



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 15, 2026 – 11:26 AM UTC

PDB ID : 7OKB / pdb_00007okb
Title : Crystal structure of Pseudomonas aeruginosa LpxA in complex with compound 45
Authors : Ryan, M.D.; Parkes, A.L.; Southey, M.; Andersen, O.A.; Zahn, M.; Barker, J.; DeJonge, B.L.M.
Deposited on : 2021-05-17
Resolution : 3.58 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

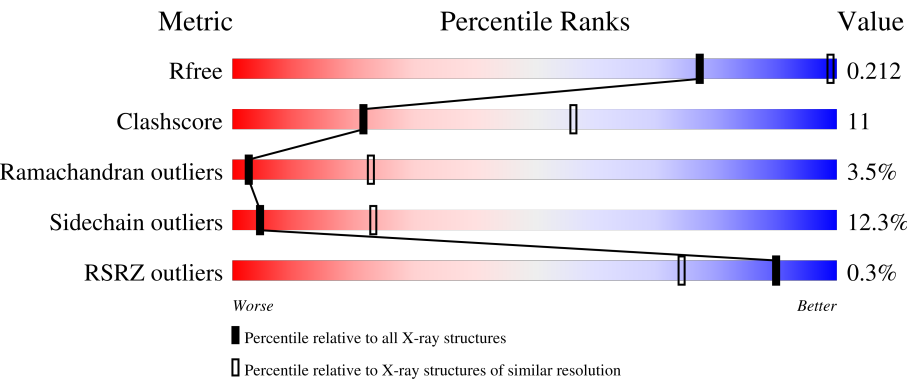
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal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

1 Overall quality at a glance i

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

The reported resolution of this entry is 3.58 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.



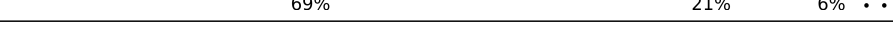
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1521 (3.66-3.50)
Clashscore	190562	1595 (3.66-3.50)
Ramachandran outliers	187476	1551 (3.66-3.50)
Sidechain outliers	187428	1551 (3.66-3.50)
RSRZ outliers	180081	1520 (3.66-3.50)

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	261	% 70% 20% 7% ..
1	B	261	69% 18% 7% ..
1	C	261	69% 21% 8% ..
1	D	261	70% 21% 5% ..

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Mol	Chain	Length	Quality of chain
1	E	261	
1	F	261	
1	G	261	
1	H	261	
1	I	261	
1	J	261	
1	K	261	
1	L	261	
1	M	261	
1	N	261	
1	O	261	
1	P	261	
1	Q	261	
1	R	261	
1	S	261	
1	T	261	
1	U	261	
1	V	261	
1	W	261	
1	X	261	
1	Y	261	
1	Z	261	
1	a	261	
1	b	261	
1	c	261	

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Mol	Chain	Length	Quality of chain
1	d	261	 69% 20% 7% . .

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	CL	C	302	-	-	X	-
2	CL	N	301	-	-	X	-
2	CL	S	301	-	-	X	-
2	CL	X	301	-	-	X	-
3	SO4	A	307	-	-	X	-
3	SO4	D	302	-	-	X	-
3	SO4	L	302	-	-	X	-
3	SO4	N	302	-	-	X	-
3	SO4	R	301	-	-	X	-
3	SO4	W	301	-	-	X	-
3	SO4	a	301	-	-	X	-

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 60243 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 Acyl-[acyl-carrier-protein]--UDP-N-acetylglucosamine O-acyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	258	Total	C	N	O	S	0	0	0
			1974	1235	364	368	7			
1	B	258	Total	C	N	O	S	0	0	0
			1974	1235	364	368	7			
1	C	258	Total	C	N	O	S	0	1	0
			1980	1239	365	369	7			
1	D	258	Total	C	N	O	S	0	0	0
			1974	1235	364	368	7			
1	E	258	Total	C	N	O	S	0	0	0
			1974	1235	364	368	7			
1	F	258	Total	C	N	O	S	0	0	0
			1974	1235	364	368	7			
1	G	257	Total	C	N	O	S	0	0	0
			1966	1230	363	367	6			
1	H	257	Total	C	N	O	S	0	0	0
			1966	1230	363	367	6			
1	I	257	Total	C	N	O	S	0	0	0
			1966	1230	363	367	6			
1	M	257	Total	C	N	O	S	0	0	0
			1966	1230	363	367	6			
1	N	257	Total	C	N	O	S	0	0	0
			1966	1230	363	367	6			
1	O	257	Total	C	N	O	S	0	0	0
			1966	1230	363	367	6			
1	J	258	Total	C	N	O	S	0	0	0
			1974	1235	364	368	7			
1	K	258	Total	C	N	O	S	0	0	0
			1974	1235	364	368	7			
1	L	258	Total	C	N	O	S	0	0	0
			1974	1235	364	368	7			
1	P	257	Total	C	N	O	S	0	0	0
			1966	1230	363	367	6			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	Q	257	Total 1966	C 1230	N 363	O 367	S 6	0	0	0
1	R	257	Total 1966	C 1230	N 363	O 367	S 6	0	0	0
1	S	258	Total 1974	C 1235	N 364	O 368	S 7	0	0	0
1	T	258	Total 1974	C 1235	N 364	O 368	S 7	0	0	0
1	U	258	Total 1974	C 1235	N 364	O 368	S 7	0	0	0
1	V	257	Total 1966	C 1230	N 363	O 367	S 6	0	0	0
1	W	257	Total 1966	C 1230	N 363	O 367	S 6	0	0	0
1	X	257	Total 1966	C 1230	N 363	O 367	S 6	0	0	0
1	Y	258	Total 1974	C 1235	N 364	O 368	S 7	0	0	0
1	Z	258	Total 1974	C 1235	N 364	O 368	S 7	0	0	0
1	a	257	Total 1966	C 1230	N 363	O 367	S 6	0	0	0
1	b	257	Total 1966	C 1230	N 363	O 367	S 6	0	0	0
1	c	258	Total 1974	C 1235	N 364	O 368	S 7	0	0	0
1	d	257	Total 1966	C 1230	N 363	O 367	S 6	0	0	0

There are 90 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	GLY	-	expression tag	UNP A0A069Q726
A	-1	SER	-	expression tag	UNP A0A069Q726
A	0	HIS	-	expression tag	UNP A0A069Q726
B	-2	GLY	-	expression tag	UNP A0A069Q726
B	-1	SER	-	expression tag	UNP A0A069Q726
B	0	HIS	-	expression tag	UNP A0A069Q726
C	-2	GLY	-	expression tag	UNP A0A069Q726
C	-1	SER	-	expression tag	UNP A0A069Q726
C	0	HIS	-	expression tag	UNP A0A069Q726
D	-2	GLY	-	expression tag	UNP A0A069Q726
D	-1	SER	-	expression tag	UNP A0A069Q726

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Chain	Residue	Modelled	Actual	Comment	Reference
D	0	HIS	-	expression tag	UNP A0A069Q726
E	-2	GLY	-	expression tag	UNP A0A069Q726
E	-1	SER	-	expression tag	UNP A0A069Q726
E	0	HIS	-	expression tag	UNP A0A069Q726
F	-2	GLY	-	expression tag	UNP A0A069Q726
F	-1	SER	-	expression tag	UNP A0A069Q726
F	0	HIS	-	expression tag	UNP A0A069Q726
G	-2	GLY	-	expression tag	UNP A0A069Q726
G	-1	SER	-	expression tag	UNP A0A069Q726
G	0	HIS	-	expression tag	UNP A0A069Q726
H	-2	GLY	-	expression tag	UNP A0A069Q726
H	-1	SER	-	expression tag	UNP A0A069Q726
H	0	HIS	-	expression tag	UNP A0A069Q726
I	-2	GLY	-	expression tag	UNP A0A069Q726
I	-1	SER	-	expression tag	UNP A0A069Q726
I	0	HIS	-	expression tag	UNP A0A069Q726
M	-2	GLY	-	expression tag	UNP A0A069Q726
M	-1	SER	-	expression tag	UNP A0A069Q726
M	0	HIS	-	expression tag	UNP A0A069Q726
N	-2	GLY	-	expression tag	UNP A0A069Q726
N	-1	SER	-	expression tag	UNP A0A069Q726
N	0	HIS	-	expression tag	UNP A0A069Q726
O	-2	GLY	-	expression tag	UNP A0A069Q726
O	-1	SER	-	expression tag	UNP A0A069Q726
O	0	HIS	-	expression tag	UNP A0A069Q726
J	-2	GLY	-	expression tag	UNP A0A069Q726
J	-1	SER	-	expression tag	UNP A0A069Q726
J	0	HIS	-	expression tag	UNP A0A069Q726
K	-2	GLY	-	expression tag	UNP A0A069Q726
K	-1	SER	-	expression tag	UNP A0A069Q726
K	0	HIS	-	expression tag	UNP A0A069Q726
L	-2	GLY	-	expression tag	UNP A0A069Q726
L	-1	SER	-	expression tag	UNP A0A069Q726
L	0	HIS	-	expression tag	UNP A0A069Q726
P	-2	GLY	-	expression tag	UNP A0A069Q726
P	-1	SER	-	expression tag	UNP A0A069Q726
P	0	HIS	-	expression tag	UNP A0A069Q726
Q	-2	GLY	-	expression tag	UNP A0A069Q726
Q	-1	SER	-	expression tag	UNP A0A069Q726
Q	0	HIS	-	expression tag	UNP A0A069Q726
R	-2	GLY	-	expression tag	UNP A0A069Q726
R	-1	SER	-	expression tag	UNP A0A069Q726

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Chain	Residue	Modelled	Actual	Comment	Reference
R	0	HIS	-	expression tag	UNP A0A069Q726
S	-2	GLY	-	expression tag	UNP A0A069Q726
S	-1	SER	-	expression tag	UNP A0A069Q726
S	0	HIS	-	expression tag	UNP A0A069Q726
T	-2	GLY	-	expression tag	UNP A0A069Q726
T	-1	SER	-	expression tag	UNP A0A069Q726
T	0	HIS	-	expression tag	UNP A0A069Q726
U	-2	GLY	-	expression tag	UNP A0A069Q726
U	-1	SER	-	expression tag	UNP A0A069Q726
U	0	HIS	-	expression tag	UNP A0A069Q726
V	-2	GLY	-	expression tag	UNP A0A069Q726
V	-1	SER	-	expression tag	UNP A0A069Q726
V	0	HIS	-	expression tag	UNP A0A069Q726
W	-2	GLY	-	expression tag	UNP A0A069Q726
W	-1	SER	-	expression tag	UNP A0A069Q726
W	0	HIS	-	expression tag	UNP A0A069Q726
X	-2	GLY	-	expression tag	UNP A0A069Q726
X	-1	SER	-	expression tag	UNP A0A069Q726
X	0	HIS	-	expression tag	UNP A0A069Q726
Y	-2	GLY	-	expression tag	UNP A0A069Q726
Y	-1	SER	-	expression tag	UNP A0A069Q726
Y	0	HIS	-	expression tag	UNP A0A069Q726
Z	-2	GLY	-	expression tag	UNP A0A069Q726
Z	-1	SER	-	expression tag	UNP A0A069Q726
Z	0	HIS	-	expression tag	UNP A0A069Q726
a	-2	GLY	-	expression tag	UNP A0A069Q726
a	-1	SER	-	expression tag	UNP A0A069Q726
a	0	HIS	-	expression tag	UNP A0A069Q726
b	-2	GLY	-	expression tag	UNP A0A069Q726
b	-1	SER	-	expression tag	UNP A0A069Q726
b	0	HIS	-	expression tag	UNP A0A069Q726
c	-2	GLY	-	expression tag	UNP A0A069Q726
c	-1	SER	-	expression tag	UNP A0A069Q726
c	0	HIS	-	expression tag	UNP A0A069Q726
d	-2	GLY	-	expression tag	UNP A0A069Q726
d	-1	SER	-	expression tag	UNP A0A069Q726
d	0	HIS	-	expression tag	UNP A0A069Q726

- Molecule 2 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

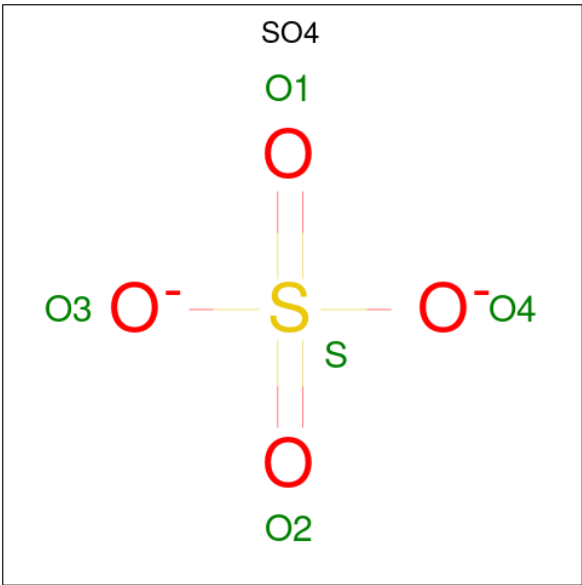
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	6	Total Cl 6 6	0	0
2	B	2	Total Cl 2 2	0	0
2	C	3	Total Cl 3 3	0	0
2	D	1	Total Cl 1 1	0	0
2	E	2	Total Cl 2 2	0	0
2	G	1	Total Cl 1 1	0	0
2	I	1	Total Cl 1 1	0	0
2	M	2	Total Cl 2 2	0	0
2	N	1	Total Cl 1 1	0	0
2	O	1	Total Cl 1 1	0	0
2	L	1	Total Cl 1 1	0	0
2	Q	1	Total Cl 1 1	0	0
2	S	1	Total Cl 1 1	0	0
2	T	1	Total Cl 1 1	0	0
2	X	2	Total Cl 2 2	0	0

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



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	C	1	Total	O	S	0	0
			5	4	1		
3	C	1	Total	O	S	0	0
			5	4	1		
3	D	1	Total	O	S	0	0
			5	4	1		
3	D	1	Total	O	S	0	0
			5	4	1		
3	D	1	Total	O	S	0	0
			5	4	1		
3	E	1	Total	O	S	0	0
			5	4	1		
3	E	1	Total	O	S	0	0
			5	4	1		
3	F	1	Total	O	S	0	0
			5	4	1		
3	F	1	Total	O	S	0	0
			5	4	1		

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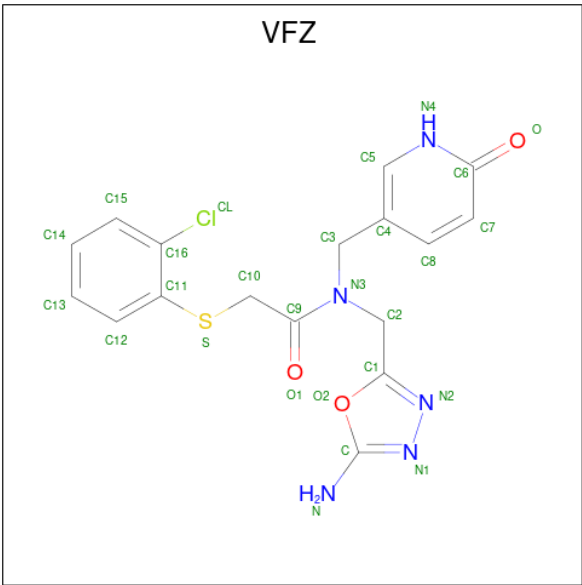
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	G	1	Total	O	S	0	0
			5	4	1		
3	G	1	Total	O	S	0	0
			5	4	1		
3	H	1	Total	O	S	0	0
			5	4	1		
3	H	1	Total	O	S	0	0
			5	4	1		
3	I	1	Total	O	S	0	0
			5	4	1		
3	I	1	Total	O	S	0	0
			5	4	1		
3	M	1	Total	O	S	0	0
			5	4	1		
3	N	1	Total	O	S	0	0
			5	4	1		
3	N	1	Total	O	S	0	0
			5	4	1		
3	N	1	Total	O	S	0	0
			5	4	1		
3	O	1	Total	O	S	0	0
			5	4	1		
3	J	1	Total	O	S	0	0
			5	4	1		
3	J	1	Total	O	S	0	0
			5	4	1		
3	K	1	Total	O	S	0	0
			5	4	1		
3	K	1	Total	O	S	0	0
			5	4	1		
3	L	1	Total	O	S	0	0
			5	4	1		
3	P	1	Total	O	S	0	0
			5	4	1		
3	P	1	Total	O	S	0	0
			5	4	1		
3	P	1	Total	O	S	0	0
			5	4	1		
3	Q	1	Total	O	S	0	0
			5	4	1		
3	R	1	Total	O	S	0	0
			5	4	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	R	1	Total	O	S	0	0
			5	4	1		
3	R	1	Total	O	S	0	0
			5	4	1		
3	S	1	Total	O	S	0	0
			5	4	1		
3	T	1	Total	O	S	0	0
			5	4	1		
3	U	1	Total	O	S	0	0
			5	4	1		
3	U	1	Total	O	S	0	0
			5	4	1		
3	U	1	Total	O	S	0	0
			5	4	1		
3	V	1	Total	O	S	0	0
			5	4	1		
3	V	1	Total	O	S	0	0
			5	4	1		
3	W	1	Total	O	S	0	0
			5	4	1		
3	X	1	Total	O	S	0	0
			5	4	1		
3	Y	1	Total	O	S	0	0
			5	4	1		
3	Y	1	Total	O	S	0	0
			5	4	1		
3	Z	1	Total	O	S	0	0
			5	4	1		
3	a	1	Total	O	S	0	0
			5	4	1		
3	b	1	Total	O	S	0	0
			5	4	1		
3	c	1	Total	O	S	0	0
			5	4	1		
3	c	1	Total	O	S	0	0
			5	4	1		
3	d	1	Total	O	S	0	0
			5	4	1		

- Molecule 4 is {N}-[(5-azanyl-1,3,4-oxadiazol-2-yl)methyl]-2-(2-chlorophenyl)sulfanyl- {N}-[(6-oxidanylidene-1 {H}-pyridin-3-yl)methyl]ethanamide (CCD ID: VFZ) (formula: C₁₇H₁₆ClN₅O₃S) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
4	A	1	Total	C	Cl	N	O	S	0	0
			27	17	1	5	3	1		
4	B	1	Total	C	Cl	N	O	S	0	0
			27	17	1	5	3	1		
4	C	1	Total	C	Cl	N	O	S	0	0
			27	17	1	5	3	1		
4	D	1	Total	C	Cl	N	O	S	0	0
			27	17	1	5	3	1		
4	E	1	Total	C	Cl	N	O	S	0	0
			27	17	1	5	3	1		
4	F	1	Total	C	Cl	N	O	S	0	0
			27	17	1	5	3	1		
4	G	1	Total	C	Cl	N	O	S	0	0
			27	17	1	5	3	1		
4	H	1	Total	C	Cl	N	O	S	0	0
			27	17	1	5	3	1		
4	I	1	Total	C	Cl	N	O	S	0	0
			27	17	1	5	3	1		
4	M	1	Total	C	Cl	N	O	S	0	0
			27	17	1	5	3	1		
4	N	1	Total	C	Cl	N	O	S	0	0
			27	17	1	5	3	1		
4	O	1	Total	C	Cl	N	O	S	0	0
			27	17	1	5	3	1		
4	J	1	Total	C	Cl	N	O	S	0	0
			27	17	1	5	3	1		
4	K	1	Total	C	Cl	N	O	S	0	0
			27	17	1	5	3	1		

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Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
4	L	1	Total 27	C 17	Cl 1	N 5	O 3	S 1	0	0
4	P	1	Total 27	C 17	Cl 1	N 5	O 3	S 1	0	0
4	Q	1	Total 27	C 17	Cl 1	N 5	O 3	S 1	0	0
4	R	1	Total 27	C 17	Cl 1	N 5	O 3	S 1	0	0
4	S	1	Total 27	C 17	Cl 1	N 5	O 3	S 1	0	0
4	T	1	Total 27	C 17	Cl 1	N 5	O 3	S 1	0	0
4	U	1	Total 27	C 17	Cl 1	N 5	O 3	S 1	0	0
4	V	1	Total 27	C 17	Cl 1	N 5	O 3	S 1	0	0
4	W	1	Total 27	C 17	Cl 1	N 5	O 3	S 1	0	0
4	X	1	Total 27	C 17	Cl 1	N 5	O 3	S 1	0	0
4	Y	1	Total 27	C 17	Cl 1	N 5	O 3	S 1	0	0
4	Z	1	Total 27	C 17	Cl 1	N 5	O 3	S 1	0	0
4	a	1	Total 27	C 17	Cl 1	N 5	O 3	S 1	0	0
4	b	1	Total 27	C 17	Cl 1	N 5	O 3	S 1	0	0
4	c	1	Total 27	C 17	Cl 1	N 5	O 3	S 1	0	0
4	d	1	Total 27	C 17	Cl 1	N 5	O 3	S 1	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total 1	O 1	0	0
5	B	1	Total 1	O 1	0	0
5	C	2	Total 2	O 2	0	0

Continued on next page...

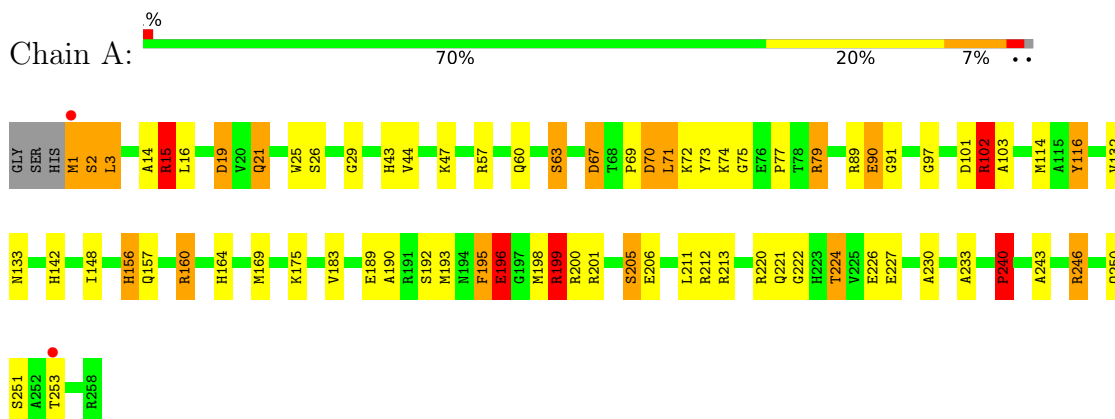
Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	D	3	Total 3	O 3	0	0
5	E	3	Total 3	O 3	0	0
5	F	1	Total 1	O 1	0	0
5	H	2	Total 2	O 2	0	0
5	M	1	Total 1	O 1	0	0
5	N	2	Total 2	O 2	0	0
5	O	1	Total 1	O 1	0	0
5	J	1	Total 1	O 1	0	0
5	K	2	Total 2	O 2	0	0
5	L	1	Total 1	O 1	0	0
5	P	2	Total 2	O 2	0	0
5	Q	1	Total 1	O 1	0	0
5	S	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	Z	1	Total 1	O 1	0	0
5	a	1	Total 1	O 1	0	0
5	c	1	Total 1	O 1	0	0

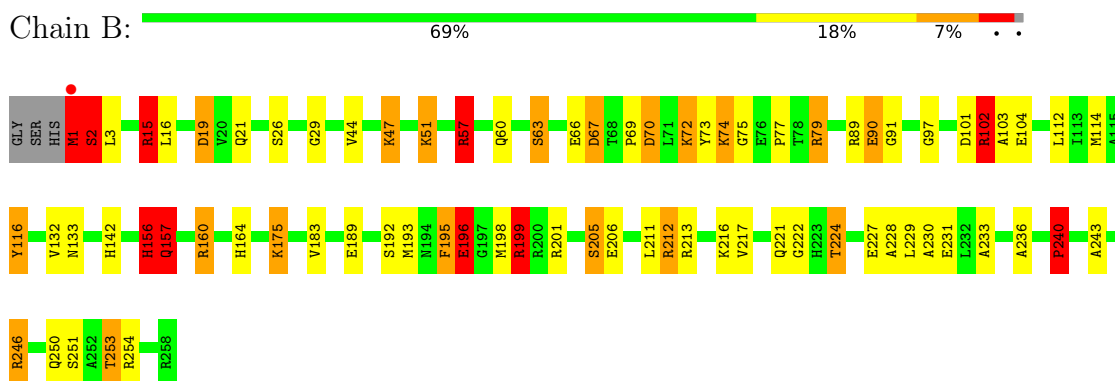
3 Residue-property plots [i](#)

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

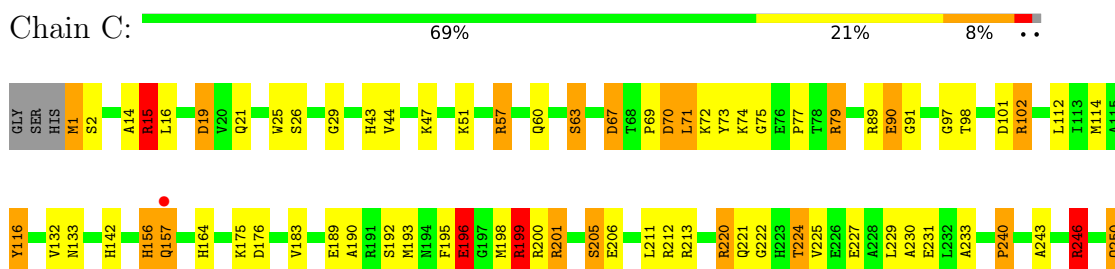
- Molecule 1: Acyl-[acyl-carrier-protein]--UDP-N-acetylglucosamine O-acyltransferase



- Molecule 1: Acyl-[acyl-carrier-protein]--UDP-N-acetylglucosamine O-acyltransferase



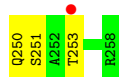
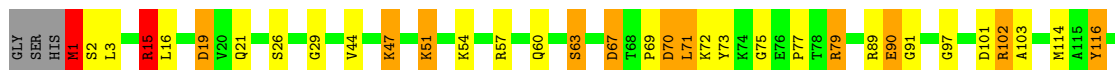
- Molecule 1: Acyl-[acyl-carrier-protein]--UDP-N-acetylglucosamine O-acyltransferase





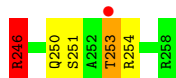
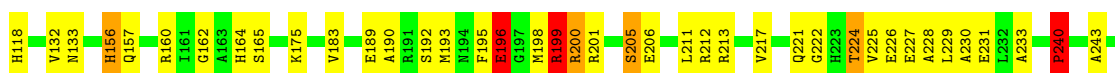
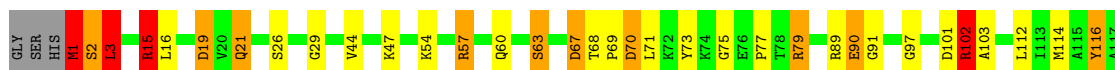
- Molecule 1: Acyl-[acyl-carrier-protein]--UDP-N-acetylglucosamine O-acyltransferase

Chain D: 70% 21% 5% ..



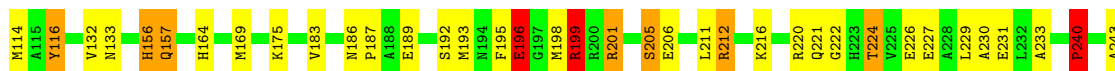
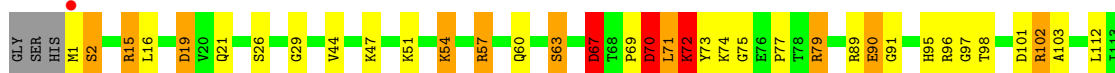
- Molecule 1: Acyl-[acyl-carrier-protein]--UDP-N-acetylglucosamine O-acyltransferase

Chain E: 69% 21% 6% ..



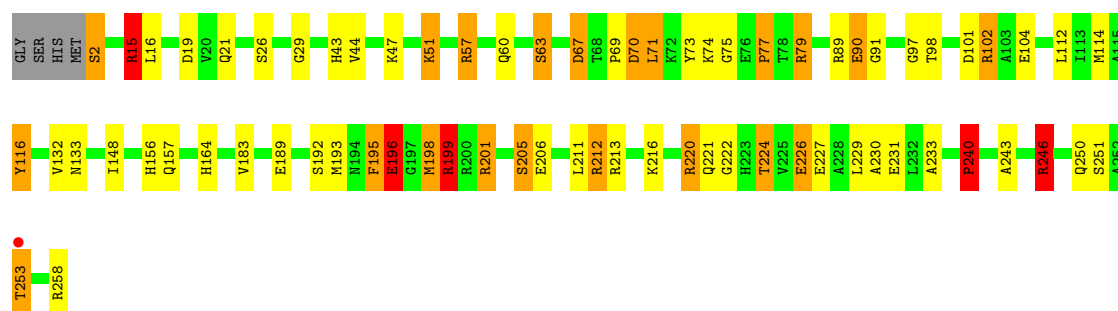
- Molecule 1: Acyl-[acyl-carrier-protein]--UDP-N-acetylglucosamine O-acyltransferase

Chain F: 69% 20% 7% ..



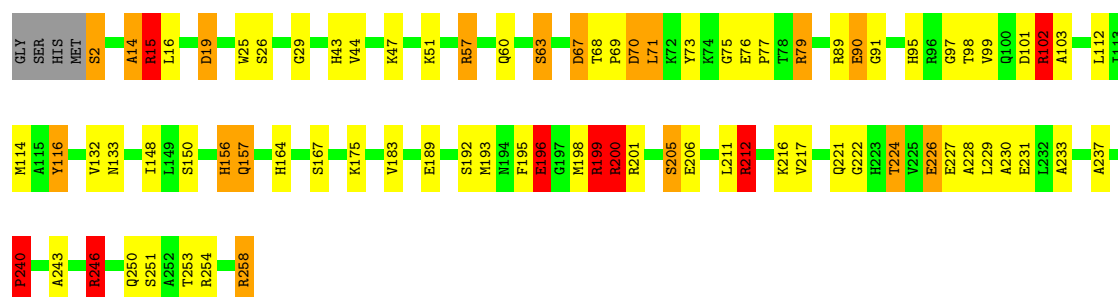
- Molecule 1: Acyl-[acyl-carrier-protein]--UDP-N-acetylglucosamine O-acyltransferase

Chain G: 71% 18% 8% ..



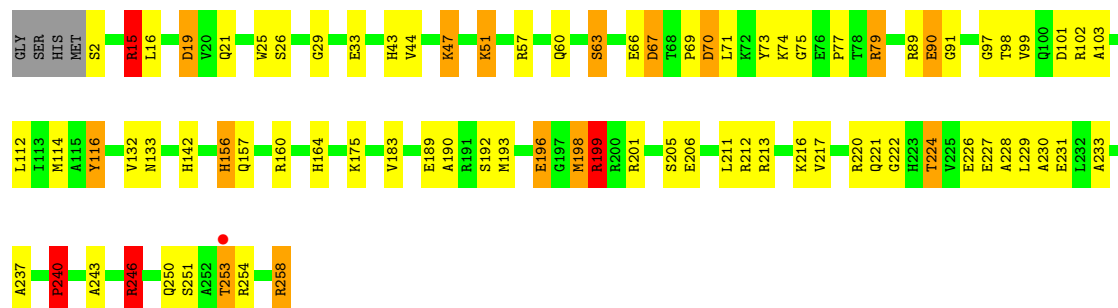
- Molecule 1: Acyl-[acyl-carrier-protein]--UDP-N-acetylglucosamine O-acyltransferase

Chain H: 67% 22% 7% . .



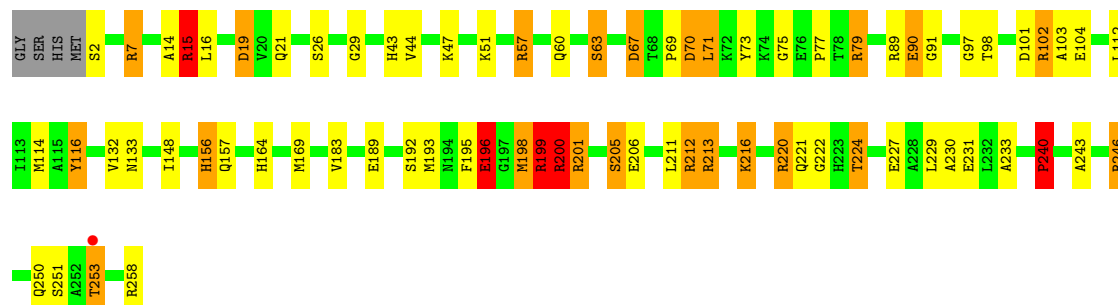
- Molecule 1: Acyl-[acyl-carrier-protein]--UDP-N-acetylglucosamine O-acyltransferase

Chain I: 67% 24% 6% . .



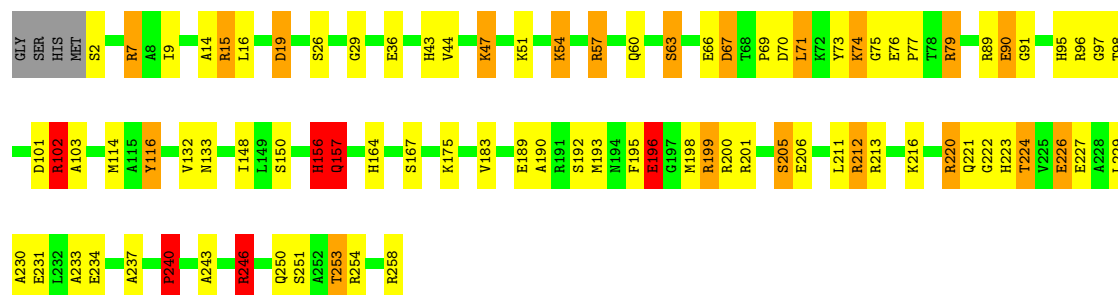
- Molecule 1: Acyl-[acyl-carrier-protein]--UDP-N-acetylglucosamine O-acyltransferase

Chain M: 70% 18% 8% . .



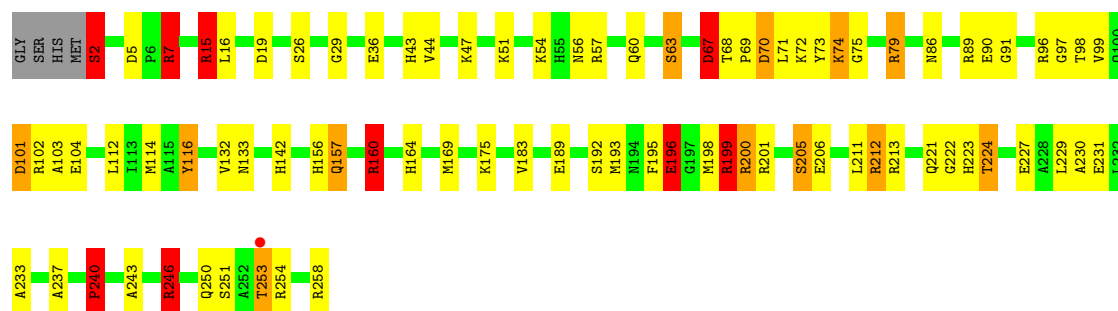
• Molecule 1: Acyl-[acyl-carrier-protein]--UDP-N-acetylglucosamine O-acyltransferase

Chain N:  65% 24% 8% . .



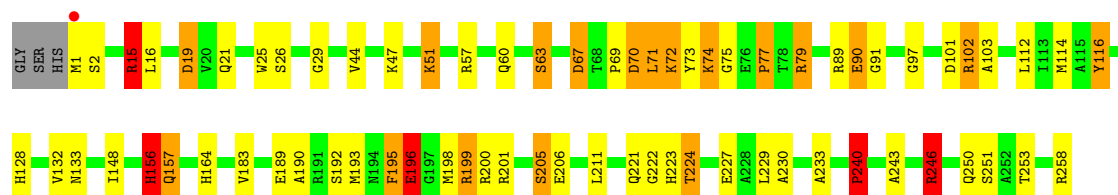
• Molecule 1: Acyl-[acyl-carrier-protein]--UDP-N-acetylglucosamine O-acyltransferase

Chain O:  66% 25% 5% . .



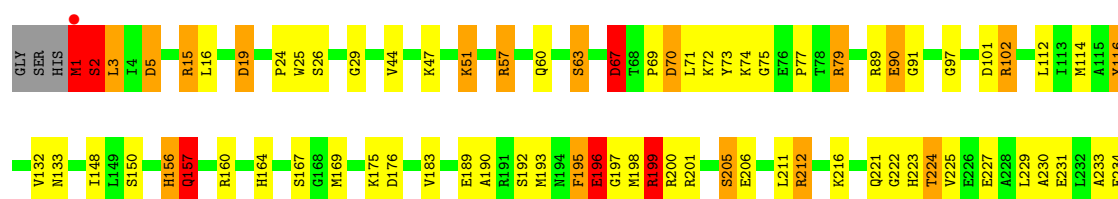
• Molecule 1: Acyl-[acyl-carrier-protein]--UDP-N-acetylglucosamine O-acyltransferase

Chain J:  72% 18% 7% . .



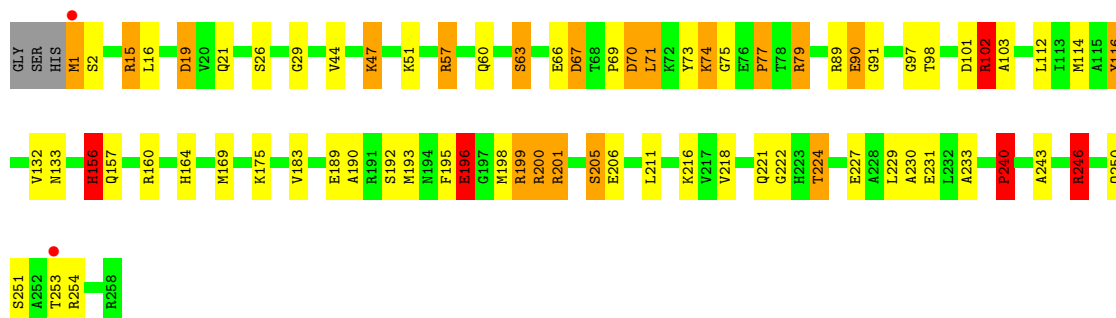
• Molecule 1: Acyl-[acyl-carrier-protein]--UDP-N-acetylglucosamine O-acyltransferase

Chain K:  67% 22% 7% . .

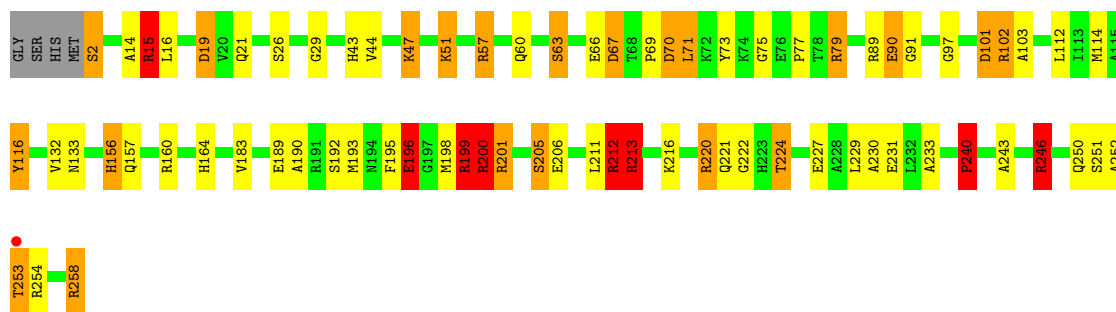




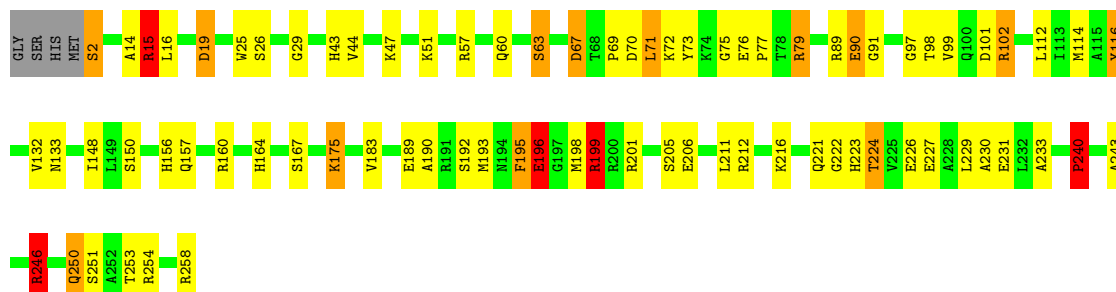
- Molecule 1: Acyl-[acyl-carrier-protein]--UDP-N-acetylglucosamine O-acyltransferase



- Molecule 1: Acyl-[acyl-carrier-protein]--UDP-N-acetylglucosamine O-acyltransferase

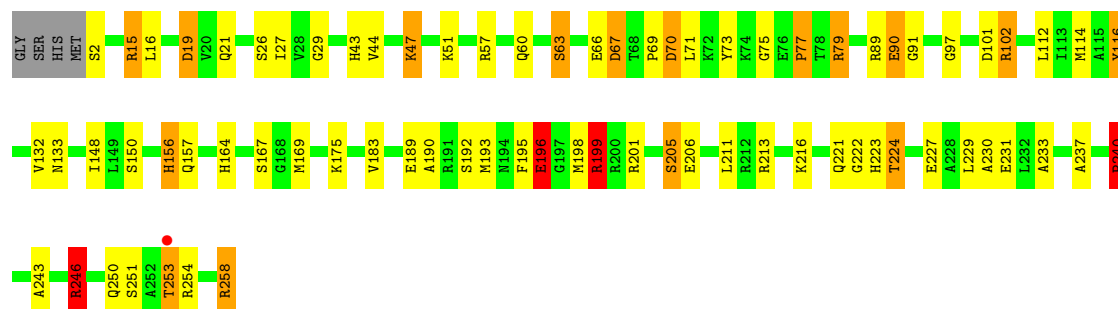


- Molecule 1: Acyl-[acyl-carrier-protein]--UDP-N-acetylglucosamine O-acyltransferase



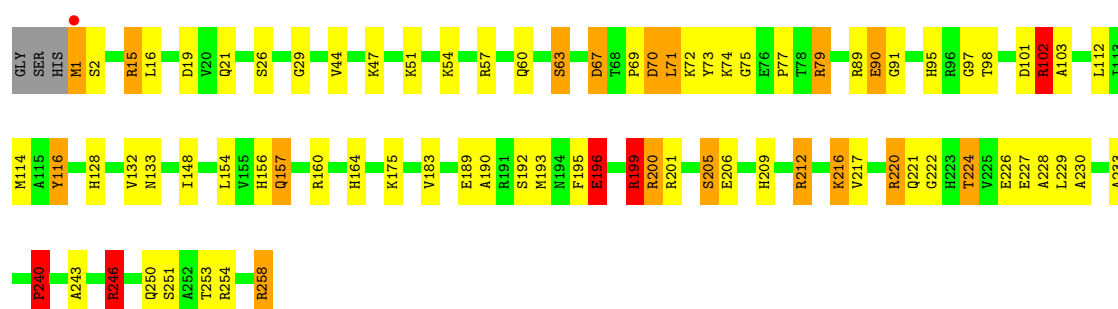
- Molecule 1: Acyl-[acyl-carrier-protein]--UDP-N-acetylglucosamine O-acyltransferase





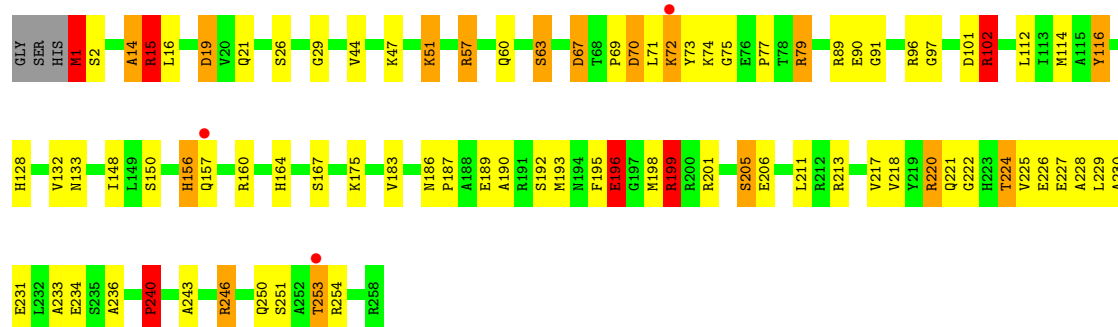
- Molecule 1: Acyl-[acyl-carrier-protein]--UDP-N-acetylglucosamine O-acyltransferase

Chain S: 68% 23% 7% ..



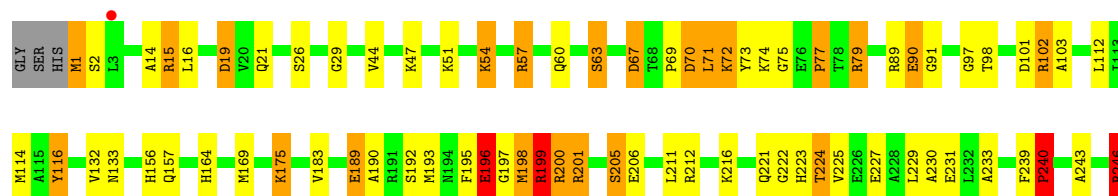
- Molecule 1: Acyl-[acyl-carrier-protein]--UDP-N-acetylglucosamine O-acyltransferase

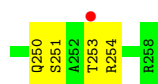
Chain T: 66% 24% 6% ..



- Molecule 1: Acyl-[acyl-carrier-protein]--UDP-N-acetylglucosamine O-acyltransferase

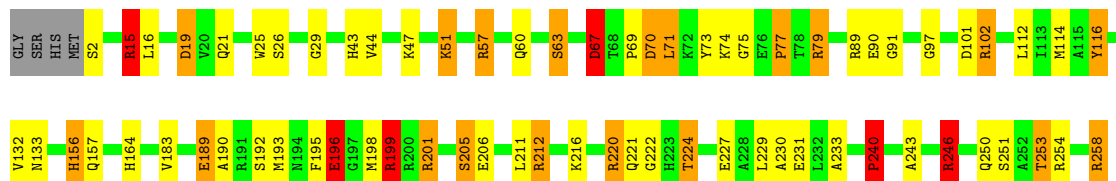
Chain U: 69% 20% 8% ..





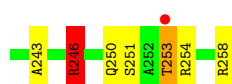
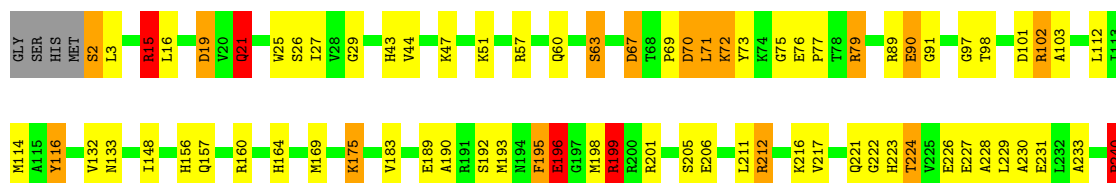
- Molecule 1: Acyl-[acyl-carrier-protein]--UDP-N-acetylglucosamine O-acyltransferase

Chain V: 72% 17% 7% ..



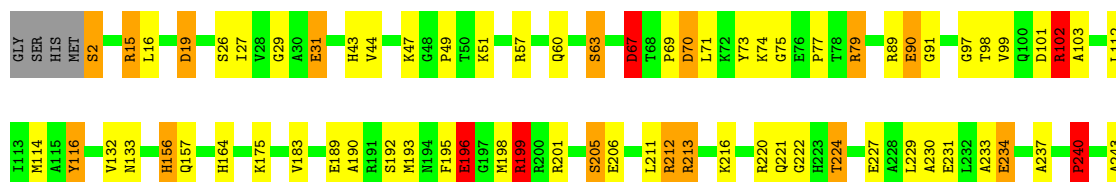
- Molecule 1: Acyl-[acyl-carrier-protein]--UDP-N-acetylglucosamine O-acyltransferase

Chain W: 67% 23% 6% ..



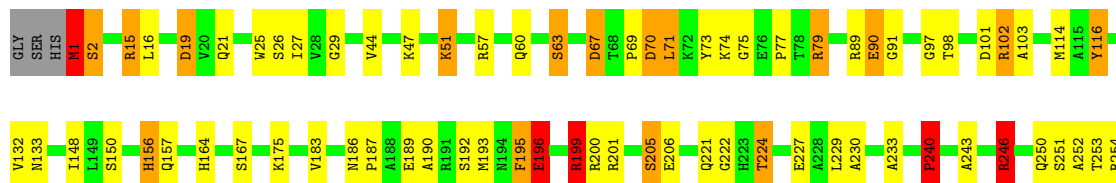
- Molecule 1: Acyl-[acyl-carrier-protein]--UDP-N-acetylglucosamine O-acyltransferase

Chain X: 69% 21% 7% ..



- Molecule 1: Acyl-[acyl-carrier-protein]--UDP-N-acetylglucosamine O-acyltransferase

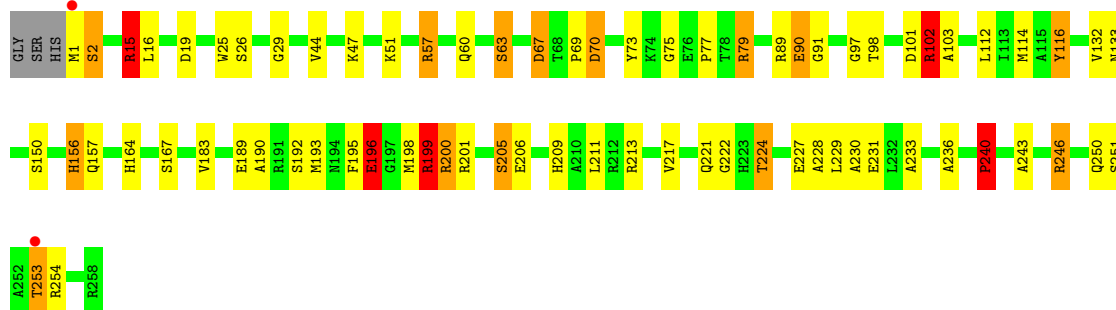
Chain Y: 70% 20% 7% ..





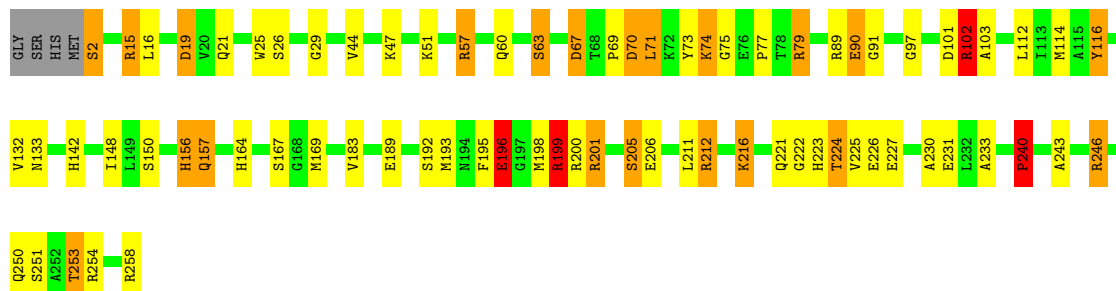
- Molecule 1: Acyl-[acyl-carrier-protein]--UDP-N-acetylglucosamine O-acyltransferase

Chain Z: 71% 21% 5% ..



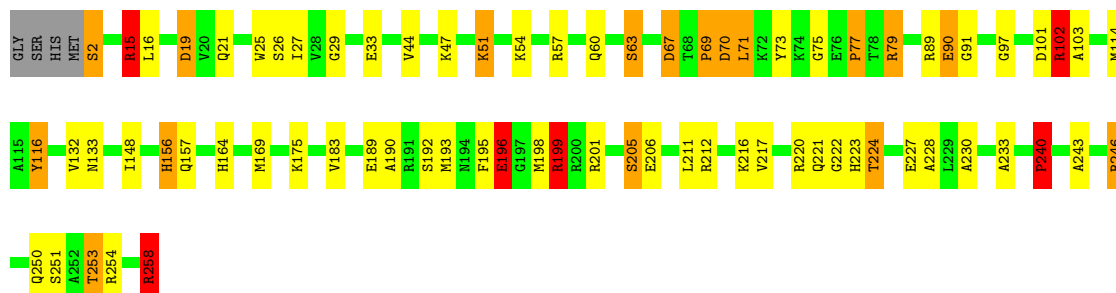
- Molecule 1: Acyl-[acyl-carrier-protein]--UDP-N-acetylglucosamine O-acyltransferase

Chain a: 69% 20% 8% ..



- Molecule 1: Acyl-[acyl-carrier-protein]--UDP-N-acetylglucosamine O-acyltransferase

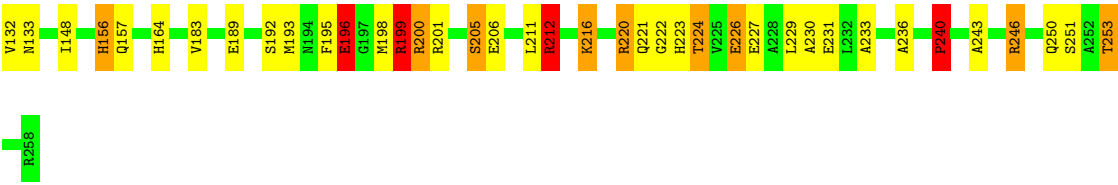
Chain b: 70% 20% 7% ..



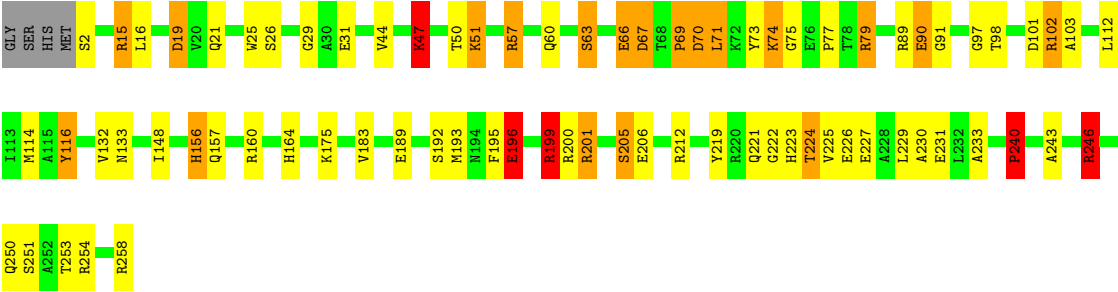
- Molecule 1: Acyl-[acyl-carrier-protein]--UDP-N-acetylglucosamine O-acyltransferase

Chain c: 71% 17% 8% ..





● Molecule 1: Acyl-[acyl-carrier-protein]--UDP-N-acetylglucosamine O-acyltransferase



4 Data and refinement statistics

Property	Value	Source
Space group	P 42 21 2	Depositor
Cell constants a, b, c, α , β , γ	378.61Å 378.61Å 264.64Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	109.08 – 3.58 109.08 – 3.58	Depositor EDS
% Data completeness (in resolution range)	100.0 (109.08-3.58) 100.0 (109.08-3.58)	Depositor EDS
R_{merge}	0.61	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.60 (at 3.58Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.195 , 0.212 0.196 , 0.212	Depositor DCC
R_{free} test set	10979 reflections (4.91%)	wwPDB-VP
Wilson B-factor (Å ²)	83.4	Xtriage
Anisotropy	0.095	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 69.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	60243	wwPDB-VP
Average B, all atoms (Å ²)	102.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.38% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: SO4, CL, VFZ

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	1.25	5/2016 (0.2%)	1.75	31/2734 (1.1%)
1	B	1.23	5/2016 (0.2%)	1.71	34/2734 (1.2%)
1	C	1.26	5/2025 (0.2%)	1.71	27/2746 (1.0%)
1	D	1.21	2/2016 (0.1%)	1.70	25/2734 (0.9%)
1	E	1.27	5/2016 (0.2%)	1.72	27/2734 (1.0%)
1	F	1.21	3/2016 (0.1%)	1.71	25/2734 (0.9%)
1	G	1.19	1/2008 (0.0%)	1.72	31/2724 (1.1%)
1	H	1.18	2/2008 (0.1%)	1.72	28/2724 (1.0%)
1	I	1.18	1/2008 (0.0%)	1.70	24/2724 (0.9%)
1	J	1.24	5/2016 (0.2%)	1.72	32/2734 (1.2%)
1	K	1.24	5/2016 (0.2%)	1.72	32/2734 (1.2%)
1	L	1.21	1/2016 (0.0%)	1.71	27/2734 (1.0%)
1	M	1.19	2/2008 (0.1%)	1.74	35/2724 (1.3%)
1	N	1.23	5/2008 (0.2%)	1.77	41/2724 (1.5%)
1	O	1.21	3/2008 (0.1%)	1.73	34/2724 (1.2%)
1	P	1.19	2/2008 (0.1%)	1.73	29/2724 (1.1%)
1	Q	1.19	2/2008 (0.1%)	1.69	24/2724 (0.9%)
1	R	1.19	2/2008 (0.1%)	1.68	22/2724 (0.8%)
1	S	1.22	4/2016 (0.2%)	1.74	31/2734 (1.1%)
1	T	1.23	6/2016 (0.3%)	1.74	34/2734 (1.2%)
1	U	1.23	3/2016 (0.1%)	1.70	29/2734 (1.1%)
1	V	1.18	1/2008 (0.0%)	1.71	28/2724 (1.0%)
1	W	1.19	1/2008 (0.0%)	1.70	26/2724 (1.0%)
1	X	1.22	3/2008 (0.1%)	1.71	27/2724 (1.0%)
1	Y	1.19	1/2016 (0.0%)	1.68	23/2734 (0.8%)
1	Z	1.20	3/2016 (0.1%)	1.70	24/2734 (0.9%)
1	a	1.20	1/2008 (0.0%)	1.71	24/2724 (0.9%)
1	b	1.20	3/2008 (0.1%)	1.71	29/2724 (1.1%)
1	c	1.20	1/2016 (0.0%)	1.72	32/2734 (1.2%)
1	d	1.19	2/2008 (0.1%)	1.71	26/2724 (1.0%)
All	All	1.21	85/60369 (0.1%)	1.72	861/81882 (1.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	B	0	2
1	D	0	2
1	F	0	1
1	G	0	1
1	H	0	1
1	K	0	2
1	L	0	1
1	O	0	2
1	P	0	1
1	Q	0	1
1	S	0	1
1	U	0	1
1	W	0	2
1	X	0	1
1	Y	0	2
1	Z	0	1
1	a	0	1
1	c	0	1
All	All	0	26

The worst 5 of 85 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	2	SER	C-O	13.46	1.40	1.24
1	U	2	SER	C-O	12.16	1.38	1.24
1	A	142	HIS	CE1-NE2	10.60	1.43	1.32
1	E	2	SER	C-O	9.62	1.36	1.24
1	E	2	SER	N-CA	8.94	1.57	1.46

The worst 5 of 861 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	P	212	ARG	CB-CG-CD	13.80	143.05	111.30
1	H	226	GLU	CB-CG-CD	10.92	131.17	112.60
1	S	2	SER	CA-C-N	10.37	135.20	120.79
1	S	2	SER	C-N-CA	10.37	135.20	120.79
1	W	72	LYS	CB-CG-CD	10.30	134.99	111.30

There are no chirality outliers.

5 of 26 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1	MET	Peptide
1	A	2	SER	Peptide
1	B	1	MET	Peptide
1	B	2	SER	Peptide
1	D	1	MET	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1974	0	1947	41	0
1	B	1974	0	1947	46	1
1	C	1980	0	1955	55	0
1	D	1974	0	1947	44	2
1	E	1974	0	1947	48	0
1	F	1974	0	1947	50	0
1	G	1966	0	1935	35	0
1	H	1966	0	1935	51	0
1	I	1966	0	1935	47	0
1	J	1974	0	1947	40	0
1	K	1974	0	1947	53	0
1	L	1974	0	1947	45	0
1	M	1966	0	1935	51	0
1	N	1966	0	1935	52	0
1	O	1966	0	1935	50	0
1	P	1966	0	1935	48	0
1	Q	1966	0	1935	48	0
1	R	1966	0	1935	44	0
1	S	1974	0	1947	44	0
1	T	1974	0	1947	49	0
1	U	1974	0	1947	42	0
1	V	1966	0	1935	44	0
1	W	1966	0	1935	50	0
1	X	1966	0	1935	54	0
1	Y	1974	0	1947	47	0
1	Z	1974	0	1947	40	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	a	1966	0	1935	44	0
1	b	1966	0	1935	46	1
1	c	1974	0	1947	45	0
1	d	1966	0	1935	53	0
2	A	6	0	0	2	0
2	B	2	0	0	2	0
2	C	3	0	0	4	0
2	D	1	0	0	1	0
2	E	2	0	0	1	0
2	G	1	0	0	1	0
2	I	1	0	0	0	0
2	L	1	0	0	0	0
2	M	2	0	0	2	0
2	N	1	0	0	2	0
2	O	1	0	0	1	0
2	Q	1	0	0	0	0
2	S	1	0	0	2	0
2	T	1	0	0	1	0
2	X	2	0	0	3	0
3	A	15	0	0	2	0
3	B	10	0	0	0	0
3	C	10	0	0	0	0
3	D	15	0	0	2	0
3	E	10	0	0	1	0
3	F	10	0	0	1	0
3	G	10	0	0	0	0
3	H	10	0	0	0	0
3	I	10	0	0	1	0
3	J	10	0	0	0	0
3	K	10	0	0	0	0
3	L	5	0	0	2	0
3	M	5	0	0	0	0
3	N	15	0	0	2	0
3	O	5	0	0	0	0
3	P	15	0	0	2	0
3	Q	5	0	0	1	0
3	R	15	0	0	2	0
3	S	5	0	0	1	0
3	T	5	0	0	0	0
3	U	15	0	0	1	0
3	V	10	0	0	0	0
3	W	5	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	X	5	0	0	0	0
3	Y	10	0	0	1	0
3	Z	5	0	0	0	0
3	a	5	0	0	2	0
3	b	5	0	0	1	0
3	c	10	0	0	0	0
3	d	5	0	0	1	0
4	A	27	0	0	3	0
4	B	27	0	0	0	0
4	C	27	0	0	0	0
4	D	27	0	0	1	0
4	E	27	0	0	1	0
4	F	27	0	0	2	0
4	G	27	0	0	0	0
4	H	27	0	0	0	0
4	I	27	0	0	1	0
4	J	27	0	0	0	0
4	K	27	0	0	0	0
4	L	27	0	0	2	0
4	M	27	0	0	0	0
4	N	27	0	0	2	0
4	O	27	0	0	0	0
4	P	27	0	0	1	0
4	Q	27	0	0	1	0
4	R	27	0	0	1	0
4	S	27	0	0	1	0
4	T	27	0	0	0	0
4	U	27	0	0	1	0
4	V	27	0	0	0	0
4	W	27	0	0	2	0
4	X	27	0	0	0	0
4	Y	27	0	0	1	0
4	Z	27	0	0	0	0
4	a	27	0	0	2	0
4	b	27	0	0	1	0
4	c	27	0	0	0	0
4	d	27	0	0	1	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
5	C	2	0	0	0	0
5	D	3	0	0	1	0
5	E	3	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	F	1	0	0	0	0
5	H	2	0	0	1	0
5	J	1	0	0	0	0
5	K	2	0	0	0	0
5	L	1	0	0	0	0
5	M	1	0	0	0	0
5	N	2	0	0	0	0
5	O	1	0	0	1	0
5	P	2	0	0	0	0
5	Q	1	0	0	0	0
5	S	2	0	0	0	0
5	T	1	0	0	0	0
5	U	1	0	0	0	0
5	Z	1	0	0	0	0
5	a	1	0	0	0	0
5	c	1	0	0	1	0
All	All	60243	0	58238	1275	2

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 11.

The worst 5 of 1275 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:N:220:ARG:NH2	2:N:301:CL:CL	1.96	1.33
1:X:220:ARG:NH2	2:X:301:CL:CL	2.14	1.17
1:C:220:ARG:NH2	2:C:302:CL:CL	2.22	1.10
1:C:156:HIS:CE1	1:C:157[B]:GLN:HG2	1.86	1.09
3:E:303:SO4:O3	4:E:305:VFZ:N	1.85	1.09

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2:SER:OG	1:D:1:MET:N[5_445]	1.90	0.30
1:D:234:GLU:OE1	1:b:212:ARG:NH2[8_555]	2.04	0.16

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	256/261 (98%)	219 (86%)	28 (11%)	9 (4%)	3	23
1	B	256/261 (98%)	217 (85%)	30 (12%)	9 (4%)	3	23
1	C	257/261 (98%)	216 (84%)	31 (12%)	10 (4%)	2	20
1	D	256/261 (98%)	220 (86%)	27 (10%)	9 (4%)	3	23
1	E	256/261 (98%)	217 (85%)	28 (11%)	11 (4%)	2	18
1	F	256/261 (98%)	219 (86%)	29 (11%)	8 (3%)	3	25
1	G	255/261 (98%)	215 (84%)	31 (12%)	9 (4%)	3	23
1	H	255/261 (98%)	216 (85%)	31 (12%)	8 (3%)	3	25
1	I	255/261 (98%)	217 (85%)	29 (11%)	9 (4%)	3	23
1	J	256/261 (98%)	218 (85%)	29 (11%)	9 (4%)	3	23
1	K	256/261 (98%)	215 (84%)	32 (12%)	9 (4%)	3	23
1	L	256/261 (98%)	220 (86%)	27 (10%)	9 (4%)	3	23
1	M	255/261 (98%)	217 (85%)	29 (11%)	9 (4%)	3	23
1	N	255/261 (98%)	217 (85%)	29 (11%)	9 (4%)	3	23
1	O	255/261 (98%)	217 (85%)	30 (12%)	8 (3%)	3	25
1	P	255/261 (98%)	215 (84%)	32 (12%)	8 (3%)	3	25
1	Q	255/261 (98%)	216 (85%)	31 (12%)	8 (3%)	3	25
1	R	255/261 (98%)	216 (85%)	30 (12%)	9 (4%)	3	23
1	S	256/261 (98%)	217 (85%)	30 (12%)	9 (4%)	3	23
1	T	256/261 (98%)	219 (86%)	28 (11%)	9 (4%)	3	23
1	U	256/261 (98%)	218 (85%)	29 (11%)	9 (4%)	3	23
1	V	255/261 (98%)	218 (86%)	28 (11%)	9 (4%)	3	23
1	W	255/261 (98%)	218 (86%)	28 (11%)	9 (4%)	3	23
1	X	255/261 (98%)	216 (85%)	30 (12%)	9 (4%)	3	23
1	Y	256/261 (98%)	217 (85%)	30 (12%)	9 (4%)	3	23

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	Z	256/261 (98%)	216 (84%)	31 (12%)	9 (4%)	3	23
1	a	255/261 (98%)	216 (85%)	30 (12%)	9 (4%)	3	23
1	b	255/261 (98%)	216 (85%)	30 (12%)	9 (4%)	3	23
1	c	256/261 (98%)	220 (86%)	27 (10%)	9 (4%)	3	23
1	d	255/261 (98%)	217 (85%)	30 (12%)	8 (3%)	3	25
All	All	7666/7830 (98%)	6515 (85%)	884 (12%)	267 (4%)	3	23

5 of 267 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	233	ALA
1	B	233	ALA
1	C	233	ALA
1	D	233	ALA
1	E	3	LEU

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	206/208 (99%)	185 (90%)	21 (10%)	7	29
1	B	206/208 (99%)	179 (87%)	27 (13%)	4	21
1	C	207/208 (100%)	182 (88%)	25 (12%)	5	24
1	D	206/208 (99%)	181 (88%)	25 (12%)	5	24
1	E	206/208 (99%)	182 (88%)	24 (12%)	5	25
1	F	206/208 (99%)	176 (85%)	30 (15%)	3	17
1	G	205/208 (99%)	177 (86%)	28 (14%)	3	20
1	H	205/208 (99%)	177 (86%)	28 (14%)	3	20
1	I	205/208 (99%)	180 (88%)	25 (12%)	5	23
1	J	206/208 (99%)	183 (89%)	23 (11%)	6	27
1	K	206/208 (99%)	180 (87%)	26 (13%)	4	22

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	L	206/208 (99%)	182 (88%)	24 (12%)	5	25
1	M	205/208 (99%)	182 (89%)	23 (11%)	6	27
1	N	205/208 (99%)	179 (87%)	26 (13%)	4	22
1	O	205/208 (99%)	181 (88%)	24 (12%)	5	25
1	P	205/208 (99%)	178 (87%)	27 (13%)	4	21
1	Q	205/208 (99%)	180 (88%)	25 (12%)	5	23
1	R	205/208 (99%)	182 (89%)	23 (11%)	6	27
1	S	206/208 (99%)	180 (87%)	26 (13%)	4	22
1	T	206/208 (99%)	182 (88%)	24 (12%)	5	25
1	U	206/208 (99%)	177 (86%)	29 (14%)	3	19
1	V	205/208 (99%)	179 (87%)	26 (13%)	4	22
1	W	205/208 (99%)	179 (87%)	26 (13%)	4	22
1	X	205/208 (99%)	180 (88%)	25 (12%)	5	23
1	Y	206/208 (99%)	183 (89%)	23 (11%)	6	27
1	Z	206/208 (99%)	185 (90%)	21 (10%)	7	29
1	a	205/208 (99%)	179 (87%)	26 (13%)	4	22
1	b	205/208 (99%)	180 (88%)	25 (12%)	5	23
1	c	206/208 (99%)	182 (88%)	24 (12%)	5	25
1	d	205/208 (99%)	177 (86%)	28 (14%)	3	20
All	All	6166/6240 (99%)	5409 (88%)	757 (12%)	4	23

5 of 757 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	S	79	ARG
1	W	192	SER
1	S	246	ARG
1	S	74	LYS
1	U	192	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 131 such sidechains are listed below:

Mol	Chain	Res	Type
1	a	55	HIS

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Mol	Chain	Res	Type
1	a	223	HIS
1	d	164	HIS
1	O	121	HIS
1	O	56	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](#)

Of 110 ligands modelled in this entry, 26 are monoatomic - leaving 84 for Mogul analysis.

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	$\# Z > 2$
3	SO4	I	302	-	4,4,4	0.35	0	6,6,6	0.13	0
4	VFZ	Z	302	-	29,29,29	0.49	0	29,39,39	0.88	2 (6%)
4	VFZ	d	302	-	29,29,29	0.46	0	29,39,39	0.99	2 (6%)
4	VFZ	G	304	-	29,29,29	0.38	0	29,39,39	0.72	1 (3%)
4	VFZ	E	305	-	29,29,29	0.39	0	29,39,39	1.37	3 (10%)
3	SO4	B	304	-	4,4,4	0.23	0	6,6,6	0.16	0
4	VFZ	X	304	-	29,29,29	0.41	0	29,39,39	1.08	3 (10%)
4	VFZ	Q	303	-	29,29,29	0.39	0	29,39,39	0.77	2 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	SO4	F	302	-	4,4,4	0.29	0	6,6,6	0.07	0
3	SO4	N	302	-	4,4,4	0.37	0	6,6,6	0.17	0
3	SO4	K	301	-	4,4,4	0.26	0	6,6,6	0.14	0
3	SO4	C	304	-	4,4,4	0.38	0	6,6,6	0.13	0
3	SO4	U	302	-	4,4,4	0.39	0	6,6,6	0.40	0
3	SO4	I	303	-	4,4,4	0.24	0	6,6,6	0.15	0
4	VFZ	S	303	-	29,29,29	0.27	0	29,39,39	0.62	0
4	VFZ	W	302	-	29,29,29	0.38	0	29,39,39	1.08	4 (13%)
4	VFZ	F	303	-	29,29,29	0.41	0	29,39,39	1.21	2 (6%)
3	SO4	V	301	-	4,4,4	0.28	0	6,6,6	0.18	0
3	SO4	Y	302	-	4,4,4	0.32	0	6,6,6	0.22	0
4	VFZ	V	303	-	29,29,29	0.39	0	29,39,39	0.74	2 (6%)
3	SO4	c	302	-	4,4,4	0.33	0	6,6,6	0.20	0
3	SO4	L	302	-	4,4,4	0.33	0	6,6,6	0.18	0
3	SO4	P	302	-	4,4,4	0.35	0	6,6,6	0.06	0
3	SO4	R	302	-	4,4,4	0.34	0	6,6,6	0.16	0
3	SO4	X	303	-	4,4,4	0.32	0	6,6,6	0.15	0
4	VFZ	J	303	-	29,29,29	0.41	0	29,39,39	0.87	1 (3%)
3	SO4	H	302	-	4,4,4	0.29	0	6,6,6	0.18	0
3	SO4	Z	301	-	4,4,4	0.32	0	6,6,6	0.16	0
3	SO4	W	301	-	4,4,4	0.33	0	6,6,6	0.19	0
3	SO4	P	301	-	4,4,4	0.30	0	6,6,6	0.23	0
3	SO4	F	301	-	4,4,4	0.35	0	6,6,6	0.14	0
4	VFZ	b	302	-	29,29,29	0.36	0	29,39,39	0.55	0
4	VFZ	M	304	-	29,29,29	0.35	0	29,39,39	0.64	1 (3%)
3	SO4	A	308	-	4,4,4	0.32	0	6,6,6	0.17	0
4	VFZ	A	310	-	29,29,29	0.49	0	29,39,39	1.24	4 (13%)
4	VFZ	a	302	-	29,29,29	0.32	0	29,39,39	0.57	0
4	VFZ	U	304	-	29,29,29	0.38	0	29,39,39	0.90	2 (6%)
4	VFZ	H	303	-	29,29,29	0.39	0	29,39,39	0.96	2 (6%)
3	SO4	P	303	-	4,4,4	0.28	0	6,6,6	0.18	0
4	VFZ	Y	303	-	29,29,29	0.33	0	29,39,39	1.07	3 (10%)
3	SO4	c	301	-	4,4,4	0.29	0	6,6,6	0.16	0
4	VFZ	N	305	-	29,29,29	0.35	0	29,39,39	0.84	2 (6%)
3	SO4	a	301	-	4,4,4	0.40	0	6,6,6	0.23	0
4	VFZ	D	305	-	29,29,29	0.49	0	29,39,39	0.79	1 (3%)
3	SO4	C	305	-	4,4,4	0.25	0	6,6,6	0.16	0
3	SO4	G	303	-	4,4,4	0.29	0	6,6,6	0.16	0
3	SO4	E	303	-	4,4,4	0.43	0	6,6,6	0.16	0
3	SO4	D	304	-	4,4,4	0.28	0	6,6,6	0.19	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	VFZ	I	304	-	29,29,29	0.31	0	29,39,39	0.67	1 (3%)
4	VFZ	C	306	-	29,29,29	0.48	0	29,39,39	1.20	2 (6%)
3	SO4	G	302	-	4,4,4	0.27	0	6,6,6	0.21	0
3	SO4	O	302	-	4,4,4	0.37	0	6,6,6	0.14	0
3	SO4	R	301	-	4,4,4	0.32	0	6,6,6	0.14	0
4	VFZ	B	305	-	29,29,29	0.32	0	29,39,39	1.02	3 (10%)
4	VFZ	P	304	-	29,29,29	0.36	0	29,39,39	0.75	1 (3%)
3	SO4	U	301	-	4,4,4	0.32	0	6,6,6	0.12	0
3	SO4	N	304	-	4,4,4	0.40	0	6,6,6	0.23	0
3	SO4	T	302	-	4,4,4	0.35	0	6,6,6	0.12	0
3	SO4	M	303	-	4,4,4	0.27	0	6,6,6	0.18	0
3	SO4	d	301	-	4,4,4	0.36	0	6,6,6	0.13	0
3	SO4	R	303	-	4,4,4	0.26	0	6,6,6	0.19	0
3	SO4	Q	302	-	4,4,4	0.30	0	6,6,6	0.12	0
3	SO4	D	302	-	4,4,4	0.31	0	6,6,6	0.15	0
3	SO4	K	302	-	4,4,4	0.27	0	6,6,6	0.20	0
3	SO4	H	301	-	4,4,4	0.36	0	6,6,6	0.17	0
3	SO4	J	301	-	4,4,4	0.28	0	6,6,6	0.23	0
3	SO4	Y	301	-	4,4,4	0.35	0	6,6,6	0.14	0
3	SO4	A	309	-	4,4,4	0.25	0	6,6,6	0.20	0
3	SO4	N	303	-	4,4,4	0.33	0	6,6,6	0.20	0
4	VFZ	c	303	-	29,29,29	0.45	0	29,39,39	0.63	0
3	SO4	S	302	-	4,4,4	0.31	0	6,6,6	0.09	0
3	SO4	V	302	-	4,4,4	0.37	0	6,6,6	0.14	0
3	SO4	A	307	-	4,4,4	0.29	0	6,6,6	0.14	0
4	VFZ	T	303	-	29,29,29	0.46	0	29,39,39	0.70	2 (6%)
4	VFZ	K	303	-	29,29,29	0.40	0	29,39,39	0.92	2 (6%)
4	VFZ	L	303	-	29,29,29	0.46	0	29,39,39	1.18	4 (13%)
3	SO4	D	303	-	4,4,4	0.27	0	6,6,6	0.24	0
4	VFZ	O	303	-	29,29,29	0.34	0	29,39,39	1.06	4 (13%)
3	SO4	J	302	-	4,4,4	0.28	0	6,6,6	0.22	0
3	SO4	U	303	-	4,4,4	0.31	0	6,6,6	0.10	0
3	SO4	B	303	-	4,4,4	0.30	0	6,6,6	0.14	0
3	SO4	b	301	-	4,4,4	0.35	0	6,6,6	0.17	0
4	VFZ	R	304	-	29,29,29	0.35	0	29,39,39	0.75	1 (3%)
3	SO4	E	304	-	4,4,4	0.29	0	6,6,6	0.08	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
4	VFZ	Z	302	-	-	1/17/17/17	0/3/3/3
4	VFZ	d	302	-	-	2/17/17/17	0/3/3/3
4	VFZ	G	304	-	-	0/17/17/17	0/3/3/3
4	VFZ	E	305	-	-	4/17/17/17	0/3/3/3
4	VFZ	J	303	-	-	1/17/17/17	0/3/3/3
4	VFZ	I	304	-	-	1/17/17/17	0/3/3/3
4	VFZ	X	304	-	-	2/17/17/17	0/3/3/3
4	VFZ	Q	303	-	-	3/17/17/17	0/3/3/3
4	VFZ	b	302	-	-	1/17/17/17	0/3/3/3
4	VFZ	C	306	-	-	2/17/17/17	0/3/3/3
4	VFZ	M	304	-	-	1/17/17/17	0/3/3/3
4	VFZ	c	303	-	-	1/17/17/17	0/3/3/3
4	VFZ	a	302	-	-	1/17/17/17	0/3/3/3
4	VFZ	A	310	-	-	2/17/17/17	0/3/3/3
4	VFZ	T	303	-	-	1/17/17/17	0/3/3/3
4	VFZ	U	304	-	-	2/17/17/17	0/3/3/3
4	VFZ	K	303	-	-	2/17/17/17	0/3/3/3
4	VFZ	B	305	-	-	3/17/17/17	0/3/3/3
4	VFZ	H	303	-	-	3/17/17/17	0/3/3/3
4	VFZ	P	304	-	-	2/17/17/17	0/3/3/3
4	VFZ	L	303	-	-	1/17/17/17	0/3/3/3
4	VFZ	Y	303	-	-	4/17/17/17	0/3/3/3
4	VFZ	S	303	-	-	1/17/17/17	0/3/3/3
4	VFZ	W	302	-	-	3/17/17/17	0/3/3/3
4	VFZ	F	303	-	-	2/17/17/17	0/3/3/3
4	VFZ	O	303	-	-	1/17/17/17	0/3/3/3
4	VFZ	N	305	-	-	1/17/17/17	0/3/3/3
4	VFZ	V	303	-	-	1/17/17/17	0/3/3/3
4	VFZ	D	305	-	-	1/17/17/17	0/3/3/3
4	VFZ	R	304	-	-	2/17/17/17	0/3/3/3

There are no bond length outliers.

The worst 5 of 57 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	E	305	VFZ	C3-N3-C2	-5.08	108.84	117.49
4	C	306	VFZ	C3-N3-C2	-4.61	109.63	117.49
4	F	303	VFZ	C3-C4-C5	-4.38	114.17	121.37
4	F	303	VFZ	C3-N3-C2	-4.11	110.49	117.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	310	VFZ	C4-C3-N3	3.95	119.78	113.77

There are no chirality outliers.

5 of 52 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	310	VFZ	N3-C3-C4-C5
4	B	305	VFZ	N3-C3-C4-C5
4	E	305	VFZ	N3-C3-C4-C5
4	I	304	VFZ	N3-C3-C4-C5
4	M	304	VFZ	N3-C3-C4-C8

There are no ring outliers.

35 monomers are involved in 29 short contacts:

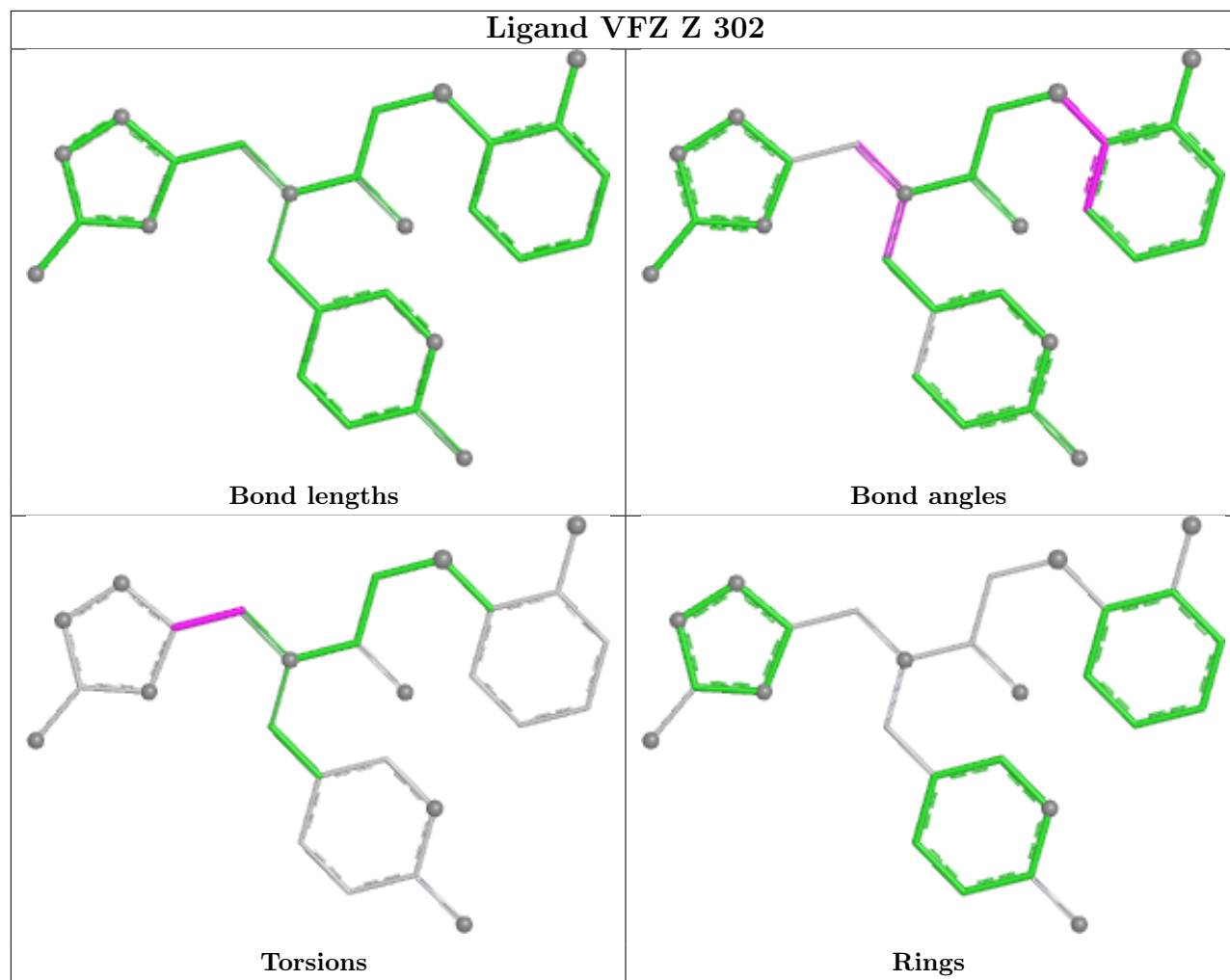
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	I	302	SO4	1	0
4	d	302	VFZ	1	0
4	E	305	VFZ	1	0
4	Q	303	VFZ	1	0
3	N	302	SO4	2	0
4	S	303	VFZ	1	0
4	W	302	VFZ	2	0
4	F	303	VFZ	2	0
3	L	302	SO4	2	0
3	P	302	SO4	1	0
3	W	301	SO4	2	0
3	P	301	SO4	1	0
3	F	301	SO4	1	0
4	b	302	VFZ	1	0
4	A	310	VFZ	3	0
4	a	302	VFZ	2	0
4	U	304	VFZ	1	0
4	Y	303	VFZ	1	0
4	N	305	VFZ	2	0
3	a	301	SO4	2	0
4	D	305	VFZ	1	0
3	E	303	SO4	1	0
4	I	304	VFZ	1	0
3	R	301	SO4	2	0
4	P	304	VFZ	1	0

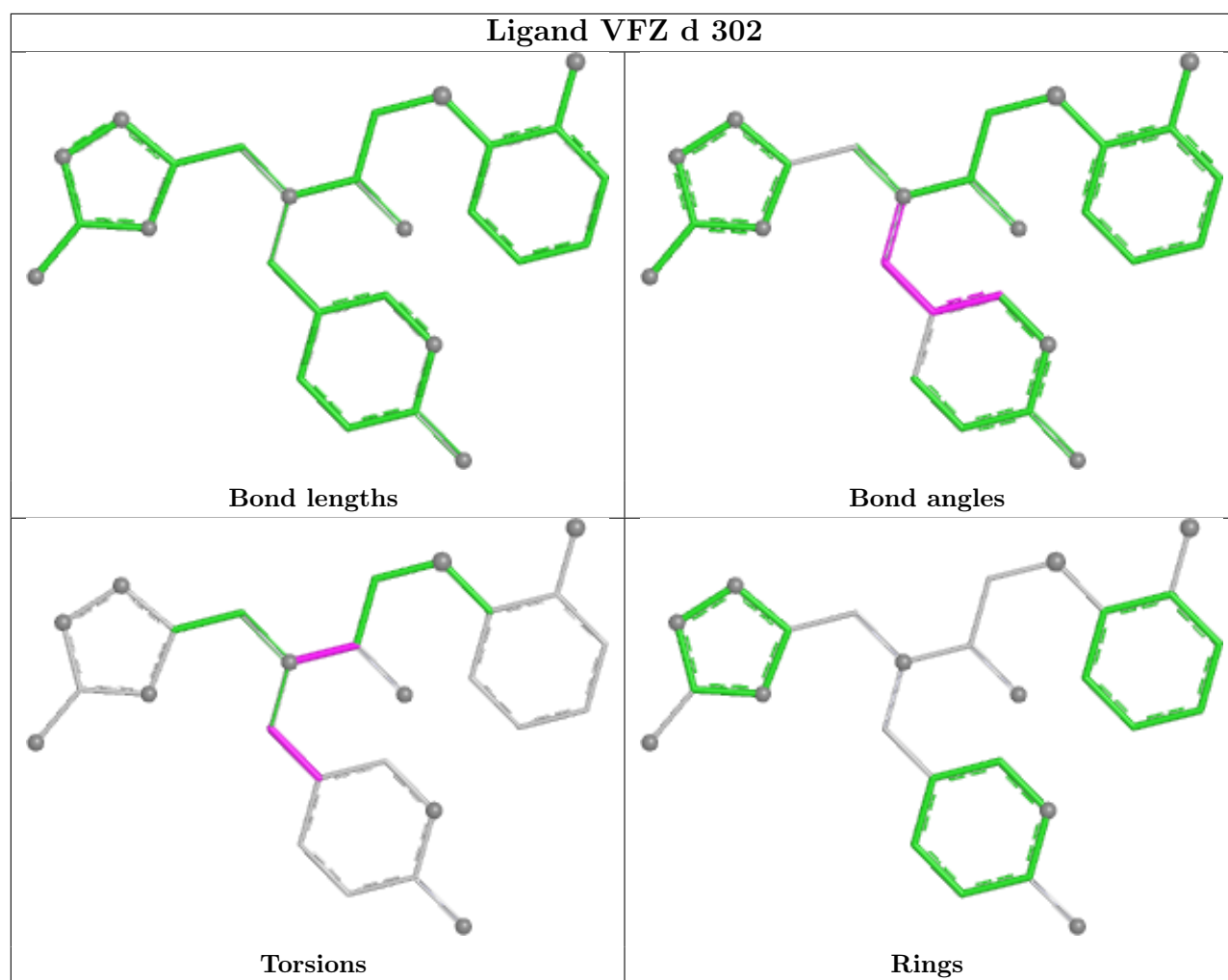
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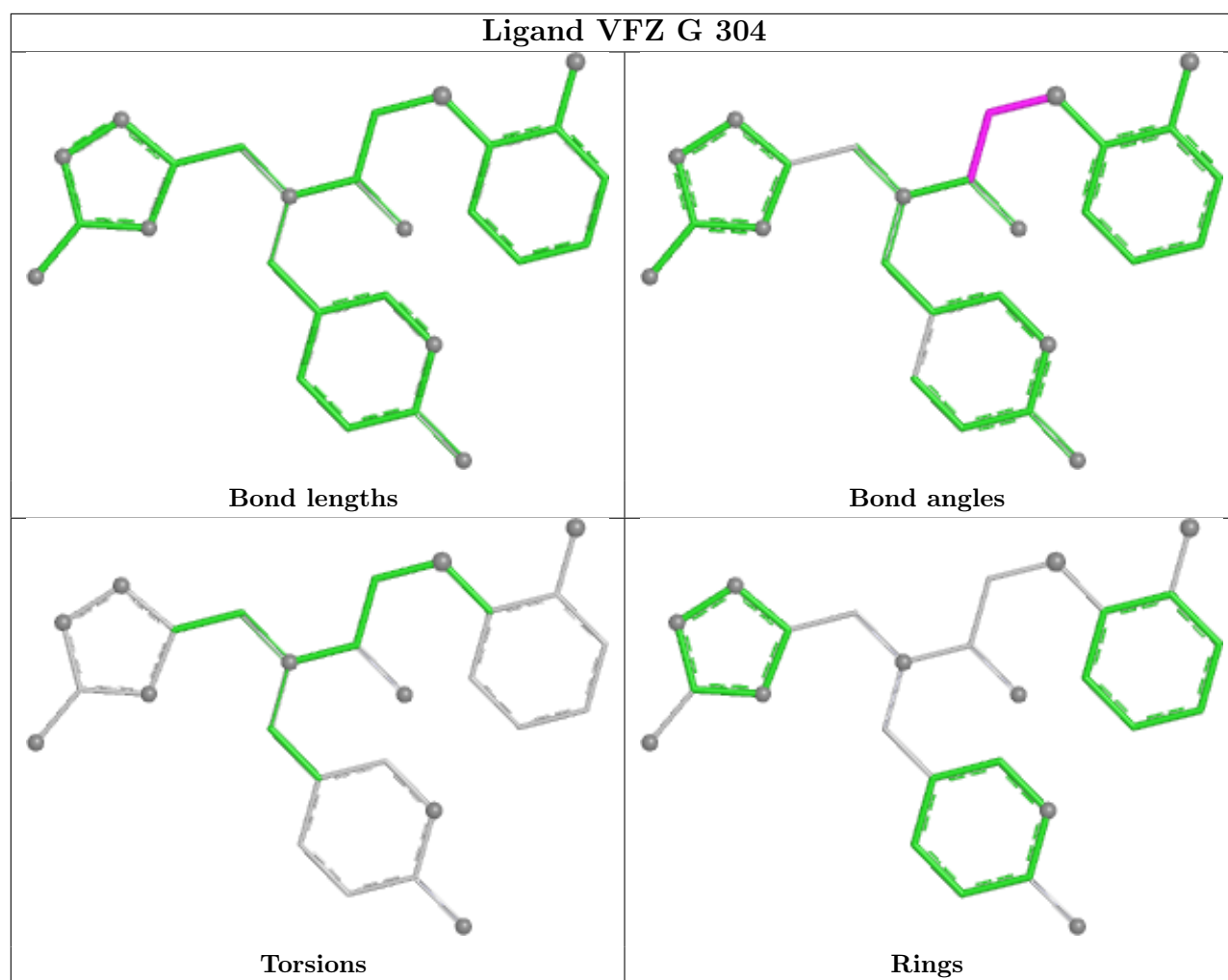
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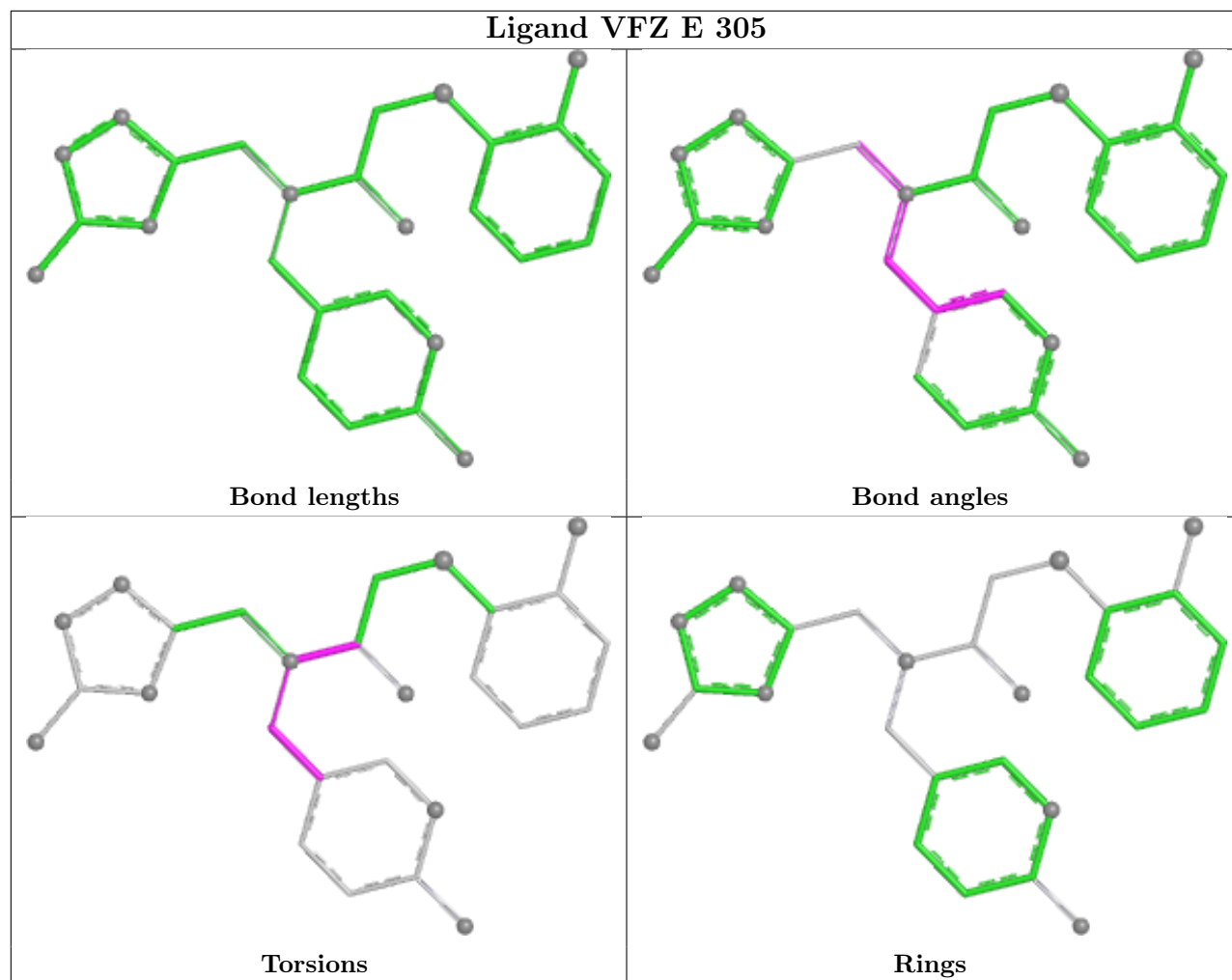
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	U	301	SO4	1	0
3	d	301	SO4	1	0
3	Q	302	SO4	1	0
3	D	302	SO4	2	0
3	Y	301	SO4	1	0
3	S	302	SO4	1	0
3	A	307	SO4	2	0
4	L	303	VFZ	2	0
3	b	301	SO4	1	0
4	R	304	VFZ	1	0

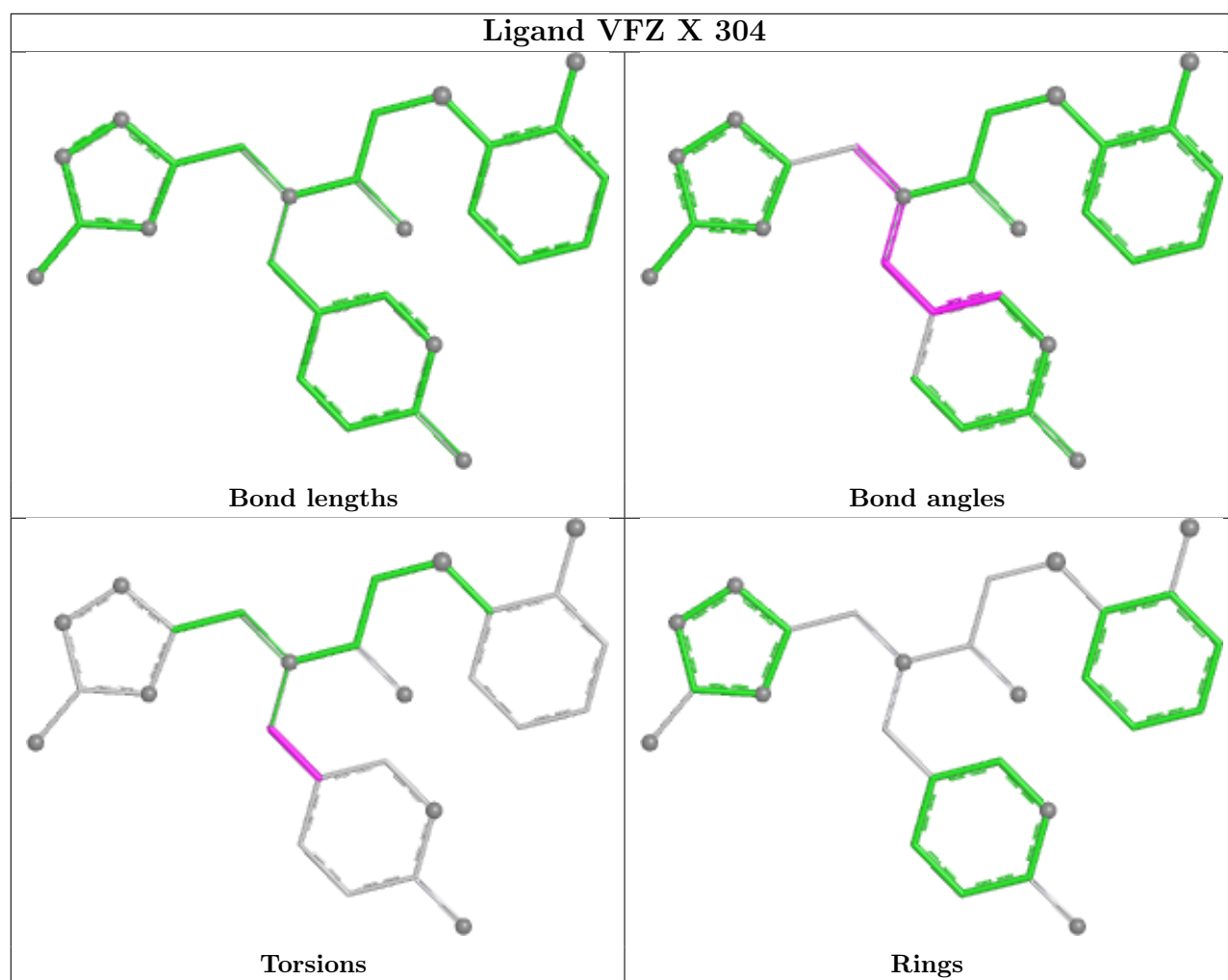
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

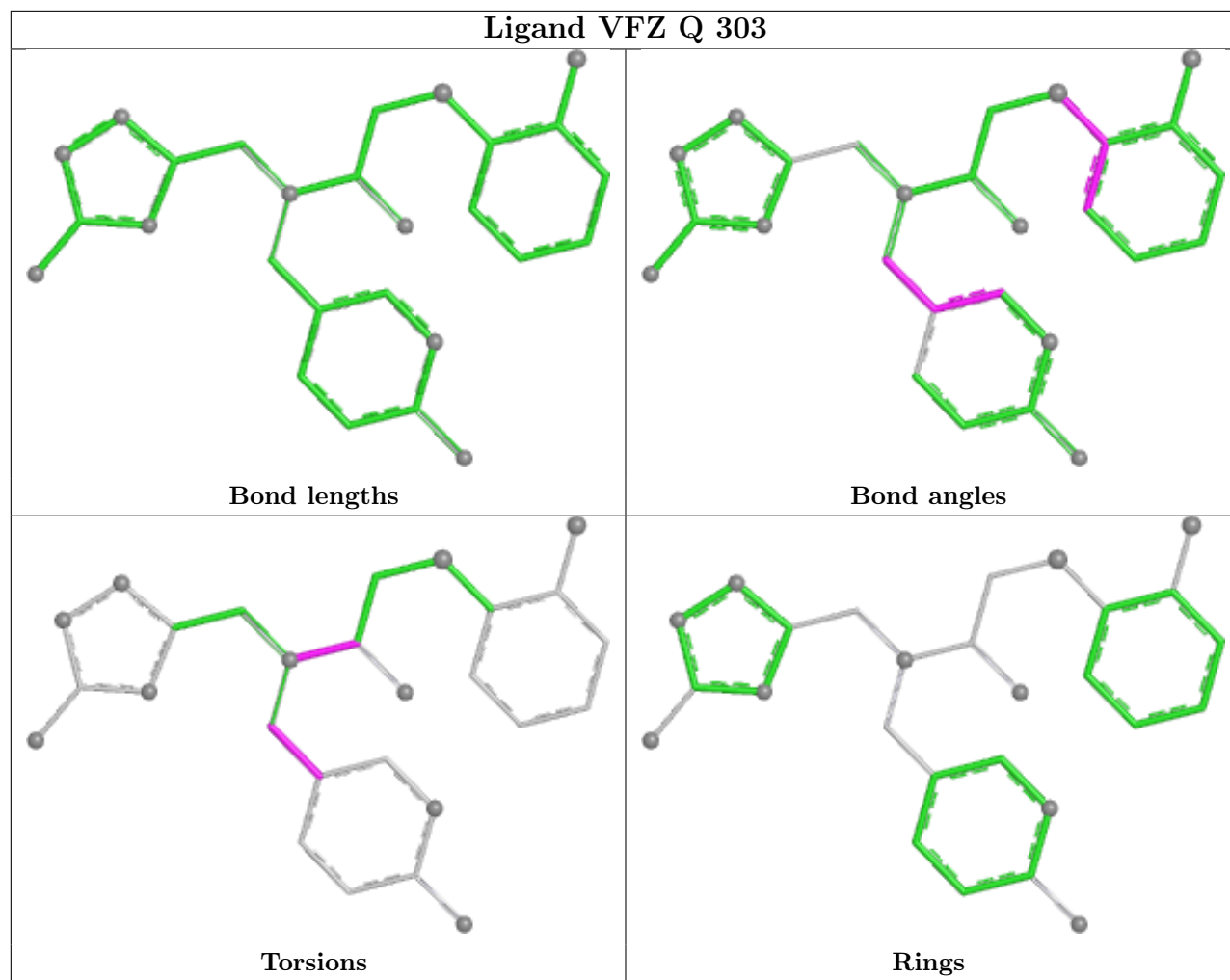


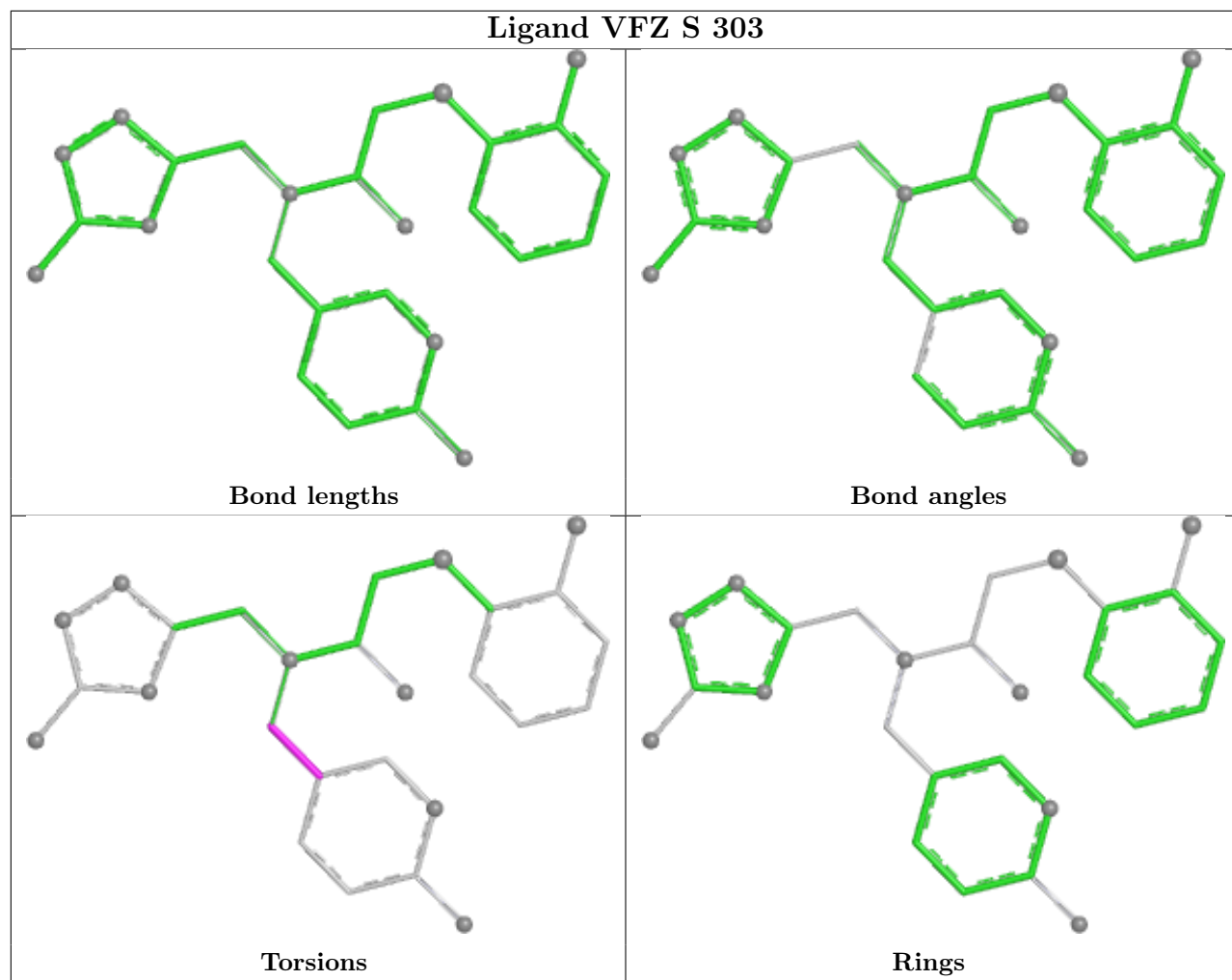


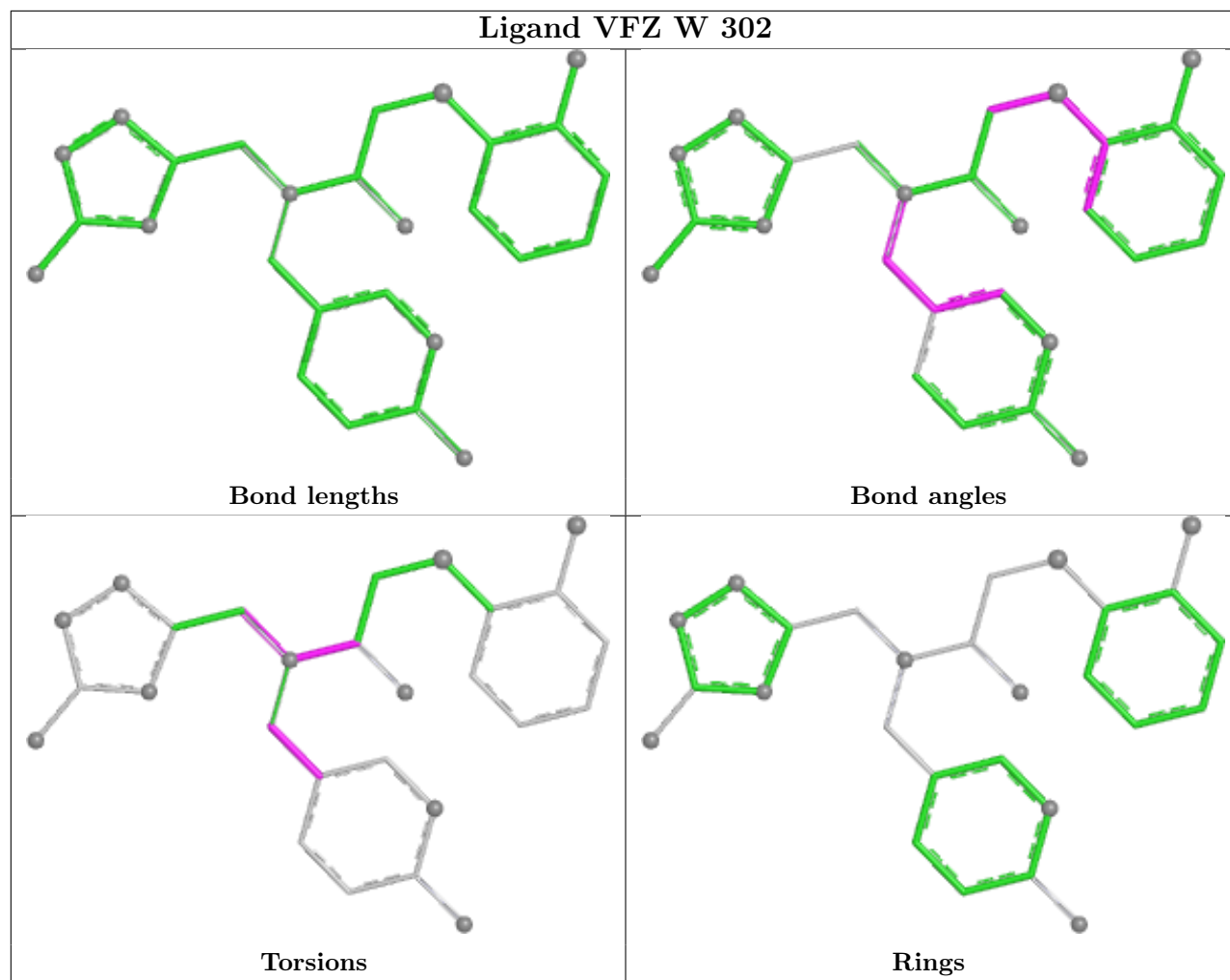


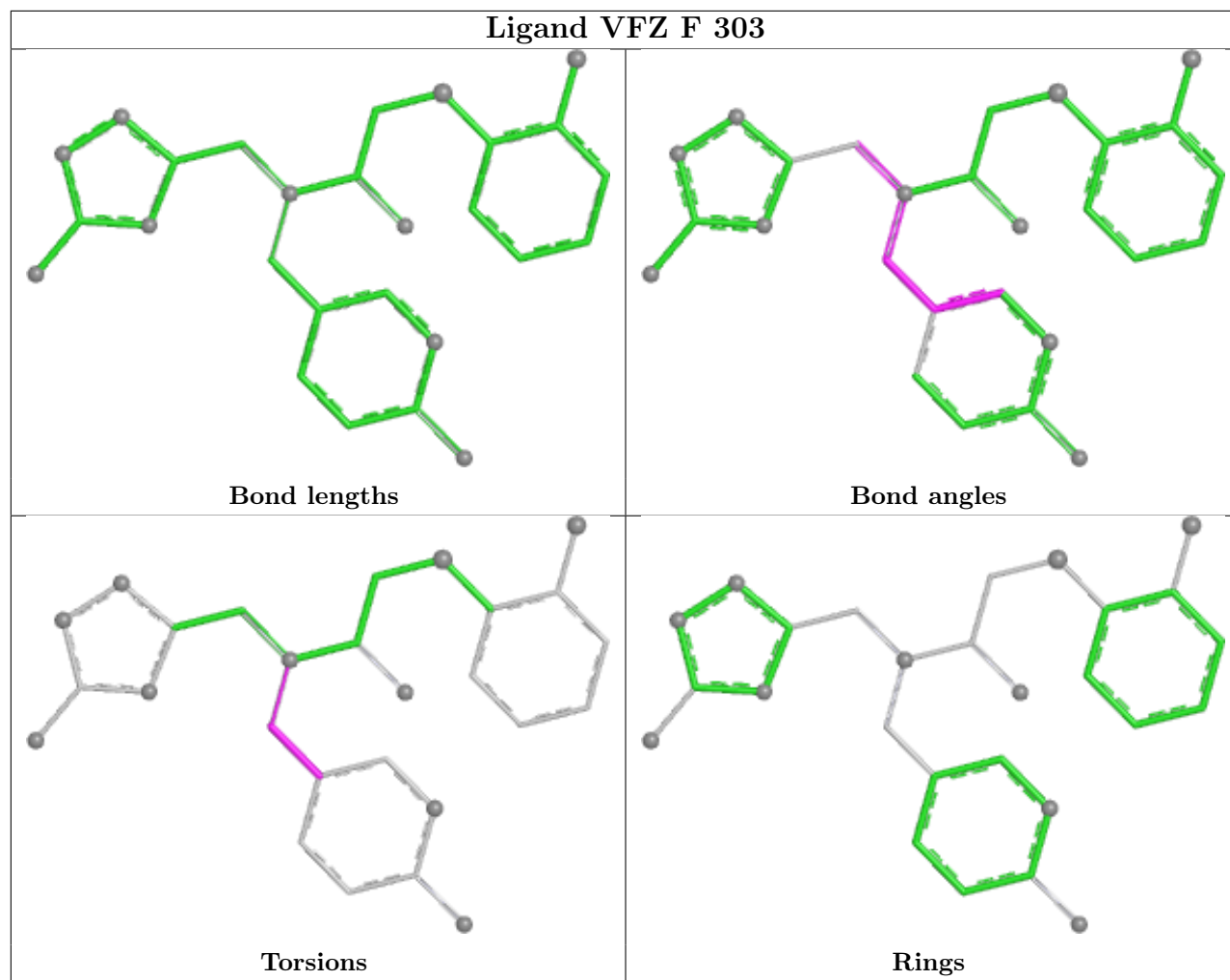


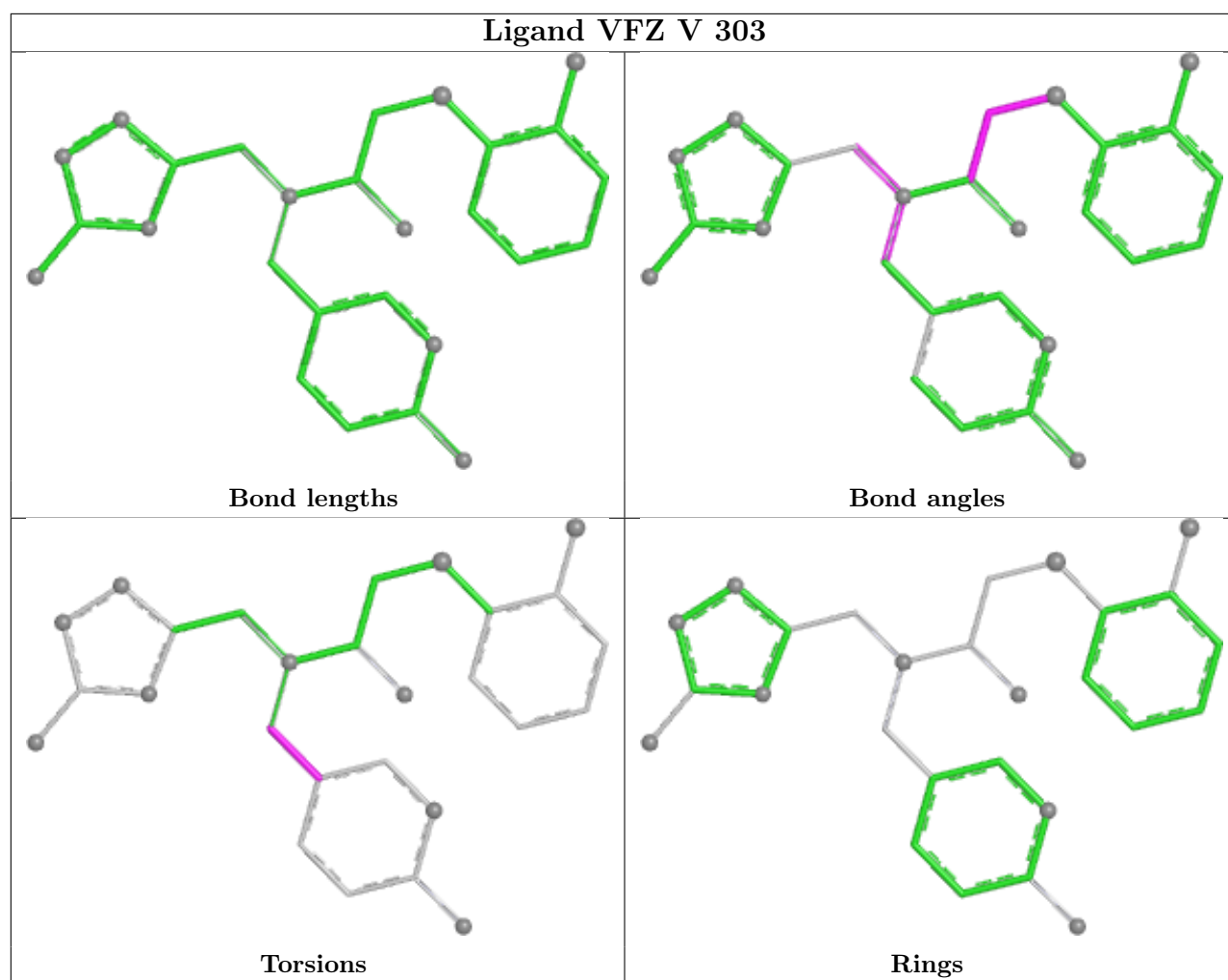


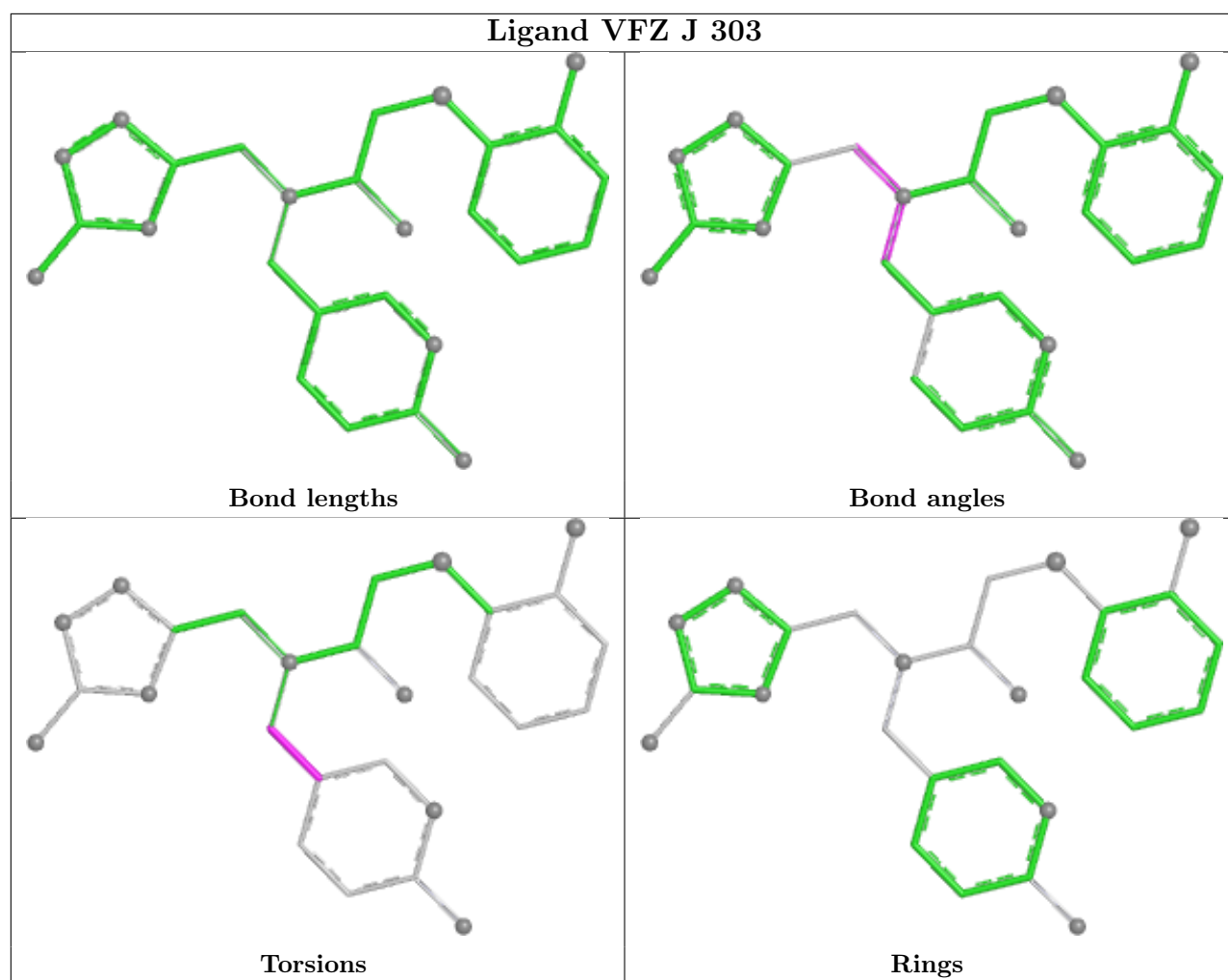


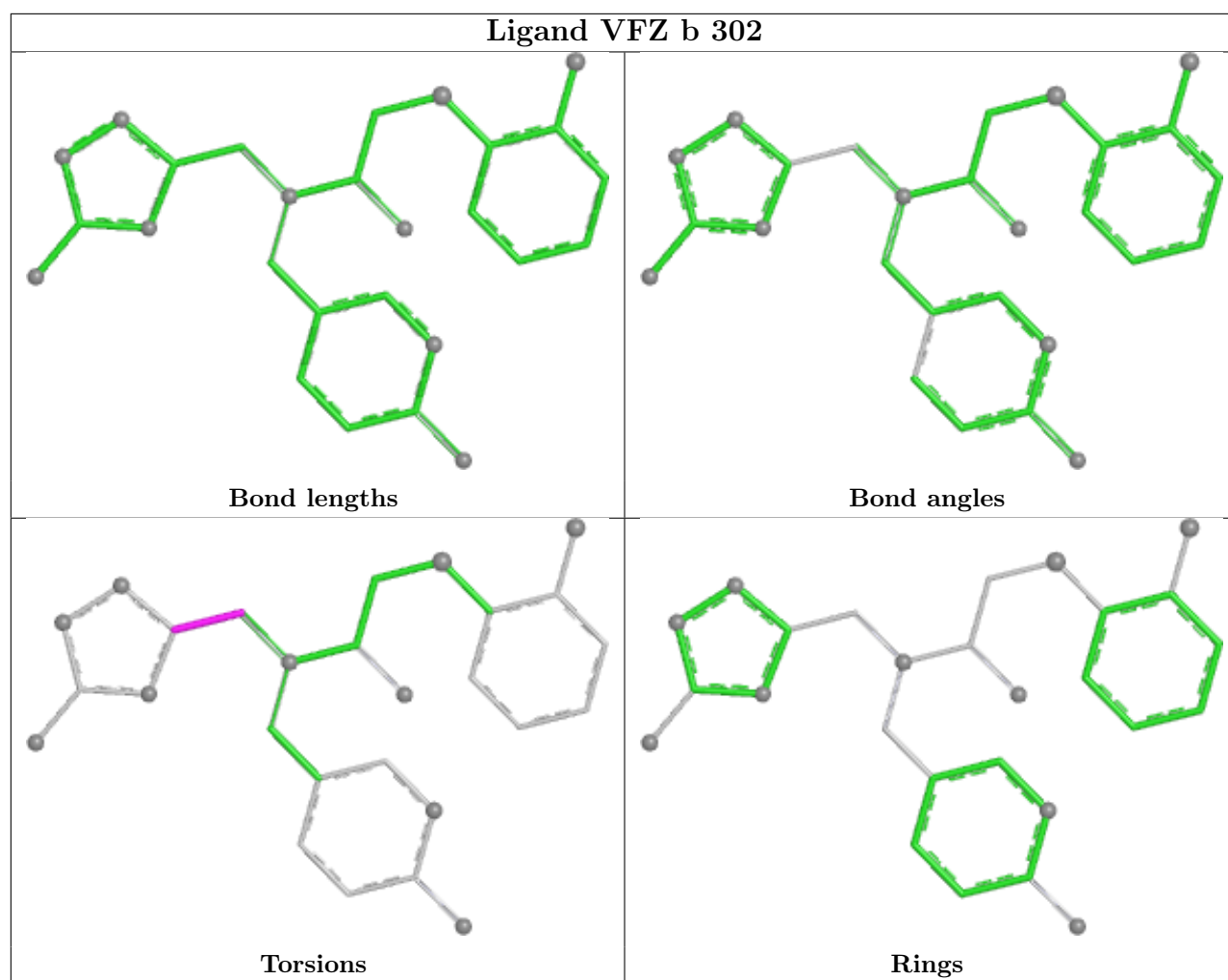


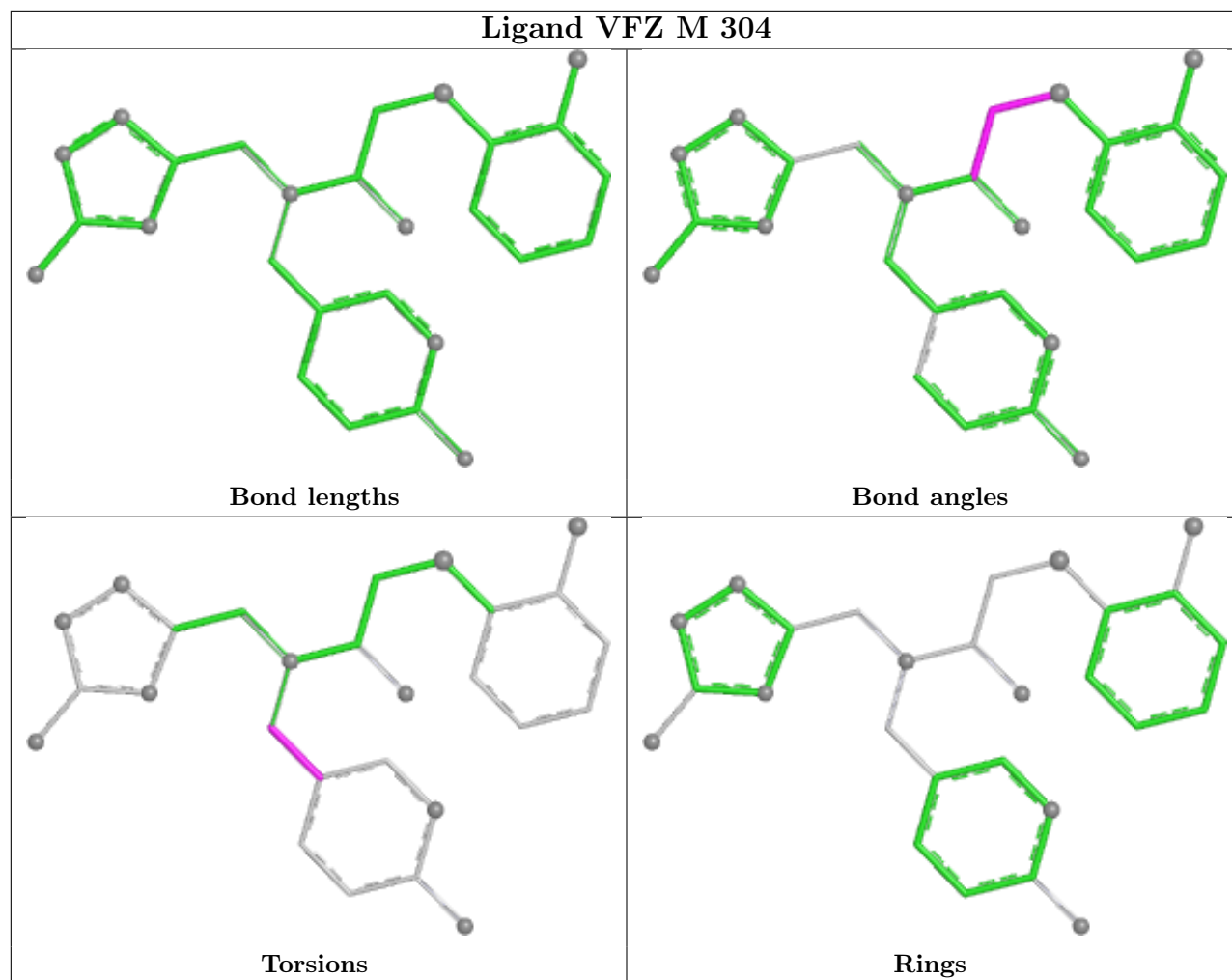


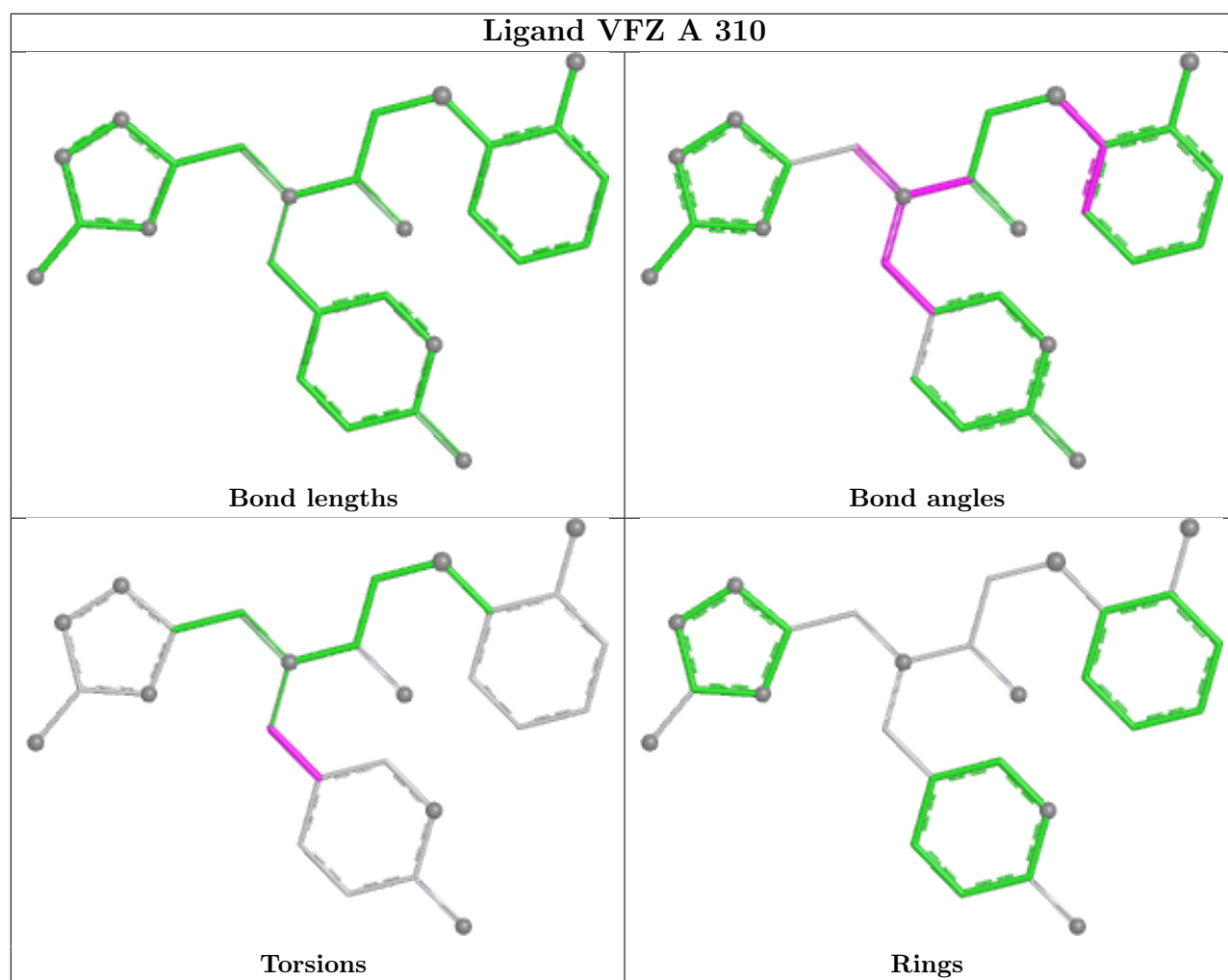


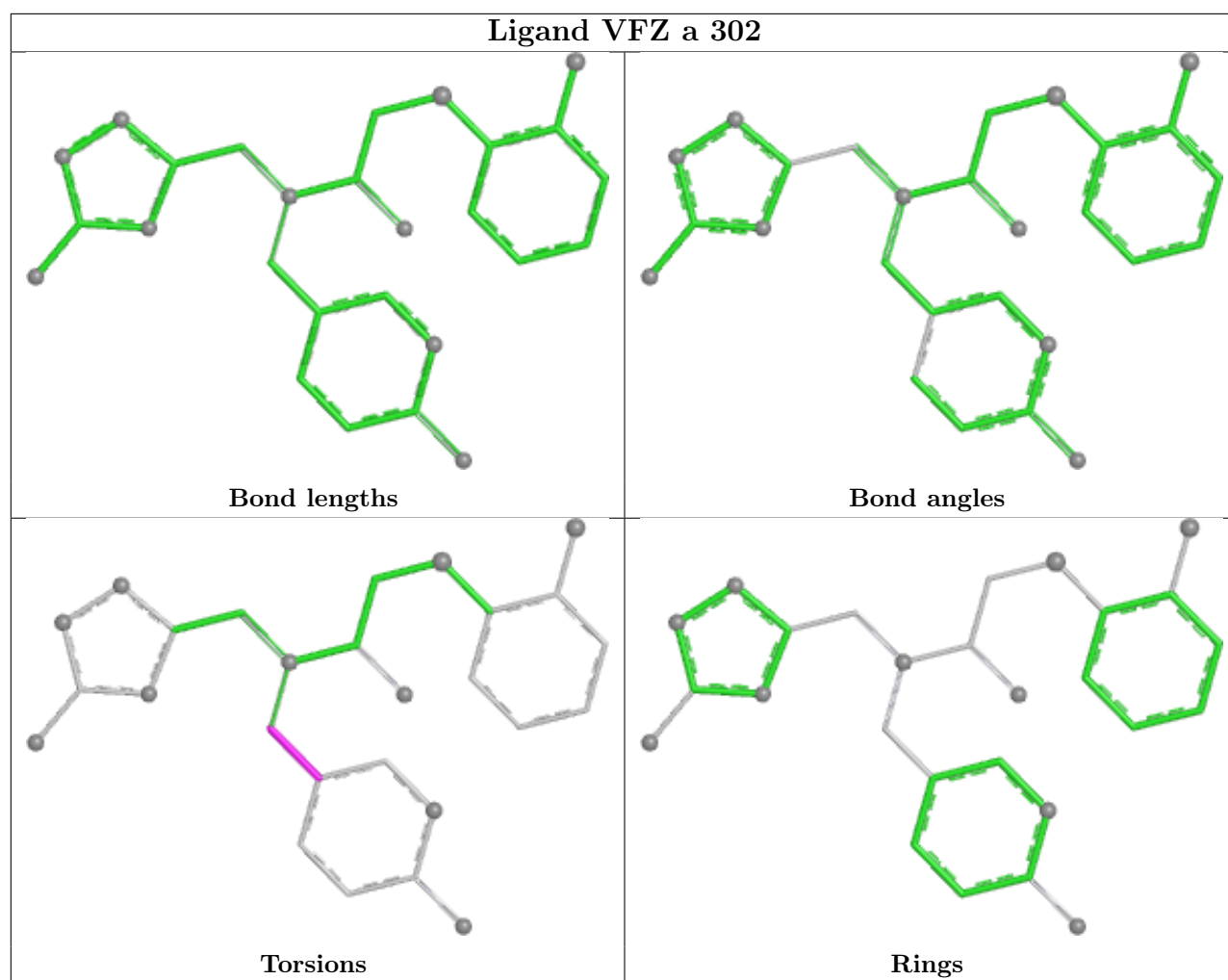


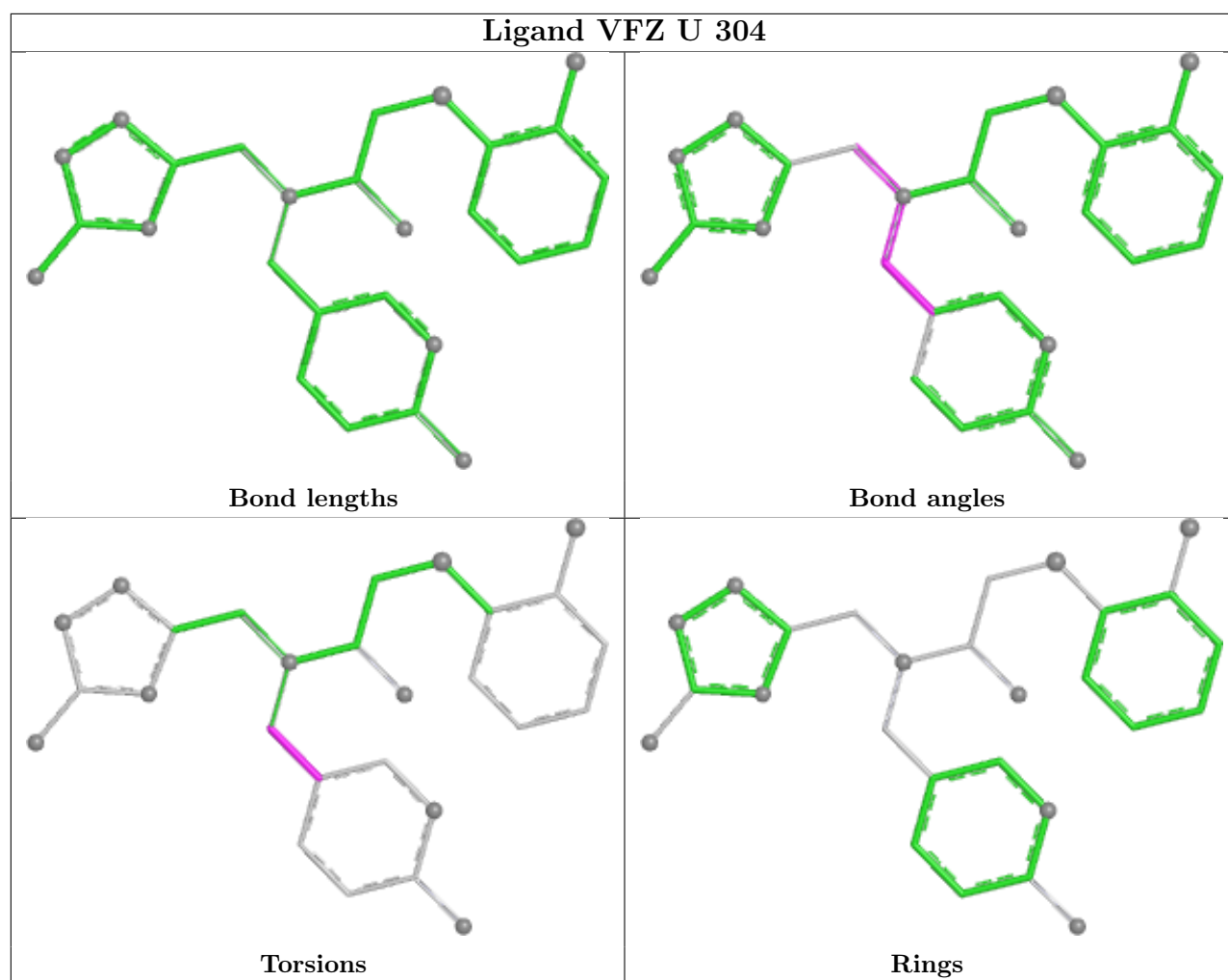


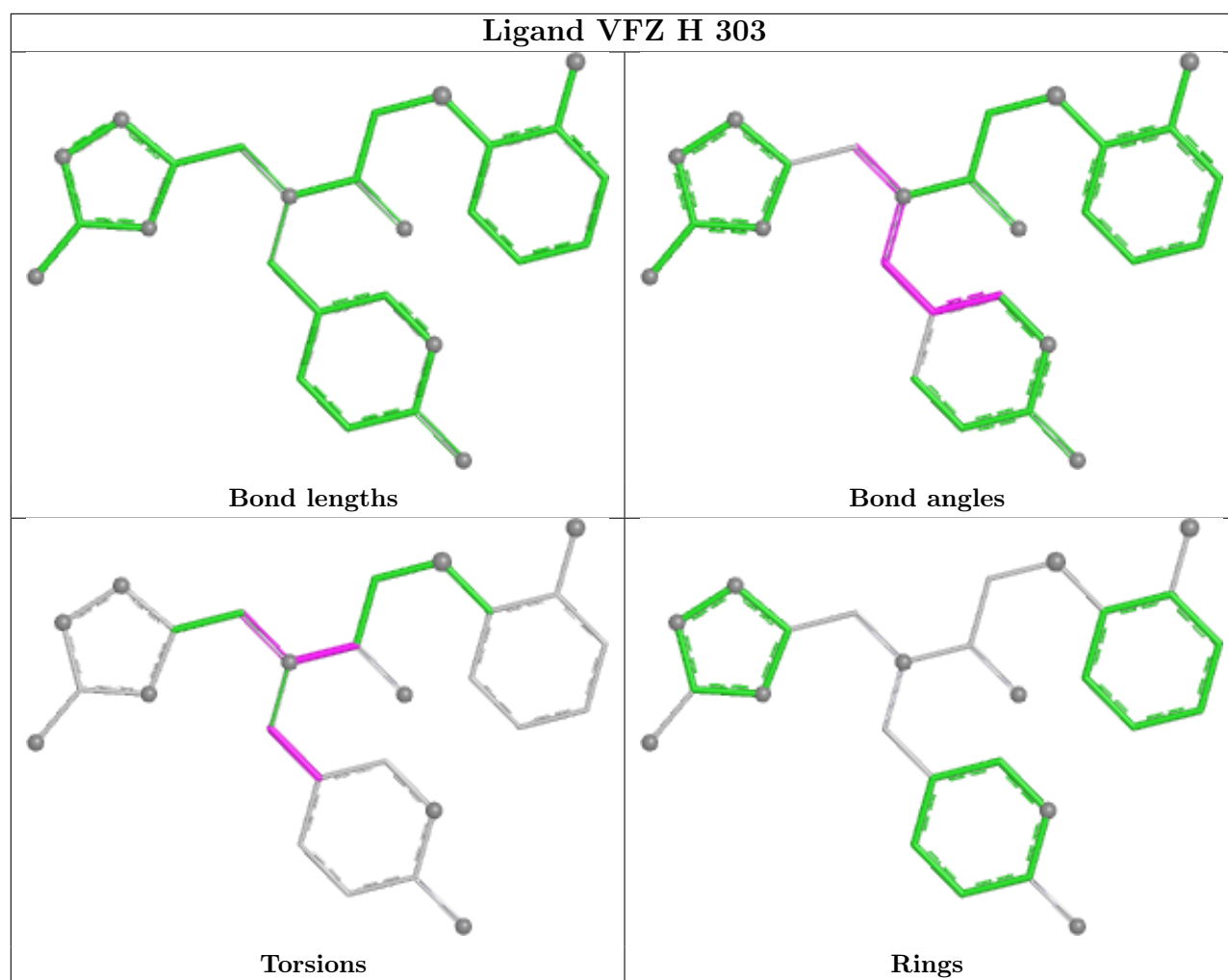


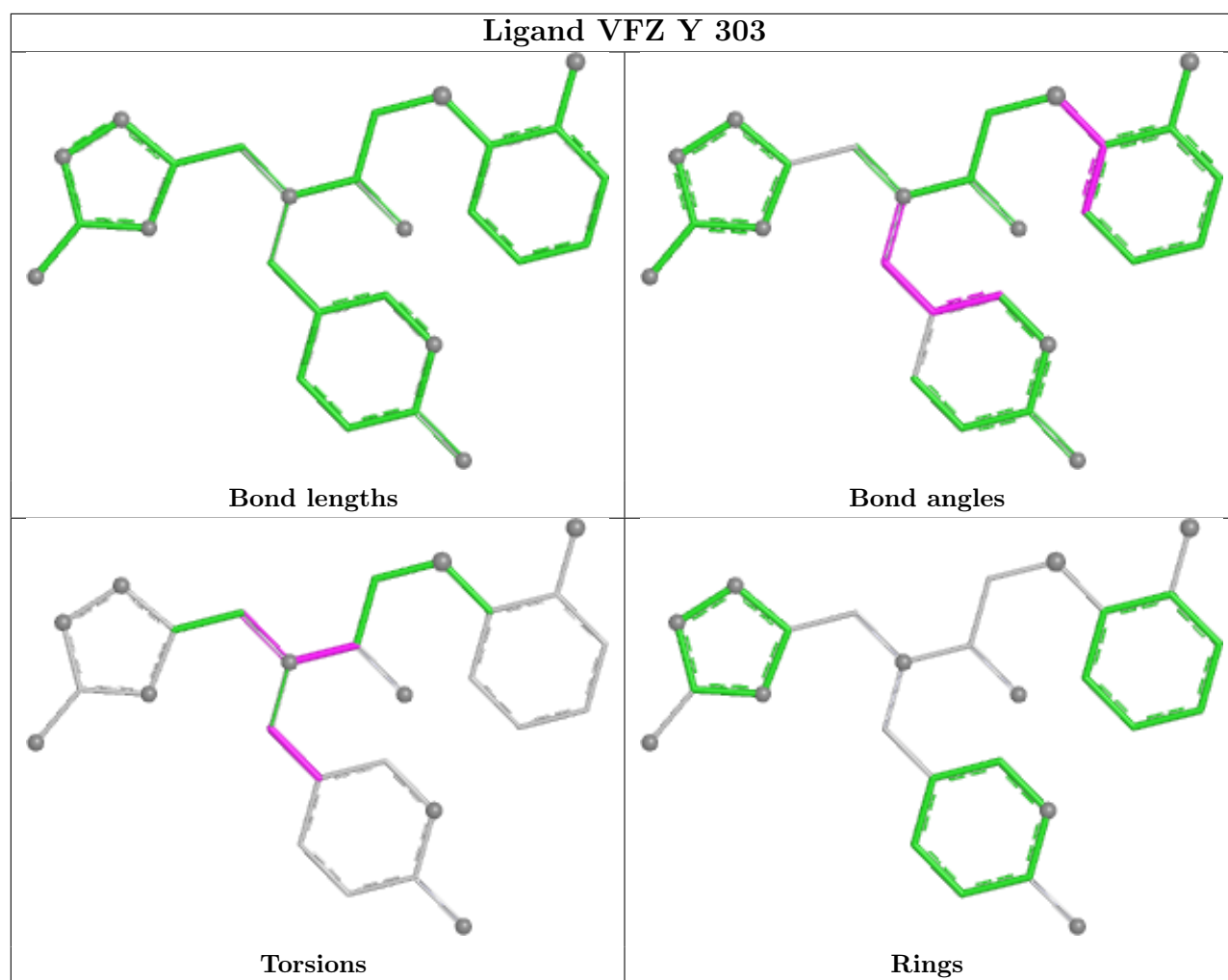


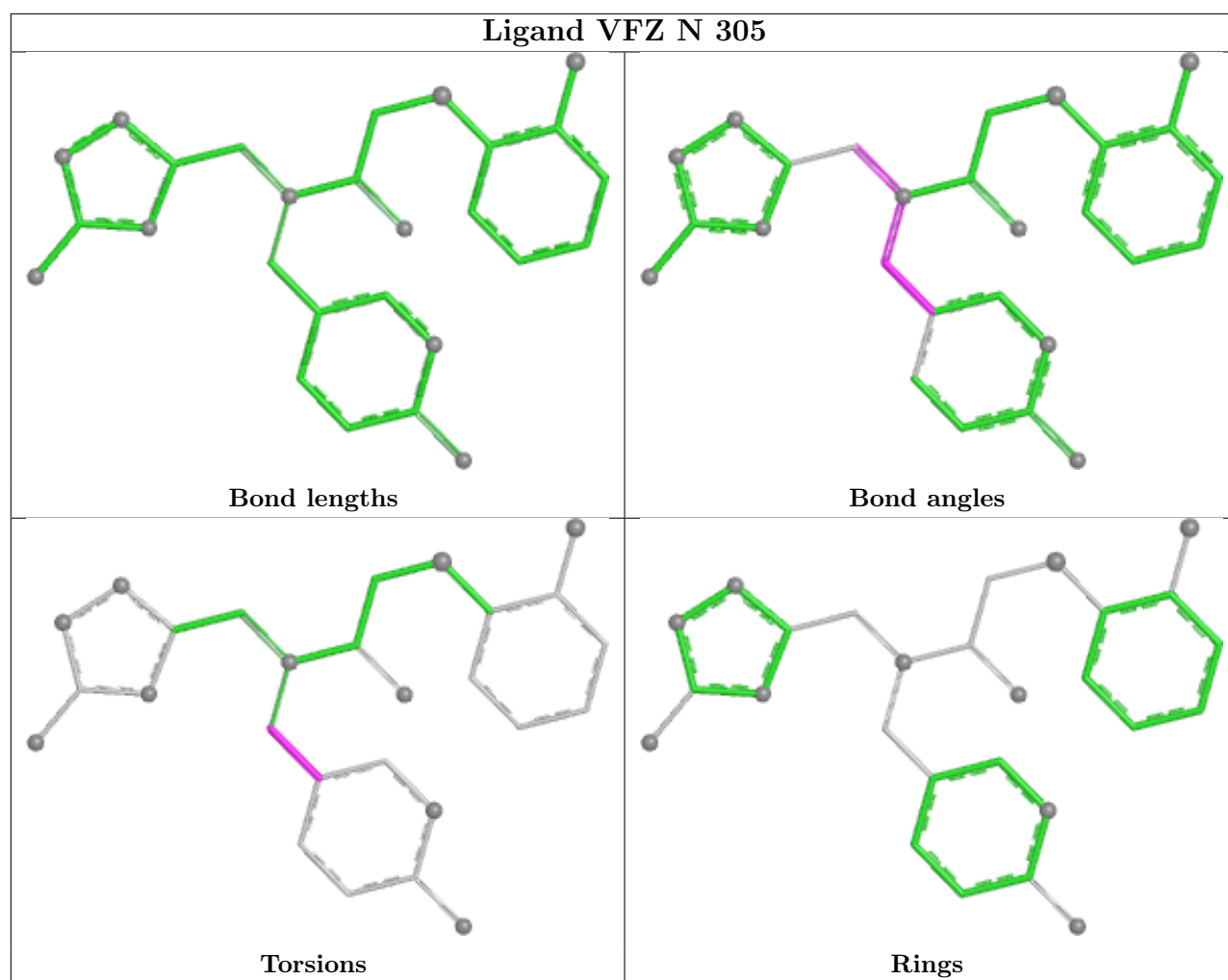


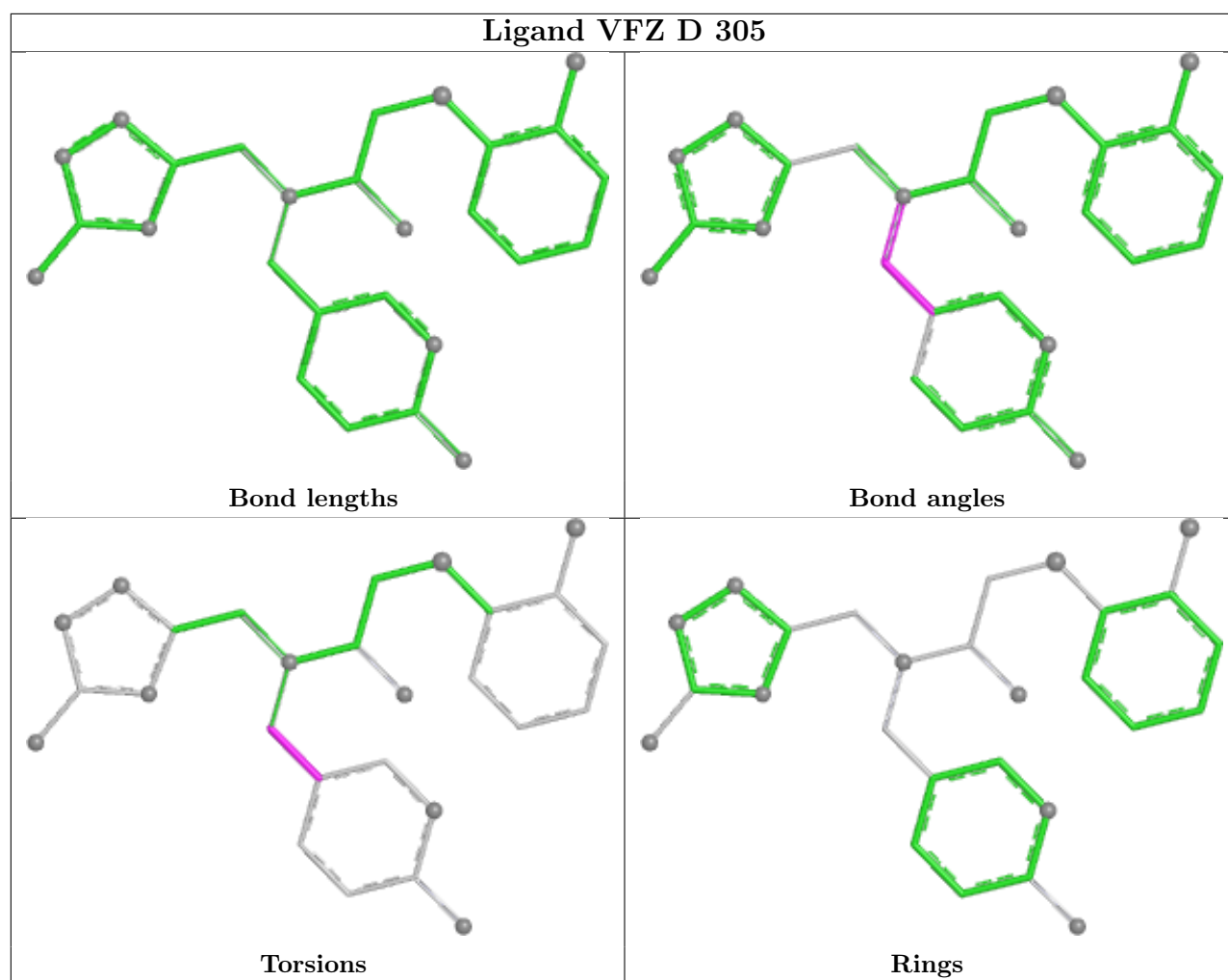


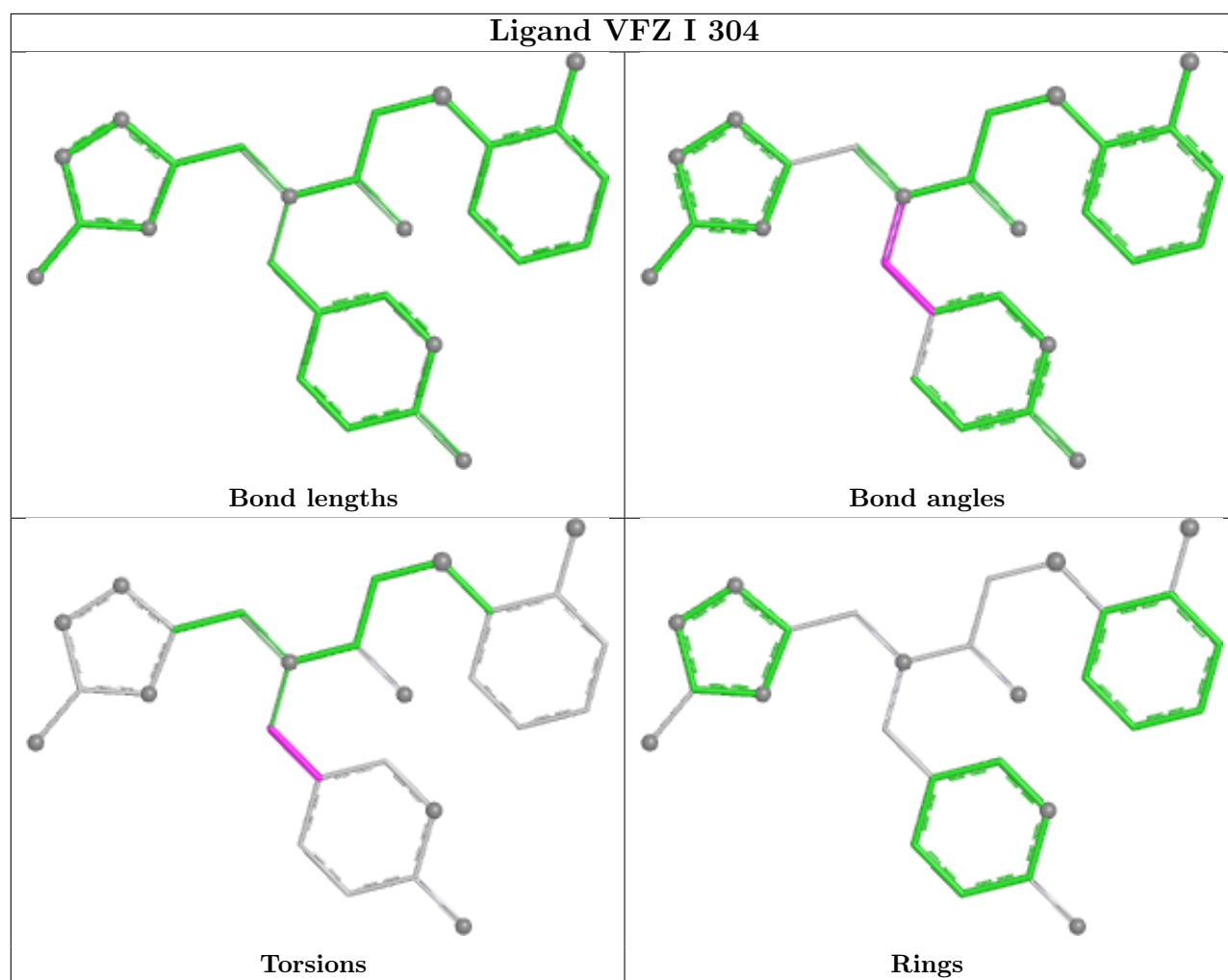


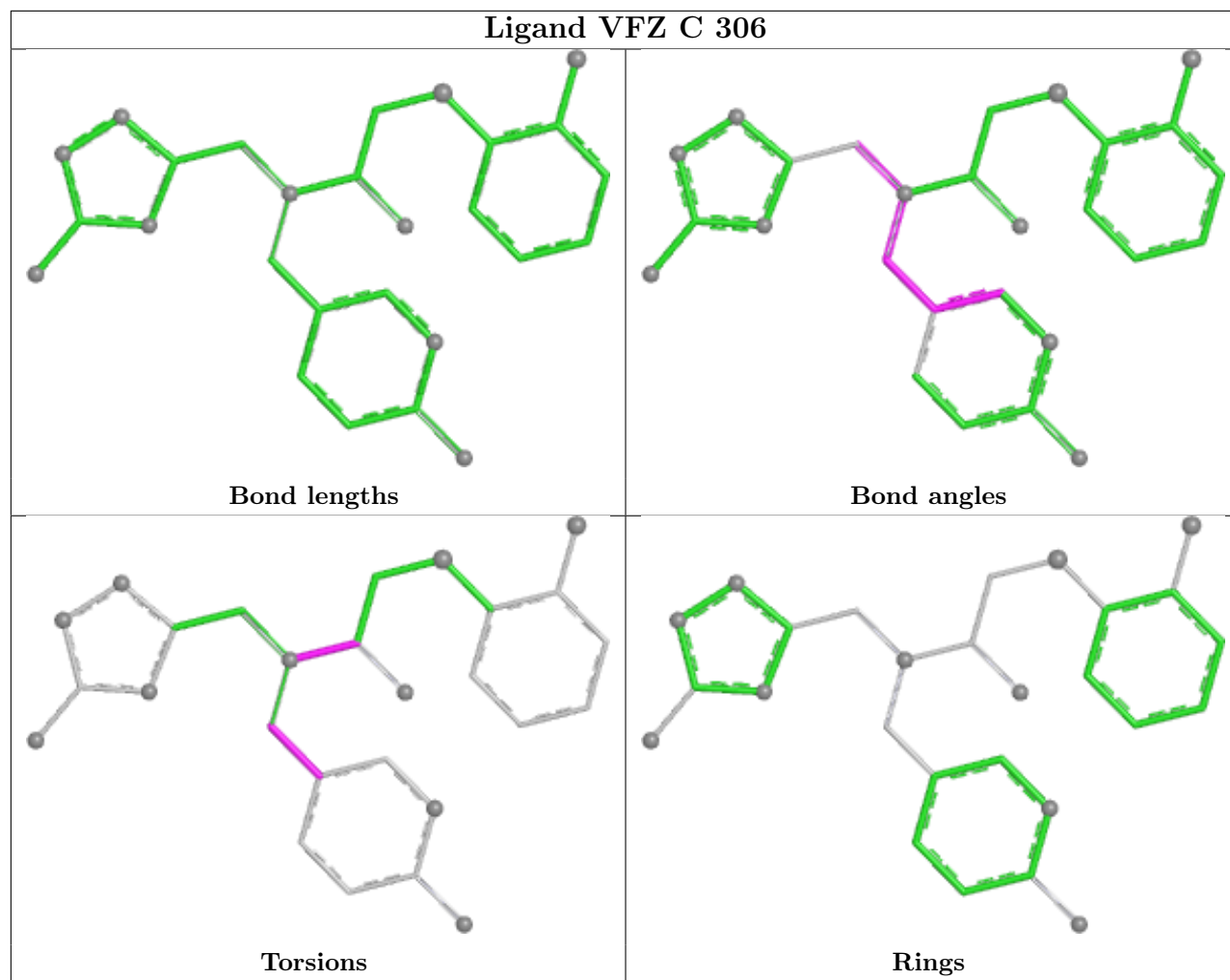


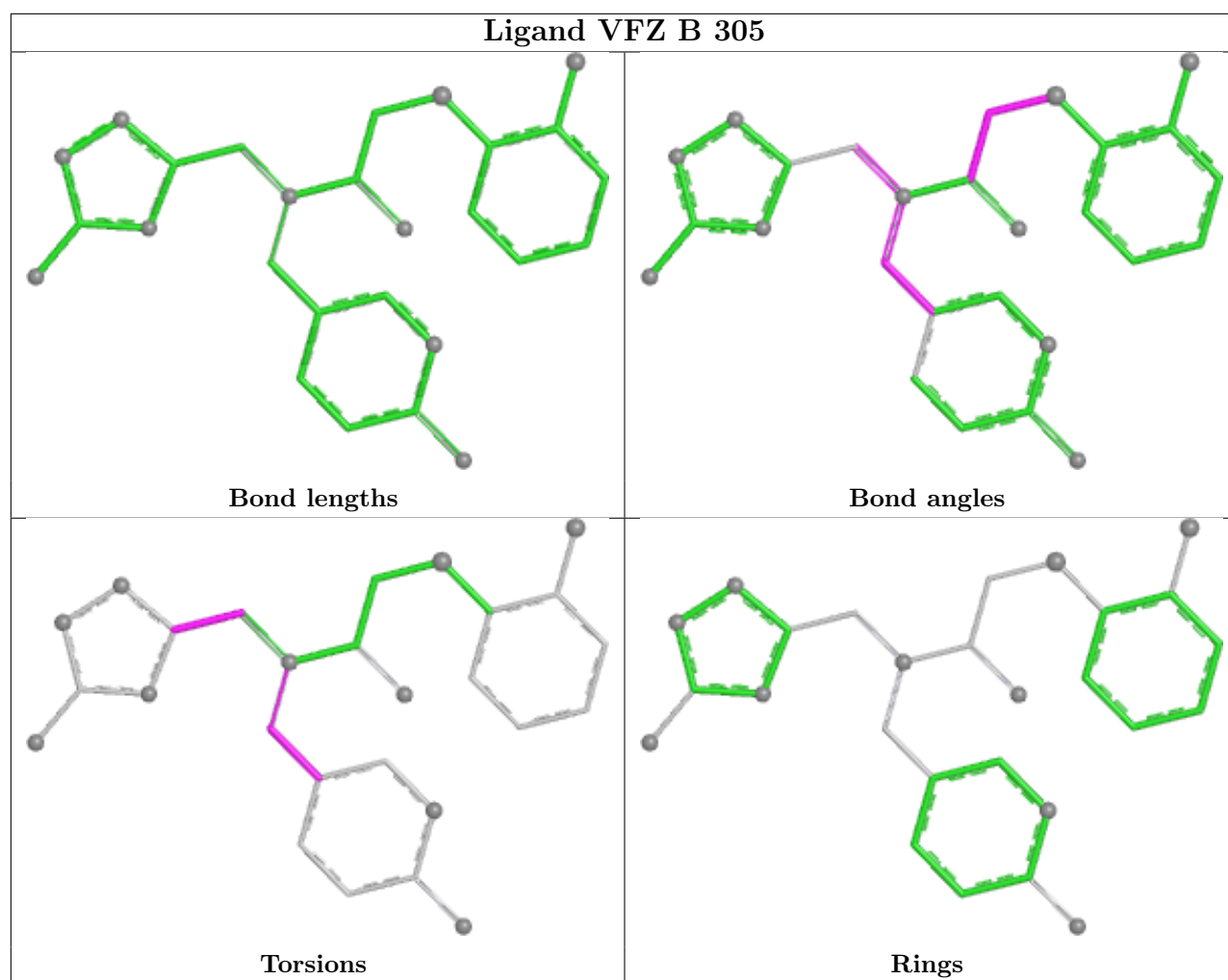












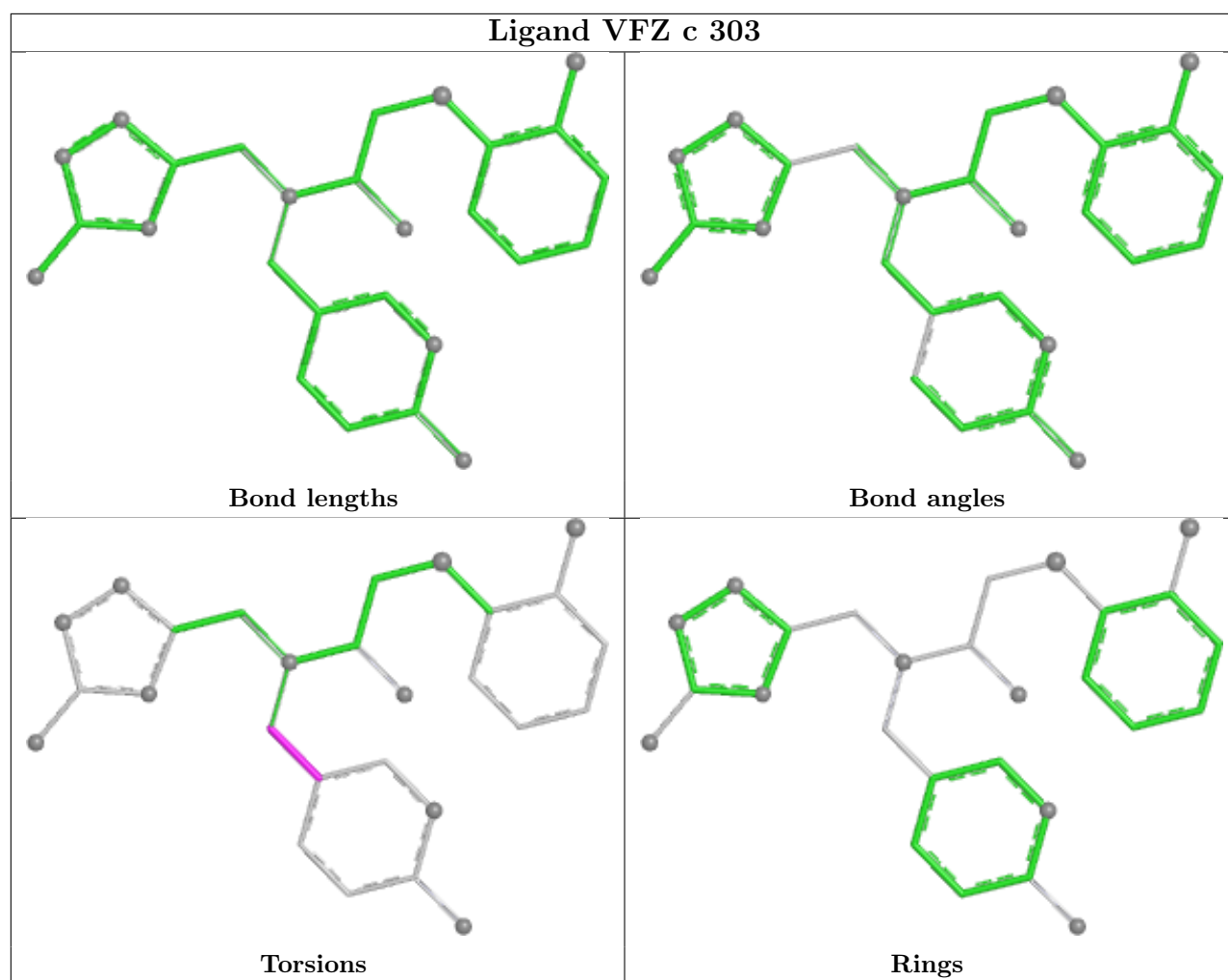
Ligand VFZ P 304

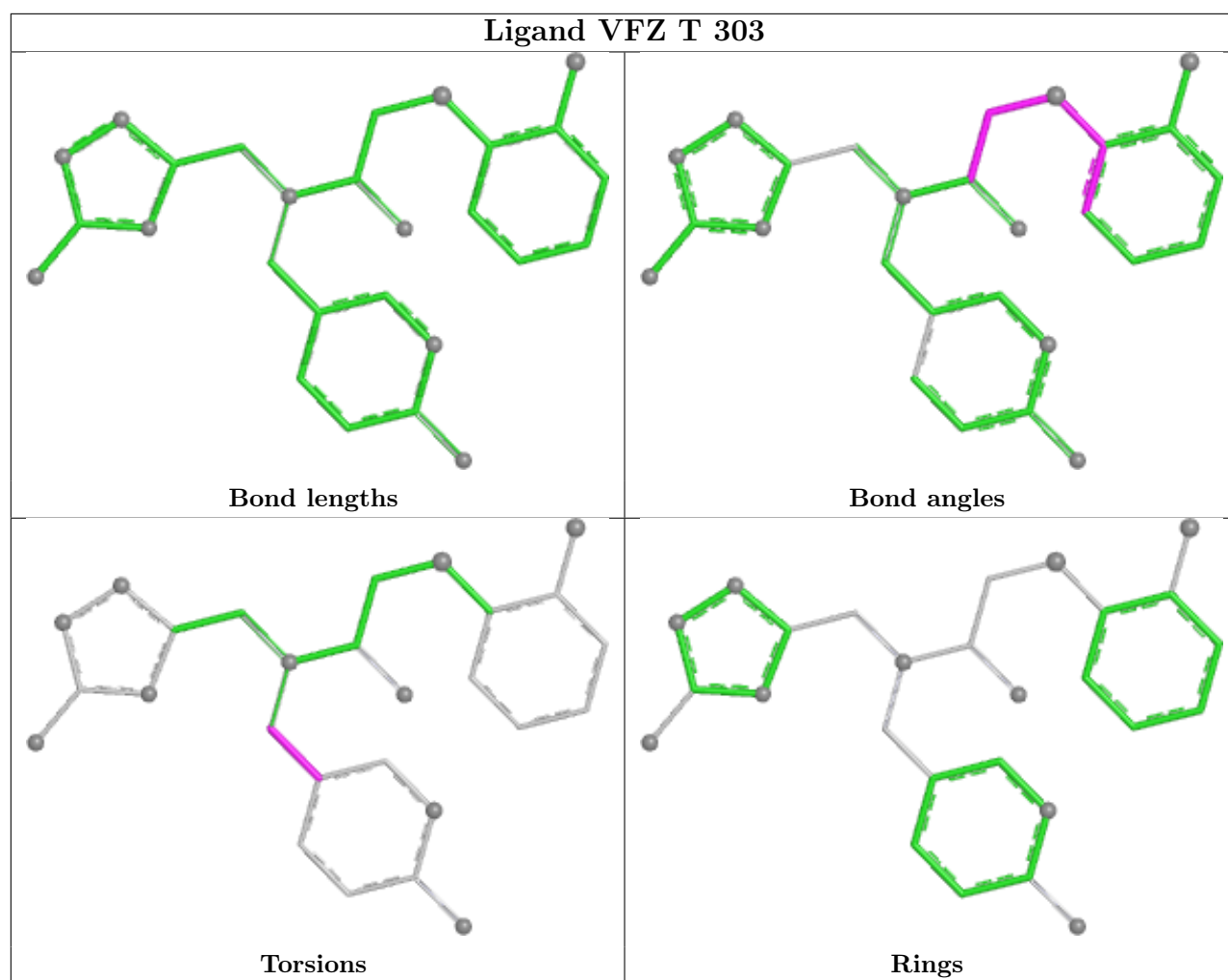
Bond lengths

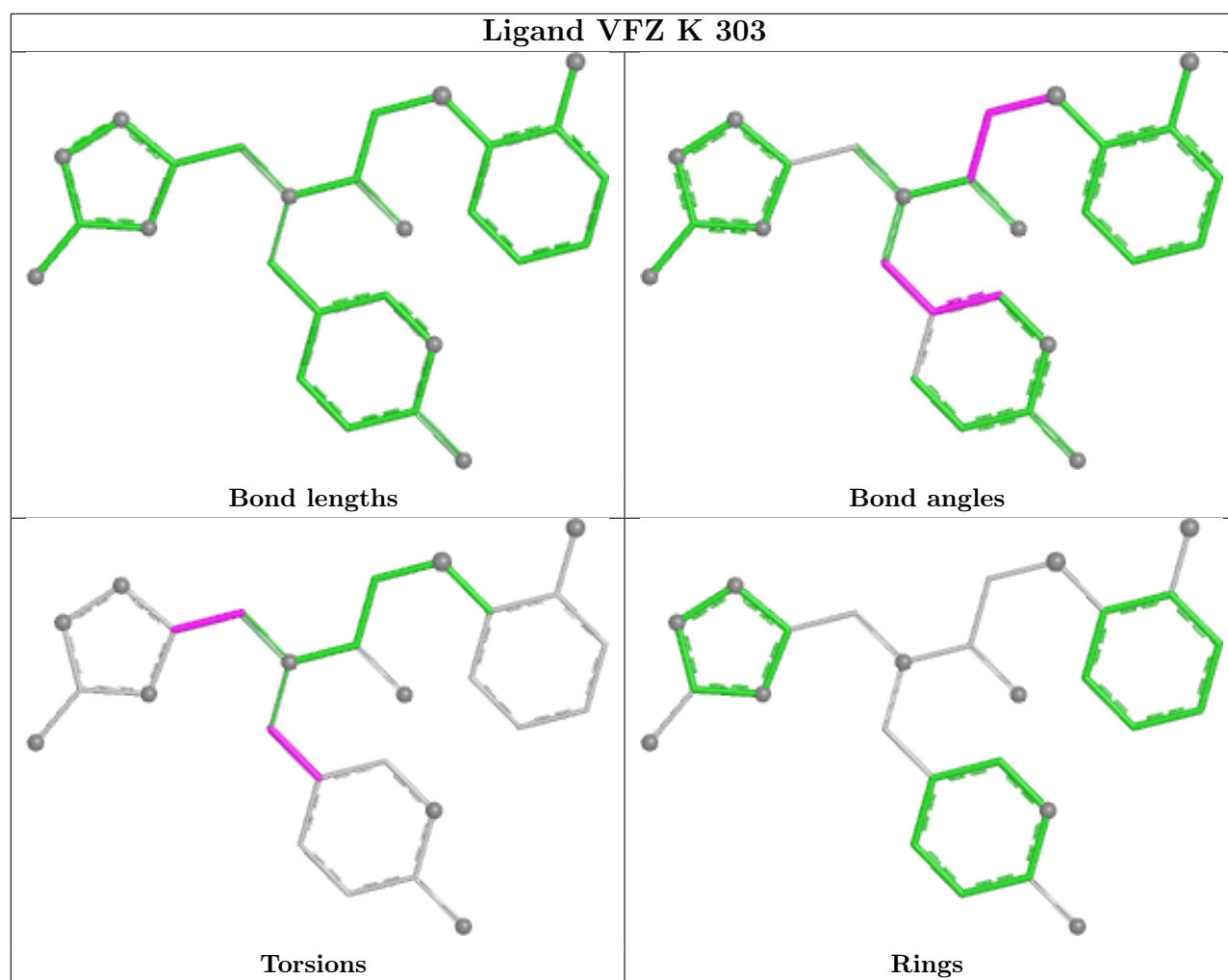
Bond angles

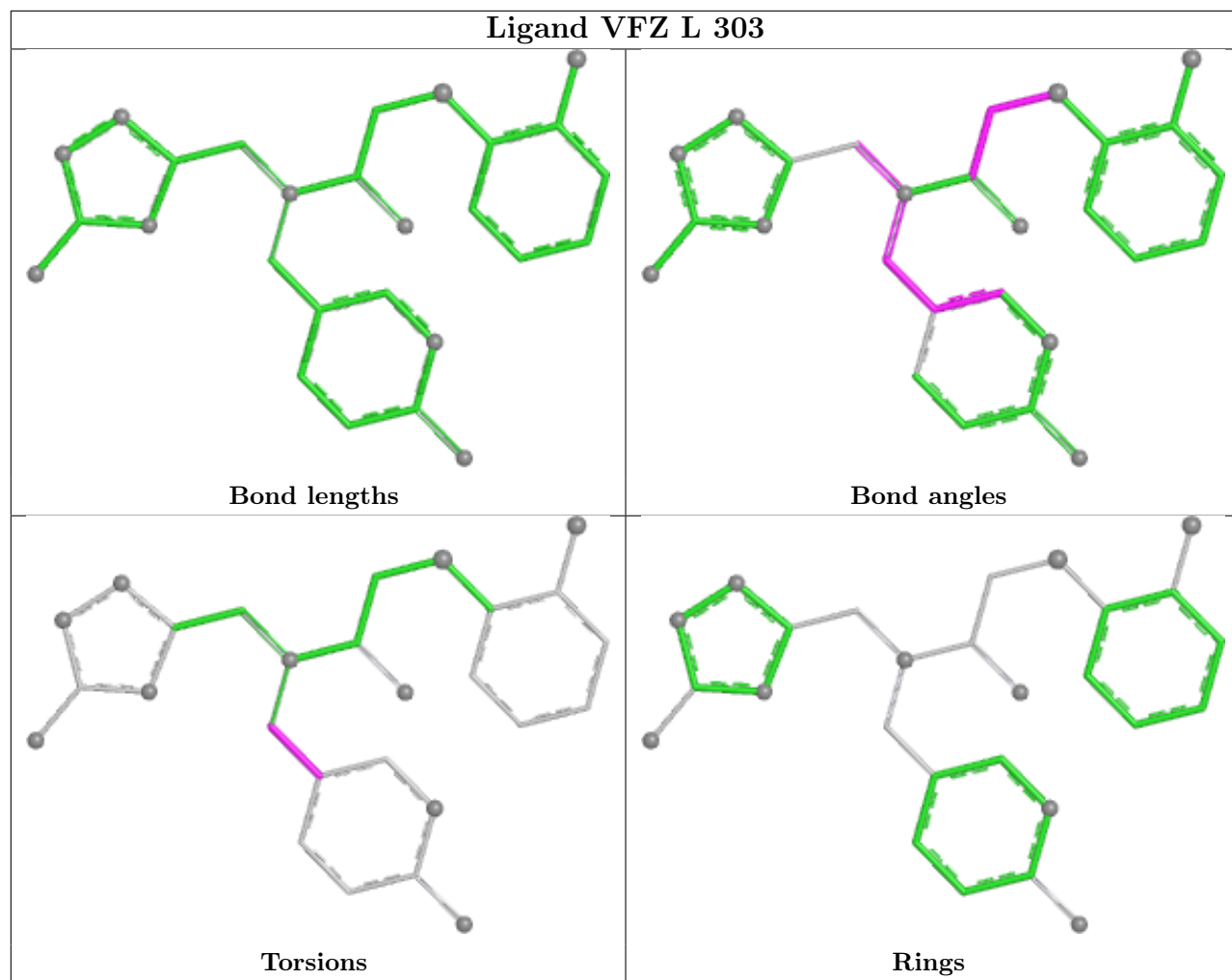
Torsions

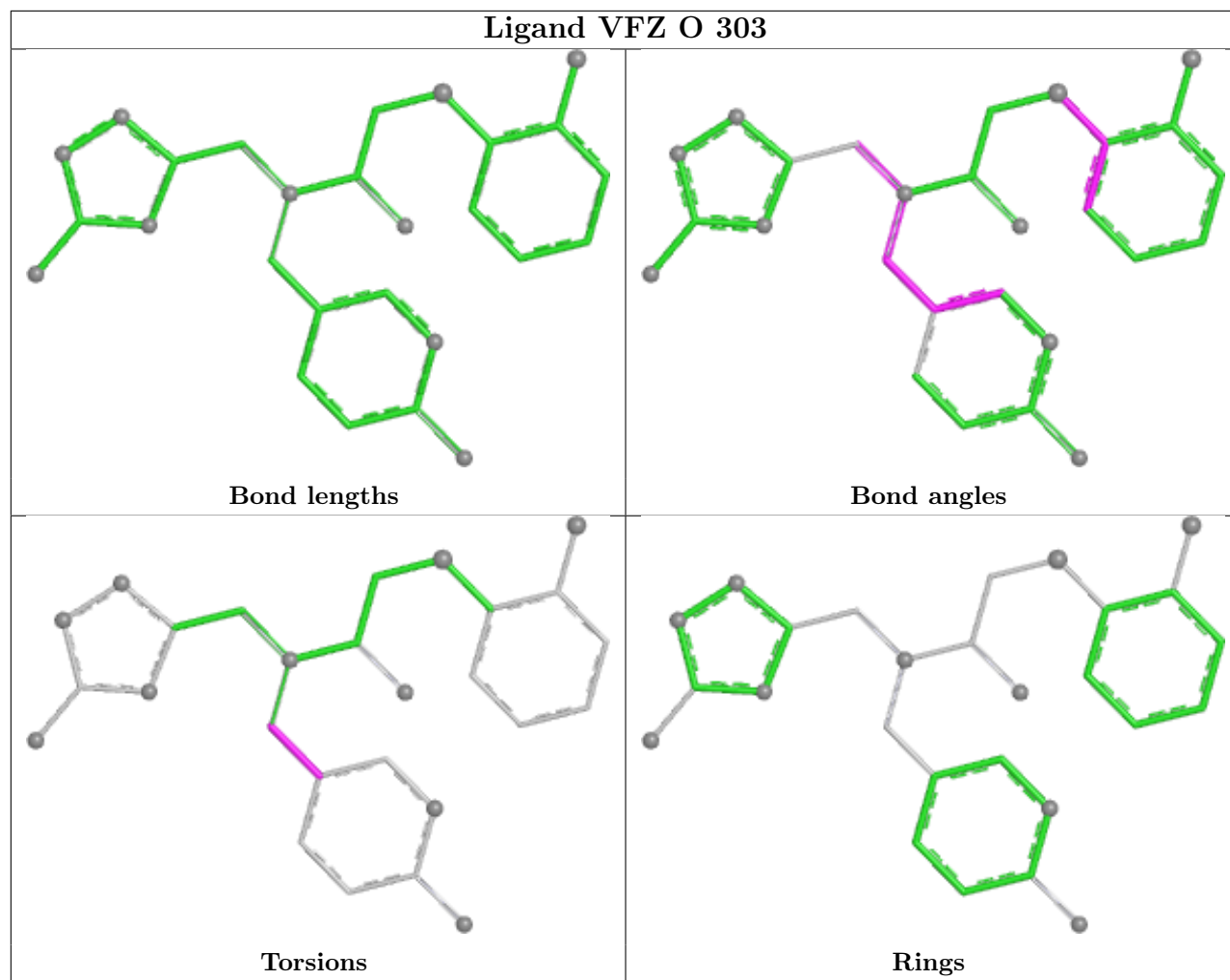
Rings

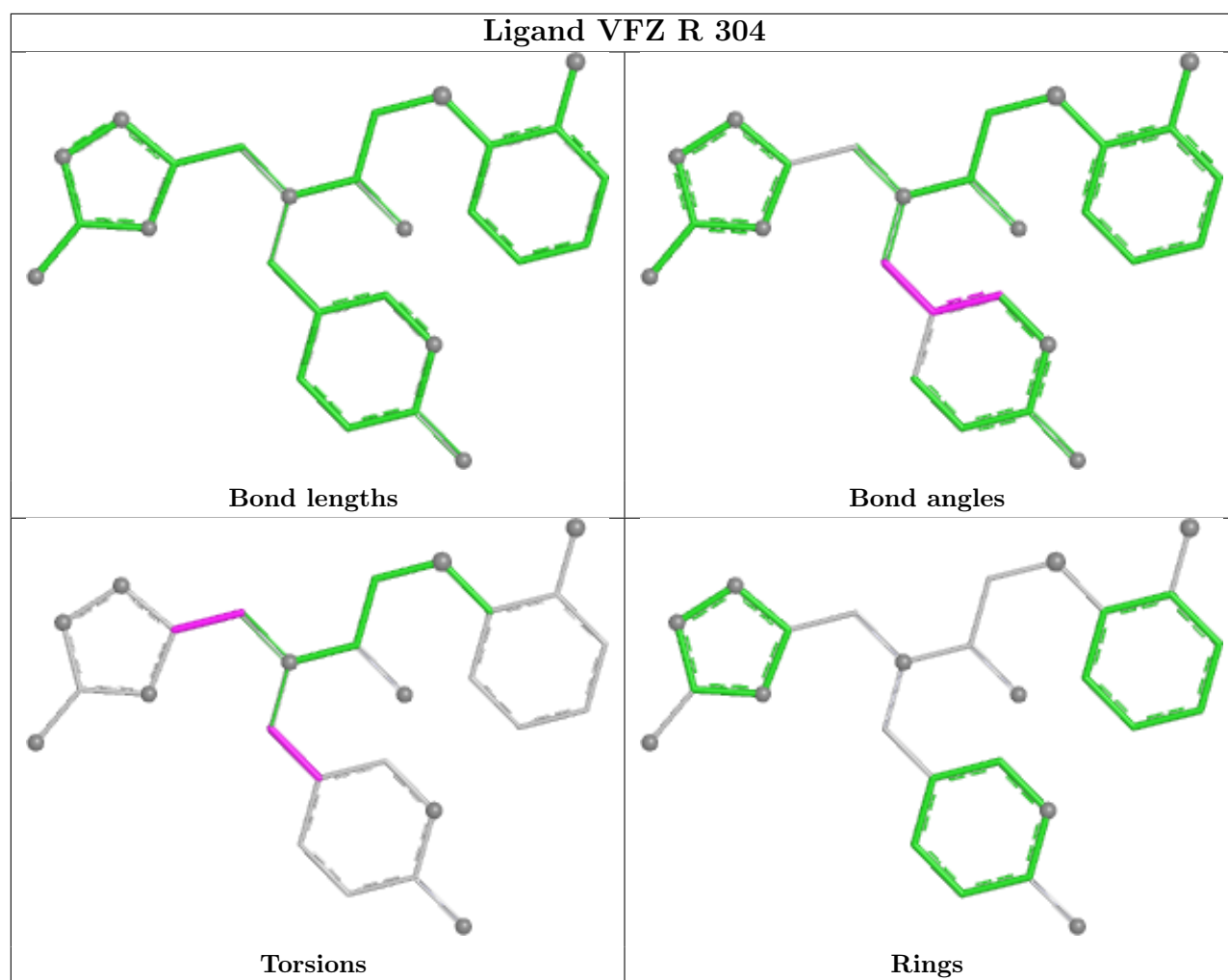












5.7 Other polymers i

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

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

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

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	258/261 (98%)	-0.43	2 (0%) 82 58	75, 92, 121, 168	0
1	B	258/261 (98%)	-0.48	1 (0%) 88 70	74, 93, 120, 154	0
1	C	258/261 (98%)	-0.46	1 (0%) 88 70	54, 91, 120, 188	1 (0%)
1	D	258/261 (98%)	-0.47	1 (0%) 88 70	69, 91, 121, 175	0
1	E	258/261 (98%)	-0.46	1 (0%) 88 70	74, 92, 122, 171	0
1	F	258/261 (98%)	-0.45	1 (0%) 88 70	70, 92, 124, 162	0
1	G	257/261 (98%)	-0.39	1 (0%) 88 70	76, 105, 131, 145	0
1	H	257/261 (98%)	-0.45	0 100 100	79, 105, 132, 149	0
1	I	257/261 (98%)	-0.47	1 (0%) 88 70	74, 104, 134, 151	0
1	J	258/261 (98%)	-0.46	1 (0%) 88 70	70, 92, 120, 143	0
1	K	258/261 (98%)	-0.40	2 (0%) 82 58	72, 94, 124, 188	0
1	L	258/261 (98%)	-0.43	2 (0%) 82 58	75, 93, 120, 151	0
1	M	257/261 (98%)	-0.40	1 (0%) 88 70	79, 106, 132, 148	0
1	N	257/261 (98%)	-0.46	0 100 100	74, 103, 131, 158	0
1	O	257/261 (98%)	-0.39	1 (0%) 88 70	81, 105, 134, 146	0
1	P	257/261 (98%)	-0.44	1 (0%) 88 70	73, 105, 132, 150	0
1	Q	257/261 (98%)	-0.43	0 100 100	78, 106, 131, 154	0
1	R	257/261 (98%)	-0.45	1 (0%) 88 70	77, 104, 130, 152	0
1	S	258/261 (98%)	-0.40	1 (0%) 88 70	74, 94, 123, 168	0
1	T	258/261 (98%)	-0.45	3 (1%) 76 49	76, 94, 123, 155	0
1	U	258/261 (98%)	-0.41	2 (0%) 82 58	78, 95, 123, 188	0
1	V	257/261 (98%)	-0.42	0 100 100	79, 105, 131, 157	0
1	W	257/261 (98%)	-0.46	1 (0%) 88 70	77, 104, 132, 148	0
1	X	257/261 (98%)	-0.49	0 100 100	72, 102, 132, 151	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	Y	258/261 (98%)	-0.47	0 100 100	75, 102, 129, 159	0
1	Z	258/261 (98%)	-0.44	2 (0%) 82 58	75, 102, 128, 158	0
1	a	257/261 (98%)	-0.49	0 100 100	72, 101, 130, 156	0
1	b	257/261 (98%)	-0.45	0 100 100	78, 101, 129, 146	0
1	c	258/261 (98%)	-0.45	0 100 100	76, 102, 132, 182	0
1	d	257/261 (98%)	-0.48	0 100 100	77, 103, 129, 147	0
All	All	7725/7830 (98%)	-0.44	27 (0%) 90 74	54, 99, 129, 188	1 (0%)

The worst 5 of 27 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	S	1	MET	4.3
1	K	253	THR	3.4
1	L	1	MET	3.1
1	I	253	THR	3.0
1	C	157[A]	GLN	2.9

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	CL	E	301	1/1	0.74	0.15	137,137,137,137	0
3	SO4	U	303	5/5	0.74	0.09	172,183,194,211	0
2	CL	G	301	1/1	0.77	0.08	131,131,131,131	0
3	SO4	N	303	5/5	0.81	0.20	103,122,138,153	5

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	CL	C	301	1/1	0.81	0.10	123,123,123,123	0
3	SO4	H	302	5/5	0.82	0.24	114,128,146,169	5
2	CL	L	301	1/1	0.82	0.08	127,127,127,127	0
3	SO4	N	304	5/5	0.82	0.09	123,126,139,150	0
3	SO4	A	309	5/5	0.82	0.23	129,133,146,155	5
2	CL	A	302	1/1	0.83	0.14	131,131,131,131	0
3	SO4	P	302	5/5	0.83	0.07	182,183,200,217	0
2	CL	M	302	1/1	0.83	0.08	118,118,118,118	0
3	SO4	R	303	5/5	0.84	0.27	114,116,135,148	5
2	CL	A	301	1/1	0.84	0.09	112,112,112,112	0
3	SO4	U	302	5/5	0.85	0.14	71,74,104,112	5
3	SO4	B	304	5/5	0.85	0.21	114,123,137,145	5
2	CL	O	301	1/1	0.86	0.07	113,113,113,113	0
3	SO4	K	302	5/5	0.86	0.17	109,124,142,151	5
2	CL	D	301	1/1	0.87	0.07	117,117,117,117	0
3	SO4	C	305	5/5	0.87	0.20	124,128,134,139	5
3	SO4	D	304	5/5	0.88	0.19	117,129,137,140	5
3	SO4	A	308	5/5	0.88	0.13	118,129,152,177	0
2	CL	I	301	1/1	0.88	0.06	115,115,115,115	0
3	SO4	a	301	5/5	0.88	0.20	127,151,163,172	0
3	SO4	c	302	5/5	0.88	0.10	103,109,133,166	0
3	SO4	P	303	5/5	0.89	0.18	122,130,145,147	5
3	SO4	A	307	5/5	0.89	0.13	102,113,129,130	5
2	CL	C	303	1/1	0.89	0.17	108,108,108,108	0
3	SO4	J	302	5/5	0.89	0.16	82,98,110,118	5
3	SO4	Y	302	5/5	0.89	0.09	104,117,140,171	0
3	SO4	C	304	5/5	0.89	0.15	149,160,181,192	0
3	SO4	I	303	5/5	0.89	0.28	101,124,131,134	5
2	CL	T	301	1/1	0.90	0.07	111,111,111,111	0
3	SO4	I	302	5/5	0.90	0.24	155,157,171,182	0
2	CL	B	302	1/1	0.90	0.14	112,112,112,112	0
3	SO4	R	302	5/5	0.90	0.08	131,141,152,169	0
3	SO4	N	302	5/5	0.90	0.14	146,157,165,182	0
2	CL	Q	301	1/1	0.90	0.08	110,110,110,110	0
3	SO4	D	303	5/5	0.90	0.12	103,126,141,162	0
3	SO4	W	301	5/5	0.90	0.17	154,163,181,186	0
3	SO4	J	301	5/5	0.90	0.18	149,155,172,195	0
2	CL	S	301	1/1	0.90	0.07	113,113,113,113	0
3	SO4	K	301	5/5	0.90	0.16	145,156,168,173	0
3	SO4	F	302	5/5	0.91	0.20	103,122,127,132	5
3	SO4	V	302	5/5	0.91	0.09	126,127,136,163	0
2	CL	X	302	1/1	0.91	0.07	107,107,107,107	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	CL	B	301	1/1	0.91	0.06	110,110,110,110	0
3	SO4	T	302	5/5	0.91	0.16	142,164,169,171	0
2	CL	A	305	1/1	0.91	0.07	120,120,120,120	0
3	SO4	H	301	5/5	0.92	0.13	154,164,169,173	0
3	SO4	Q	302	5/5	0.92	0.14	154,165,177,178	0
3	SO4	D	302	5/5	0.92	0.14	141,151,171,176	0
3	SO4	F	301	5/5	0.92	0.12	159,160,182,182	0
3	SO4	X	303	5/5	0.92	0.14	129,168,181,184	0
3	SO4	S	302	5/5	0.92	0.14	162,170,183,183	0
3	SO4	B	303	5/5	0.92	0.16	130,152,167,175	0
3	SO4	U	301	5/5	0.92	0.13	159,160,171,172	0
2	CL	A	304	1/1	0.93	0.09	92,92,92,92	0
3	SO4	E	303	5/5	0.93	0.12	163,166,184,192	0
3	SO4	E	304	5/5	0.93	0.21	110,121,128,134	5
3	SO4	L	302	5/5	0.93	0.13	107,118,130,134	5
3	SO4	V	301	5/5	0.93	0.12	108,116,129,134	5
3	SO4	M	303	5/5	0.93	0.12	103,109,133,139	5
2	CL	X	301	1/1	0.93	0.05	110,110,110,110	0
2	CL	C	302	1/1	0.93	0.06	144,144,144,144	0
3	SO4	Y	301	5/5	0.93	0.16	150,162,167,184	0
3	SO4	G	302	5/5	0.93	0.07	108,126,141,151	0
3	SO4	Z	301	5/5	0.93	0.16	148,163,172,181	0
3	SO4	O	302	5/5	0.93	0.18	141,144,170,176	0
3	SO4	c	301	5/5	0.93	0.14	118,121,135,138	5
2	CL	A	303	1/1	0.93	0.06	129,129,129,129	0
3	SO4	d	301	5/5	0.93	0.14	157,172,174,176	0
3	SO4	b	301	5/5	0.94	0.12	139,162,171,176	0
3	SO4	P	301	5/5	0.94	0.11	106,114,129,130	5
3	SO4	G	303	5/5	0.94	0.11	97,99,111,117	5
3	SO4	R	301	5/5	0.94	0.10	139,148,165,175	0
2	CL	N	301	1/1	0.95	0.07	126,126,126,126	0
2	CL	A	306	1/1	0.95	0.07	110,110,110,110	0
4	VFZ	B	305	27/27	0.95	0.10	72,90,147,154	0
4	VFZ	F	303	27/27	0.95	0.10	75,94,158,170	0
4	VFZ	M	304	27/27	0.95	0.12	84,102,174,184	0
4	VFZ	T	303	27/27	0.95	0.11	78,97,159,172	0
4	VFZ	X	304	27/27	0.95	0.12	80,99,195,221	0
4	VFZ	d	302	27/27	0.95	0.12	67,92,179,181	0
4	VFZ	H	303	27/27	0.96	0.12	79,97,166,217	0
4	VFZ	I	304	27/27	0.96	0.11	77,103,159,176	0
4	VFZ	C	306	27/27	0.96	0.11	75,93,173,184	0
4	VFZ	N	305	27/27	0.96	0.11	77,106,163,172	0

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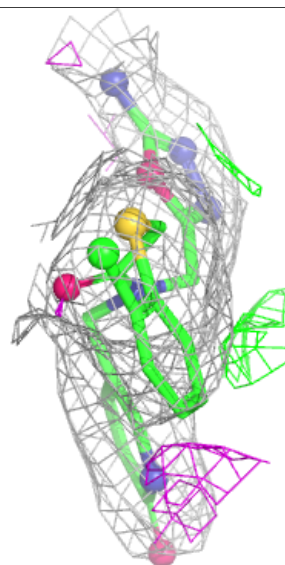
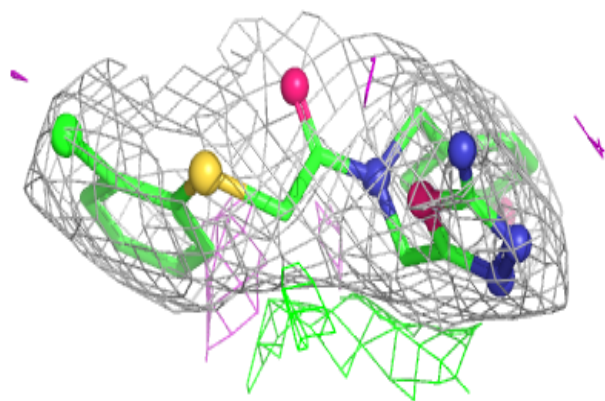
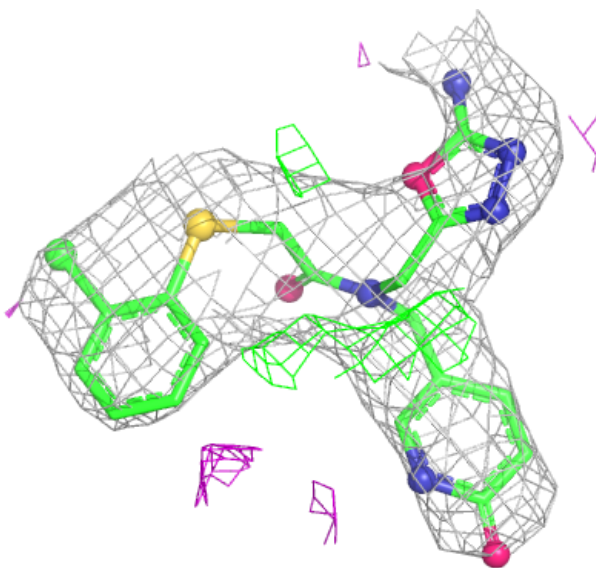
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	VFZ	K	303	27/27	0.96	0.11	78,96,158,176	0
4	VFZ	P	304	27/27	0.96	0.11	74,99,162,167	0
4	VFZ	Q	303	27/27	0.96	0.10	84,102,151,159	0
4	VFZ	R	304	27/27	0.96	0.11	83,103,178,243	0
4	VFZ	S	303	27/27	0.96	0.11	78,97,168,187	0
4	VFZ	E	305	27/27	0.96	0.09	66,90,147,150	0
4	VFZ	V	303	27/27	0.96	0.11	82,100,166,182	0
4	VFZ	W	302	27/27	0.96	0.10	76,94,182,200	0
2	CL	M	301	1/1	0.96	0.06	100,100,100,100	0
4	VFZ	Y	303	27/27	0.96	0.11	75,101,157,166	0
4	VFZ	Z	302	27/27	0.96	0.12	72,106,176,200	0
4	VFZ	a	302	27/27	0.96	0.10	77,101,174,197	0
4	VFZ	b	302	27/27	0.96	0.11	71,99,166,182	0
4	VFZ	c	303	27/27	0.96	0.10	72,99,168,189	0
4	VFZ	G	304	27/27	0.96	0.10	82,96,146,167	0
4	VFZ	D	305	27/27	0.97	0.10	64,85,161,161	0
4	VFZ	L	303	27/27	0.97	0.10	61,91,149,157	0
4	VFZ	U	304	27/27	0.97	0.10	69,91,148,155	0
2	CL	E	302	1/1	0.97	0.08	88,88,88,88	0
4	VFZ	O	303	27/27	0.97	0.11	78,100,166,177	0
4	VFZ	J	303	27/27	0.97	0.10	72,93,147,153	0
4	VFZ	A	310	27/27	0.98	0.09	76,88,149,155	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.

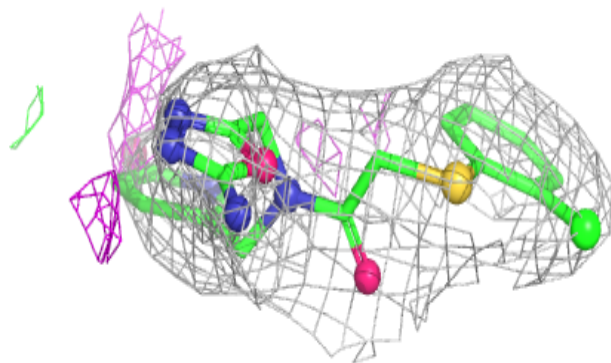
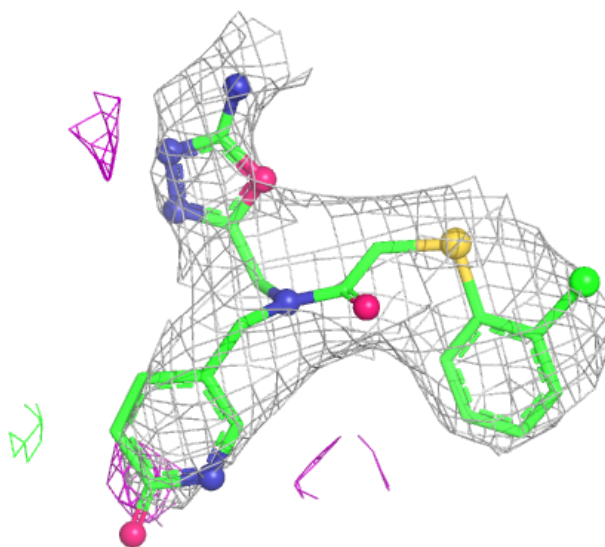
Electron density around VFZ B 305:

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



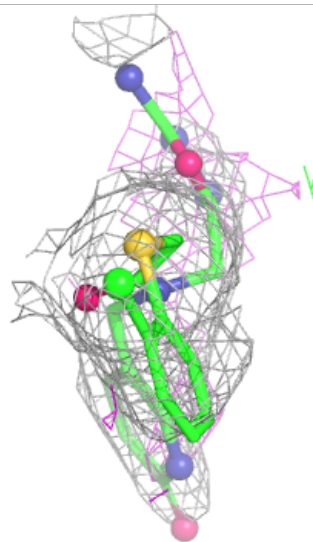
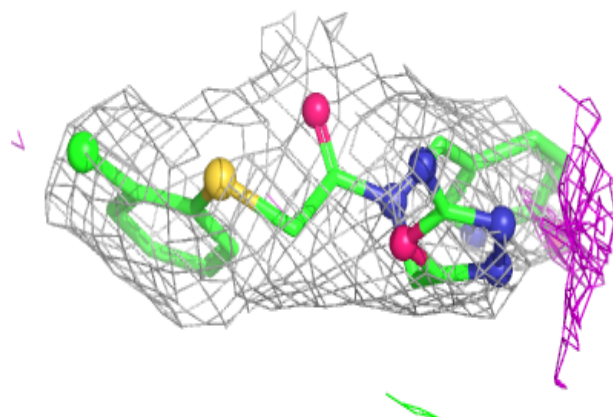
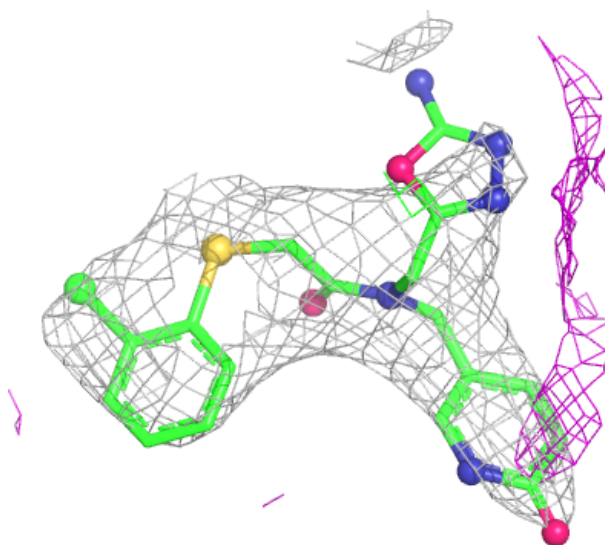
Electron density around VFZ F 303:

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and green (positive)



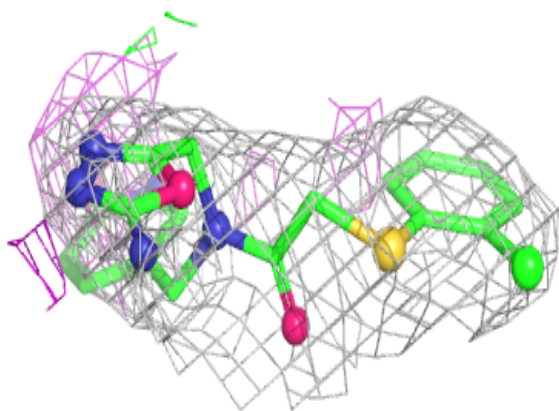
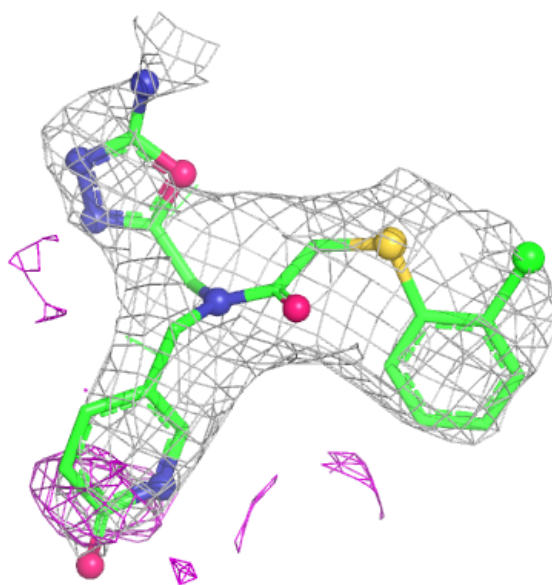
Electron density around VFZ M 304:

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and green (positive)



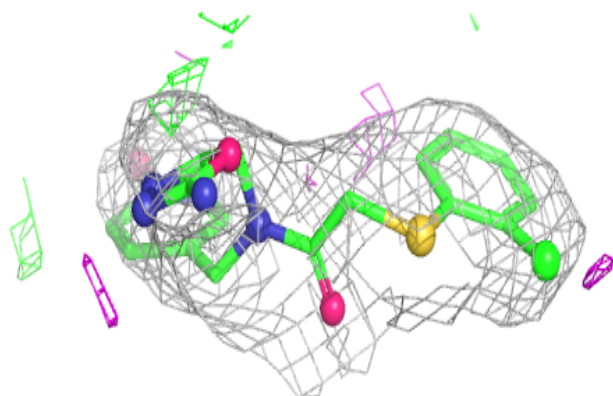
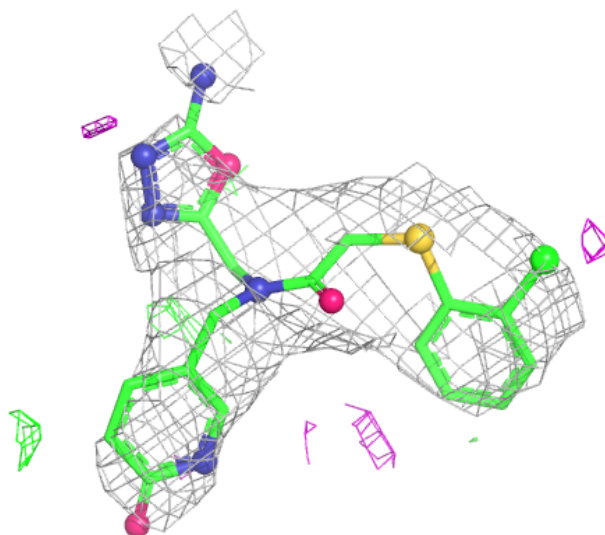
Electron density around VFZ T 303:

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and green (positive)



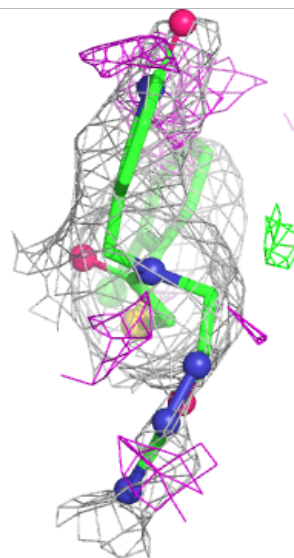
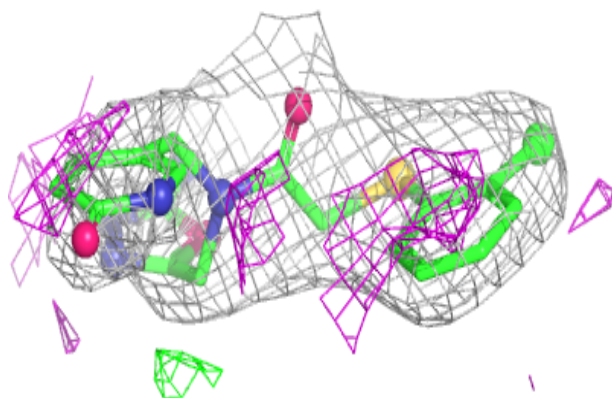
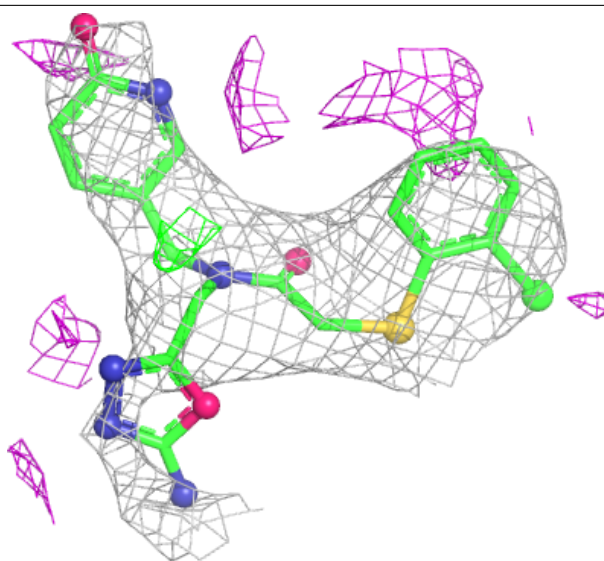
Electron density around VFZ X 304:

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and green (positive)



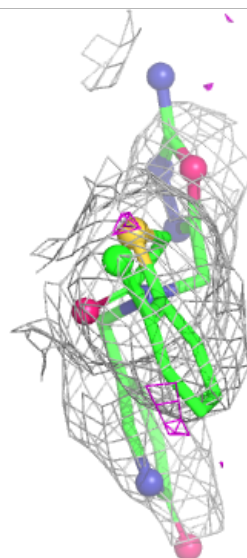
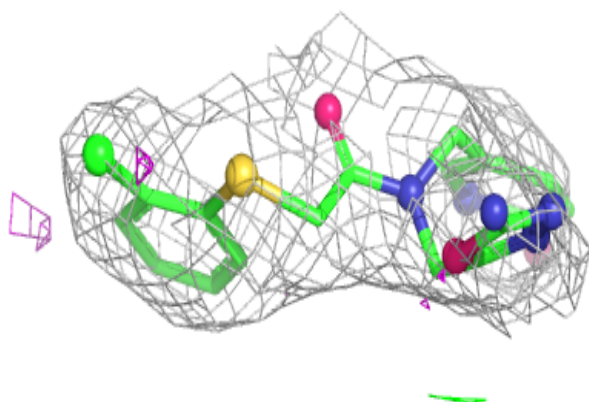
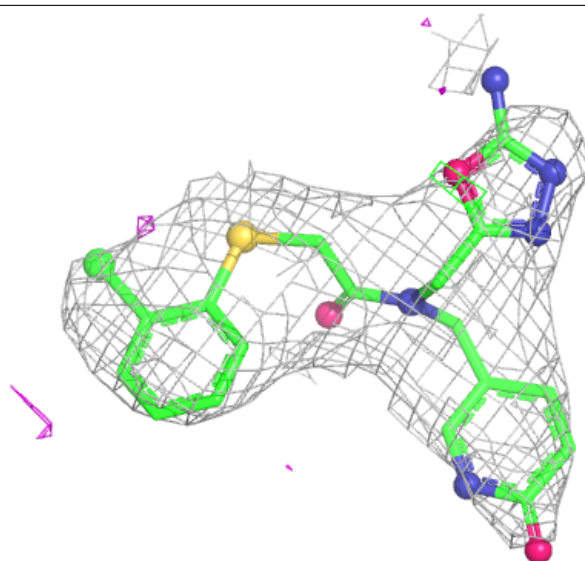
Electron density around VFZ d 302:

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and green (positive)



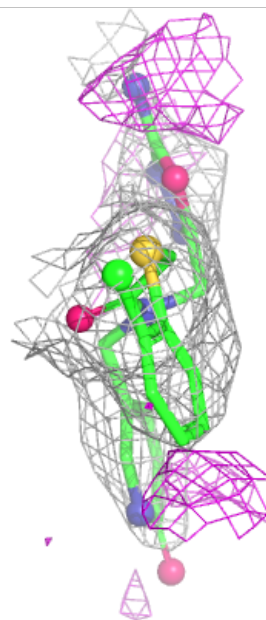
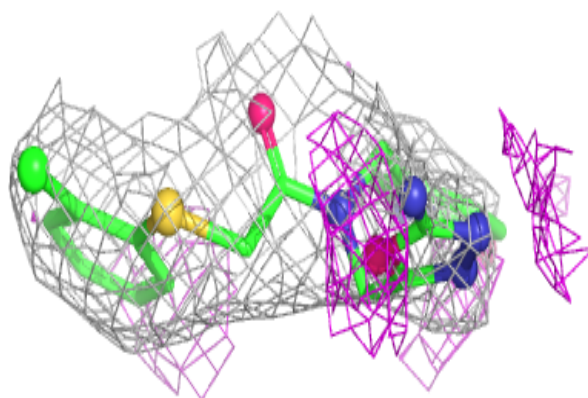
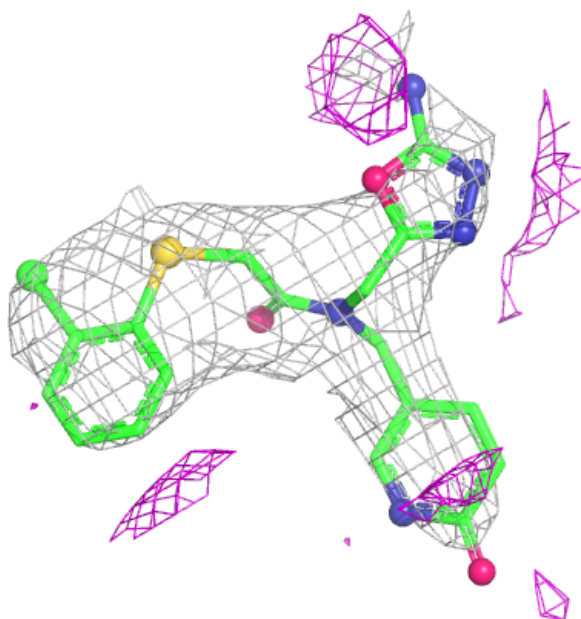
Electron density around VFZ H 303:

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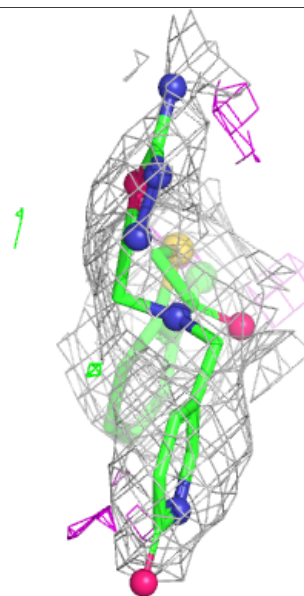
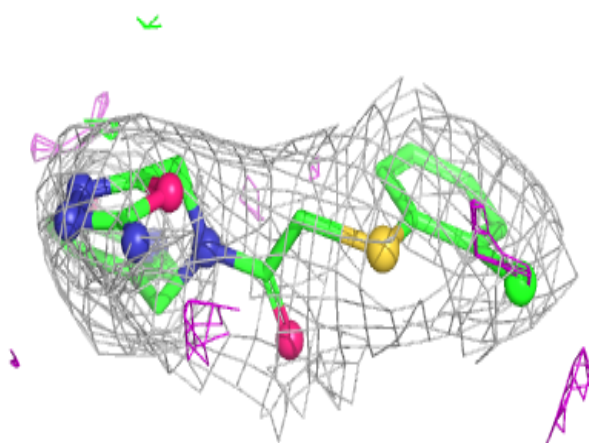
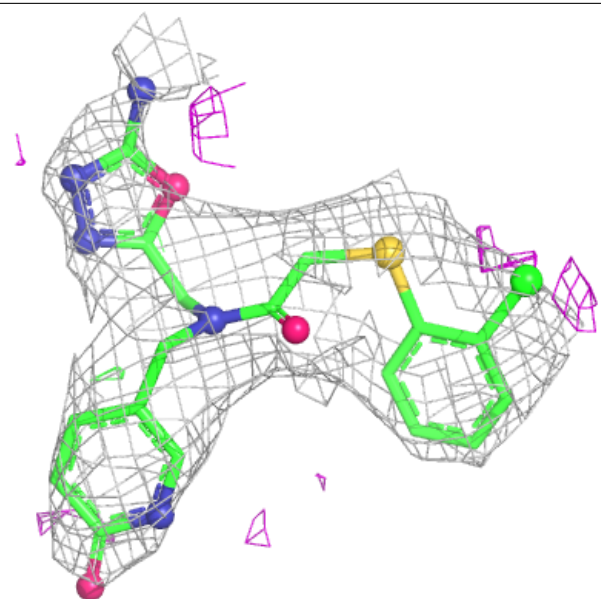
Electron density around VFZ I 304:

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and green (positive)



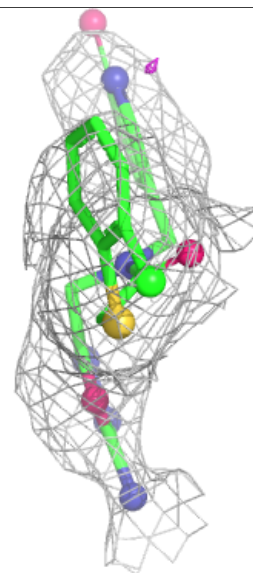
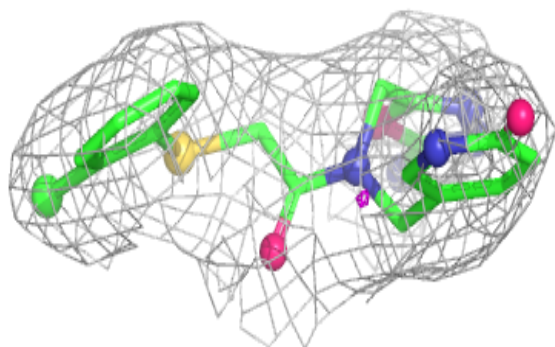
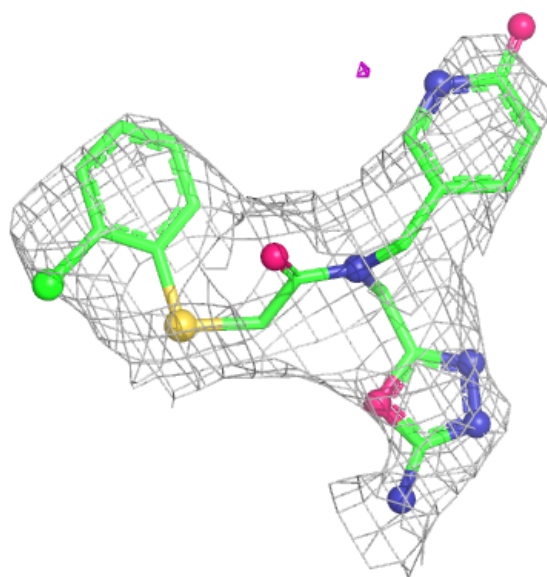
Electron density around VFZ C 306:

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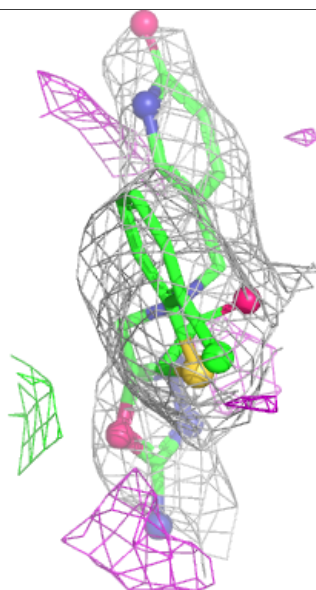
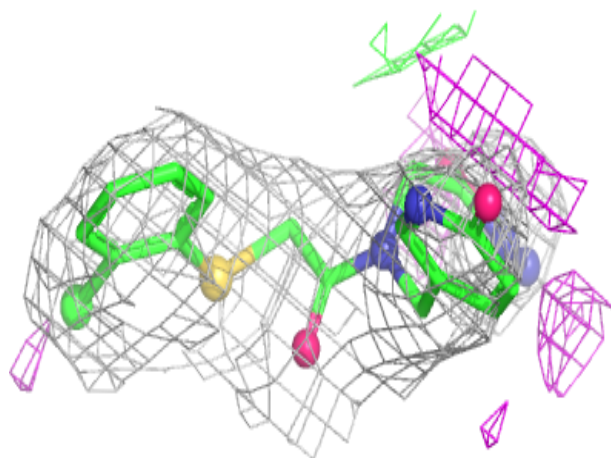
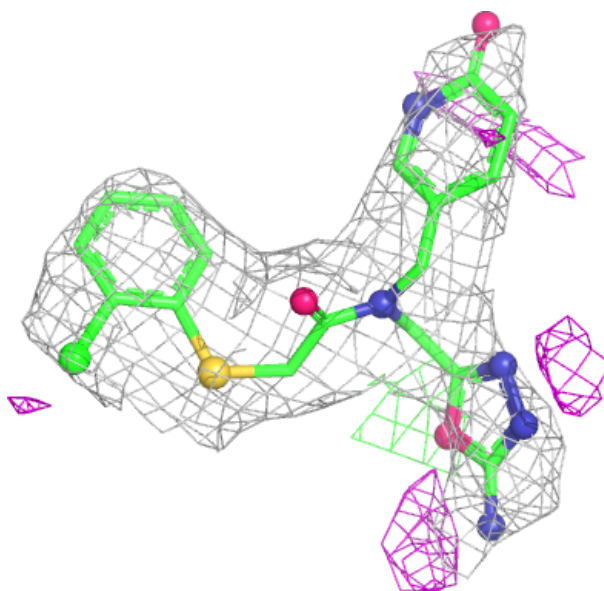
Electron density around VFZ N 305:

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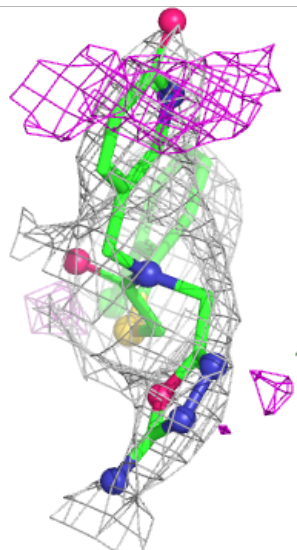
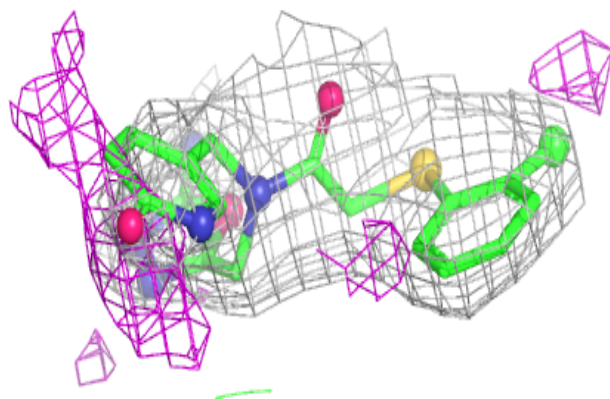
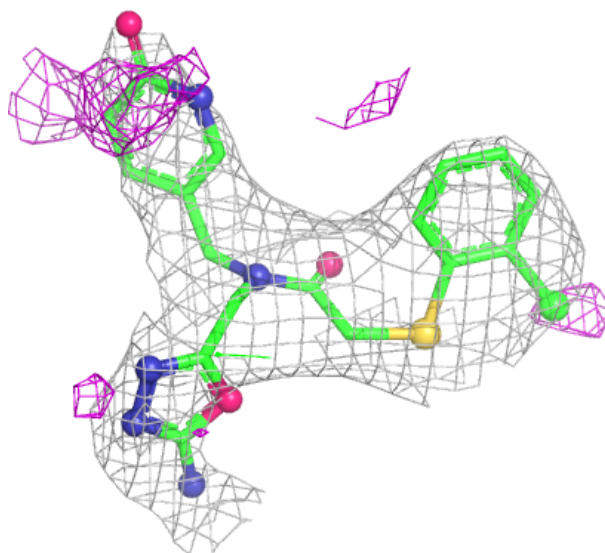
Electron density around VFZ K 303:

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and green (positive)



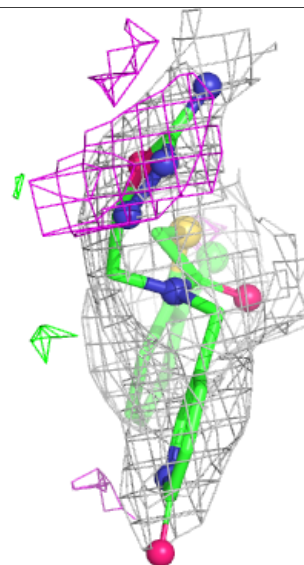
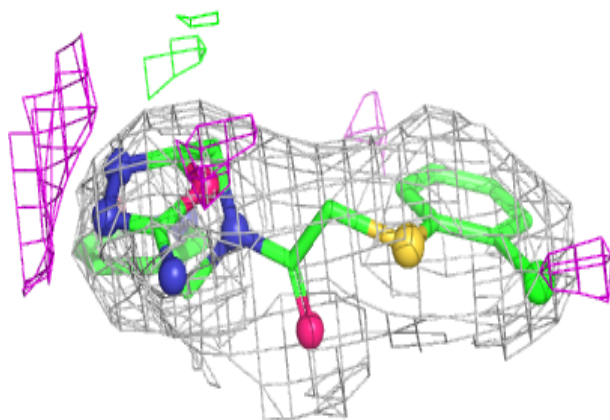
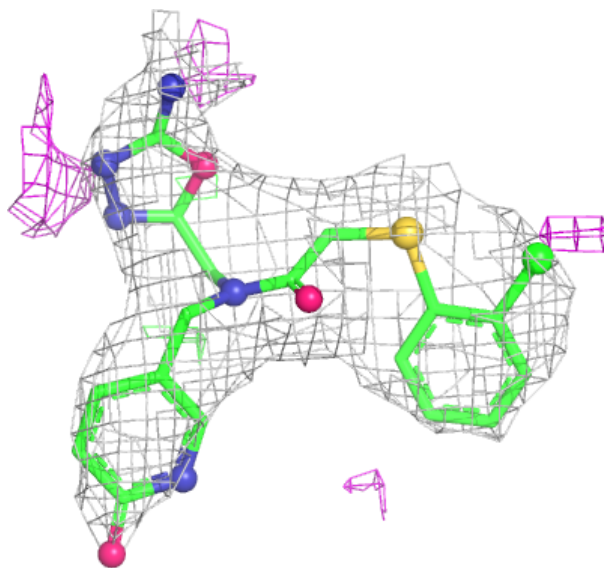
Electron density around VFZ P 304:

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and green (positive)



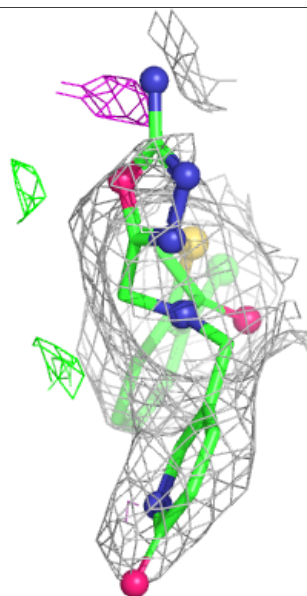
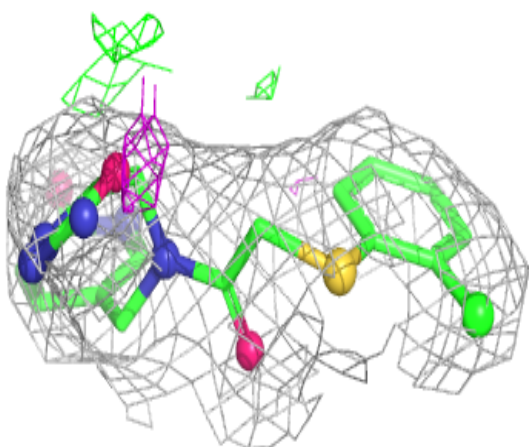
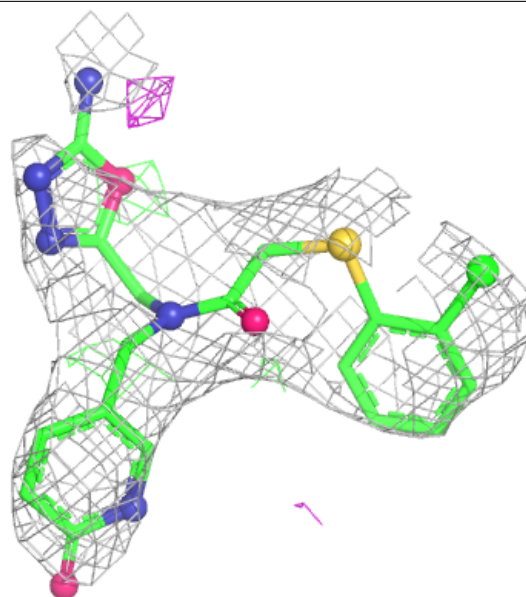
Electron density around VFZ Q 303:

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and green (positive)



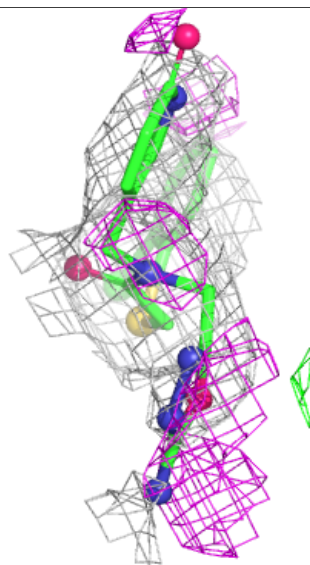
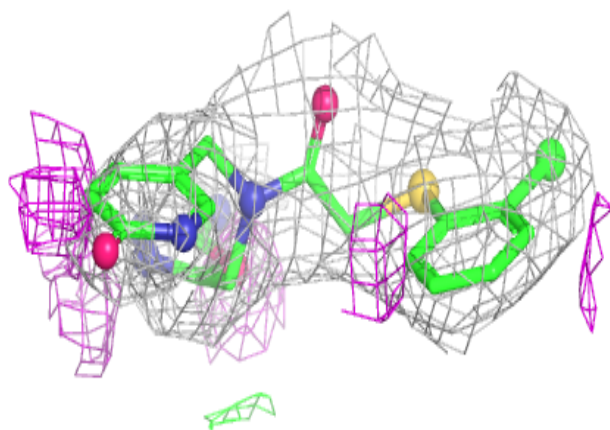
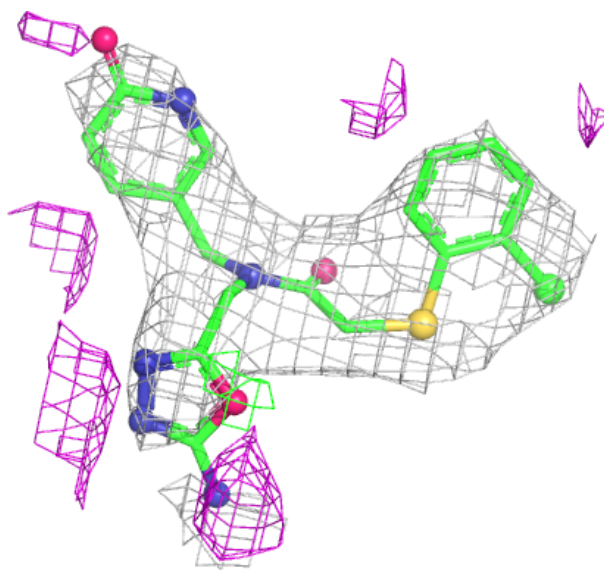
Electron density around VFZ R 304:

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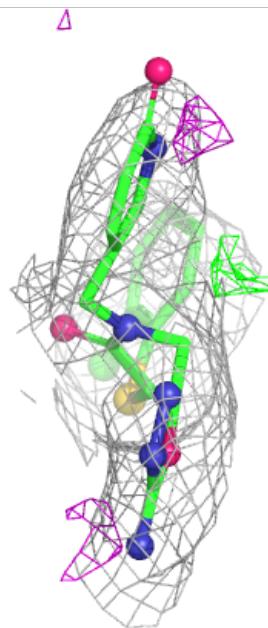
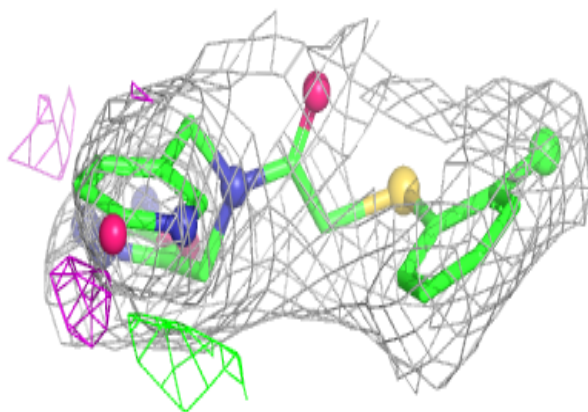
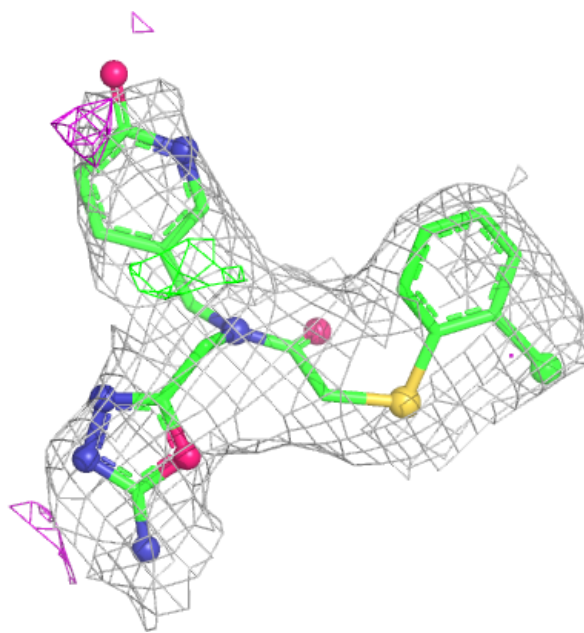
Electron density around VFZ S 303:

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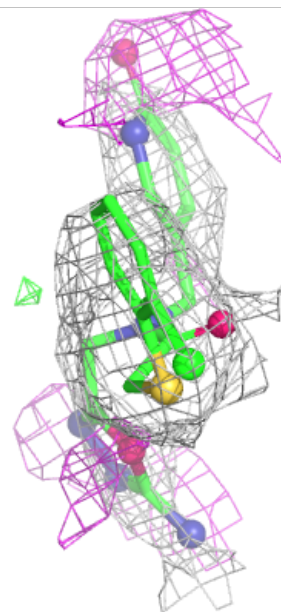
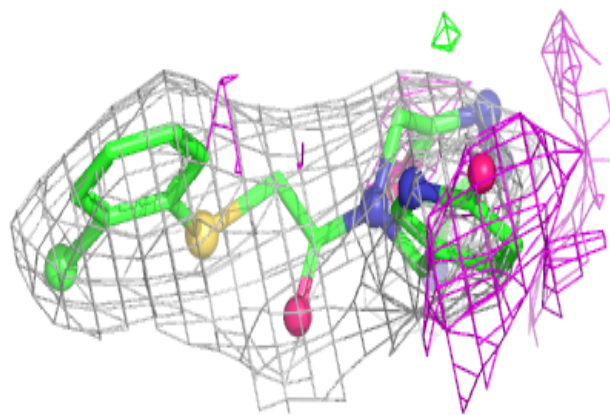
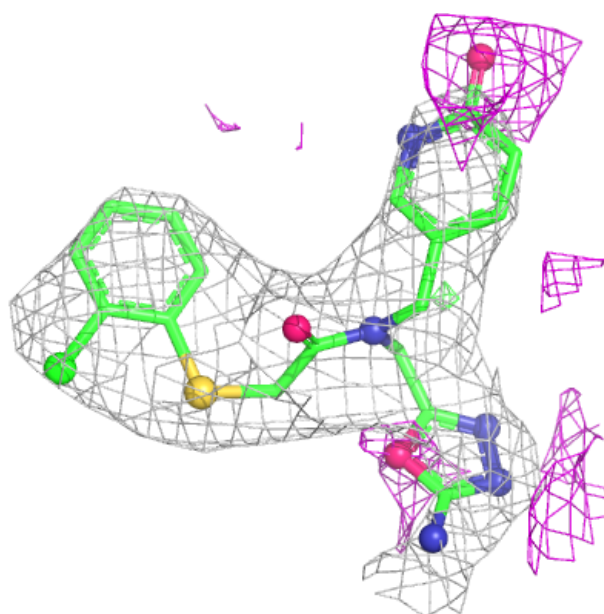
Electron density around VFZ E 305:

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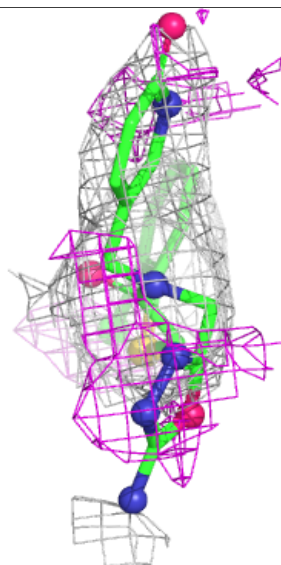
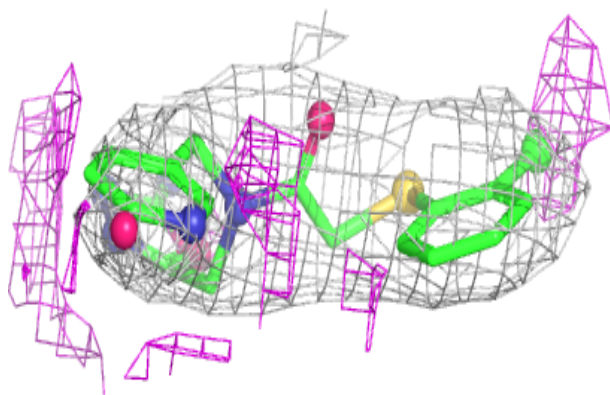
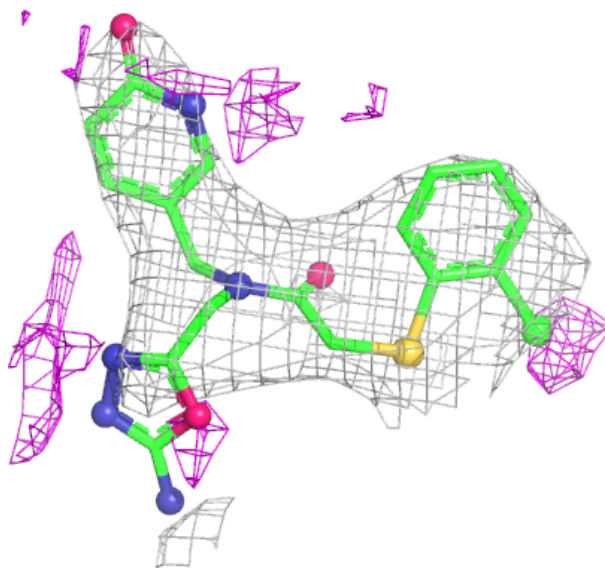
Electron density around VFZ V 303:

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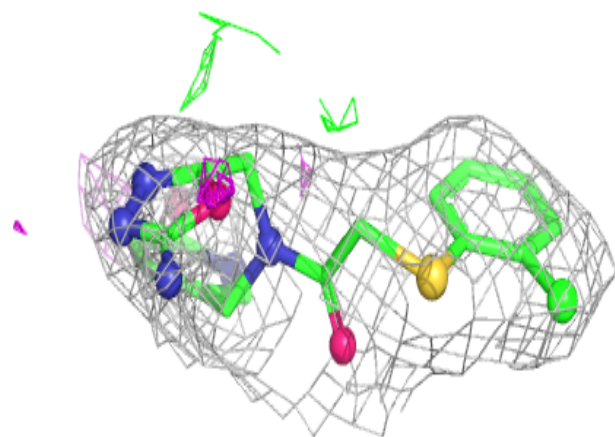
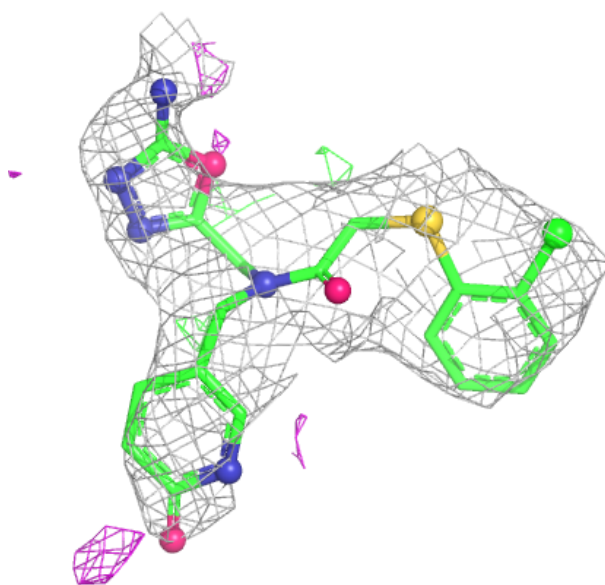
Electron density around VFZ W 302:

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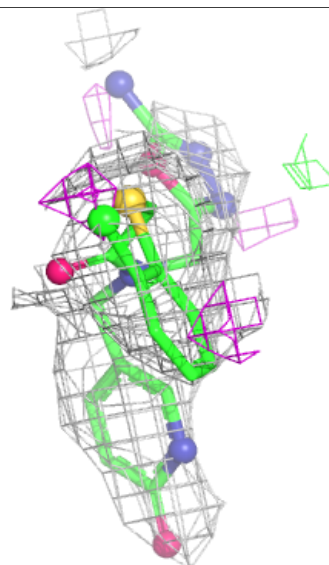
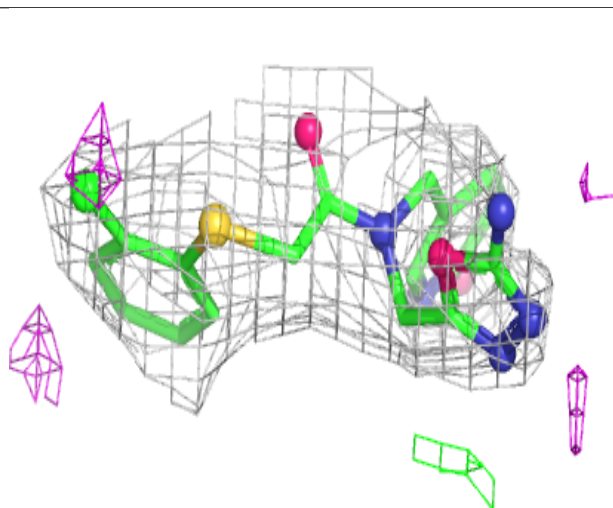
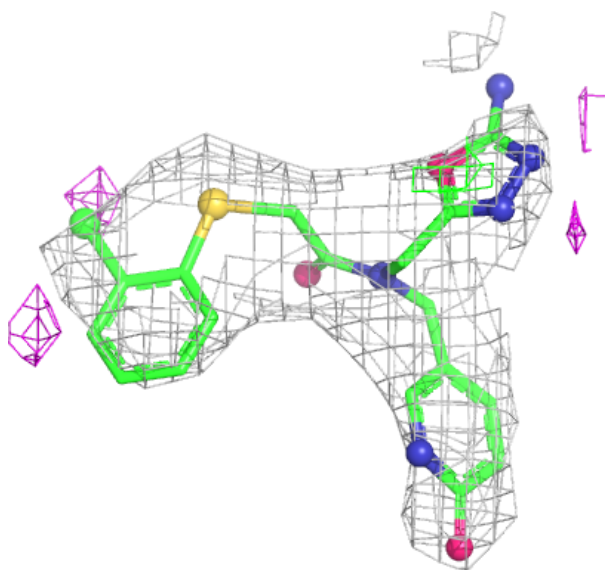
Electron density around VFZ Y 303:

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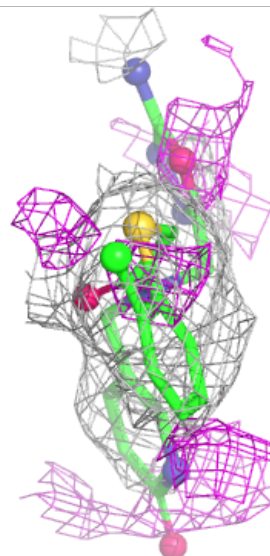
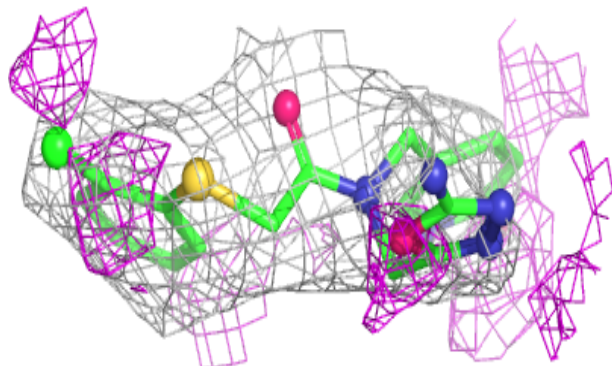
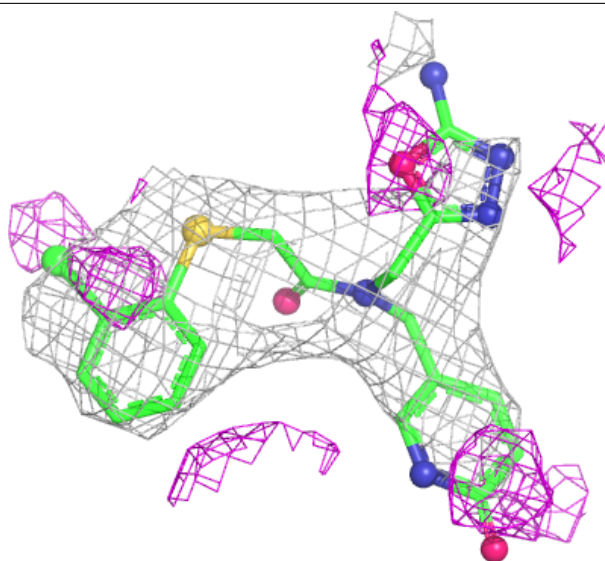
Electron density around VFZ Z 302:

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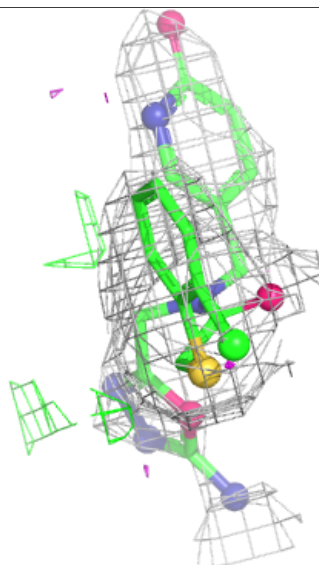
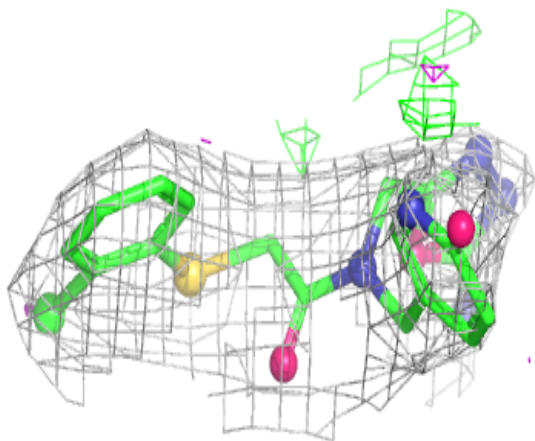
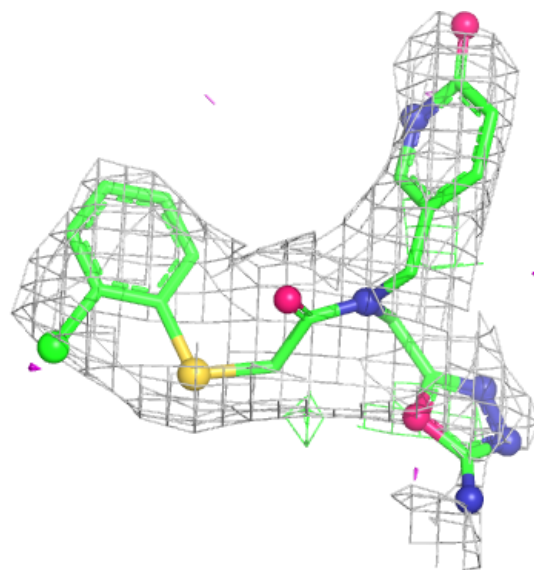
Electron density around VFZ a 302:

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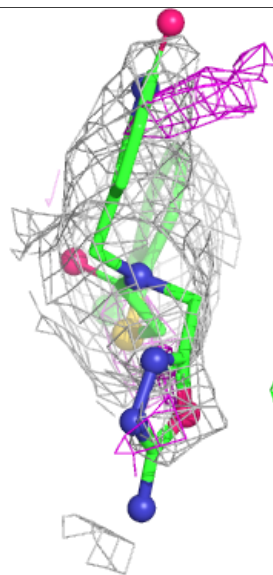
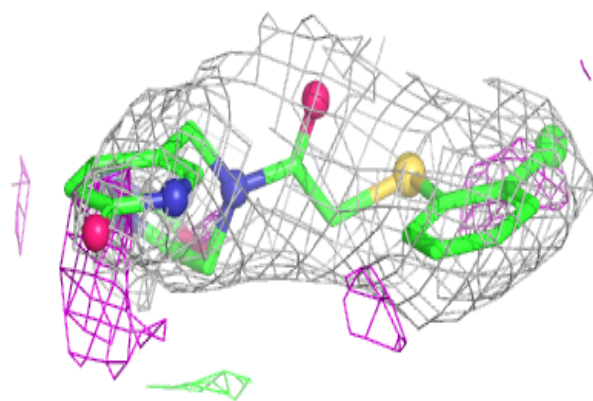
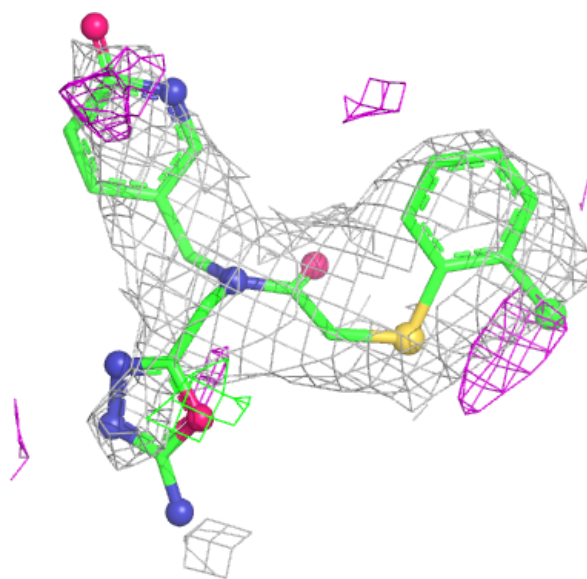
Electron density around VFZ b 302:

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



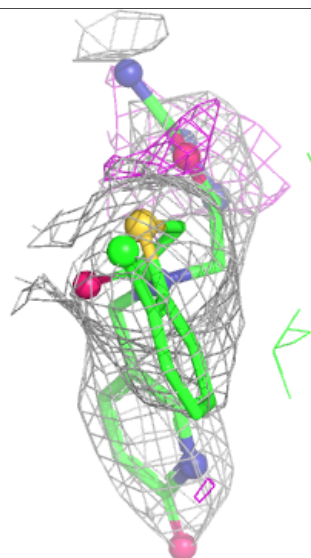
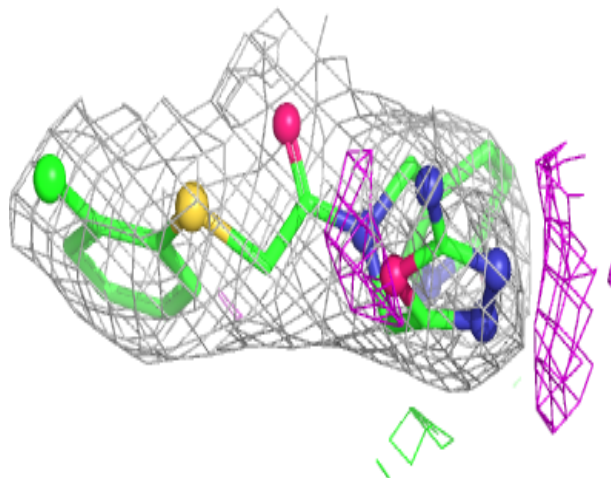
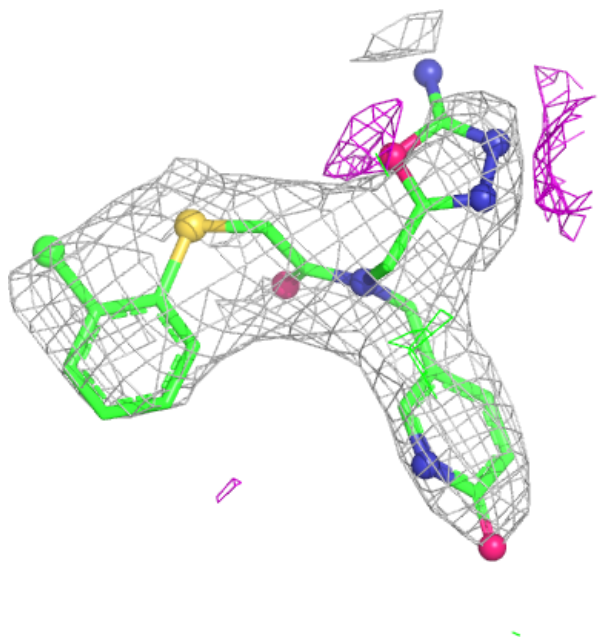
Electron density around VFZ c 303:

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



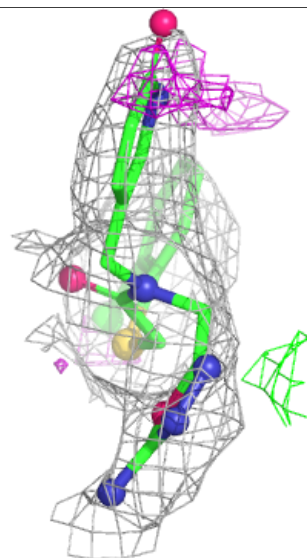
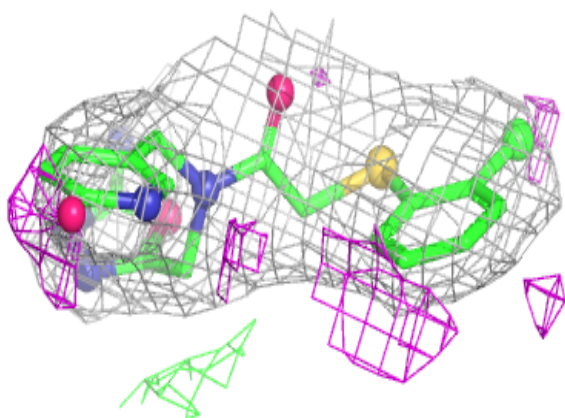
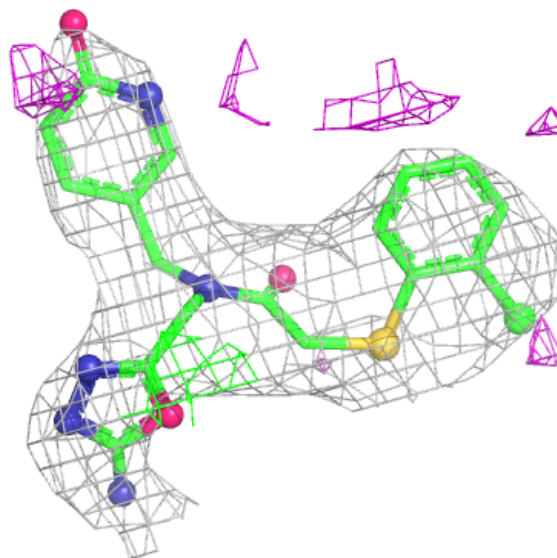
Electron density around VFZ G 304:

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



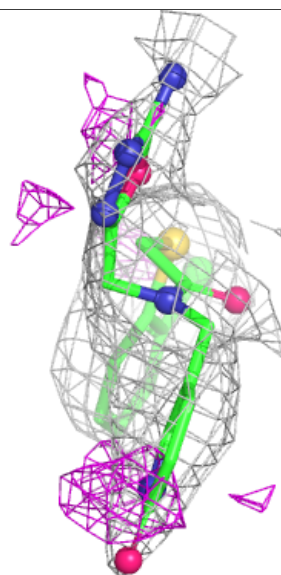
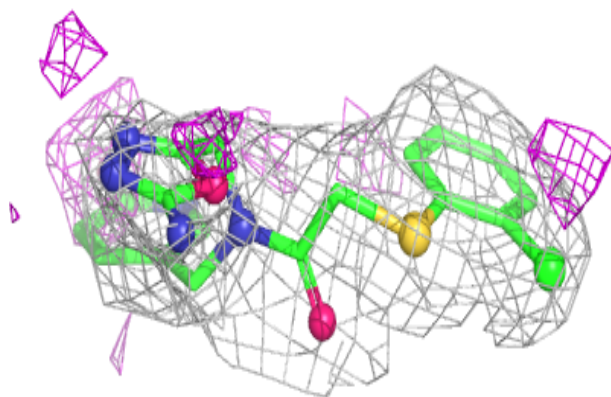
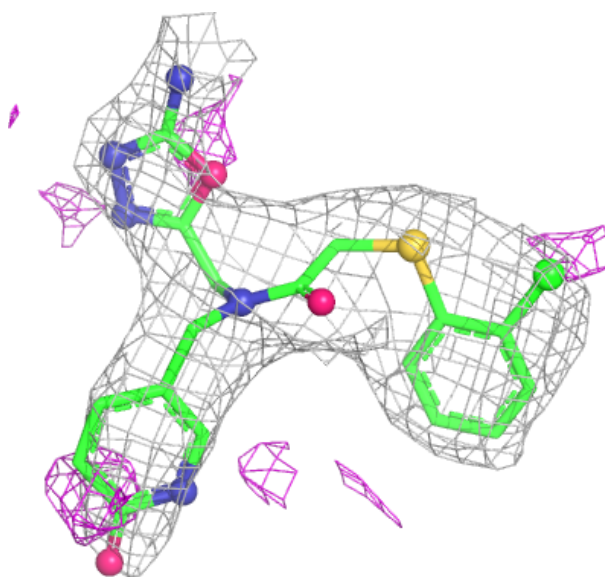
Electron density around VFZ D 305:

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



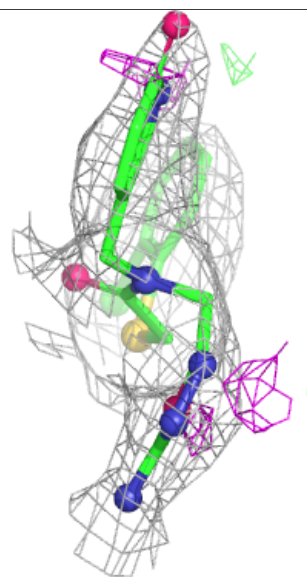
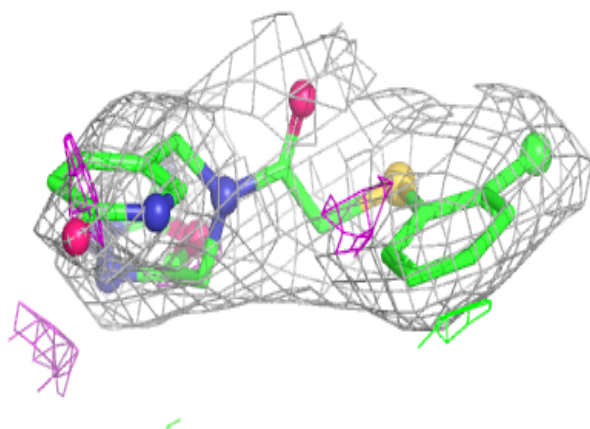
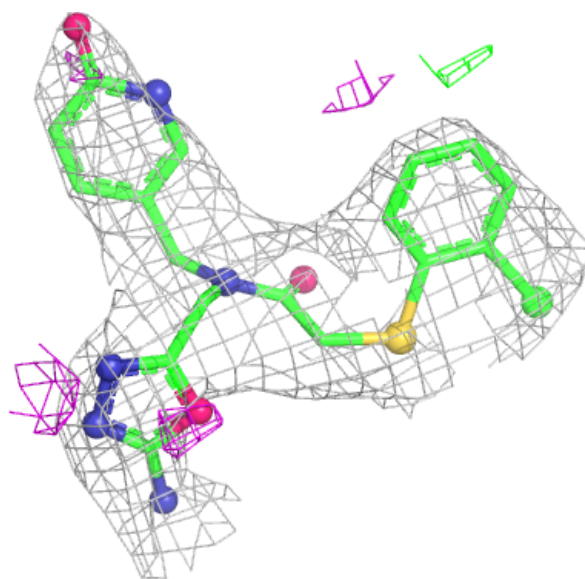
Electron density around VFZ L 303:

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



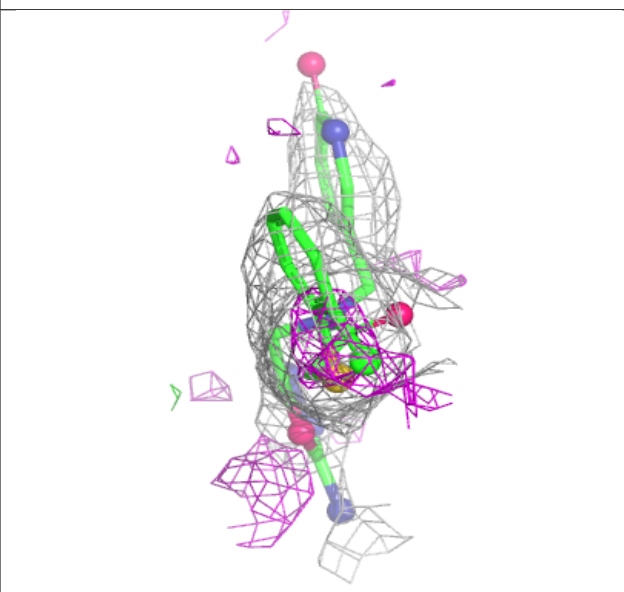
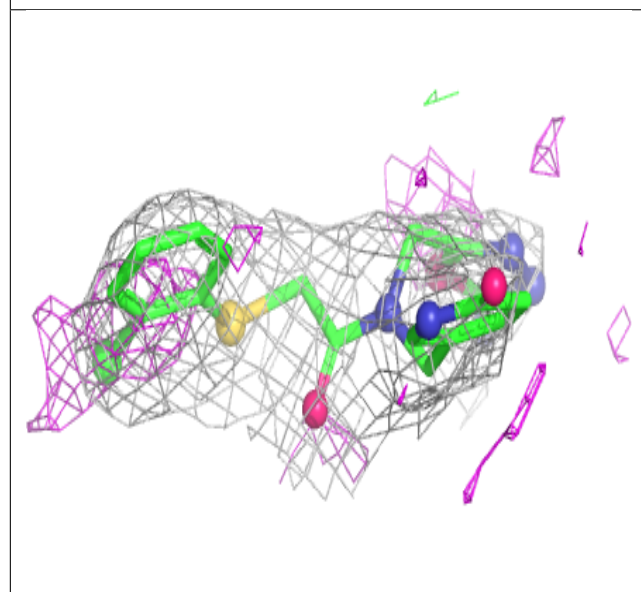
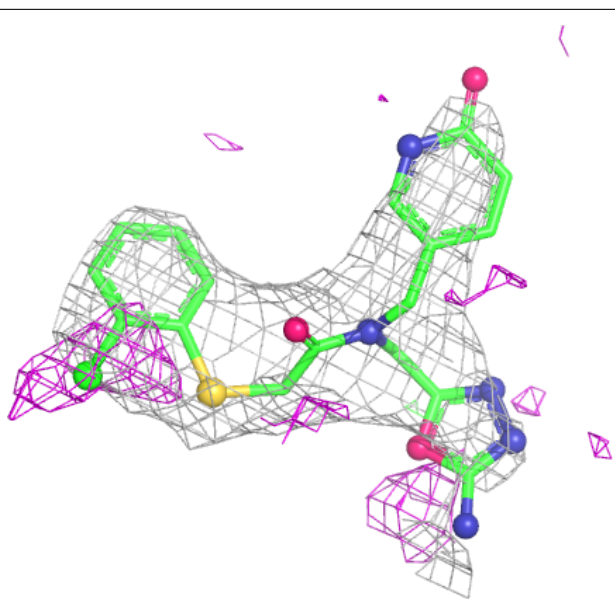
Electron density around VFZ U 304:

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



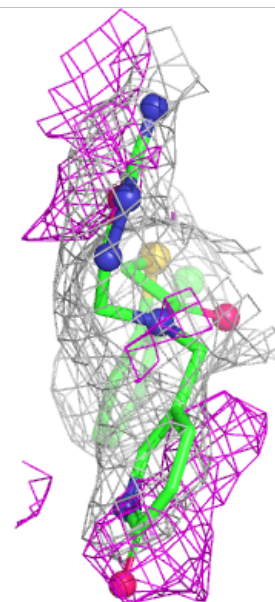
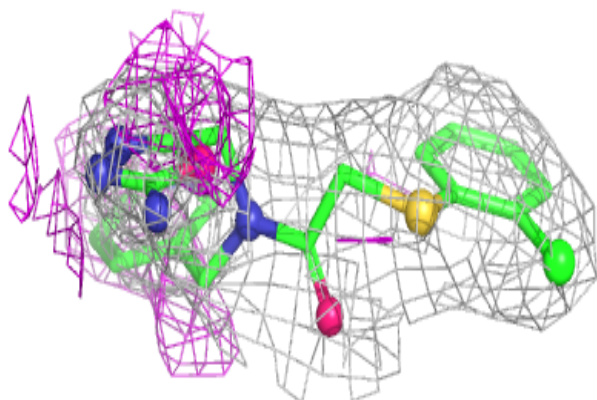
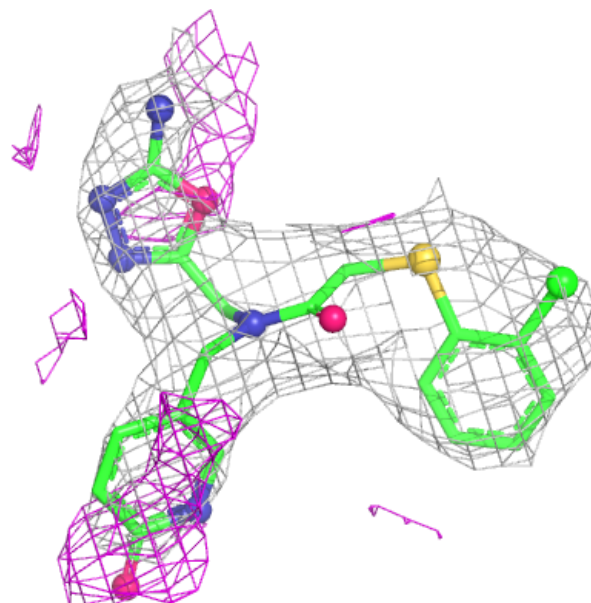
Electron density around VFZ O 303:

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



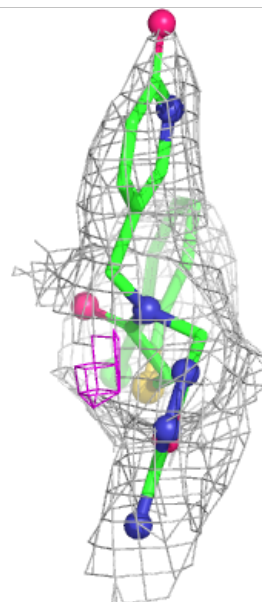
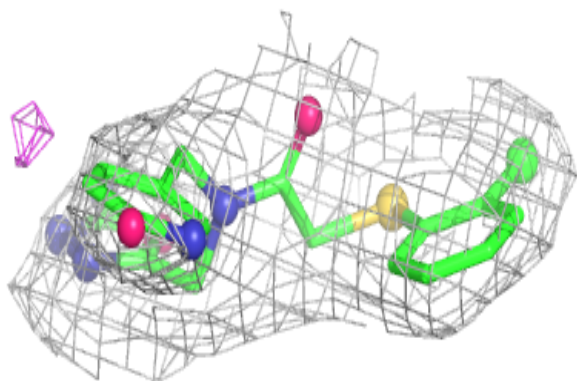
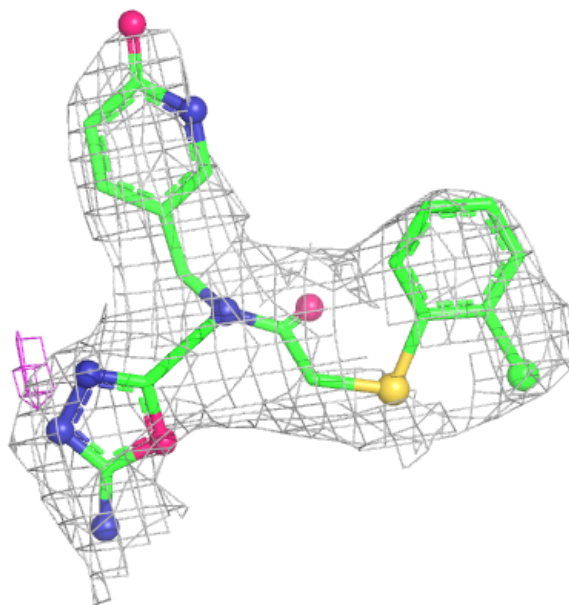
Electron density around VFZ J 303:

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



Electron density around VFZ A 310:

$2mF_o - DF_c$ (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.