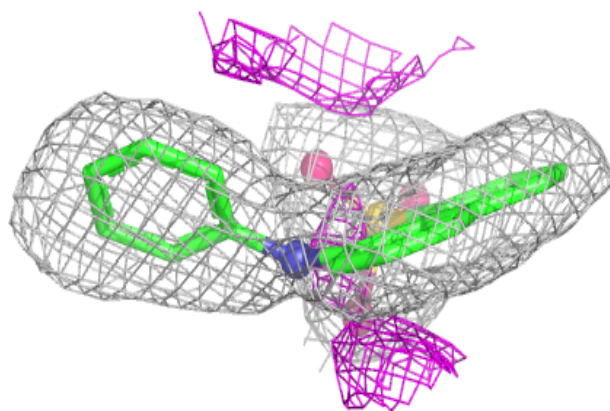
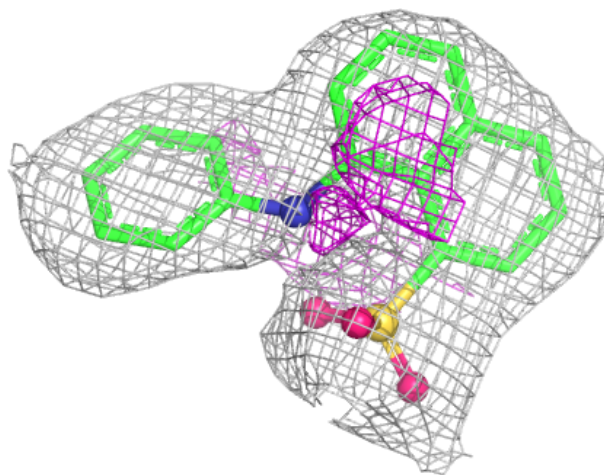
Electron density around 2AN M 203:

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



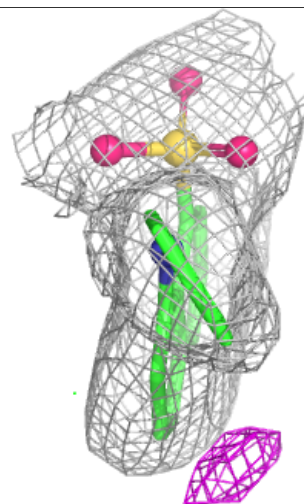
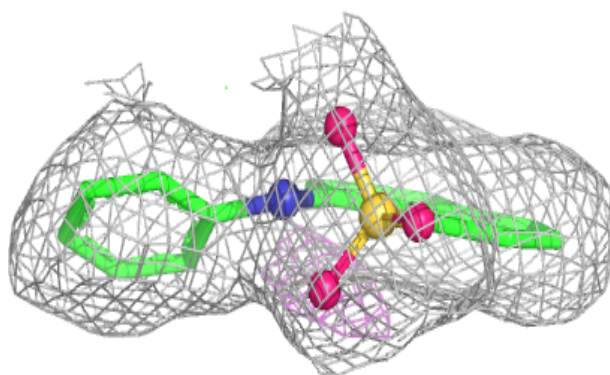
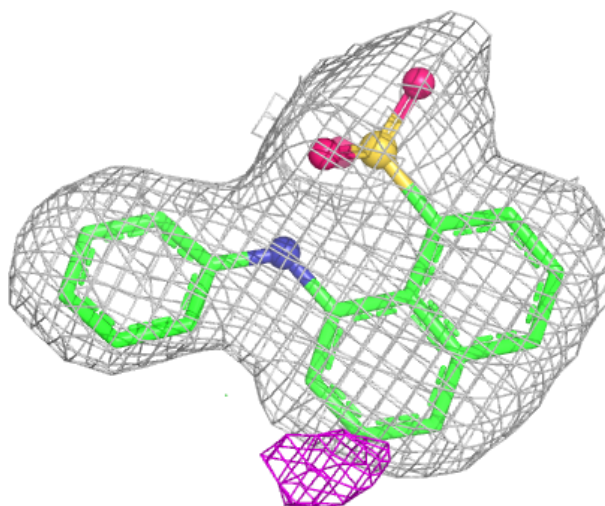
Electron density around 2AN N 201:

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



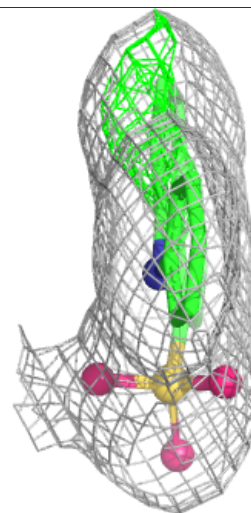
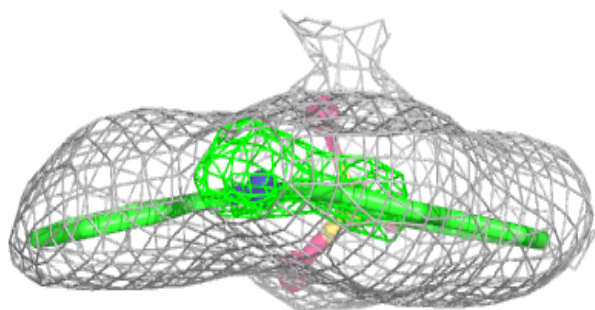
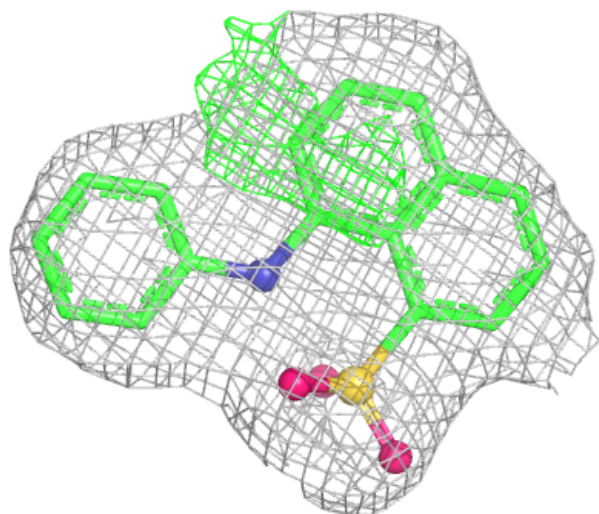
Electron density around 2AN N 202:

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



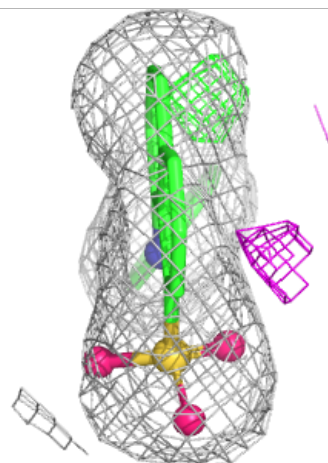
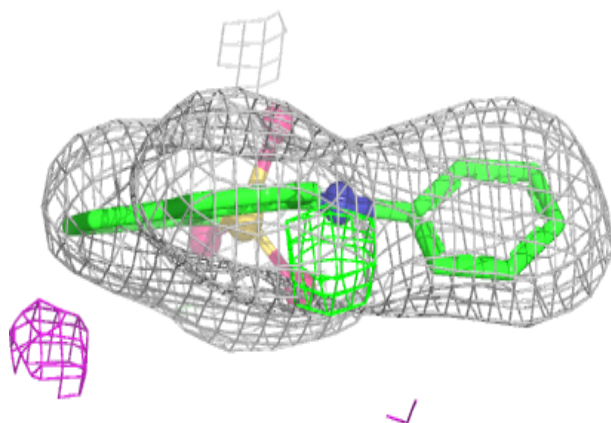
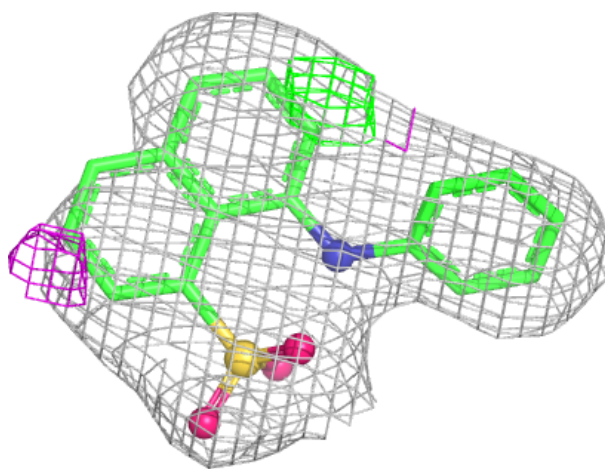
Electron density around 2AN E 203:

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



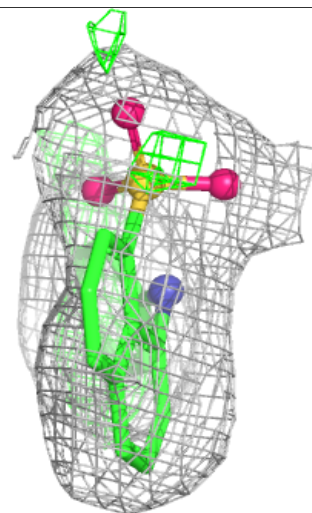
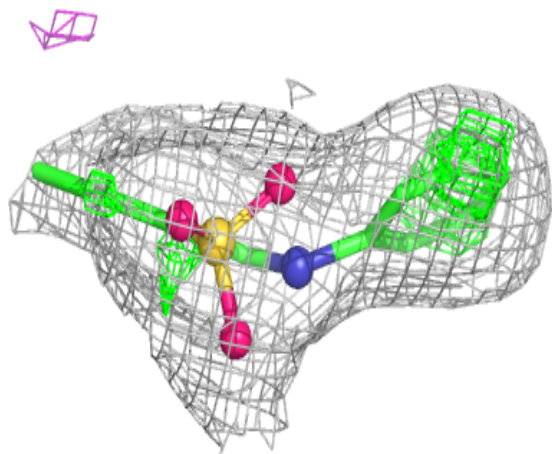
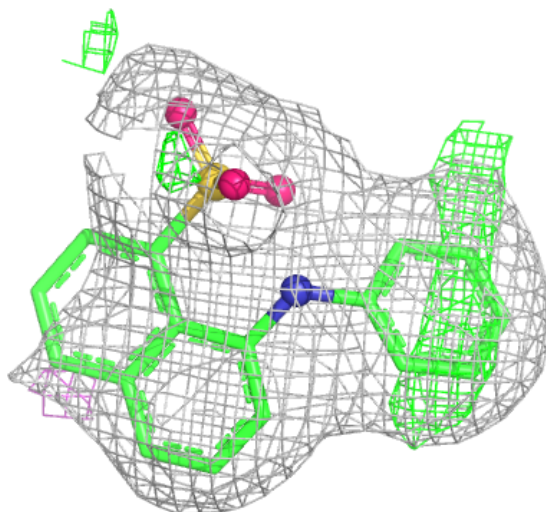
Electron density around 2AN E 204:

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



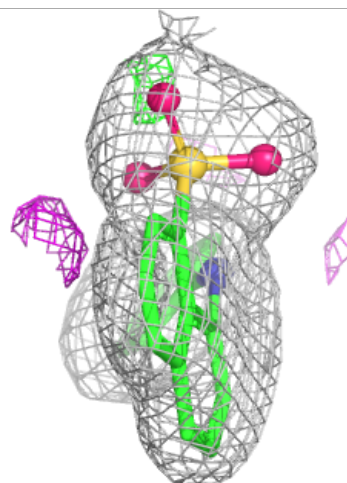
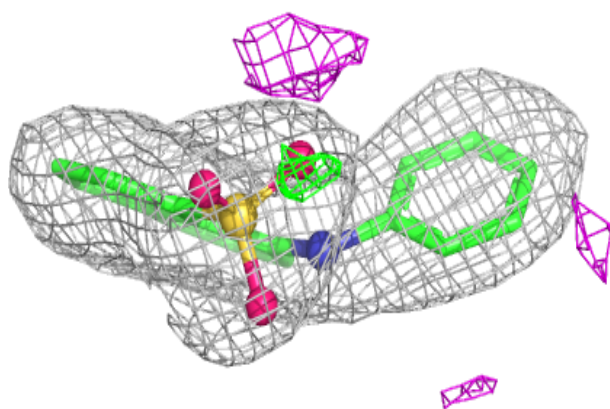
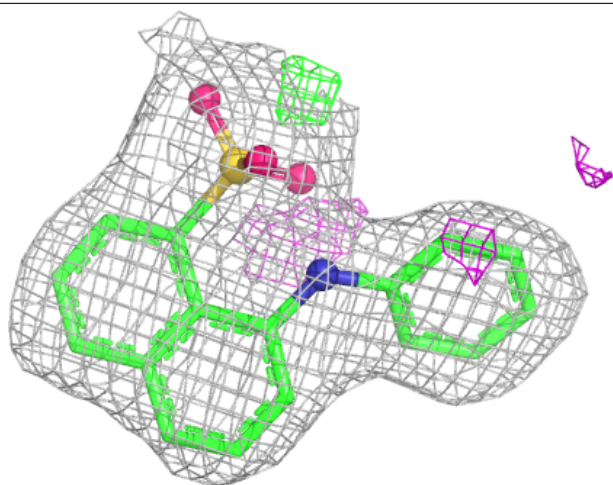
Electron density around 2AN E 205:

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



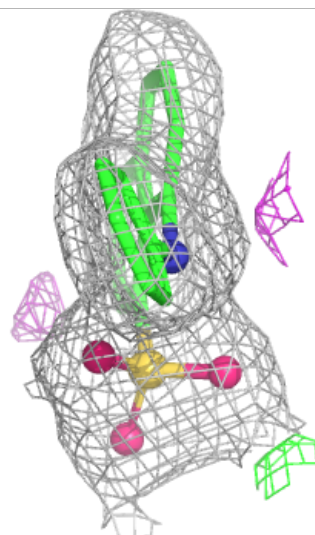
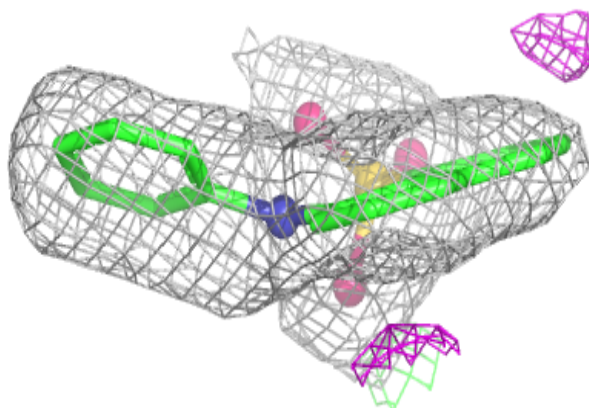
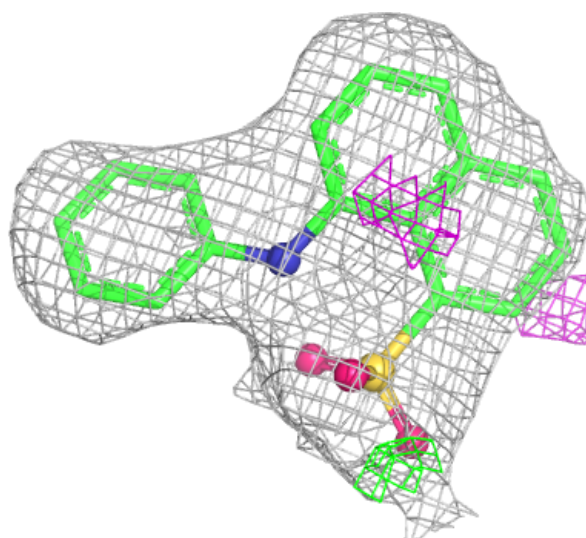
Electron density around 2AN O 202:

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



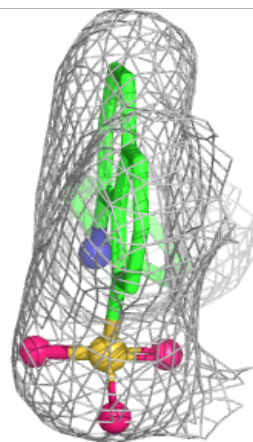
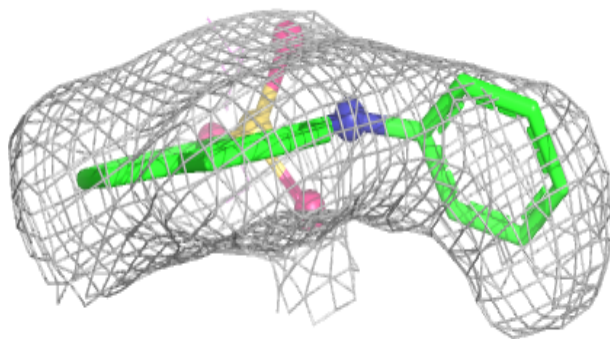
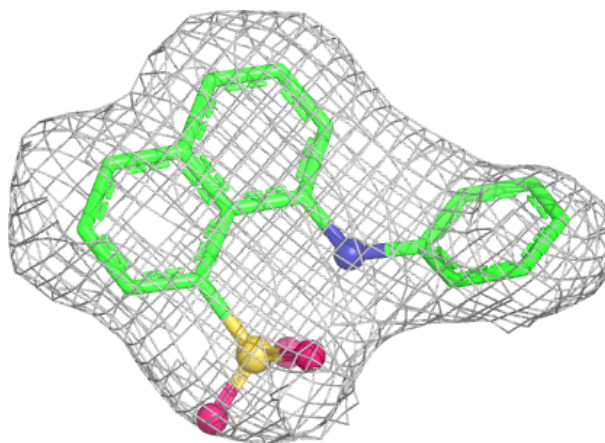
Electron density around 2AN P 201:

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



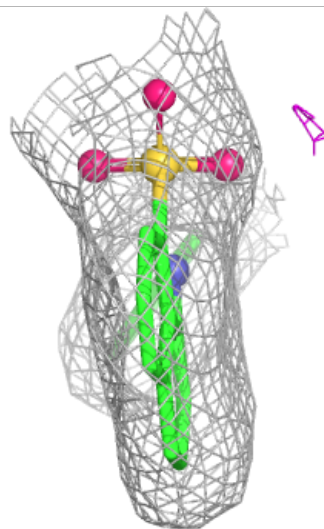
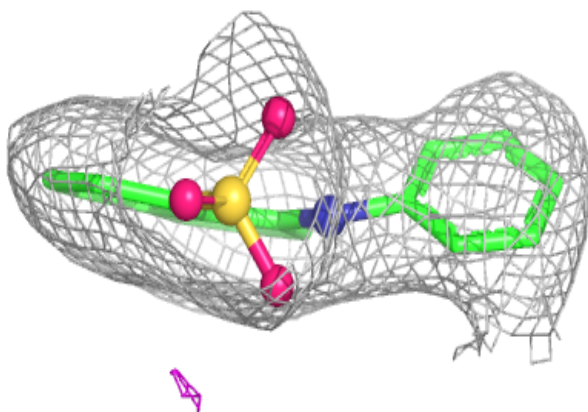
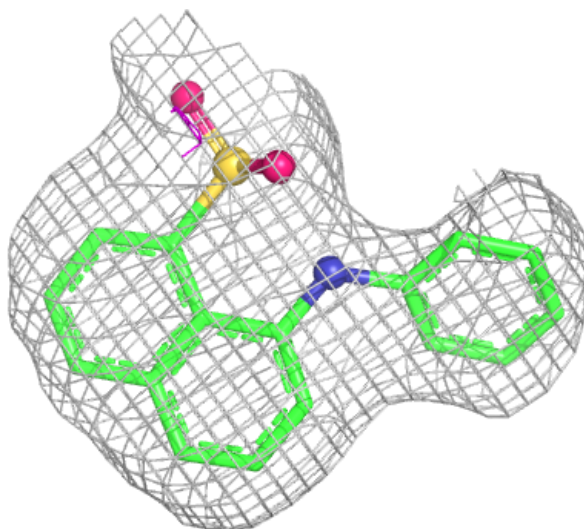
Electron density around 2AN P 202:

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



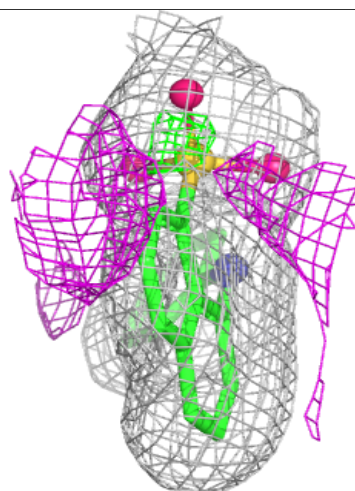
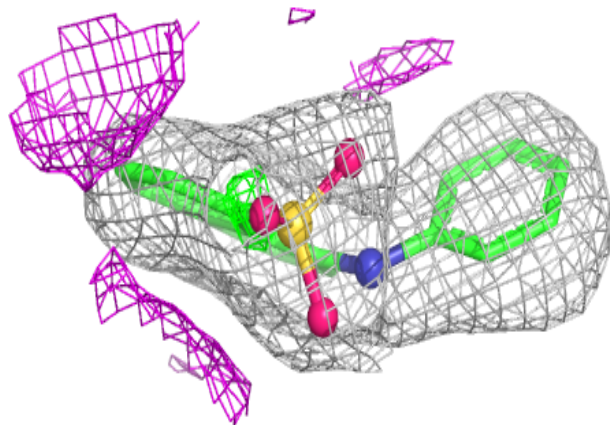
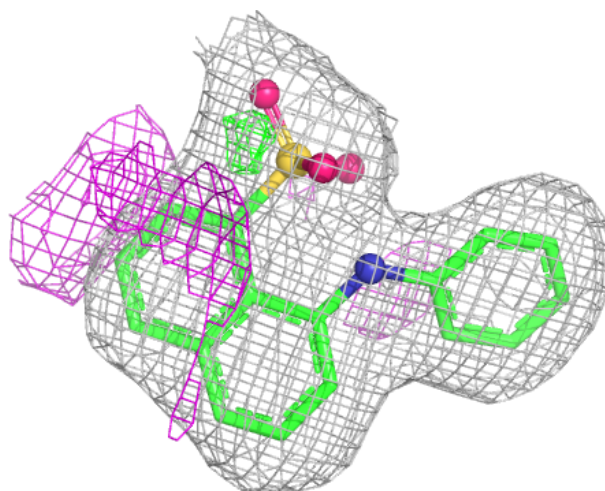
Electron density around 2AN Q 201:

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



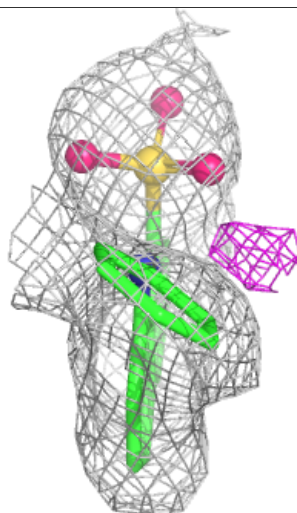
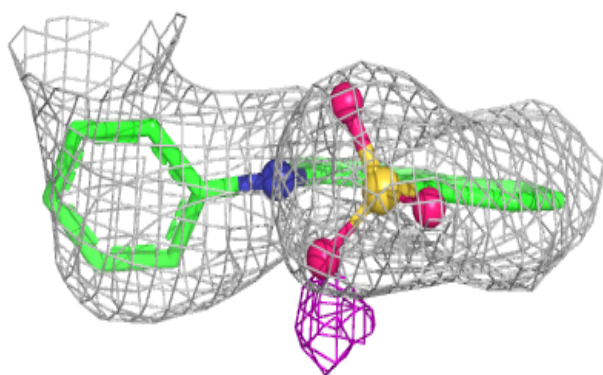
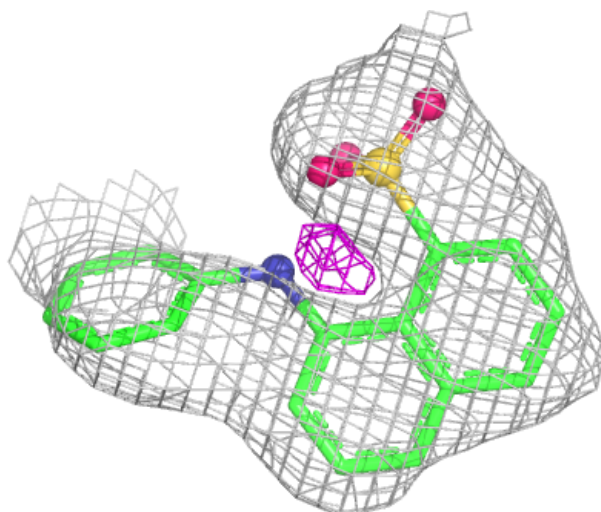
Electron density around 2AN G 201:

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



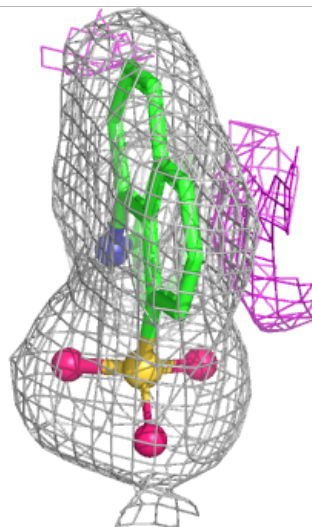
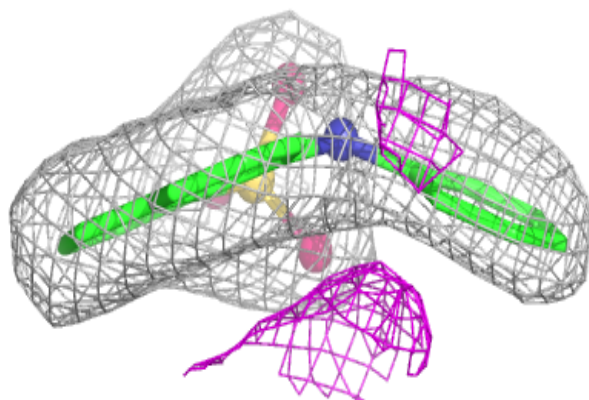
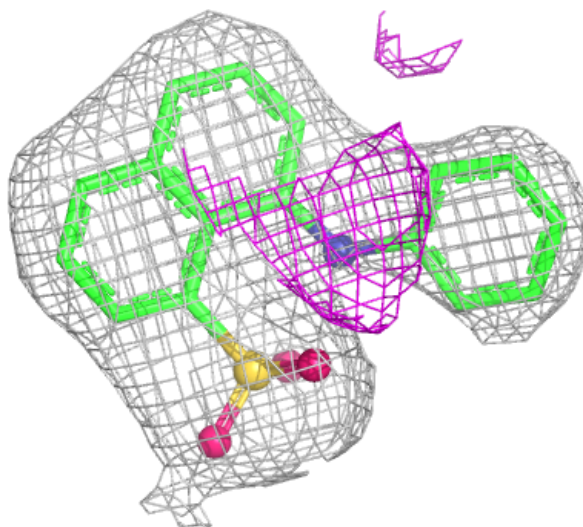
Electron density around 2AN R 201:

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



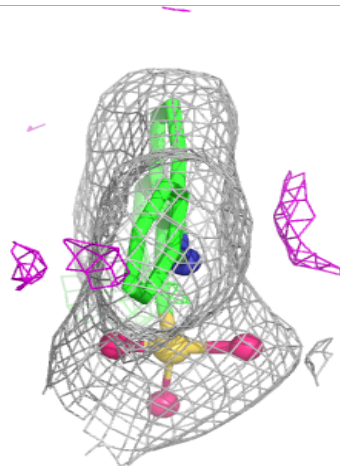
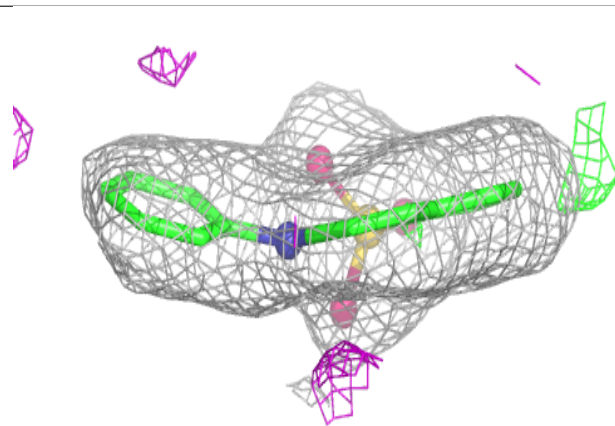
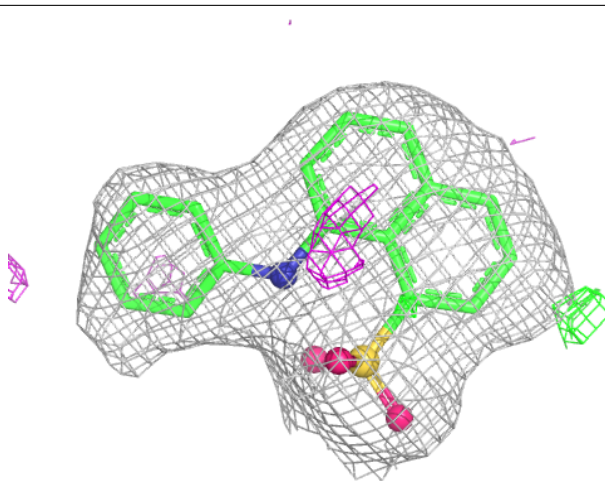
Electron density around 2AN R 202:

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



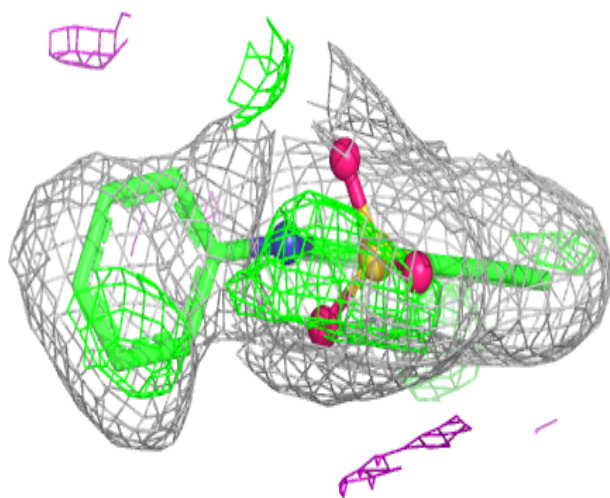
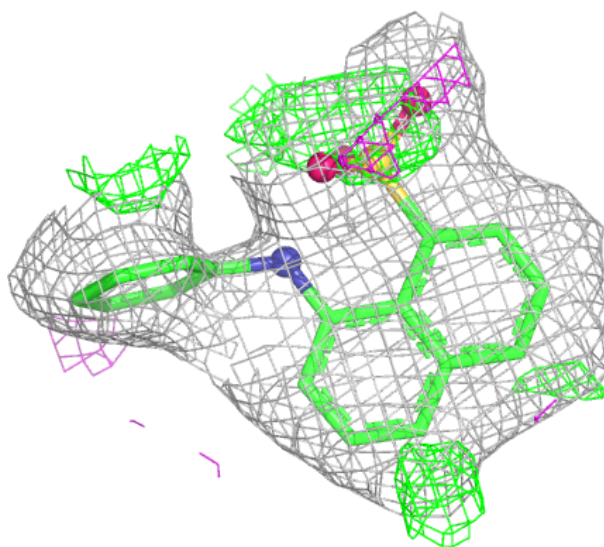
Electron density around 2AN G 202:

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



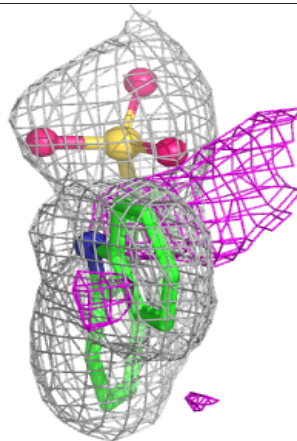
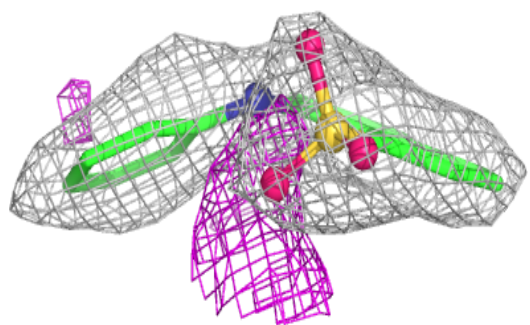
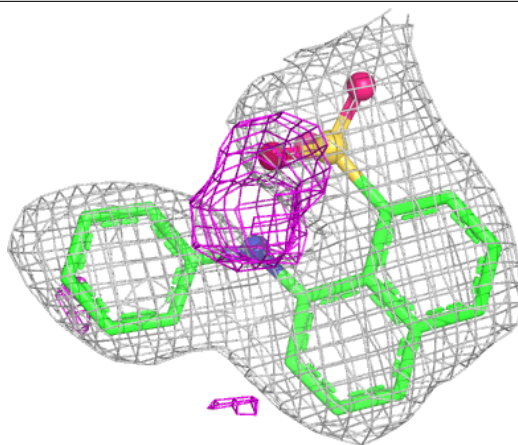
Electron density around 2AN R 204:

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



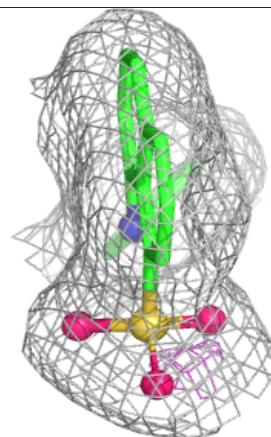
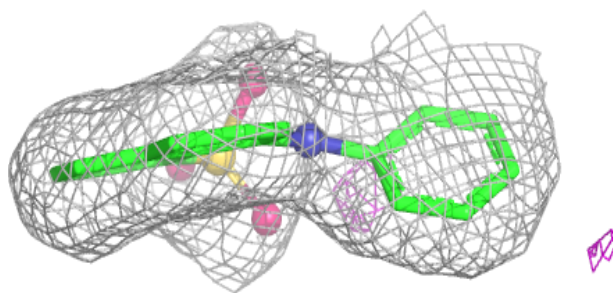
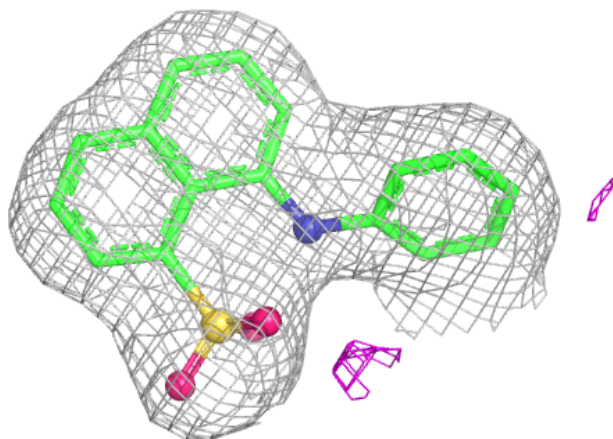
Electron density around 2AN S 201:

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



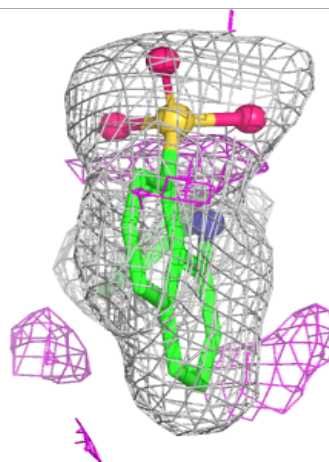
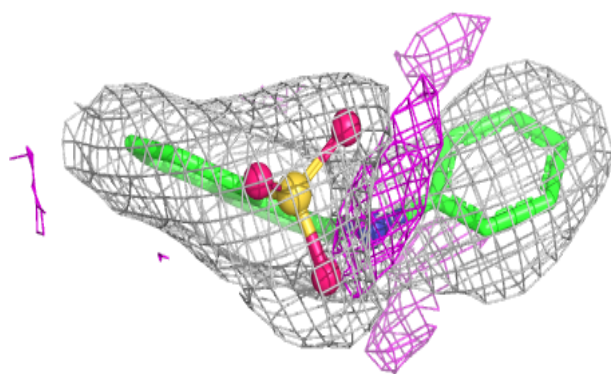
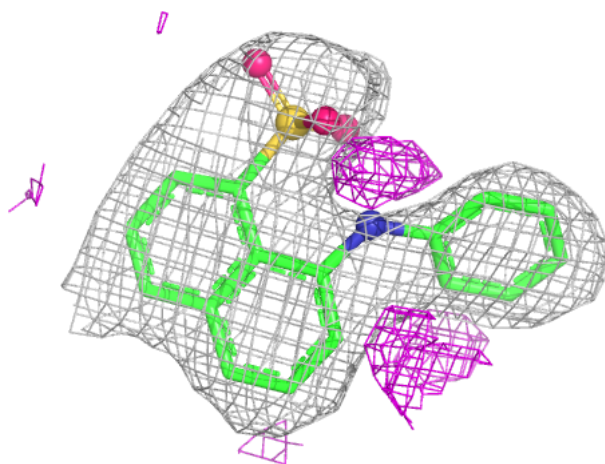
Electron density around 2AN U 201:

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



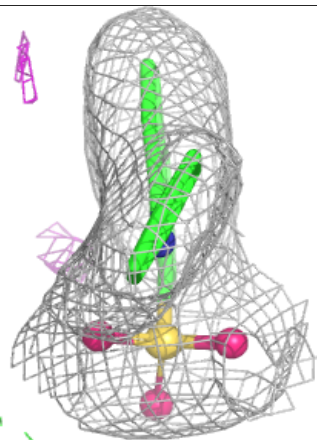
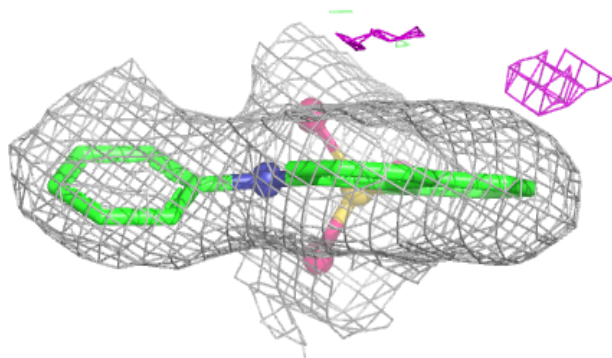
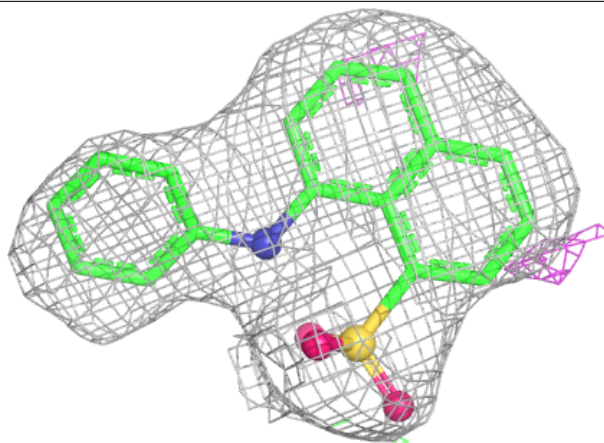
Electron density around 2AN U 202:

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



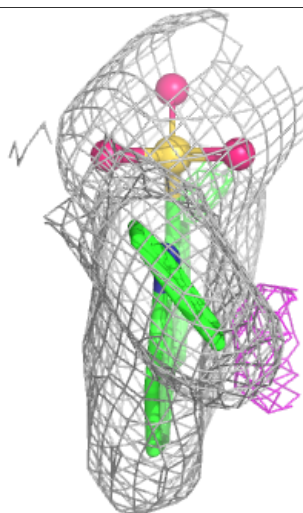
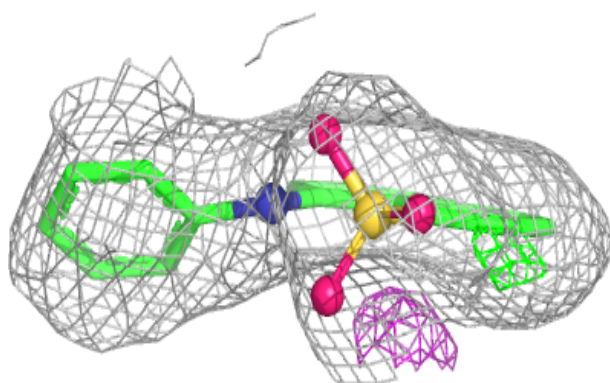
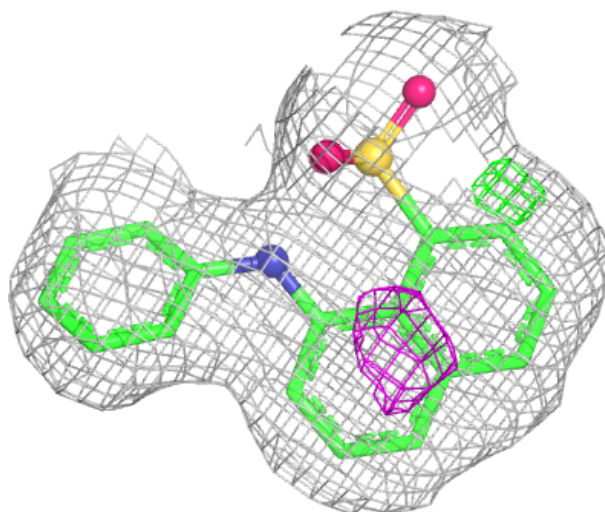
Electron density around 2AN U 203:

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



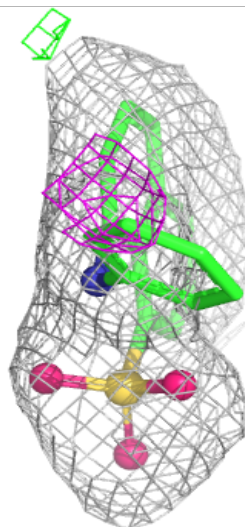
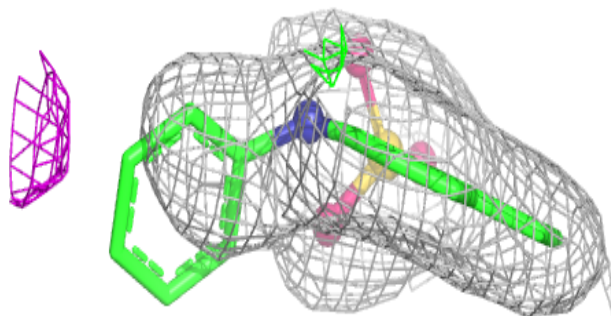
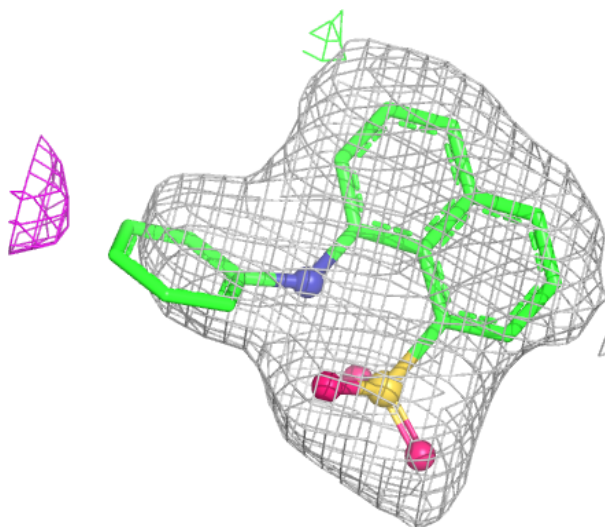
Electron density around 2AN B 202:

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



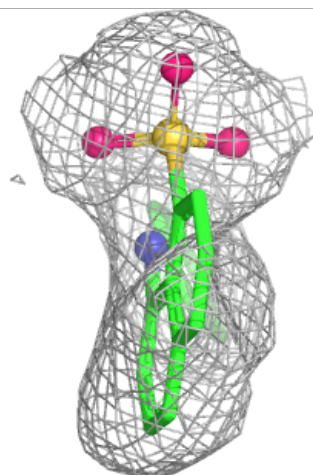
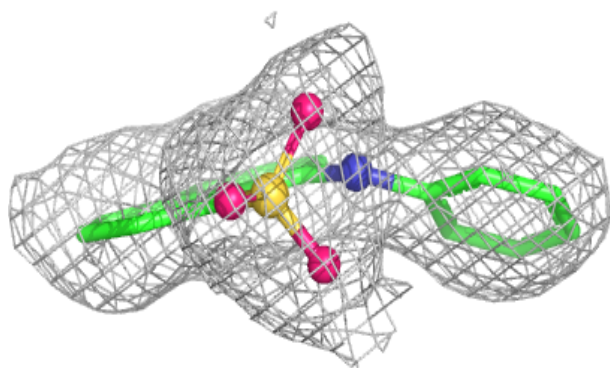
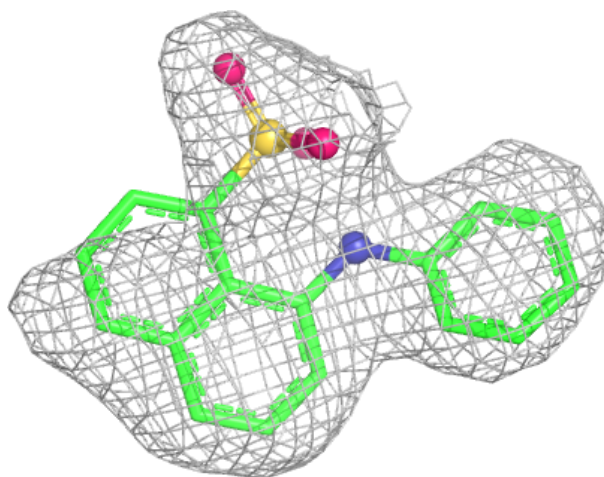
Electron density around 2AN V 202:

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



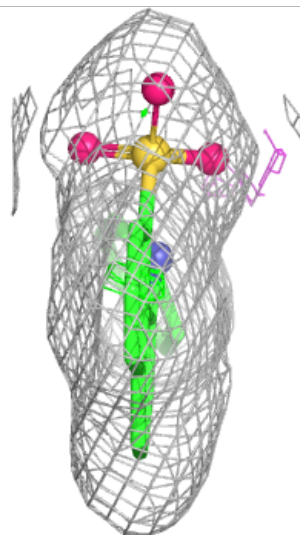
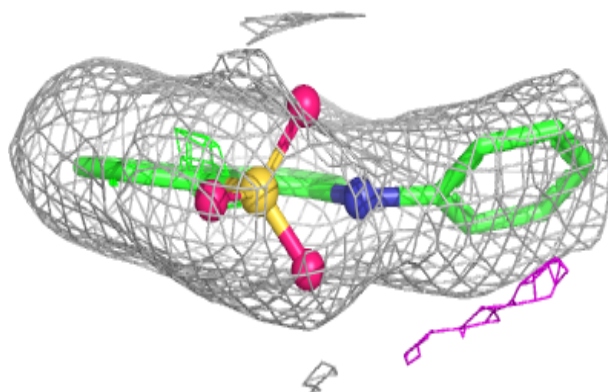
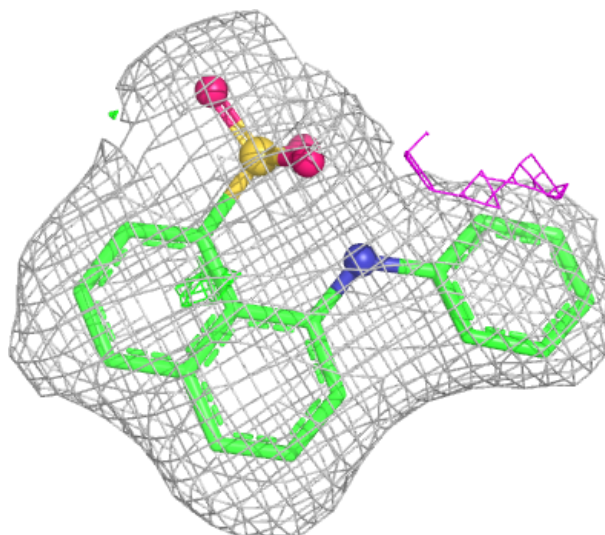
Electron density around 2AN B 204:

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



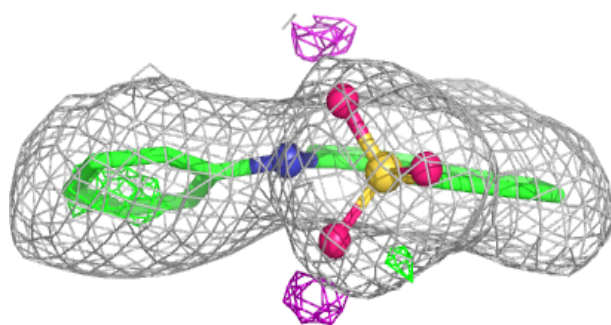
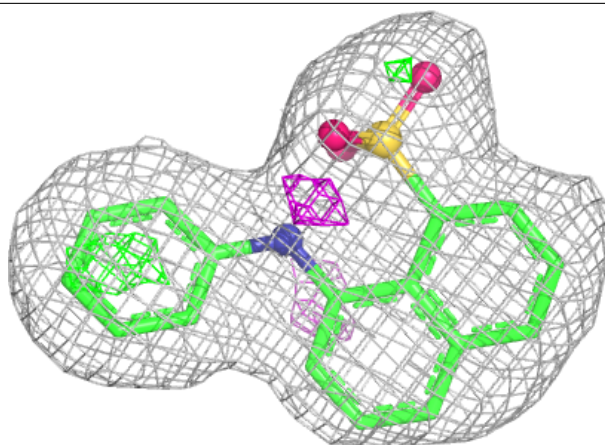
Electron density around 2AN A 201:

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



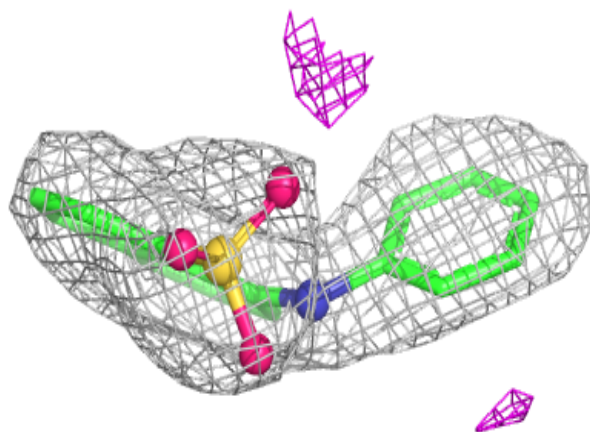
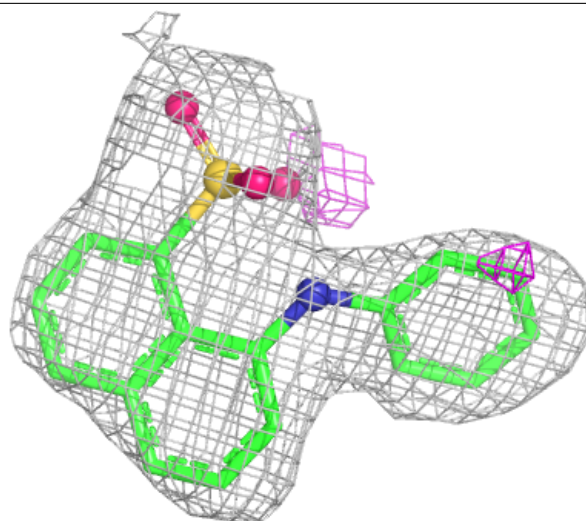
Electron density around 2AN H 203:

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



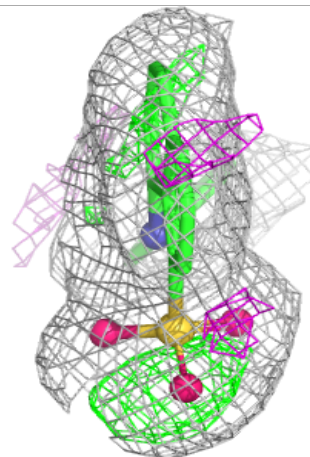
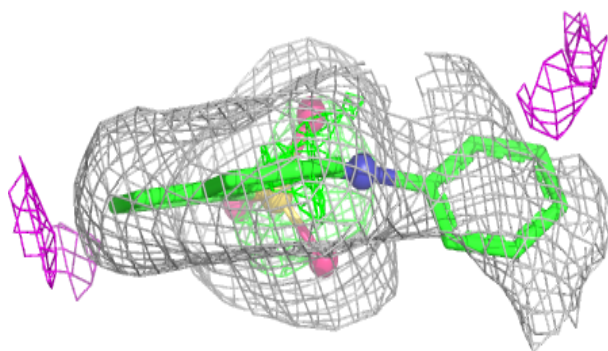
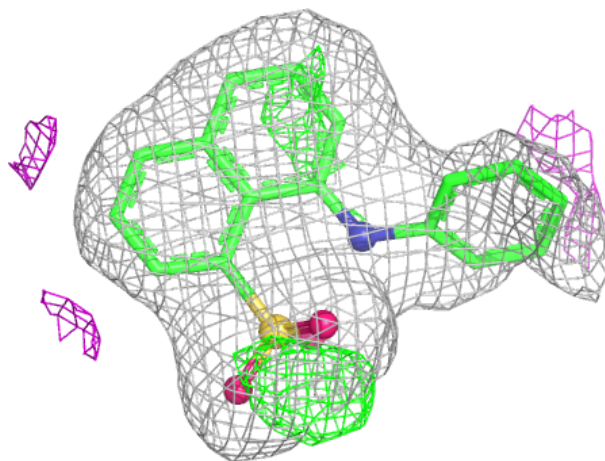
Electron density around 2AN X 201:

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



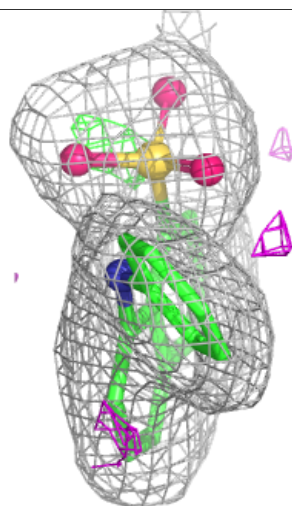
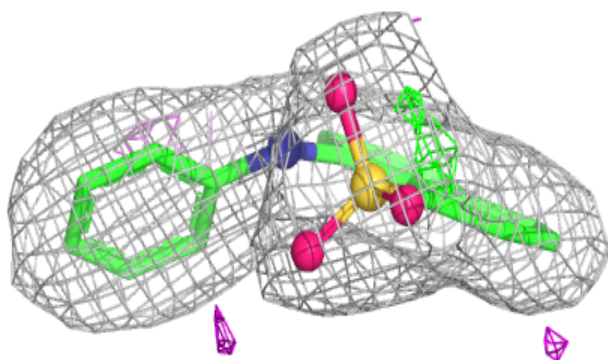
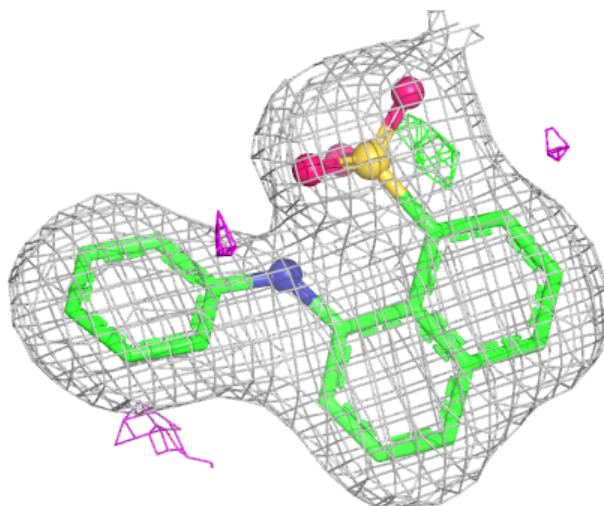
Electron density around 2AN X 203:

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



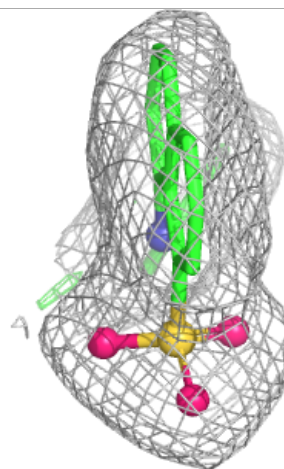
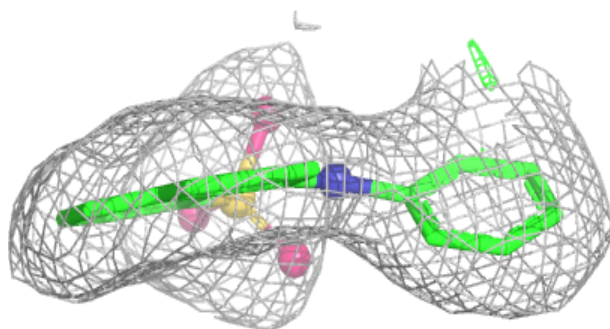
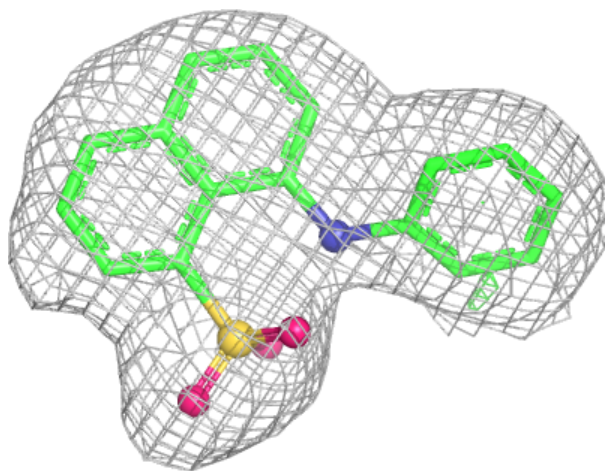
Electron density around 2AN Y 201:

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



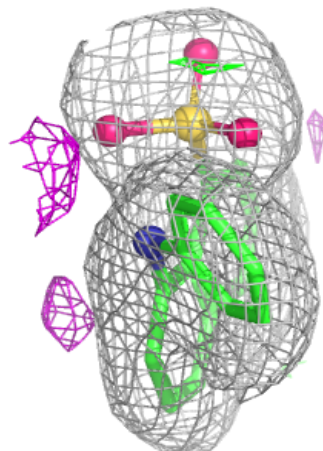
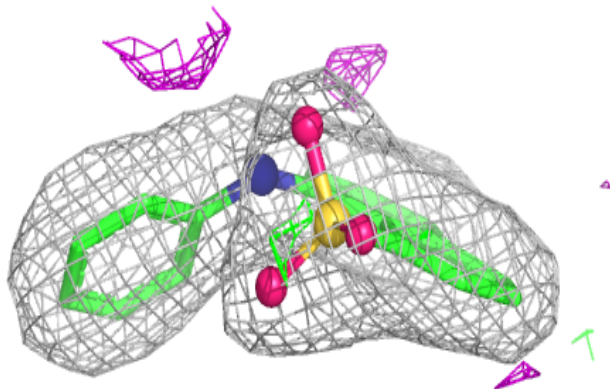
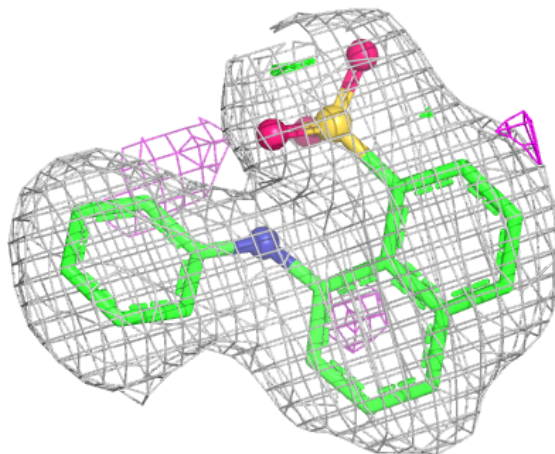
Electron density around 2AN Y 202:

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



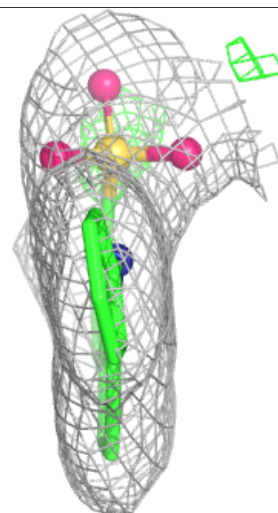
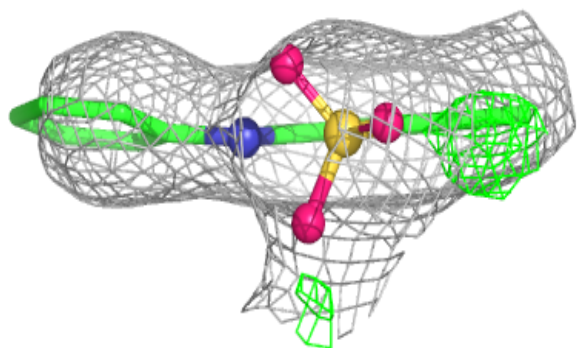
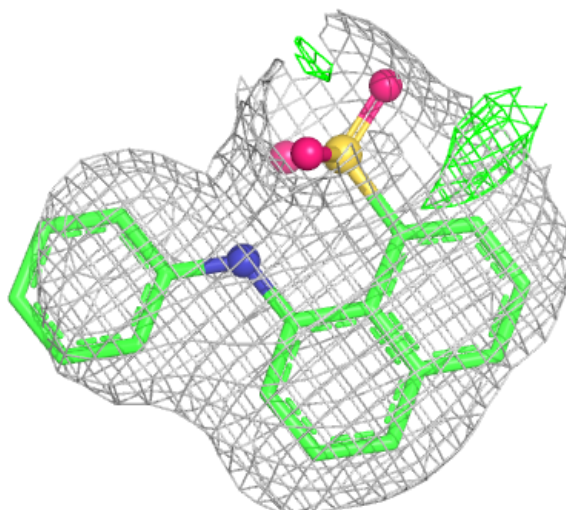
Electron density around 2AN I 202:

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



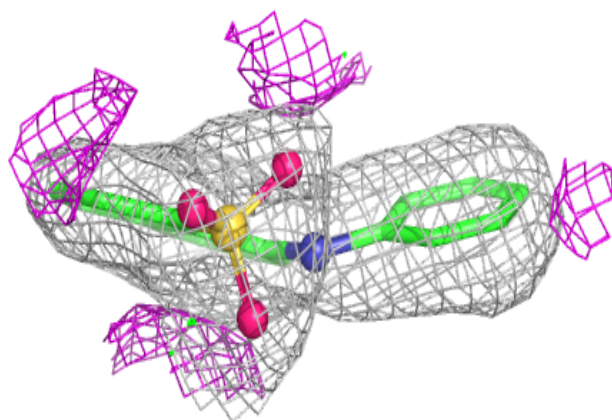
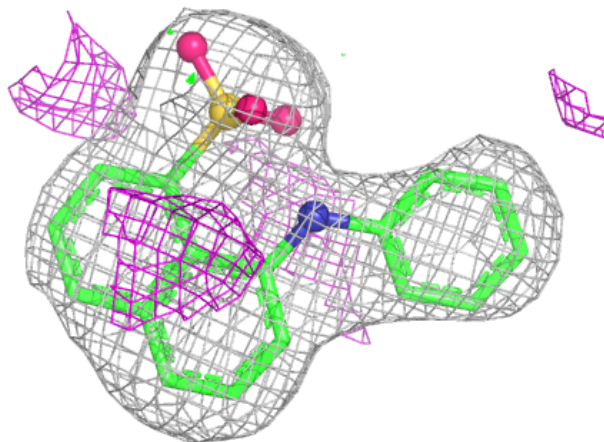
Electron density around 2AN I 203:

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



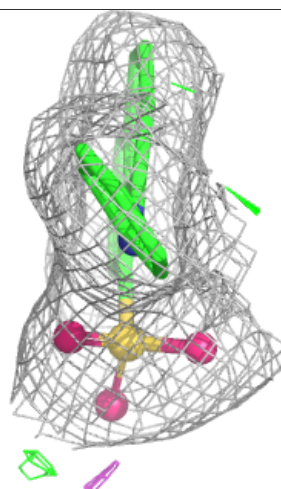
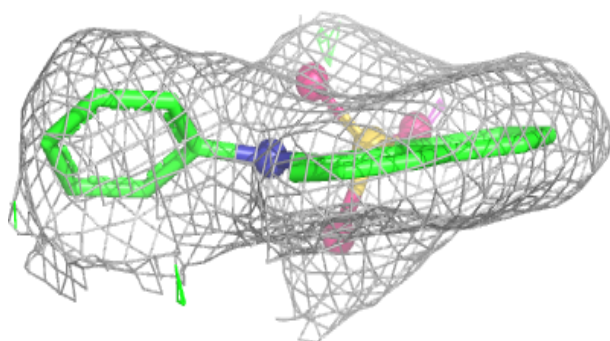
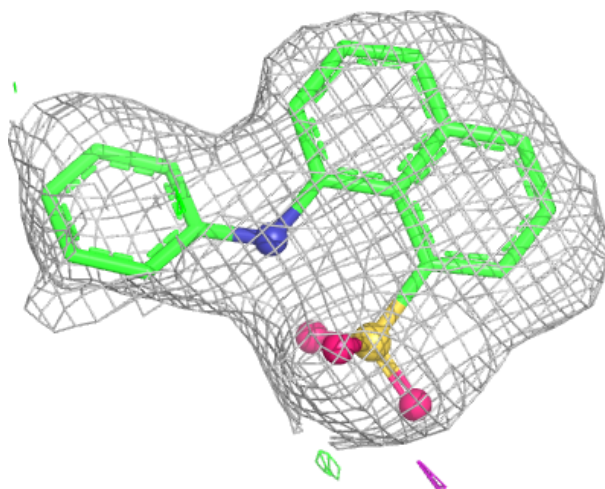
Electron density around 2AN Z 201:

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



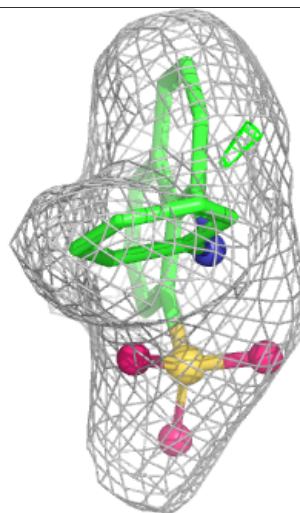
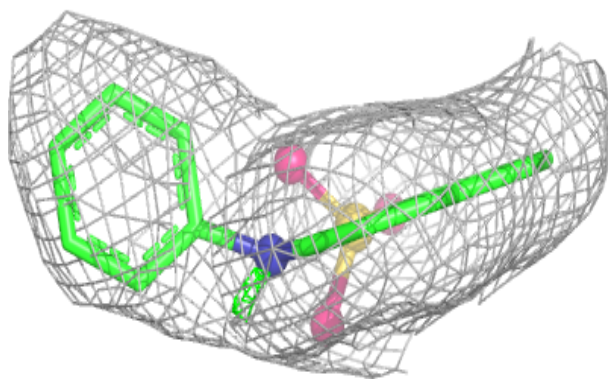
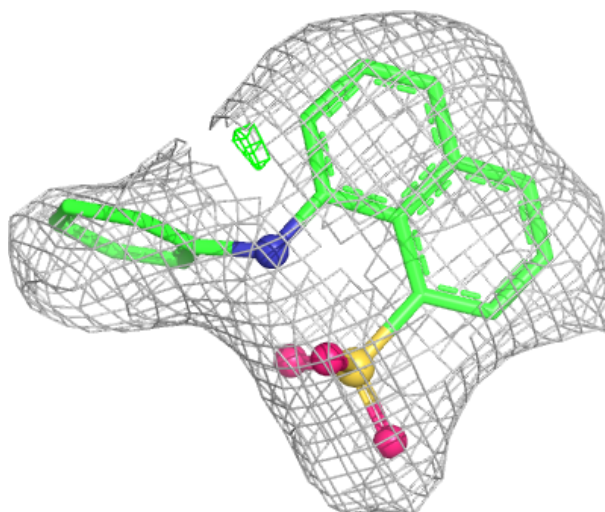
Electron density around 2AN C 202:

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



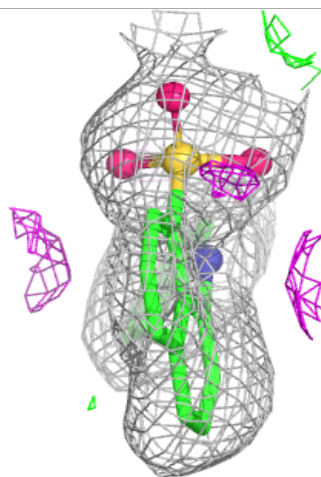
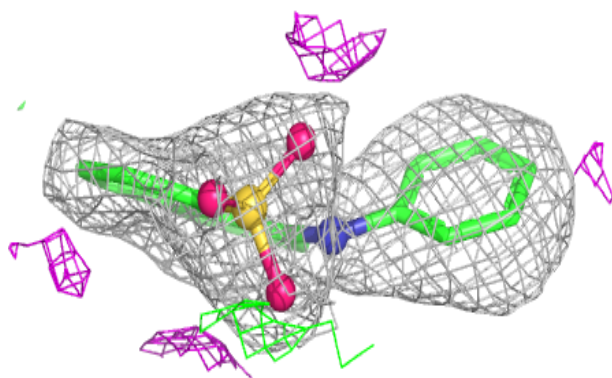
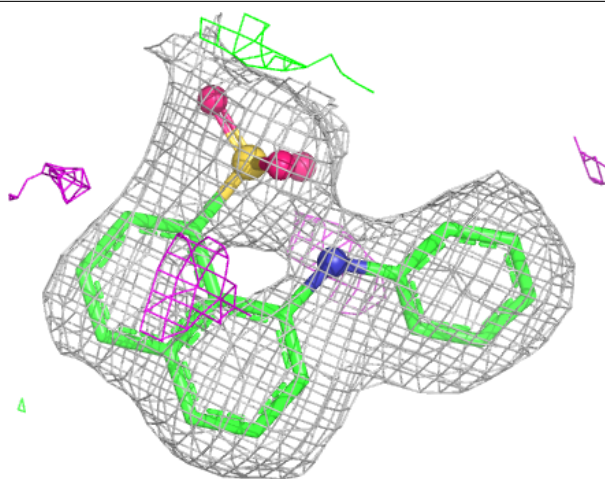
Electron density around 2AN C 203:

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



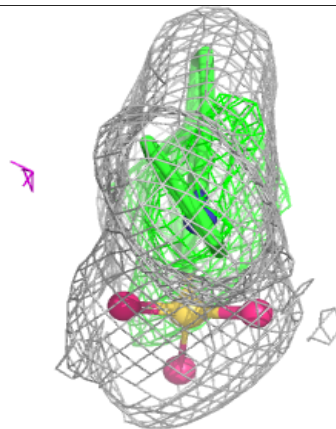
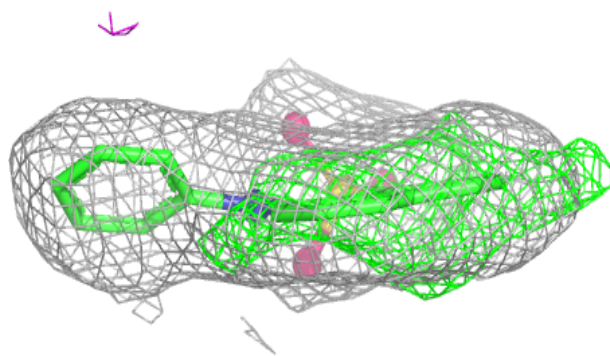
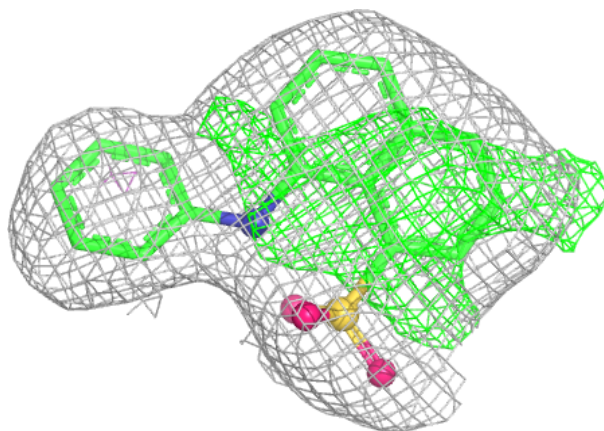
Electron density around 2AN J 201:

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



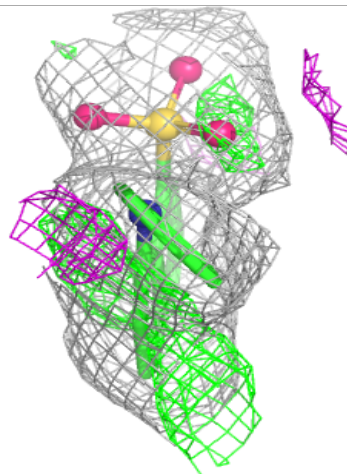
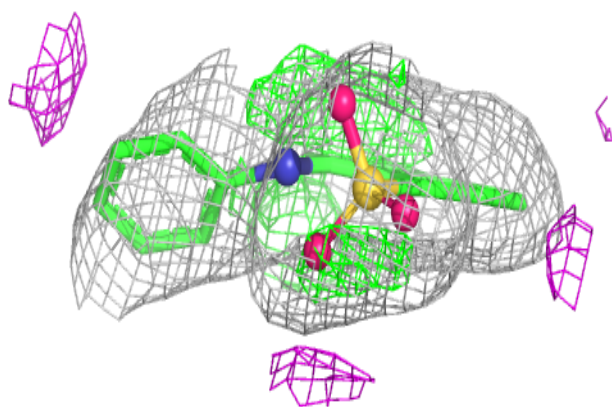
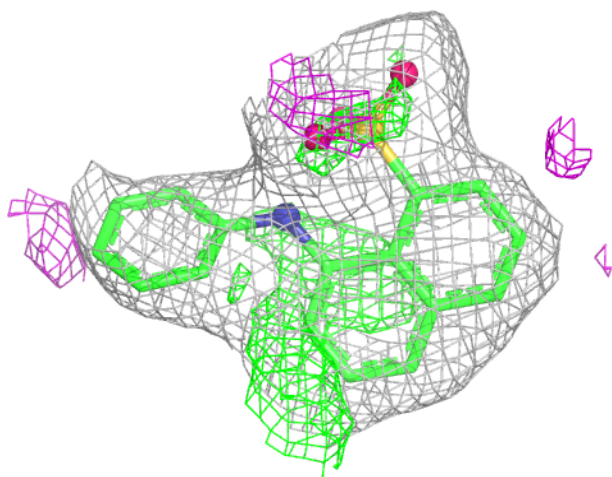
Electron density around 2AN J 202:

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



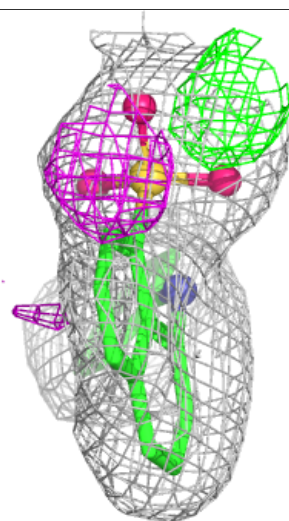
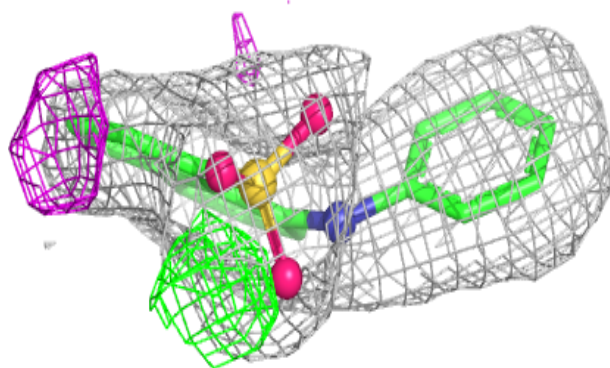
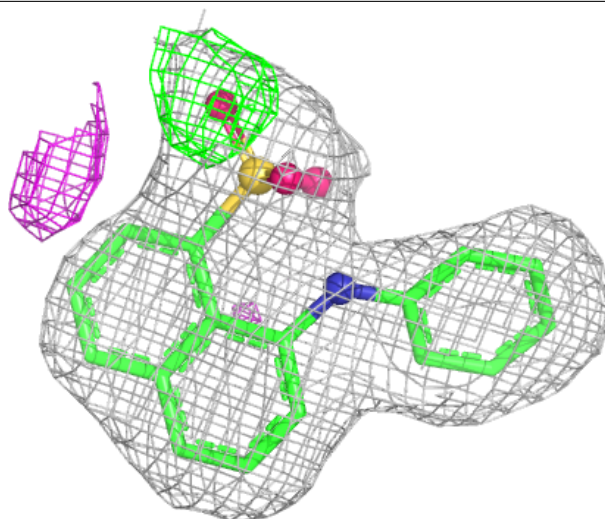
Electron density around 2AN b 203:

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



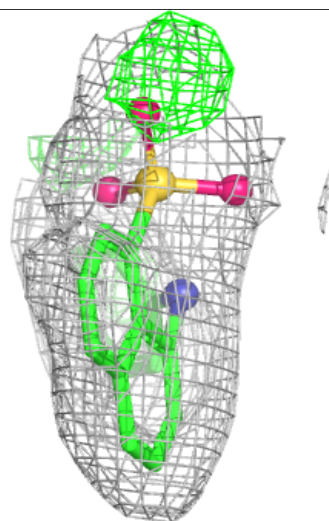
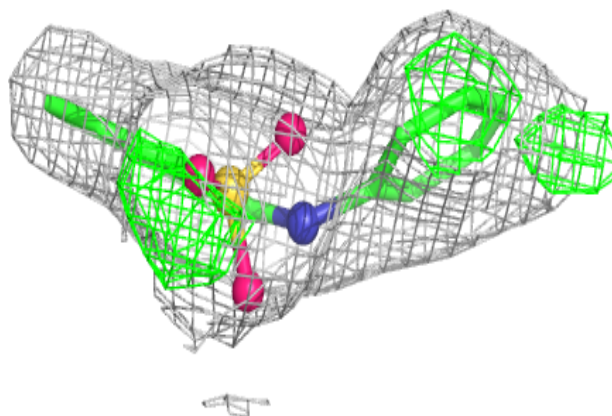
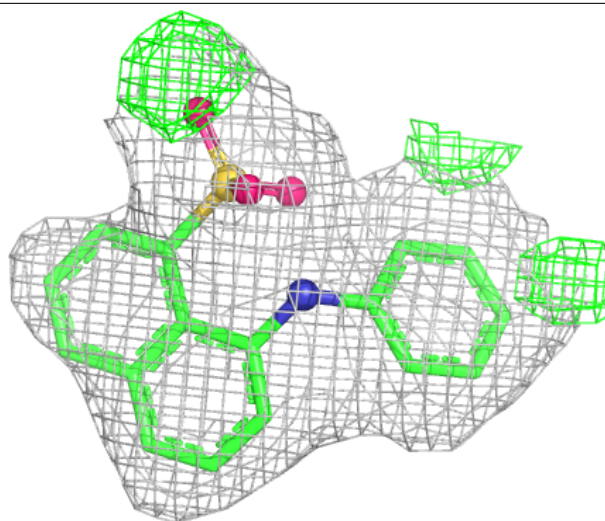
Electron density around 2AN K 201:

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



Electron density around 2AN 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)



6.5 Other polymers [i](#)

There are no such residues in this entry.