Full wwPDB X-ray Structure Validation Report ⓘ

Oct 20, 2021 – 02:49 pm BST

PDB ID	:	7OKB
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 Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

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

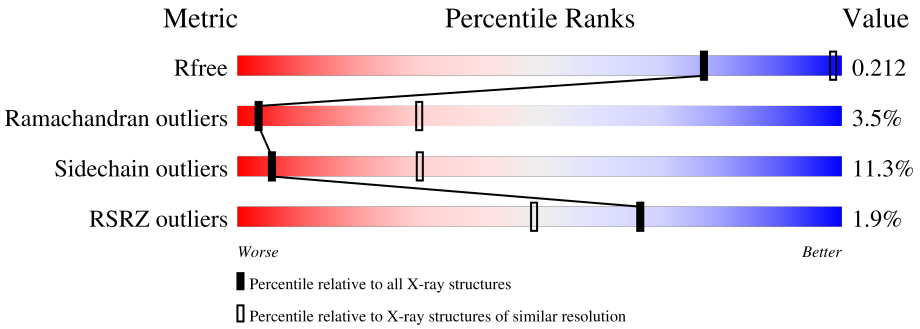
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.23.2
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0267
CCP4	:	7.1.010 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.23.2

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}	130704	1094 (3.66-3.50)
Ramachandran outliers	138981	1143 (3.66-3.50)
Sidechain outliers	138945	1143 (3.66-3.50)
RSRZ outliers	127900	1012 (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 <=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	84% 12%
1	B	261	84% 11%
1	C	261	84% 13%
1	D	261	85% 12%
1	E	261	85% 12%
1	F	261	84% 12%
1	G	261	5% 84% 12%

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Mol	Chain	Length	Quality of chain
1	H	261	3% 84% 13%
1	I	261	3% 84% 13%
1	J	261	% 84% 12%
1	K	261	84% 12%
1	L	261	84% 13%
1	M	261	5% 83% 13%
1	N	261	3% 82% 13%
1	O	261	3% 84% 11%
1	P	261	% 85% 11%
1	Q	261	5% 84% 13%
1	R	261	3% 85% 13%
1	S	261	83% 13%
1	T	261	85% 11%
1	U	261	82% 14%
1	V	261	4% 85% 11%
1	W	261	6% 84% 12%
1	X	261	2% 85% 11%
1	Y	261	4% 84% 13%
1	Z	261	% 85% 12%
1	a	261	3% 84% 12%
1	b	261	83% 13%
1	c	261	85% 12%
1	d	261	3% 84% 11%

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	A	304	-	-	-	X
3	SO4	A	307	-	-	-	X
3	SO4	A	309	-	-	-	X
3	SO4	B	304	-	-	-	X
3	SO4	C	304	-	-	-	X
3	SO4	C	305	-	-	-	X
3	SO4	D	304	-	-	-	X
3	SO4	E	304	-	-	-	X
3	SO4	F	301	-	-	-	X
3	SO4	F	302	-	-	-	X
3	SO4	H	301	-	-	-	X
3	SO4	H	302	-	-	-	X
3	SO4	I	303	-	-	-	X
3	SO4	J	301	-	-	-	X
3	SO4	K	301	-	-	-	X
3	SO4	K	302	-	-	-	X
3	SO4	M	303	-	-	-	X
3	SO4	N	302	-	-	-	X
3	SO4	N	303	-	-	-	X
3	SO4	O	302	-	-	-	X
3	SO4	P	303	-	-	-	X
3	SO4	Q	302	-	-	-	X
3	SO4	R	303	-	-	-	X
3	SO4	S	302	-	-	-	X
3	SO4	T	302	-	-	-	X
3	SO4	W	301	-	-	-	X
3	SO4	X	303	-	-	-	X
3	SO4	c	301	-	-	-	X
3	SO4	d	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	C	N	O	S	0	0	0
			1966	1230	363	367	6			
1	R	257	Total	C	N	O	S	0	0	0
			1966	1230	363	367	6			
1	S	258	Total	C	N	O	S	0	0	0
			1974	1235	364	368	7			
1	T	258	Total	C	N	O	S	0	0	0
			1974	1235	364	368	7			
1	U	258	Total	C	N	O	S	0	0	0
			1974	1235	364	368	7			
1	V	257	Total	C	N	O	S	0	0	0
			1966	1230	363	367	6			
1	W	257	Total	C	N	O	S	0	0	0
			1966	1230	363	367	6			
1	X	257	Total	C	N	O	S	0	0	0
			1966	1230	363	367	6			
1	Y	258	Total	C	N	O	S	0	0	0
			1974	1235	364	368	7			
1	Z	258	Total	C	N	O	S	0	0	0
			1974	1235	364	368	7			
1	a	257	Total	C	N	O	S	0	0	0
			1966	1230	363	367	6			
1	b	257	Total	C	N	O	S	0	0	0
			1966	1230	363	367	6			
1	c	258	Total	C	N	O	S	0	0	0
			1974	1235	364	368	7			
1	d	257	Total	C	N	O	S	0	0	0
			1966	1230	363	367	6			

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 (three-letter code: CL) (formula: Cl).

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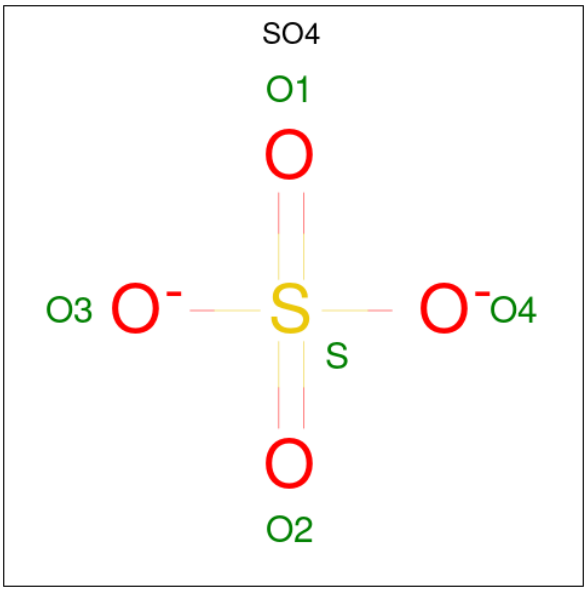
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf

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 (three-letter code: SO4) (formula: O_4S).



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

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

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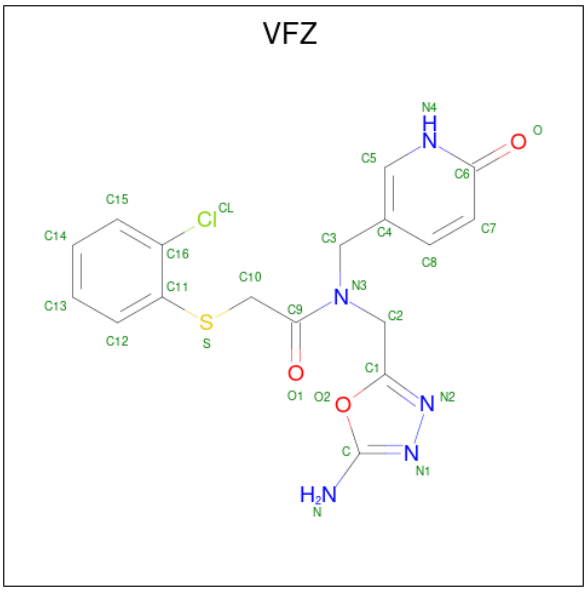
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	R	1	Total O S 5 4 1	0	0
3	R	1	Total O S 5 4 1	0	0
3	S	1	Total O S 5 4 1	0	0
3	T	1	Total O S 5 4 1	0	0
3	U	1	Total O S 5 4 1	0	0
3	U	1	Total O S 5 4 1	0	0
3	U	1	Total O S 5 4 1	0	0
3	V	1	Total O S 5 4 1	0	0
3	V	1	Total O S 5 4 1	0	0
3	W	1	Total O S 5 4 1	0	0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

- 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 (three-letter code: VFZ) (formula: $C_{17}H_{16}ClN_5O_3S$) (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	C	Cl	N	O	S	0	0
			27	17	1	5	3	1		
4	P	1	Total	C	Cl	N	O	S	0	0
			27	17	1	5	3	1		
4	Q	1	Total	C	Cl	N	O	S	0	0
			27	17	1	5	3	1		
4	R	1	Total	C	Cl	N	O	S	0	0
			27	17	1	5	3	1		
4	S	1	Total	C	Cl	N	O	S	0	0
			27	17	1	5	3	1		
4	T	1	Total	C	Cl	N	O	S	0	0
			27	17	1	5	3	1		
4	U	1	Total	C	Cl	N	O	S	0	0
			27	17	1	5	3	1		
4	V	1	Total	C	Cl	N	O	S	0	0
			27	17	1	5	3	1		
4	W	1	Total	C	Cl	N	O	S	0	0
			27	17	1	5	3	1		
4	X	1	Total	C	Cl	N	O	S	0	0
			27	17	1	5	3	1		
4	Y	1	Total	C	Cl	N	O	S	0	0
			27	17	1	5	3	1		
4	Z	1	Total	C	Cl	N	O	S	0	0
			27	17	1	5	3	1		
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		

- Molecule 5 is water.

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

Continued on next page...

Continued from previous page...

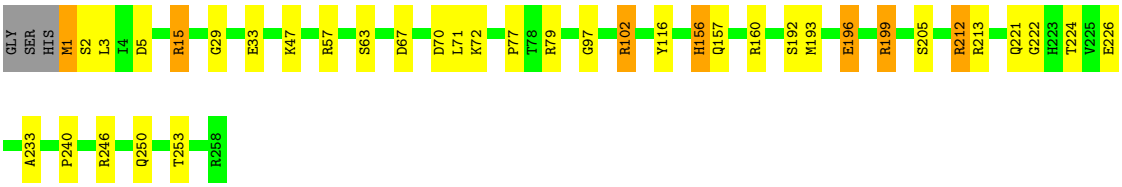
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	D	3	Total O 3 3	0	0
5	E	3	Total O 3 3	0	0
5	F	1	Total O 1 1	0	0
5	H	2	Total O 2 2	0	0
5	M	1	Total O 1 1	0	0
5	N	2	Total O 2 2	0	0
5	O	1	Total O 1 1	0	0
5	J	1	Total O 1 1	0	0
5	K	2	Total O 2 2	0	0
5	L	1	Total O 1 1	0	0
5	P	2	Total O 2 2	0	0
5	Q	1	Total O 1 1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

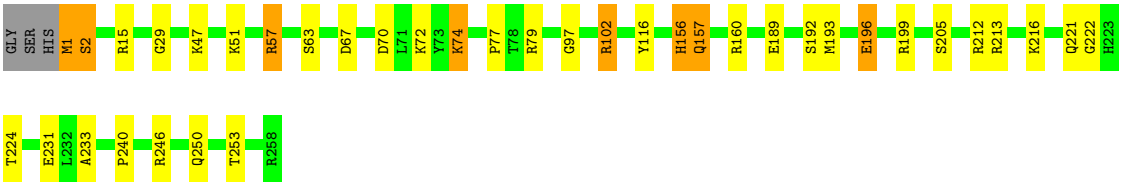
• Molecule 1: Acyl-[acyl-carrier-protein]--UDP-N-acetylglucosamine O-acyltransferase

Chain A:



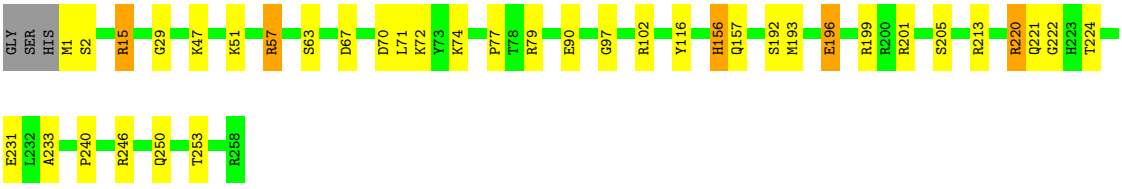
• Molecule 1: Acyl-[acyl-carrier-protein]--UDP-N-acetylglucosamine O-acyltransferase

Chain B:



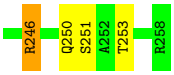
• Molecule 1: Acyl-[acyl-carrier-protein]--UDP-N-acetylglucosamine O-acyltransferase

Chain C:



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

Chain D:



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

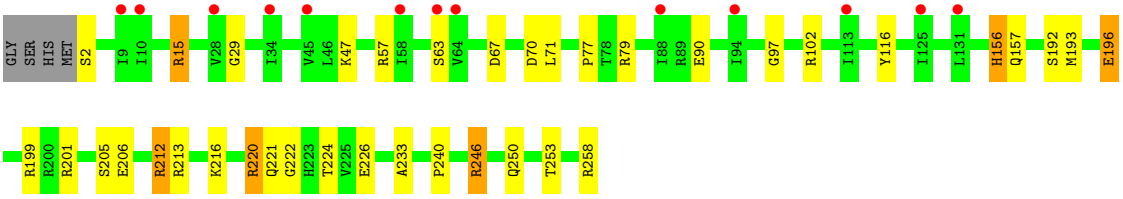
Chain E:

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

Chain F:

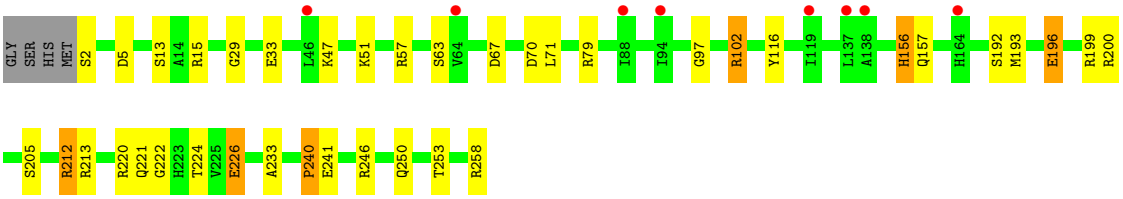
• Molecule 1: Acyl-[acyl-carrier-protein]--UDP-N-acetylglucosamine O-acyltransferase

Chain G:



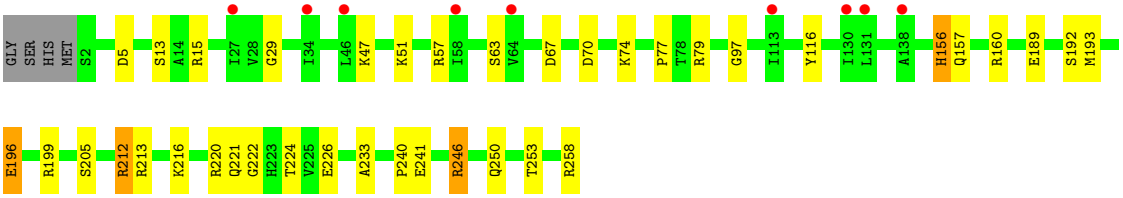
• Molecule 1: Acyl-[acyl-carrier-protein]--UDP-N-acetylglucosamine O-acyltransferase

Chain H:

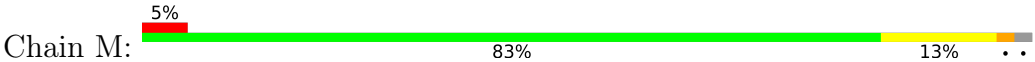


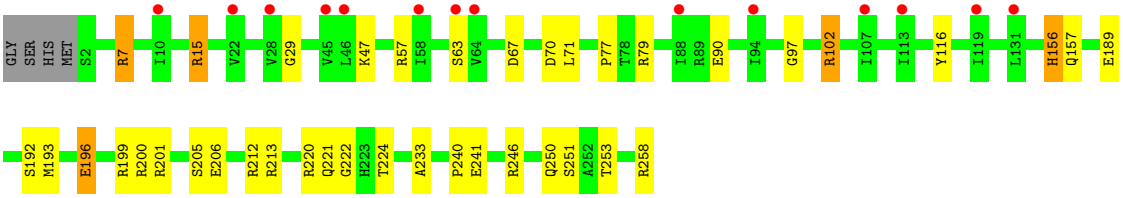
• Molecule 1: Acyl-[acyl-carrier-protein]--UDP-N-acetylglucosamine O-acyltransferase

Chain I:

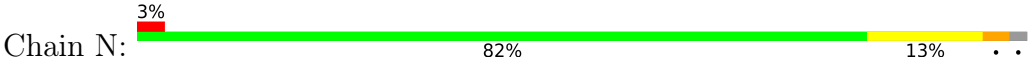


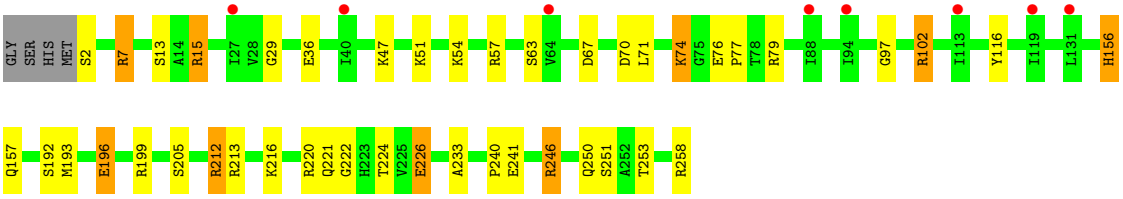
• Molecule 1: Acyl-[acyl-carrier-protein]--UDP-N-acetylglucosamine O-acyltransferase



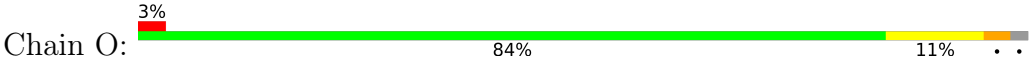


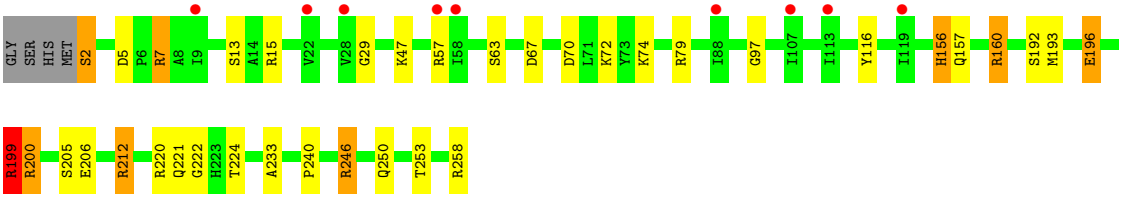
• Molecule 1: Acyl-[acyl-carrier-protein]--UDP-N-acetylglucosamine O-acyltransferase



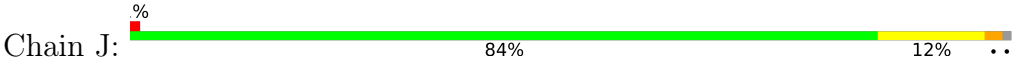


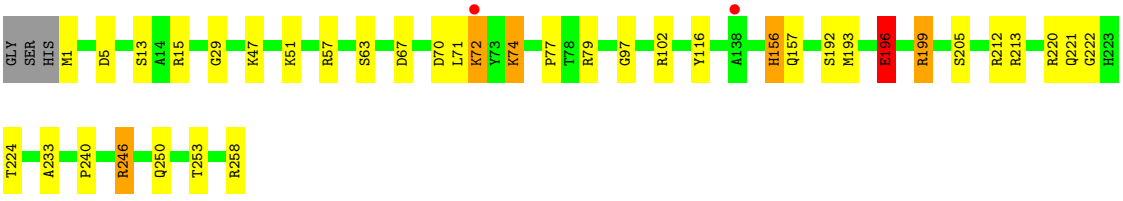
• Molecule 1: Acyl-[acyl-carrier-protein]--UDP-N-acetylglucosamine O-acyltransferase





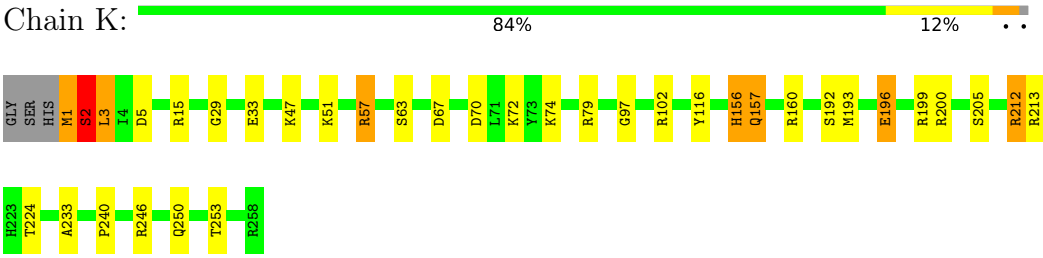
• Molecule 1: Acyl-[acyl-carrier-protein]--UDP-N-acetylglucosamine O-acyltransferase





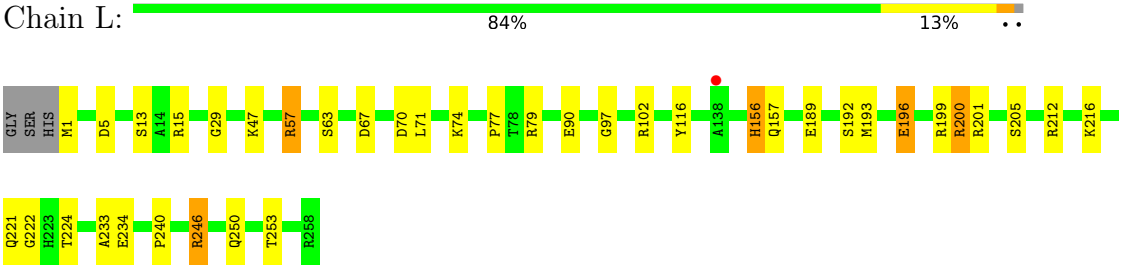
• Molecule 1: Acyl-[acyl-carrier-protein]--UDP-N-acetylglucosamine O-acyltransferase

Chain K:



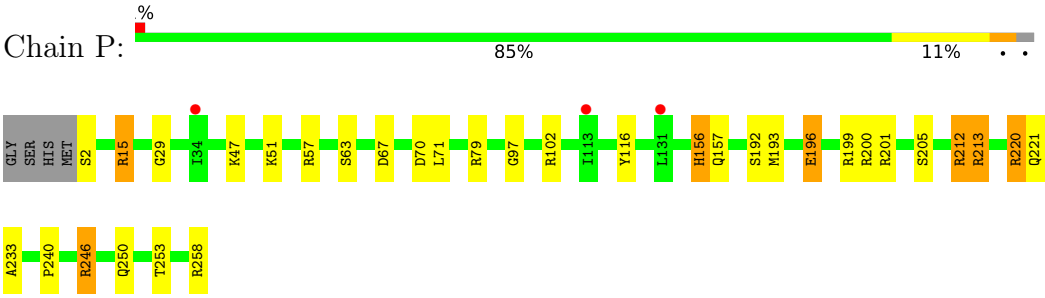
• Molecule 1: Acyl-[acyl-carrier-protein]--UDP-N-acetylglucosamine O-acyltransferase

Chain L:



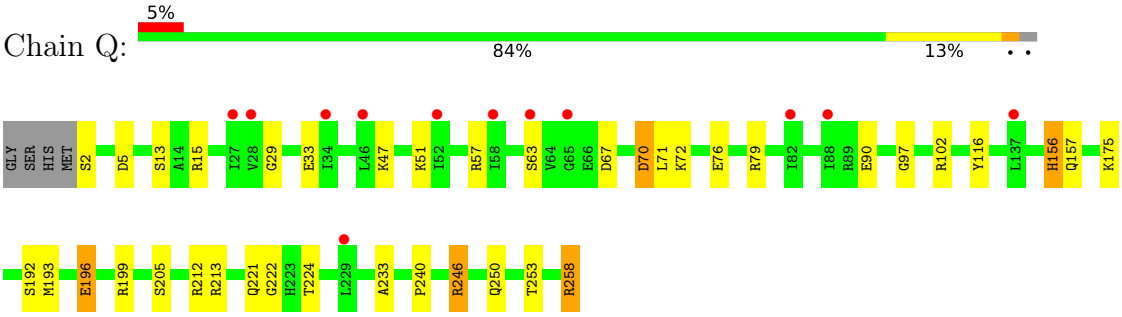
• Molecule 1: Acyl-[acyl-carrier-protein]--UDP-N-acetylglucosamine O-acyltransferase

Chain P:



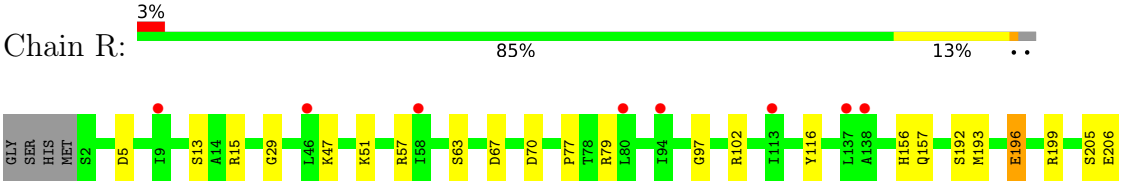
• Molecule 1: Acyl-[acyl-carrier-protein]--UDP-N-acetylglucosamine O-acyltransferase

Chain Q:



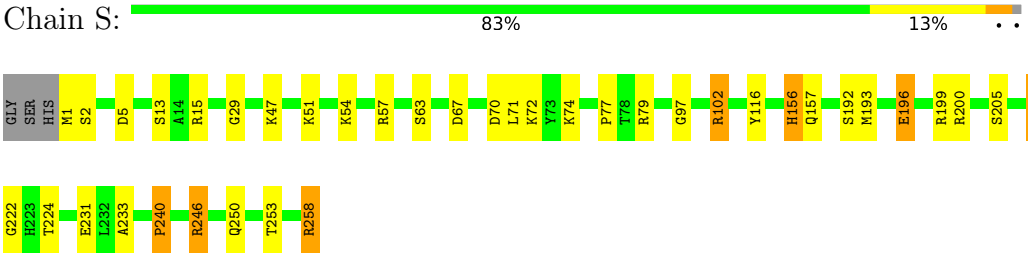
• Molecule 1: Acyl-[acyl-carrier-protein]--UDP-N-acetylglucosamine O-acyltransferase

Chain R:



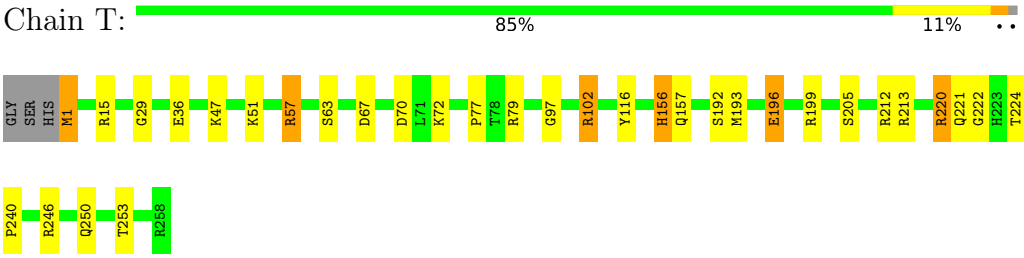
• Molecule 1: Acyl-[acyl-carrier-protein]--UDP-N-acetylglucosamine O-acyltransferase

Chain S:



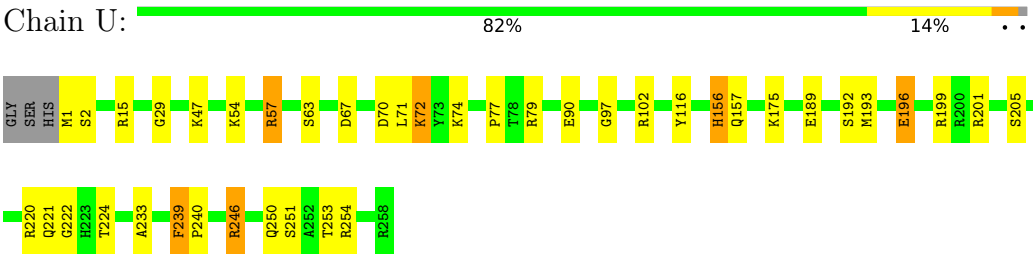
• Molecule 1: Acyl-[acyl-carrier-protein]--UDP-N-acetylglucosamine O-acyltransferase

Chain T:



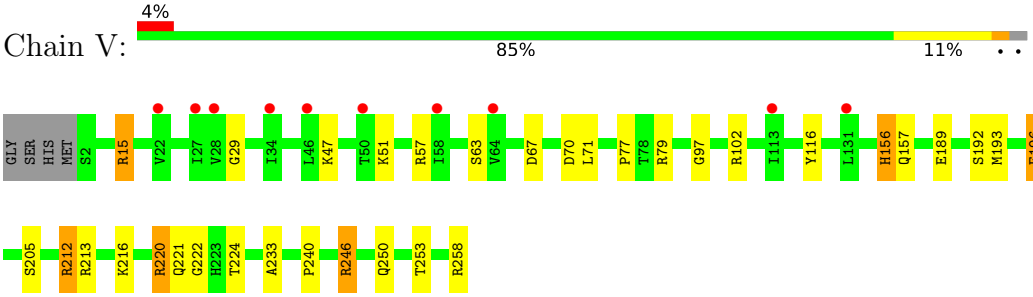
• Molecule 1: Acyl-[acyl-carrier-protein]--UDP-N-acetylglucosamine O-acyltransferase

Chain U:



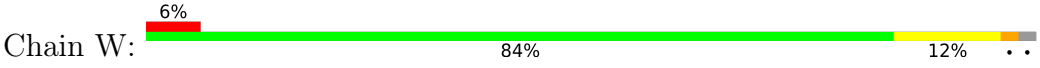
• Molecule 1: Acyl-[acyl-carrier-protein]--UDP-N-acetylglucosamine O-acyltransferase

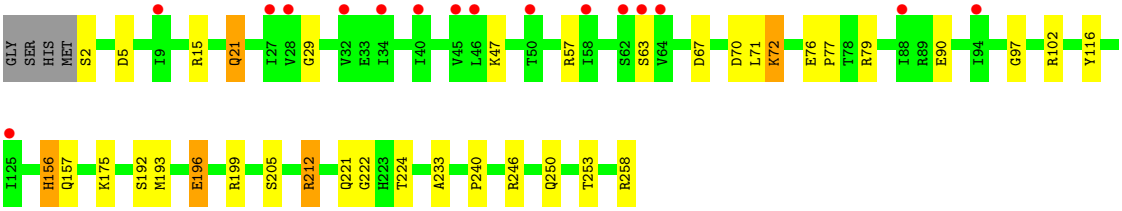
Chain V:



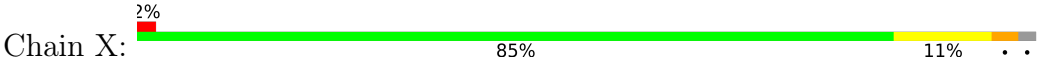
• Molecule 1: Acyl-[acyl-carrier-protein]--UDP-N-acetylglucosamine O-acyltransferase

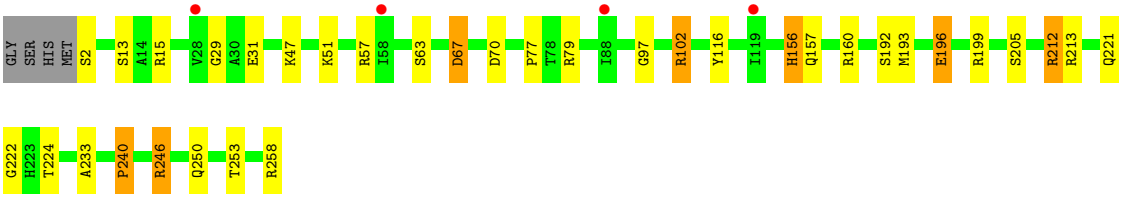
Chain W:



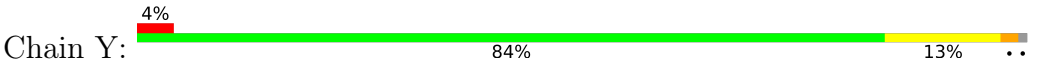


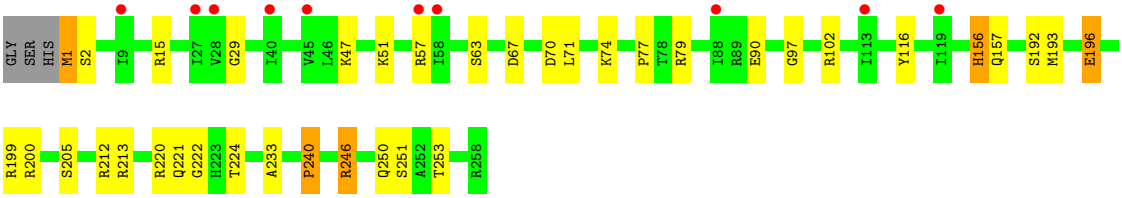
• Molecule 1: Acyl-[acyl-carrier-protein]--UDP-N-acetylglucosamine O-acyltransferase



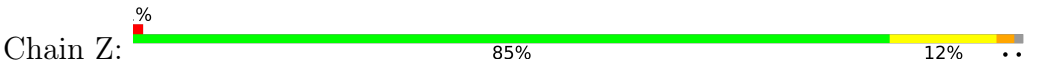


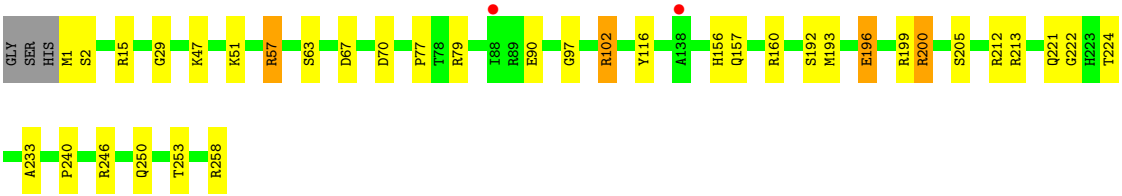
• Molecule 1: Acyl-[acyl-carrier-protein]--UDP-N-acetylglucosamine O-acyltransferase



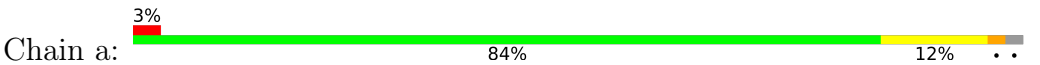


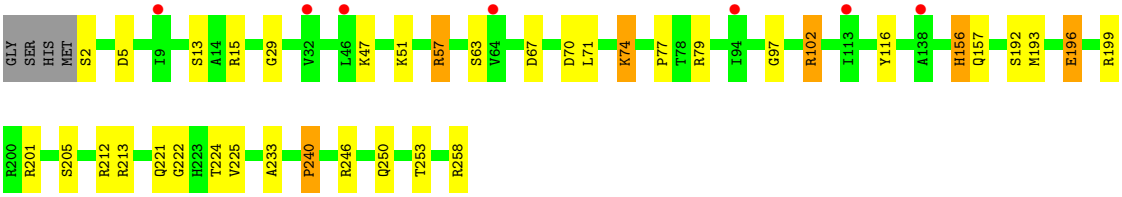
• Molecule 1: Acyl-[acyl-carrier-protein]--UDP-N-acetylglucosamine O-acyltransferase





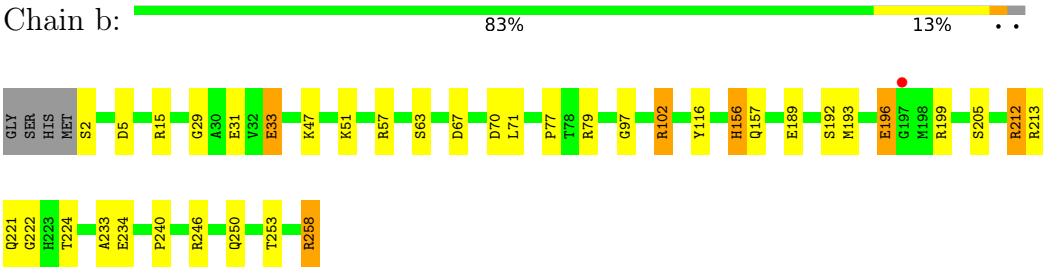
• Molecule 1: Acyl-[acyl-carrier-protein]--UDP-N-acetylglucosamine O-acyltransferase





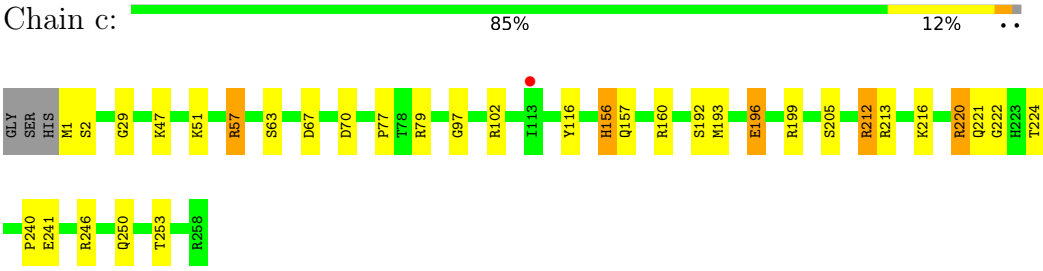
• Molecule 1: Acyl-[acyl-carrier-protein]--UDP-N-acetylglucosamine O-acyltransferase

Chain b:



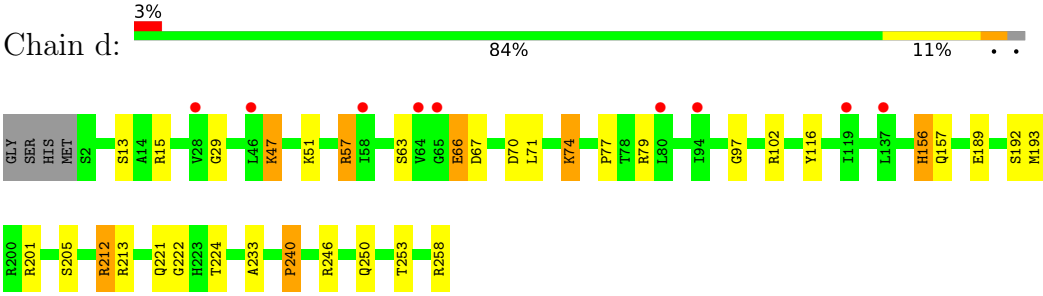
• Molecule 1: Acyl-[acyl-carrier-protein]--UDP-N-acetylglucosamine O-acyltransferase

Chain c:



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

Chain d:



4 Data and refinement statistics (i)

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
$< I/\sigma(I) >$ [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)	(Not available) , (Not available)	EDS
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.29$	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	0.90	2/2016 (0.1%)	1.30	20/2734 (0.7%)
1	B	0.91	2/2016 (0.1%)	1.23	13/2734 (0.5%)
1	C	0.91	4/2025 (0.2%)	1.24	14/2746 (0.5%)
1	D	0.88	2/2016 (0.1%)	1.22	11/2734 (0.4%)
1	E	0.95	8/2016 (0.4%)	1.26	14/2734 (0.5%)
1	F	0.87	0/2016	1.21	10/2734 (0.4%)
1	G	0.88	2/2008 (0.1%)	1.23	14/2724 (0.5%)
1	H	0.87	2/2008 (0.1%)	1.22	18/2724 (0.7%)
1	I	0.88	3/2008 (0.1%)	1.21	10/2724 (0.4%)
1	J	0.91	3/2016 (0.1%)	1.24	18/2734 (0.7%)
1	K	0.92	5/2016 (0.2%)	1.25	14/2734 (0.5%)
1	L	0.89	3/2016 (0.1%)	1.23	10/2734 (0.4%)
1	M	0.89	4/2008 (0.2%)	1.29	20/2724 (0.7%)
1	N	0.94	5/2008 (0.2%)	1.31	22/2724 (0.8%)
1	O	0.88	2/2008 (0.1%)	1.25	19/2724 (0.7%)
1	P	0.86	0/2008	1.26	16/2724 (0.6%)
1	Q	0.90	3/2008 (0.1%)	1.20	15/2724 (0.6%)
1	R	0.86	2/2008 (0.1%)	1.18	7/2724 (0.3%)
1	S	0.88	2/2016 (0.1%)	1.25	19/2734 (0.7%)
1	T	0.90	3/2016 (0.1%)	1.26	16/2734 (0.6%)
1	U	0.93	3/2016 (0.1%)	1.23	13/2734 (0.5%)
1	V	0.88	1/2008 (0.0%)	1.23	15/2724 (0.6%)
1	W	0.89	2/2008 (0.1%)	1.20	11/2724 (0.4%)
1	X	0.90	2/2008 (0.1%)	1.24	13/2724 (0.5%)
1	Y	0.87	2/2016 (0.1%)	1.21	13/2734 (0.5%)
1	Z	0.88	1/2016 (0.0%)	1.23	12/2734 (0.4%)
1	a	0.88	0/2008	1.22	12/2724 (0.4%)
1	b	0.91	5/2008 (0.2%)	1.22	13/2724 (0.5%)
1	c	0.87	1/2016 (0.0%)	1.25	14/2734 (0.5%)
1	d	0.88	1/2008 (0.0%)	1.21	14/2724 (0.5%)
All	All	0.89	75/60369 (0.1%)	1.24	430/81882 (0.5%)

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

All (75) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	W	76	GLU	CD-OE2	-13.05	1.11	1.25
1	U	189	GLU	CD-OE1	-13.01	1.11	1.25
1	V	189	GLU	CD-OE1	10.98	1.37	1.25
1	N	76	GLU	CD-OE2	-10.97	1.13	1.25
1	Z	90	GLU	CD-OE2	10.83	1.37	1.25
1	Q	76	GLU	CD-OE1	-10.64	1.14	1.25
1	C	2	SER	C-O	8.92	1.40	1.23
1	B	189	GLU	CD-OE1	-8.62	1.16	1.25
1	I	189	GLU	CD-OE1	-8.34	1.16	1.25
1	E	206	GLU	CD-OE1	-8.13	1.16	1.25
1	U	2	SER	C-O	8.06	1.38	1.23
1	X	67	ASP	CG-OD1	-7.33	1.08	1.25
1	K	33	GLU	CD-OE1	7.28	1.33	1.25
1	b	189	GLU	CD-OE1	-7.14	1.17	1.25
1	M	241	GLU	CD-OE1	7.13	1.33	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	c	241	GLU	CD-OE1	7.06	1.33	1.25
1	G	206	GLU	CD-OE1	-7.02	1.18	1.25
1	I	241	GLU	CD-OE1	6.94	1.33	1.25
1	E	2	SER	CA-CB	6.87	1.63	1.52
1	E	2	SER	C-O	6.71	1.36	1.23
1	d	189	GLU	CD-OE1	-6.63	1.18	1.25
1	D	234	GLU	CD-OE2	-6.58	1.18	1.25
1	C	231	GLU	CD-OE2	-6.44	1.18	1.25
1	T	36	GLU	CD-OE1	-6.36	1.18	1.25
1	H	33	GLU	CD-OE2	-6.35	1.18	1.25
1	J	57	ARG	NE-CZ	6.35	1.41	1.33
1	K	2	SER	CB-OG	6.34	1.50	1.42
1	J	196	GLU	CD-OE2	-6.27	1.18	1.25
1	D	57	ARG	NE-CZ	6.13	1.41	1.33
1	M	189	GLU	CD-OE2	-6.09	1.19	1.25
1	N	36	GLU	CD-OE1	-6.08	1.19	1.25
1	b	33	GLU	CD-OE2	6.05	1.32	1.25
1	M	90	GLU	CD-OE1	6.03	1.32	1.25
1	E	2	SER	CB-OG	6.01	1.50	1.42
1	J	1	MET	CG-SD	5.96	1.96	1.81
1	A	226	GLU	CD-OE1	5.94	1.32	1.25
1	O	57	ARG	NE-CZ	5.89	1.40	1.33
1	N	241	GLU	CD-OE1	5.84	1.32	1.25
1	C	90	GLU	CD-OE1	5.78	1.32	1.25
1	T	1	MET	CG-SD	5.72	1.96	1.81
1	b	234	GLU	CD-OE2	-5.71	1.19	1.25
1	E	2	SER	N-CA	5.69	1.57	1.46
1	L	189	GLU	CD-OE1	-5.67	1.19	1.25
1	S	57	ARG	NE-CZ	5.63	1.40	1.33
1	E	57	ARG	NE-CZ	5.61	1.40	1.33
1	M	7	ARG	NE-CZ	5.60	1.40	1.33
1	Q	90	GLU	CD-OE1	5.59	1.31	1.25
1	A	33	GLU	CD-OE1	-5.59	1.19	1.25
1	b	57	ARG	NE-CZ	5.56	1.40	1.33
1	E	226	GLU	CD-OE2	5.53	1.31	1.25
1	G	90	GLU	CD-OE1	5.52	1.31	1.25
1	R	57	ARG	NE-CZ	5.51	1.40	1.33
1	Q	33	GLU	CD-OE1	-5.51	1.19	1.25
1	Y	57	ARG	NE-CZ	5.49	1.40	1.33
1	I	57	ARG	NE-CZ	5.49	1.40	1.33
1	N	7	ARG	NE-CZ	5.49	1.40	1.33
1	K	2	SER	CA-CB	5.49	1.61	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	K	33	GLU	CD-OE2	-5.43	1.19	1.25
1	U	90	GLU	CD-OE1	5.43	1.31	1.25
1	L	234	GLU	CD-OE2	5.39	1.31	1.25
1	E	206	GLU	CD-OE2	-5.35	1.19	1.25
1	B	231	GLU	CD-OE1	-5.31	1.19	1.25
1	K	3	LEU	N-CA	5.24	1.56	1.46
1	O	206	GLU	CD-OE1	5.23	1.31	1.25
1	b	31	GLU	CD-OE2	5.18	1.31	1.25
1	S	231	GLU	CD-OE2	-5.16	1.20	1.25
1	N	226	GLU	CD-OE2	-5.14	1.20	1.25
1	T	1	MET	N-CA	5.14	1.56	1.46
1	C	57	ARG	NE-CZ	5.13	1.39	1.33
1	W	90	GLU	CD-OE1	5.11	1.31	1.25
1	L	90	GLU	CD-OE1	5.10	1.31	1.25
1	R	206	GLU	CD-OE1	5.07	1.31	1.25
1	X	57	ARG	NE-CZ	5.05	1.39	1.33
1	Y	90	GLU	CD-OE1	5.05	1.31	1.25
1	H	241	GLU	CD-OE1	5.03	1.31	1.25

All (430) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	N	7	ARG	NE-CZ-NH2	14.33	127.46	120.30
1	M	7	ARG	NE-CZ-NH2	13.51	127.05	120.30
1	X	67	ASP	CB-CG-OD1	-13.47	106.18	118.30
1	A	160	ARG	NE-CZ-NH1	13.14	126.87	120.30
1	P	213	ARG	NE-CZ-NH1	12.50	126.55	120.30
1	P	212	ARG	CB-CG-CD	12.10	143.05	111.60
1	N	7	ARG	NE-CZ-NH1	-11.83	114.39	120.30
1	A	57	ARG	CG-CD-NE	-10.60	89.55	111.80
1	A	15	ARG	NE-CZ-NH1	10.45	125.52	120.30
1	E	246	ARG	NE-CZ-NH1	10.36	125.48	120.30
1	c	220	ARG	NE-CZ-NH2	10.34	125.47	120.30
1	M	7	ARG	CD-NE-CZ	10.29	138.00	123.60
1	C	57	ARG	NE-CZ-NH2	10.25	125.42	120.30
1	X	67	ASP	CB-CG-OD2	9.88	127.19	118.30
1	Y	220	ARG	NE-CZ-NH1	9.83	125.22	120.30
1	J	57	ARG	NE-CZ-NH2	9.81	125.21	120.30
1	T	102	ARG	CG-CD-NE	-9.75	91.32	111.80
1	N	7	ARG	CD-NE-CZ	9.71	137.19	123.60
1	I	220	ARG	CG-CD-NE	9.53	131.82	111.80
1	M	7	ARG	NE-CZ-NH1	-9.20	115.70	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	W	72	LYS	CB-CG-CD	8.99	134.99	111.60
1	H	212	ARG	NE-CZ-NH1	-8.98	115.81	120.30
1	L	201	ARG	CG-CD-NE	-8.87	93.18	111.80
1	O	212	ARG	CB-CG-CD	8.84	134.57	111.60
1	O	200	ARG	CB-CG-CD	8.82	134.54	111.60
1	G	201	ARG	CG-CD-NE	-8.72	93.48	111.80
1	M	201	ARG	CG-CD-NE	-8.72	93.48	111.80
1	G	212	ARG	CB-CG-CD	8.69	134.21	111.60
1	a	201	ARG	CG-CD-NE	-8.65	93.64	111.80
1	F	201	ARG	CG-CD-NE	-8.63	93.67	111.80
1	U	201	ARG	CG-CD-NE	-8.62	93.70	111.80
1	d	201	ARG	CG-CD-NE	-8.61	93.72	111.80
1	V	201	ARG	CG-CD-NE	-8.60	93.74	111.80
1	P	201	ARG	CG-CD-NE	-8.52	93.91	111.80
1	C	201	ARG	CG-CD-NE	-8.52	93.91	111.80
1	N	220	ARG	CG-CD-NE	8.46	129.57	111.80
1	c	220	ARG	NH1-CZ-NH2	-8.36	110.20	119.40
1	A	3	LEU	CB-CG-CD2	8.34	125.17	111.00
1	c	212	ARG	NE-CZ-NH1	-8.27	116.17	120.30
1	T	220	ARG	NE-CZ-NH2	8.26	124.43	120.30
1	C	57	ARG	CB-CG-CD	7.91	132.17	111.60
1	Y	213	ARG	NE-CZ-NH1	7.91	124.25	120.30
1	a	102	ARG	CB-CG-CD	7.84	131.97	111.60
1	N	2	SER	CA-C-O	-7.80	103.72	120.10
1	A	57	ARG	CB-CA-C	7.77	125.94	110.40
1	Z	200	ARG	CB-CG-CD	7.62	131.42	111.60
1	V	189	GLU	CG-CD-OE1	7.57	133.43	118.30
1	a	213	ARG	NE-CZ-NH1	7.56	124.08	120.30
1	D	57	ARG	CB-CA-C	7.54	125.48	110.40
1	V	15	ARG	NE-CZ-NH2	7.53	124.06	120.30
1	b	220	ARG	NE-CZ-NH2	7.50	124.05	120.30
1	B	160	ARG	NE-CZ-NH1	7.48	124.04	120.30
1	I	212	ARG	NE-CZ-NH1	-7.48	116.56	120.30
1	G	57	ARG	CB-CA-C	7.47	125.35	110.40
1	E	246	ARG	NH1-CZ-NH2	-7.47	111.18	119.40
1	J	213	ARG	NE-CZ-NH1	7.47	124.03	120.30
1	S	57	ARG	CB-CA-C	7.45	125.30	110.40
1	V	57	ARG	CB-CA-C	7.44	125.29	110.40
1	J	57	ARG	CB-CA-C	7.40	125.20	110.40
1	V	57	ARG	CB-CG-CD	7.40	130.84	111.60
1	G	57	ARG	CB-CG-CD	7.40	130.84	111.60
1	R	57	ARG	CB-CA-C	7.39	125.19	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	b	57	ARG	CB-CA-C	7.38	125.16	110.40
1	H	57	ARG	CB-CA-C	7.37	125.15	110.40
1	I	213	ARG	CG-CD-NE	-7.37	96.31	111.80
1	R	213	ARG	CG-CD-NE	-7.36	96.34	111.80
1	W	57	ARG	CD-NE-CZ	7.36	133.90	123.60
1	M	57	ARG	CB-CA-C	7.35	125.11	110.40
1	P	57	ARG	CB-CA-C	7.35	125.10	110.40
1	W	57	ARG	CB-CA-C	7.31	125.03	110.40
1	I	57	ARG	CB-CA-C	7.30	125.00	110.40
1	Y	57	ARG	CB-CA-C	7.30	125.00	110.40
1	B	57	ARG	CB-CA-C	7.29	124.97	110.40
1	O	57	ARG	CB-CA-C	7.28	124.96	110.40
1	Q	57	ARG	CB-CA-C	7.28	124.96	110.40
1	X	57	ARG	CB-CA-C	7.28	124.95	110.40
1	N	57	ARG	CB-CA-C	7.27	124.94	110.40
1	J	220	ARG	NE-CZ-NH1	7.27	123.93	120.30
1	V	212	ARG	NE-CZ-NH2	7.24	123.92	120.30
1	b	258	ARG	CG-CD-NE	7.24	127.01	111.80
1	P	57	ARG	CB-CG-CD	7.23	130.39	111.60
1	d	212	ARG	NE-CZ-NH1	-7.20	116.70	120.30
1	Z	102	ARG	CB-CG-CD	7.15	130.19	111.60
1	Q	57	ARG	CD-NE-CZ	7.14	133.60	123.60
1	Q	70	ASP	CB-CG-OD2	7.07	124.66	118.30
1	E	2	SER	N-CA-CB	7.05	121.07	110.50
1	c	220	ARG	NE-CZ-NH1	7.05	123.82	120.30
1	X	102	ARG	CB-CG-CD	7.03	129.88	111.60
1	D	212	ARG	NE-CZ-NH1	-7.03	116.79	120.30
1	M	57	ARG	CB-CG-CD	7.02	129.85	111.60
1	E	57	ARG	CB-CA-C	6.96	124.31	110.40
1	K	57	ARG	CB-CA-C	6.95	124.29	110.40
1	S	57	ARG	NE-CZ-NH2	6.94	123.77	120.30
1	Z	57	ARG	CB-CA-C	6.93	124.26	110.40
1	M	7	ARG	CG-CD-NE	-6.93	97.25	111.80
1	F	72	LYS	CA-CB-CG	6.92	128.63	113.40
1	T	57	ARG	CB-CA-C	6.91	124.21	110.40
1	Y	200	ARG	CB-CG-CD	6.91	129.55	111.60
1	A	15	ARG	CA-CB-CG	6.90	128.57	113.40
1	M	15	ARG	NE-CZ-NH2	6.89	123.75	120.30
1	F	57	ARG	CB-CA-C	6.86	124.13	110.40
1	X	213	ARG	CG-CD-NE	-6.86	97.39	111.80
1	V	189	GLU	OE1-CD-OE2	-6.86	115.07	123.30
1	H	57	ARG	CB-CG-CD	6.84	129.40	111.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	V	213	ARG	NE-CZ-NH1	6.84	123.72	120.30
1	c	57	ARG	CB-CA-C	6.84	124.08	110.40
1	U	57	ARG	CB-CA-C	6.83	124.06	110.40
1	d	57	ARG	CB-CA-C	6.83	124.05	110.40
1	L	57	ARG	CB-CA-C	6.79	123.97	110.40
1	a	57	ARG	CB-CA-C	6.79	123.97	110.40
1	N	57	ARG	CD-NE-CZ	6.78	133.10	123.60
1	K	213	ARG	NE-CZ-NH1	6.76	123.68	120.30
1	O	220	ARG	NE-CZ-NH1	6.76	123.68	120.30
1	H	220	ARG	NE-CZ-NH2	6.75	123.67	120.30
1	M	213	ARG	NE-CZ-NH1	6.75	123.67	120.30
1	O	57	ARG	NE-CZ-NH2	6.75	123.67	120.30
1	N	7	ARG	CG-CD-NE	-6.74	97.66	111.80
1	J	74	LYS	CB-CG-CD	6.72	129.07	111.60
1	D	57	ARG	NE-CZ-NH2	6.71	123.65	120.30
1	P	220	ARG	NE-CZ-NH2	6.70	123.65	120.30
1	d	213	ARG	NE-CZ-NH1	6.68	123.64	120.30
1	S	5	ASP	CB-CG-OD2	-6.67	112.30	118.30
1	N	102	ARG	CB-CG-CD	6.67	128.93	111.60
1	O	7	ARG	CA-CB-CG	-6.62	98.83	113.40
1	P	15	ARG	NE-CZ-NH2	6.60	123.60	120.30
1	C	57	ARG	CB-CA-C	6.59	123.59	110.40
1	G	213	ARG	NE-CZ-NH1	6.58	123.59	120.30
1	b	102	ARG	CB-CG-CD	6.58	128.70	111.60
1	J	116	TYR	CB-CG-CD2	6.57	124.94	121.00
1	T	226	GLU	OE1-CD-OE2	6.55	131.16	123.30
1	C	57	ARG	NH1-CZ-NH2	-6.54	112.20	119.40
1	N	226	GLU	CB-CG-CD	-6.54	96.54	114.20
1	M	57	ARG	CD-NE-CZ	6.51	132.72	123.60
1	U	220	ARG	NE-CZ-NH2	6.50	123.55	120.30
1	L	116	TYR	CB-CG-CD2	6.50	124.90	121.00
1	N	57	ARG	CB-CG-CD	6.50	128.49	111.60
1	P	220	ARG	CG-CD-NE	6.47	125.39	111.80
1	c	213	ARG	NE-CZ-NH1	6.44	123.52	120.30
1	M	200	ARG	CB-CG-CD	6.42	128.29	111.60
1	H	226	GLU	CA-CB-CG	6.41	127.51	113.40
1	U	72	LYS	CB-CG-CD	6.40	128.23	111.60
1	U	212	ARG	NE-CZ-NH2	6.39	123.50	120.30
1	O	5	ASP	CB-CG-OD2	-6.37	112.57	118.30
1	N	212	ARG	NE-CZ-NH1	-6.35	117.12	120.30
1	S	72	LYS	CG-CD-CE	6.35	130.96	111.90
1	W	57	ARG	CB-CG-CD	6.35	128.12	111.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	P	213	ARG	CB-CG-CD	6.34	128.08	111.60
1	G	15	ARG	CA-CB-CG	6.33	127.34	113.40
1	Q	57	ARG	CB-CG-CD	6.33	128.05	111.60
1	U	213	ARG	NE-CZ-NH1	6.32	123.46	120.30
1	B	156	HIS	CB-CA-C	6.30	123.01	110.40
1	T	246	ARG	CG-CD-NE	-6.30	98.56	111.80
1	H	213	ARG	NE-CZ-NH2	6.30	123.45	120.30
1	H	226	GLU	CB-CG-CD	6.29	131.17	114.20
1	A	212	ARG	CB-CG-CD	6.28	127.94	111.60
1	K	212	ARG	CB-CG-CD	6.28	127.93	111.60
1	B	213	ARG	NE-CZ-NH1	6.27	123.44	120.30
1	T	220	ARG	NH1-CZ-NH2	-6.27	112.50	119.40
1	B	102	ARG	CG-CD-NE	-6.27	98.63	111.80
1	J	258	ARG	CG-CD-NE	6.25	124.93	111.80
1	V	116	TYR	CB-CG-CD2	6.22	124.73	121.00
1	K	116	TYR	CB-CG-CD2	6.18	124.71	121.00
1	A	72	LYS	CG-CD-CE	6.16	130.37	111.90
1	b	213	ARG	NE-CZ-NH1	6.15	123.38	120.30
1	B	246	ARG	CG-CD-NE	-6.15	98.88	111.80
1	H	57	ARG	CD-NE-CZ	6.13	132.18	123.60
1	S	213	ARG	NE-CZ-NH1	6.13	123.36	120.30
1	O	199	ARG	NH1-CZ-NH2	-6.12	112.66	119.40
1	W	116	TYR	CB-CG-CD2	6.11	124.67	121.00
1	Z	246	ARG	CG-CD-NE	-6.11	98.97	111.80
1	M	7	ARG	CB-CG-CD	-6.10	95.74	111.60
1	C	72	LYS	CG-CD-CE	6.09	130.18	111.90
1	O	7	ARG	NE-CZ-NH2	-6.08	117.26	120.30
1	A	116	TYR	CB-CG-CD2	6.05	124.63	121.00
1	T	116	TYR	CB-CG-CD2	6.04	124.63	121.00
1	O	116	TYR	CB-CG-CD2	6.04	124.62	121.00
1	X	57	ARG	NE-CZ-NH2	6.04	123.32	120.30
1	L	116	TYR	CB-CA-C	6.02	122.45	110.40
1	Q	72	LYS	CG-CD-CE	6.02	129.97	111.90
1	D	116	TYR	CB-CG-CD2	6.02	124.61	121.00
1	Q	70	ASP	CB-CG-OD1	-6.01	112.89	118.30
1	E	246	ARG	NE-CZ-NH2	5.99	123.29	120.30
1	K	246	ARG	CG-CD-NE	-5.98	99.24	111.80
1	R	57	ARG	CB-CG-CD	5.97	127.13	111.60
1	M	212	ARG	NE-CZ-NH2	5.96	123.28	120.30
1	N	7	ARG	CB-CG-CD	-5.95	96.13	111.60
1	I	116	TYR	CB-CG-CD2	5.94	124.56	121.00
1	c	246	ARG	CG-CD-NE	-5.93	99.34	111.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	V	220	ARG	CG-CD-NE	5.93	124.25	111.80
1	O	7	ARG	CB-CG-CD	5.93	127.01	111.60
1	A	160	ARG	NH1-CZ-NH2	-5.92	112.88	119.40
1	Q	5	ASP	CB-CG-OD2	-5.92	112.97	118.30
1	T	116	TYR	CB-CA-C	5.91	122.22	110.40
1	G	206	GLU	CB-CG-CD	-5.91	98.26	114.20
1	P	116	TYR	CB-CG-CD2	5.90	124.54	121.00
1	K	116	TYR	CB-CA-C	5.89	122.17	110.40
1	S	102	ARG	CB-CG-CD	5.89	126.90	111.60
1	Z	160	ARG	NE-CZ-NH1	5.88	123.24	120.30
1	I	5	ASP	CB-CG-OD2	-5.87	113.02	118.30
1	L	57	ARG	CA-CB-CG	5.87	126.31	113.40
1	B	213	ARG	NE-CZ-NH2	-5.87	117.37	120.30
1	I	57	ARG	CB-CG-CD	5.86	126.84	111.60
1	b	116	TYR	CB-CG-CD2	5.85	124.51	121.00
1	C	15	ARG	NE-CZ-NH2	5.84	123.22	120.30
1	d	74	LYS	CB-CG-CD	5.84	126.78	111.60
1	D	116	TYR	CB-CA-C	5.82	122.05	110.40
1	O	57	ARG	CB-CG-CD	5.81	126.70	111.60
1	S	258	ARG	NE-CZ-NH1	5.79	123.20	120.30
1	T	213	ARG	NE-CZ-NH1	5.79	123.19	120.30
1	S	57	ARG	CB-CG-CD	5.79	126.64	111.60
1	Z	116	TYR	CB-CA-C	5.79	121.97	110.40
1	a	116	TYR	CB-CA-C	5.78	121.96	110.40
1	W	116	TYR	CB-CA-C	5.77	121.94	110.40
1	E	213	ARG	NE-CZ-NH1	5.77	123.18	120.30
1	K	1	MET	CG-SD-CE	5.77	109.43	100.20
1	O	116	TYR	CB-CA-C	5.76	121.93	110.40
1	S	116	TYR	CB-CA-C	5.76	121.92	110.40
1	J	57	ARG	CB-CG-CD	5.76	126.58	111.60
1	G	220	ARG	CG-CD-NE	5.76	123.89	111.80
1	Y	57	ARG	NE-CZ-NH1	5.76	123.18	120.30
1	O	160	ARG	CB-CG-CD	5.75	126.56	111.60
1	G	116	TYR	CB-CA-C	5.75	121.90	110.40
1	S	258	ARG	CG-CD-NE	5.74	123.86	111.80
1	X	57	ARG	CB-CG-CD	5.73	126.50	111.60
1	b	116	TYR	CB-CA-C	5.73	121.86	110.40
1	Z	213	ARG	NE-CZ-NH1	5.73	123.16	120.30
1	c	116	TYR	CB-CA-C	5.72	121.84	110.40
1	d	47	LYS	CG-CD-CE	5.72	129.05	111.90
1	P	57	ARG	CD-NE-CZ	5.70	131.58	123.60
1	H	116	TYR	CB-CA-C	5.70	121.80	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	J	72	LYS	CB-CG-CD	5.70	126.42	111.60
1	C	116	TYR	CB-CG-CD2	5.70	124.42	121.00
1	A	213	ARG	NE-CZ-NH2	-5.70	117.45	120.30
1	J	57	ARG	NH1-CZ-NH2	-5.70	113.14	119.40
1	d	66	GLU	CA-CB-CG	5.69	125.92	113.40
1	P	116	TYR	CB-CA-C	5.68	121.77	110.40
1	A	57	ARG	CD-NE-CZ	5.68	131.55	123.60
1	C	213	ARG	NE-CZ-NH1	5.67	123.14	120.30
1	Y	116	TYR	CB-CA-C	5.67	121.74	110.40
1	B	74	LYS	CB-CG-CD	5.66	126.32	111.60
1	Z	116	TYR	CB-CG-CD2	5.66	124.40	121.00
1	L	200	ARG	CB-CG-CD	5.65	126.30	111.60
1	R	116	TYR	CB-CA-C	5.65	121.70	110.40
1	F	57	ARG	NE-CZ-NH2	5.65	123.12	120.30
1	E	116	TYR	CB-CA-C	5.65	121.69	110.40
1	U	239	PHE	CB-CG-CD2	-5.65	116.85	120.80
1	N	116	TYR	CB-CA-C	5.64	121.69	110.40
1	J	116	TYR	CB-CA-C	5.64	121.69	110.40
1	I	116	TYR	CB-CA-C	5.63	121.66	110.40
1	Q	116	TYR	CB-CA-C	5.63	121.66	110.40
1	A	116	TYR	CB-CA-C	5.62	121.65	110.40
1	G	57	ARG	CD-NE-CZ	5.62	131.47	123.60
1	C	116	TYR	CB-CA-C	5.62	121.63	110.40
1	K	57	ARG	CA-CB-CG	5.61	125.75	113.40
1	d	116	TYR	CB-CA-C	5.61	121.62	110.40
1	W	212	ARG	NE-CZ-NH2	5.60	123.10	120.30
1	U	116	TYR	CB-CA-C	5.60	121.60	110.40
1	a	57	ARG	NE-CZ-NH2	5.60	123.10	120.30
1	T	57	ARG	CA-CB-CG	5.59	125.69	113.40
1	V	116	TYR	CB-CA-C	5.59	121.57	110.40
1	a	57	ARG	CA-CB-CG	5.58	125.68	113.40
1	X	116	TYR	CB-CA-C	5.58	121.56	110.40
1	F	116	TYR	CB-CA-C	5.57	121.54	110.40
1	R	116	TYR	CB-CG-CD2	5.56	124.34	121.00
1	J	258	ARG	NE-CZ-NH1	5.55	123.08	120.30
1	P	200	ARG	CG-CD-NE	-5.55	100.14	111.80
1	M	116	TYR	CB-CA-C	5.55	121.50	110.40
1	T	220	ARG	NE-CZ-NH1	5.54	123.07	120.30
1	N	2	SER	CA-C-N	5.54	129.39	117.20
1	P	213	ARG	NH1-CZ-NH2	-5.54	113.31	119.40
1	K	200	ARG	NE-CZ-NH2	5.53	123.07	120.30
1	D	1	MET	CA-C-O	-5.53	108.48	120.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	H	200	ARG	CB-CG-CD	5.53	125.98	111.60
1	F	57	ARG	CA-CB-CG	5.53	125.56	113.40
1	E	5	ASP	CB-CG-OD1	-5.52	113.33	118.30
1	O	72	LYS	CB-CA-C	5.52	121.44	110.40
1	b	57	ARG	CB-CG-CD	5.51	125.92	111.60
1	X	212	ARG	NE-CZ-NH1	-5.50	117.55	120.30
1	D	47	LYS	CG-CD-CE	5.50	128.39	111.90
1	S	258	ARG	NE-CZ-NH2	-5.50	117.55	120.30
1	S	258	ARG	CA-C-O	5.49	131.62	120.10
1	B	116	TYR	CB-CA-C	5.48	121.36	110.40
1	c	116	TYR	CB-CG-CD2	5.47	124.28	121.00
1	S	258	ARG	CB-CG-CD	5.47	125.81	111.60
1	A	5	ASP	CB-CG-OD2	-5.46	113.39	118.30
1	H	5	ASP	CB-CG-OD2	-5.46	113.39	118.30
1	Y	116	TYR	CB-CG-CD2	5.46	124.28	121.00
1	D	57	ARG	CB-CG-CD	5.44	125.74	111.60
1	M	206	GLU	N-CA-CB	5.43	120.38	110.60
1	W	212	ARG	NE-CZ-NH1	-5.43	117.58	120.30
1	F	156	HIS	CB-CA-C	5.43	121.26	110.40
1	G	116	TYR	CB-CG-CD2	5.42	124.25	121.00
1	Q	213	ARG	NE-CZ-NH1	-5.42	117.59	120.30
1	D	72	LYS	CB-CA-C	5.42	121.25	110.40
1	N	213	ARG	CG-CD-NE	-5.42	100.42	111.80
1	N	216	LYS	CD-CE-NZ	-5.41	99.25	111.70
1	Z	57	ARG	NE-CZ-NH2	5.40	123.00	120.30
1	S	2	SER	C-N-CA	5.40	135.20	121.70
1	N	74	LYS	N-CA-CB	-5.40	100.89	110.60
1	K	72	LYS	CB-CA-C	5.39	121.19	110.40
1	a	5	ASP	CB-CG-OD1	-5.39	113.44	118.30
1	Z	258	ARG	NE-CZ-NH1	5.39	123.00	120.30
1	V	57	ARG	CD-NE-CZ	5.39	131.14	123.60
1	J	220	ARG	NH1-CZ-NH2	-5.38	113.49	119.40
1	W	156	HIS	CB-CA-C	5.37	121.15	110.40
1	M	246	ARG	CB-CG-CD	5.37	125.56	111.60
1	a	246	ARG	CB-CG-CD	5.37	125.56	111.60
1	E	57	ARG	CA-CB-CG	5.37	125.20	113.40
1	Q	72	LYS	CB-CA-C	5.37	121.13	110.40
1	b	220	ARG	NH1-CZ-NH2	-5.37	113.50	119.40
1	b	246	ARG	CB-CG-CD	5.37	125.55	111.60
1	A	3	LEU	CB-CG-CD1	5.36	120.12	111.00
1	c	160	ARG	NE-CZ-NH1	5.36	122.98	120.30
1	Q	258	ARG	NE-CZ-NH2	-5.36	117.62	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	246	ARG	CB-CG-CD	5.35	125.52	111.60
1	X	116	TYR	CB-CG-CD2	5.35	124.21	121.00
1	F	116	TYR	CB-CG-CD2	5.35	124.21	121.00
1	b	5	ASP	CB-CG-OD2	-5.34	113.50	118.30
1	T	1	MET	CG-SD-CE	5.33	108.72	100.20
1	U	156	HIS	CB-CA-C	5.33	121.06	110.40
1	c	246	ARG	CB-CG-CD	5.33	125.45	111.60
1	K	156	HIS	CG-ND1-CE1	5.33	115.66	108.20
1	A	199	ARG	CB-CG-CD	5.32	125.44	111.60
1	E	116	TYR	CB-CG-CD2	5.32	124.19	121.00
1	d	77	PRO	N-CA-CB	-5.31	96.76	102.60
1	a	74	LYS	CA-CB-CG	5.30	125.07	113.40
1	W	72	LYS	CD-CE-NZ	5.30	123.89	111.70
1	L	57	ARG	NE-CZ-NH2	5.30	122.95	120.30
1	d	57	ARG	CD-NE-CZ	5.30	131.02	123.60
1	T	246	ARG	CB-CG-CD	5.29	125.36	111.60
1	Q	213	ARG	NE-CZ-NH2	5.29	122.94	120.30
1	M	57	ARG	CG-CD-NE	-5.28	100.71	111.80
1	S	116	TYR	CB-CG-CD2	5.28	124.17	121.00
1	V	57	ARG	CG-CD-NE	-5.28	100.72	111.80
1	B	72	LYS	CG-CD-CE	5.27	127.70	111.90
1	K	246	ARG	CB-CG-CD	5.27	125.30	111.60
1	C	156	HIS	CB-CA-C	5.26	120.92	110.40
1	N	15	ARG	CB-CG-CD	5.26	125.27	111.60
1	c	216	LYS	CG-CD-CE	-5.25	96.16	111.90
1	Q	116	TYR	CB-CG-CD2	5.24	124.15	121.00
1	J	199	ARG	NE-CZ-NH2	5.24	122.92	120.30
1	V	246	ARG	CB-CG-CD	5.24	125.22	111.60
1	d	156	HIS	CB-CA-C	5.24	120.87	110.40
1	E	102	ARG	CG-CD-NE	-5.23	100.82	111.80
1	Q	156	HIS	CB-CA-C	5.23	120.85	110.40
1	Y	156	HIS	CB-CA-C	5.22	120.84	110.40
1	G	246	ARG	CB-CG-CD	5.21	125.16	111.60
1	d	57	ARG	CA-CB-CG	5.21	124.87	113.40
1	A	246	ARG	CB-CG-CD	5.21	125.15	111.60
1	F	246	ARG	CB-CG-CD	5.21	125.15	111.60
1	C	246	ARG	CB-CG-CD	5.21	125.14	111.60
1	O	246	ARG	CB-CG-CD	5.21	125.14	111.60
1	X	246	ARG	CB-CG-CD	5.21	125.13	111.60
1	N	156	HIS	CB-CA-C	5.20	120.79	110.40
1	A	102	ARG	CG-CD-NE	-5.19	100.89	111.80
1	O	57	ARG	NH1-CZ-NH2	-5.19	113.69	119.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	J	156	HIS	CB-CA-C	5.18	120.77	110.40
1	B	102	ARG	CB-CG-CD	5.18	125.07	111.60
1	Y	220	ARG	CG-CD-NE	5.18	122.68	111.80
1	G	57	ARG	CG-CD-NE	-5.18	100.93	111.80
1	H	57	ARG	CG-CD-NE	-5.17	100.94	111.80
1	S	240	PRO	N-CA-CB	-5.17	96.91	102.60
1	M	212	ARG	CB-CG-CD	5.17	125.05	111.60
1	T	57	ARG	NE-CZ-NH2	5.17	122.89	120.30
1	J	1	MET	CG-SD-CE	5.17	108.47	100.20
1	J	246	ARG	CB-CG-CD	5.17	125.03	111.60
1	b	258	ARG	CB-CA-C	5.17	120.73	110.40
1	H	116	TYR	CB-CG-CD2	5.16	124.10	121.00
1	D	213	ARG	NE-CZ-NH1	5.16	122.88	120.30
1	H	102	ARG	CB-CG-CD	5.16	125.00	111.60
1	Y	220	ARG	NH1-CZ-NH2	-5.16	113.73	119.40
1	B	116	TYR	CB-CG-CD2	5.15	124.09	121.00
1	c	57	ARG	CA-CB-CG	5.15	124.74	113.40
1	H	240	PRO	N-CA-CB	-5.15	96.94	102.60
1	N	246	ARG	CB-CG-CD	5.14	124.97	111.60
1	K	1	MET	C-N-CA	5.14	134.56	121.70
1	L	5	ASP	CB-CG-OD1	-5.14	113.68	118.30
1	I	156	HIS	CB-CA-C	5.14	120.67	110.40
1	U	254	ARG	NE-CZ-NH1	5.13	122.87	120.30
1	H	246	ARG	CB-CG-CD	5.13	124.94	111.60
1	a	240	PRO	N-CA-CB	-5.13	96.95	102.60
1	c	156	HIS	CB-CA-C	5.13	120.65	110.40
1	O	156	HIS	CB-CA-C	5.12	120.65	110.40
1	L	246	ARG	CB-CG-CD	5.12	124.92	111.60
1	O	7	ARG	CG-CD-NE	-5.12	101.05	111.80
1	L	156	HIS	CB-CA-C	5.12	120.64	110.40
1	T	72	LYS	CG-CD-CE	5.12	127.26	111.90
1	D	246	ARG	CB-CG-CD	5.12	124.91	111.60
1	R	5	ASP	CB-CG-OD2	-5.12	113.69	118.30
1	R	246	ARG	CB-CG-CD	5.12	124.90	111.60
1	C	72	LYS	CB-CA-C	5.12	120.63	110.40
1	E	57	ARG	NE-CZ-NH2	5.11	122.86	120.30
1	d	116	TYR	CB-CG-CD2	5.11	124.07	121.00
1	A	1	MET	CG-SD-CE	5.11	108.37	100.20
1	I	246	ARG	CB-CG-CD	5.10	124.86	111.60
1	Y	57	ARG	CB-CG-CD	5.10	124.86	111.60
1	E	2	SER	C-N-CA	5.09	134.43	121.70
1	F	157	GLN	CB-CG-CD	-5.09	98.35	111.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	G	156	HIS	CB-CA-C	5.09	120.59	110.40
1	H	156	HIS	CB-CA-C	5.09	120.58	110.40
1	P	246	ARG	CB-CG-CD	5.09	124.84	111.60
1	C	220	ARG	NE-CZ-NH2	-5.09	117.76	120.30
1	V	156	HIS	CB-CA-C	5.09	120.57	110.40
1	X	240	PRO	N-CA-CB	-5.09	97.00	102.60
1	P	156	HIS	CB-CA-C	5.08	120.57	110.40
1	a	156	HIS	CB-CA-C	5.08	120.57	110.40
1	S	156	HIS	CB-CA-C	5.08	120.56	110.40
1	A	156	HIS	CB-CA-C	5.08	120.56	110.40
1	N	213	ARG	NE-CZ-NH1	-5.08	117.76	120.30
1	M	102	ARG	CG-CD-NE	-5.07	101.15	111.80
1	S	246	ARG	CB-CG-CD	5.07	124.79	111.60
1	b	156	HIS	CB-CA-C	5.07	120.55	110.40
1	J	5	ASP	CB-CG-OD2	-5.06	113.74	118.30
1	S	212	ARG	CB-CG-CD	5.06	124.76	111.60
1	M	156	HIS	CB-CA-C	5.05	120.51	110.40
1	U	246	ARG	CB-CG-CD	5.05	124.74	111.60
1	d	240	PRO	N-CA-CB	-5.05	97.04	102.60
1	H	220	ARG	NH1-CZ-NH2	-5.04	113.86	119.40
1	T	156	HIS	CB-CA-C	5.03	120.46	110.40
1	W	5	ASP	CB-CG-OD2	-5.03	113.77	118.30
1	K	160	ARG	NE-CZ-NH1	5.03	122.81	120.30
1	Z	246	ARG	CB-CG-CD	5.03	124.67	111.60
1	U	220	ARG	NH1-CZ-NH2	-5.02	113.88	119.40
1	E	160	ARG	NE-CZ-NH1	5.02	122.81	120.30
1	U	57	ARG	CA-CB-CG	5.01	124.43	113.40
1	Y	240	PRO	N-CA-CB	-5.01	97.09	102.60
1	Z	57	ARG	CA-CB-CG	5.01	124.42	113.40
1	Q	246	ARG	CB-CG-CD	5.01	124.62	111.60
1	X	156	HIS	CB-CA-C	5.01	120.41	110.40
1	Y	246	ARG	CB-CG-CD	5.00	124.61	111.60

There are no chirality outliers.

All (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

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Mol	Chain	Res	Type	Group
1	D	2	SER	Peptide
1	F	2	SER	Peptide
1	G	2	SER	Peptide
1	H	2	SER	Mainchain
1	K	2	SER	Peptide
1	K	5	ASP	Sidechain
1	L	1	MET	Peptide
1	O	199	ARG	Sidechain
1	O	2	SER	Peptide
1	P	2	SER	Peptide
1	Q	2	SER	Peptide
1	S	1	MET	Peptide
1	U	239	PHE	Sidechain
1	W	2	SER	Peptide
1	W	21	GLN	Sidechain
1	X	67	ASP	Sidechain
1	Y	1	MET	Peptide
1	Y	2	SER	Peptide
1	Z	2	SER	Peptide
1	a	2	SER	Peptide
1	c	2	SER	Peptide

5.2 Too-close contacts (i)

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

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	256/261 (98%)	219 (86%)	28 (11%)	9 (4%)	3 30
1	B	256/261 (98%)	217 (85%)	30 (12%)	9 (4%)	3 30

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	257/261 (98%)	216 (84%)	31 (12%)	10 (4%)	3	27
1	D	256/261 (98%)	220 (86%)	27 (10%)	9 (4%)	3	30
1	E	256/261 (98%)	217 (85%)	28 (11%)	11 (4%)	2	24
1	F	256/261 (98%)	219 (86%)	29 (11%)	8 (3%)	4	32
1	G	255/261 (98%)	215 (84%)	31 (12%)	9 (4%)	3	30
1	H	255/261 (98%)	216 (85%)	31 (12%)	8 (3%)	4	32
1	I	255/261 (98%)	217 (85%)	29 (11%)	9 (4%)	3	30
1	J	256/261 (98%)	218 (85%)	29 (11%)	9 (4%)	3	30
1	K	256/261 (98%)	215 (84%)	32 (12%)	9 (4%)	3	30
1	L	256/261 (98%)	220 (86%)	27 (10%)	9 (4%)	3	30
1	M	255/261 (98%)	217 (85%)	29 (11%)	9 (4%)	3	30
1	N	255/261 (98%)	217 (85%)	29 (11%)	9 (4%)	3	30
1	O	255/261 (98%)	217 (85%)	30 (12%)	8 (3%)	4	32
1	P	255/261 (98%)	215 (84%)	32 (12%)	8 (3%)	4	32
1	Q	255/261 (98%)	216 (85%)	31 (12%)	8 (3%)	4	32
1	R	255/261 (98%)	216 (85%)	30 (12%)	9 (4%)	3	30
1	S	256/261 (98%)	217 (85%)	30 (12%)	9 (4%)	3	30
1	T	256/261 (98%)	219 (86%)	28 (11%)	9 (4%)	3	30
1	U	256/261 (98%)	218 (85%)	29 (11%)	9 (4%)	3	30
1	V	255/261 (98%)	218 (86%)	28 (11%)	9 (4%)	3	30
1	W	255/261 (98%)	218 (86%)	28 (11%)	9 (4%)	3	30
1	X	255/261 (98%)	216 (85%)	30 (12%)	9 (4%)	3	30
1	Y	256/261 (98%)	217 (85%)	30 (12%)	9 (4%)	3	30
1	Z	256/261 (98%)	216 (84%)	31 (12%)	9 (4%)	3	30
1	a	255/261 (98%)	216 (85%)	30 (12%)	9 (4%)	3	30
1	b	255/261 (98%)	216 (85%)	30 (12%)	9 (4%)	3	30
1	c	256/261 (98%)	220 (86%)	27 (10%)	9 (4%)	3	30
1	d	255/261 (98%)	217 (85%)	30 (12%)	8 (3%)	4	32
All	All	7666/7830 (98%)	6515 (85%)	884 (12%)	267 (4%)	3	30

All (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
1	E	233	ALA
1	F	233	ALA
1	G	233	ALA
1	H	233	ALA
1	I	233	ALA
1	M	233	ALA
1	N	233	ALA
1	O	233	ALA
1	J	233	ALA
1	K	3	LEU
1	K	233	ALA
1	L	233	ALA
1	P	233	ALA
1	Q	233	ALA
1	R	233	ALA
1	S	233	ALA
1	T	233	ALA
1	U	233	ALA
1	V	233	ALA
1	W	233	ALA
1	X	233	ALA
1	Y	233	ALA
1	Z	233	ALA
1	a	233	ALA
1	b	233	ALA
1	c	233	ALA
1	d	233	ALA
1	A	97	GLY
1	A	250	GLN
1	B	29	GLY
1	B	97	GLY
1	B	250	GLN
1	C	97	GLY
1	C	250	GLN
1	D	97	GLY
1	D	250	GLN
1	E	2	SER
1	E	97	GLY

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Mol	Chain	Res	Type
1	E	250	GLN
1	F	97	GLY
1	F	250	GLN
1	G	97	GLY
1	G	250	GLN
1	H	97	GLY
1	H	250	GLN
1	I	97	GLY
1	I	250	GLN
1	M	97	GLY
1	M	250	GLN
1	N	97	GLY
1	N	250	GLN
1	O	97	GLY
1	O	250	GLN
1	J	97	GLY
1	J	250	GLN
1	K	97	GLY
1	K	250	GLN
1	L	97	GLY
1	L	250	GLN
1	P	97	GLY
1	P	250	GLN
1	Q	97	GLY
1	Q	250	GLN
1	R	97	GLY
1	R	250	GLN
1	S	97	GLY
1	S	250	GLN
1	T	97	GLY
1	T	250	GLN
1	U	97	GLY
1	U	250	GLN
1	V	97	GLY
1	V	250	GLN
1	W	97	GLY
1	W	250	GLN
1	X	97	GLY
1	X	250	GLN
1	Y	97	GLY
1	Y	250	GLN
1	Z	97	GLY

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Mol	Chain	Res	Type
1	Z	250	GLN
1	a	97	GLY
1	a	250	GLN
1	b	97	GLY
1	b	250	GLN
1	c	97	GLY
1	c	250	GLN
1	d	29	GLY
1	d	97	GLY
1	d	250	GLN
1	A	29	GLY
1	A	196	GLU
1	B	196	GLU
1	C	29	GLY
1	C	196	GLU
1	D	196	GLU
1	E	29	GLY
1	E	196	GLU
1	F	29	GLY
1	F	196	GLU
1	G	196	GLU
1	H	196	GLU
1	I	196	GLU
1	M	196	GLU
1	N	196	GLU
1	O	196	GLU
1	J	196	GLU
1	K	196	GLU
1	L	29	GLY
1	L	196	GLU
1	P	196	GLU
1	Q	196	GLU
1	R	196	GLU
1	S	29	GLY
1	S	196	GLU
1	T	29	GLY
1	T	196	GLU
1	U	196	GLU
1	V	29	GLY
1	V	196	GLU
1	W	29	GLY
1	W	196	GLU

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Mol	Chain	Res	Type
1	X	196	GLU
1	Y	196	GLU
1	Z	29	GLY
1	Z	196	GLU
1	a	196	GLU
1	b	29	GLY
1	b	196	GLU
1	c	29	GLY
1	c	196	GLU
1	d	196	GLU
1	A	224	THR
1	B	224	THR
1	C	224	THR
1	D	29	GLY
1	D	157	GLN
1	D	224	THR
1	E	224	THR
1	F	224	THR
1	G	29	GLY
1	G	224	THR
1	H	29	GLY
1	H	224	THR
1	I	29	GLY
1	M	224	THR
1	N	29	GLY
1	N	224	THR
1	O	29	GLY
1	O	224	THR
1	J	29	GLY
1	K	29	GLY
1	K	157	GLN
1	L	157	GLN
1	L	224	THR
1	P	29	GLY
1	P	224	THR
1	Q	29	GLY
1	Q	224	THR
1	R	29	GLY
1	R	224	THR
1	S	222	GLY
1	S	224	THR
1	U	29	GLY

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Mol	Chain	Res	Type
1	U	222	GLY
1	U	224	THR
1	V	224	THR
1	W	224	THR
1	X	29	GLY
1	X	224	THR
1	Y	29	GLY
1	Y	157	GLN
1	Y	224	THR
1	Z	224	THR
1	a	29	GLY
1	a	157	GLN
1	b	224	THR
1	c	157	GLN
1	c	224	THR
1	d	157	GLN
1	d	224	THR
1	A	157	GLN
1	A	222	GLY
1	B	157	GLN
1	B	222	GLY
1	C	157[A]	GLN
1	C	157[B]	GLN
1	C	222	GLY
1	E	157	GLN
1	E	222	GLY
1	G	157	GLN
1	G	222	GLY
1	H	157	GLN
1	I	157	GLN
1	I	224	THR
1	M	29	GLY
1	M	157	GLN
1	N	157	GLN
1	N	222	GLY
1	O	157	GLN
1	J	157	GLN
1	J	224	THR
1	K	222	GLY
1	K	224	THR
1	P	157	GLN
1	P	222	GLY

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Mol	Chain	Res	Type
1	Q	157	GLN
1	Q	222	GLY
1	R	157	GLN
1	S	157	GLN
1	T	157	GLN
1	T	222	GLY
1	T	224	THR
1	U	157	GLN
1	V	157	GLN
1	W	157	GLN
1	W	222	GLY
1	X	157	GLN
1	Z	157	GLN
1	a	224	THR
1	b	157	GLN
1	b	222	GLY
1	d	222	GLY
1	D	222	GLY
1	F	222	GLY
1	I	222	GLY
1	M	222	GLY
1	O	222	GLY
1	J	222	GLY
1	L	222	GLY
1	R	222	GLY
1	Y	222	GLY
1	Z	222	GLY
1	a	222	GLY
1	c	222	GLY
1	H	222	GLY
1	V	222	GLY
1	X	222	GLY
1	A	77	PRO
1	B	77	PRO
1	E	77	PRO
1	D	77	PRO
1	F	77	PRO
1	T	77	PRO
1	C	77	PRO
1	G	77	PRO
1	I	77	PRO
1	M	77	PRO

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Mol	Chain	Res	Type
1	J	77	PRO
1	L	77	PRO
1	S	77	PRO
1	U	77	PRO
1	V	77	PRO
1	W	77	PRO
1	Y	77	PRO
1	Z	77	PRO
1	c	77	PRO
1	N	77	PRO
1	R	77	PRO
1	X	77	PRO
1	a	77	PRO
1	b	77	PRO

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	206/208 (99%)	188 (91%)	18 (9%)	10 41
1	B	206/208 (99%)	183 (89%)	23 (11%)	6 31
1	C	207/208 (100%)	185 (89%)	22 (11%)	6 33
1	D	206/208 (99%)	183 (89%)	23 (11%)	6 31
1	E	206/208 (99%)	185 (90%)	21 (10%)	7 34
1	F	206/208 (99%)	178 (86%)	28 (14%)	3 22
1	G	205/208 (99%)	182 (89%)	23 (11%)	6 31
1	H	205/208 (99%)	183 (89%)	22 (11%)	6 33
1	I	205/208 (99%)	181 (88%)	24 (12%)	5 29
1	J	206/208 (99%)	183 (89%)	23 (11%)	6 31
1	K	206/208 (99%)	182 (88%)	24 (12%)	5 29
1	L	206/208 (99%)	182 (88%)	24 (12%)	5 29
1	M	205/208 (99%)	184 (90%)	21 (10%)	7 34

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	N	205/208 (99%)	178 (87%)	27 (13%)	4	23
1	O	205/208 (99%)	181 (88%)	24 (12%)	5	29
1	P	205/208 (99%)	182 (89%)	23 (11%)	6	31
1	Q	205/208 (99%)	182 (89%)	23 (11%)	6	31
1	R	205/208 (99%)	183 (89%)	22 (11%)	6	33
1	S	206/208 (99%)	180 (87%)	26 (13%)	4	24
1	T	206/208 (99%)	185 (90%)	21 (10%)	7	34
1	U	206/208 (99%)	179 (87%)	27 (13%)	4	23
1	V	205/208 (99%)	182 (89%)	23 (11%)	6	31
1	W	205/208 (99%)	182 (89%)	23 (11%)	6	31
1	X	205/208 (99%)	182 (89%)	23 (11%)	6	31
1	Y	206/208 (99%)	183 (89%)	23 (11%)	6	31
1	Z	206/208 (99%)	185 (90%)	21 (10%)	7	34
1	a	205/208 (99%)	181 (88%)	24 (12%)	5	29
1	b	205/208 (99%)	182 (89%)	23 (11%)	6	31
1	c	206/208 (99%)	185 (90%)	21 (10%)	7	34
1	d	205/208 (99%)	180 (88%)	25 (12%)	5	26
All	All	6166/6240 (99%)	5471 (89%)	695 (11%)	6	30

All (695) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	15	ARG
1	A	47	LYS
1	A	63	SER
1	A	67	ASP
1	A	70	ASP
1	A	71	LEU
1	A	79	ARG
1	A	102	ARG
1	A	156	HIS
1	A	192	SER
1	A	193	MET
1	A	196	GLU
1	A	199	ARG
1	A	205	SER

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Mol	Chain	Res	Type
1	A	212	ARG
1	A	221	GLN
1	A	240	PRO
1	A	253	THR
1	B	1	MET
1	B	15	ARG
1	B	47	LYS
1	B	51	LYS
1	B	57	ARG
1	B	63	SER
1	B	67	ASP
1	B	70	ASP
1	B	74	LYS
1	B	79	ARG
1	B	102	ARG
1	B	156	HIS
1	B	157	GLN
1	B	192	SER
1	B	193	MET
1	B	196	GLU
1	B	199	ARG
1	B	205	SER
1	B	212	ARG
1	B	216	LYS
1	B	221	GLN
1	B	240	PRO
1	B	253	THR
1	C	1	MET
1	C	15	ARG
1	C	47	LYS
1	C	51	LYS
1	C	57	ARG
1	C	63	SER
1	C	67	ASP
1	C	70	ASP
1	C	71	LEU
1	C	74	LYS
1	C	79	ARG
1	C	102	ARG
1	C	156	HIS
1	C	192	SER
1	C	193	MET

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Mol	Chain	Res	Type
1	C	196	GLU
1	C	199	ARG
1	C	205	SER
1	C	220	ARG
1	C	221	GLN
1	C	240	PRO
1	C	253	THR
1	D	1	MET
1	D	15	ARG
1	D	47	LYS
1	D	51	LYS
1	D	63	SER
1	D	67	ASP
1	D	70	ASP
1	D	71	LEU
1	D	79	ARG
1	D	102	ARG
1	D	156	HIS
1	D	192	SER
1	D	193	MET
1	D	196	GLU
1	D	199	ARG
1	D	205	SER
1	D	212	ARG
1	D	216	LYS
1	D	221	GLN
1	D	240	PRO
1	D	246	ARG
1	D	251	SER
1	D	253	THR
1	E	1	MET
1	E	47	LYS
1	E	54	LYS
1	E	57	ARG
1	E	63	SER
1	E	67	ASP
1	E	70	ASP
1	E	79	ARG
1	E	102	ARG
1	E	156	HIS
1	E	192	SER
1	E	193	MET

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Mol	Chain	Res	Type
1	E	196	GLU
1	E	199	ARG
1	E	205	SER
1	E	212	ARG
1	E	221	GLN
1	E	240	PRO
1	E	246	ARG
1	E	251	SER
1	E	253	THR
1	F	1	MET
1	F	13	SER
1	F	15	ARG
1	F	47	LYS
1	F	54	LYS
1	F	57	ARG
1	F	63	SER
1	F	67	ASP
1	F	70	ASP
1	F	71	LEU
1	F	72	LYS
1	F	74	LYS
1	F	79	ARG
1	F	156	HIS
1	F	157	GLN
1	F	192	SER
1	F	193	MET
1	F	196	GLU
1	F	199	ARG
1	F	205	SER
1	F	212	ARG
1	F	216	LYS
1	F	220	ARG
1	F	221	GLN
1	F	240	PRO
1	F	246	ARG
1	F	251	SER
1	F	253	THR
1	G	15	ARG
1	G	47	LYS
1	G	63	SER
1	G	67	ASP
1	G	70	ASP

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Mol	Chain	Res	Type
1	G	71	LEU
1	G	79	ARG
1	G	102	ARG
1	G	156	HIS
1	G	192	SER
1	G	193	MET
1	G	196	GLU
1	G	199	ARG
1	G	205	SER
1	G	212	ARG
1	G	216	LYS
1	G	220	ARG
1	G	221	GLN
1	G	226	GLU
1	G	240	PRO
1	G	246	ARG
1	G	253	THR
1	G	258	ARG
1	H	13	SER
1	H	15	ARG
1	H	47	LYS
1	H	51	LYS
1	H	63	SER
1	H	67	ASP
1	H	70	ASP
1	H	71	LEU
1	H	79	ARG
1	H	102	ARG
1	H	156	HIS
1	H	192	SER
1	H	193	MET
1	H	196	GLU
1	H	199	ARG
1	H	205	SER
1	H	212	ARG
1	H	221	GLN
1	H	226	GLU
1	H	240	PRO
1	H	253	THR
1	H	258	ARG
1	I	13	SER
1	I	15	ARG

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Mol	Chain	Res	Type
1	I	47	LYS
1	I	51	LYS
1	I	63	SER
1	I	67	ASP
1	I	70	ASP
1	I	74	LYS
1	I	79	ARG
1	I	156	HIS
1	I	160	ARG
1	I	192	SER
1	I	193	MET
1	I	196	GLU
1	I	199	ARG
1	I	205	SER
1	I	212	ARG
1	I	216	LYS
1	I	221	GLN
1	I	226	GLU
1	I	240	PRO
1	I	246	ARG
1	I	253	THR
1	I	258	ARG
1	M	7	ARG
1	M	15	ARG
1	M	47	LYS
1	M	63	SER
1	M	67	ASP
1	M	70	ASP
1	M	71	LEU
1	M	79	ARG
1	M	102	ARG
1	M	156	HIS
1	M	192	SER
1	M	193	MET
1	M	196	GLU
1	M	199	ARG
1	M	205	SER
1	M	220	ARG
1	M	221	GLN
1	M	240	PRO
1	M	251	SER
1	M	253	THR

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Mol	Chain	Res	Type
1	M	258	ARG
1	N	7	ARG
1	N	13	SER
1	N	15	ARG
1	N	47	LYS
1	N	51	LYS
1	N	54	LYS
1	N	63	SER
1	N	67	ASP
1	N	70	ASP
1	N	71	LEU
1	N	74	LYS
1	N	79	ARG
1	N	102	ARG
1	N	156	HIS
1	N	192	SER
1	N	193	MET
1	N	196	GLU
1	N	199	ARG
1	N	205	SER
1	N	212	ARG
1	N	221	GLN
1	N	226	GLU
1	N	240	PRO
1	N	246	ARG
1	N	251	SER
1	N	253	THR
1	N	258	ARG
1	O	2	SER
1	O	7	ARG
1	O	13	SER
1	O	15	ARG
1	O	47	LYS
1	O	63	SER
1	O	67	ASP
1	O	70	ASP
1	O	74	LYS
1	O	79	ARG
1	O	156	HIS
1	O	160	ARG
1	O	192	SER
1	O	193	MET

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Mol	Chain	Res	Type
1	O	196	GLU
1	O	199	ARG
1	O	200	ARG
1	O	205	SER
1	O	212	ARG
1	O	221	GLN
1	O	240	PRO
1	O	246	ARG
1	O	253	THR
1	O	258	ARG
1	J	13	SER
1	J	15	ARG
1	J	47	LYS
1	J	51	LYS
1	J	63	SER
1	J	67	ASP
1	J	70	ASP
1	J	71	LEU
1	J	72	LYS
1	J	74	LYS
1	J	79	ARG
1	J	102	ARG
1	J	156	HIS
1	J	192	SER
1	J	193	MET
1	J	196	GLU
1	J	199	ARG
1	J	205	SER
1	J	212	ARG
1	J	221	GLN
1	J	240	PRO
1	J	246	ARG
1	J	253	THR
1	K	1	MET
1	K	2	SER
1	K	15	ARG
1	K	47	LYS
1	K	51	LYS
1	K	57	ARG
1	K	63	SER
1	K	67	ASP
1	K	70	ASP

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Mol	Chain	Res	Type
1	K	74	LYS
1	K	79	ARG
1	K	102	ARG
1	K	156	HIS
1	K	157	GLN
1	K	192	SER
1	K	193	MET
1	K	196	GLU
1	K	199	ARG
1	K	205	SER
1	K	212	ARG
1	K	220	ARG
1	K	221	GLN
1	K	240	PRO
1	K	253	THR
1	L	13	SER
1	L	15	ARG
1	L	47	LYS
1	L	57	ARG
1	L	63	SER
1	L	67	ASP
1	L	70	ASP
1	L	71	LEU
1	L	74	LYS
1	L	79	ARG
1	L	102	ARG
1	L	156	HIS
1	L	192	SER
1	L	193	MET
1	L	196	GLU
1	L	199	ARG
1	L	200	ARG
1	L	205	SER
1	L	212	ARG
1	L	216	LYS
1	L	221	GLN
1	L	240	PRO
1	L	246	ARG
1	L	253	THR
1	P	15	ARG
1	P	47	LYS
1	P	51	LYS

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Mol	Chain	Res	Type
1	P	63	SER
1	P	67	ASP
1	P	70	ASP
1	P	71	LEU
1	P	79	ARG
1	P	102	ARG
1	P	156	HIS
1	P	192	SER
1	P	193	MET
1	P	196	GLU
1	P	199	ARG
1	P	205	SER
1	P	212	ARG
1	P	213	ARG
1	P	220	ARG
1	P	221	GLN
1	P	240	PRO
1	P	246	ARG
1	P	253	THR
1	P	258	ARG
1	Q	13	SER
1	Q	15	ARG
1	Q	47	LYS
1	Q	51	LYS
1	Q	63	SER
1	Q	67	ASP
1	Q	70	ASP
1	Q	71	LEU
1	Q	79	ARG
1	Q	102	ARG
1	Q	156	HIS
1	Q	175	LYS
1	Q	192	SER
1	Q	193	MET
1	Q	196	GLU
1	Q	199	ARG
1	Q	205	SER
1	Q	212	ARG
1	Q	221	GLN
1	Q	240	PRO
1	Q	246	ARG
1	Q	253	THR

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Mol	Chain	Res	Type
1	Q	258	ARG
1	R	13	SER
1	R	15	ARG
1	R	47	LYS
1	R	51	LYS
1	R	63	SER
1	R	67	ASP
1	R	70	ASP
1	R	79	ARG
1	R	102	ARG
1	R	156	HIS
1	R	192	SER
1	R	193	MET
1	R	196	GLU
1	R	199	ARG
1	R	205	SER
1	R	212	ARG
1	R	216	LYS
1	R	221	GLN
1	R	240	PRO
1	R	246	ARG
1	R	253	THR
1	R	258	ARG
1	S	13	SER
1	S	15	ARG
1	S	47	LYS
1	S	51	LYS
1	S	54	LYS
1	S	63	SER
1	S	67	ASP
1	S	70	ASP
1	S	71	LEU
1	S	74	LYS
1	S	79	ARG
1	S	102	ARG
1	S	156	HIS
1	S	192	SER
1	S	193	MET
1	S	196	GLU
1	S	199	ARG
1	S	200	ARG
1	S	205	SER

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Mol	Chain	Res	Type
1	S	212	ARG
1	S	220	ARG
1	S	221	GLN
1	S	240	PRO
1	S	246	ARG
1	S	253	THR
1	S	258	ARG
1	T	1	MET
1	T	15	ARG
1	T	47	LYS
1	T	51	LYS
1	T	57	ARG
1	T	63	SER
1	T	67	ASP
1	T	70	ASP
1	T	79	ARG
1	T	102	ARG
1	T	156	HIS
1	T	192	SER
1	T	193	MET
1	T	196	GLU
1	T	199	ARG
1	T	205	SER
1	T	212	ARG
1	T	220	ARG
1	T	221	GLN
1	T	240	PRO
1	T	253	THR
1	U	1	MET
1	U	15	ARG
1	U	47	LYS
1	U	54	LYS
1	U	57	ARG
1	U	63	SER
1	U	67	ASP
1	U	70	ASP
1	U	71	LEU
1	U	72	LYS
1	U	74	LYS
1	U	79	ARG
1	U	102	ARG
1	U	156	HIS

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Mol	Chain	Res	Type
1	U	175	LYS
1	U	192	SER
1	U	193	MET
1	U	196	GLU
1	U	199	ARG
1	U	205	SER
1	U	212	ARG
1	U	216	LYS
1	U	221	GLN
1	U	240	PRO
1	U	246	ARG
1	U	251	SER
1	U	253	THR
1	V	15	ARG
1	V	47	LYS
1	V	51	LYS
1	V	63	SER
1	V	67	ASP
1	V	70	ASP
1	V	71	LEU
1	V	79	ARG
1	V	102	ARG
1	V	156	HIS
1	V	192	SER
1	V	193	MET
1	V	196	GLU
1	V	199	ARG
1	V	205	SER
1	V	212	ARG
1	V	216	LYS
1	V	220	ARG
1	V	221	GLN
1	V	240	PRO
1	V	246	ARG
1	V	253	THR
1	V	258	ARG
1	W	15	ARG
1	W	21	GLN
1	W	47	LYS
1	W	63	SER
1	W	67	ASP
1	W	70	ASP

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Mol	Chain	Res	Type
1	W	71	LEU
1	W	72	LYS
1	W	79	ARG
1	W	102	ARG
1	W	156	HIS
1	W	175	LYS
1	W	192	SER
1	W	193	MET
1	W	196	GLU
1	W	199	ARG
1	W	205	SER
1	W	212	ARG
1	W	221	GLN
1	W	240	PRO
1	W	246	ARG
1	W	253	THR
1	W	258	ARG
1	X	2	SER
1	X	13	SER
1	X	15	ARG
1	X	31	GLU
1	X	47	LYS
1	X	51	LYS
1	X	63	SER
1	X	70	ASP
1	X	79	ARG
1	X	102	ARG
1	X	156	HIS
1	X	160	ARG
1	X	192	SER
1	X	193	MET
1	X	196	GLU
1	X	199	ARG
1	X	205	SER
1	X	212	ARG
1	X	221	GLN
1	X	240	PRO
1	X	246	ARG
1	X	253	THR
1	X	258	ARG
1	Y	1	MET
1	Y	15	ARG

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Mol	Chain	Res	Type
1	Y	47	LYS
1	Y	51	LYS
1	Y	63	SER
1	Y	67	ASP
1	Y	70	ASP
1	Y	71	LEU
1	Y	74	LYS
1	Y	79	ARG
1	Y	102	ARG
1	Y	156	HIS
1	Y	192	SER
1	Y	193	MET
1	Y	196	GLU
1	Y	199	ARG
1	Y	205	SER
1	Y	212	ARG
1	Y	221	GLN
1	Y	240	PRO
1	Y	246	ARG
1	Y	251	SER
1	Y	253	THR
1	Z	1	MET
1	Z	15	ARG
1	Z	47	LYS
1	Z	51	LYS
1	Z	57	ARG
1	Z	63	SER
1	Z	67	ASP
1	Z	70	ASP
1	Z	79	ARG
1	Z	102	ARG
1	Z	156	HIS
1	Z	192	SER
1	Z	193	MET
1	Z	196	GLU
1	Z	199	ARG
1	Z	200	ARG
1	Z	205	SER
1	Z	212	ARG
1	Z	221	GLN
1	Z	240	PRO
1	Z	253	THR

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Mol	Chain	Res	Type
1	a	13	SER
1	a	15	ARG
1	a	47	LYS
1	a	51	LYS
1	a	57	ARG
1	a	63	SER
1	a	67	ASP
1	a	70	ASP
1	a	71	LEU
1	a	74	LYS
1	a	79	ARG
1	a	102	ARG
1	a	156	HIS
1	a	192	SER
1	a	193	MET
1	a	196	GLU
1	a	199	ARG
1	a	205	SER
1	a	212	ARG
1	a	221	GLN
1	a	225	VAL
1	a	240	PRO
1	a	253	THR
1	a	258	ARG
1	b	2	SER
1	b	15	ARG
1	b	33	GLU
1	b	47	LYS
1	b	51	LYS
1	b	63	SER
1	b	67	ASP
1	b	70	ASP
1	b	71	LEU
1	b	79	ARG
1	b	102	ARG
1	b	156	HIS
1	b	192	SER
1	b	193	MET
1	b	196	GLU
1	b	199	ARG
1	b	205	SER
1	b	212	ARG

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Mol	Chain	Res	Type
1	b	216	LYS
1	b	221	GLN
1	b	240	PRO
1	b	253	THR
1	b	258	ARG
1	c	1	MET
1	c	47	LYS
1	c	51	LYS
1	c	57	ARG
1	c	63	SER
1	c	67	ASP
1	c	70	ASP
1	c	79	ARG
1	c	102	ARG
1	c	156	HIS
1	c	192	SER
1	c	193	MET
1	c	196	GLU
1	c	199	ARG
1	c	205	SER
1	c	212	ARG
1	c	220	ARG
1	c	221	GLN
1	c	226	GLU
1	c	240	PRO
1	c	253	THR
1	d	13	SER
1	d	15	ARG
1	d	47	LYS
1	d	51	LYS
1	d	57	ARG
1	d	63	SER
1	d	66	GLU
1	d	67	ASP
1	d	70	ASP
1	d	71	LEU
1	d	74	LYS
1	d	79	ARG
1	d	102	ARG
1	d	156	HIS
1	d	192	SER
1	d	193	MET

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Mol	Chain	Res	Type
1	d	196	GLU
1	d	199	ARG
1	d	205	SER
1	d	212	ARG
1	d	221	GLN
1	d	240	PRO
1	d	246	ARG
1	d	253	THR
1	d	258	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (108) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	55	HIS
1	A	121	HIS
1	A	164	HIS
1	B	85	HIS
1	B	121	HIS
1	B	164	HIS
1	C	85	HIS
1	C	121	HIS
1	C	164	HIS
1	D	85	HIS
1	D	121	HIS
1	D	164	HIS
1	E	55	HIS
1	E	121	HIS
1	E	164	HIS
1	F	85	HIS
1	F	121	HIS
1	F	164	HIS
1	G	43	HIS
1	G	55	HIS
1	G	121	HIS
1	G	164	HIS
1	H	55	HIS
1	H	95	HIS
1	H	121	HIS
1	H	164	HIS
1	I	43	HIS
1	I	55	HIS
1	I	164	HIS

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Mol	Chain	Res	Type
1	I	223	HIS
1	M	43	HIS
1	M	55	HIS
1	M	164	HIS
1	M	223	HIS
1	N	55	HIS
1	N	121	HIS
1	N	164	HIS
1	N	223	HIS
1	O	43	HIS
1	O	55	HIS
1	O	56	ASN
1	O	121	HIS
1	O	164	HIS
1	O	223	HIS
1	J	85	HIS
1	J	121	HIS
1	J	164	HIS
1	J	223	HIS
1	K	85	HIS
1	K	121	HIS
1	K	157	GLN
1	K	164	HIS
1	K	223	HIS
1	L	85	HIS
1	L	121	HIS
1	L	164	HIS
1	L	223	HIS
1	P	43	HIS
1	P	85	HIS
1	P	121	HIS
1	P	164	HIS
1	Q	55	HIS
1	Q	164	HIS
1	R	43	HIS
1	R	55	HIS
1	R	121	HIS
1	R	164	HIS
1	R	223	HIS
1	S	85	HIS
1	S	121	HIS
1	S	164	HIS

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Mol	Chain	Res	Type
1	T	85	HIS
1	T	121	HIS
1	T	164	HIS
1	U	55	HIS
1	U	121	HIS
1	U	164	HIS
1	V	43	HIS
1	V	85	HIS
1	V	121	HIS
1	V	164	HIS
1	V	223	HIS
1	W	55	HIS
1	W	121	HIS
1	W	164	HIS
1	W	223	HIS
1	X	43	HIS
1	X	55	HIS
1	X	164	HIS
1	X	223	HIS
1	Y	85	HIS
1	Y	164	HIS
1	Z	55	HIS
1	Z	164	HIS
1	Z	223	HIS
1	a	55	HIS
1	a	121	HIS
1	a	164	HIS
1	a	223	HIS
1	b	55	HIS
1	b	121	HIS
1	b	164	HIS
1	c	55	HIS
1	c	121	HIS
1	c	164	HIS
1	d	55	HIS
1	d	121	HIS
1	d	164	HIS

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

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	303	-	4,4,4	0.30	0	6,6,6	0.14	0
3	SO4	F	301	-	4,4,4	0.35	0	6,6,6	0.13	0
4	VFZ	A	310	-	24,29,29	1.22	2 (8%)	25,39,39	2.01	5 (20%)
3	SO4	B	303	-	4,4,4	0.36	0	6,6,6	0.14	0
3	SO4	R	301	-	4,4,4	0.35	0	6,6,6	0.17	0
4	VFZ	H	303	-	24,29,29	1.09	2 (8%)	25,39,39	1.87	4 (16%)
3	SO4	D	304	-	4,4,4	0.33	0	6,6,6	0.17	0
3	SO4	Y	302	-	4,4,4	0.29	0	6,6,6	0.25	0
3	SO4	U	303	-	4,4,4	0.35	0	6,6,6	0.09	0
3	SO4	F	302	-	4,4,4	0.30	0	6,6,6	0.09	0
4	VFZ	I	304	-	24,29,29	1.17	2 (8%)	25,39,39	1.76	3 (12%)
3	SO4	G	303	-	4,4,4	0.34	0	6,6,6	0.19	0
3	SO4	E	304	-	4,4,4	0.30	0	6,6,6	0.07	0
3	SO4	T	302	-	4,4,4	0.35	0	6,6,6	0.12	0
3	SO4	A	308	-	4,4,4	0.30	0	6,6,6	0.22	0
4	VFZ	B	305	-	24,29,29	1.15	2 (8%)	25,39,39	1.80	4 (16%)
3	SO4	D	302	-	4,4,4	0.38	0	6,6,6	0.15	0
3	SO4	J	301	-	4,4,4	0.33	0	6,6,6	0.23	0
4	VFZ	W	302	-	24,29,29	1.06	2 (8%)	25,39,39	2.00	7 (28%)
3	SO4	A	309	-	4,4,4	0.35	0	6,6,6	0.20	0
3	SO4	C	304	-	4,4,4	0.36	0	6,6,6	0.13	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	SO4	D	303	-	4,4,4	0.28	0	6,6,6	0.22	0
3	SO4	A	307	-	4,4,4	0.33	0	6,6,6	0.15	0
3	SO4	K	302	-	4,4,4	0.29	0	6,6,6	0.18	0
4	VFZ	C	306	-	24,29,29	1.07	1 (4%)	25,39,39	1.95	5 (20%)
4	VFZ	N	305	-	24,29,29	1.06	1 (4%)	25,39,39	1.85	4 (16%)
3	SO4	B	304	-	4,4,4	0.28	0	6,6,6	0.18	0
3	SO4	N	302	-	4,4,4	0.38	0	6,6,6	0.19	0
4	VFZ	G	304	-	24,29,29	1.10	2 (8%)	25,39,39	1.71	3 (12%)
3	SO4	G	302	-	4,4,4	0.34	0	6,6,6	0.22	0
3	SO4	H	302	-	4,4,4	0.34	0	6,6,6	0.18	0
4	VFZ	c	303	-	24,29,29	1.13	2 (8%)	25,39,39	1.72	2 (8%)
3	SO4	P	303	-	4,4,4	0.29	0	6,6,6	0.17	0
3	SO4	E	303	-	4,4,4	0.45	0	6,6,6	0.16	0
3	SO4	C	305	-	4,4,4	0.27	0	6,6,6	0.15	0
4	VFZ	M	304	-	24,29,29	1.13	2 (8%)	25,39,39	1.72	3 (12%)

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	B	305	-	-	1/16/17/17	0/3/3/3
4	VFZ	G	304	-	-	0/16/17/17	0/3/3/3
4	VFZ	A	310	-	-	0/16/17/17	0/3/3/3
4	VFZ	H	303	-	-	1/16/17/17	0/3/3/3
4	VFZ	W	302	-	-	1/16/17/17	0/3/3/3
4	VFZ	I	304	-	-	0/16/17/17	0/3/3/3
4	VFZ	N	305	-	-	0/16/17/17	0/3/3/3
4	VFZ	c	303	-	-	0/16/17/17	0/3/3/3
4	VFZ	C	306	-	-	1/16/17/17	0/3/3/3
4	VFZ	M	304	-	-	0/16/17/17	0/3/3/3

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	310	VFZ	C8-C4	3.26	1.45	1.38
4	I	304	VFZ	C8-C4	3.19	1.45	1.38
4	c	303	VFZ	C8-C4	3.05	1.45	1.38
4	N	305	VFZ	C8-C4	3.04	1.45	1.38
4	H	303	VFZ	C8-C4	3.00	1.45	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	M	304	VFZ	C8-C4	2.96	1.45	1.38
4	B	305	VFZ	C8-C4	2.93	1.45	1.38
4	A	310	VFZ	C6-N4	2.89	1.38	1.33
4	G	304	VFZ	C8-C4	2.88	1.45	1.38
4	c	303	VFZ	C6-N4	2.72	1.37	1.33
4	M	304	VFZ	C6-N4	2.69	1.37	1.33
4	W	302	VFZ	C8-C4	2.68	1.44	1.38
4	C	306	VFZ	C8-C4	2.60	1.44	1.38
4	G	304	VFZ	C6-N4	2.60	1.37	1.33
4	B	305	VFZ	C6-N4	2.54	1.37	1.33
4	I	304	VFZ	C6-N4	2.45	1.37	1.33
4	H	303	VFZ	C6-N4	2.27	1.37	1.33
4	W	302	VFZ	C6-N4	2.01	1.36	1.33

All (40) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	C	306	VFZ	C7-C6-N4	-5.66	115.07	124.79
4	H	303	VFZ	C7-C6-N4	-5.61	115.15	124.79
4	A	310	VFZ	C7-C6-N4	-5.59	115.19	124.79
4	N	305	VFZ	C7-C6-N4	-5.58	115.20	124.79
4	c	303	VFZ	C7-C6-N4	-5.58	115.21	124.79
4	W	302	VFZ	C7-C6-N4	-5.58	115.21	124.79
4	M	304	VFZ	C7-C6-N4	-5.58	115.22	124.79
4	G	304	VFZ	C7-C6-N4	-5.54	115.27	124.79
4	B	305	VFZ	C7-C6-N4	-5.46	115.43	124.79
4	N	305	VFZ	C5-N4-C6	5.45	124.45	116.79
4	C	306	VFZ	C5-N4-C6	5.45	124.44	116.79
4	B	305	VFZ	C5-N4-C6	5.43	124.41	116.79
4	H	303	VFZ	C5-N4-C6	5.40	124.37	116.79
4	M	304	VFZ	C5-N4-C6	5.40	124.37	116.79
4	I	304	VFZ	C5-N4-C6	5.37	124.33	116.79
4	I	304	VFZ	C7-C6-N4	-5.36	115.60	124.79
4	A	310	VFZ	C5-N4-C6	5.35	124.31	116.79
4	W	302	VFZ	C5-N4-C6	5.35	124.30	116.79
4	c	303	VFZ	C5-N4-C6	5.33	124.28	116.79
4	G	304	VFZ	C5-N4-C6	5.27	124.19	116.79
4	A	310	VFZ	C4-C3-N3	4.14	119.78	113.13
4	H	303	VFZ	C3-C4-C8	3.72	127.76	120.77
4	A	310	VFZ	C12-C11-S	3.33	129.57	121.46
4	C	306	VFZ	C3-C4-C8	3.29	126.95	120.77
4	W	302	VFZ	C10-S-C11	-2.93	98.12	102.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	N	305	VFZ	C4-C3-N3	2.86	117.72	113.13
4	W	302	VFZ	C1-C2-N3	-2.85	108.86	113.64
4	W	302	VFZ	C12-C11-S	2.75	128.17	121.46
4	I	304	VFZ	C4-C3-N3	2.71	117.49	113.13
4	M	304	VFZ	C1-C2-N3	-2.70	109.11	113.64
4	N	305	VFZ	C3-C4-C8	2.54	125.54	120.77
4	C	306	VFZ	C3-N3-C2	-2.47	109.63	115.88
4	G	304	VFZ	C1-C2-N3	-2.46	109.51	113.64
4	H	303	VFZ	C3-C4-C5	-2.46	115.10	120.80
4	W	302	VFZ	C3-C4-C8	2.42	125.32	120.77
4	B	305	VFZ	C1-C2-N3	-2.41	109.60	113.64
4	B	305	VFZ	C4-C3-N3	-2.27	109.48	113.13
4	C	306	VFZ	C3-C4-C5	-2.10	115.93	120.80
4	W	302	VFZ	C4-C3-N3	-2.04	109.86	113.13
4	A	310	VFZ	C3-N3-C9	2.01	127.11	121.91

There are no chirality outliers.

All (4) torsion outliers are listed below:

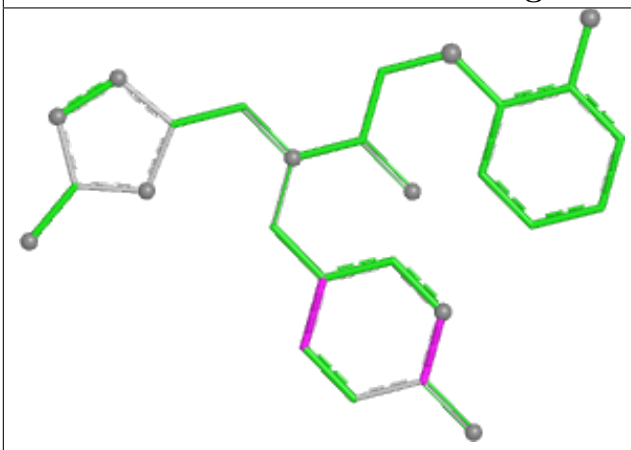
Mol	Chain	Res	Type	Atoms
4	B	305	VFZ	N2-C1-C2-N3
4	H	303	VFZ	C10-C9-N3-C3
4	W	302	VFZ	C10-C9-N3-C3
4	C	306	VFZ	C10-C9-N3-C3

There are no ring outliers.

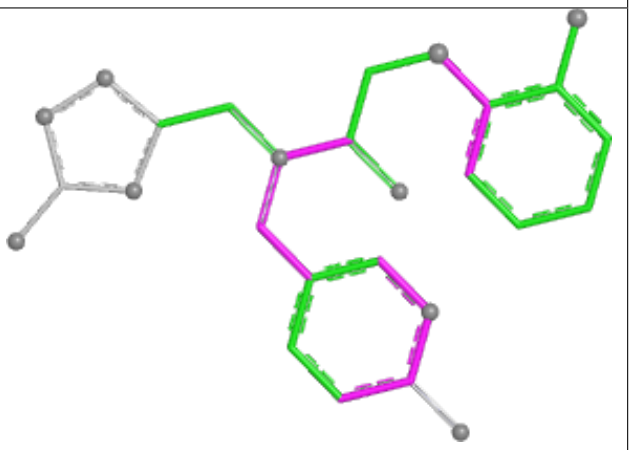
No monomer is involved in short contacts.

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

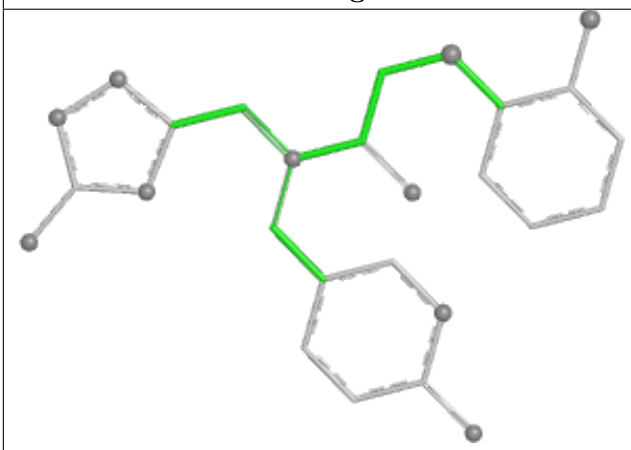
Ligand VFZ A 310



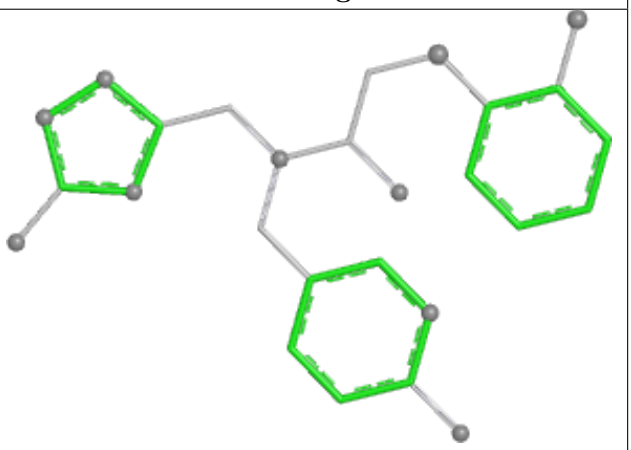
Bond lengths



Bond angles

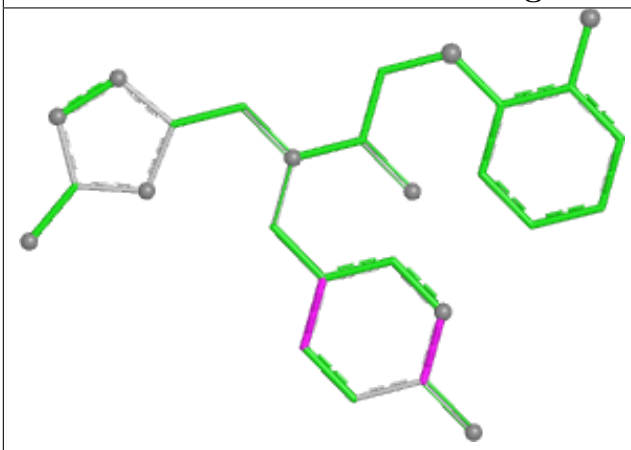


Torsions



Rings

Ligand VFZ H 303



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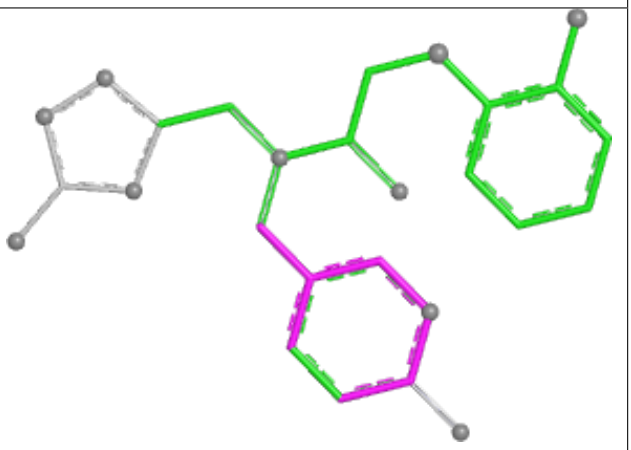
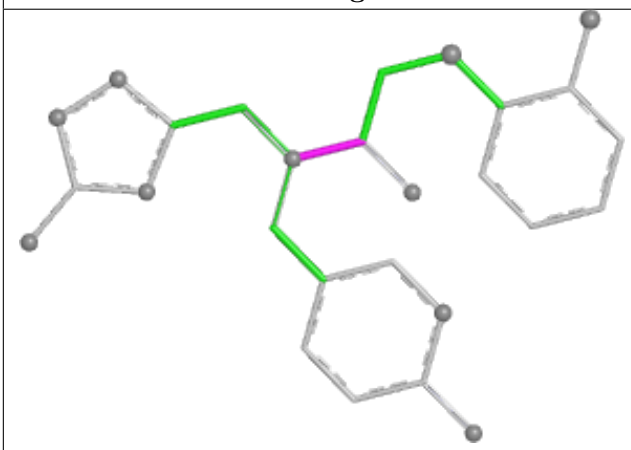


Bond angles



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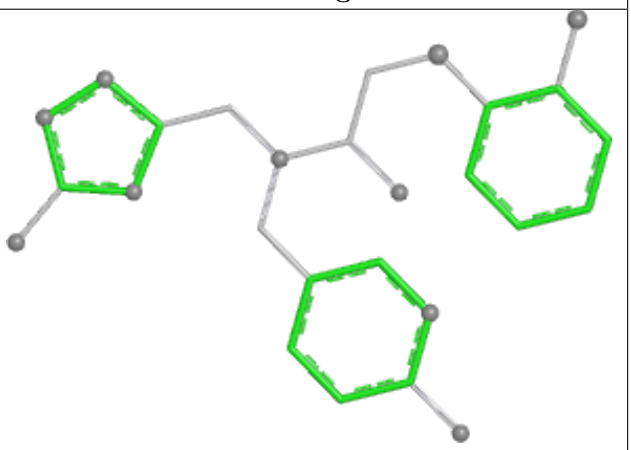
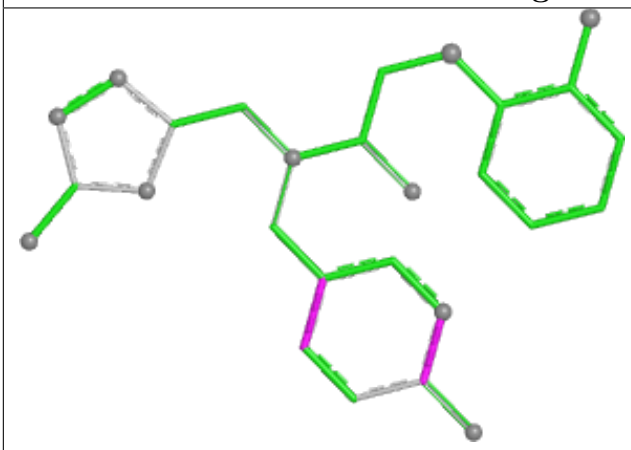


Rings

Ligand VFZ I 304



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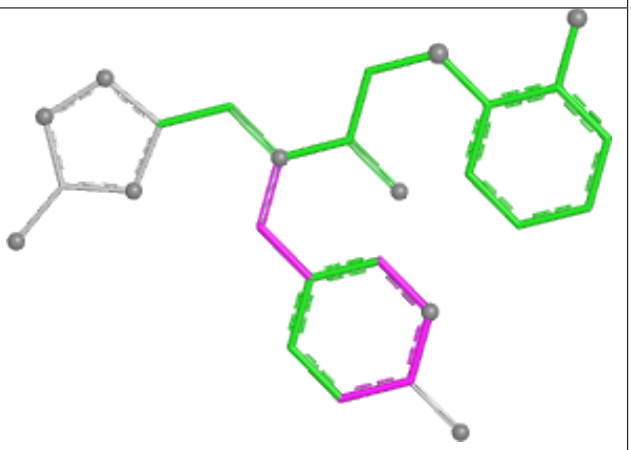
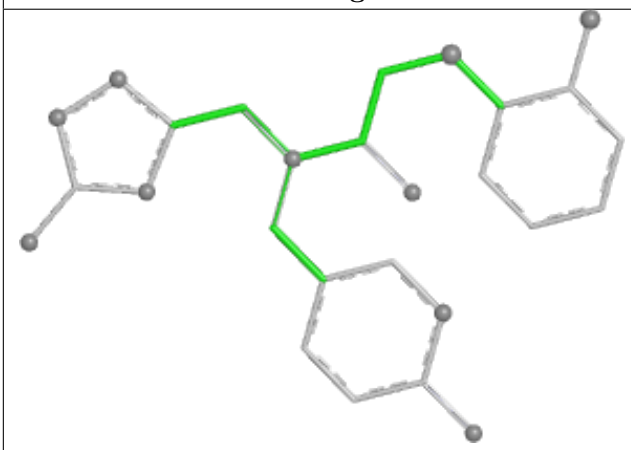


Bond angles



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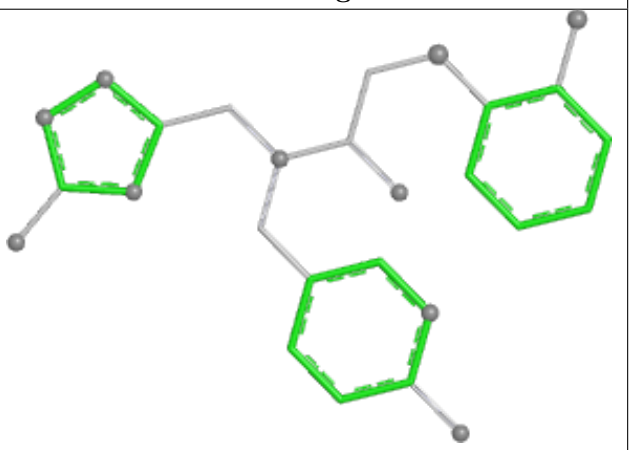
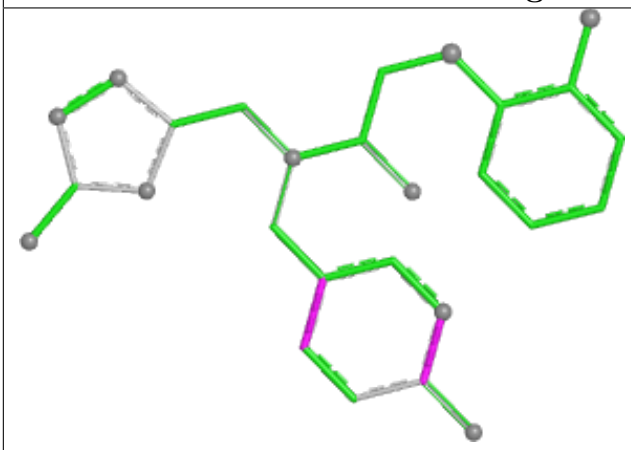


Rings

Ligand VFZ B 305



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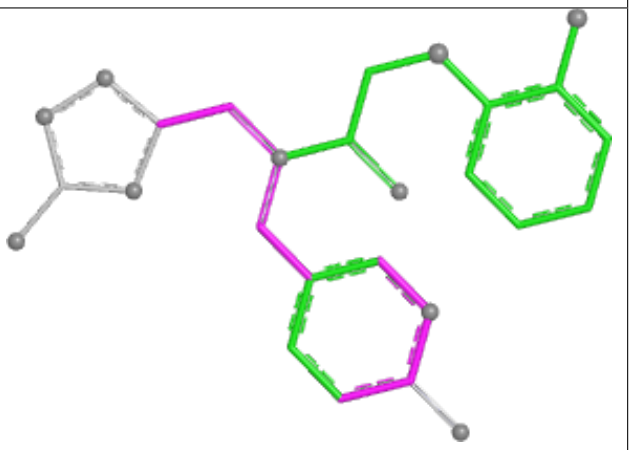

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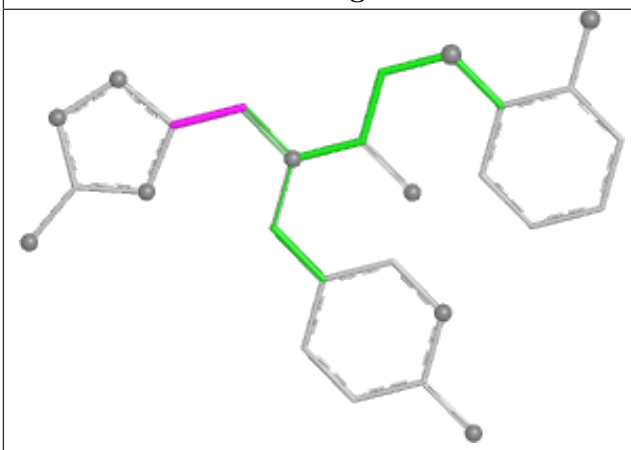

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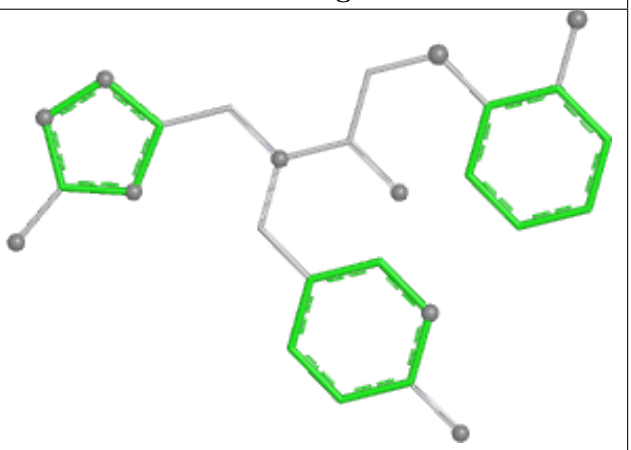
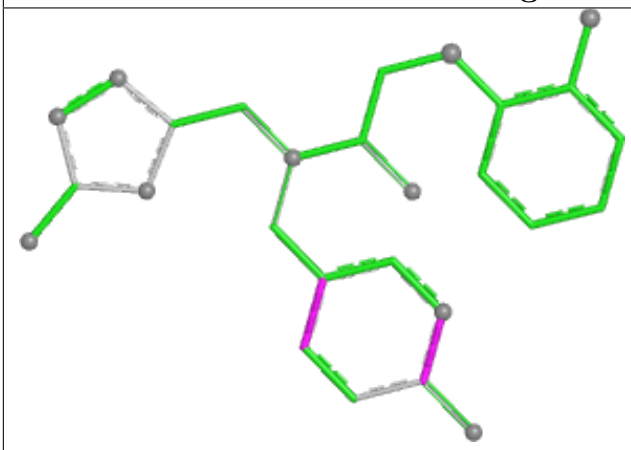


Rings

Ligand VFZ W 302



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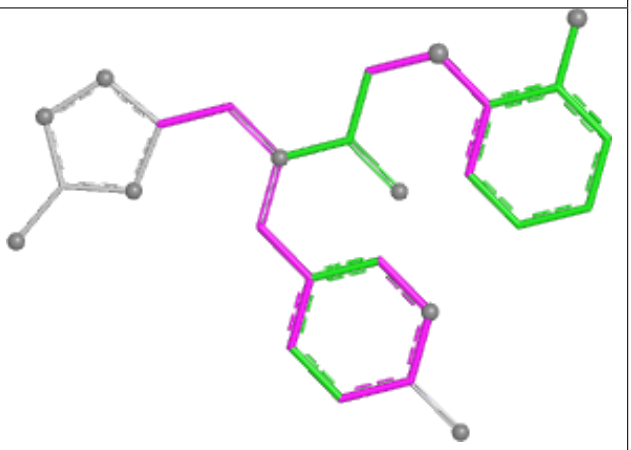

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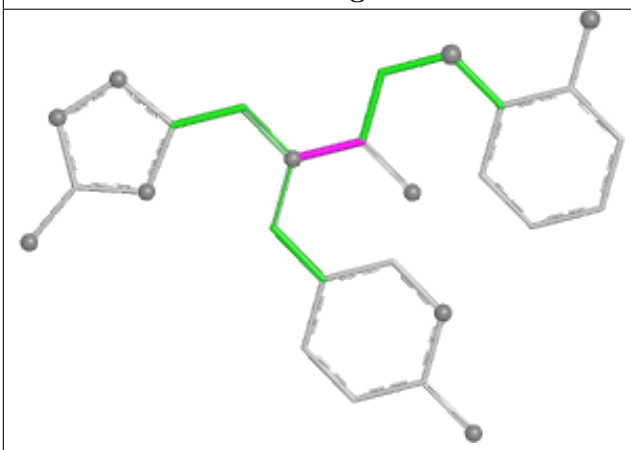

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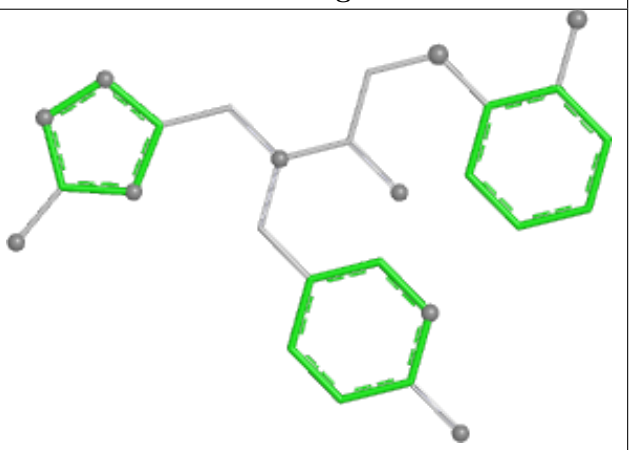

Rings

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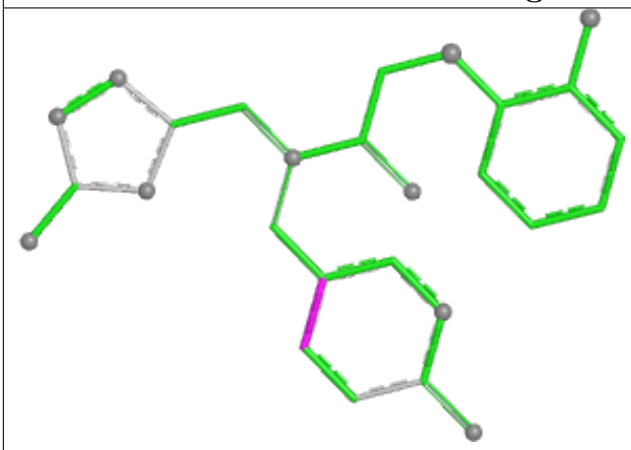

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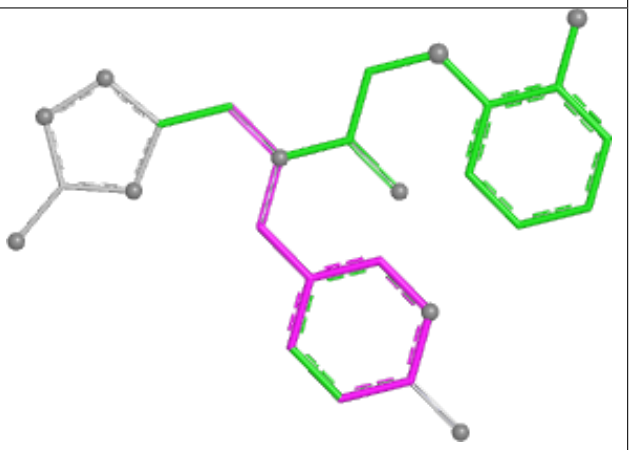

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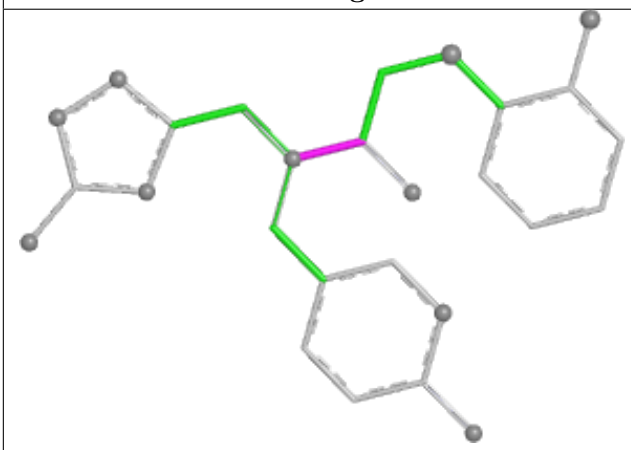

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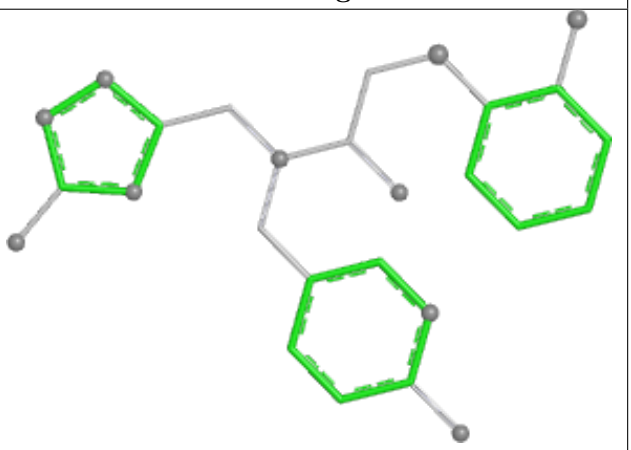

Rings

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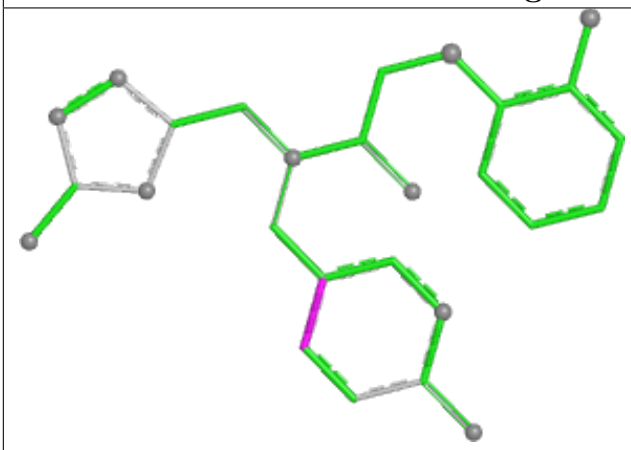

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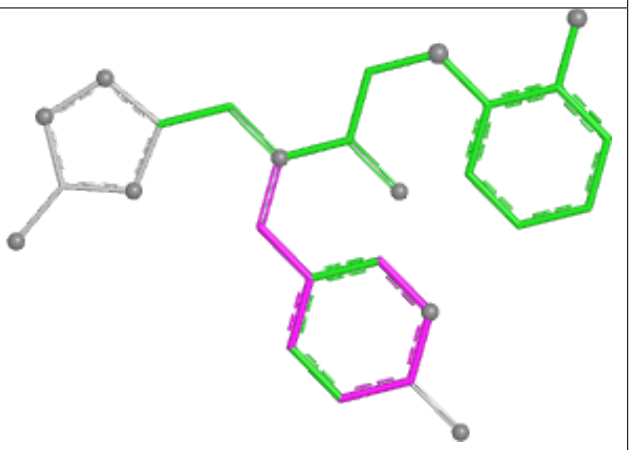

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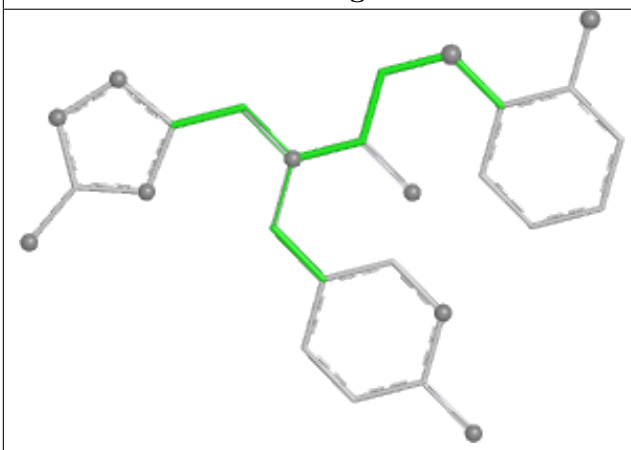

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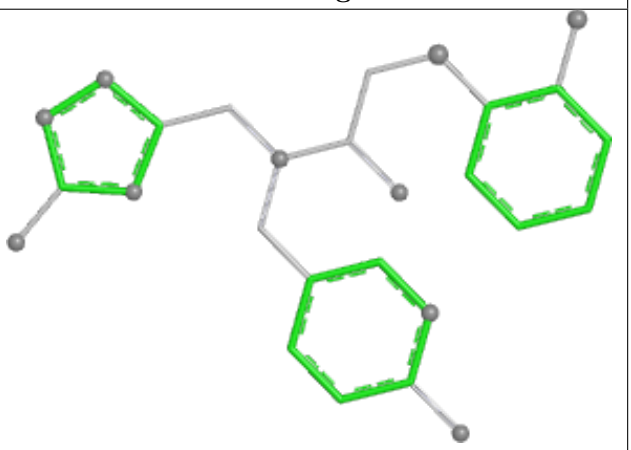
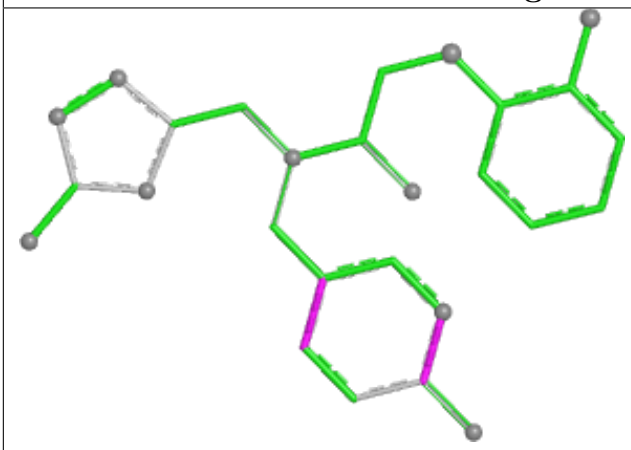


Rings

Ligand VFZ G 304



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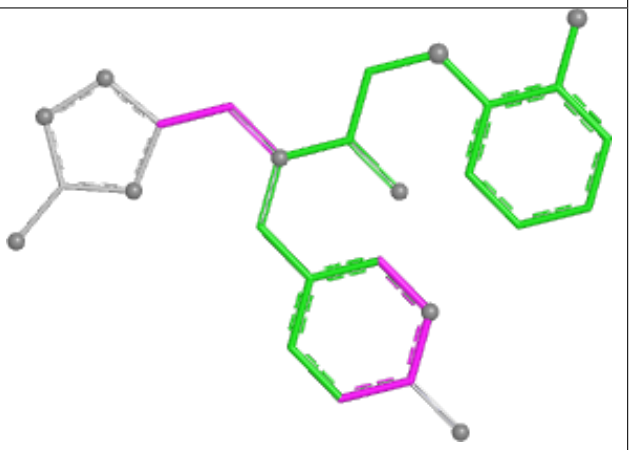

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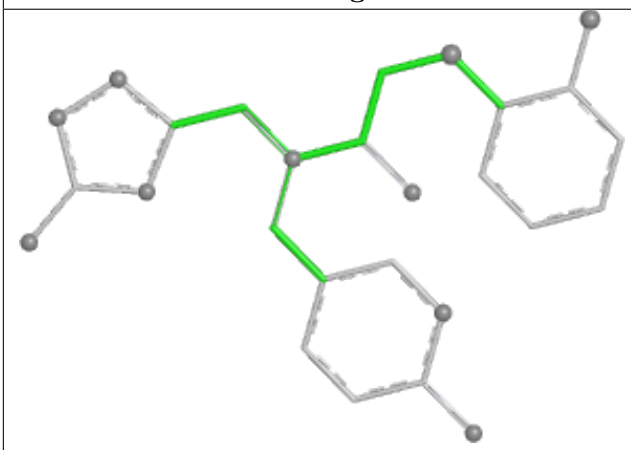

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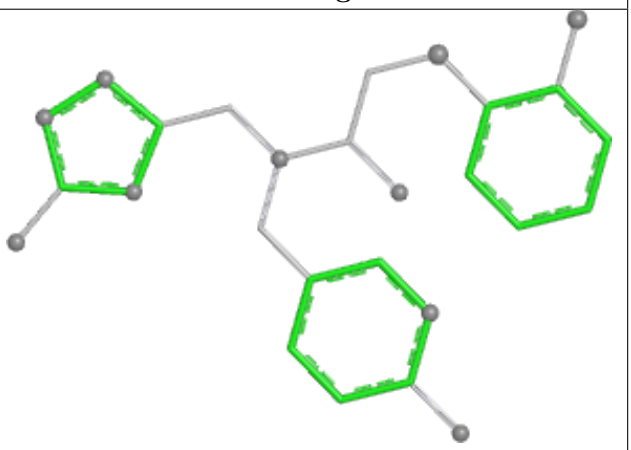
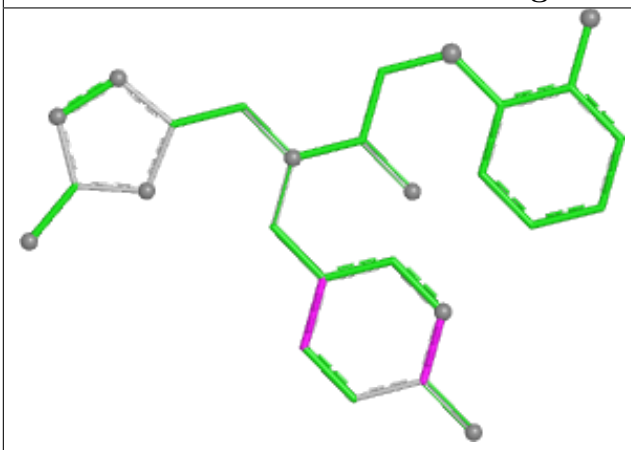


Rings

Ligand VFZ c 303



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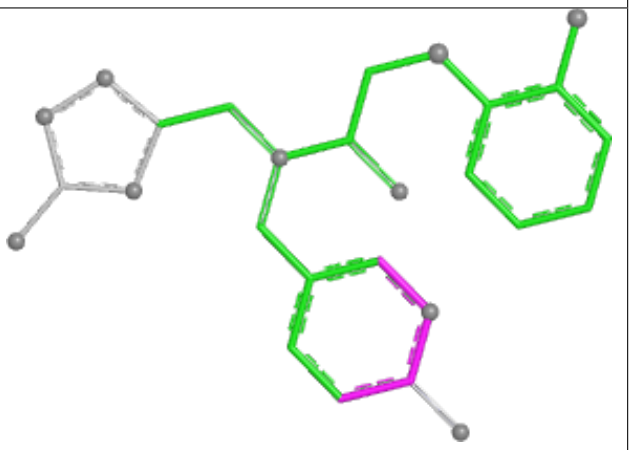
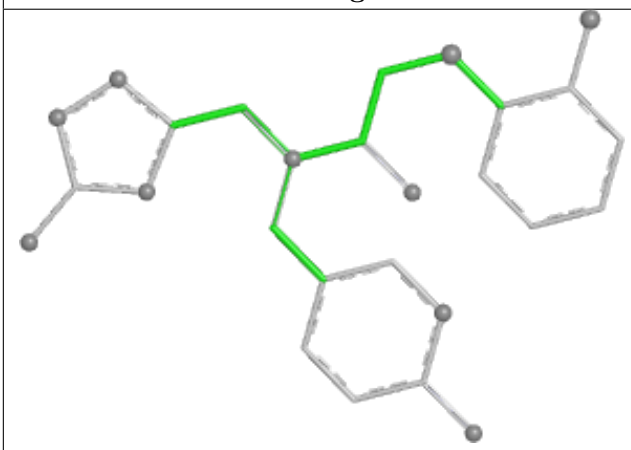


Bond angles



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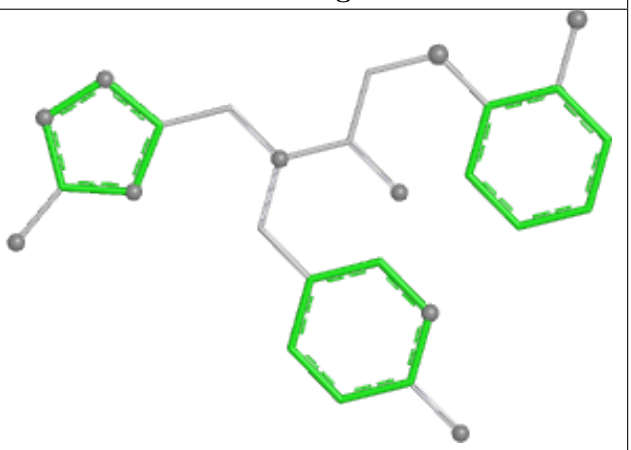
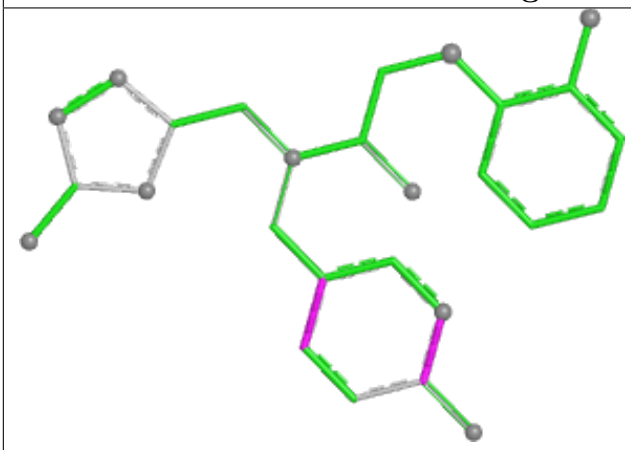


Rings

Ligand VFZ M 304



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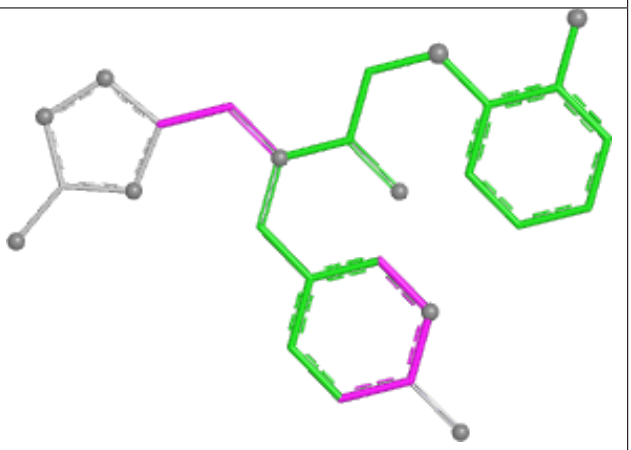

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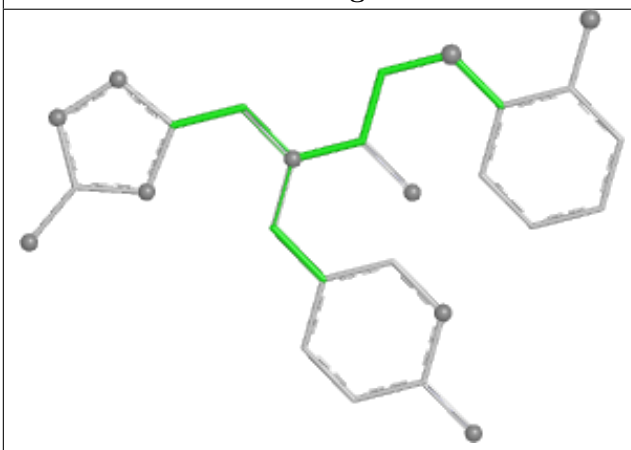

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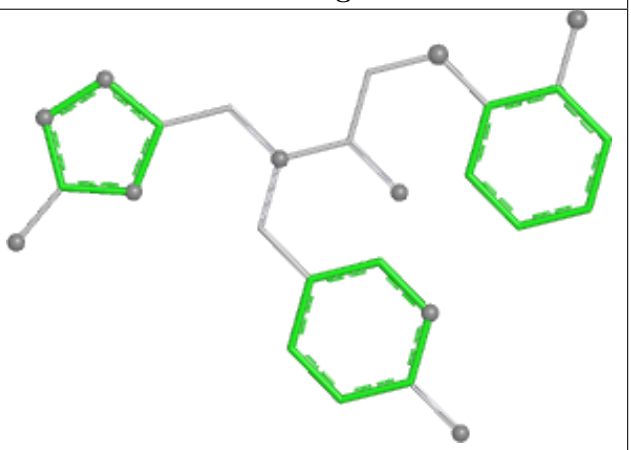
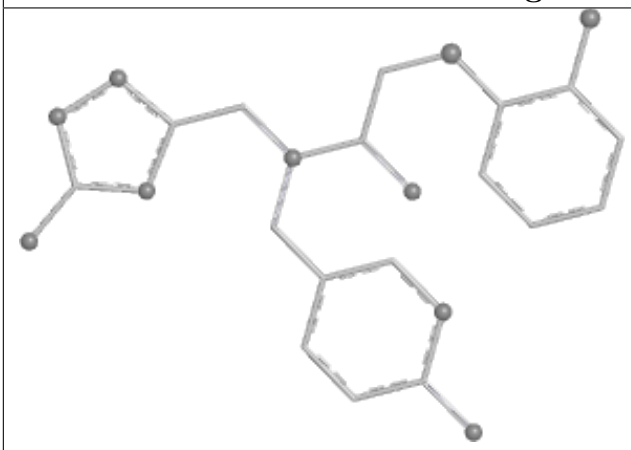


Rings

Ligand VFZ D 305



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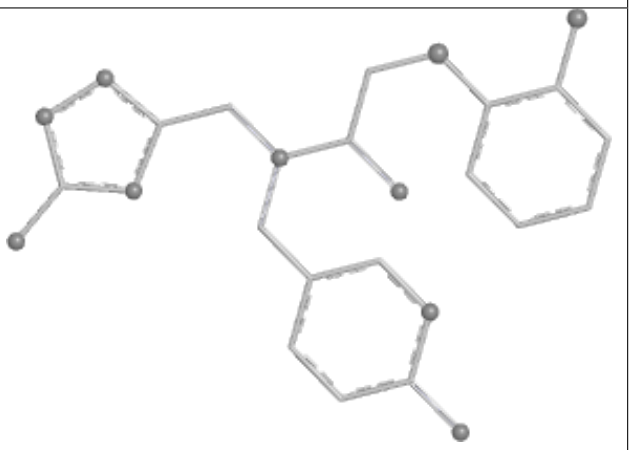

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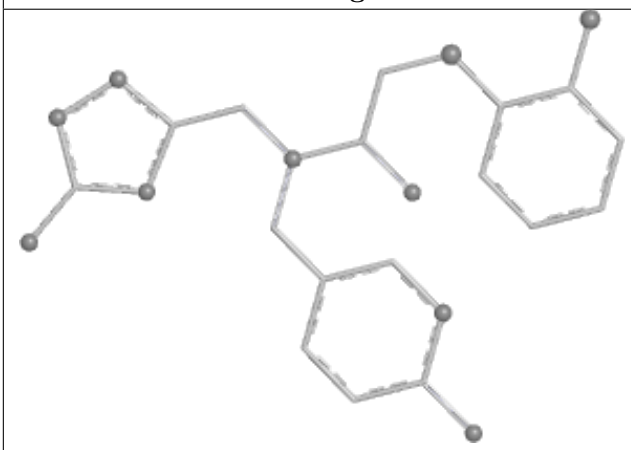

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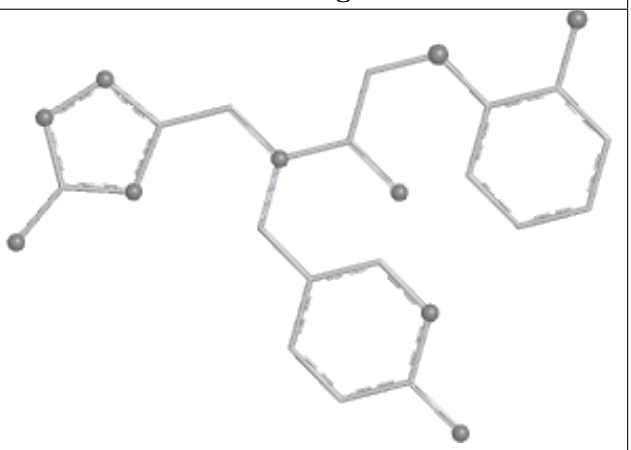
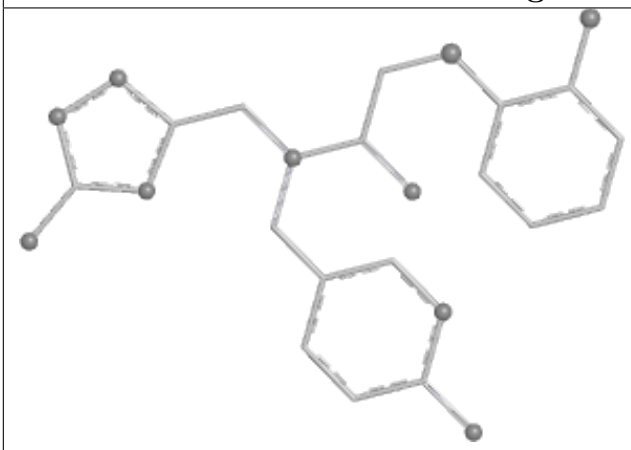


Rings

Ligand VFZ E 305



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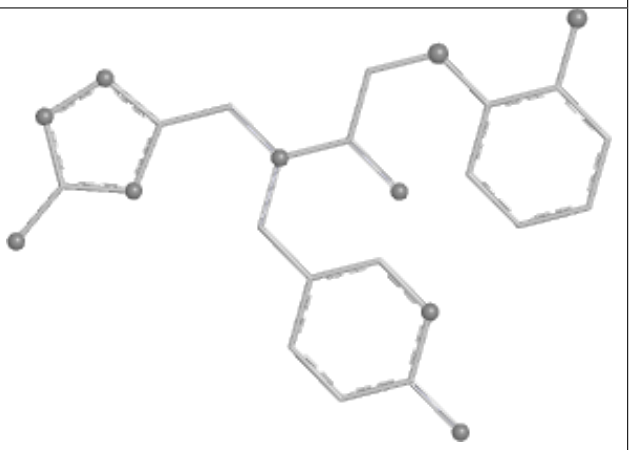
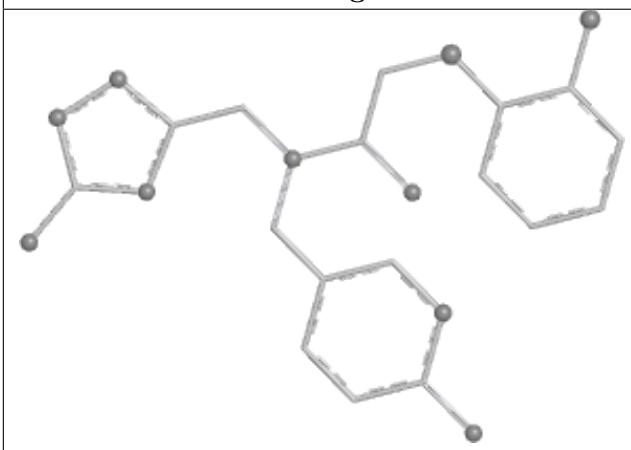


Bond angles



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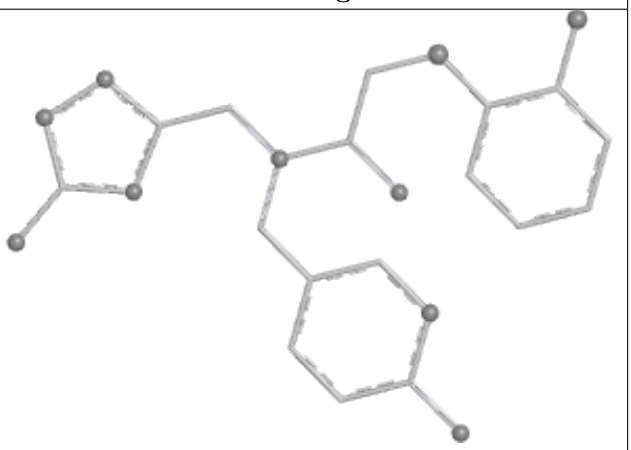
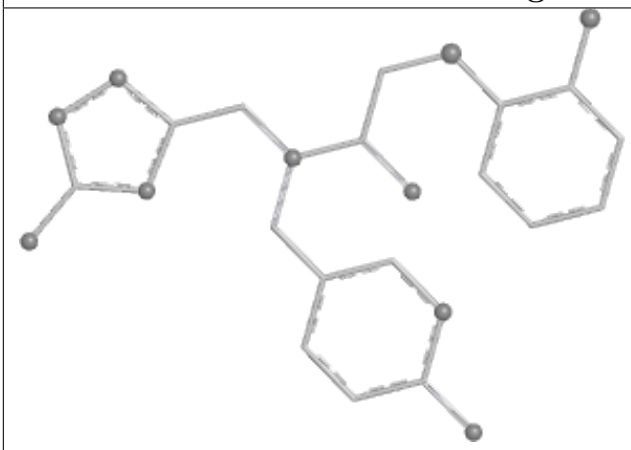


Rings

Ligand VFZ F 303



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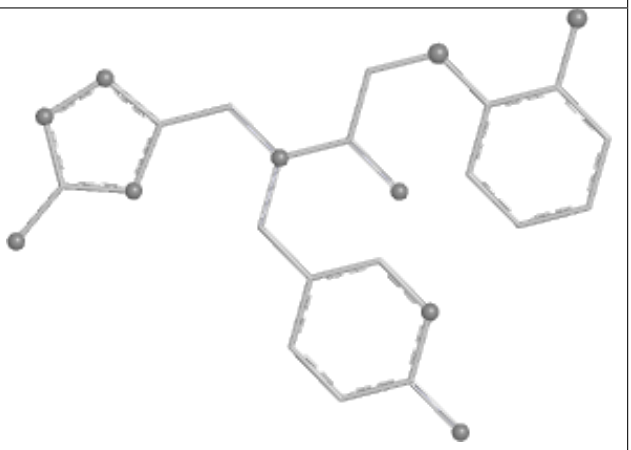
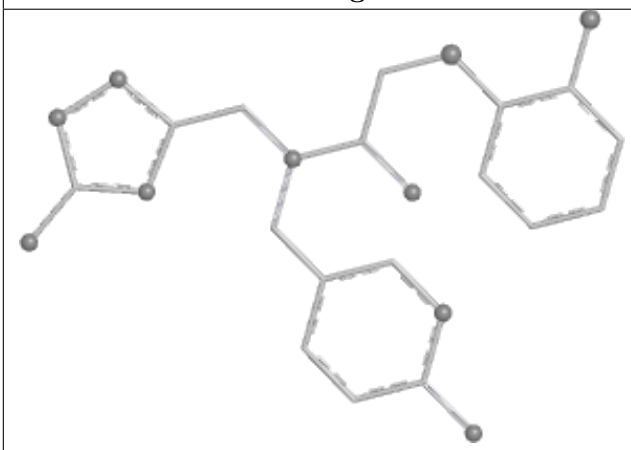
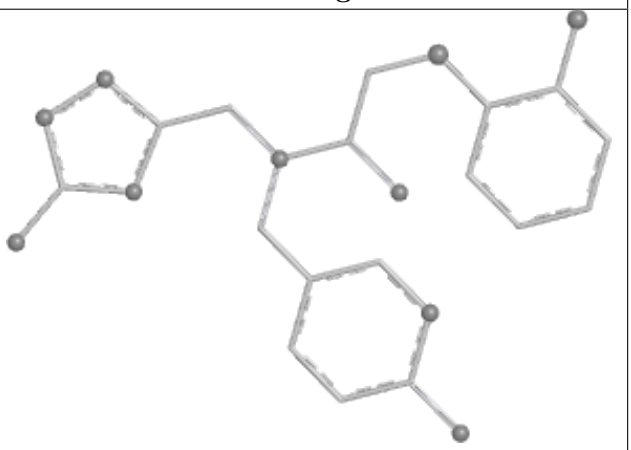


Bond angles

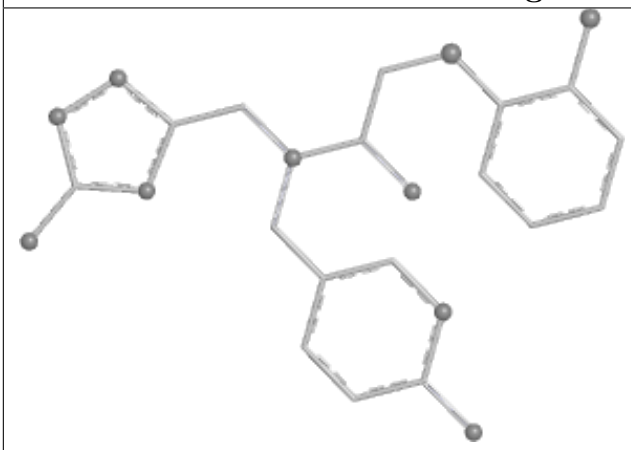


Torsions



Rings

Ligand VFZ O 303



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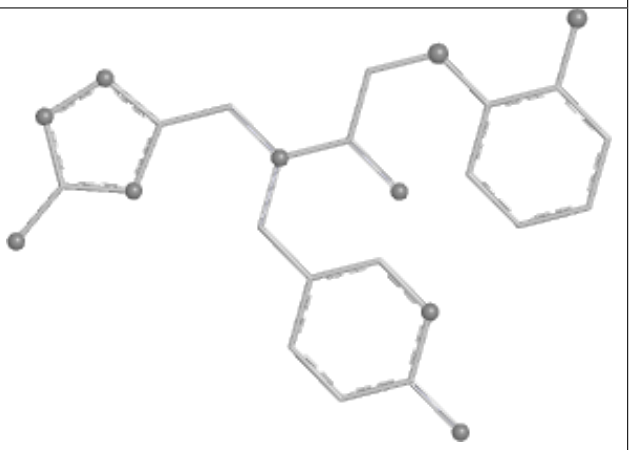

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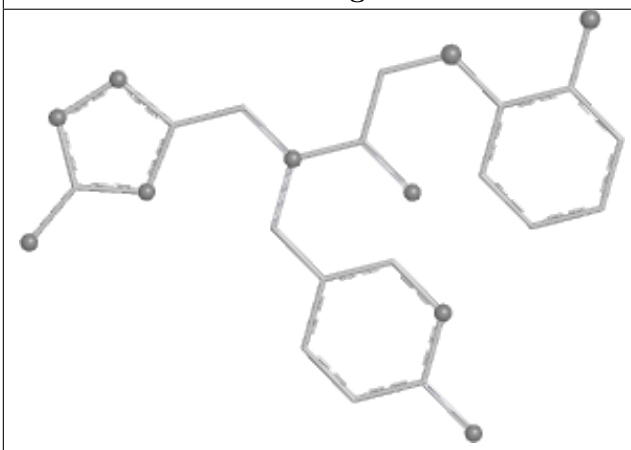
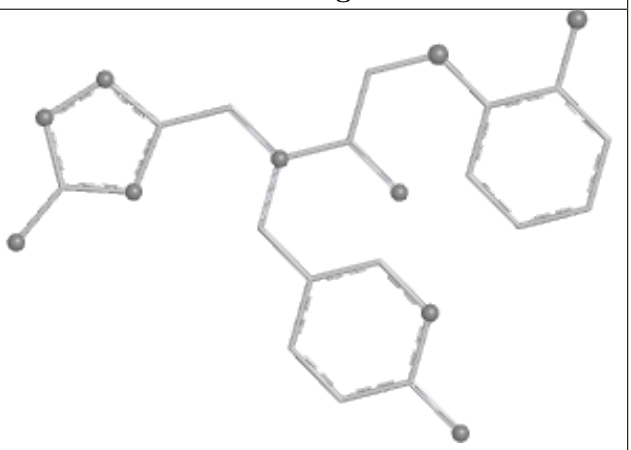


Torsions



Rings

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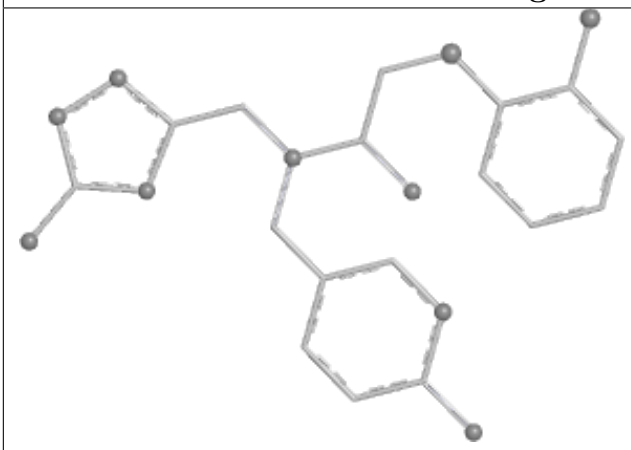

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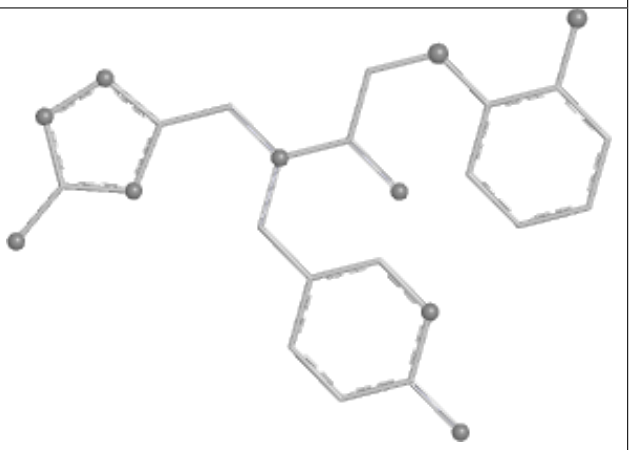

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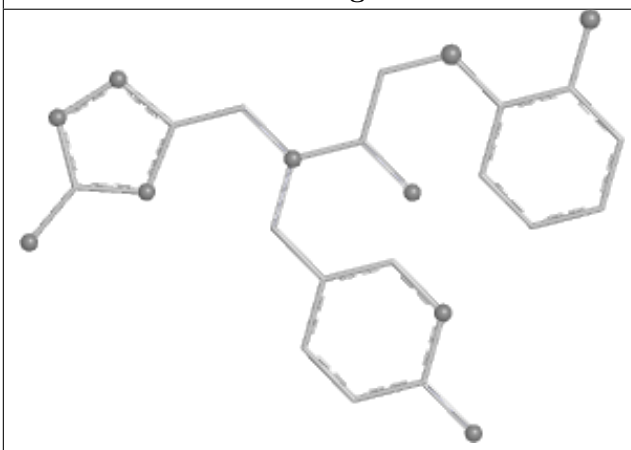

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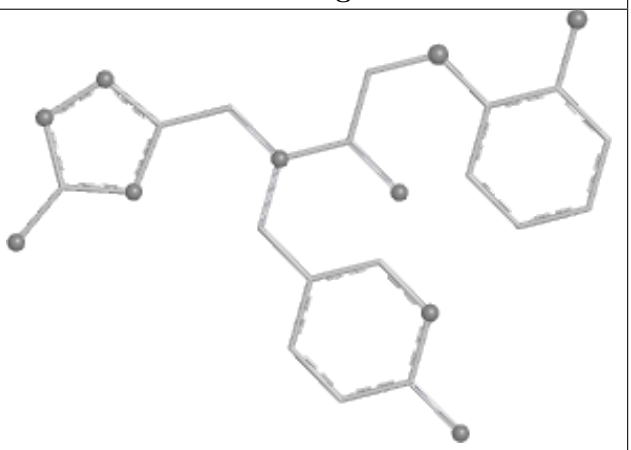

Rings

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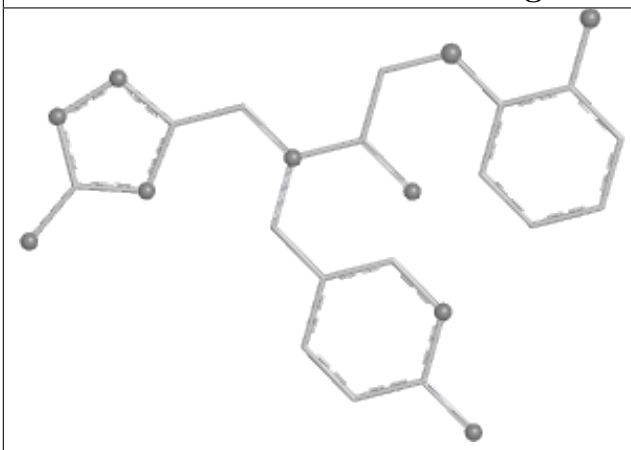

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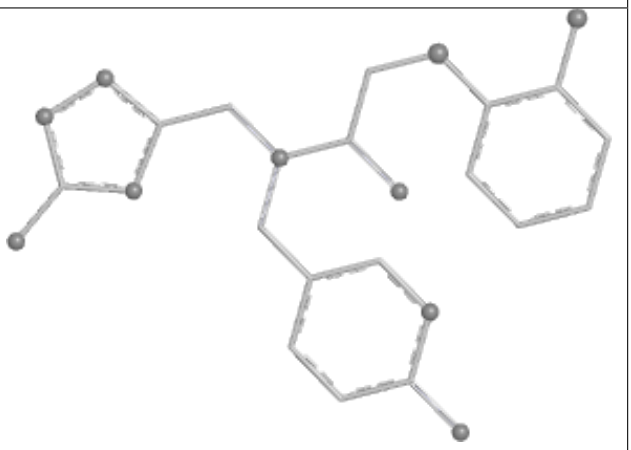

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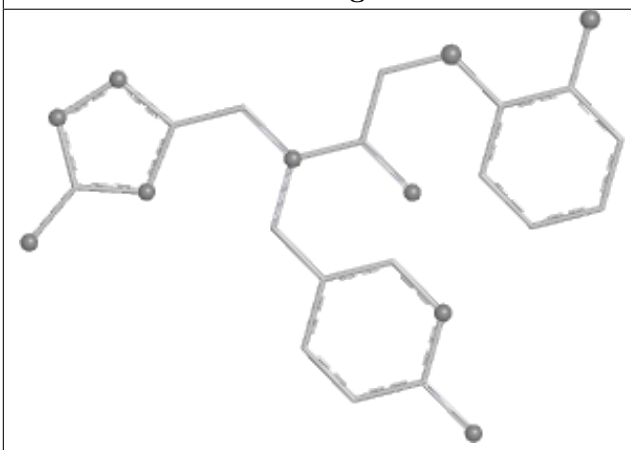

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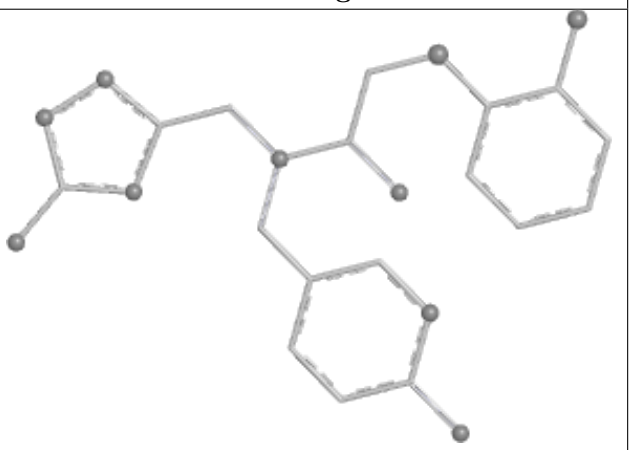

Rings

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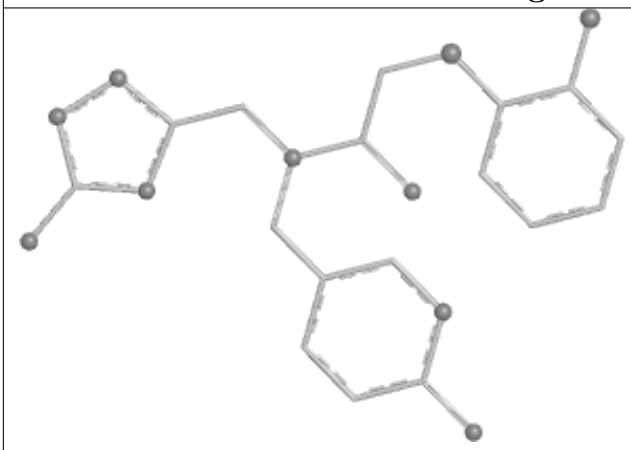

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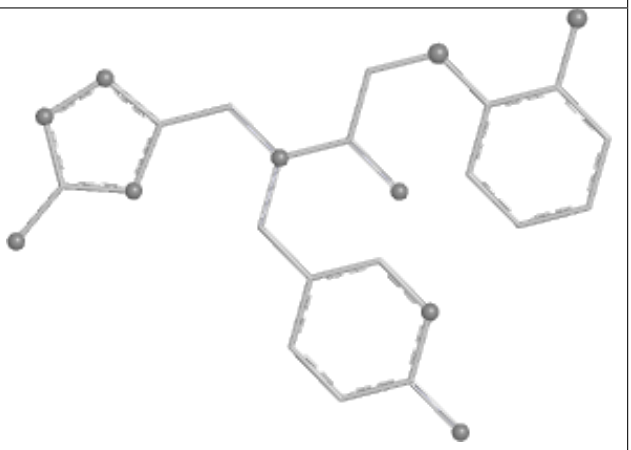

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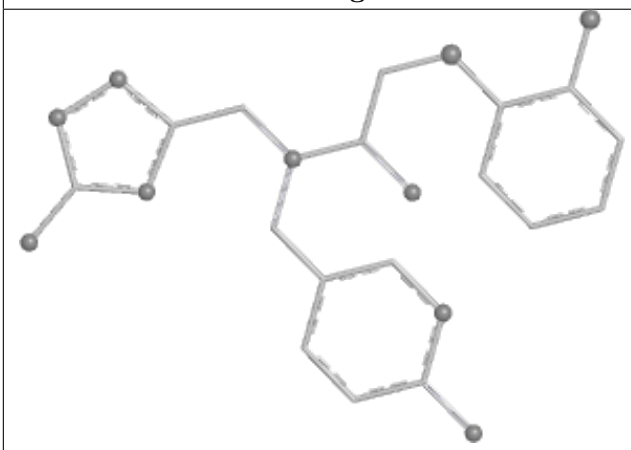

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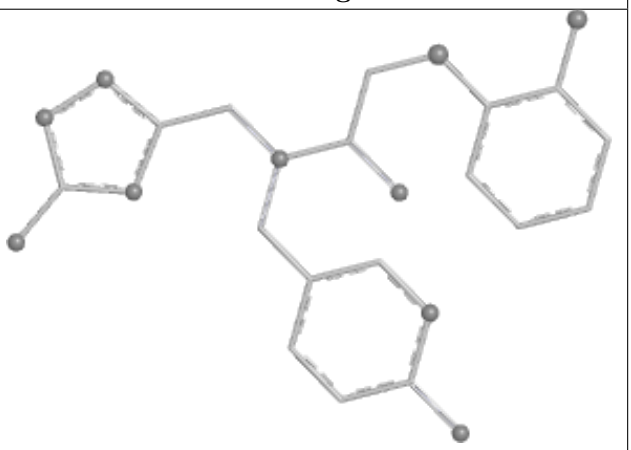

Rings

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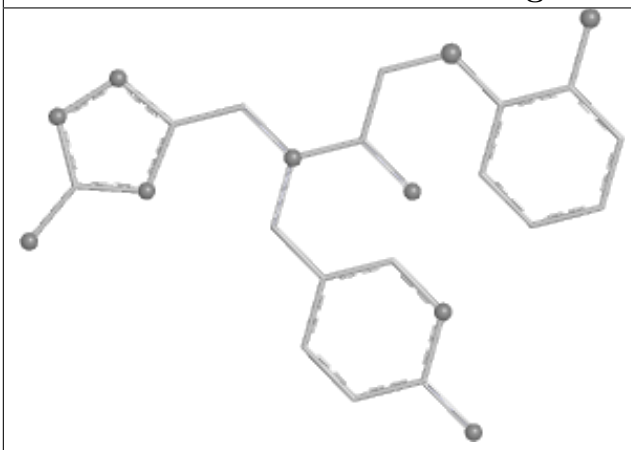

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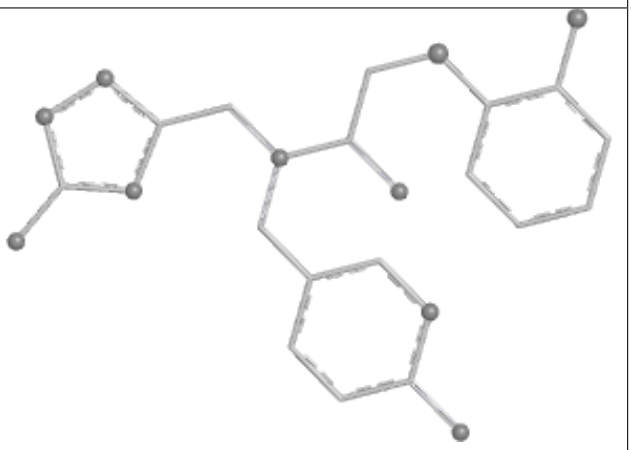

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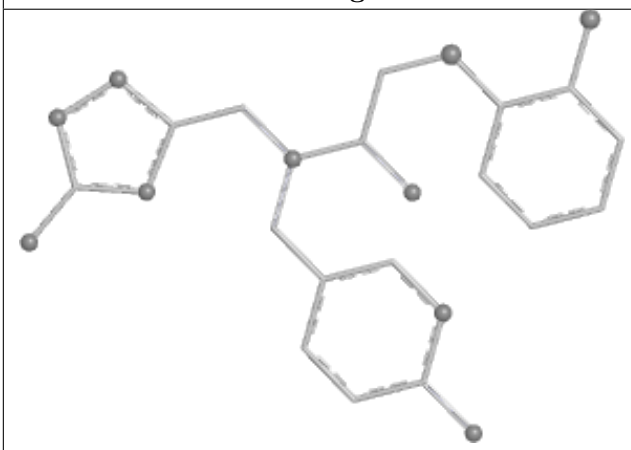

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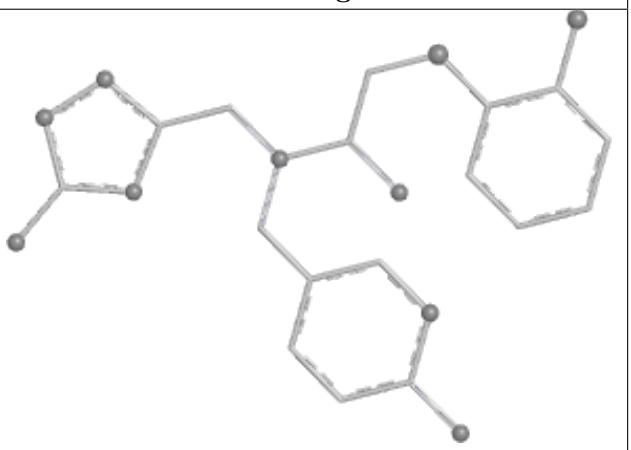

Rings

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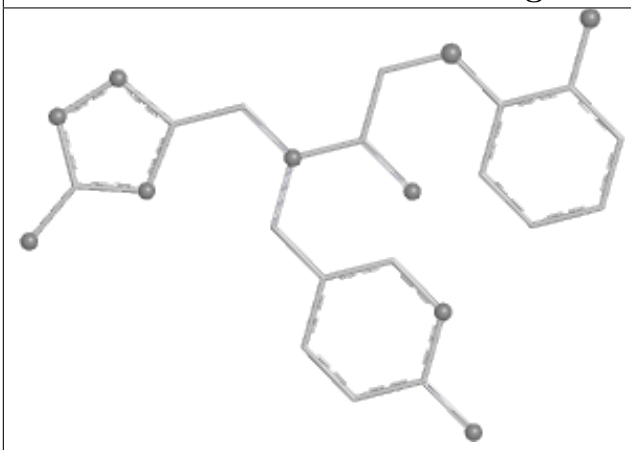

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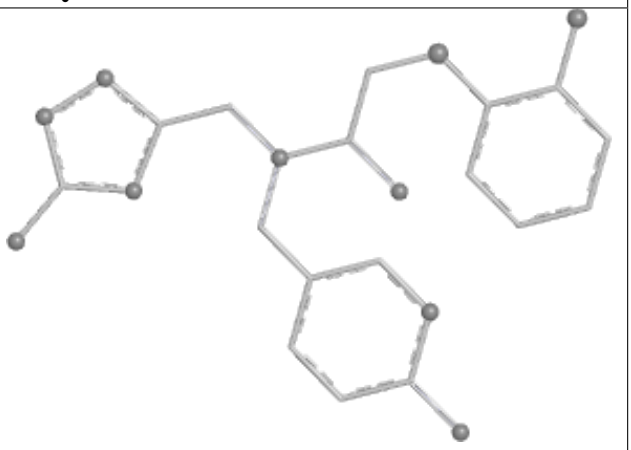

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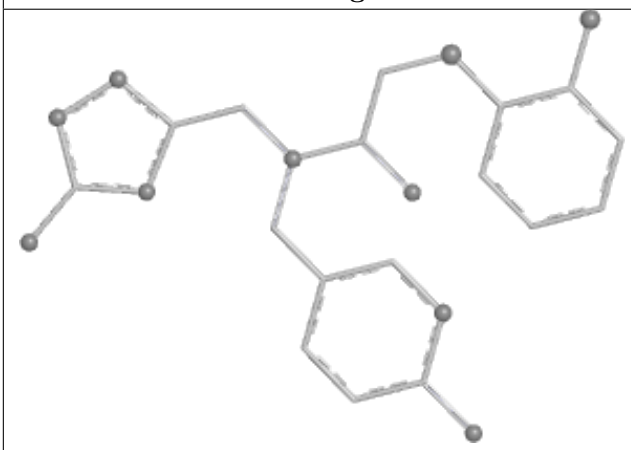

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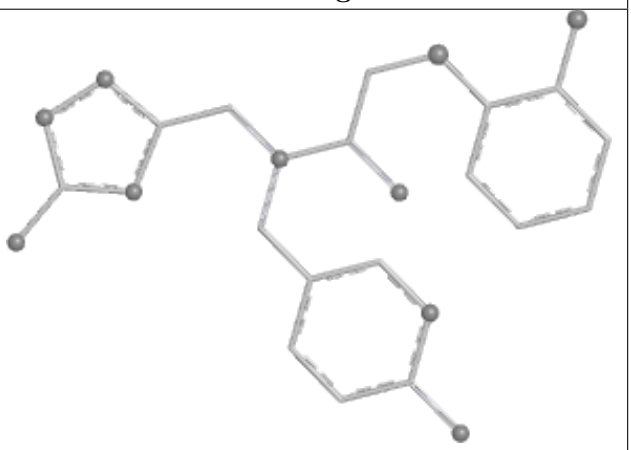

Rings

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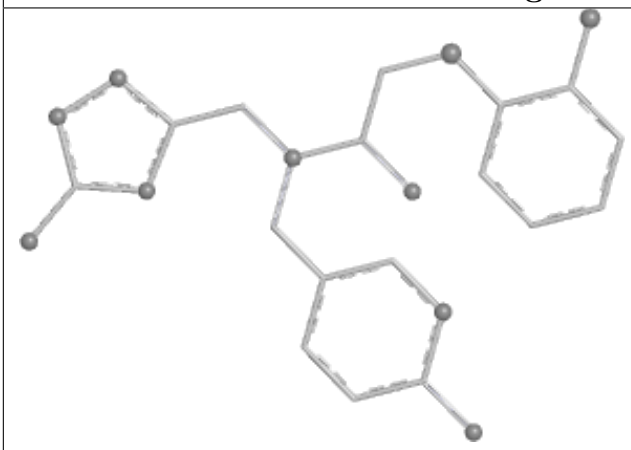

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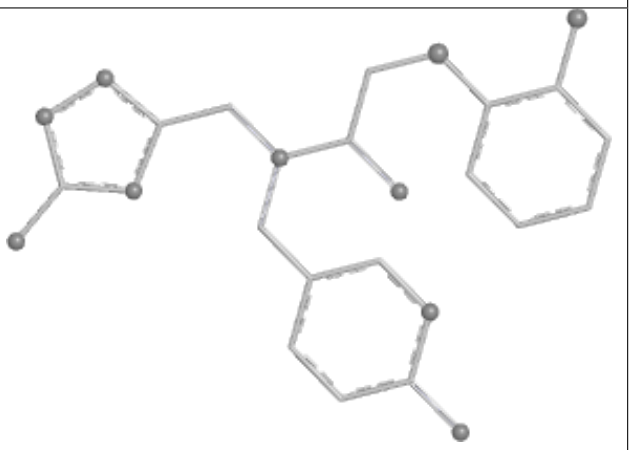

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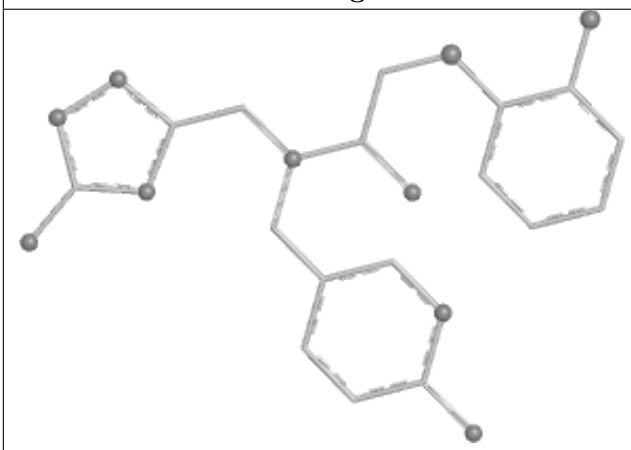

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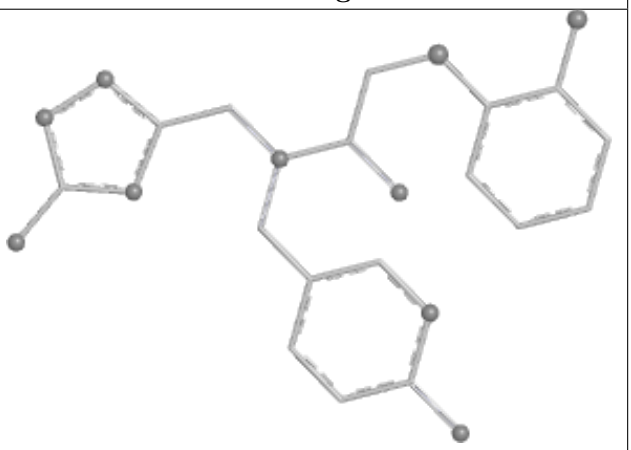

Rings

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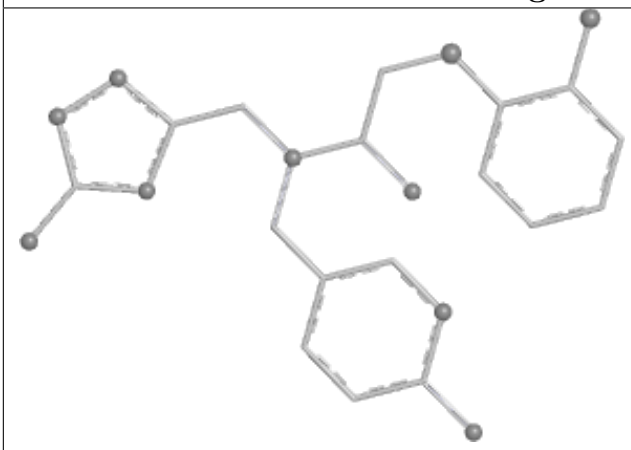

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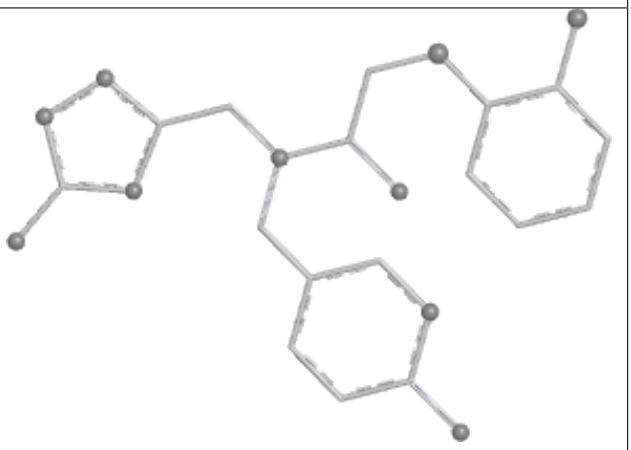

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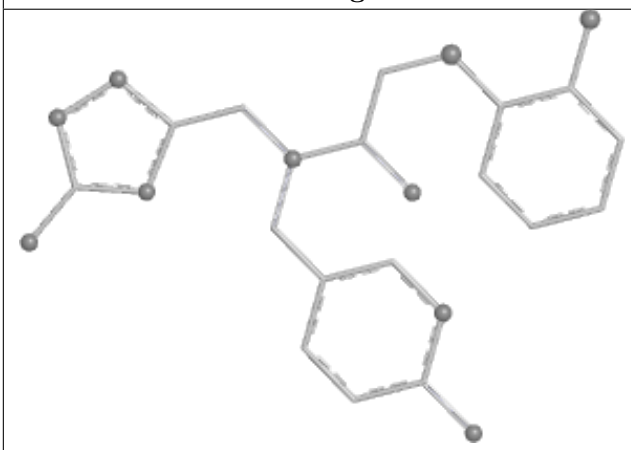

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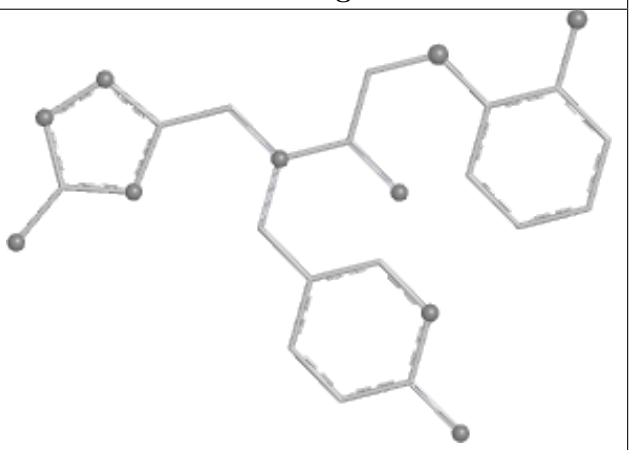

Rings

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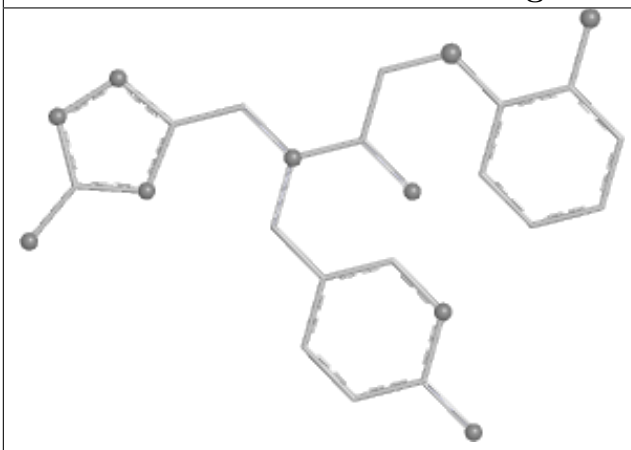

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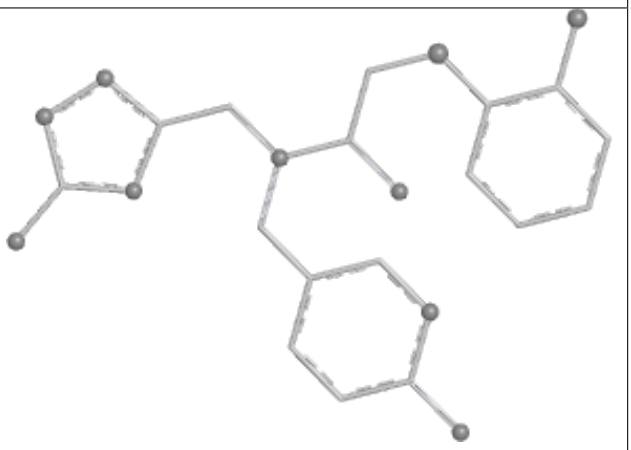

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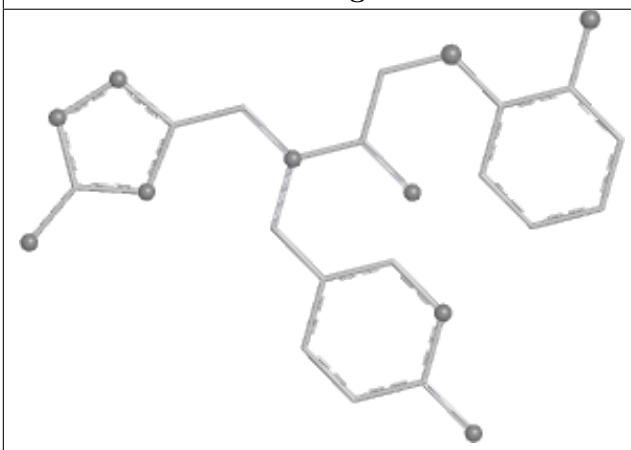

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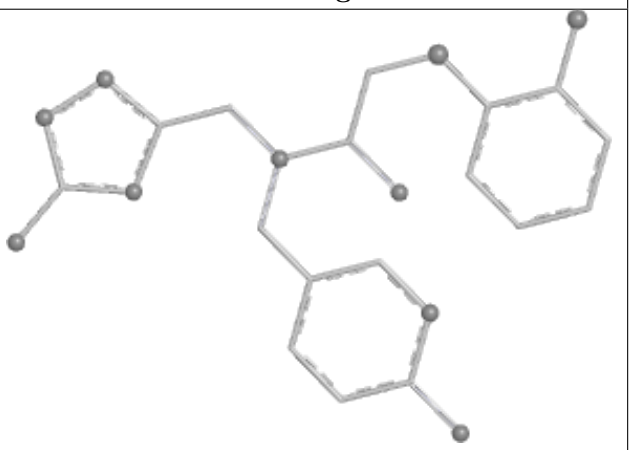

Rings

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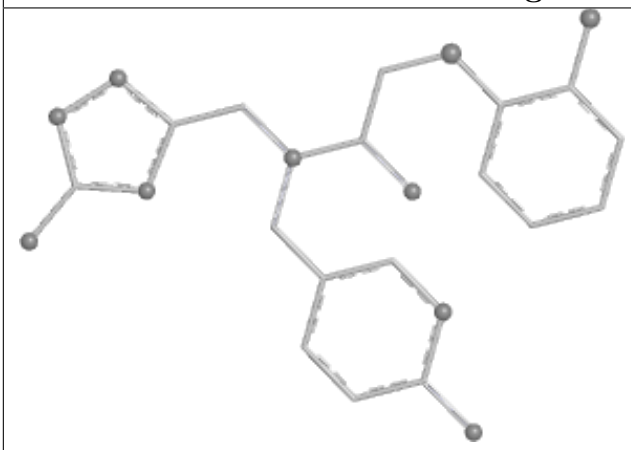

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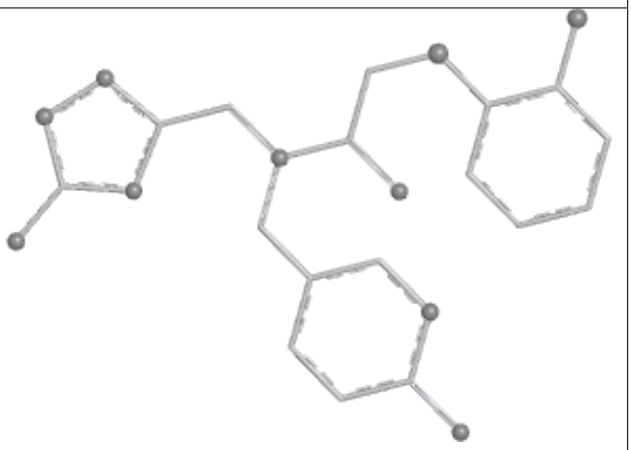

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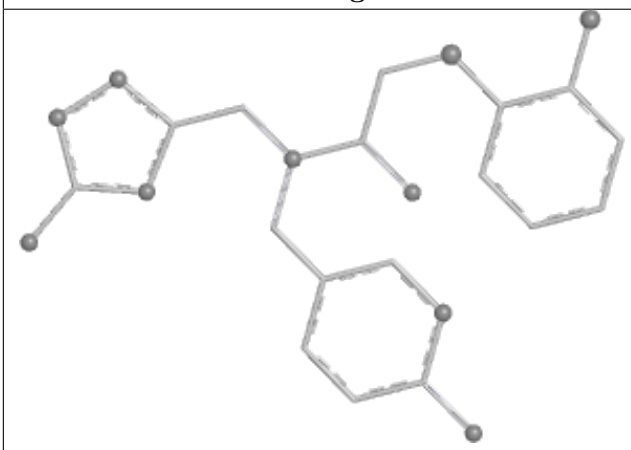

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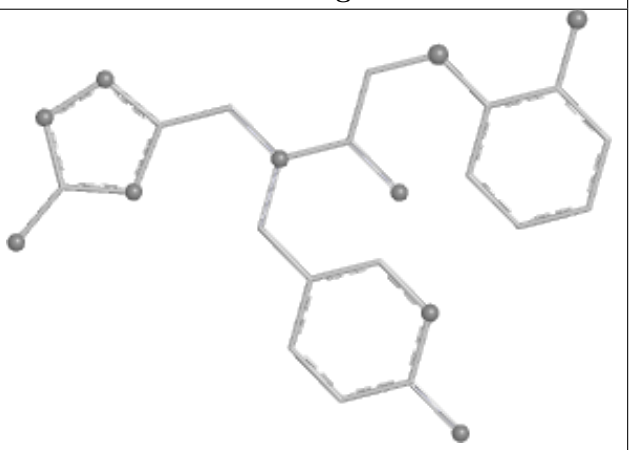
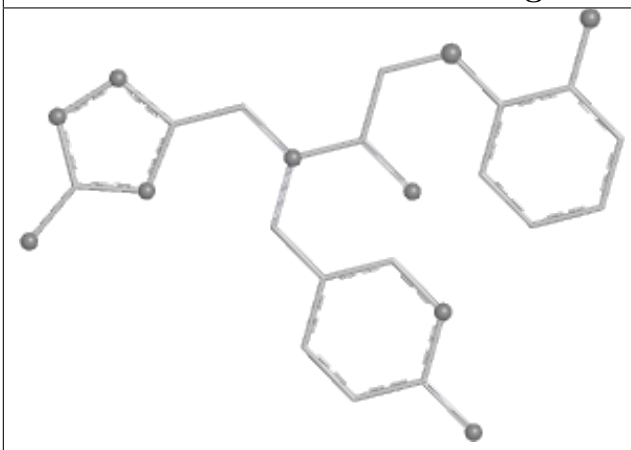


Rings

Ligand VFZ V 303



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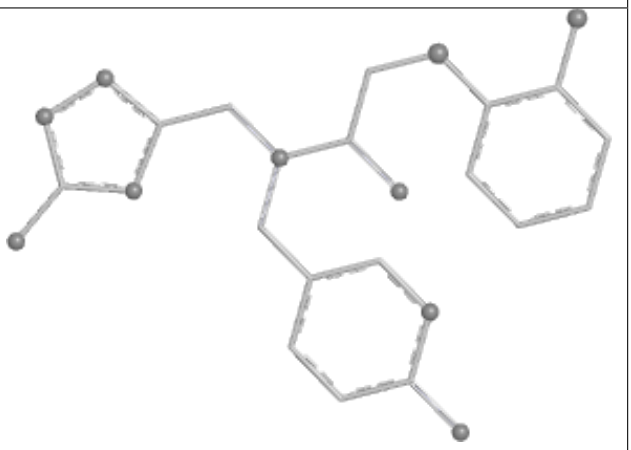

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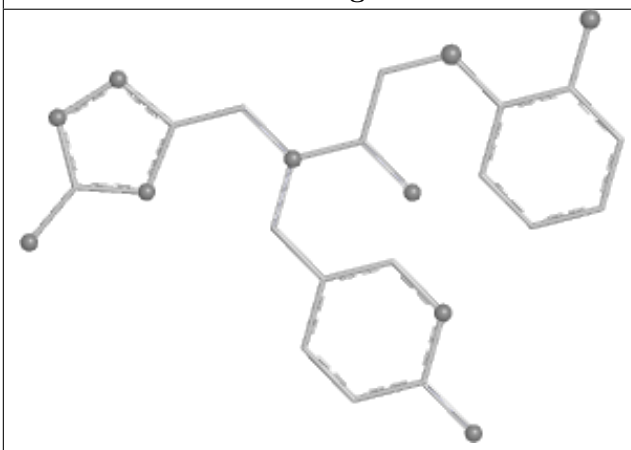

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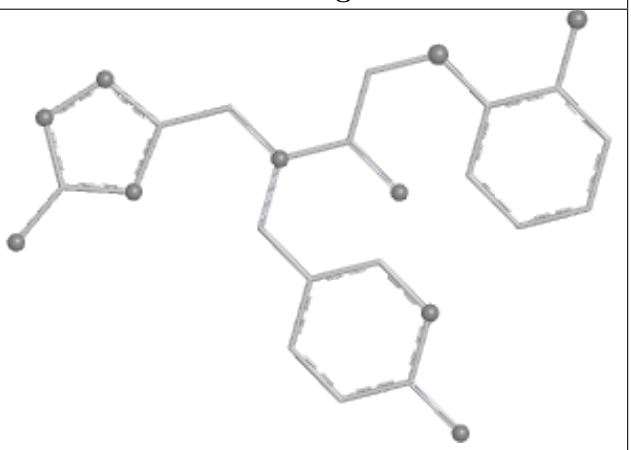
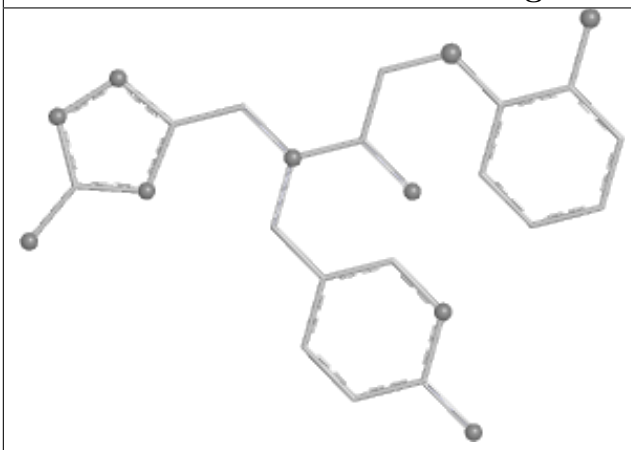


Rings

Ligand VFZ X 304



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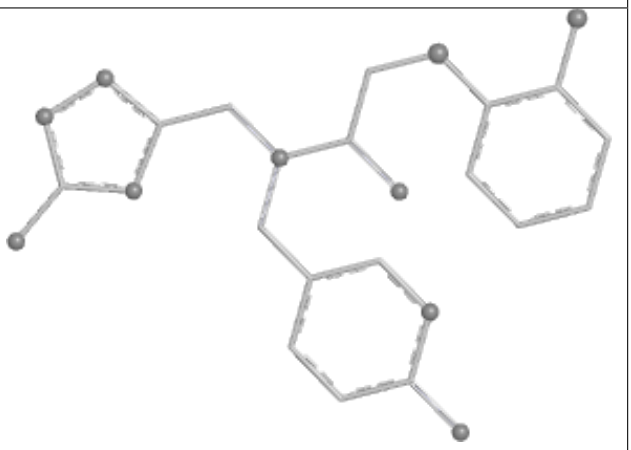

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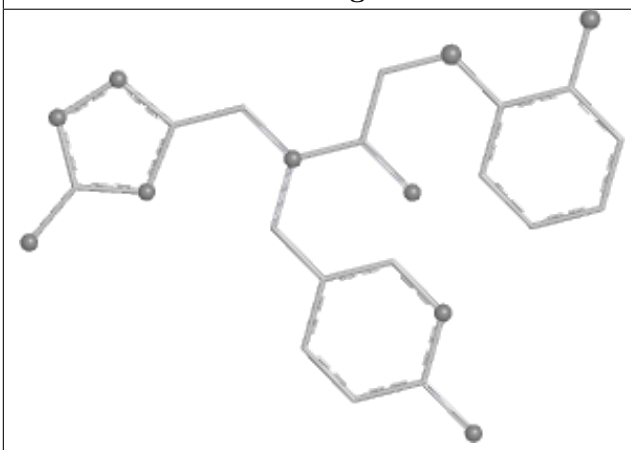

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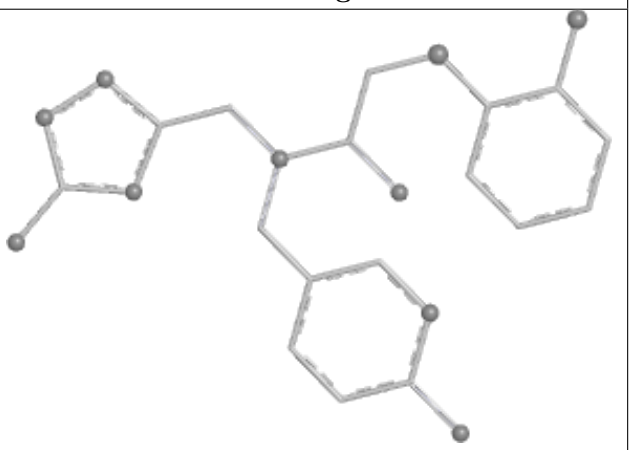
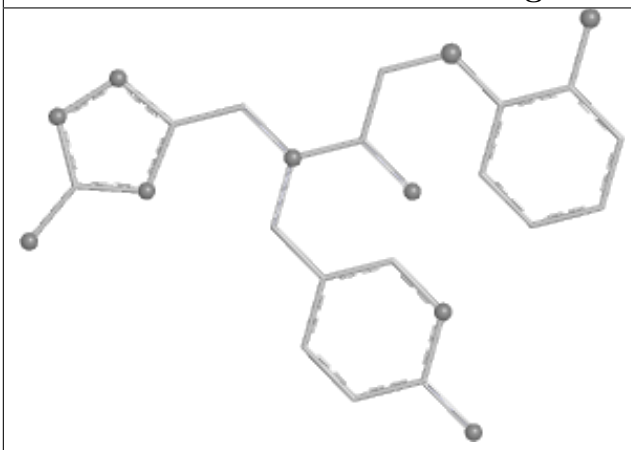


Rings

Ligand VFZ Y 303



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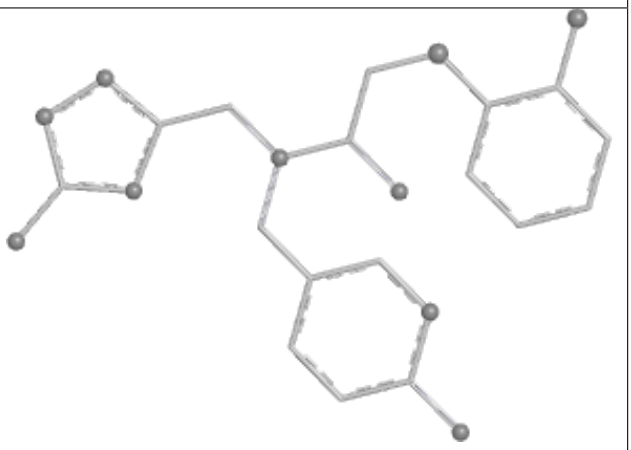

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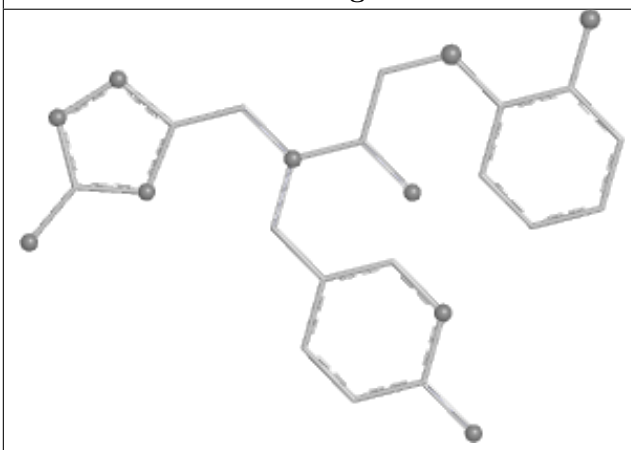

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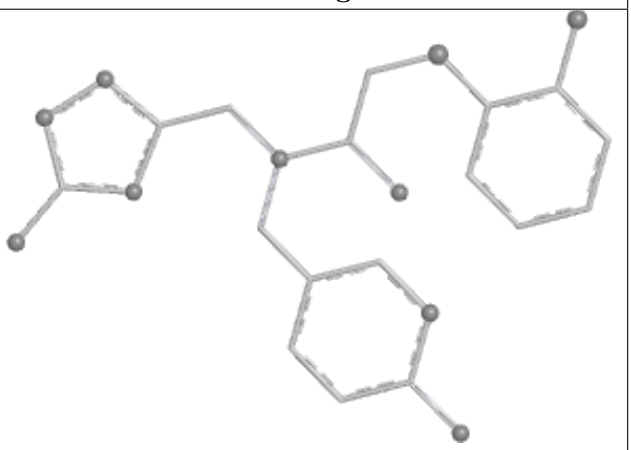
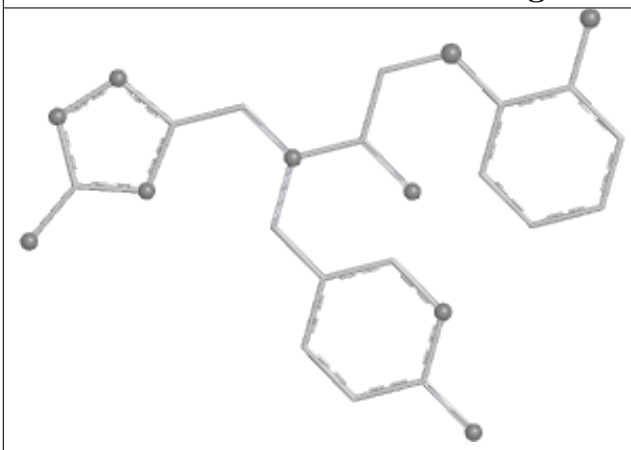


Rings

Ligand VFZ Z 302



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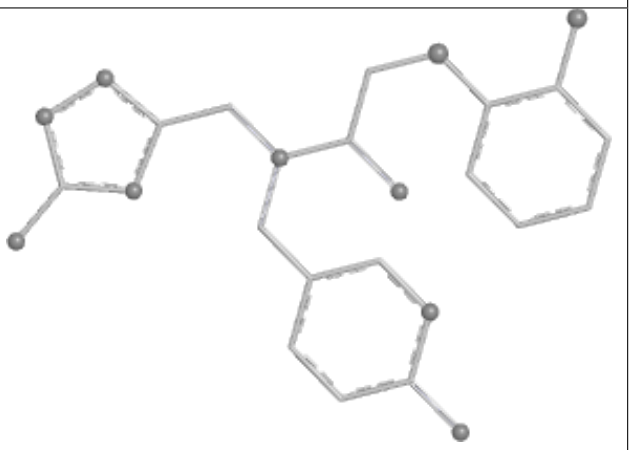
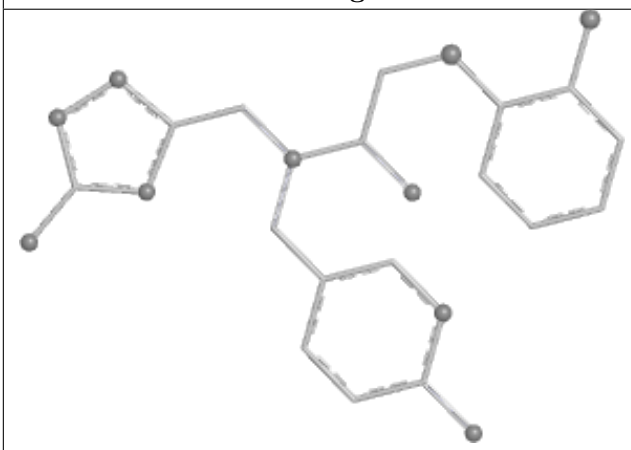


Bond angles



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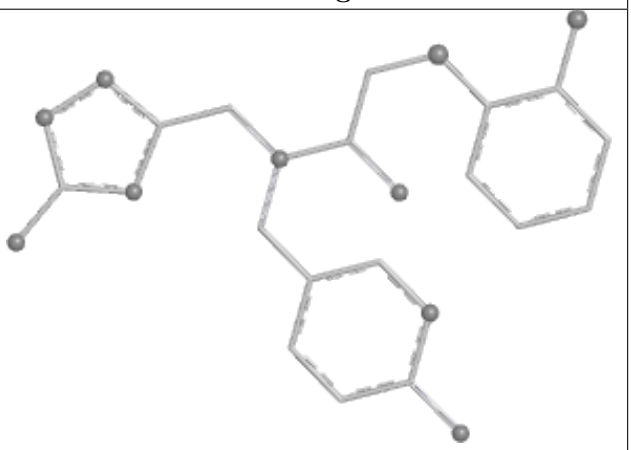
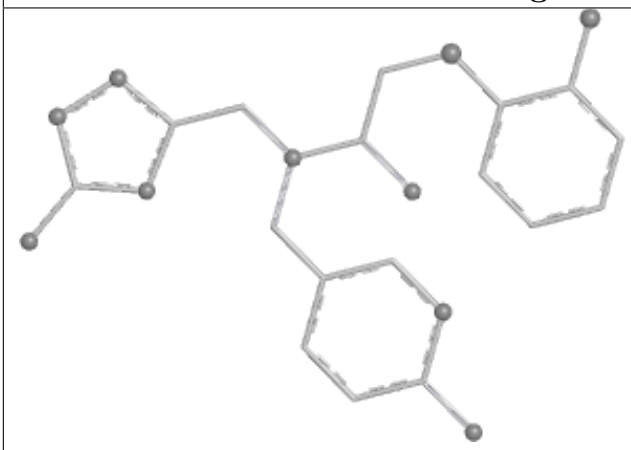


Rings

Ligand VFZ a 302



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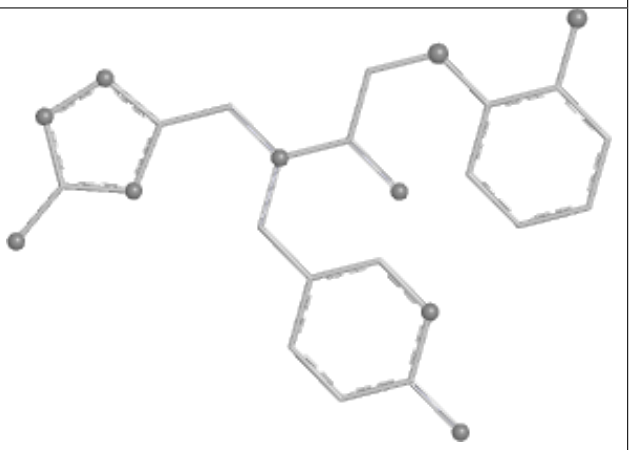

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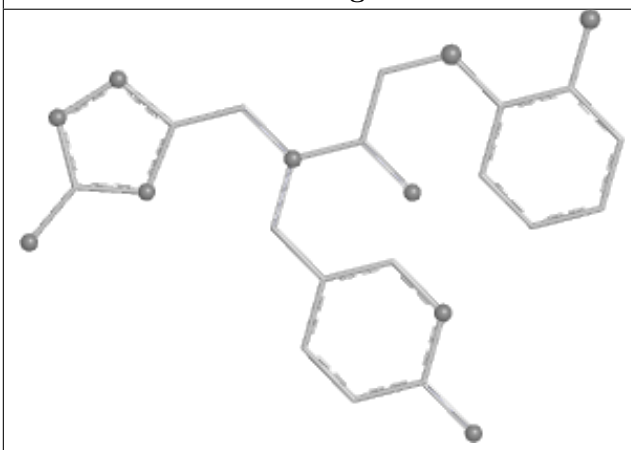
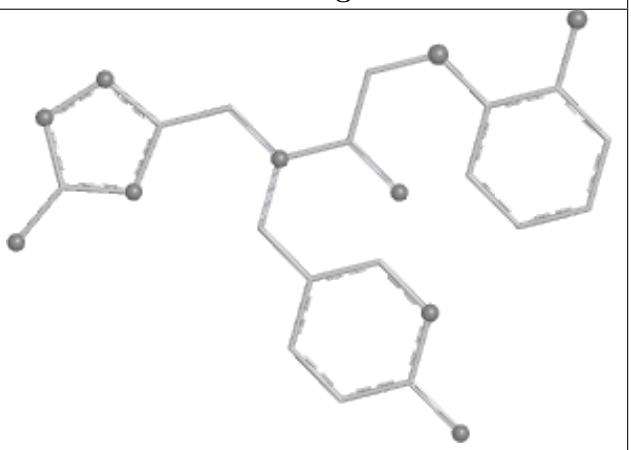
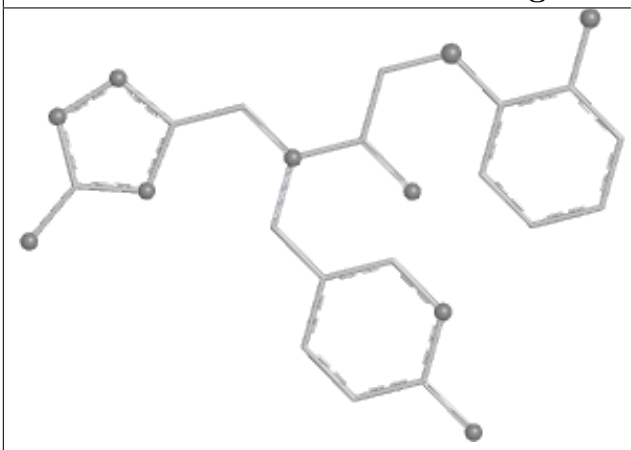


Torsions

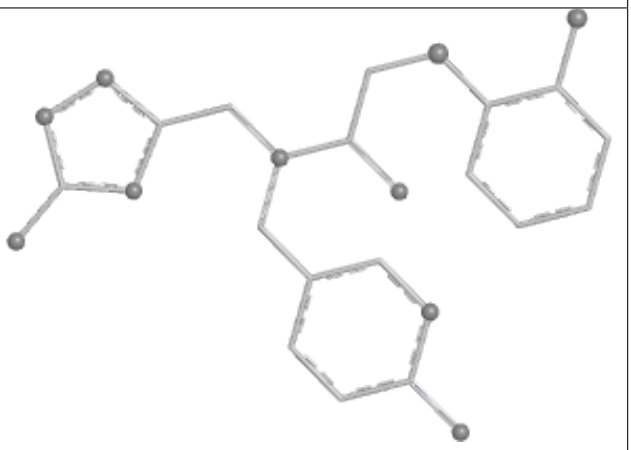


Rings

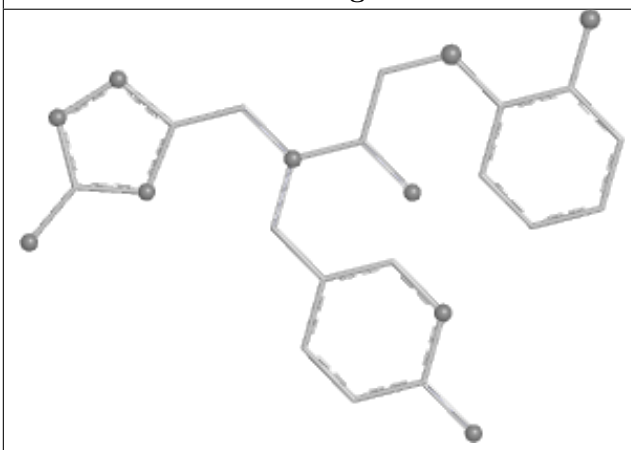
Ligand VFZ b 302



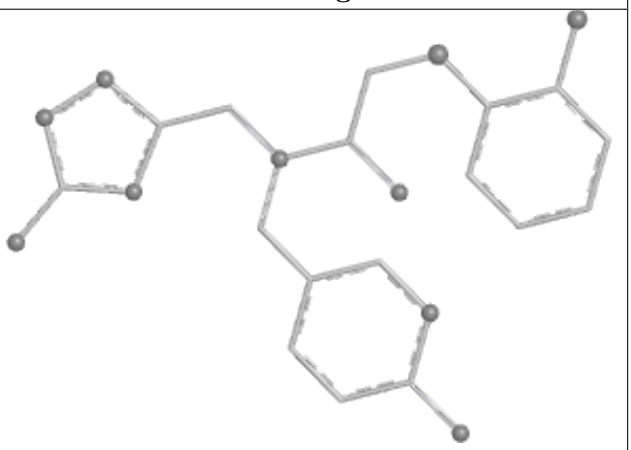
Bond lengths



Bond angles

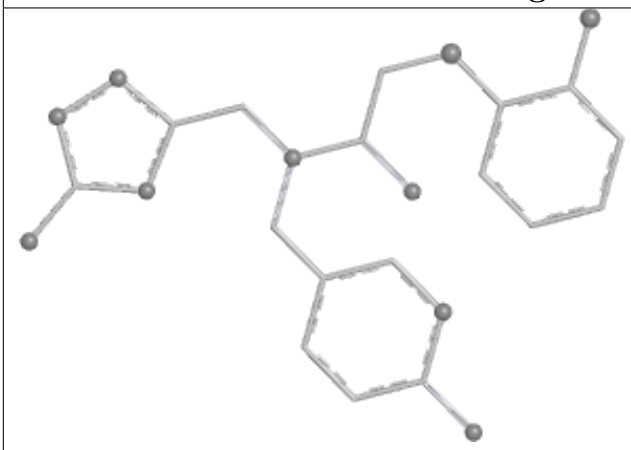


Torsions

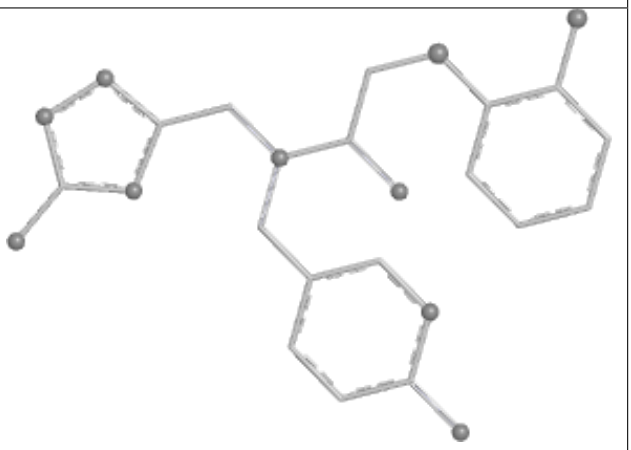


Rings

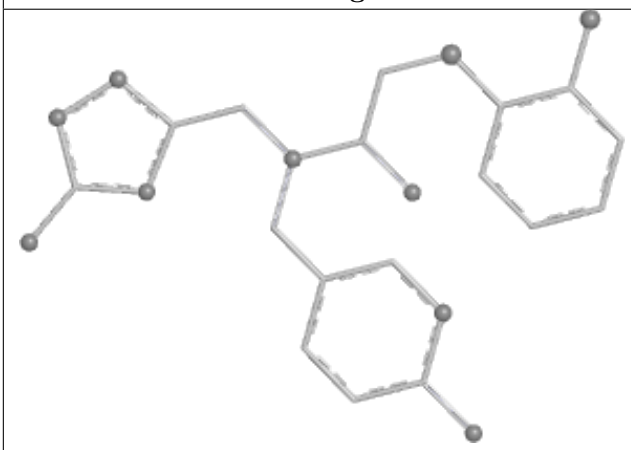
Ligand VFZ d 302



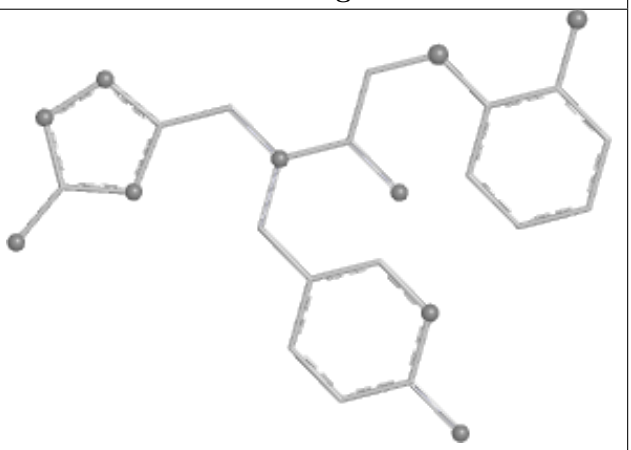
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers

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

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, 95^{th} 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%)	0.29	0 100 100	75, 92, 121, 168	0
1	B	258/261 (98%)	0.24	0 100 100	74, 93, 120, 154	0
1	C	258/261 (98%)	0.22	0 100 100	70, 91, 120, 188	0
1	D	258/261 (98%)	0.27	0 100 100	69, 91, 121, 175	0
1	E	258/261 (98%)	0.27	0 100 100	74, 92, 122, 171	0
1	F	258/261 (98%)	0.23	0 100 100	70, 92, 124, 162	0
1	G	257/261 (98%)	0.50	13 (5%) 28 16	76, 105, 131, 145	0
1	H	257/261 (98%)	0.46	8 (3%) 49 31	79, 105, 132, 149	0
1	I	257/261 (98%)	0.44	9 (3%) 44 28	74, 104, 134, 151	0
1	J	258/261 (98%)	0.24	2 (0%) 86 73	70, 92, 120, 143	0
1	K	258/261 (98%)	0.22	0 100 100	72, 94, 124, 188	0
1	L	258/261 (98%)	0.24	1 (0%) 92 86	75, 93, 120, 151	0
1	M	257/261 (98%)	0.48	14 (5%) 25 14	79, 106, 132, 148	0
1	N	257/261 (98%)	0.43	8 (3%) 49 31	74, 103, 131, 158	0
1	O	257/261 (98%)	0.43	9 (3%) 44 28	81, 105, 134, 146	0
1	P	257/261 (98%)	0.37	3 (1%) 79 64	73, 105, 132, 150	0
1	Q	257/261 (98%)	0.54	12 (4%) 31 18	78, 106, 131, 154	0
1	R	257/261 (98%)	0.37	8 (3%) 49 31	77, 104, 130, 152	0
1	S	258/261 (98%)	0.26	0 100 100	74, 94, 123, 168	0
1	T	258/261 (98%)	0.21	0 100 100	76, 94, 123, 155	0
1	U	258/261 (98%)	0.23	0 100 100	78, 95, 123, 188	0
1	V	257/261 (98%)	0.48	10 (3%) 39 24	79, 105, 131, 157	0
1	W	257/261 (98%)	0.56	16 (6%) 20 10	77, 104, 132, 148	0
1	X	257/261 (98%)	0.40	4 (1%) 72 55	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%)	0.57	10 (3%) 39 24	75, 102, 129, 159	0
1	Z	258/261 (98%)	0.35	2 (0%) 86 73	75, 102, 128, 158	0
1	a	257/261 (98%)	0.39	7 (2%) 54 36	72, 101, 130, 156	0
1	b	257/261 (98%)	0.32	1 (0%) 92 86	78, 101, 129, 146	0
1	c	258/261 (98%)	0.36	1 (0%) 92 86	76, 102, 132, 182	0
1	d	257/261 (98%)	0.50	9 (3%) 44 28	77, 103, 129, 147	0
All	All	7725/7830 (98%)	0.36	147 (1%) 66 49	69, 99, 129, 188	0

All (147) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	58	ILE	3.2
1	G	88	ILE	2.9
1	O	58	ILE	2.8
1	Y	88	ILE	2.8
1	Y	58	ILE	2.7
1	a	64	VAL	2.7
1	W	9	ILE	2.7
1	Q	58	ILE	2.7
1	a	94	ILE	2.6
1	d	64	VAL	2.6
1	W	63	SER	2.6
1	W	88	ILE	2.6
1	W	34	ILE	2.6
1	R	46	LEU	2.6
1	b	197	GLY	2.5
1	G	131	LEU	2.5
1	H	137	LEU	2.5
1	M	45	VAL	2.5
1	O	113	ILE	2.5
1	H	46	LEU	2.5
1	Q	27	ILE	2.4
1	W	94	ILE	2.4
1	Q	46	LEU	2.4
1	W	45	VAL	2.4
1	Y	28	VAL	2.4
1	P	113	ILE	2.4
1	G	28	VAL	2.4
1	N	94	ILE	2.4
1	W	27	ILE	2.4

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Mol	Chain	Res	Type	RSRZ
1	V	28	VAL	2.4
1	G	94	ILE	2.4
1	Y	113	ILE	2.4
1	d	119	ILE	2.4
1	W	58	ILE	2.4
1	Q	28	VAL	2.4
1	P	131	LEU	2.4
1	G	9	ILE	2.4
1	X	88	ILE	2.4
1	W	40	ILE	2.3
1	Y	119	ILE	2.3
1	H	138	ALA	2.3
1	H	94	ILE	2.3
1	M	58	ILE	2.3
1	I	64	VAL	2.3
1	N	40	ILE	2.3
1	d	46	LEU	2.3
1	d	80	LEU	2.3
1	V	22	VAL	2.3
1	V	46	LEU	2.3
1	a	46	LEU	2.3
1	G	63	SER	2.3
1	M	94	ILE	2.3
1	V	27	ILE	2.3
1	M	64	VAL	2.3
1	O	88	ILE	2.3
1	M	28	VAL	2.3
1	N	88	ILE	2.3
1	R	138	ALA	2.3
1	I	131	LEU	2.2
1	V	131	LEU	2.2
1	N	113	ILE	2.2
1	O	57	ARG	2.2
1	N	27	ILE	2.2
1	R	137	LEU	2.2
1	Q	52	ILE	2.2
1	X	28	VAL	2.2
1	Y	9	ILE	2.2
1	Q	65	GLY	2.2
1	a	138	ALA	2.2
1	G	34	ILE	2.2
1	M	10	ILE	2.2

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Mol	Chain	Res	Type	RSRZ
1	R	9	ILE	2.2
1	a	9	ILE	2.2
1	d	65	GLY	2.2
1	Y	27	ILE	2.2
1	M	63	SER	2.2
1	N	131	LEU	2.2
1	Y	40	ILE	2.2
1	d	137	LEU	2.2
1	I	113	ILE	2.2
1	M	119	ILE	2.2
1	a	32	VAL	2.2
1	M	46	LEU	2.2
1	P	34	ILE	2.2
1	I	130	ILE	2.2
1	Q	88	ILE	2.2
1	V	58	ILE	2.2
1	J	138	ALA	2.2
1	R	113	ILE	2.2
1	R	80	LEU	2.1
1	M	107	ILE	2.1
1	O	119	ILE	2.1
1	N	64	VAL	2.1
1	Z	138	ALA	2.1
1	X	58	ILE	2.1
1	J	72	LYS	2.1
1	G	64	VAL	2.1
1	c	113	ILE	2.1
1	Y	45	VAL	2.1
1	H	119	ILE	2.1
1	Y	57	ARG	2.1
1	d	28	VAL	2.1
1	I	58	ILE	2.1
1	O	28	VAL	2.1
1	H	164	HIS	2.1
1	V	50	THR	2.1
1	O	9	ILE	2.1
1	L	138	ALA	2.1
1	W	32	VAL	2.1
1	G	10	ILE	2.1
1	Q	82	ILE	2.1
1	V	64	VAL	2.1
1	Q	63	SER	2.1

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Mol	Chain	Res	Type	RSRZ
1	G	45	VAL	2.1
1	O	22	VAL	2.1
1	G	125	ILE	2.1
1	M	113	ILE	2.1
1	R	94	ILE	2.1
1	V	113	ILE	2.1
1	Z	88	ILE	2.1
1	H	88	ILE	2.1
1	d	94	ILE	2.1
1	W	64	VAL	2.1
1	I	27	ILE	2.1
1	I	46	LEU	2.1
1	G	113	ILE	2.0
1	I	34	ILE	2.0
1	Q	34	ILE	2.0
1	H	64	VAL	2.0
1	M	131	LEU	2.0
1	W	46	LEU	2.0
1	W	125	ILE	2.0
1	I	138	ALA	2.0
1	M	88	ILE	2.0
1	R	58	ILE	2.0
1	a	113	ILE	2.0
1	d	58	ILE	2.0
1	V	34	ILE	2.0
1	W	62	SER	2.0
1	Q	137	LEU	2.0
1	W	50	THR	2.0
1	W	28	VAL	2.0
1	N	119	ILE	2.0
1	O	107	ILE	2.0
1	M	22	VAL	2.0
1	X	119	ILE	2.0
1	Q	229	LEU	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} 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	I	301	1/1	0.14	0.25	115,115,115,115	0
2	CL	C	301	1/1	0.16	0.26	123,123,123,123	0
2	CL	L	301	1/1	0.22	0.26	127,127,127,127	0
2	CL	A	302	1/1	0.26	0.32	131,131,131,131	0
2	CL	A	301	1/1	0.30	0.27	112,112,112,112	0
2	CL	E	301	1/1	0.38	0.36	137,137,137,137	0
2	CL	M	302	1/1	0.42	0.23	118,118,118,118	0
2	CL	S	301	1/1	0.42	0.17	113,113,113,113	0
2	CL	G	301	1/1	0.44	0.28	131,131,131,131	0
2	CL	A	306	1/1	0.46	0.23	110,110,110,110	0
3	SO4	K	302	5/5	0.47	0.69	109,124,142,151	5
3	SO4	N	303	5/5	0.48	0.88	103,122,138,153	5
2	CL	Q	301	1/1	0.49	0.19	110,110,110,110	0
2	CL	N	301	1/1	0.49	0.24	126,126,126,126	0
2	CL	C	303	1/1	0.51	0.19	108,108,108,108	0
3	SO4	H	302	5/5	0.51	1.09	114,128,146,169	5
3	SO4	A	309	5/5	0.52	0.95	129,133,146,155	5
3	SO4	R	303	5/5	0.53	0.83	114,116,135,148	5
2	CL	A	305	1/1	0.54	0.29	120,120,120,120	0
3	SO4	D	304	5/5	0.54	0.77	117,129,137,140	5
2	CL	X	302	1/1	0.54	0.24	107,107,107,107	0
3	SO4	P	303	5/5	0.55	0.68	122,130,145,147	5
3	SO4	B	304	5/5	0.56	0.70	114,123,137,145	5
3	SO4	P	302	5/5	0.57	0.27	182,183,200,217	0
2	CL	T	301	1/1	0.57	0.15	111,111,111,111	0
2	CL	C	302	1/1	0.57	0.23	144,144,144,144	0
2	CL	A	303	1/1	0.60	0.30	129,129,129,129	0
3	SO4	E	304	5/5	0.60	0.67	110,121,128,134	5
3	SO4	U	303	5/5	0.60	0.25	172,183,194,211	0
3	SO4	C	305	5/5	0.63	0.73	124,128,134,139	5
2	CL	D	301	1/1	0.63	0.17	117,117,117,117	0
3	SO4	F	302	5/5	0.65	0.60	103,122,127,132	5

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	SO4	I	303	5/5	0.65	0.82	101,124,131,134	5
2	CL	M	301	1/1	0.66	0.25	100,100,100,100	0
2	CL	B	301	1/1	0.67	0.18	110,110,110,110	0
2	CL	O	301	1/1	0.68	0.20	113,113,113,113	0
3	SO4	V	301	5/5	0.68	0.39	108,116,129,134	5
2	CL	E	302	1/1	0.69	0.37	88,88,88,88	0
3	SO4	T	302	5/5	0.69	0.51	142,164,169,171	0
3	SO4	B	303	5/5	0.70	0.38	130,152,167,175	0
3	SO4	d	301	5/5	0.71	0.44	157,172,174,176	0
3	SO4	F	301	5/5	0.72	0.45	159,160,182,182	0
3	SO4	c	301	5/5	0.72	0.66	118,121,135,138	5
3	SO4	S	302	5/5	0.72	0.50	162,170,183,183	0
3	SO4	M	303	5/5	0.73	0.44	103,109,133,139	5
3	SO4	C	304	5/5	0.73	0.41	149,160,181,192	0
2	CL	A	304	1/1	0.74	0.41	92,92,92,92	0
3	SO4	A	307	5/5	0.75	0.40	102,113,129,130	5
3	SO4	O	302	5/5	0.75	0.49	141,144,170,176	0
3	SO4	Q	302	5/5	0.75	0.41	154,165,177,178	0
3	SO4	K	301	5/5	0.75	0.51	145,156,168,173	0
3	SO4	E	303	5/5	0.75	0.31	163,166,184,192	0
3	SO4	Y	301	5/5	0.76	0.35	150,162,167,184	0
3	SO4	H	301	5/5	0.77	0.48	154,164,169,173	0
3	SO4	D	302	5/5	0.77	0.38	141,151,171,176	0
3	SO4	N	302	5/5	0.77	0.42	146,157,165,182	0
3	SO4	X	303	5/5	0.78	0.44	129,168,181,184	0
3	SO4	W	301	5/5	0.78	0.43	154,163,181,186	0
3	SO4	J	301	5/5	0.80	0.58	149,155,172,195	0
3	SO4	b	301	5/5	0.80	0.34	139,162,171,176	0
3	SO4	a	301	5/5	0.82	0.47	127,151,163,172	0
3	SO4	Z	301	5/5	0.82	0.43	148,163,172,181	0
3	SO4	J	302	5/5	0.83	0.45	82,98,110,118	5
3	SO4	R	301	5/5	0.84	0.29	139,148,165,175	0
3	SO4	P	301	5/5	0.84	0.41	106,114,129,130	5
3	SO4	I	302	5/5	0.85	0.42	155,157,171,182	0
3	SO4	L	302	5/5	0.86	0.31	107,118,130,134	5
3	SO4	U	301	5/5	0.86	0.36	159,160,171,172	0
3	SO4	G	303	5/5	0.86	0.43	97,99,111,117	5
2	CL	B	302	1/1	0.87	0.65	112,112,112,112	0
3	SO4	R	302	5/5	0.87	0.23	131,141,152,169	0
3	SO4	N	304	5/5	0.89	0.19	123,126,139,150	0
3	SO4	A	308	5/5	0.89	0.23	118,129,152,177	0
2	CL	X	301	1/1	0.89	0.22	110,110,110,110	0

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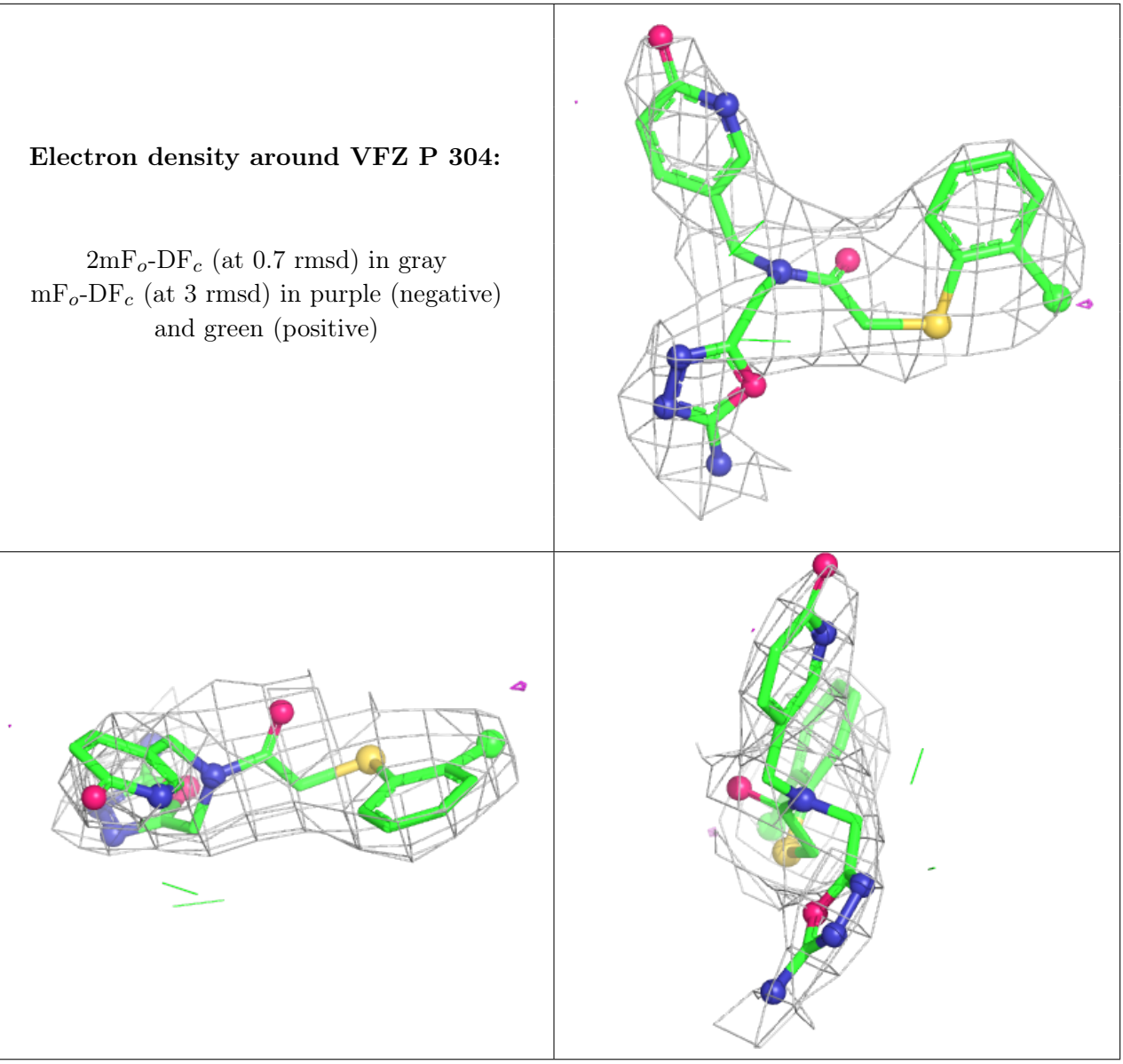
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	SO4	Y	302	5/5	0.90	0.20	104,117,140,171	0
3	SO4	U	302	5/5	0.90	0.24	71,74,104,112	5
3	SO4	D	303	5/5	0.90	0.27	103,126,141,162	0
4	VFZ	P	304	27/27	0.91	0.62	74,99,162,167	0
4	VFZ	Y	303	27/27	0.91	0.52	75,101,157,166	0
4	VFZ	b	302	27/27	0.91	0.59	71,99,166,182	0
4	VFZ	d	302	27/27	0.91	0.61	67,92,179,181	0
4	VFZ	T	303	27/27	0.92	0.64	78,97,159,172	0
4	VFZ	V	303	27/27	0.92	0.57	82,100,166,182	0
4	VFZ	X	304	27/27	0.92	0.54	80,99,195,221	0
4	VFZ	I	304	27/27	0.92	0.64	77,103,159,176	0
4	VFZ	Z	302	27/27	0.92	0.55	72,106,176,200	0
4	VFZ	a	302	27/27	0.92	0.70	77,101,174,197	0
4	VFZ	O	303	27/27	0.92	0.66	78,100,166,177	0
3	SO4	V	302	5/5	0.92	0.30	126,127,136,163	0
4	VFZ	Q	303	27/27	0.93	0.58	84,102,151,159	0
4	VFZ	R	304	27/27	0.93	0.54	83,103,178,243	0
4	VFZ	D	305	27/27	0.93	0.55	64,85,161,161	0
4	VFZ	H	303	27/27	0.93	0.56	79,97,166,217	0
3	SO4	G	302	5/5	0.93	0.23	108,126,141,151	0
4	VFZ	M	304	27/27	0.93	0.69	84,102,174,184	0
4	VFZ	N	305	27/27	0.93	0.60	77,106,163,172	0
4	VFZ	B	305	27/27	0.93	0.53	72,90,147,154	0
4	VFZ	L	303	27/27	0.93	0.58	61,91,149,157	0
4	VFZ	c	303	27/27	0.93	0.63	72,99,168,189	0
4	VFZ	C	306	27/27	0.93	0.52	75,93,173,184	0
4	VFZ	K	303	27/27	0.94	0.61	78,96,158,176	0
4	VFZ	G	304	27/27	0.94	0.63	82,96,146,167	0
4	VFZ	U	304	27/27	0.94	0.57	69,91,148,155	0
4	VFZ	A	310	27/27	0.94	0.48	76,88,149,155	0
4	VFZ	W	302	27/27	0.94	0.69	76,94,182,200	0
4	VFZ	J	303	27/27	0.94	0.61	72,93,147,153	0
4	VFZ	S	303	27/27	0.95	0.61	78,97,168,187	0
3	SO4	c	302	5/5	0.95	0.19	103,109,133,166	0
4	VFZ	E	305	27/27	0.95	0.45	66,90,147,150	0
4	VFZ	F	303	27/27	0.95	0.53	75,94,158,170	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.

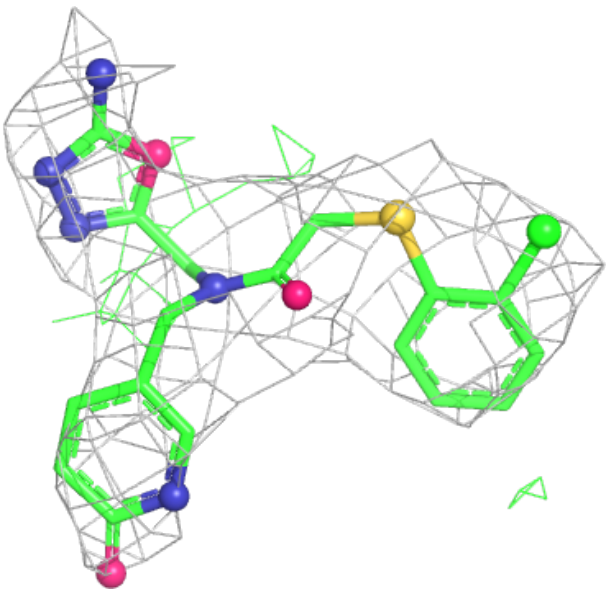
Electron density around VFZ P 304:

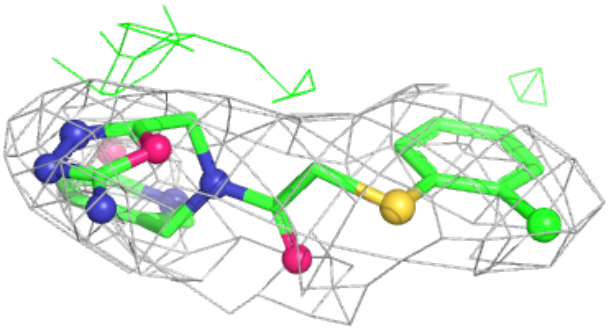
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

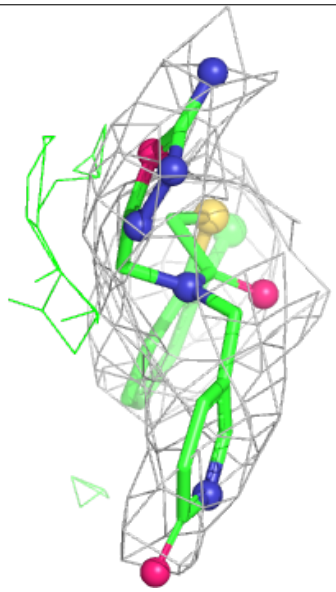


Electron density around VFZ Y 303:

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

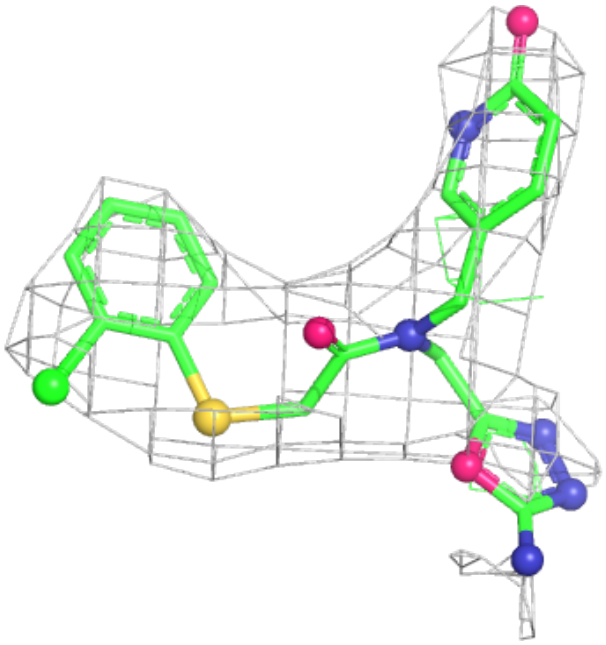


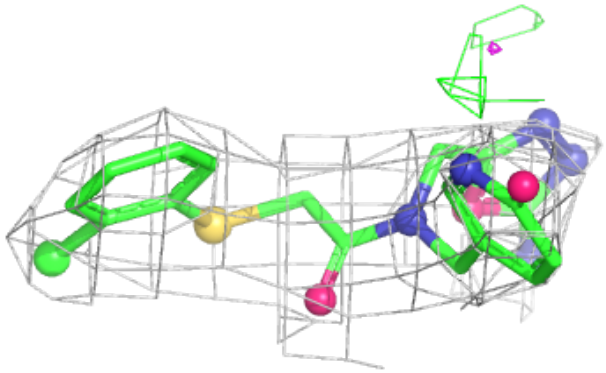


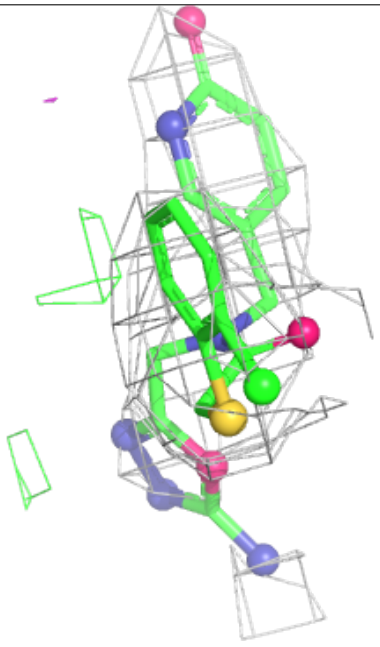


Electron density around VFZ b 302:

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

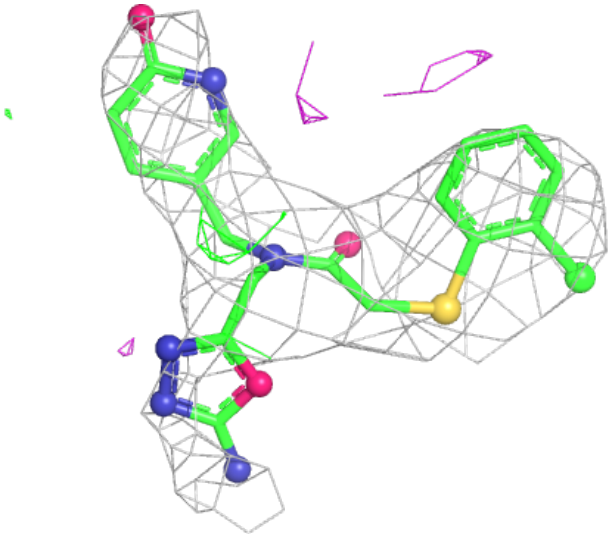


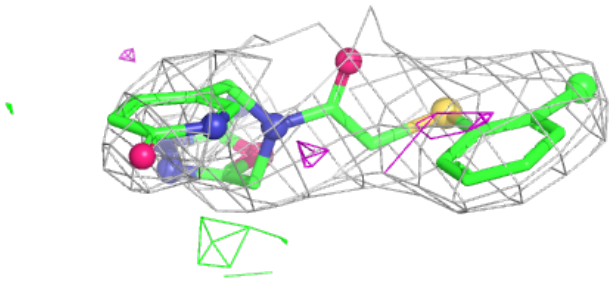


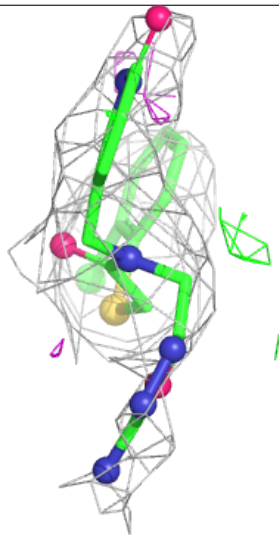


Electron density around VFZ d 302:

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

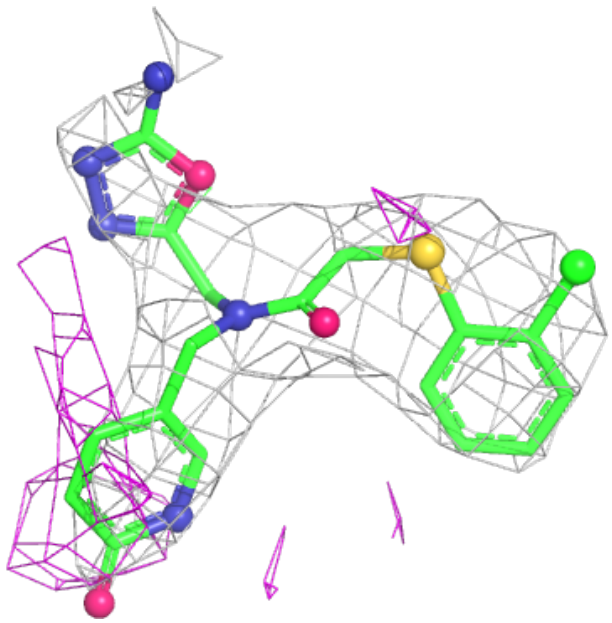


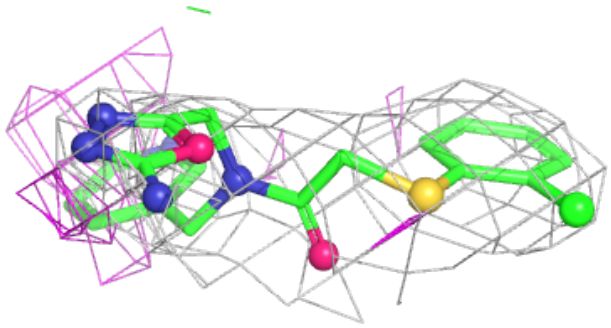


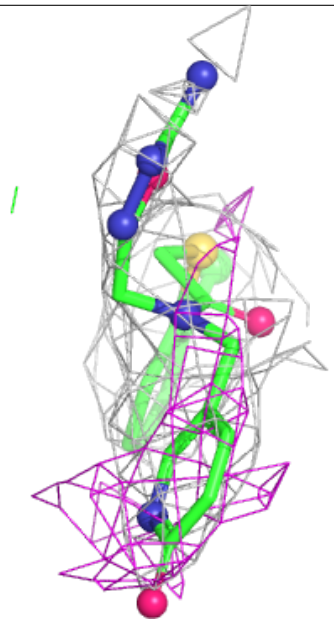


Electron density around VFZ T 303:

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

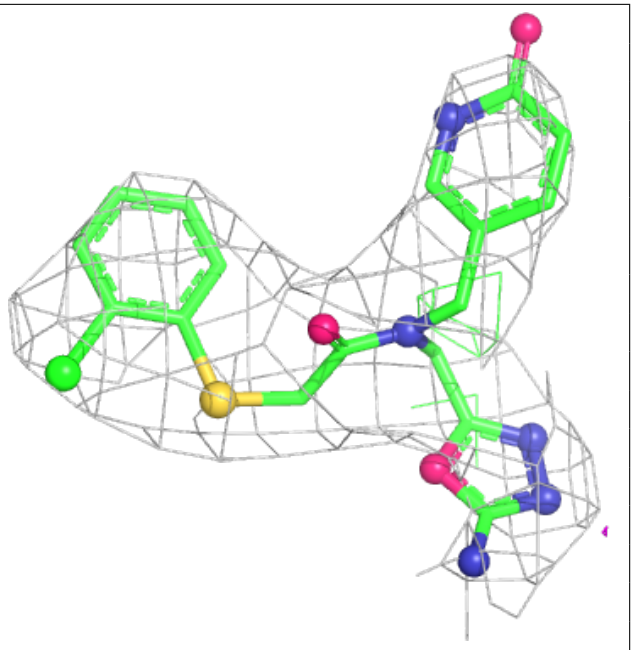


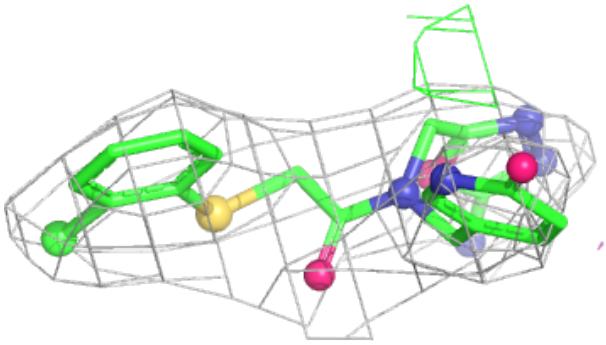


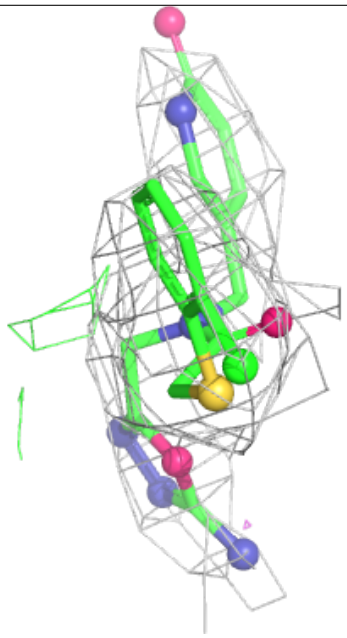


Electron density around VFZ V 303:

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

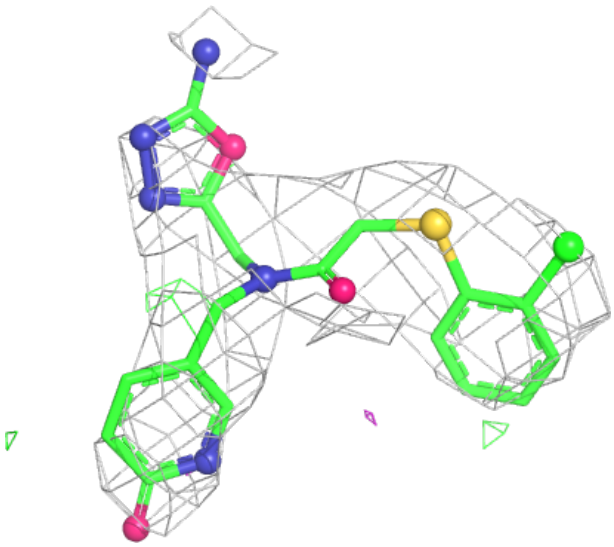


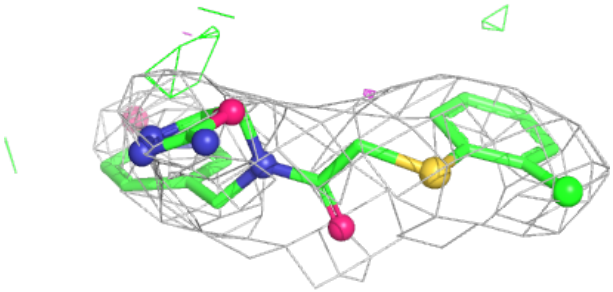


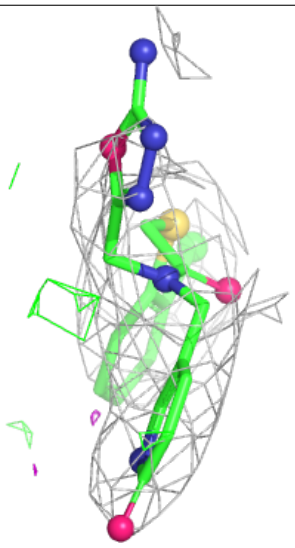


Electron density around VFZ X 304:

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

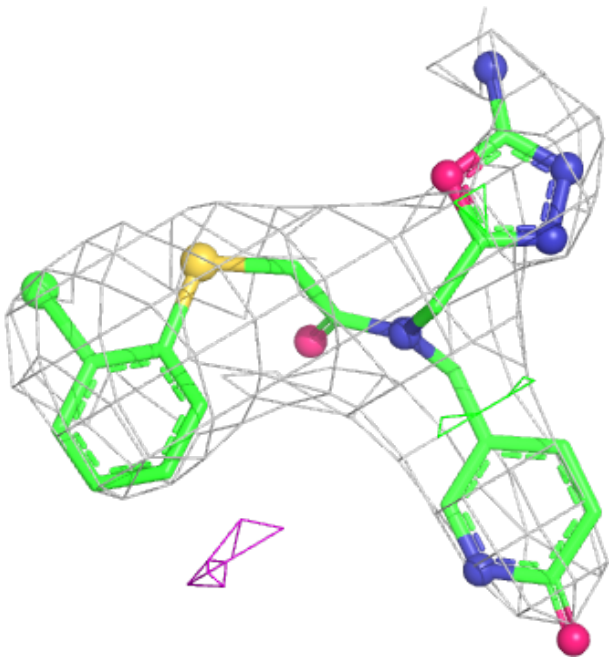


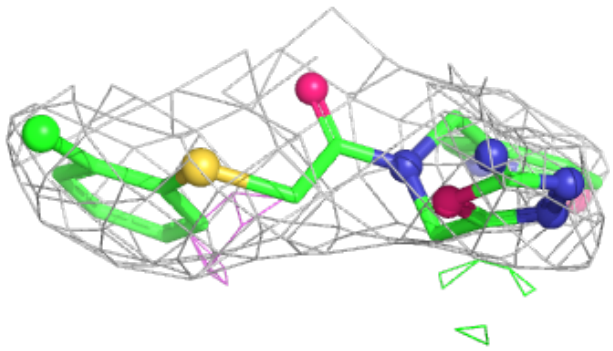


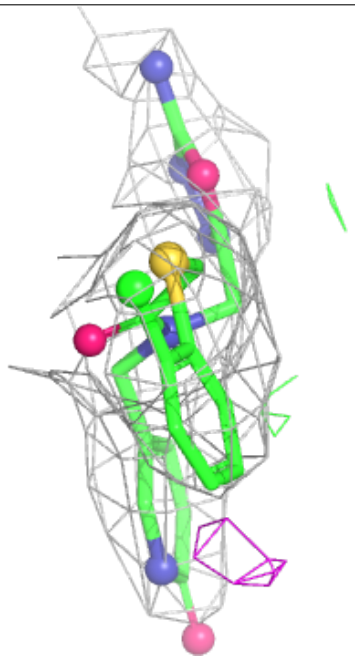


Electron density around VFZ I 304:

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

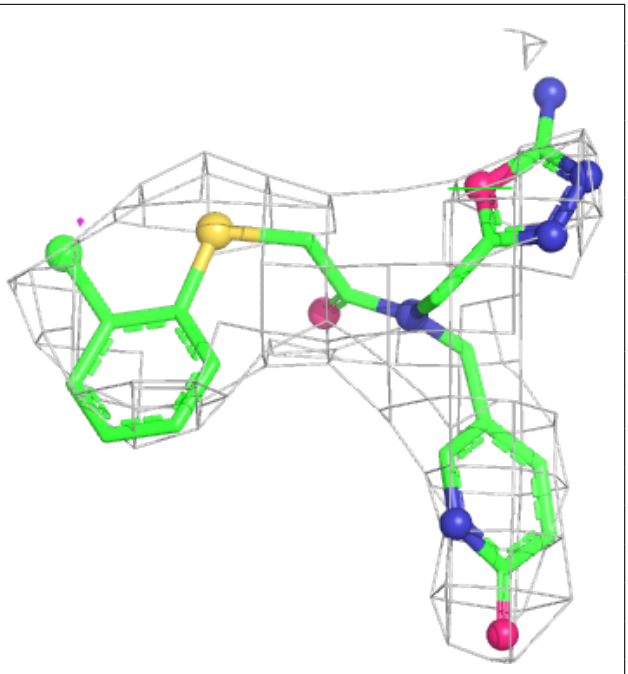


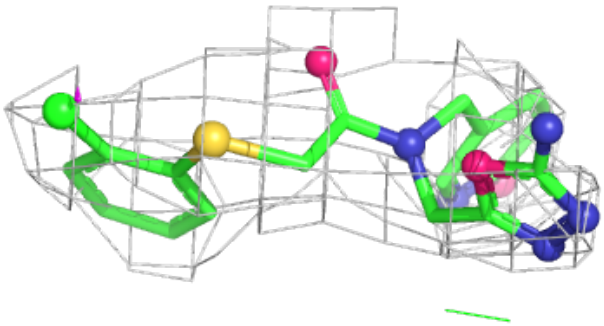


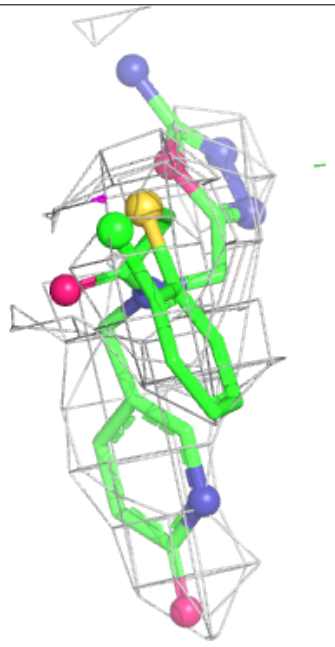


Electron density around VFZ Z 302:

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

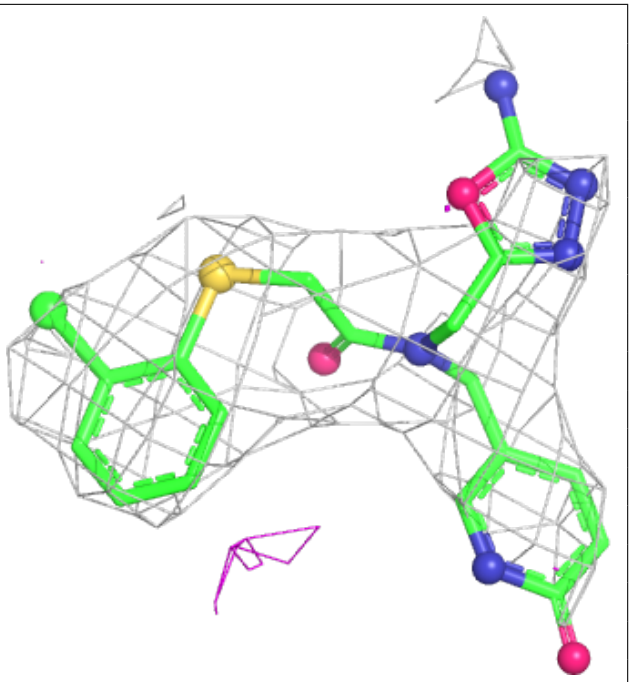


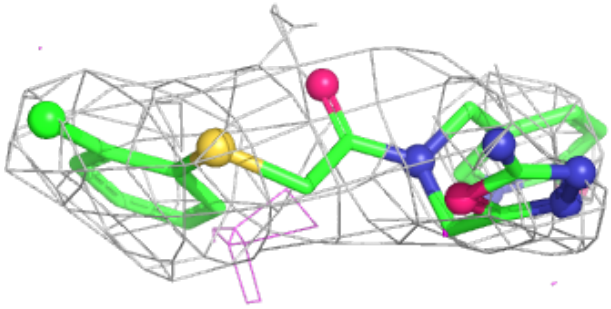


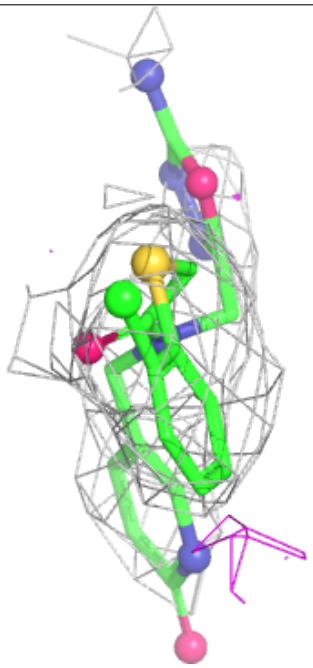


Electron density around VFZ a 302:

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

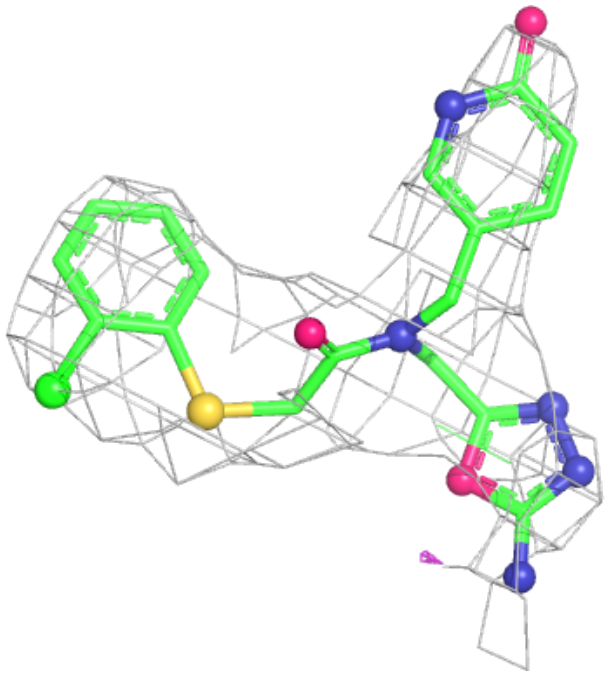


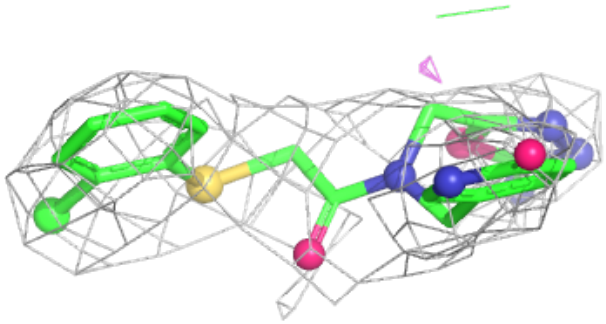


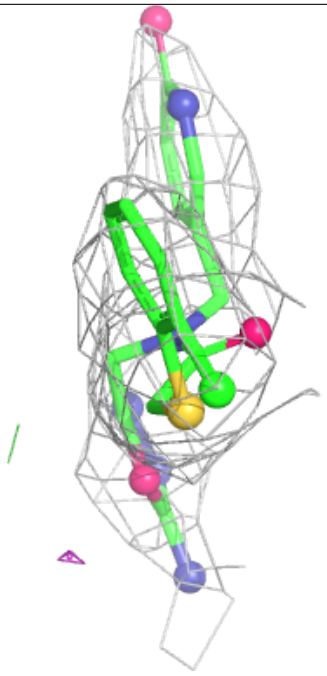


Electron density around VFZ O 303:

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

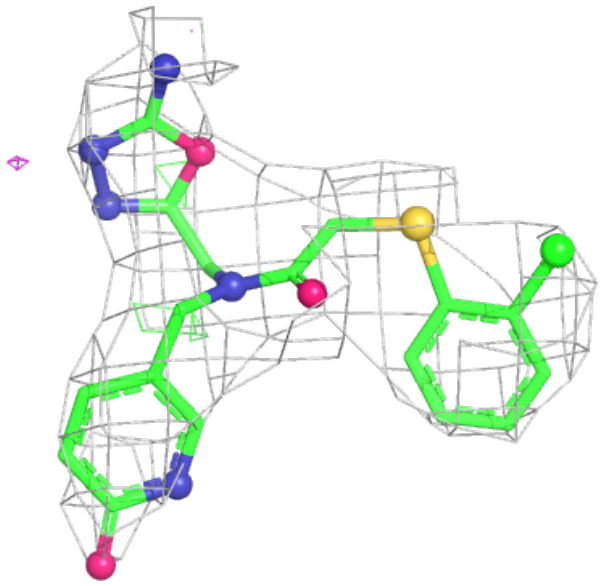


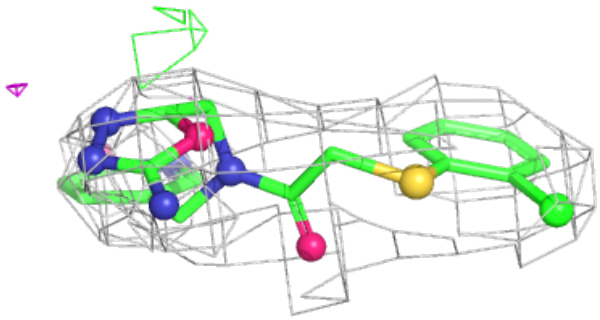


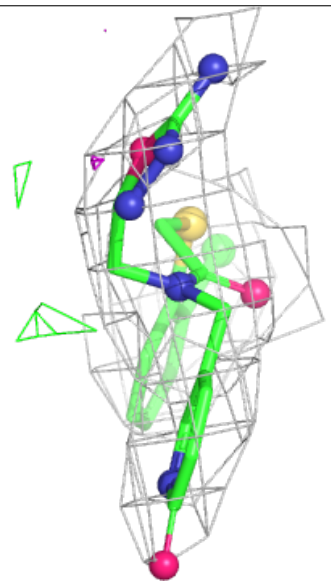


Electron density around VFZ Q 303:

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

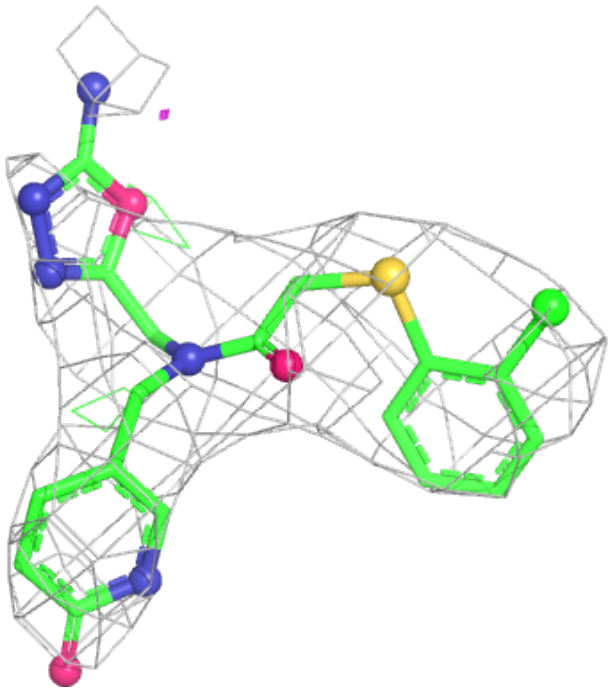


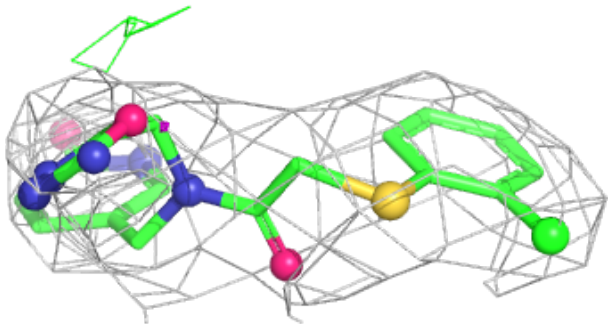


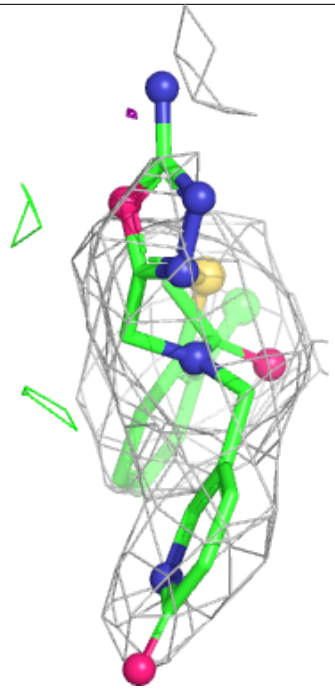


Electron density around VFZ R 304:

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

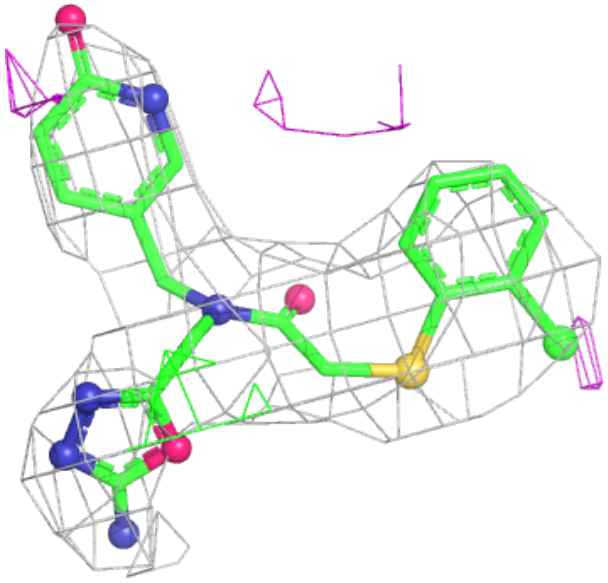


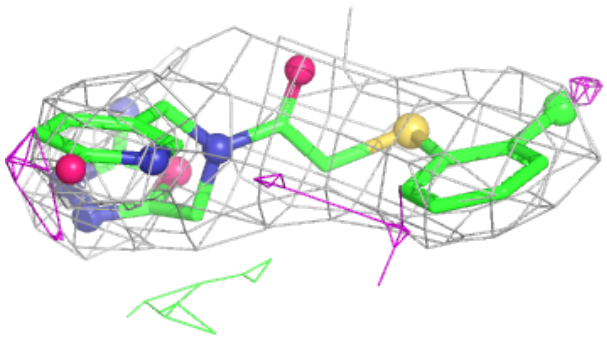


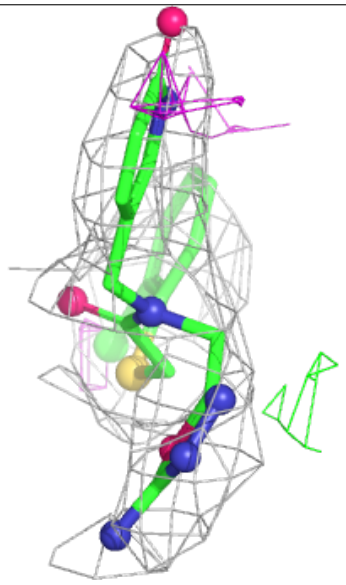


Electron density around VFZ D 305:

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

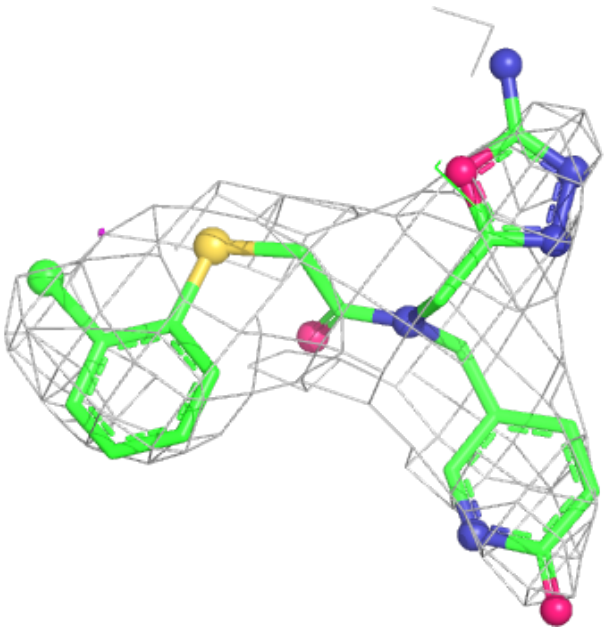


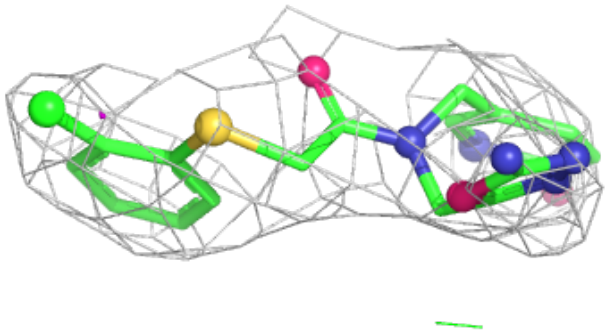


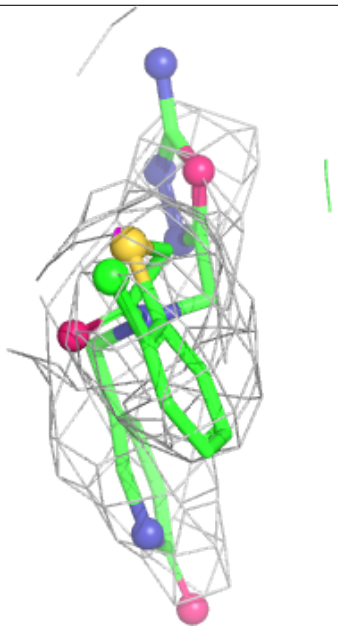


Electron density around VFZ H 303:

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

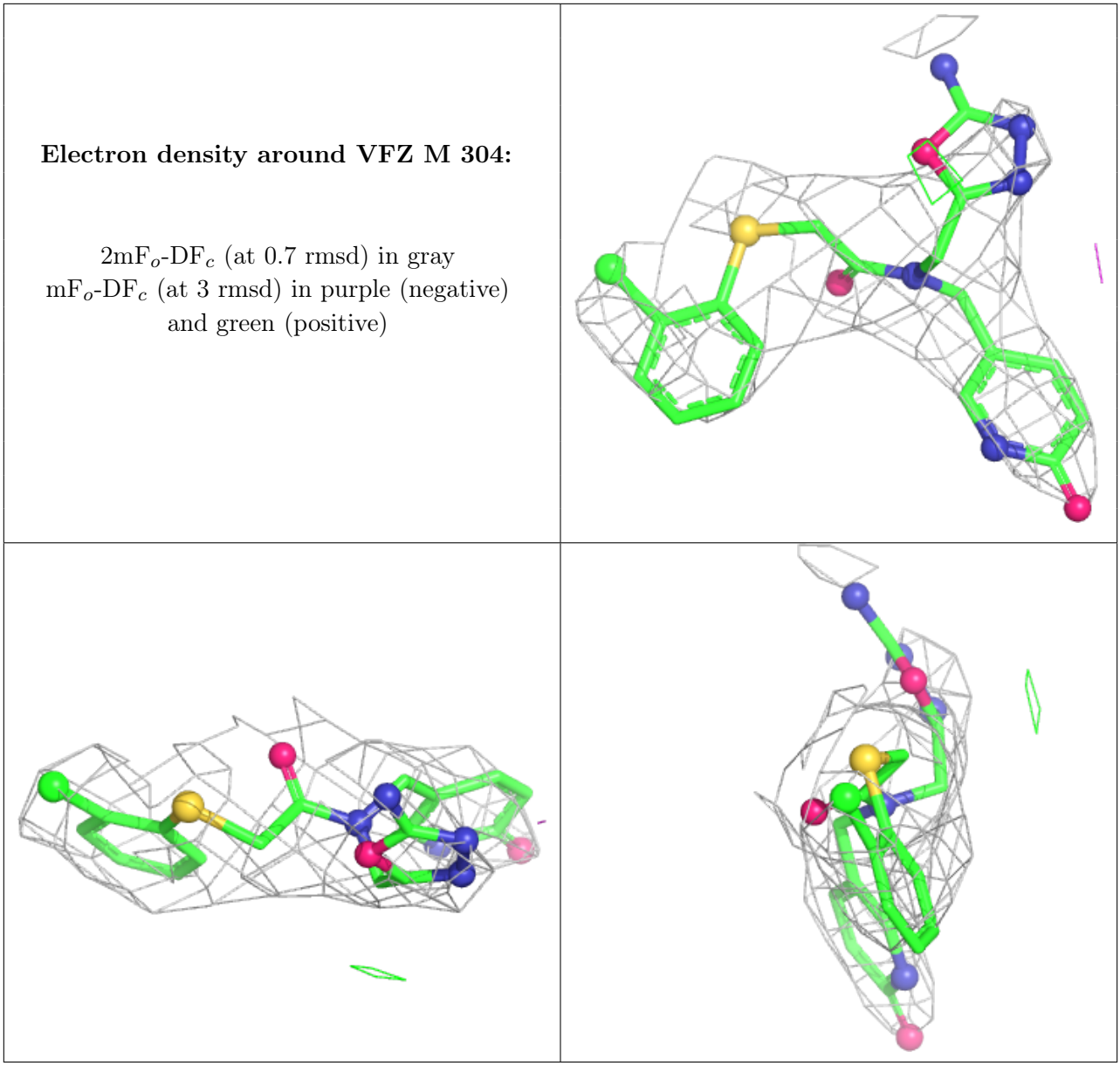






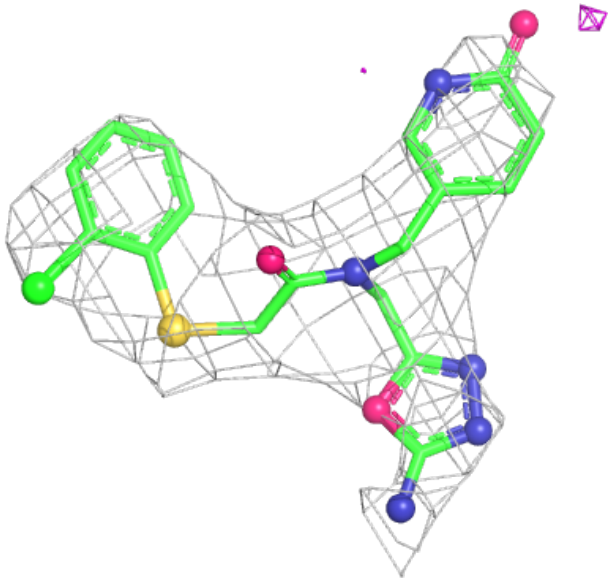
Electron density around VFZ M 304:

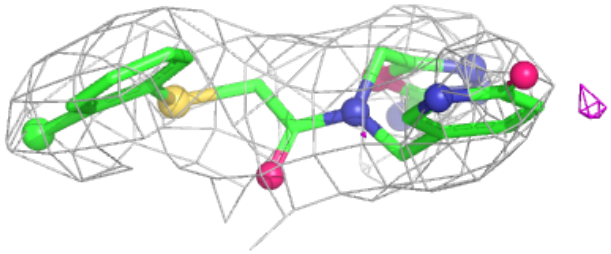
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

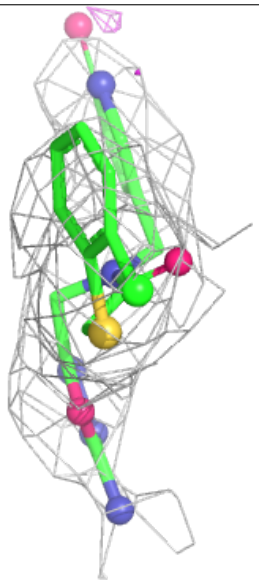


Electron density around VFZ N 305:

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

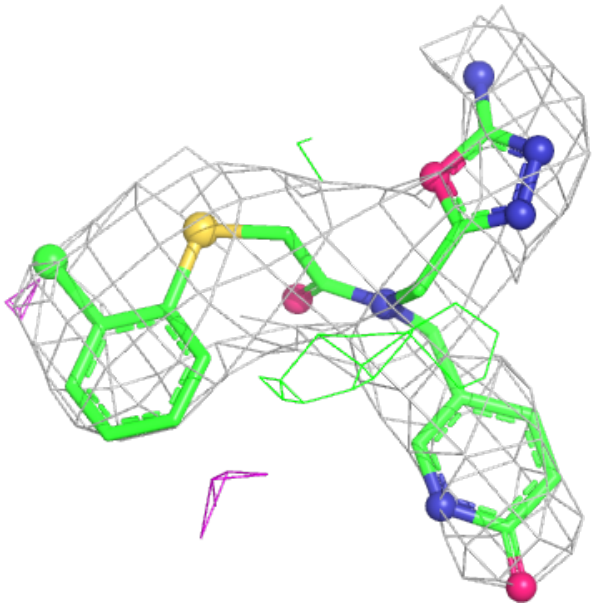


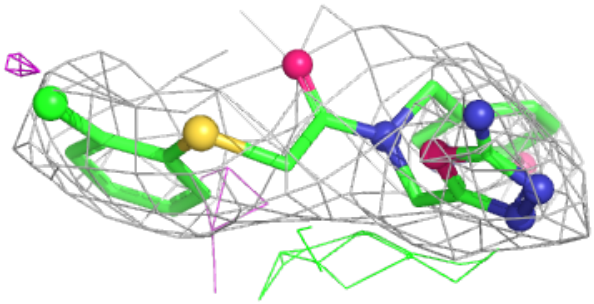




Electron density around VFZ B 305:

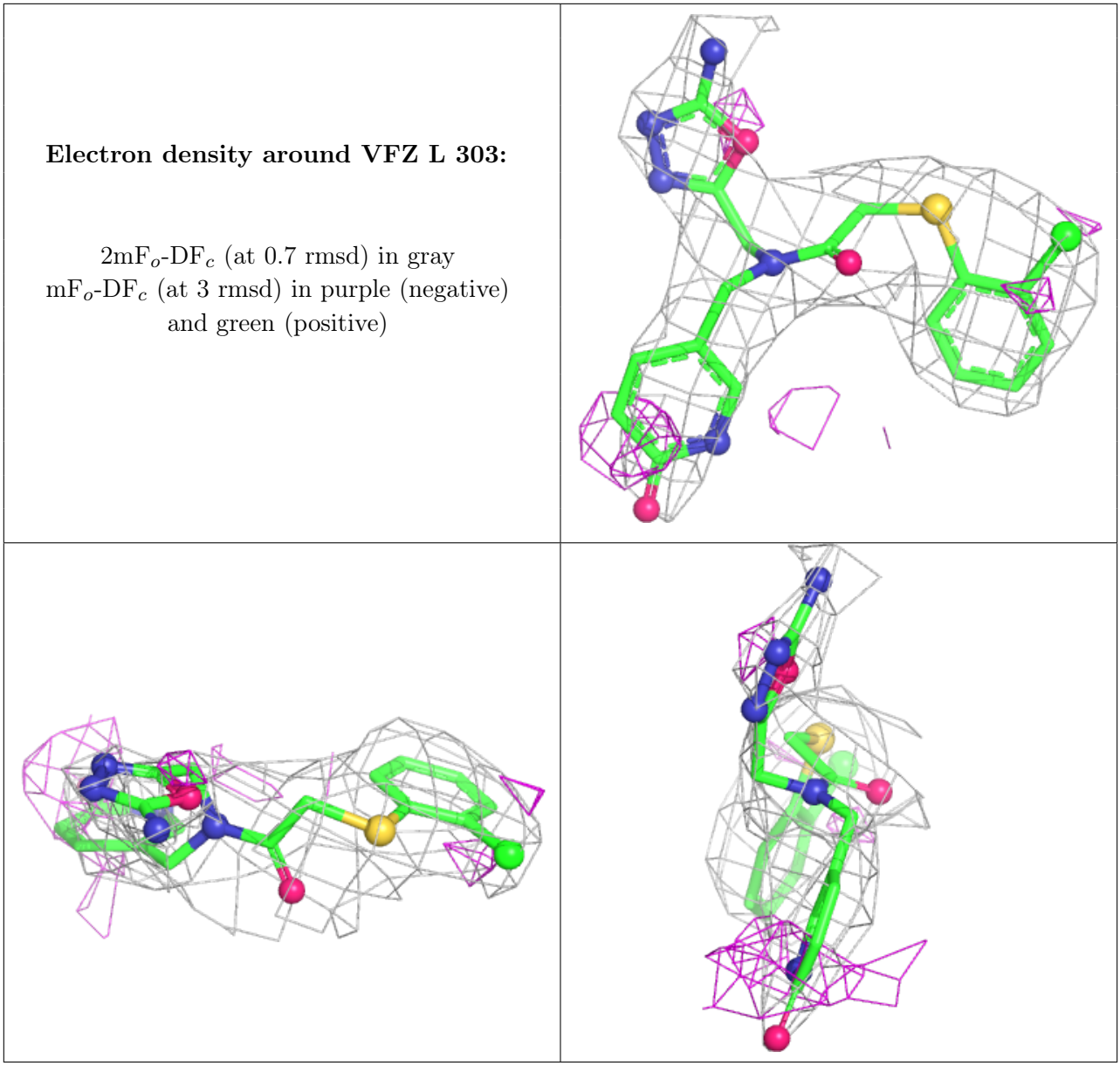
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)





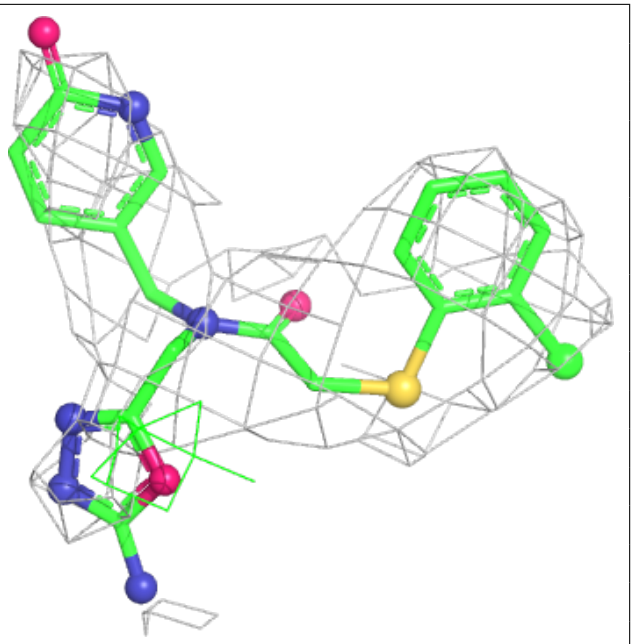
Electron density around VFZ L 303:

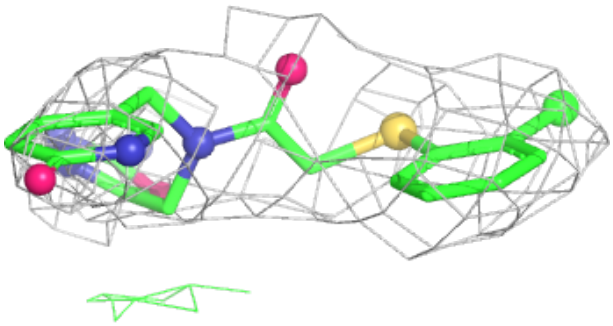
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

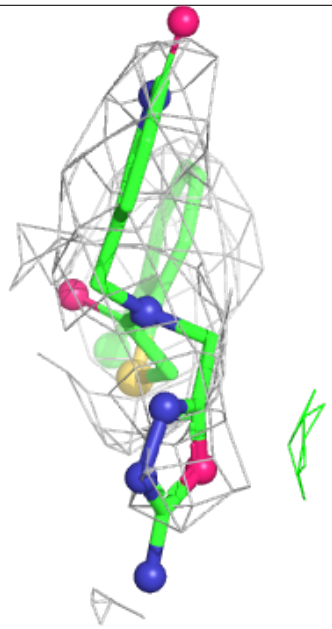


Electron density around VFZ c 303:

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

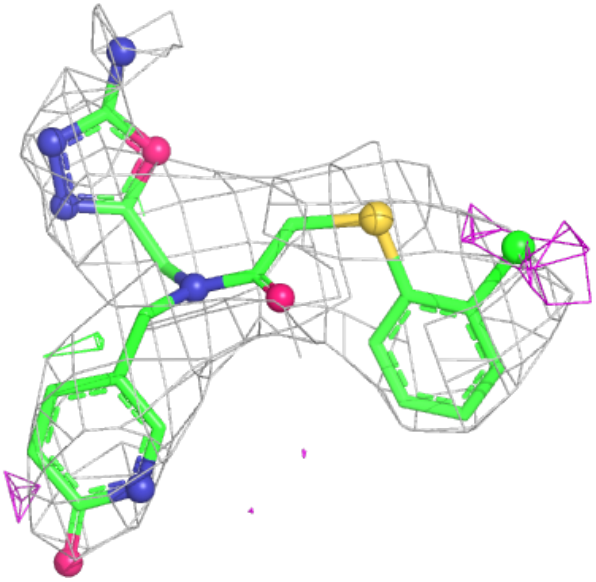


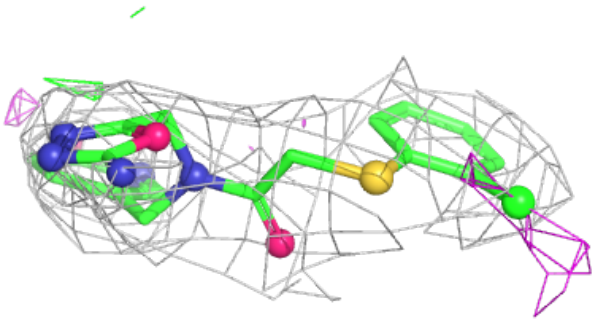


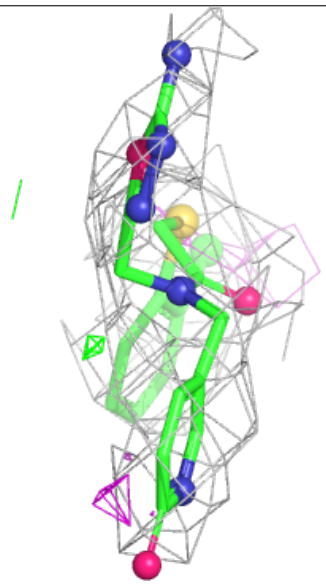


Electron density around VFZ C 306:

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

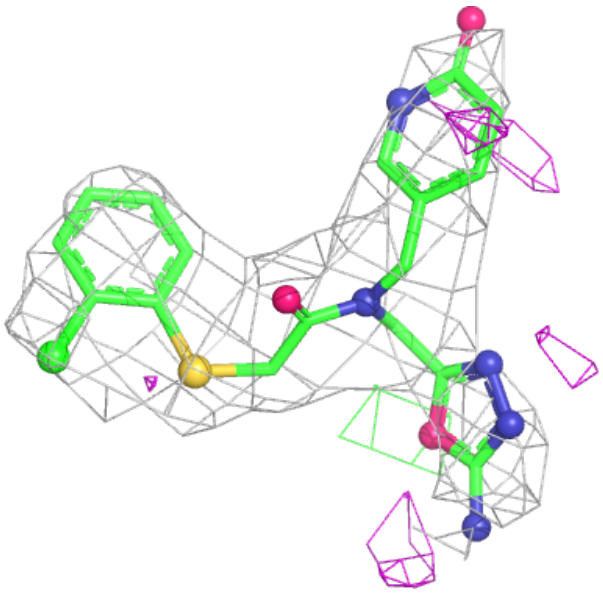


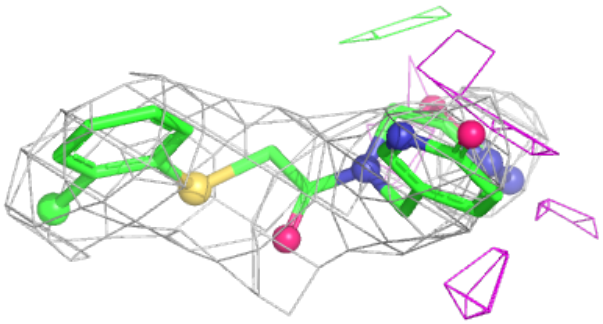


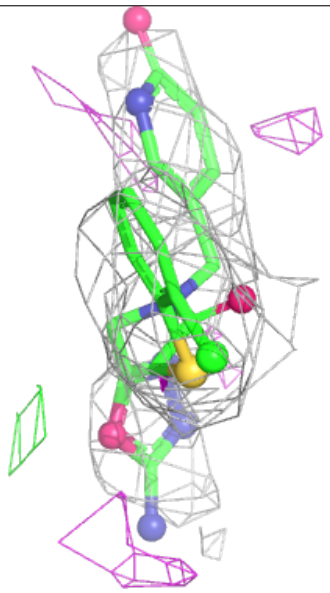


Electron density around VFZ K 303:

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

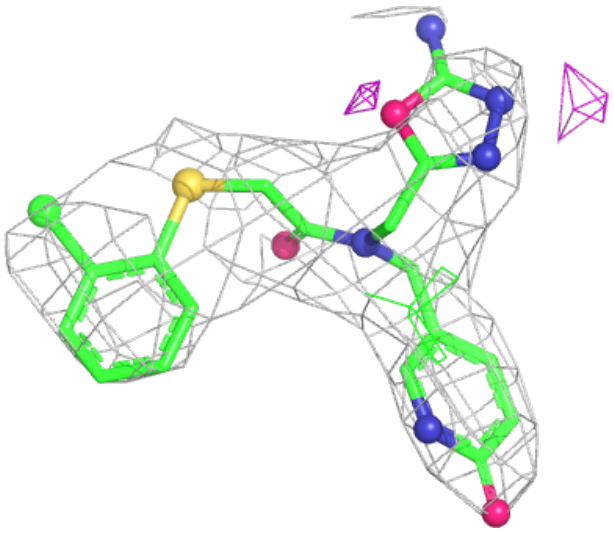


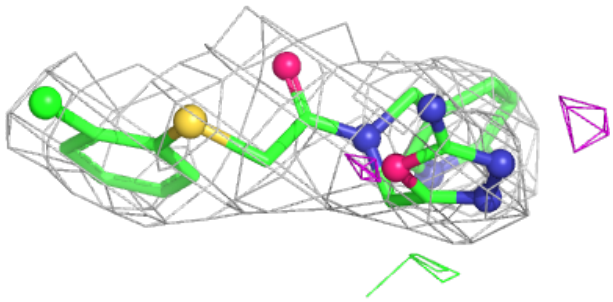


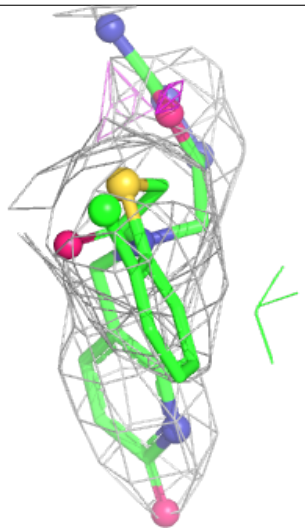


Electron density around VFZ G 304:

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

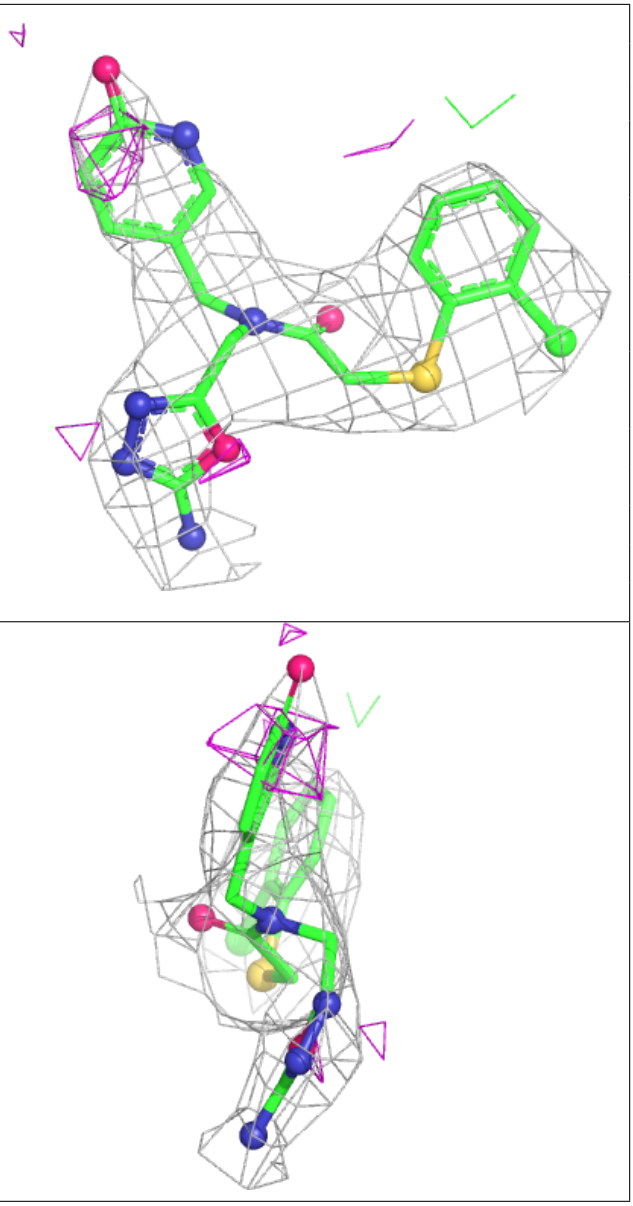






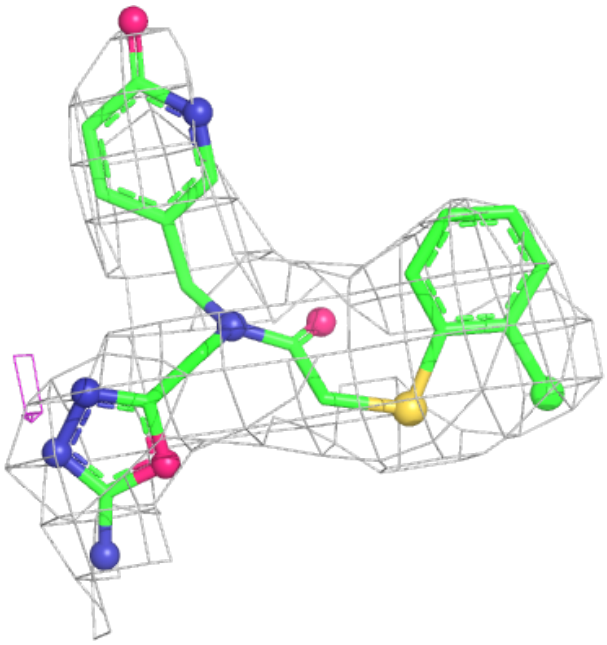
Electron density around VFZ U 304:

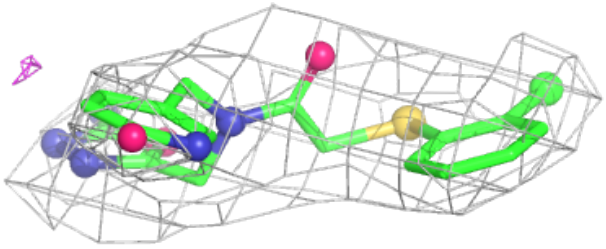
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

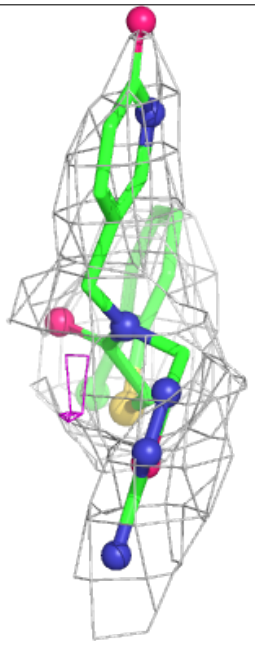


Electron density around VFZ A 310:

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

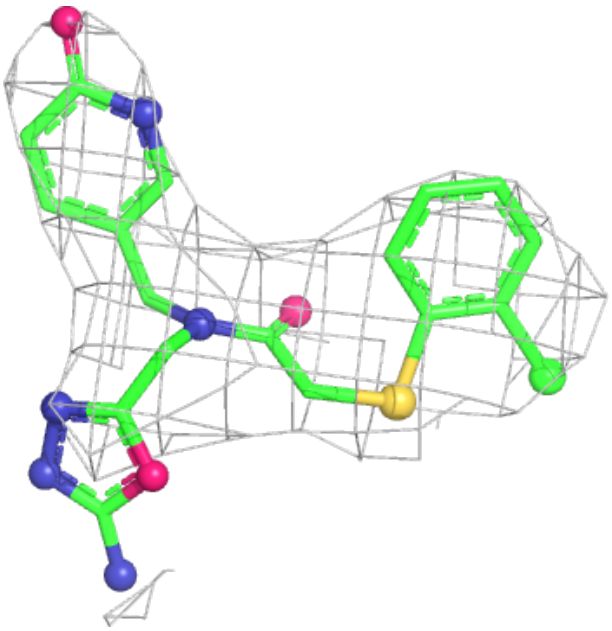


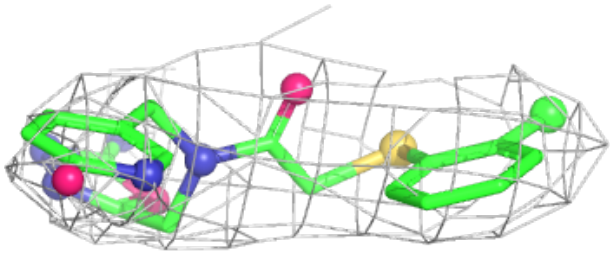


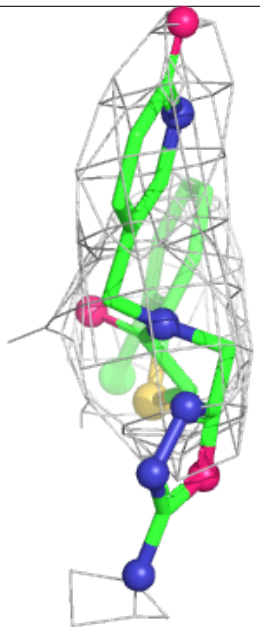


Electron density around VFZ W 302:

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

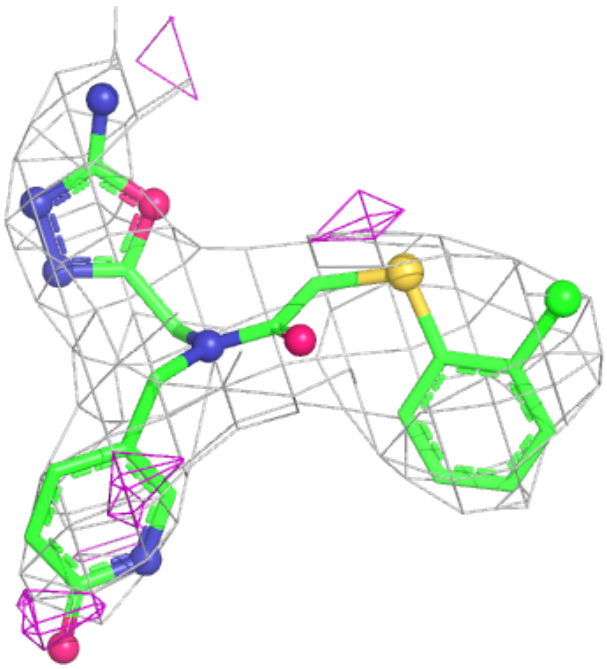


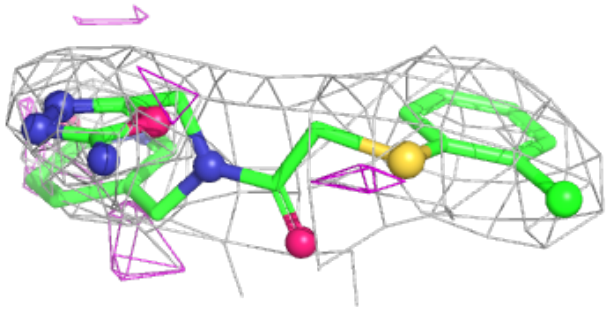


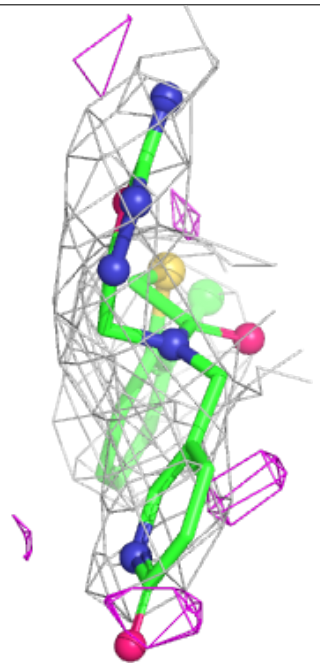


Electron density around VFZ J 303:

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

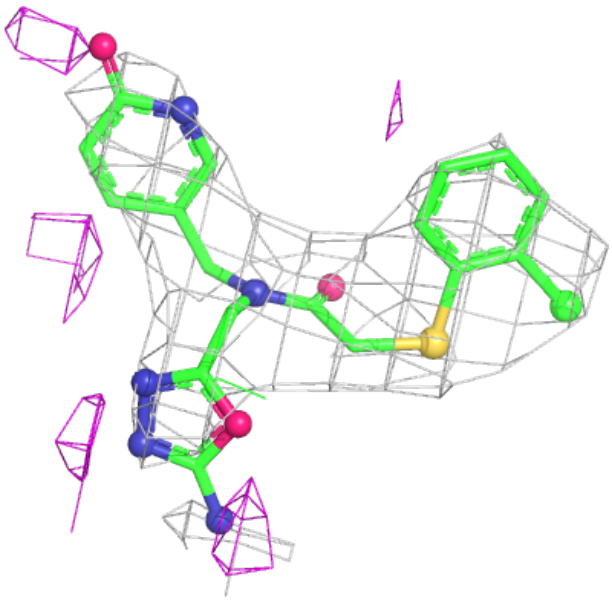


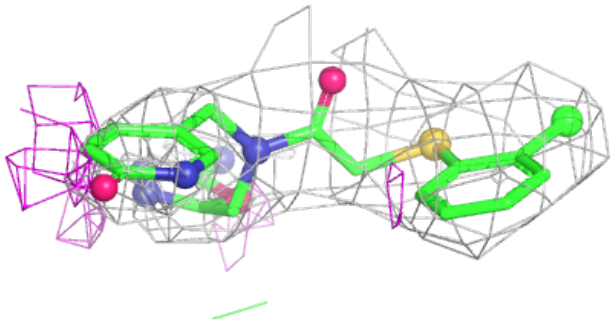


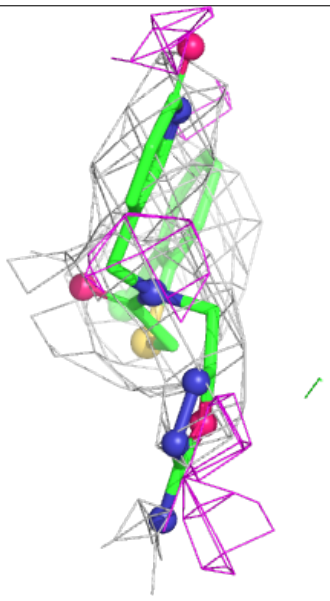


Electron density around VFZ S 303:

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

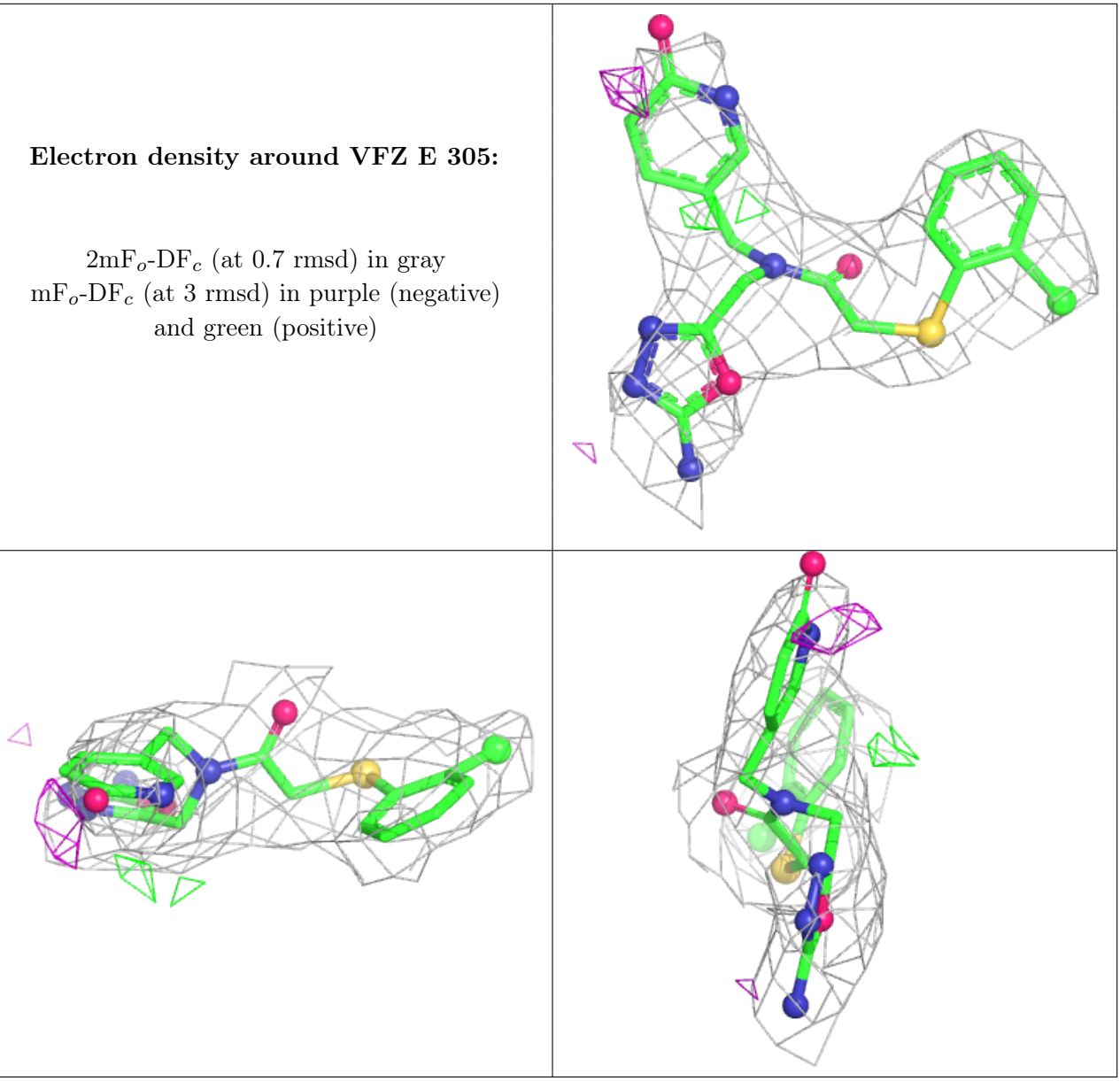






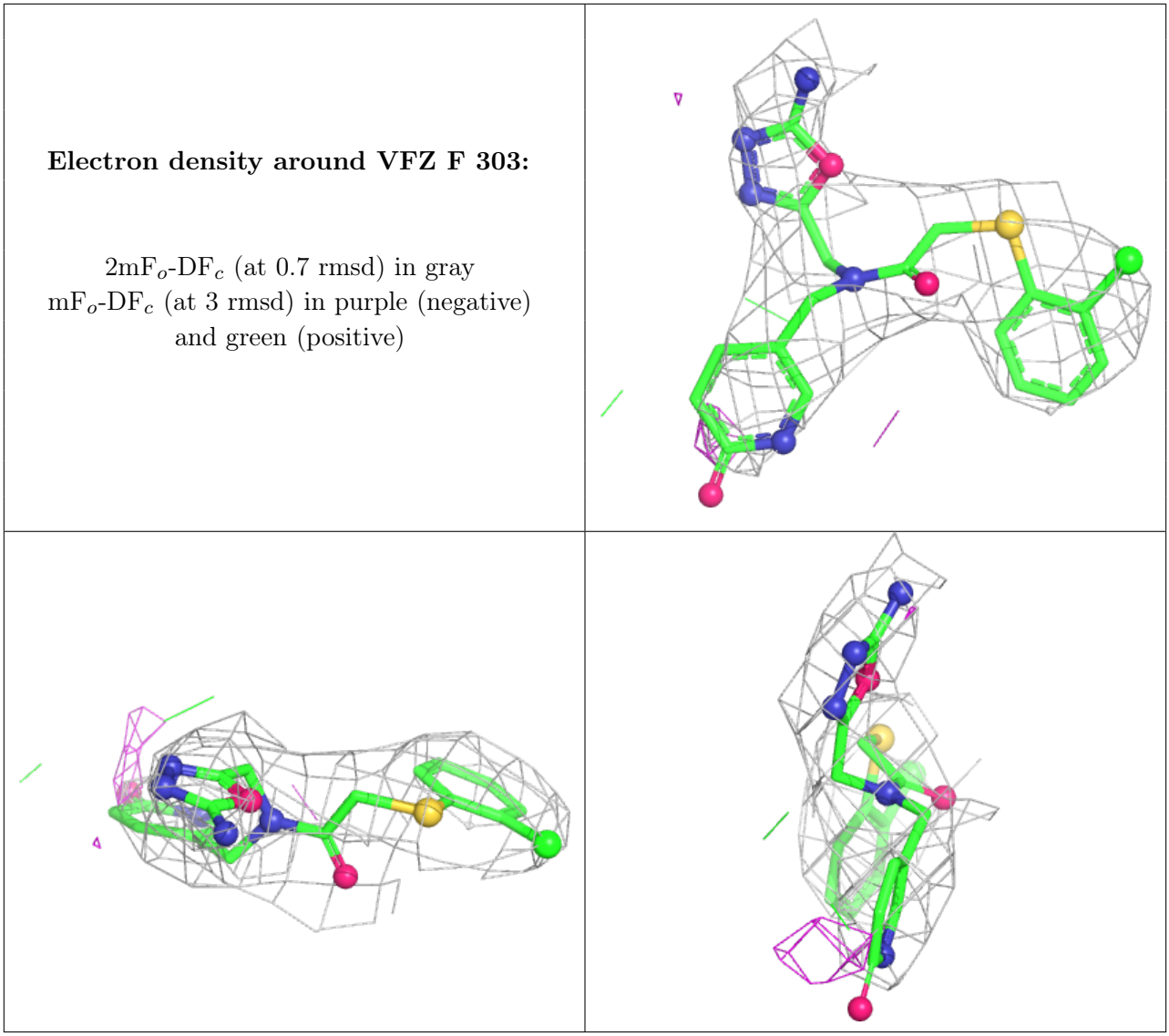
Electron density around VFZ E 305:

$2mF_o$-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:

$2mF_o$-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.