Full wwPDB X-ray Structure Validation Report ⓘ

Jan 22, 2024 – 12:11 am GMT

PDB ID	:	7OK2
Title	:	Crystal structure of Pseudomonas aeruginosa LpxA in complex with compound 3
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	:	2.89 Å(reported)

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

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

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

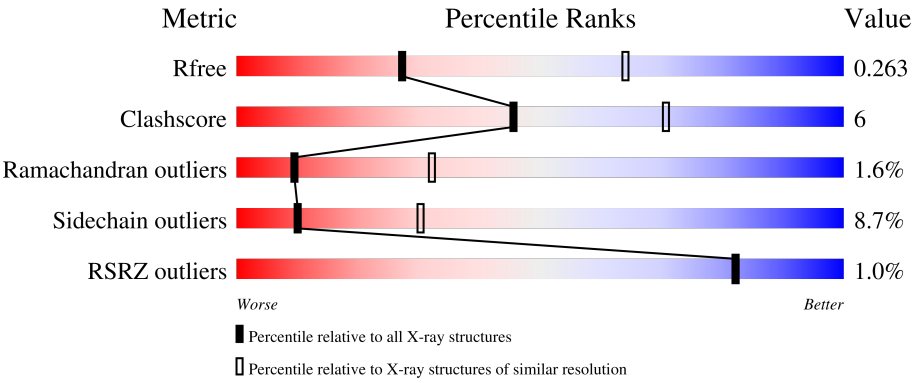
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.89 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	1957 (2.90-2.90)
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (2.90-2.90)

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	1	261	80% 18%
1	2	261	81% 16%
1	3	261	75% 22%
1	4	261	82% 14%

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Mol	Chain	Length	Quality of chain
1	A	261	78% 19%
1	B	261	75% 23%
1	C	261	82% 16%
1	D	261	74% 22%
1	E	261	81% 17%
1	F	261	77% 20%
1	G	261	75% 20%
1	H	261	74% 23%
1	I	261	79% 16%
1	J	261	73% 23%
1	K	261	78% 19%
1	L	261	74% 21%
1	M	261	76% 21%
1	N	261	79% 18%
1	O	261	76% 20%
1	P	261	74% 22%
1	Q	261	77% 20%
1	R	261	76% 20%
1	S	261	79% 18%
1	T	261	75% 21%
1	U	261	75% 22%
1	V	261	78% 20%
1	W	261	82% 15%
1	X	261	77% 20%
1	Y	261	76% 20%

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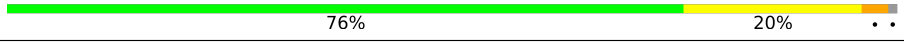
Mol	Chain	Length	Quality of chain
1	Z	261	

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 60216 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	1	258	Total	C	N	O	S	0	0	0
			1974	1235	364	368	7			
1	2	258	Total	C	N	O	S	0	0	0
			1974	1235	364	368	7			
1	3	258	Total	C	N	O	S	0	0	0
			1974	1235	364	368	7			
1	4	258	Total	C	N	O	S	0	0	0
			1974	1235	364	368	7			
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	0	0
			1974	1235	364	368	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	258	Total	C	N	O	S	0	0	0
			1974	1235	364	368	7			
1	H	258	Total	C	N	O	S	0	0	0
			1974	1235	364	368	7			
1	I	258	Total	C	N	O	S	0	0	0
			1974	1235	364	368	7			
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			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	M	258	Total	C	N	O	S	0	0	0
			1974	1235	364	368	7			
1	N	258	Total	C	N	O	S	0	0	0
			1974	1235	364	368	7			
1	O	258	Total	C	N	O	S	0	0	0
			1974	1235	364	368	7			
1	P	258	Total	C	N	O	S	0	0	0
			1974	1235	364	368	7			
1	Q	258	Total	C	N	O	S	0	0	0
			1974	1235	364	368	7			
1	R	258	Total	C	N	O	S	0	0	0
			1974	1235	364	368	7			
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	258	Total	C	N	O	S	0	0	0
			1974	1235	364	368	7			
1	W	258	Total	C	N	O	S	0	0	0
			1974	1235	364	368	7			
1	X	258	Total	C	N	O	S	0	0	0
			1974	1235	364	368	7			
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			

There are 90 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
1	-2	GLY	-	expression tag	UNP A6V1E4
1	-1	SER	-	expression tag	UNP A6V1E4
1	0	HIS	-	expression tag	UNP A6V1E4
2	-2	GLY	-	expression tag	UNP A6V1E4
2	-1	SER	-	expression tag	UNP A6V1E4
2	0	HIS	-	expression tag	UNP A6V1E4
3	-2	GLY	-	expression tag	UNP A6V1E4
3	-1	SER	-	expression tag	UNP A6V1E4
3	0	HIS	-	expression tag	UNP A6V1E4
4	-2	GLY	-	expression tag	UNP A6V1E4
4	-1	SER	-	expression tag	UNP A6V1E4

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Chain	Residue	Modelled	Actual	Comment	Reference
4	0	HIS	-	expression tag	UNP A6V1E4
A	-2	GLY	-	expression tag	UNP A6V1E4
A	-1	SER	-	expression tag	UNP A6V1E4
A	0	HIS	-	expression tag	UNP A6V1E4
B	-2	GLY	-	expression tag	UNP A6V1E4
B	-1	SER	-	expression tag	UNP A6V1E4
B	0	HIS	-	expression tag	UNP A6V1E4
C	-2	GLY	-	expression tag	UNP A6V1E4
C	-1	SER	-	expression tag	UNP A6V1E4
C	0	HIS	-	expression tag	UNP A6V1E4
D	-2	GLY	-	expression tag	UNP A6V1E4
D	-1	SER	-	expression tag	UNP A6V1E4
D	0	HIS	-	expression tag	UNP A6V1E4
E	-2	GLY	-	expression tag	UNP A6V1E4
E	-1	SER	-	expression tag	UNP A6V1E4
E	0	HIS	-	expression tag	UNP A6V1E4
F	-2	GLY	-	expression tag	UNP A6V1E4
F	-1	SER	-	expression tag	UNP A6V1E4
F	0	HIS	-	expression tag	UNP A6V1E4
G	-2	GLY	-	expression tag	UNP A6V1E4
G	-1	SER	-	expression tag	UNP A6V1E4
G	0	HIS	-	expression tag	UNP A6V1E4
H	-2	GLY	-	expression tag	UNP A6V1E4
H	-1	SER	-	expression tag	UNP A6V1E4
H	0	HIS	-	expression tag	UNP A6V1E4
I	-2	GLY	-	expression tag	UNP A6V1E4
I	-1	SER	-	expression tag	UNP A6V1E4
I	0	HIS	-	expression tag	UNP A6V1E4
J	-2	GLY	-	expression tag	UNP A6V1E4
J	-1	SER	-	expression tag	UNP A6V1E4
J	0	HIS	-	expression tag	UNP A6V1E4
K	-2	GLY	-	expression tag	UNP A6V1E4
K	-1	SER	-	expression tag	UNP A6V1E4
K	0	HIS	-	expression tag	UNP A6V1E4
L	-2	GLY	-	expression tag	UNP A6V1E4
L	-1	SER	-	expression tag	UNP A6V1E4
L	0	HIS	-	expression tag	UNP A6V1E4
M	-2	GLY	-	expression tag	UNP A6V1E4
M	-1	SER	-	expression tag	UNP A6V1E4
M	0	HIS	-	expression tag	UNP A6V1E4
N	-2	GLY	-	expression tag	UNP A6V1E4
N	-1	SER	-	expression tag	UNP A6V1E4

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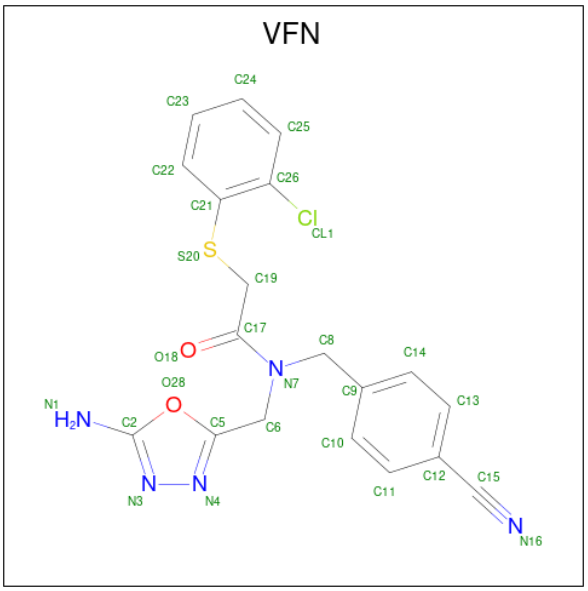
Chain	Residue	Modelled	Actual	Comment	Reference
N	0	HIS	-	expression tag	UNP A6V1E4
O	-2	GLY	-	expression tag	UNP A6V1E4
O	-1	SER	-	expression tag	UNP A6V1E4
O	0	HIS	-	expression tag	UNP A6V1E4
P	-2	GLY	-	expression tag	UNP A6V1E4
P	-1	SER	-	expression tag	UNP A6V1E4
P	0	HIS	-	expression tag	UNP A6V1E4
Q	-2	GLY	-	expression tag	UNP A6V1E4
Q	-1	SER	-	expression tag	UNP A6V1E4
Q	0	HIS	-	expression tag	UNP A6V1E4
R	-2	GLY	-	expression tag	UNP A6V1E4
R	-1	SER	-	expression tag	UNP A6V1E4
R	0	HIS	-	expression tag	UNP A6V1E4
S	-2	GLY	-	expression tag	UNP A6V1E4
S	-1	SER	-	expression tag	UNP A6V1E4
S	0	HIS	-	expression tag	UNP A6V1E4
T	-2	GLY	-	expression tag	UNP A6V1E4
T	-1	SER	-	expression tag	UNP A6V1E4
T	0	HIS	-	expression tag	UNP A6V1E4
U	-2	GLY	-	expression tag	UNP A6V1E4
U	-1	SER	-	expression tag	UNP A6V1E4
U	0	HIS	-	expression tag	UNP A6V1E4
V	-2	GLY	-	expression tag	UNP A6V1E4
V	-1	SER	-	expression tag	UNP A6V1E4
V	0	HIS	-	expression tag	UNP A6V1E4
W	-2	GLY	-	expression tag	UNP A6V1E4
W	-1	SER	-	expression tag	UNP A6V1E4
W	0	HIS	-	expression tag	UNP A6V1E4
X	-2	GLY	-	expression tag	UNP A6V1E4
X	-1	SER	-	expression tag	UNP A6V1E4
X	0	HIS	-	expression tag	UNP A6V1E4
Y	-2	GLY	-	expression tag	UNP A6V1E4
Y	-1	SER	-	expression tag	UNP A6V1E4
Y	0	HIS	-	expression tag	UNP A6V1E4
Z	-2	GLY	-	expression tag	UNP A6V1E4
Z	-1	SER	-	expression tag	UNP A6V1E4
Z	0	HIS	-	expression tag	UNP A6V1E4

- Molecule 2 is {N}-[(5-azanyl-1,3,4-oxadiazol-2-yl)methyl]-2-(2-chlorophenyl)sulfanyl- {N}-[(4-cyanophenyl)methyl]ethanamide (three-letter code: VFN) (formula: $C_{19}H_{16}ClN_5O_2S$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	1	1	Total	C	Cl	N	O	S	0	0
			28	19	1	5	2	1		
2	1	1	Total	C	Cl	N	O	S	0	0
			28	19	1	5	2	1		
2	2	1	Total	C	Cl	N	O	S	0	0
			28	19	1	5	2	1		
2	3	1	Total	C	Cl	N	O	S	0	0
			28	19	1	5	2	1		
2	3	1	Total	C	Cl	N	O	S	0	0
			28	19	1	5	2	1		
2	A	1	Total	C	Cl	N	O	S	0	0
			28	19	1	5	2	1		
2	A	1	Total	C	Cl	N	O	S	0	0
			28	19	1	5	2	1		
2	B	1	Total	C	Cl	N	O	S	0	0
			28	19	1	5	2	1		
2	D	1	Total	C	Cl	N	O	S	0	0
			28	19	1	5	2	1		
2	D	1	Total	C	Cl	N	O	S	0	0
			28	19	1	5	2	1		
2	F	1	Total	C	Cl	N	O	S	0	0
			28	19	1	5	2	1		
2	G	1	Total	C	Cl	N	O	S	0	0
			28	19	1	5	2	1		
2	H	1	Total	C	Cl	N	O	S	0	0
			28	19	1	5	2	1		
2	H	1	Total	C	Cl	N	O	S	0	0
			28	19	1	5	2	1		

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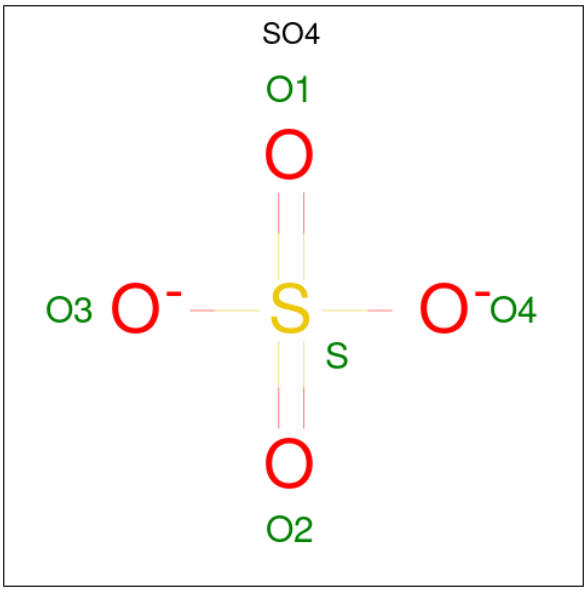
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	J	1	Total	C	Cl	N	O	S	0	0
			28	19	1	5	2	1		
2	K	1	Total	C	Cl	N	O	S	0	0
			28	19	1	5	2	1		
2	L	1	Total	C	Cl	N	O	S	0	0
			28	19	1	5	2	1		
2	N	1	Total	C	Cl	N	O	S	0	0
			28	19	1	5	2	1		
2	O	1	Total	C	Cl	N	O	S	0	0
			28	19	1	5	2	1		
2	O	1	Total	C	Cl	N	O	S	0	0
			28	19	1	5	2	1		
2	P	1	Total	C	Cl	N	O	S	0	0
			28	19	1	5	2	1		
2	P	1	Total	C	Cl	N	O	S	0	0
			28	19	1	5	2	1		
2	R	1	Total	C	Cl	N	O	S	0	0
			28	19	1	5	2	1		
2	S	1	Total	C	Cl	N	O	S	0	0
			28	19	1	5	2	1		
2	S	1	Total	C	Cl	N	O	S	0	0
			28	19	1	5	2	1		
2	T	1	Total	C	Cl	N	O	S	0	0
			28	19	1	5	2	1		
2	V	1	Total	C	Cl	N	O	S	0	0
			28	19	1	5	2	1		
2	W	1	Total	C	Cl	N	O	S	0	0
			28	19	1	5	2	1		
2	W	1	Total	C	Cl	N	O	S	0	0
			28	19	1	5	2	1		
2	Z	1	Total	C	Cl	N	O	S	0	0
			28	19	1	5	2	1		

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	1	1	Total O S 5 4 1	0	0
3	2	1	Total O S 5 4 1	0	0
3	3	1	Total O S 5 4 1	0	0
3	4	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
3	E	1	Total O S 5 4 1	0	0
3	F	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	I	1	Total O S 5 4 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	J	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	M	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	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
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	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	Z	1	Total O S 5 4 1	0	0

- Molecule 4 is water.

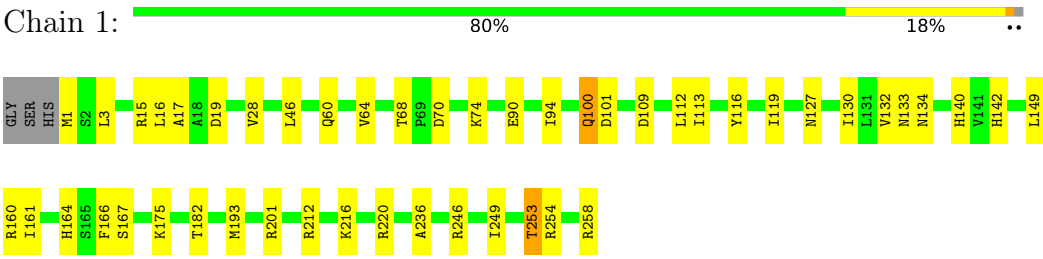
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	1	Total O 1 1	0	0

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.

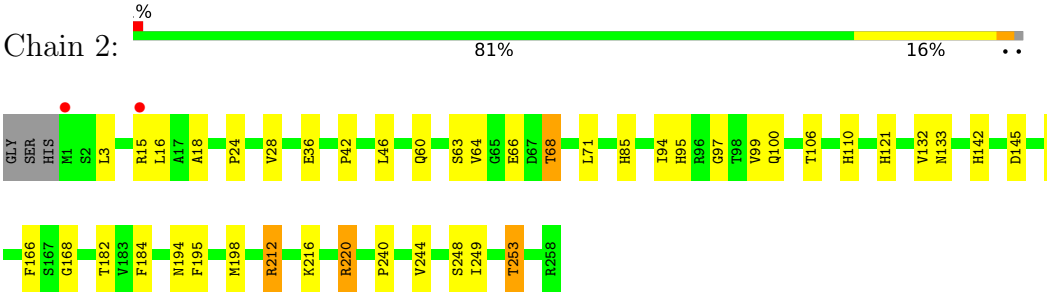
• Molecule 1: Acyl-[acyl-carrier-protein]-UDP-N-acetylglucosamine O-acyltransferase

Chain 1:



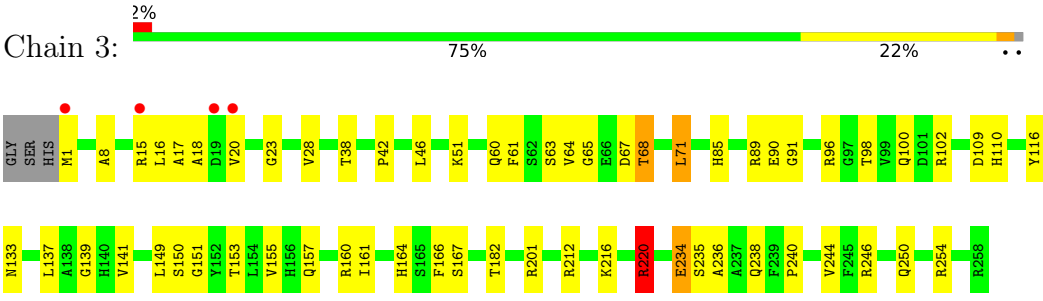
• Molecule 1: Acyl-[acyl-carrier-protein]-UDP-N-acetylglucosamine O-acyltransferase

Chain 2:



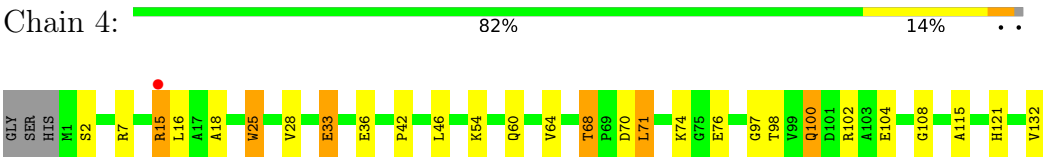
• Molecule 1: Acyl-[acyl-carrier-protein]-UDP-N-acetylglucosamine O-acyltransferase

Chain 3:



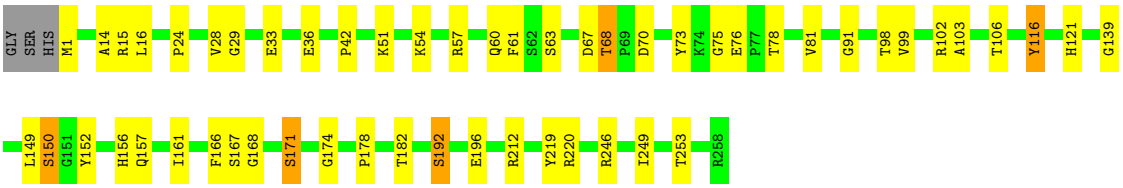
• Molecule 1: Acyl-[acyl-carrier-protein]-UDP-N-acetylglucosamine O-acyltransferase

Chain 4:



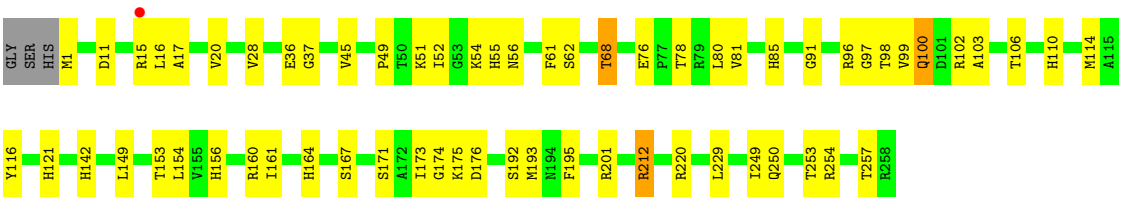
• Molecule 1: Acyl-[acyl-carrier-protein]-UDP-N-acetylglucosamine O-acyltransferase

Chain A:



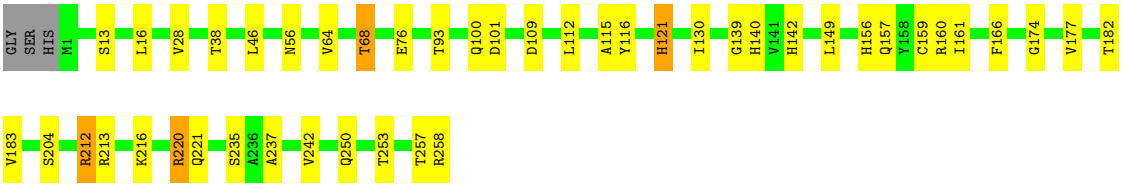
• Molecule 1: Acyl-[acyl-carrier-protein]-UDP-N-acetylglucosamine O-acyltransferase

Chain B:



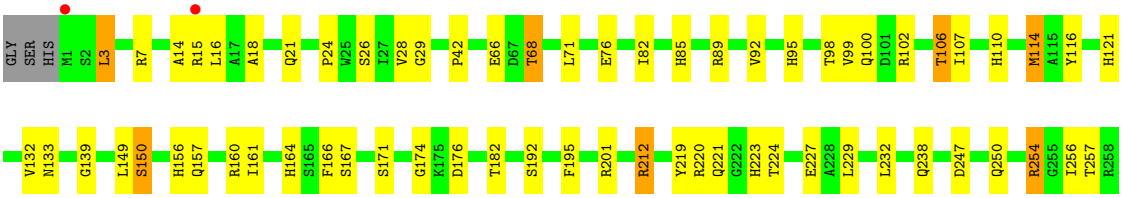
• Molecule 1: Acyl-[acyl-carrier-protein]-UDP-N-acetylglucosamine O-acyltransferase

Chain C:



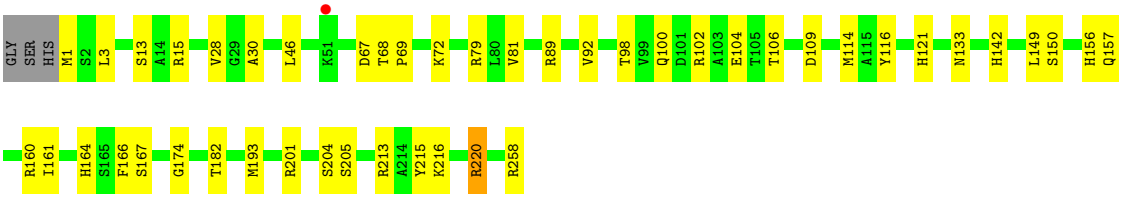
• Molecule 1: Acyl-[acyl-carrier-protein]-UDP-N-acetylglucosamine O-acyltransferase

Chain D:



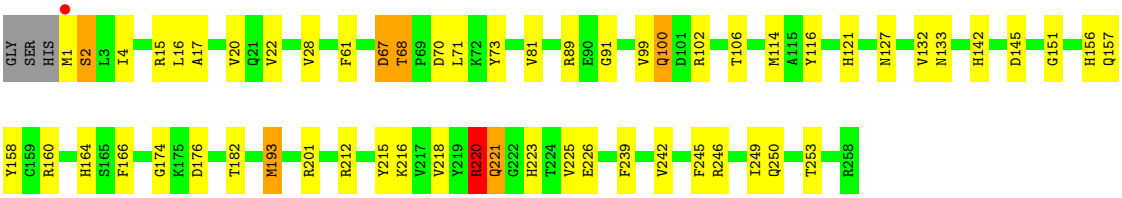
• Molecule 1: Acyl-[acyl-carrier-protein]-UDP-N-acetylglucosamine O-acyltransferase

Chain E:



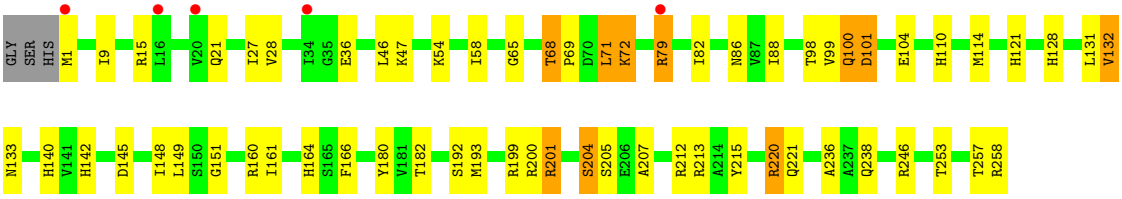
• Molecule 1: Acyl-[acyl-carrier-protein]-UDP-N-acetylglucosamine O-acyltransferase

Chain F:



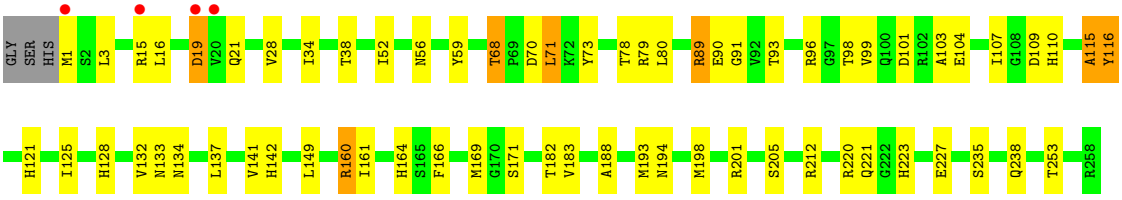
• Molecule 1: Acyl-[acyl-carrier-protein]-UDP-N-acetylglucosamine O-acyltransferase

Chain G:



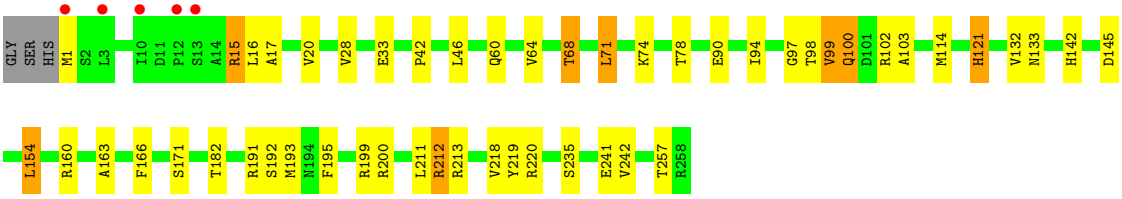
• Molecule 1: Acyl-[acyl-carrier-protein]-UDP-N-acetylglucosamine O-acyltransferase

Chain H:



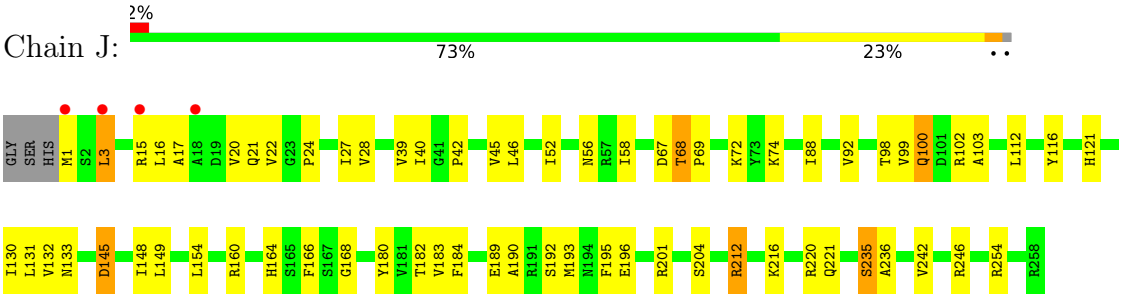
• Molecule 1: Acyl-[acyl-carrier-protein]-UDP-N-acetylglucosamine O-acyltransferase

Chain I:



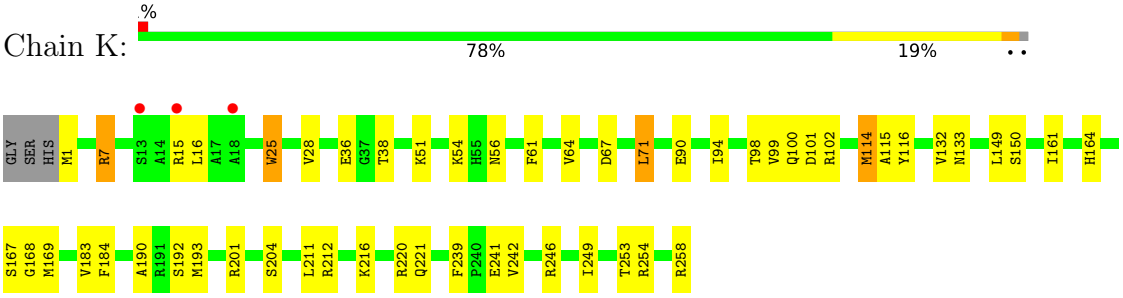
• Molecule 1: Acyl-[acyl-carrier-protein]-UDP-N-acetylglucosamine O-acyltransferase

Chain J:



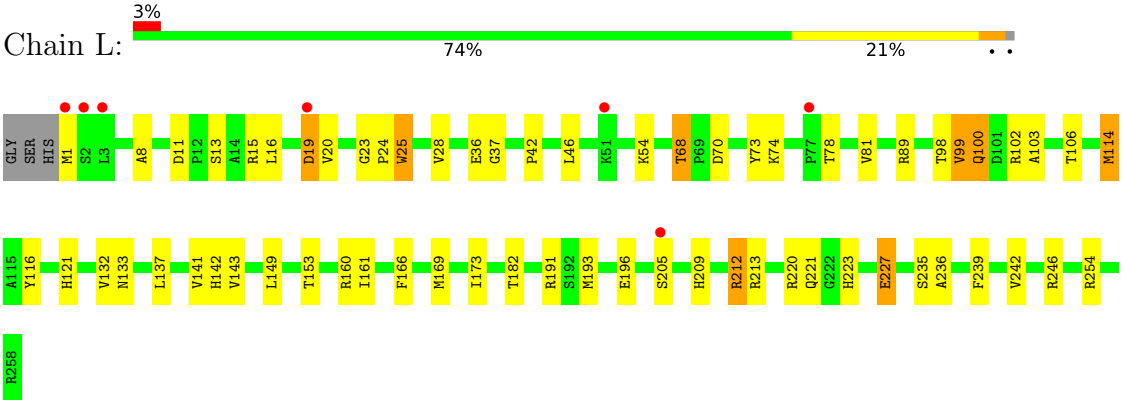
• Molecule 1: Acyl-[acyl-carrier-protein]-UDP-N-acetylglucosamine O-acyltransferase

Chain K:



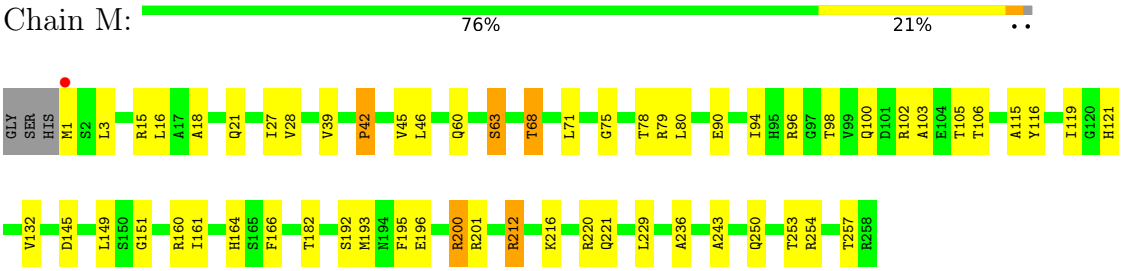
• Molecule 1: Acyl-[acyl-carrier-protein]-UDP-N-acetylglucosamine O-acyltransferase

Chain L:



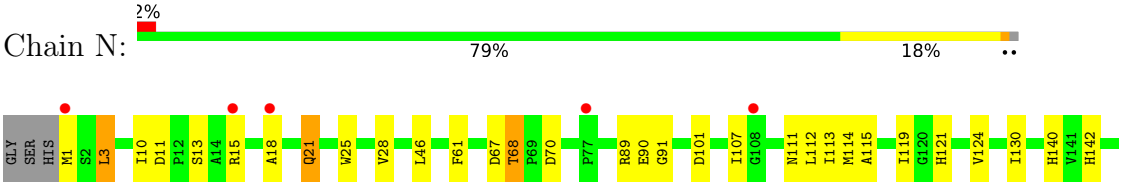
• Molecule 1: Acyl-[acyl-carrier-protein]-UDP-N-acetylglucosamine O-acyltransferase

Chain M:



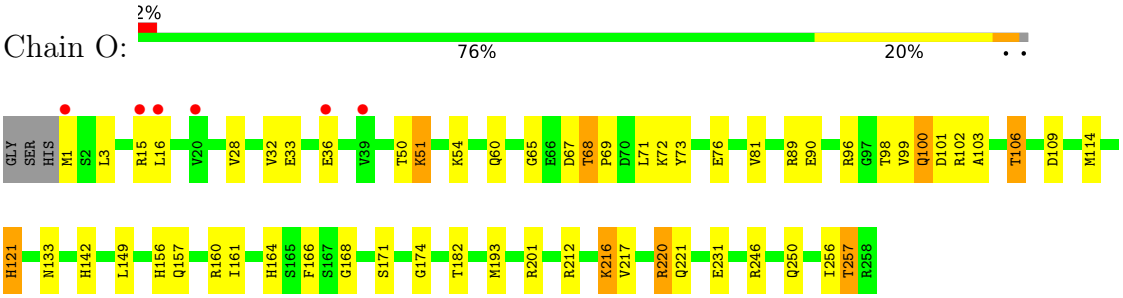
• Molecule 1: Acyl-[acyl-carrier-protein]-UDP-N-acetylglucosamine O-acyltransferase

Chain N:



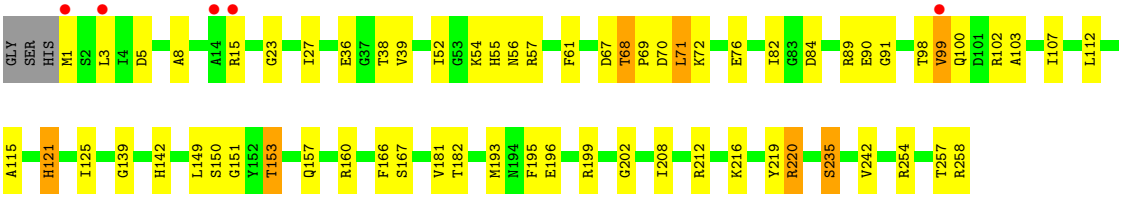
• Molecule 1: Acyl-[acyl-carrier-protein]-UDP-N-acetylglucosamine O-acyltransferase

Chain O:



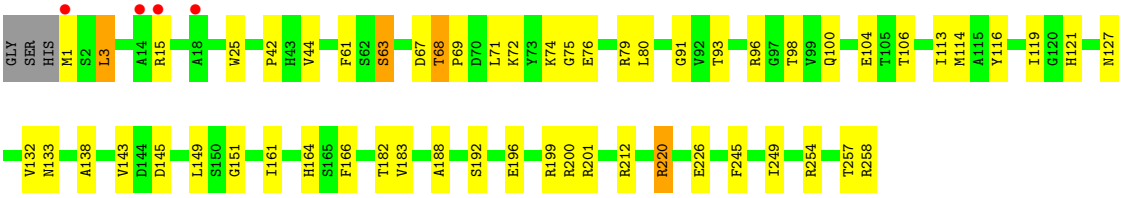
• Molecule 1: Acyl-[acyl-carrier-protein]-UDP-N-acetylglucosamine O-acyltransferase

Chain P:



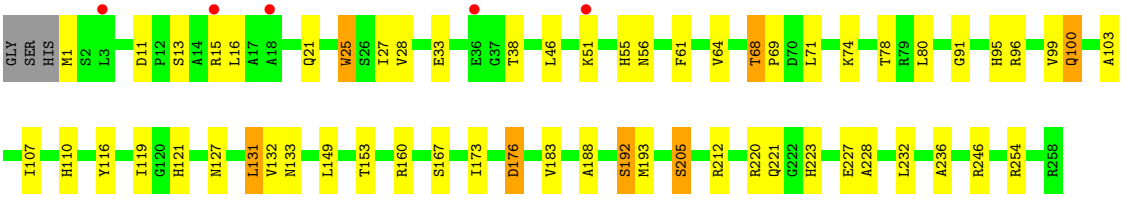
• Molecule 1: Acyl-[acyl-carrier-protein]-UDP-N-acetylglucosamine O-acyltransferase

Chain Q:



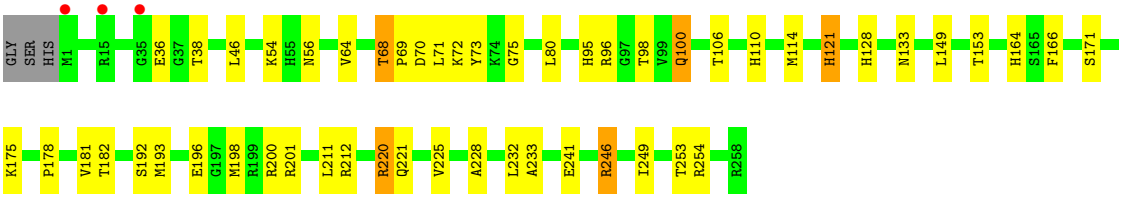
• Molecule 1: Acyl-[acyl-carrier-protein]-UDP-N-acetylglucosamine O-acyltransferase

Chain R:



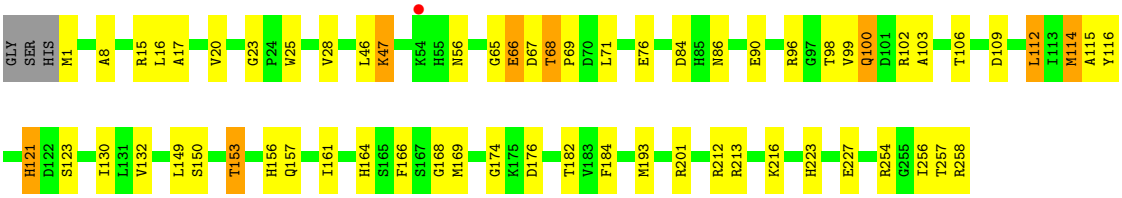
• Molecule 1: Acyl-[acyl-carrier-protein]-UDP-N-acetylglucosamine O-acyltransferase

Chain S:



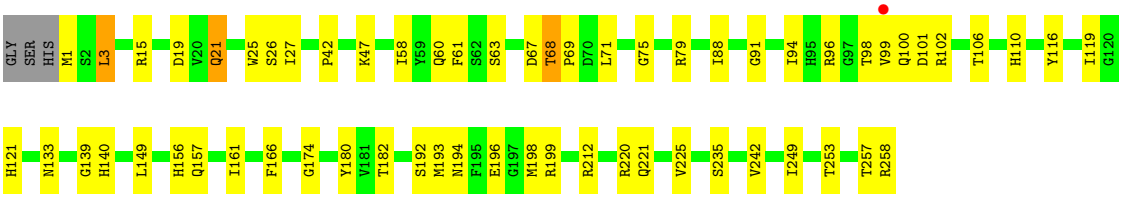
• Molecule 1: Acyl-[acyl-carrier-protein]-UDP-N-acetylglucosamine O-acyltransferase

Chain T:



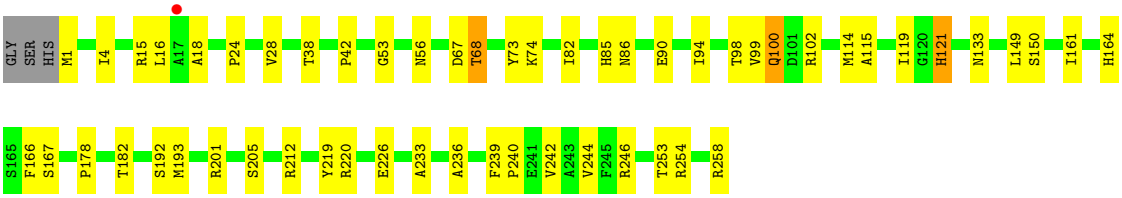
• Molecule 1: Acyl-[acyl-carrier-protein]-UDP-N-acetylglucosamine O-acyltransferase

Chain U:



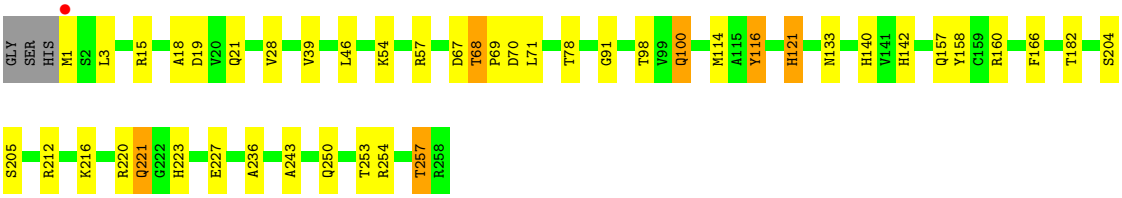
• Molecule 1: Acyl-[acyl-carrier-protein]-UDP-N-acetylglucosamine O-acyltransferase

Chain V:



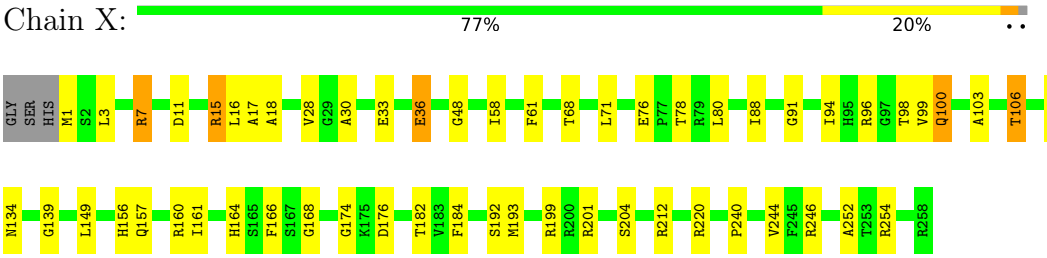
• Molecule 1: Acyl-[acyl-carrier-protein]-UDP-N-acetylglucosamine O-acyltransferase

Chain W:



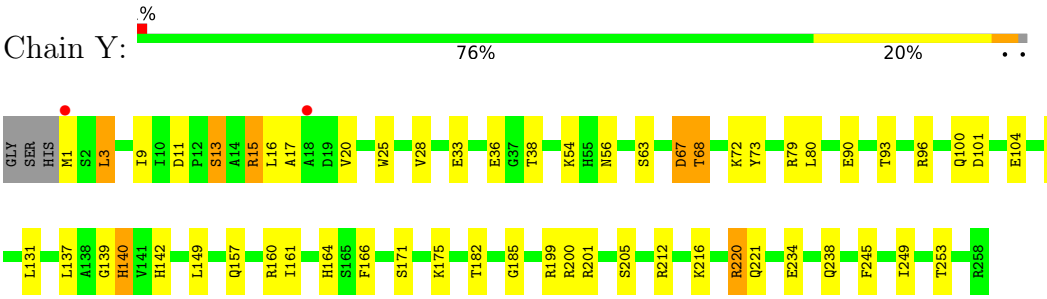
• Molecule 1: Acyl-[acyl-carrier-protein]-UDP-N-acetylglucosamine O-acyltransferase

Chain X:



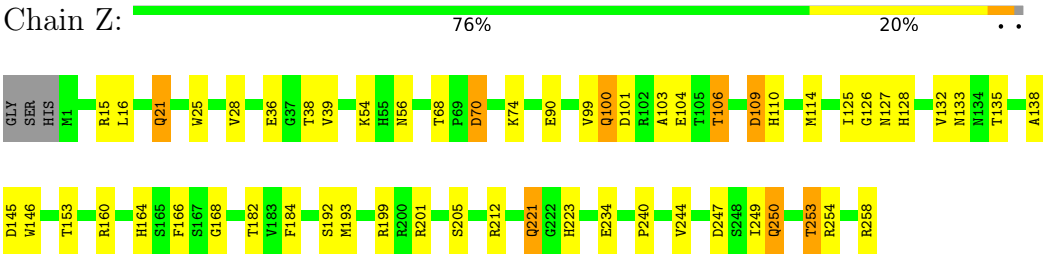
• Molecule 1: Acyl-[acyl-carrier-protein]-UDP-N-acetylglucosamine O-acyltransferase

Chain Y:



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

Chain Z:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	247.29Å 367.65Å 372.08Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.45 – 2.89 49.45 – 2.89	Depositor EDS
% Data completeness (in resolution range)	99.8 (49.45-2.89) 99.8 (49.45-2.89)	Depositor EDS
R_{merge}	0.59	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.37 (at 2.91Å)	Xtriage
Refinement program	BUSTER 2.11.7	Depositor
R, R_{free}	0.192 , 0.231 0.225 , 0.263	Depositor DCC
R_{free} test set	18696 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	66.5	Xtriage
Anisotropy	0.266	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 48.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.43$, $< L^2 > = 0.25$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	60216	wwPDB-VP
Average B, all atoms (Å^2)	71.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.37% 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: SO4, VFN

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	1	0.53	0/2016	0.78	0/2734
1	2	0.53	0/2016	0.78	0/2734
1	3	0.52	0/2016	0.79	0/2734
1	4	0.53	0/2016	0.79	0/2734
1	A	0.52	0/2016	0.78	0/2734
1	B	0.51	0/2016	0.78	0/2734
1	C	0.51	0/2016	0.76	0/2734
1	D	0.55	0/2016	0.81	0/2734
1	E	0.54	0/2016	0.80	0/2734
1	F	0.51	0/2016	0.78	0/2734
1	G	0.52	0/2016	0.76	0/2734
1	H	0.49	0/2016	0.75	0/2734
1	I	0.51	0/2016	0.75	0/2734
1	J	0.52	0/2016	0.77	0/2734
1	K	0.50	0/2016	0.74	0/2734
1	L	0.48	0/2016	0.75	0/2734
1	M	0.52	0/2016	0.75	0/2734
1	N	0.50	0/2016	0.75	0/2734
1	O	0.51	0/2016	0.76	0/2734
1	P	0.50	0/2016	0.77	0/2734
1	Q	0.50	0/2016	0.77	0/2734
1	R	0.51	0/2016	0.78	0/2734
1	S	0.52	0/2016	0.78	0/2734
1	T	0.50	0/2016	0.77	0/2734
1	U	0.53	0/2016	0.80	0/2734
1	V	0.53	0/2016	0.80	0/2734
1	W	0.52	0/2016	0.78	0/2734
1	X	0.54	0/2016	0.81	0/2734
1	Y	0.52	0/2016	0.79	0/2734
1	Z	0.54	0/2016	0.79	0/2734
All	All	0.52	0/60480	0.78	0/82020

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1	1974	0	1947	23	0
1	2	1974	0	1947	20	0
1	3	1974	0	1947	35	0
1	4	1974	0	1947	20	0
1	A	1974	0	1947	22	0
1	B	1974	0	1947	32	0
1	C	1974	0	1947	19	0
1	D	1974	0	1947	34	0
1	E	1974	0	1947	20	0
1	F	1974	0	1947	34	0
1	G	1974	0	1947	33	0
1	H	1974	0	1947	29	0
1	I	1974	0	1947	23	0
1	J	1974	0	1947	36	0
1	K	1974	0	1947	23	0
1	L	1974	0	1947	33	0
1	M	1974	0	1947	28	0
1	N	1974	0	1947	18	0
1	O	1974	0	1947	29	0
1	P	1974	0	1947	34	0
1	Q	1974	0	1947	25	0
1	R	1974	0	1947	30	0
1	S	1974	0	1947	27	0
1	T	1974	0	1947	32	0
1	U	1974	0	1947	21	0
1	V	1974	0	1947	23	0
1	W	1974	0	1947	20	0
1	X	1974	0	1947	26	0
1	Y	1974	0	1947	28	0
1	Z	1974	0	1947	27	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	1	56	0	0	0	0
2	2	28	0	0	1	0
2	3	56	0	0	3	0
2	A	56	0	0	0	0
2	B	28	0	0	0	0
2	D	56	0	0	0	0
2	F	28	0	0	0	0
2	G	28	0	0	1	0
2	H	56	0	0	3	0
2	J	28	0	0	0	0
2	K	28	0	0	1	0
2	L	28	0	0	0	0
2	N	28	0	0	1	0
2	O	56	0	0	0	0
2	P	56	0	0	3	0
2	R	28	0	0	1	0
2	S	56	0	0	0	0
2	T	28	0	0	0	0
2	V	28	0	0	0	0
2	W	56	0	0	1	0
2	Z	28	0	0	0	0
3	1	5	0	0	0	0
3	2	5	0	0	0	0
3	3	5	0	0	0	0
3	4	5	0	0	0	0
3	A	5	0	0	0	0
3	B	5	0	0	0	0
3	C	10	0	0	0	0
3	D	5	0	0	0	0
3	E	5	0	0	0	0
3	F	5	0	0	0	0
3	G	5	0	0	0	0
3	H	5	0	0	0	0
3	I	5	0	0	0	0
3	J	5	0	0	0	0
3	K	5	0	0	0	0
3	L	5	0	0	0	0
3	M	5	0	0	0	0
3	N	5	0	0	0	0
3	O	5	0	0	0	0
3	P	5	0	0	0	0
3	Q	5	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	R	5	0	0	0	0
3	S	5	0	0	0	0
3	T	5	0	0	0	0
3	U	5	0	0	0	0
3	V	5	0	0	0	0
3	W	5	0	0	0	0
3	X	5	0	0	0	0
3	Y	5	0	0	0	0
3	Z	5	0	0	0	0
4	B	1	0	0	0	0
All	All	60216	0	58410	757	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 6.

All (757) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:68:THR:HG21	1:C:121:HIS:HD2	1.36	0.89
1:H:164:HIS:CE1	1:H:201:ARG:HG3	2.09	0.88
1:3:98:THR:HB	1:3:100:GLN:HE21	1.38	0.88
1:1:249:ILE:O	1:1:253:THR:HG22	1.76	0.86
1:H:164:HIS:HE1	1:H:201:ARG:HG3	1.40	0.84
1:R:100:GLN:H	1:R:100:GLN:HE21	1.28	0.82
1:X:132:VAL:HG12	1:X:133:ASN:H	1.45	0.81
1:S:164:HIS:HE1	1:S:201:ARG:HG3	1.46	0.80
1:C:68:THR:HG21	1:C:121:HIS:CD2	2.18	0.79
1:1:150:SER:HB2	1:1:167:SER:O	1.83	0.78
1:3:98:THR:HB	1:3:100:GLN:NE2	1.98	0.78
1:Z:38:THR:HG23	1:Z:56:ASN:HB2	1.66	0.77
1:F:164:HIS:CE1	1:F:201:ARG:HG3	2.20	0.77
1:T:164:HIS:HE1	1:T:201:ARG:HG3	1.51	0.76
1:F:166:PHE:HB3	1:F:182:THR:HG22	1.68	0.76
1:J:164:HIS:HE1	1:J:201:ARG:HG3	1.50	0.75
1:V:254:ARG:HH21	1:V:254:ARG:HB3	1.51	0.75
1:X:149:LEU:HD21	1:X:161:ILE:HG21	1.69	0.75
1:T:164:HIS:CE1	1:T:201:ARG:HG3	2.22	0.75
1:W:100:GLN:H	1:W:100:GLN:HE21	1.36	0.74
1:D:149:LEU:HD21	1:D:161:ILE:HG21	1.71	0.73
1:R:16:LEU:HD11	1:R:28:VAL:HG11	1.70	0.72
1:E:142:HIS:HB2	1:E:160:ARG:HG2	1.72	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Z:100:GLN:H	1:Z:100:GLN:HE21	1.38	0.72
1:O:164:HIS:HE1	1:O:201:ARG:HG3	1.54	0.72
1:4:164:HIS:CE1	1:4:201:ARG:HG3	2.24	0.72
1:A:150:SER:HB2	1:A:167:SER:O	1.90	0.72
1:V:98:THR:HB	1:V:100:GLN:HE21	1.54	0.72
1:T:201:ARG:HG2	1:T:201:ARG:HH11	1.55	0.71
1:Z:164:HIS:HE1	1:Z:201:ARG:HG3	1.56	0.71
1:J:27:ILE:HD11	1:L:25:TRP:HZ3	1.56	0.70
1:F:16:LEU:HD11	1:F:28:VAL:HG11	1.72	0.70
1:M:80:LEU:HB2	1:M:96:ARG:HG2	1.74	0.70
1:J:52:ILE:HG23	1:J:56:ASN:HD22	1.57	0.69
1:Y:164:HIS:HE1	1:Y:201:ARG:HG3	1.56	0.69
1:F:164:HIS:HE1	1:F:201:ARG:HG3	1.54	0.69
1:M:21:GLN:HB2	1:M:39:VAL:HG22	1.74	0.69
1:M:254:ARG:HH11	1:Z:160:ARG:HD2	1.58	0.69
1:B:36:GLU:HB2	1:B:54:LYS:HG2	1.74	0.69
1:C:149:LEU:HD21	1:C:161:ILE:HG21	1.74	0.68
1:E:164:HIS:HE1	1:E:201:ARG:HG3	1.57	0.68
1:H:132:VAL:HG12	1:H:133:ASN:H	1.59	0.68
1:B:85:HIS:O	1:B:110:HIS:HA	1.94	0.68
1:D:166:PHE:HB3	1:D:182:THR:HG22	1.76	0.68
1:T:223:HIS:HB3	1:T:227:GLU:HB3	1.76	0.68
1:G:98:THR:HB	1:G:100:GLN:HE21	1.58	0.67
1:M:80:LEU:HD11	1:M:94:ILE:HG22	1.75	0.67
1:V:24:PRO:HD2	1:V:42:PRO:HB3	1.76	0.67
1:M:63:SER:HB3	1:O:60:GLN:HE21	1.59	0.66
1:U:149:LEU:HD21	1:U:161:ILE:HG21	1.75	0.66
1:D:98:THR:HB	1:D:100:GLN:NE2	2.11	0.66
1:J:130:ILE:HD12	1:J:148:ILE:HG12	1.76	0.66
1:E:13:SER:OG	1:E:30:ALA:HA	1.95	0.66
1:M:28:VAL:HG22	1:M:46:LEU:HD12	1.78	0.66
1:V:166:PHE:O	1:V:182:THR:HA	1.95	0.66
1:2:166:PHE:HB3	1:2:182:THR:HG22	1.79	0.65
1:4:164:HIS:HE1	1:4:201:ARG:HG3	1.61	0.65
1:E:201:ARG:HG2	1:E:201:ARG:HH11	1.61	0.65
1:P:166:PHE:HB3	1:P:182:THR:HG22	1.77	0.65
1:V:239:PHE:HB2	1:V:242:VAL:HG23	1.78	0.65
1:I:195:PHE:HZ	1:I:212:ARG:HG2	1.61	0.65
1:J:166:PHE:HB3	1:J:182:THR:HG22	1.78	0.65
1:X:132:VAL:HG12	1:X:133:ASN:N	2.12	0.65
1:G:164:HIS:CE1	1:G:201:ARG:HG2	2.32	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:3:164:HIS:HE1	1:3:201:ARG:HG3	1.62	0.64
1:1:100:GLN:H	1:1:100:GLN:HE21	1.46	0.64
1:4:149:LEU:HD21	1:4:161:ILE:HG21	1.79	0.64
1:S:211:LEU:HD11	1:S:241:GLU:HB3	1.80	0.63
1:3:164:HIS:CE1	1:3:201:ARG:HG3	2.33	0.63
1:J:183:VAL:HG12	1:J:190:ALA:HA	1.81	0.63
1:T:16:LEU:HD11	1:T:28:VAL:HG11	1.81	0.63
1:B:164:HIS:HE1	1:B:201:ARG:HG3	1.64	0.63
1:3:254:ARG:HH11	1:J:160:ARG:HD2	1.64	0.63
1:4:166:PHE:HB3	1:4:182:THR:HG22	1.79	0.63
1:A:166:PHE:HB3	1:A:182:THR:HG22	1.81	0.63
1:S:73:TYR:HB2	1:S:98:THR:HG22	1.80	0.63
1:3:166:PHE:HB3	1:3:182:THR:HG22	1.81	0.62
1:C:156:HIS:HB2	1:C:174:GLY:HA2	1.82	0.62
1:4:68:THR:HG21	1:4:121:HIS:ND1	2.15	0.62
1:O:81:VAL:HB	1:O:106:THR:HG23	1.82	0.62
1:F:132:VAL:HG12	1:F:133:ASN:H	1.65	0.62
1:G:132:VAL:HG12	1:G:133:ASN:H	1.65	0.62
1:U:94:ILE:HG12	1:U:119:ILE:HD12	1.82	0.61
1:M:80:LEU:HD12	1:M:105:THR:HB	1.82	0.61
1:R:160:ARG:HD2	1:W:254:ARG:HH11	1.64	0.61
1:Y:15:ARG:HH11	1:Y:33:GLU:HB2	1.65	0.61
1:A:68:THR:HG21	1:A:121:HIS:ND1	2.16	0.61
1:N:166:PHE:HB3	1:N:182:THR:HG22	1.82	0.60
1:G:164:HIS:HE1	1:G:201:ARG:HG2	1.64	0.60
1:T:201:ARG:HG2	1:T:201:ARG:NH1	2.16	0.60
1:E:258:ARG:HH22	1:S:225:VAL:HG22	1.67	0.60
1:J:166:PHE:O	1:J:182:THR:HA	2.01	0.60
1:T:25:TRP:HZ3	1:U:27:ILE:HD11	1.66	0.60
1:4:201:ARG:HG2	1:4:201:ARG:HH11	1.67	0.60
1:D:160:ARG:HB2	1:D:176:ASP:OD2	2.00	0.60
1:L:223:HIS:HB3	1:L:227:GLU:HB3	1.82	0.60
1:S:166:PHE:HB3	1:S:182:THR:HG22	1.84	0.60
1:3:16:LEU:HD11	1:3:28:VAL:HG11	1.84	0.60
1:G:98:THR:HB	1:G:100:GLN:NE2	2.16	0.59
1:E:164:HIS:CE1	1:E:201:ARG:HG3	2.37	0.59
1:1:236:ALA:HB1	1:1:246:ARG:NH1	2.18	0.59
1:H:142:HIS:HB2	1:H:160:ARG:HG3	1.83	0.59
1:Y:38:THR:HG23	1:Y:56:ASN:HB2	1.83	0.59
1:3:65:GLY:O	1:3:96:ARG:HD3	2.02	0.59
1:K:98:THR:HB	1:K:100:GLN:NE2	2.17	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Z:164:HIS:CE1	1:Z:201:ARG:HG3	2.37	0.59
1:O:98:THR:HB	1:O:100:GLN:NE2	2.17	0.59
1:P:196:GLU:OE2	1:P:199:ARG:HD3	2.01	0.59
1:Q:68:THR:HG21	1:Q:121:HIS:ND1	2.17	0.59
1:V:254:ARG:HB3	1:V:254:ARG:NH2	2.17	0.59
1:X:166:PHE:O	1:X:182:THR:HA	2.03	0.59
1:1:236:ALA:HB1	1:1:246:ARG:HH11	1.68	0.59
1:B:195:PHE:HZ	1:B:212:ARG:HG2	1.67	0.59
1:M:166:PHE:HB3	1:M:182:THR:HG22	1.84	0.59
1:V:240:PRO:O	1:V:244:VAL:HG23	2.03	0.58
1:Q:149:LEU:HD21	1:Q:161:ILE:HG21	1.85	0.58
1:I:99:VAL:HA	1:I:103:ALA:HB2	1.85	0.58
1:O:164:HIS:CE1	1:O:201:ARG:HG3	2.37	0.58
1:3:132:VAL:HG12	1:3:133:ASN:H	1.68	0.58
1:F:1:MET:HG2	1:F:2:SER:N	2.18	0.58
1:M:16:LEU:HD11	1:M:28:VAL:HG11	1.85	0.58
1:E:28:VAL:HG22	1:E:46:LEU:HD12	1.86	0.58
1:1:28:VAL:HG22	1:1:46:LEU:HD12	1.86	0.58
1:T:17:ALA:HB3	1:T:20:VAL:HG23	1.85	0.58
1:F:239:PHE:HB2	1:F:242:VAL:HG23	1.85	0.58
1:2:149:LEU:HD21	1:2:161:ILE:HG21	1.86	0.58
1:X:166:PHE:HB3	1:X:182:THR:HG22	1.85	0.58
1:1:142:HIS:HB2	1:1:160:ARG:HG2	1.85	0.57
1:N:10:ILE:HG12	1:N:28:VAL:HB	1.86	0.57
1:T:149:LEU:HD21	1:T:161:ILE:HG21	1.85	0.57
1:C:38:THR:HG23	1:C:56:ASN:HB2	1.87	0.57
1:L:137:LEU:HD22	1:L:141:VAL:HG11	1.85	0.57
1:3:68:THR:HG21	1:3:121:HIS:ND1	2.20	0.57
1:O:16:LEU:HD11	1:O:28:VAL:HG11	1.86	0.57
1:Y:11:ASP:OD1	1:Y:13:SER:HB3	2.04	0.57
1:F:81:VAL:HB	1:F:106:THR:HG22	1.87	0.57
1:A:149:LEU:HD21	1:A:161:ILE:HG21	1.86	0.57
1:K:149:LEU:HD21	1:K:161:ILE:HG21	1.87	0.57
1:K:164:HIS:HE1	1:K:201:ARG:HG3	1.70	0.57
1:L:209:HIS:NE2	1:L:213:ARG:HD3	2.20	0.57
1:V:98:THR:HB	1:V:100:GLN:NE2	2.19	0.57
1:E:166:PHE:HB3	1:E:182:THR:HG22	1.87	0.56
1:K:249:ILE:O	1:K:253:THR:HG22	2.04	0.56
1:N:3:LEU:HB3	1:N:21:GLN:HG3	1.85	0.56
1:I:28:VAL:HG22	1:I:46:LEU:HD12	1.87	0.56
1:S:164:HIS:CE1	1:S:201:ARG:HG3	2.34	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:150:SER:HB2	1:D:167:SER:O	2.04	0.56
1:G:204:SER:HB2	1:G:207:ALA:H	1.70	0.56
1:J:235:SER:HB3	1:J:242:VAL:HG11	1.86	0.56
1:R:131:LEU:HG	1:R:149:LEU:HD12	1.87	0.56
1:H:194:ASN:O	1:H:198:MET:HG3	2.06	0.56
1:O:166:PHE:HB3	1:O:182:THR:HG22	1.87	0.56
1:P:71:LEU:HD22	2:P:302:VFN:N16	2.20	0.56
1:T:166:PHE:HB3	1:T:182:THR:HG22	1.87	0.56
1:H:107:ILE:HG12	1:H:125:ILE:HD12	1.88	0.56
1:R:38:THR:HG23	1:R:56:ASN:HB2	1.86	0.56
1:R:69:PRO:HD3	1:R:95:HIS:CE1	2.41	0.56
1:V:16:LEU:HD11	1:V:28:VAL:HG11	1.88	0.56
1:L:100:GLN:H	1:L:100:GLN:HE21	1.51	0.56
1:P:98:THR:HB	1:P:100:GLN:HE21	1.71	0.56
1:Z:249:ILE:O	1:Z:253:THR:HG22	2.06	0.56
1:C:166:PHE:HB3	1:C:182:THR:HG22	1.87	0.56
1:U:156:HIS:HB2	1:U:174:GLY:HA2	1.87	0.56
1:H:91:GLY:O	1:H:116:TYR:HA	2.06	0.55
1:R:160:ARG:HD2	1:W:254:ARG:NH1	2.22	0.55
1:K:98:THR:HB	1:K:100:GLN:HE21	1.71	0.55
1:S:246:ARG:HB3	1:S:246:ARG:HH11	1.70	0.55
1:W:142:HIS:HB2	1:W:160:ARG:HG2	1.87	0.55
1:I:166:PHE:HB3	1:I:182:THR:HG22	1.88	0.55
1:L:142:HIS:HB2	1:L:160:ARG:HG2	1.88	0.55
1:Z:68:THR:HG22	1:Z:70:ASP:H	1.72	0.55
1:N:68:THR:HG21	1:N:121:HIS:ND1	2.21	0.55
1:X:58:ILE:HG12	1:X:88:ILE:HB	1.87	0.55
1:L:132:VAL:HG12	1:L:133:ASN:H	1.71	0.55
1:Z:104:GLU:HG2	1:Z:106:THR:HG22	1.89	0.55
1:A:61:PHE:O	1:A:91:GLY:HA2	2.07	0.55
1:B:149:LEU:HD11	1:B:161:ILE:HG21	1.89	0.55
1:N:112:LEU:HD23	1:N:130:ILE:HG23	1.88	0.55
1:L:36:GLU:HB3	1:L:54:LYS:HG2	1.89	0.55
1:L:16:LEU:HD23	1:L:20:VAL:HG11	1.89	0.54
1:D:132:VAL:HG12	1:D:133:ASN:N	2.22	0.54
1:Y:166:PHE:HB3	1:Y:182:THR:HG22	1.89	0.54
1:F:246:ARG:HH21	1:F:250:GLN:HE21	1.55	0.54
1:O:98:THR:HB	1:O:100:GLN:HE21	1.71	0.54
1:D:156:HIS:HB2	1:D:174:GLY:HA2	1.90	0.54
1:1:101:ASP:HB2	1:1:140:HIS:CE1	2.43	0.54
1:3:149:LEU:HD23	1:3:153:THR:HG21	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:16:LEU:HD11	1:B:28:VAL:HG11	1.90	0.53
1:H:78:THR:HG22	1:H:103:ALA:HB1	1.90	0.53
1:H:149:LEU:HD21	1:H:161:ILE:HG21	1.89	0.53
1:T:84:ASP:O	1:T:109:ASP:HA	2.08	0.53
1:A:16:LEU:HD11	1:A:28:VAL:HG11	1.91	0.53
1:I:142:HIS:HB2	1:I:160:ARG:HG2	1.90	0.53
1:Q:132:VAL:HG12	1:Q:133:ASN:H	1.72	0.53
1:V:149:LEU:HD21	1:V:161:ILE:HG21	1.90	0.53
1:B:195:PHE:CZ	1:B:212:ARG:HG2	2.43	0.53
1:G:132:VAL:HG12	1:G:133:ASN:N	2.22	0.53
1:I:195:PHE:CZ	1:I:212:ARG:HG2	2.42	0.53
1:J:68:THR:HG21	1:J:121:HIS:HB3	1.91	0.53
1:M:98:THR:HB	1:M:100:GLN:NE2	2.24	0.53
1:B:98:THR:HB	1:B:100:GLN:HE21	1.73	0.53
1:F:127:ASN:O	1:F:145:ASP:HA	2.09	0.53
1:K:132:VAL:HG12	1:K:133:ASN:H	1.74	0.53
1:W:78:THR:HG21	1:W:98:THR:HA	1.91	0.53
1:D:66:GLU:HB3	1:D:95:HIS:HD2	1.73	0.53
1:Q:98:THR:HB	1:Q:100:GLN:HE21	1.72	0.53
1:R:99:VAL:HA	1:R:103:ALA:HB2	1.91	0.53
1:2:16:LEU:HD11	1:2:28:VAL:HG11	1.91	0.53
1:F:17:ALA:HB3	1:F:20:VAL:HG23	1.90	0.53
1:H:132:VAL:HG12	1:H:133:ASN:N	2.24	0.53
1:D:229:LEU:HA	1:D:232:LEU:HD12	1.91	0.52
1:O:168:GLY:O	1:O:171:SER:HB2	2.08	0.52
1:R:100:GLN:HE21	1:R:100:GLN:N	2.04	0.52
1:V:38:THR:HG23	1:V:56:ASN:HB2	1.91	0.52
1:Z:21:GLN:HB2	1:Z:39:VAL:HG22	1.91	0.52
1:N:113:ILE:HG21	1:N:119:ILE:HD11	1.92	0.52
1:P:181:VAL:HG22	1:P:193:MET:HE1	1.91	0.52
1:S:249:ILE:O	1:S:253:THR:HG22	2.09	0.52
1:F:249:ILE:O	1:F:253:THR:HG22	2.08	0.52
1:Z:135:THR:HG23	1:Z:153:THR:HB	1.91	0.52
1:2:85:HIS:O	1:2:110:HIS:HA	2.09	0.52
1:F:1:MET:HG2	1:F:2:SER:H	1.75	0.52
1:G:151:GLY:HA3	2:H:301:VFN:CL1	2.46	0.52
1:A:168:GLY:O	1:A:171:SER:HB2	2.09	0.52
1:L:239:PHE:HB2	1:L:242:VAL:HG23	1.91	0.52
1:3:240:PRO:O	1:3:244:VAL:HG23	2.09	0.52
1:W:98:THR:HB	1:W:100:GLN:NE2	2.25	0.52
1:3:46:LEU:HD23	1:3:64:VAL:HB	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:246:ARG:HH11	1:J:246:ARG:HB3	1.74	0.52
1:A:249:ILE:O	1:A:253:THR:HG22	2.10	0.52
1:1:113:ILE:HG21	1:1:119:ILE:HD11	1.91	0.51
1:L:149:LEU:HD21	1:L:161:ILE:HG21	1.90	0.51
1:T:156:HIS:HB2	1:T:174:GLY:HA2	1.92	0.51
1:Z:110:HIS:O	1:Z:128:HIS:HA	2.10	0.51
1:1:109:ASP:O	1:1:127:ASN:HA	2.10	0.51
1:P:98:THR:HB	1:P:100:GLN:NE2	2.25	0.51
1:V:68:THR:HG21	1:V:121:HIS:ND1	2.26	0.51
1:Z:221:GLN:HB3	1:Z:223:HIS:ND1	2.25	0.51
1:C:101:ASP:HB2	1:C:140:HIS:CE1	2.45	0.51
1:2:142:HIS:HB2	1:2:160:ARG:HG2	1.91	0.51
1:H:68:THR:HG21	1:H:121:HIS:HB3	1.91	0.51
1:R:33:GLU:HB3	1:R:51:LYS:HG2	1.93	0.51
1:S:36:GLU:HB3	1:S:54:LYS:HG2	1.93	0.51
1:G:79:ARG:HB2	1:G:104:GLU:HG3	1.93	0.51
1:G:193:MET:HE3	1:G:215:TYR:HB2	1.92	0.51
1:J:69:PRO:HG2	1:L:114:MET:HG2	1.93	0.51
1:N:101:ASP:HB2	1:N:140:HIS:CE1	2.46	0.51
1:Q:151:GLY:HA3	2:R:301:VFN:CL1	2.47	0.51
1:Y:68:THR:HG21	1:Y:121:HIS:ND1	2.25	0.51
1:3:234:GLU:HG3	1:L:212:ARG:HG3	1.92	0.51
1:3:160:ARG:HD2	1:J:254:ARG:NH1	2.26	0.51
1:B:254:ARG:NH1	1:O:160:ARG:HD2	2.26	0.51
1:C:16:LEU:HD11	1:C:28:VAL:HG11	1.93	0.51
1:Q:25:TRP:HZ3	1:R:27:ILE:HD11	1.75	0.51
1:2:28:VAL:HG22	1:2:46:LEU:HD12	1.92	0.51
1:I:78:THR:HG22	1:I:103:ALA:HB1	1.92	0.51
1:L:81:VAL:HB	1:L:106:THR:HG22	1.93	0.51
1:R:223:HIS:HB3	1:R:227:GLU:HB2	1.92	0.51
1:U:166:PHE:HB3	1:U:182:THR:HG22	1.92	0.51
1:4:102:ARG:HE	1:4:104:GLU:HB3	1.75	0.51
1:Y:139:GLY:O	1:Y:157:GLN:HA	2.10	0.51
1:1:100:GLN:HE21	1:1:100:GLN:N	2.09	0.50
1:D:102:ARG:HH21	1:D:106:THR:HG21	1.74	0.50
1:O:149:LEU:HD21	1:O:161:ILE:HG21	1.92	0.50
1:Y:149:LEU:HD21	1:Y:161:ILE:HG21	1.93	0.50
1:1:16:LEU:HD11	1:1:28:VAL:HG11	1.93	0.50
1:K:16:LEU:HD11	1:K:28:VAL:HG11	1.93	0.50
1:R:132:VAL:HG12	1:R:133:ASN:H	1.76	0.50
1:1:149:LEU:HD21	1:1:161:ILE:HG21	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:59:TYR:HB2	1:H:89:ARG:C	2.31	0.50
1:A:24:PRO:HD2	1:A:42:PRO:HB3	1.93	0.50
1:D:166:PHE:O	1:D:182:THR:HA	2.11	0.50
1:G:149:LEU:HD21	1:G:161:ILE:HG21	1.93	0.50
1:P:90:GLU:HG3	1:Q:93:THR:HG21	1.93	0.50
1:Q:166:PHE:HB3	1:Q:182:THR:HG22	1.93	0.50
1:V:254:ARG:HH21	1:V:254:ARG:CB	2.22	0.50
1:2:64:VAL:HG22	1:2:94:ILE:HD12	1.94	0.50
1:L:166:PHE:HB3	1:L:182:THR:HG22	1.92	0.50
1:Y:80:LEU:HB2	1:Y:96:ARG:HG2	1.94	0.50
1:2:249:ILE:O	1:2:253:THR:HG22	2.12	0.50
1:B:175:LYS:HB2	1:O:257:THR:HG23	1.94	0.50
1:E:201:ARG:HG2	1:E:201:ARG:NH1	2.27	0.50
1:I:16:LEU:HD11	1:I:28:VAL:HG11	1.93	0.50
1:I:42:PRO:O	1:I:60:GLN:HA	2.11	0.50
1:I:98:THR:HB	1:I:100:GLN:HE21	1.75	0.50
1:H:71:LEU:HD22	2:H:301:VFN:N16	2.27	0.50
1:Y:234:GLU:O	1:Y:238:GLN:HG3	2.12	0.50
1:1:164:HIS:CE1	1:1:201:ARG:HG3	2.47	0.50
1:4:46:LEU:HD23	1:4:64:VAL:HB	1.94	0.50
1:B:164:HIS:CE1	1:B:201:ARG:HG3	2.44	0.50
1:L:24:PRO:HD2	1:L:42:PRO:HB3	1.93	0.50
1:1:166:PHE:HB3	1:1:182:THR:HG22	1.94	0.49
1:S:228:ALA:O	1:S:232:LEU:HG	2.11	0.49
1:Y:249:ILE:O	1:Y:253:THR:HG22	2.12	0.49
2:2:301:VFN:C14	1:4:132:VAL:HG21	2.42	0.49
1:3:254:ARG:NH1	1:J:160:ARG:HD2	2.25	0.49
1:N:114:MET:HG2	1:O:69:PRO:HG2	1.94	0.49
1:Q:183:VAL:HB	1:Q:188:ALA:HB1	1.92	0.49
1:C:46:LEU:HD23	1:C:64:VAL:HB	1.93	0.49
1:F:246:ARG:HH21	1:F:250:GLN:NE2	2.10	0.49
1:K:38:THR:HG23	1:K:56:ASN:HB2	1.95	0.49
1:L:161:ILE:HD11	1:L:173:ILE:HG21	1.94	0.49
1:E:79:ARG:HB2	1:E:104:GLU:HG3	1.94	0.49
1:O:142:HIS:HB2	1:O:160:ARG:HG2	1.94	0.49
1:G:9:ILE:HB	1:G:27:ILE:HG12	1.93	0.49
1:H:223:HIS:HB3	1:H:227:GLU:HB2	1.94	0.49
1:M:68:THR:HG21	1:M:121:HIS:ND1	2.27	0.49
1:Y:199:ARG:HH12	1:Y:200:ARG:CZ	2.26	0.49
1:Z:36:GLU:HB3	1:Z:54:LYS:HG2	1.94	0.49
1:F:67:ASP:HB3	1:F:73:TYR:CE2	2.48	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:V:236:ALA:HB1	1:V:246:ARG:HH11	1.78	0.49
1:4:16:LEU:HD11	1:4:28:VAL:HG11	1.94	0.49
1:G:131:LEU:HG	1:G:149:LEU:HD12	1.95	0.49
1:M:90:GLU:O	1:M:115:ALA:HA	2.13	0.49
1:J:212:ARG:HD3	1:J:216:LYS:HD2	1.94	0.49
1:X:132:VAL:CG1	1:X:133:ASN:H	2.21	0.48
1:1:201:ARG:HH11	1:1:201:ARG:HG2	1.78	0.48
1:A:60:GLN:HG3	1:B:45:VAL:HG21	1.95	0.48
1:A:81:VAL:HB	1:A:106:THR:HG22	1.95	0.48
1:G:71:LEU:HD22	2:G:301:VFN:N16	2.28	0.48
1:G:193:MET:CE	1:G:215:TYR:HB2	2.43	0.48
1:K:168:GLY:HA3	1:K:184:PHE:CD2	2.49	0.48
1:E:149:LEU:HD21	1:E:161:ILE:HG21	1.95	0.48
1:F:142:HIS:HB2	1:F:160:ARG:HG2	1.93	0.48
1:M:27:ILE:HD13	1:M:45:VAL:HG22	1.95	0.48
1:W:166:PHE:HB3	1:W:182:THR:HG22	1.95	0.48
1:X:246:ARG:HB3	1:X:246:ARG:HH11	1.78	0.48
1:Z:127:ASN:O	1:Z:145:ASP:HA	2.14	0.48
1:3:132:VAL:HG12	1:3:133:ASN:N	2.28	0.48
1:4:36:GLU:HB3	1:4:54:LYS:HG2	1.96	0.48
1:B:49:PRO:HD2	1:B:78:THR:O	2.13	0.48
1:J:164:HIS:CE1	1:J:201:ARG:HG3	2.40	0.48
1:O:156:HIS:HB2	1:O:174:GLY:HA2	1.95	0.48
1:2:132:VAL:HG12	1:2:133:ASN:H	1.78	0.48
1:G:101:ASP:HB2	1:G:140:HIS:CE1	2.48	0.48
1:S:68:THR:HG21	1:S:121:HIS:ND1	2.29	0.48
1:H:166:PHE:HB3	1:H:182:THR:HG22	1.95	0.48
1:J:28:VAL:HG22	1:J:46:LEU:HD12	1.96	0.48
1:L:100:GLN:HE21	1:L:100:GLN:N	2.11	0.48
1:Y:79:ARG:HB2	1:Y:104:GLU:HG3	1.95	0.48
1:Z:168:GLY:HA3	1:Z:184:PHE:CD2	2.49	0.48
1:S:201:ARG:HH11	1:S:201:ARG:HG2	1.79	0.48
1:A:78:THR:HG22	1:A:103:ALA:HB1	1.96	0.48
1:I:235:SER:HB3	1:I:242:VAL:HG11	1.96	0.48
1:L:132:VAL:HG12	1:L:133:ASN:N	2.29	0.48
1:M:196:GLU:HB3	1:M:200:ARG:HH11	1.79	0.48
1:P:82:ILE:HG12	1:P:107:ILE:HD12	1.96	0.48
1:V:82:ILE:HG23	1:V:86:ASN:HD22	1.78	0.48
1:D:254:ARG:HH11	1:P:160:ARG:HD2	1.79	0.48
1:U:42:PRO:HD2	1:U:60:GLN:HB3	1.96	0.48
1:3:151:GLY:HA3	2:3:302:VFN:CL1	2.51	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:80:LEU:HB2	1:B:96:ARG:HG2	1.96	0.47
1:B:254:ARG:HH11	1:O:160:ARG:HD2	1.78	0.47
1:D:238:GLN:HB3	1:R:205:SER:HB3	1.96	0.47
1:Q:245:PHE:O	1:Q:249:ILE:HD12	2.14	0.47
1:U:3:LEU:HB3	1:U:21:GLN:HG2	1.96	0.47
1:Y:142:HIS:HB2	1:Y:160:ARG:HG3	1.96	0.47
1:Z:99:VAL:HA	1:Z:103:ALA:HB2	1.95	0.47
1:S:100:GLN:H	1:S:100:GLN:HE21	1.61	0.47
1:T:150:SER:O	1:T:153:THR:HB	2.14	0.47
1:Z:166:PHE:HB3	1:Z:182:THR:HG22	1.96	0.47
1:C:212:ARG:HD3	1:C:216:LYS:HE3	1.97	0.47
1:D:114:MET:HG3	1:E:69:PRO:HG2	1.97	0.47
1:K:239:PHE:HB2	1:K:242:VAL:HG23	1.95	0.47
1:Q:113:ILE:HG21	1:Q:119:ILE:HD11	1.96	0.47
1:U:180:TYR:HB2	1:U:193:MET:CE	2.45	0.47
1:2:166:PHE:O	1:2:182:THR:HA	2.13	0.47
1:U:166:PHE:O	1:U:182:THR:HA	2.14	0.47
1:W:100:GLN:H	1:W:100:GLN:NE2	2.07	0.47
1:X:61:PHE:O	1:X:91:GLY:HA2	2.14	0.47
1:A:15:ARG:O	1:A:33:GLU:HA	2.15	0.47
1:S:69:PRO:HD3	1:S:95:HIS:CE1	2.50	0.47
1:W:91:GLY:O	1:W:116:TYR:HA	2.14	0.47
1:G:166:PHE:HB3	1:G:182:THR:HG22	1.97	0.47
1:V:166:PHE:HB3	1:V:182:THR:HG22	1.97	0.47
1:M:78:THR:HG22	1:M:103:ALA:HB1	1.97	0.47
1:T:98:THR:HB	1:T:100:GLN:HE21	1.78	0.47
1:U:249:ILE:O	1:U:253:THR:HG22	2.15	0.47
1:F:89:ARG:HB2	1:F:114:MET:HA	1.97	0.47
1:J:236:ALA:HB1	1:J:246:ARG:NH1	2.30	0.47
1:O:166:PHE:O	1:O:182:THR:HA	2.15	0.47
1:P:68:THR:OG1	1:P:121:HIS:HB3	2.13	0.47
1:I:68:THR:HG21	1:I:121:HIS:ND1	2.29	0.47
1:T:99:VAL:HA	1:T:103:ALA:HB2	1.97	0.47
1:W:223:HIS:HB3	1:W:227:GLU:HB2	1.96	0.47
1:J:168:GLY:HA3	1:J:184:PHE:CD2	2.50	0.47
1:S:46:LEU:HD23	1:S:64:VAL:HB	1.97	0.47
1:S:80:LEU:HB2	1:S:96:ARG:HG2	1.97	0.47
1:X:15:ARG:O	1:X:33:GLU:HA	2.15	0.47
1:G:69:PRO:HG2	1:I:114:MET:HG2	1.96	0.46
1:G:199:ARG:HH21	1:G:200:ARG:HG2	1.79	0.46
1:P:39:VAL:HB	1:P:57:ARG:HD2	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:127:ASN:O	1:Q:145:ASP:HA	2.15	0.46
1:J:17:ALA:HB3	1:J:20:VAL:HG23	1.96	0.46
1:F:160:ARG:HH21	1:L:254:ARG:HH12	1.62	0.46
1:F:166:PHE:O	1:F:182:THR:HA	2.15	0.46
1:O:33:GLU:HB3	1:O:51:LYS:HE2	1.97	0.46
1:O:73:TYR:HB2	1:O:98:THR:HG22	1.96	0.46
1:Q:42:PRO:O	1:Q:44:VAL:HG23	2.16	0.46
1:T:68:THR:HG21	1:T:121:HIS:ND1	2.30	0.46
1:B:52:ILE:HG23	1:B:56:ASN:HD22	1.80	0.46
1:C:166:PHE:O	1:C:182:THR:HA	2.15	0.46
1:F:100:GLN:H	1:F:100:GLN:HE21	1.62	0.46
1:G:28:VAL:HG22	1:G:46:LEU:HD12	1.96	0.46
1:R:132:VAL:HG12	1:R:133:ASN:N	2.30	0.46
1:V:94:ILE:HG12	1:V:119:ILE:HD12	1.97	0.46
1:3:150:SER:HB2	1:3:167:SER:O	2.15	0.46
1:X:16:LEU:HD11	1:X:28:VAL:HG11	1.98	0.46
1:X:80:LEU:HB2	1:X:96:ARG:HG2	1.97	0.46
1:X:88:ILE:HG12	1:X:94:ILE:HD11	1.97	0.46
1:4:98:THR:HB	1:4:100:GLN:NE2	2.31	0.46
1:C:142:HIS:HB2	1:C:160:ARG:HG2	1.97	0.46
1:G:58:ILE:HG12	1:G:88:ILE:HB	1.98	0.46
1:J:154:LEU:HB2	1:L:169:MET:HE3	1.98	0.46
1:Q:63:SER:HB2	1:Q:93:THR:HG22	1.97	0.46
1:U:61:PHE:O	1:U:91:GLY:HA2	2.16	0.46
1:2:168:GLY:HA3	1:2:184:PHE:CD2	2.51	0.46
1:D:24:PRO:HG2	1:D:42:PRO:HB3	1.97	0.46
1:J:131:LEU:HG	1:J:149:LEU:HD12	1.98	0.46
1:M:236:ALA:HB1	1:M:243:ALA:HA	1.97	0.46
1:P:61:PHE:O	1:P:91:GLY:HA2	2.16	0.46
1:Y:16:LEU:HD11	1:Y:28:VAL:HG11	1.98	0.46
1:F:68:THR:HG21	1:F:121:HIS:ND1	2.31	0.46
1:L:68:THR:HG21	1:L:121:HIS:ND1	2.30	0.46
1:W:28:VAL:HG22	1:W:46:LEU:HD12	1.98	0.46
1:K:36:GLU:HB3	1:K:54:LYS:HG2	1.98	0.46
1:O:32:VAL:HG22	1:O:50:THR:HB	1.97	0.46
1:P:36:GLU:HB3	1:P:54:LYS:HG2	1.98	0.46
1:U:98:THR:HB	1:U:100:GLN:NE2	2.31	0.46
1:B:98:THR:HB	1:B:100:GLN:NE2	2.32	0.45
1:E:156:HIS:HB2	1:E:174:GLY:HA2	1.97	0.45
1:G:36:GLU:HB3	1:G:54:LYS:HG2	1.98	0.45
1:N:236:ALA:HB1	1:N:243:ALA:HA	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:164:HIS:HE1	1:Q:201:ARG:HG3	1.80	0.45
1:T:65:GLY:O	1:T:96:ARG:HG3	2.16	0.45
1:X:17:ALA:HB3	1:X:36:GLU:N	2.31	0.45
1:4:201:ARG:HG2	1:4:201:ARG:NH1	2.32	0.45
1:K:132:VAL:HG12	1:K:133:ASN:N	2.31	0.45
1:M:132:VAL:HG23	1:M:149:LEU:O	2.17	0.45
1:O:65:GLY:O	1:O:96:ARG:HG3	2.16	0.45
1:P:100:GLN:NE2	1:P:100:GLN:H	2.14	0.45
1:Q:166:PHE:O	1:Q:182:THR:HA	2.17	0.45
1:R:188:ALA:HB3	1:W:257:THR:HG21	1.97	0.45
1:S:196:GLU:O	1:S:200:ARG:HG3	2.16	0.45
1:K:64:VAL:HG22	1:K:94:ILE:HD12	1.99	0.45
1:R:46:LEU:HA	1:R:64:VAL:O	2.17	0.45
1:1:60:GLN:HE21	1:Y:63:SER:HB3	1.81	0.45
1:3:238:GLN:HB3	1:L:205:SER:HB2	1.98	0.45
1:4:15:ARG:CZ	1:4:33:GLU:HB2	2.47	0.45
1:G:72:LYS:HD3	1:G:98:THR:HG21	1.97	0.45
1:L:19:ASP:HB2	1:L:37:GLY:HA2	1.97	0.45
1:M:166:PHE:O	1:M:182:THR:HA	2.16	0.45
1:P:107:ILE:HG12	1:P:125:ILE:HD12	1.98	0.45
1:U:68:THR:HG21	1:U:121:HIS:ND1	2.31	0.45
1:U:235:SER:HB3	1:U:242:VAL:HG11	1.98	0.45
1:X:78:THR:HG22	1:X:103:ALA:HB1	1.98	0.45
1:3:89:ARG:HB3	1:3:90:GLU:OE1	2.16	0.45
1:J:27:ILE:HD13	1:J:45:VAL:HG22	1.98	0.45
1:X:7:ARG:HE	1:X:7:ARG:HB2	1.24	0.45
1:Y:171:SER:HA	1:Y:185:GLY:O	2.17	0.45
1:2:24:PRO:HD2	1:2:42:PRO:HB3	1.99	0.45
1:F:61:PHE:O	1:F:91:GLY:HA2	2.17	0.45
1:G:148:ILE:HB	1:G:166:PHE:HD1	1.82	0.45
1:O:100:GLN:HE21	1:O:100:GLN:H	1.65	0.45
1:D:3:LEU:HB3	1:D:21:GLN:HG2	1.98	0.45
1:G:82:ILE:HG23	1:G:86:ASN:HD22	1.82	0.45
1:P:68:THR:HG22	1:P:69:PRO:CD	2.46	0.45
1:P:235:SER:HB3	1:P:242:VAL:HG11	1.98	0.45
1:Z:109:ASP:O	1:Z:127:ASN:HA	2.17	0.45
1:D:132:VAL:HG12	1:D:133:ASN:H	1.81	0.45
1:G:68:THR:HG21	1:G:121:HIS:ND1	2.32	0.45
1:M:94:ILE:HG12	1:M:119:ILE:HD12	1.99	0.45
1:X:98:THR:HB	1:X:100:GLN:HE21	1.80	0.45
1:3:236:ALA:CB	1:3:246:ARG:HH11	2.30	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:82:ILE:HG12	1:D:107:ILE:HD12	1.99	0.45
1:J:3:LEU:H	1:J:3:LEU:HG	1.63	0.45
1:N:164:HIS:CE1	1:N:201:ARG:HG3	2.52	0.45
1:D:224:THR:HG23	1:D:227:GLU:OE1	2.17	0.45
1:E:160:ARG:HD2	1:S:254:ARG:NH1	2.31	0.45
1:J:88:ILE:HG23	1:J:92:VAL:HG11	1.98	0.45
1:J:180:TYR:HB2	1:J:193:MET:CE	2.47	0.45
1:V:73:TYR:HB2	1:V:98:THR:HG22	1.99	0.45
1:B:68:THR:HG21	1:B:121:HIS:ND1	2.32	0.44
1:L:73:TYR:HB2	1:L:98:THR:HG22	1.98	0.44
1:N:160:ARG:HD2	1:Q:254:ARG:HH11	1.81	0.44
1:R:236:ALA:HB1	1:R:246:ARG:NH1	2.32	0.44
1:X:139:GLY:O	1:X:157:GLN:HA	2.17	0.44
1:Y:101:ASP:HB2	1:Y:140:HIS:HD1	1.82	0.44
1:3:17:ALA:O	1:3:20:VAL:HG23	2.17	0.44
1:L:28:VAL:HG22	1:L:46:LEU:HD12	1.99	0.44
1:V:150:SER:HB3	2:W:301:VFN:O18	2.17	0.44
1:V:164:HIS:HE1	1:V:201:ARG:HG3	1.82	0.44
1:W:39:VAL:HB	1:W:57:ARG:HD2	1.99	0.44
1:X:164:HIS:HE1	1:X:201:ARG:HG3	1.82	0.44
1:C:139:GLY:O	1:C:157:GLN:HA	2.17	0.44
1:F:221:GLN:HB3	1:F:223:HIS:CE1	2.52	0.44
1:K:7:ARG:HD2	1:K:25:TRP:HE1	1.83	0.44
1:M:42:PRO:HD2	1:M:60:GLN:HB3	1.99	0.44
1:Q:132:VAL:HG12	1:Q:133:ASN:N	2.31	0.44
1:R:61:PHE:O	1:R:91:GLY:HA2	2.18	0.44
1:R:167:SER:HB2	1:R:173:ILE:HD11	1.98	0.44
1:S:153:THR:HG23	1:S:171:SER:HB2	2.00	0.44
1:2:60:GLN:HE21	1:3:63:SER:HB3	1.83	0.44
1:2:194:ASN:O	1:2:198:MET:HG3	2.18	0.44
1:J:99:VAL:HA	1:J:103:ALA:HB2	1.98	0.44
1:K:211:LEU:HD11	1:K:241:GLU:HB3	1.99	0.44
1:Q:98:THR:HB	1:Q:100:GLN:NE2	2.33	0.44
1:3:139:GLY:O	1:3:157:GLN:HA	2.17	0.44
1:J:132:VAL:HG12	1:J:133:ASN:H	1.83	0.44
1:3:155:VAL:HG11	1:3:161:ILE:HD11	2.00	0.44
1:M:151:GLY:HA3	2:N:301:VFN:CL1	2.55	0.44
1:O:216:LYS:HA	1:O:220:ARG:HB2	2.00	0.44
1:R:149:LEU:HD22	1:R:153:THR:HG21	2.00	0.44
1:S:110:HIS:O	1:S:128:HIS:HA	2.17	0.44
1:T:8:ALA:HB2	1:T:23:GLY:O	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:4:196:GLU:O	1:4:200:ARG:HG3	2.17	0.44
1:B:142:HIS:HB2	1:B:160:ARG:HG2	2.00	0.44
1:F:91:GLY:HA3	1:F:116:TYR:CE1	2.52	0.44
1:G:132:VAL:CG1	1:G:133:ASN:H	2.29	0.44
1:L:99:VAL:HA	1:L:103:ALA:HB2	2.00	0.44
1:Q:79:ARG:O	1:Q:104:GLU:HA	2.18	0.44
1:W:21:GLN:HB2	1:W:39:VAL:HG13	1.99	0.44
1:Y:245:PHE:CZ	1:Y:249:ILE:HD11	2.53	0.44
1:J:24:PRO:HD2	1:J:42:PRO:HB3	2.00	0.44
1:R:80:LEU:HB2	1:R:96:ARG:HG2	1.99	0.44
1:2:240:PRO:O	1:2:244:VAL:HG23	2.18	0.43
1:3:71:LEU:HD22	2:3:301:VFN:N16	2.32	0.43
1:B:36:GLU:O	1:B:54:LYS:HA	2.18	0.43
1:K:183:VAL:HG12	1:K:190:ALA:HA	1.99	0.43
1:W:221:GLN:HB3	1:W:223:HIS:ND1	2.33	0.43
1:Z:16:LEU:HD11	1:Z:28:VAL:HG11	2.00	0.43
1:C:156:HIS:O	1:C:159:CYS:HB2	2.18	0.43
1:F:91:GLY:HA3	1:F:116:TYR:CD1	2.53	0.43
1:H:38:THR:HG23	1:H:56:ASN:HB2	2.01	0.43
1:L:8:ALA:HB2	1:L:23:GLY:O	2.17	0.43
1:L:89:ARG:HB2	1:L:114:MET:HA	2.00	0.43
1:W:236:ALA:O	1:W:243:ALA:HB2	2.19	0.43
1:3:85:HIS:O	1:3:110:HIS:HA	2.17	0.43
1:G:166:PHE:O	1:G:182:THR:HA	2.18	0.43
1:H:80:LEU:HB2	1:H:96:ARG:HG2	1.99	0.43
1:J:98:THR:HB	1:J:100:GLN:HE21	1.83	0.43
1:N:89:ARG:HB2	1:N:114:MET:HA	2.00	0.43
1:T:98:THR:HB	1:T:100:GLN:NE2	2.33	0.43
1:2:68:THR:HG21	1:2:121:HIS:ND1	2.34	0.43
1:3:137:LEU:HD22	1:3:141:VAL:HG11	2.00	0.43
1:4:157:GLN:HB3	1:4:158:TYR:CD2	2.52	0.43
1:A:73:TYR:HB2	1:A:98:THR:HG22	2.00	0.43
1:C:177:VAL:HG22	1:C:183:VAL:HG11	1.99	0.43
1:H:90:GLU:O	1:H:115:ALA:HA	2.18	0.43
1:H:169:MET:HE3	1:I:154:LEU:HB2	2.00	0.43
1:S:198:MET:HE1	1:S:211:LEU:HD13	2.00	0.43
1:V:115:ALA:HB3	1:V:133:ASN:ND2	2.33	0.43
1:P:89:ARG:HD3	1:Q:69:PRO:HB3	2.00	0.43
1:U:194:ASN:O	1:U:198:MET:HG3	2.17	0.43
1:X:240:PRO:O	1:X:244:VAL:HG23	2.18	0.43
1:1:132:VAL:HG12	1:1:133:ASN:H	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:68:THR:HG21	1:D:121:HIS:ND1	2.34	0.43
1:D:85:HIS:O	1:D:110:HIS:HA	2.18	0.43
1:L:236:ALA:HB1	1:L:246:ARG:NH1	2.34	0.43
1:M:229:LEU:HD11	1:M:253:THR:HG21	2.00	0.43
1:O:99:VAL:HA	1:O:103:ALA:HB2	2.00	0.43
1:S:201:ARG:HG2	1:S:201:ARG:NH1	2.34	0.43
1:A:99:VAL:HA	1:A:103:ALA:HB2	1.99	0.43
1:B:17:ALA:HB3	1:B:20:VAL:HG23	2.00	0.43
1:K:150:SER:HB2	1:K:167:SER:O	2.18	0.43
1:M:149:LEU:HD11	1:M:161:ILE:HG21	2.01	0.43
1:R:254:ARG:NH1	1:W:160:ARG:HD2	2.34	0.43
1:W:140:HIS:O	1:W:158:TYR:HA	2.18	0.43
1:2:195:PHE:HZ	1:2:212:ARG:HG2	1.84	0.43
1:F:132:VAL:HG12	1:F:133:ASN:N	2.32	0.43
1:I:17:ALA:HB3	1:I:20:VAL:HG23	2.00	0.43
1:3:61:PHE:O	1:3:91:GLY:HA2	2.19	0.43
1:3:216:LYS:HA	1:3:220:ARG:HB2	2.00	0.43
1:4:229:LEU:HD23	1:4:246:ARG:HG3	2.01	0.43
1:T:47:LYS:HD2	1:T:66:GLU:HA	2.00	0.43
1:D:160:ARG:HD2	1:P:254:ARG:NH1	2.34	0.43
1:E:216:LYS:HE3	1:E:220:ARG:NH1	2.34	0.43
1:F:216:LYS:HE2	1:F:220:ARG:NH1	2.34	0.43
1:P:70:ASP:HA	2:P:302:VFN:N16	2.33	0.43
1:U:101:ASP:HB2	1:U:140:HIS:CE1	2.54	0.43
1:U:139:GLY:O	1:U:157:GLN:HA	2.18	0.43
1:Y:216:LYS:HA	1:Y:220:ARG:HB2	2.00	0.43
1:Z:240:PRO:O	1:Z:244:VAL:HG23	2.18	0.43
1:1:112:LEU:HD23	1:1:130:ILE:HG23	2.00	0.42
1:H:235:SER:HA	1:H:238:GLN:OE1	2.19	0.42
1:O:89:ARG:HB3	1:O:90:GLU:OE1	2.19	0.42
1:T:28:VAL:HG22	1:T:46:LEU:HD12	1.99	0.42
1:T:90:GLU:O	1:T:115:ALA:HA	2.19	0.42
1:T:114:MET:HG3	1:U:69:PRO:HG2	2.00	0.42
1:Y:17:ALA:HB3	1:Y:20:VAL:HG23	2.01	0.42
1:A:156:HIS:HB2	1:A:174:GLY:HA2	2.01	0.42
1:D:98:THR:HB	1:D:100:GLN:HE21	1.82	0.42
1:D:195:PHE:HZ	1:D:212:ARG:HG2	1.84	0.42
1:H:73:TYR:HB2	1:H:98:THR:HG22	2.00	0.42
1:J:16:LEU:HD11	1:J:28:VAL:HG11	2.00	0.42
1:O:217:VAL:HG11	1:O:231:GLU:HB3	2.00	0.42
1:P:38:THR:HG23	1:P:56:ASN:HB2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:61:PHE:O	1:Q:91:GLY:HA2	2.19	0.42
1:A:14:ALA:HB2	1:A:29:GLY:O	2.19	0.42
2:H:302:VFN:N16	1:I:71:LEU:HD22	2.34	0.42
1:I:211:LEU:HD11	1:I:241:GLU:HB3	2.01	0.42
1:J:22:VAL:HA	1:J:40:ILE:HB	1.99	0.42
1:M:195:PHE:HZ	1:M:212:ARG:HG2	1.84	0.42
1:X:106:THR:HG23	1:X:124:VAL:HG22	2.01	0.42
1:Z:142:HIS:HB2	1:Z:160:ARG:HG2	2.02	0.42
1:1:64:VAL:HG22	1:1:94:ILE:HD12	2.02	0.42
2:3:302:VFN:N16	1:4:71:LEU:HD22	2.35	0.42
1:D:14:ALA:HB2	1:D:29:GLY:O	2.19	0.42
1:H:79:ARG:HB2	1:H:104:GLU:HG3	1.99	0.42
1:H:183:VAL:HB	1:H:188:ALA:HB1	2.01	0.42
1:I:15:ARG:O	1:I:33:GLU:HA	2.20	0.42
1:U:58:ILE:HG12	1:U:88:ILE:HB	2.01	0.42
1:2:42:PRO:O	1:2:60:GLN:HA	2.19	0.42
1:A:139:GLY:O	1:A:157:GLN:HA	2.18	0.42
1:A:152:TYR:HB2	1:B:154:LEU:HD11	2.02	0.42
1:P:99:VAL:HA	1:P:103:ALA:HB2	2.00	0.42
1:R:107:ILE:HD11	1:R:119:ILE:HG21	2.01	0.42
1:S:38:THR:HG23	1:S:56:ASN:HB2	2.02	0.42
1:T:114:MET:CG	1:U:69:PRO:HG2	2.49	0.42
1:X:168:GLY:HA3	1:X:184:PHE:CD1	2.54	0.42
1:3:235:SER:HA	1:3:238:GLN:OE1	2.19	0.42
1:B:78:THR:HG22	1:B:103:ALA:HB1	2.01	0.42
1:C:235:SER:OG	1:C:242:VAL:HG11	2.20	0.42
1:E:193:MET:HE3	1:E:215:TYR:HB2	2.01	0.42
1:F:160:ARG:HB2	1:F:176:ASP:OD2	2.19	0.42
1:G:180:TYR:HB2	1:G:193:MET:SD	2.59	0.42
1:H:34:ILE:HG12	1:H:52:ILE:HD13	2.02	0.42
1:H:137:LEU:HD22	1:H:141:VAL:HG11	1.99	0.42
1:J:132:VAL:HG12	1:J:133:ASN:N	2.35	0.42
1:N:124:VAL:HB	1:N:142:HIS:ND1	2.33	0.42
1:P:68:THR:HG22	1:P:69:PRO:HD2	2.01	0.42
1:P:150:SER:HB2	1:P:167:SER:O	2.20	0.42
1:B:149:LEU:HA	1:B:167:SER:OG	2.20	0.42
1:C:237:ALA:HB2	1:J:195:PHE:HB3	2.01	0.42
1:D:114:MET:HE1	1:D:132:VAL:HG22	2.01	0.42
1:I:98:THR:HB	1:I:100:GLN:NE2	2.35	0.42
1:K:216:LYS:HA	1:K:220:ARG:HB2	2.01	0.42
1:Y:90:GLU:O	1:Y:115:ALA:HA	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:58:ILE:HG12	1:J:88:ILE:HB	2.01	0.42
1:L:236:ALA:HB1	1:L:246:ARG:HH11	1.84	0.42
1:1:201:ARG:HG2	1:1:201:ARG:NH1	2.34	0.42
1:E:68:THR:HG21	1:E:121:HIS:HB3	2.02	0.42
1:Q:143:VAL:HG13	1:Q:161:ILE:HB	2.02	0.42
1:R:228:ALA:O	1:R:232:LEU:HG	2.20	0.42
1:S:114:MET:HG2	1:T:69:PRO:HG2	2.02	0.42
1:T:168:GLY:HA3	1:T:184:PHE:CD2	2.55	0.42
1:4:42:PRO:HD2	1:4:60:GLN:HB3	2.02	0.42
1:H:110:HIS:O	1:H:128:HIS:HA	2.20	0.42
1:N:107:ILE:HG23	1:N:111:ASN:HD22	1.85	0.42
1:R:78:THR:HG22	1:R:103:ALA:HB1	2.01	0.42
1:T:169:MET:HG2	1:U:156:HIS:CE1	2.54	0.42
1:X:98:THR:HB	1:X:100:GLN:NE2	2.35	0.42
1:Z:247:ASP:HA	1:Z:250:GLN:HB3	2.02	0.42
1:3:236:ALA:HB1	1:3:246:ARG:HH11	1.85	0.41
1:A:178:PRO:HB3	1:A:249:ILE:HG13	2.01	0.41
1:B:99:VAL:HA	1:B:103:ALA:HB2	2.02	0.41
1:P:142:HIS:HB2	1:P:160:ARG:HG2	2.02	0.41
1:P:151:GLY:HA3	2:P:301:VFN:CL1	2.57	0.41
1:S:178:PRO:HB2	1:S:181:VAL:CG2	2.50	0.41
1:F:193:MET:SD	1:F:215:TYR:HB2	2.60	0.41
1:K:114:MET:HB2	1:K:132:VAL:HA	2.02	0.41
1:O:68:THR:HG21	1:O:121:HIS:ND1	2.34	0.41
1:S:68:THR:HB	1:S:70:ASP:H	1.84	0.41
1:4:7:ARG:HD2	1:4:25:TRP:NE1	2.35	0.41
1:C:112:LEU:HD23	1:C:130:ILE:HG23	2.02	0.41
1:I:145:ASP:O	1:I:163:ALA:HA	2.20	0.41
1:M:164:HIS:CE1	1:M:201:ARG:HG3	2.56	0.41
1:Q:196:GLU:O	1:Q:200:ARG:HG3	2.20	0.41
1:B:61:PHE:O	1:B:91:GLY:HA2	2.19	0.41
1:B:156:HIS:HB2	1:B:174:GLY:HA2	2.02	0.41
1:I:166:PHE:O	1:I:182:THR:HA	2.20	0.41
1:T:100:GLN:NE2	1:T:100:GLN:H	2.19	0.41
1:T:114:MET:HB2	1:T:132:VAL:HA	2.02	0.41
1:3:42:PRO:HD2	1:3:60:GLN:HB3	2.01	0.41
1:B:167:SER:HB3	1:B:173:ILE:HD11	2.02	0.41
1:D:16:LEU:HD11	1:D:28:VAL:HG11	2.03	0.41
1:D:223:HIS:HB3	1:D:227:GLU:HB2	2.03	0.41
1:E:150:SER:HB2	1:E:167:SER:O	2.20	0.41
1:F:4:ILE:HG23	1:F:22:VAL:HB	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:7:ARG:HD2	1:K:25:TRP:NE1	2.36	0.41
1:K:71:LEU:HD22	2:K:301:VFN:N16	2.34	0.41
1:V:90:GLU:O	1:V:115:ALA:HA	2.19	0.41
1:X:30:ALA:O	1:X:48:GLY:HA3	2.21	0.41
1:Z:145:ASP:HB3	1:Z:146:TRP:CD1	2.55	0.41
1:1:90:GLU:HG3	1:Y:93:THR:HG21	2.03	0.41
1:2:132:VAL:HG12	1:2:133:ASN:N	2.35	0.41
1:3:8:ALA:HB2	1:3:23:GLY:O	2.20	0.41
1:D:164:HIS:HE1	1:D:201:ARG:HG3	1.86	0.41
1:F:157:GLN:HB3	1:F:158:TYR:CD2	2.56	0.41
1:F:218:VAL:HG21	1:F:245:PHE:CE2	2.56	0.41
1:N:156:HIS:HB2	1:N:174:GLY:HA2	2.03	0.41
1:2:66:GLU:HB3	1:2:95:HIS:HD2	1.84	0.41
1:B:229:LEU:HD21	1:B:249:ILE:HG22	2.02	0.41
1:H:132:VAL:CG1	1:H:133:ASN:H	2.30	0.41
1:P:27:ILE:HD11	1:R:25:TRP:HZ3	1.85	0.41
1:R:183:VAL:HB	1:R:188:ALA:HB1	2.02	0.41
1:Y:164:HIS:CE1	1:Y:201:ARG:HG3	2.43	0.41
1:D:66:GLU:HB3	1:D:95:HIS:CD2	2.55	0.41
1:F:133:ASN:O	1:F:151:GLY:HA2	2.20	0.41
1:F:156:HIS:HD2	1:F:174:GLY:HA2	1.85	0.41
1:M:250:GLN:HA	1:M:253:THR:HG22	2.02	0.41
1:P:149:LEU:HD22	1:P:153:THR:HG21	2.03	0.41
1:Y:3:LEU:H	1:Y:3:LEU:HG	1.50	0.41
1:Y:36:GLU:HB2	1:Y:54:LYS:HG2	2.02	0.41
1:G:110:HIS:O	1:G:128:HIS:HA	2.20	0.41
1:H:16:LEU:HD11	1:H:28:VAL:HG11	2.03	0.41
1:J:216:LYS:NZ	1:J:220:ARG:HH11	2.19	0.41
1:K:90:GLU:O	1:K:115:ALA:HA	2.21	0.41
1:M:160:ARG:HD2	1:Z:254:ARG:HH11	1.85	0.41
1:P:195:PHE:HD1	1:P:208:ILE:HG23	1.86	0.41
1:T:112:LEU:HD23	1:T:130:ILE:HG23	2.03	0.41
1:X:156:HIS:HB2	1:X:174:GLY:HA2	2.03	0.41
1:Y:67:ASP:HB3	1:Y:73:TYR:CE2	2.56	0.41
1:D:139:GLY:O	1:D:157:GLN:HA	2.21	0.41
1:G:47:LYS:HB3	1:G:65:GLY:O	2.21	0.41
1:M:254:ARG:NH1	1:Z:160:ARG:HD2	2.32	0.41
1:N:61:PHE:O	1:N:91:GLY:HA2	2.21	0.41
1:N:223:HIS:HD2	1:N:227:GLU:HB3	1.85	0.41
1:R:160:ARG:HB2	1:R:176:ASP:OD2	2.21	0.41
1:W:157:GLN:HB3	1:W:158:TYR:CD2	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:54:LYS:HB3	1:B:55:HIS:CD2	2.56	0.40
1:D:247:ASP:HA	1:D:250:GLN:HB3	2.03	0.40
1:B:81:VAL:HB	1:B:106:THR:HG22	2.03	0.40
1:C:160:ARG:HD2	1:K:254:ARG:HH11	1.86	0.40
1:D:89:ARG:O	1:D:92:VAL:HG23	2.21	0.40
1:E:89:ARG:O	1:E:92:VAL:HG23	2.21	0.40
1:G:236:ALA:HB1	1:G:246:ARG:HH11	1.86	0.40
1:I:64:VAL:HG13	1:I:94:ILE:HB	2.02	0.40
1:L:166:PHE:O	1:L:182:THR:HA	2.21	0.40
1:N:90:GLU:O	1:N:115:ALA:HA	2.20	0.40
1:P:52:ILE:HG23	1:P:56:ASN:HD22	1.86	0.40
1:R:68:THR:HG21	1:R:121:HIS:HB3	2.03	0.40
1:T:56:ASN:OD1	1:T:86:ASN:HB2	2.22	0.40
1:Z:125:ILE:HG12	1:Z:143:VAL:HB	2.03	0.40
1:G:142:HIS:HB2	1:G:160:ARG:HG2	2.03	0.40
1:O:36:GLU:HB3	1:O:54:LYS:HG2	2.02	0.40
1:V:178:PRO:HG2	1:V:219:TYR:OH	2.22	0.40
1:X:164:HIS:CE1	1:X:201:ARG:HG3	2.56	0.40
1:Y:131:LEU:HD21	1:Y:137:LEU:HD11	2.03	0.40
1:B:249:ILE:O	1:B:253:THR:HG22	2.21	0.40
1:D:219:TYR:HE1	1:P:258:ARG:HB3	1.86	0.40
1:L:78:THR:HG22	1:L:103:ALA:HB1	2.03	0.40
1:O:246:ARG:HH21	1:O:250:GLN:HE21	1.68	0.40
1:P:139:GLY:O	1:P:157:GLN:HA	2.21	0.40
1:P:166:PHE:O	1:P:182:THR:HA	2.20	0.40
1:T:100:GLN:HE21	1:T:100:GLN:H	1.68	0.40
1:W:68:THR:HG21	1:W:121:HIS:HB3	2.03	0.40
1:Z:132:VAL:HG12	1:Z:133:ASN:N	2.37	0.40
1:1:216:LYS:HA	1:1:220:ARG:HB2	2.04	0.40
1:A:36:GLU:HB3	1:A:54:LYS:HG2	2.03	0.40
1:A:91:GLY:O	1:A:116:TYR:HA	2.22	0.40
1:E:98:THR:HB	1:E:100:GLN:HE21	1.86	0.40
1:H:166:PHE:O	1:H:182:THR:HA	2.21	0.40
1:I:132:VAL:HG12	1:I:133:ASN:H	1.87	0.40
1:P:8:ALA:HB2	1:P:23:GLY:O	2.21	0.40
1:Q:80:LEU:HB2	1:Q:96:ARG:HG2	2.04	0.40
1:S:198:MET:CE	1:S:211:LEU:HD13	2.51	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	1	256/261 (98%)	225 (88%)	28 (11%)	3 (1%)	13 40
1	2	256/261 (98%)	224 (88%)	28 (11%)	4 (2%)	9 32
1	3	256/261 (98%)	220 (86%)	31 (12%)	5 (2%)	7 27
1	4	256/261 (98%)	218 (85%)	32 (12%)	6 (2%)	6 23
1	A	256/261 (98%)	229 (90%)	22 (9%)	5 (2%)	7 27
1	B	256/261 (98%)	222 (87%)	29 (11%)	5 (2%)	7 27
1	C	256/261 (98%)	224 (88%)	28 (11%)	4 (2%)	9 32
1	D	256/261 (98%)	221 (86%)	33 (13%)	2 (1%)	19 51
1	E	256/261 (98%)	223 (87%)	29 (11%)	4 (2%)	9 32
1	F	256/261 (98%)	230 (90%)	24 (9%)	2 (1%)	19 51
1	G	256/261 (98%)	225 (88%)	27 (10%)	4 (2%)	9 32
1	H	256/261 (98%)	227 (89%)	22 (9%)	7 (3%)	5 19
1	I	256/261 (98%)	226 (88%)	25 (10%)	5 (2%)	7 27
1	J	256/261 (98%)	219 (86%)	35 (14%)	2 (1%)	19 51
1	K	256/261 (98%)	218 (85%)	34 (13%)	4 (2%)	9 32
1	L	256/261 (98%)	229 (90%)	26 (10%)	1 (0%)	34 66
1	M	256/261 (98%)	225 (88%)	26 (10%)	5 (2%)	7 27
1	N	256/261 (98%)	228 (89%)	26 (10%)	2 (1%)	19 51
1	O	256/261 (98%)	223 (87%)	30 (12%)	3 (1%)	13 40
1	P	256/261 (98%)	223 (87%)	26 (10%)	7 (3%)	5 19
1	Q	256/261 (98%)	218 (85%)	31 (12%)	7 (3%)	5 19
1	R	256/261 (98%)	223 (87%)	28 (11%)	5 (2%)	7 27
1	S	256/261 (98%)	231 (90%)	20 (8%)	5 (2%)	7 27
1	T	256/261 (98%)	223 (87%)	31 (12%)	2 (1%)	19 51
1	U	256/261 (98%)	219 (86%)	31 (12%)	6 (2%)	6 23

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	V	256/261 (98%)	225 (88%)	26 (10%)	5 (2%)	7 27
1	W	256/261 (98%)	224 (88%)	28 (11%)	4 (2%)	9 32
1	X	256/261 (98%)	226 (88%)	27 (10%)	3 (1%)	13 40
1	Y	256/261 (98%)	228 (89%)	26 (10%)	2 (1%)	19 51
1	Z	256/261 (98%)	223 (87%)	29 (11%)	4 (2%)	9 32
All	All	7680/7830 (98%)	6719 (88%)	838 (11%)	123 (2%)	9 32

All (123) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	2	18	ALA
1	3	18	ALA
1	3	220	ARG
1	C	220	ARG
1	D	18	ALA
1	H	3	LEU
1	I	121	HIS
1	M	3	LEU
1	M	18	ALA
1	N	18	ALA
1	P	3	LEU
1	Q	3	LEU
1	Q	138	ALA
1	Q	220	ARG
1	U	220	ARG
1	V	18	ALA
1	V	85	HIS
1	X	18	ALA
1	Y	116	TYR
1	2	71	LEU
1	2	220	ARG
1	3	38	THR
1	4	18	ALA
1	A	220	ARG
1	B	116	TYR
1	C	116	TYR
1	C	121	HIS
1	E	3	LEU
1	F	220	ARG
1	H	116	TYR

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Mol	Chain	Res	Type
1	M	75	GLY
1	M	220	ARG
1	O	133	ASN
1	P	55	HIS
1	P	220	ARG
1	Q	116	TYR
1	R	220	ARG
1	S	121	HIS
1	S	220	ARG
1	T	121	HIS
1	U	133	ASN
1	W	133	ASN
1	X	252	ALA
1	Y	220	ARG
1	1	17	ALA
1	1	116	TYR
1	4	115	ALA
1	B	220	ARG
1	E	116	TYR
1	E	220	ARG
1	H	19	ASP
1	H	101	ASP
1	H	134	ASN
1	I	192	SER
1	J	116	TYR
1	N	254	ARG
1	O	101	ASP
1	P	121	HIS
1	R	116	TYR
1	U	75	GLY
1	U	110	HIS
1	U	116	TYR
1	V	121	HIS
1	V	233	ALA
1	W	18	ALA
1	W	116	TYR
1	X	134	ASN
1	1	134	ASN
1	3	116	TYR
1	3	121	HIS
1	4	192	SER
1	A	116	TYR

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Mol	Chain	Res	Type
1	B	97	GLY
1	E	133	ASN
1	G	220	ARG
1	H	115	ALA
1	J	145	ASP
1	K	61	PHE
1	K	101	ASP
1	K	116	TYR
1	L	116	TYR
1	M	116	TYR
1	O	121	HIS
1	P	219	TYR
1	Q	192	SER
1	R	192	SER
1	S	133	ASN
1	S	233	ALA
1	W	121	HIS
1	Z	101	ASP
1	Z	138	ALA
1	Z	192	SER
1	A	219	TYR
1	B	37	GLY
1	B	192	SER
1	D	116	TYR
1	F	2	SER
1	G	101	ASP
1	H	89	ARG
1	K	192	SER
1	P	202	GLY
1	R	110	HIS
1	T	116	TYR
1	U	192	SER
1	A	75	GLY
1	A	192	SER
1	C	115	ALA
1	G	192	SER
1	I	219	TYR
1	P	115	ALA
1	R	55	HIS
1	S	75	GLY
1	I	97	GLY
1	Z	126	GLY

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Mol	Chain	Res	Type
1	4	108	GLY
1	G	132	VAL
1	I	218	VAL
1	Q	75	GLY
1	V	53	GLY
1	2	97	GLY
1	Q	76	GLU
1	4	76	GLU
1	4	97	GLY

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	1	206/208 (99%)	190 (92%)	16 (8%)	12 34
1	2	206/208 (99%)	192 (93%)	14 (7%)	16 42
1	3	206/208 (99%)	194 (94%)	12 (6%)	20 50
1	4	206/208 (99%)	193 (94%)	13 (6%)	18 46
1	A	206/208 (99%)	191 (93%)	15 (7%)	14 38
1	B	206/208 (99%)	189 (92%)	17 (8%)	11 32
1	C	206/208 (99%)	191 (93%)	15 (7%)	14 38
1	D	206/208 (99%)	187 (91%)	19 (9%)	9 27
1	E	206/208 (99%)	193 (94%)	13 (6%)	18 46
1	F	206/208 (99%)	192 (93%)	14 (7%)	16 42
1	G	206/208 (99%)	184 (89%)	22 (11%)	6 20
1	H	206/208 (99%)	188 (91%)	18 (9%)	10 30
1	I	206/208 (99%)	187 (91%)	19 (9%)	9 27
1	J	206/208 (99%)	186 (90%)	20 (10%)	8 25
1	K	206/208 (99%)	189 (92%)	17 (8%)	11 32
1	L	206/208 (99%)	183 (89%)	23 (11%)	6 18
1	M	206/208 (99%)	189 (92%)	17 (8%)	11 32

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	N	206/208 (99%)	187 (91%)	19 (9%)	9 27
1	O	206/208 (99%)	184 (89%)	22 (11%)	6 20
1	P	206/208 (99%)	188 (91%)	18 (9%)	10 30
1	Q	206/208 (99%)	189 (92%)	17 (8%)	11 32
1	R	206/208 (99%)	188 (91%)	18 (9%)	10 30
1	S	206/208 (99%)	193 (94%)	13 (6%)	18 46
1	T	206/208 (99%)	181 (88%)	25 (12%)	5 15
1	U	206/208 (99%)	182 (88%)	24 (12%)	5 16
1	V	206/208 (99%)	187 (91%)	19 (9%)	9 27
1	W	206/208 (99%)	185 (90%)	21 (10%)	7 22
1	X	206/208 (99%)	185 (90%)	21 (10%)	7 22
1	Y	206/208 (99%)	191 (93%)	15 (7%)	14 38
1	Z	206/208 (99%)	187 (91%)	19 (9%)	9 27
All	All	6180/6240 (99%)	5645 (91%)	535 (9%)	10 30

All (535) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	1	1	MET
1	1	3	LEU
1	1	15	ARG
1	1	19	ASP
1	1	68	THR
1	1	70	ASP
1	1	74	LYS
1	1	100	GLN
1	1	150	SER
1	1	157	GLN
1	1	175	LYS
1	1	193	MET
1	1	212	ARG
1	1	253	THR
1	1	254	ARG
1	1	258	ARG
1	2	3	LEU
1	2	15	ARG
1	2	36	GLU

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Mol	Chain	Res	Type
1	2	63	SER
1	2	68	THR
1	2	99	VAL
1	2	100	GLN
1	2	106	THR
1	2	145	ASP
1	2	212	ARG
1	2	216	LYS
1	2	220	ARG
1	2	248	SER
1	2	253	THR
1	3	1	MET
1	3	15	ARG
1	3	51	LYS
1	3	67	ASP
1	3	68	THR
1	3	71	LEU
1	3	102	ARG
1	3	109	ASP
1	3	212	ARG
1	3	220	ARG
1	3	234	GLU
1	3	250	GLN
1	4	2	SER
1	4	15	ARG
1	4	25	TRP
1	4	33	GLU
1	4	68	THR
1	4	70	ASP
1	4	71	LEU
1	4	74	LYS
1	4	100	GLN
1	4	189	GLU
1	4	196	GLU
1	4	212	ARG
1	4	250	GLN
1	A	1	MET
1	A	51	LYS
1	A	57	ARG
1	A	63	SER
1	A	67	ASP
1	A	68	THR

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Mol	Chain	Res	Type
1	A	70	ASP
1	A	76	GLU
1	A	102	ARG
1	A	150	SER
1	A	171	SER
1	A	192	SER
1	A	196	GLU
1	A	212	ARG
1	A	246	ARG
1	B	1	MET
1	B	11	ASP
1	B	15	ARG
1	B	51	LYS
1	B	62	SER
1	B	68	THR
1	B	76	GLU
1	B	100	GLN
1	B	102	ARG
1	B	114	MET
1	B	153	THR
1	B	171	SER
1	B	176	ASP
1	B	193	MET
1	B	212	ARG
1	B	250	GLN
1	B	257	THR
1	C	13	SER
1	C	68	THR
1	C	76	GLU
1	C	93	THR
1	C	100	GLN
1	C	109	ASP
1	C	204	SER
1	C	212	ARG
1	C	213	ARG
1	C	220	ARG
1	C	221	GLN
1	C	250	GLN
1	C	253	THR
1	C	257	THR
1	C	258	ARG
1	D	3	LEU

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Mol	Chain	Res	Type
1	D	7	ARG
1	D	15	ARG
1	D	26	SER
1	D	68	THR
1	D	71	LEU
1	D	76	GLU
1	D	99	VAL
1	D	106	THR
1	D	114	MET
1	D	150	SER
1	D	171	SER
1	D	192	SER
1	D	212	ARG
1	D	220	ARG
1	D	221	GLN
1	D	254	ARG
1	D	256	ILE
1	D	257	THR
1	E	1	MET
1	E	15	ARG
1	E	67	ASP
1	E	72	LYS
1	E	81	VAL
1	E	102	ARG
1	E	106	THR
1	E	109	ASP
1	E	114	MET
1	E	157	GLN
1	E	204	SER
1	E	205	SER
1	E	213	ARG
1	F	15	ARG
1	F	67	ASP
1	F	68	THR
1	F	70	ASP
1	F	71	LEU
1	F	99	VAL
1	F	100	GLN
1	F	102	ARG
1	F	193	MET
1	F	212	ARG
1	F	220	ARG

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Mol	Chain	Res	Type
1	F	221	GLN
1	F	225	VAL
1	F	226	GLU
1	G	1	MET
1	G	15	ARG
1	G	21	GLN
1	G	68	THR
1	G	71	LEU
1	G	72	LYS
1	G	79	ARG
1	G	99	VAL
1	G	100	GLN
1	G	114	MET
1	G	145	ASP
1	G	201	ARG
1	G	204	SER
1	G	205	SER
1	G	212	ARG
1	G	213	ARG
1	G	220	ARG
1	G	221	GLN
1	G	238	GLN
1	G	253	THR
1	G	257	THR
1	G	258	ARG
1	H	1	MET
1	H	15	ARG
1	H	19	ASP
1	H	21	GLN
1	H	68	THR
1	H	70	ASP
1	H	71	LEU
1	H	93	THR
1	H	99	VAL
1	H	109	ASP
1	H	160	ARG
1	H	171	SER
1	H	193	MET
1	H	205	SER
1	H	212	ARG
1	H	220	ARG
1	H	221	GLN

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Mol	Chain	Res	Type
1	H	253	THR
1	I	1	MET
1	I	15	ARG
1	I	68	THR
1	I	71	LEU
1	I	74	LYS
1	I	90	GLU
1	I	99	VAL
1	I	100	GLN
1	I	102	ARG
1	I	154	LEU
1	I	171	SER
1	I	191	ARG
1	I	193	MET
1	I	199	ARG
1	I	200	ARG
1	I	212	ARG
1	I	213	ARG
1	I	220	ARG
1	I	257	THR
1	J	1	MET
1	J	3	LEU
1	J	15	ARG
1	J	21	GLN
1	J	39	VAL
1	J	67	ASP
1	J	68	THR
1	J	72	LYS
1	J	74	LYS
1	J	100	GLN
1	J	102	ARG
1	J	112	LEU
1	J	145	ASP
1	J	189	GLU
1	J	192	SER
1	J	196	GLU
1	J	204	SER
1	J	212	ARG
1	J	221	GLN
1	J	235	SER
1	K	1	MET
1	K	7	ARG

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Mol	Chain	Res	Type
1	K	15	ARG
1	K	25	TRP
1	K	51	LYS
1	K	67	ASP
1	K	71	LEU
1	K	99	VAL
1	K	102	ARG
1	K	114	MET
1	K	169	MET
1	K	193	MET
1	K	204	SER
1	K	212	ARG
1	K	221	GLN
1	K	246	ARG
1	K	258	ARG
1	L	1	MET
1	L	11	ASP
1	L	13	SER
1	L	15	ARG
1	L	19	ASP
1	L	25	TRP
1	L	68	THR
1	L	70	ASP
1	L	74	LYS
1	L	99	VAL
1	L	100	GLN
1	L	102	ARG
1	L	114	MET
1	L	143	VAL
1	L	153	THR
1	L	191	ARG
1	L	193	MET
1	L	196	GLU
1	L	212	ARG
1	L	220	ARG
1	L	221	GLN
1	L	227	GLU
1	L	235	SER
1	M	1	MET
1	M	15	ARG
1	M	42	PRO
1	M	63	SER

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Mol	Chain	Res	Type
1	M	68	THR
1	M	71	LEU
1	M	79	ARG
1	M	102	ARG
1	M	106	THR
1	M	145	ASP
1	M	192	SER
1	M	193	MET
1	M	200	ARG
1	M	212	ARG
1	M	216	LYS
1	M	221	GLN
1	M	257	THR
1	N	1	MET
1	N	3	LEU
1	N	11	ASP
1	N	13	SER
1	N	15	ARG
1	N	21	GLN
1	N	25	TRP
1	N	46	LEU
1	N	67	ASP
1	N	68	THR
1	N	70	ASP
1	N	145	ASP
1	N	157	GLN
1	N	193	MET
1	N	212	ARG
1	N	220	ARG
1	N	226	GLU
1	N	250	GLN
1	N	257	THR
1	O	1	MET
1	O	3	LEU
1	O	15	ARG
1	O	51	LYS
1	O	67	ASP
1	O	68	THR
1	O	71	LEU
1	O	72	LYS
1	O	76	GLU
1	O	100	GLN

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Mol	Chain	Res	Type
1	O	102	ARG
1	O	106	THR
1	O	109	ASP
1	O	114	MET
1	O	157	GLN
1	O	193	MET
1	O	212	ARG
1	O	216	LYS
1	O	220	ARG
1	O	221	GLN
1	O	256	ILE
1	O	257	THR
1	P	1	MET
1	P	5	ASP
1	P	15	ARG
1	P	67	ASP
1	P	68	THR
1	P	71	LEU
1	P	72	LYS
1	P	76	GLU
1	P	84	ASP
1	P	99	VAL
1	P	102	ARG
1	P	112	LEU
1	P	153	THR
1	P	212	ARG
1	P	216	LYS
1	P	220	ARG
1	P	235	SER
1	P	257	THR
1	Q	1	MET
1	Q	3	LEU
1	Q	15	ARG
1	Q	63	SER
1	Q	67	ASP
1	Q	68	THR
1	Q	71	LEU
1	Q	72	LYS
1	Q	74	LYS
1	Q	106	THR
1	Q	114	MET
1	Q	199	ARG

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Mol	Chain	Res	Type
1	Q	212	ARG
1	Q	220	ARG
1	Q	226	GLU
1	Q	257	THR
1	Q	258	ARG
1	R	1	MET
1	R	11	ASP
1	R	13	SER
1	R	15	ARG
1	R	21	GLN
1	R	25	TRP
1	R	68	THR
1	R	71	LEU
1	R	74	LYS
1	R	100	GLN
1	R	127	ASN
1	R	131	LEU
1	R	176	ASP
1	R	192	SER
1	R	193	MET
1	R	205	SER
1	R	212	ARG
1	R	221	GLN
1	S	68	THR
1	S	71	LEU
1	S	72	LYS
1	S	100	GLN
1	S	106	THR
1	S	149	LEU
1	S	175	LYS
1	S	192	SER
1	S	193	MET
1	S	212	ARG
1	S	220	ARG
1	S	221	GLN
1	S	246	ARG
1	T	1	MET
1	T	15	ARG
1	T	47	LYS
1	T	66	GLU
1	T	67	ASP
1	T	68	THR

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Mol	Chain	Res	Type
1	T	71	LEU
1	T	76	GLU
1	T	100	GLN
1	T	102	ARG
1	T	106	THR
1	T	112	LEU
1	T	114	MET
1	T	123	SER
1	T	153	THR
1	T	157	GLN
1	T	176	ASP
1	T	193	MET
1	T	212	ARG
1	T	213	ARG
1	T	216	LYS
1	T	254	ARG
1	T	256	ILE
1	T	257	THR
1	T	258	ARG
1	U	1	MET
1	U	3	LEU
1	U	15	ARG
1	U	19	ASP
1	U	21	GLN
1	U	25	TRP
1	U	26	SER
1	U	47	LYS
1	U	63	SER
1	U	67	ASP
1	U	68	THR
1	U	71	LEU
1	U	79	ARG
1	U	96	ARG
1	U	99	VAL
1	U	102	ARG
1	U	106	THR
1	U	196	GLU
1	U	199	ARG
1	U	212	ARG
1	U	221	GLN
1	U	225	VAL
1	U	257	THR

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Mol	Chain	Res	Type
1	U	258	ARG
1	V	1	MET
1	V	4	ILE
1	V	15	ARG
1	V	67	ASP
1	V	68	THR
1	V	74	LYS
1	V	99	VAL
1	V	100	GLN
1	V	102	ARG
1	V	114	MET
1	V	167	SER
1	V	192	SER
1	V	193	MET
1	V	205	SER
1	V	212	ARG
1	V	220	ARG
1	V	226	GLU
1	V	253	THR
1	V	258	ARG
1	W	1	MET
1	W	3	LEU
1	W	15	ARG
1	W	19	ASP
1	W	54	LYS
1	W	67	ASP
1	W	68	THR
1	W	69	PRO
1	W	70	ASP
1	W	71	LEU
1	W	100	GLN
1	W	114	MET
1	W	204	SER
1	W	205	SER
1	W	212	ARG
1	W	216	LYS
1	W	220	ARG
1	W	221	GLN
1	W	250	GLN
1	W	253	THR
1	W	257	THR
1	X	1	MET

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Mol	Chain	Res	Type
1	X	3	LEU
1	X	7	ARG
1	X	11	ASP
1	X	15	ARG
1	X	36	GLU
1	X	68	THR
1	X	71	LEU
1	X	76	GLU
1	X	99	VAL
1	X	100	GLN
1	X	106	THR
1	X	160	ARG
1	X	176	ASP
1	X	192	SER
1	X	193	MET
1	X	199	ARG
1	X	204	SER
1	X	212	ARG
1	X	220	ARG
1	X	254	ARG
1	Y	1	MET
1	Y	3	LEU
1	Y	9	ILE
1	Y	13	SER
1	Y	15	ARG
1	Y	25	TRP
1	Y	67	ASP
1	Y	68	THR
1	Y	72	LYS
1	Y	100	GLN
1	Y	140	HIS
1	Y	175	LYS
1	Y	205	SER
1	Y	212	ARG
1	Y	221	GLN
1	Z	15	ARG
1	Z	21	GLN
1	Z	25	TRP
1	Z	70	ASP
1	Z	74	LYS
1	Z	90	GLU
1	Z	100	GLN

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Mol	Chain	Res	Type
1	Z	106	THR
1	Z	109	ASP
1	Z	114	MET
1	Z	193	MET
1	Z	199	ARG
1	Z	205	SER
1	Z	212	ARG
1	Z	221	GLN
1	Z	234	GLU
1	Z	250	GLN
1	Z	253	THR
1	Z	258	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (93) such sidechains are listed below:

Mol	Chain	Res	Type
1	1	100	GLN
1	1	157	GLN
1	1	164	HIS
1	2	95	HIS
1	2	100	GLN
1	2	157	GLN
1	2	221	GLN
1	2	223	HIS
1	2	250	GLN
1	3	100	GLN
1	3	142	HIS
1	3	164	HIS
1	3	186	ASN
1	4	100	GLN
1	4	164	HIS
1	4	194	ASN
1	4	223	HIS
1	A	164	HIS
1	B	100	GLN
1	B	142	HIS
1	B	164	HIS
1	C	85	HIS
1	C	100	GLN
1	C	142	HIS
1	D	100	GLN
1	D	164	HIS

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Mol	Chain	Res	Type
1	E	100	GLN
1	E	164	HIS
1	F	100	GLN
1	F	157	GLN
1	F	164	HIS
1	F	221	GLN
1	F	223	HIS
1	F	250	GLN
1	G	100	GLN
1	G	164	HIS
1	H	21	GLN
1	H	60	GLN
1	H	100	GLN
1	H	164	HIS
1	I	100	GLN
1	I	164	HIS
1	J	100	GLN
1	J	164	HIS
1	K	55	HIS
1	K	100	GLN
1	K	118	HIS
1	K	164	HIS
1	L	95	HIS
1	L	100	GLN
1	L	164	HIS
1	M	100	GLN
1	M	164	HIS
1	N	157	GLN
1	N	164	HIS
1	O	100	GLN
1	O	157	GLN
1	O	164	HIS
1	O	250	GLN
1	P	100	GLN
1	P	118	HIS
1	P	164	HIS
1	Q	100	GLN
1	Q	142	HIS
1	Q	157	GLN
1	Q	164	HIS
1	R	100	GLN
1	R	156	HIS

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Mol	Chain	Res	Type
1	R	223	HIS
1	S	21	GLN
1	S	100	GLN
1	S	164	HIS
1	T	100	GLN
1	T	118	HIS
1	T	157	GLN
1	T	164	HIS
1	U	100	GLN
1	V	100	GLN
1	V	142	HIS
1	V	164	HIS
1	V	221	GLN
1	V	223	HIS
1	V	250	GLN
1	W	100	GLN
1	W	156	HIS
1	W	164	HIS
1	X	100	GLN
1	X	164	HIS
1	Y	100	GLN
1	Y	164	HIS
1	Z	55	HIS
1	Z	100	GLN
1	Z	164	HIS

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

61 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	SO4	C	302	-	4,4,4	0.22	0	6,6,6	0.18	0
3	SO4	J	302	-	4,4,4	0.28	0	6,6,6	0.24	0
2	VFN	J	301	-	26,30,30	1.01	1 (3%)	28,40,40	0.90	0
2	VFN	2	301	-	26,30,30	0.93	1 (3%)	28,40,40	0.86	1 (3%)
2	VFN	P	302	-	26,30,30	0.87	1 (3%)	28,40,40	1.03	1 (3%)
2	VFN	T	301	-	26,30,30	0.96	1 (3%)	28,40,40	1.06	1 (3%)
2	VFN	H	302	-	26,30,30	0.97	2 (7%)	28,40,40	1.14	2 (7%)
3	SO4	K	302	-	4,4,4	0.16	0	6,6,6	0.08	0
3	SO4	M	301	-	4,4,4	0.14	0	6,6,6	0.15	0
3	SO4	S	303	-	4,4,4	0.20	0	6,6,6	0.22	0
3	SO4	G	302	-	4,4,4	0.22	0	6,6,6	0.17	0
2	VFN	B	301	-	26,30,30	0.89	0	28,40,40	0.83	0
3	SO4	V	302	-	4,4,4	0.11	0	6,6,6	0.22	0
2	VFN	V	301	-	26,30,30	0.98	1 (3%)	28,40,40	1.05	1 (3%)
3	SO4	U	301	-	4,4,4	0.12	0	6,6,6	0.29	0
2	VFN	1	301	-	26,30,30	0.91	1 (3%)	28,40,40	0.88	0
2	VFN	P	301	-	26,30,30	0.94	2 (7%)	28,40,40	0.86	0
3	SO4	P	303	-	4,4,4	0.25	0	6,6,6	0.15	0
3	SO4	O	303	-	4,4,4	0.19	0	6,6,6	0.09	0
2	VFN	W	302	-	26,30,30	0.88	1 (3%)	28,40,40	1.25	4 (14%)
3	SO4	Q	301	-	4,4,4	0.15	0	6,6,6	0.22	0
3	SO4	X	301	-	4,4,4	0.24	0	6,6,6	0.13	0
2	VFN	H	301	-	26,30,30	1.00	2 (7%)	28,40,40	1.06	2 (7%)
2	VFN	F	301	-	26,30,30	0.96	2 (7%)	28,40,40	1.05	1 (3%)
2	VFN	O	302	-	26,30,30	0.92	1 (3%)	28,40,40	0.83	1 (3%)
3	SO4	D	303	-	4,4,4	0.28	0	6,6,6	0.26	0
3	SO4	R	302	-	4,4,4	0.21	0	6,6,6	0.29	0
3	SO4	Y	301	-	4,4,4	0.19	0	6,6,6	0.17	0
3	SO4	4	301	-	4,4,4	0.07	0	6,6,6	0.22	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	SO4	L	302	-	4,4,4	0.09	0	6,6,6	0.19	0
3	SO4	N	302	-	4,4,4	0.20	0	6,6,6	0.24	0
3	SO4	T	302	-	4,4,4	0.15	0	6,6,6	0.24	0
2	VFN	K	301	-	26,30,30	0.98	2 (7%)	28,40,40	0.95	1 (3%)
3	SO4	3	303	-	4,4,4	0.16	0	6,6,6	0.14	0
2	VFN	N	301	-	26,30,30	0.85	1 (3%)	28,40,40	0.85	1 (3%)
2	VFN	A	301	-	26,30,30	0.92	2 (7%)	28,40,40	0.90	1 (3%)
2	VFN	G	301	-	26,30,30	0.98	0	28,40,40	0.82	0
2	VFN	W	301	-	26,30,30	1.00	1 (3%)	28,40,40	1.18	3 (10%)
2	VFN	L	301	-	26,30,30	0.90	2 (7%)	28,40,40	0.90	1 (3%)
3	SO4	B	302	-	4,4,4	0.23	0	6,6,6	0.22	0
2	VFN	D	301	-	26,30,30	0.96	2 (7%)	28,40,40	0.88	0
2	VFN	S	302	-	26,30,30	1.00	2 (7%)	28,40,40	0.95	1 (3%)
3	SO4	2	302	-	4,4,4	0.25	0	6,6,6	0.29	0
3	SO4	F	302	-	4,4,4	0.25	0	6,6,6	0.15	0
2	VFN	O	301	-	26,30,30	0.87	1 (3%)	28,40,40	0.94	1 (3%)
3	SO4	I	301	-	4,4,4	0.20	0	6,6,6	0.15	0
3	SO4	C	301	-	4,4,4	0.10	0	6,6,6	0.21	0
3	SO4	W	303	-	4,4,4	0.23	0	6,6,6	0.13	0
3	SO4	E	301	-	4,4,4	0.18	0	6,6,6	0.16	0
3	SO4	A	303	-	4,4,4	0.20	0	6,6,6	0.18	0
2	VFN	Z	301	-	26,30,30	0.96	1 (3%)	28,40,40	0.91	1 (3%)
3	SO4	Z	302	-	4,4,4	0.15	0	6,6,6	0.19	0
2	VFN	1	302	-	26,30,30	1.07	2 (7%)	28,40,40	1.21	4 (14%)
2	VFN	3	302	-	26,30,30	0.99	2 (7%)	28,40,40	0.59	0
3	SO4	H	303	-	4,4,4	0.18	0	6,6,6	0.18	0
2	VFN	A	302	-	26,30,30	0.89	1 (3%)	28,40,40	0.86	1 (3%)
2	VFN	R	301	-	26,30,30	0.94	2 (7%)	28,40,40	1.07	2 (7%)
2	VFN	3	301	-	26,30,30	0.88	1 (3%)	28,40,40	0.85	1 (3%)
2	VFN	S	301	-	26,30,30	0.85	0	28,40,40	0.97	1 (3%)
3	SO4	1	303	-	4,4,4	0.16	0	6,6,6	0.13	0
2	VFN	D	302	-	26,30,30	0.81	1 (3%)	28,40,40	0.83	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	VFN	J	301	-	-	0/18/19/19	0/3/3/3
2	VFN	2	301	-	-	1/18/19/19	0/3/3/3
2	VFN	P	302	-	-	0/18/19/19	0/3/3/3
2	VFN	T	301	-	-	1/18/19/19	0/3/3/3
2	VFN	H	302	-	-	0/18/19/19	0/3/3/3
2	VFN	B	301	-	-	0/18/19/19	0/3/3/3
2	VFN	V	301	-	-	0/18/19/19	0/3/3/3
2	VFN	1	301	-	-	0/18/19/19	0/3/3/3
2	VFN	P	301	-	-	0/18/19/19	0/3/3/3
2	VFN	W	302	-	-	0/18/19/19	0/3/3/3
2	VFN	H	301	-	-	0/18/19/19	0/3/3/3
2	VFN	F	301	-	-	0/18/19/19	0/3/3/3
2	VFN	O	302	-	-	0/18/19/19	0/3/3/3
2	VFN	K	301	-	-	0/18/19/19	0/3/3/3
2	VFN	N	301	-	-	0/18/19/19	0/3/3/3
2	VFN	A	301	-	-	1/18/19/19	0/3/3/3
2	VFN	G	301	-	-	0/18/19/19	0/3/3/3
2	VFN	W	301	-	-	0/18/19/19	0/3/3/3
2	VFN	L	301	-	-	0/18/19/19	0/3/3/3
2	VFN	D	301	-	-	0/18/19/19	0/3/3/3
2	VFN	S	302	-	-	0/18/19/19	0/3/3/3
2	VFN	O	301	-	-	0/18/19/19	0/3/3/3
2	VFN	Z	301	-	-	0/18/19/19	0/3/3/3
2	VFN	1	302	-	-	0/18/19/19	0/3/3/3
2	VFN	3	302	-	-	0/18/19/19	0/3/3/3
2	VFN	A	302	-	-	0/18/19/19	0/3/3/3
2	VFN	R	301	-	-	0/18/19/19	0/3/3/3
2	VFN	3	301	-	-	0/18/19/19	0/3/3/3
2	VFN	S	301	-	-	0/18/19/19	0/3/3/3
2	VFN	D	302	-	-	0/18/19/19	0/3/3/3

All (39) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	1	302	VFN	C6-C5	-3.01	1.47	1.51
2	H	302	VFN	C6-C5	-3.01	1.47	1.51
2	3	302	VFN	C6-C5	-2.90	1.47	1.51
2	J	301	VFN	C6-C5	-2.86	1.47	1.51
2	V	301	VFN	C6-C5	-2.77	1.48	1.51
2	2	301	VFN	C6-C5	-2.71	1.48	1.51
2	S	302	VFN	C6-C5	-2.64	1.48	1.51
2	Z	301	VFN	C6-C5	-2.56	1.48	1.51
2	3	302	VFN	C17-N7	2.54	1.40	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	301	VFN	C6-C5	-2.53	1.48	1.51
2	O	302	VFN	C17-N7	2.50	1.40	1.35
2	S	302	VFN	C17-N7	2.49	1.40	1.35
2	T	301	VFN	C6-C5	-2.44	1.48	1.51
2	1	302	VFN	C17-N7	2.43	1.40	1.35
2	A	301	VFN	C6-C5	-2.41	1.48	1.51
2	A	302	VFN	C6-C5	-2.39	1.48	1.51
2	D	301	VFN	C6-C5	-2.39	1.48	1.51
2	3	301	VFN	C17-N7	2.37	1.40	1.35
2	K	301	VFN	C6-C5	-2.34	1.48	1.51
2	P	301	VFN	C17-N7	2.31	1.39	1.35
2	O	301	VFN	C17-N7	2.28	1.39	1.35
2	L	301	VFN	C17-N7	2.28	1.39	1.35
2	P	301	VFN	C6-C5	-2.26	1.48	1.51
2	K	301	VFN	C17-N7	2.23	1.39	1.35
2	L	301	VFN	C6-C5	-2.23	1.48	1.51
2	D	302	VFN	C17-N7	2.20	1.39	1.35
2	W	302	VFN	C17-N7	2.19	1.39	1.35
2	R	301	VFN	C6-C5	-2.18	1.48	1.51
2	H	302	VFN	C17-N7	2.15	1.39	1.35
2	W	301	VFN	C17-N7	2.11	1.39	1.35
2	D	301	VFN	C17-N7	2.10	1.39	1.35
2	F	301	VFN	C17-N7	2.09	1.39	1.35
2	F	301	VFN	C6-C5	-2.08	1.48	1.51
2	R	301	VFN	C17-N7	2.05	1.39	1.35
2	1	301	VFN	C17-N7	2.05	1.39	1.35
2	H	301	VFN	C17-N7	2.03	1.39	1.35
2	A	301	VFN	C8-C9	-2.02	1.47	1.51
2	P	302	VFN	C17-N7	2.01	1.39	1.35
2	N	301	VFN	C6-C5	-2.00	1.49	1.51

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	F	301	VFN	C19-S20-C21	3.65	108.21	102.61
2	V	301	VFN	C5-C6-N7	-3.33	108.05	113.64
2	H	301	VFN	C5-C6-N7	-3.13	108.39	113.64
2	S	302	VFN	C5-C6-N7	-3.07	108.48	113.64
2	A	301	VFN	C9-C8-N7	-2.84	108.56	113.13
2	H	302	VFN	C13-C12-C15	-2.82	115.28	119.99
2	H	302	VFN	C5-C6-N7	-2.79	108.95	113.64
2	H	301	VFN	C19-S20-C21	2.77	106.87	102.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	T	301	VFN	C5-C6-N7	-2.74	109.04	113.64
2	1	302	VFN	C5-C6-N7	-2.70	109.10	113.64
2	W	302	VFN	C19-S20-C21	2.67	106.72	102.61
2	O	301	VFN	C19-S20-C21	2.54	106.51	102.61
2	2	301	VFN	C9-C8-N7	-2.47	109.16	113.13
2	Z	301	VFN	C5-C6-N7	-2.45	109.53	113.64
2	R	301	VFN	C19-S20-C21	2.44	106.36	102.61
2	W	301	VFN	C19-S20-C21	2.41	106.31	102.61
2	1	302	VFN	C19-S20-C21	2.39	106.29	102.61
2	W	301	VFN	C8-N7-C17	-2.36	115.81	121.91
2	W	301	VFN	C21-C26-CL1	2.27	123.67	119.69
2	P	302	VFN	C9-C8-N7	-2.24	109.54	113.13
2	A	302	VFN	C8-N7-C17	-2.21	116.17	121.91
2	W	302	VFN	C14-C13-C12	-2.21	117.49	120.35
2	W	302	VFN	C8-N7-C17	-2.19	116.22	121.91
2	3	301	VFN	C8-N7-C17	-2.19	116.23	121.91
2	R	301	VFN	C8-N7-C17	-2.18	116.25	121.91
2	1	302	VFN	C14-C13-C12	-2.17	117.55	120.35
2	W	302	VFN	C9-C8-N7	-2.17	109.65	113.13
2	L	301	VFN	C5-C6-N7	-2.08	110.15	113.64
2	O	302	VFN	C9-C8-N7	-2.08	109.80	113.13
2	S	301	VFN	C13-C12-C15	-2.04	116.59	119.99
2	K	301	VFN	C5-C6-N7	-2.02	110.25	113.64
2	1	302	VFN	C23-C22-C21	2.02	123.14	119.63
2	N	301	VFN	C19-S20-C21	2.02	105.71	102.61

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	301	VFN	N4-C5-C6-N7
2	2	301	VFN	C11-C12-C15-N16
2	T	301	VFN	C11-C12-C15-N16

There are no ring outliers.

12 monomers are involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	2	301	VFN	1	0
2	P	302	VFN	2	0
2	H	302	VFN	1	0

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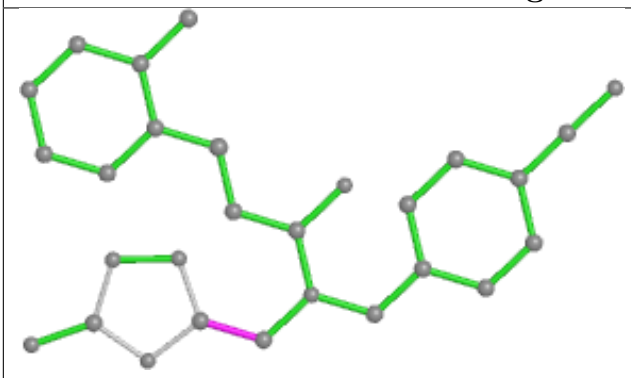
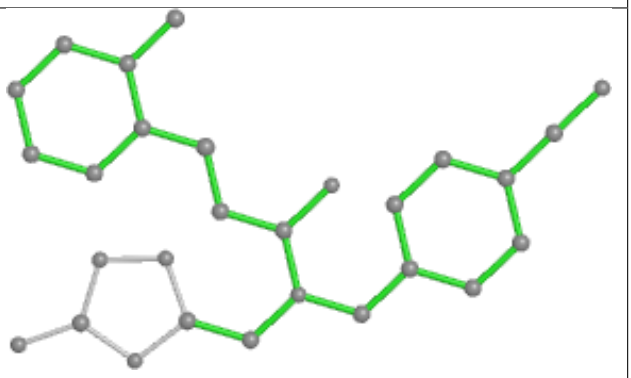
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	P	301	VFN	1	0
2	H	301	VFN	2	0
2	K	301	VFN	1	0
2	N	301	VFN	1	0
2	G	301	VFN	1	0
2	W	301	VFN	1	0
2	3	302	VFN	2	0
2	R	301	VFN	1	0
2	3	301	VFN	1	0

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

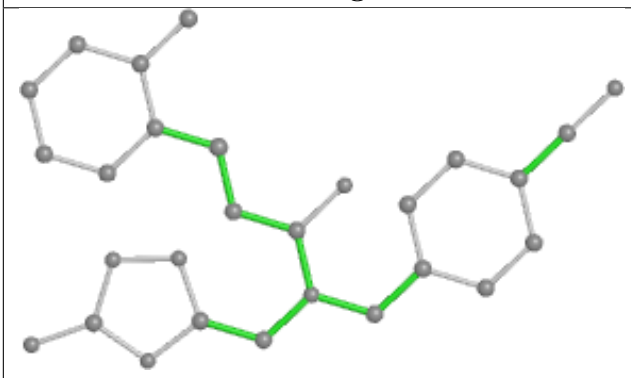
Ligand VFN J 301



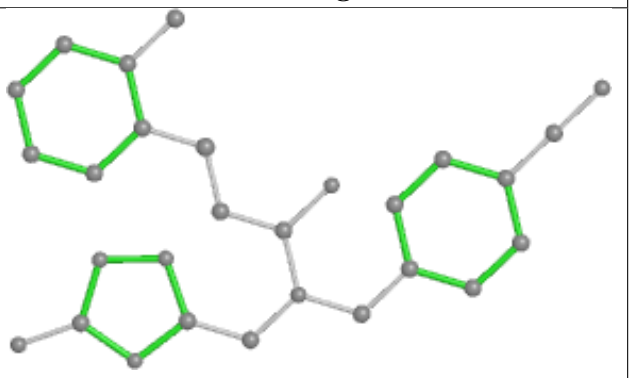
Bond lengths



Bond angles

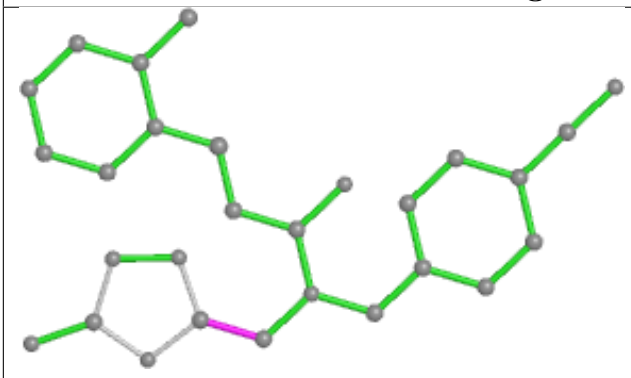


Torsions



Rings

Ligand VFN 2 301



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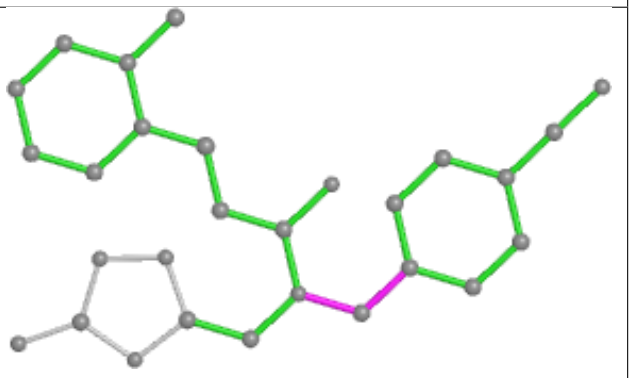

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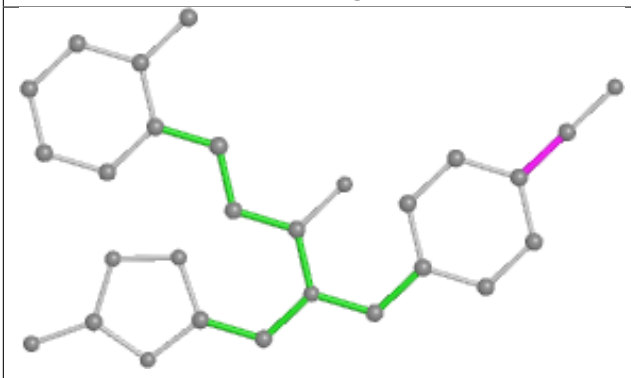

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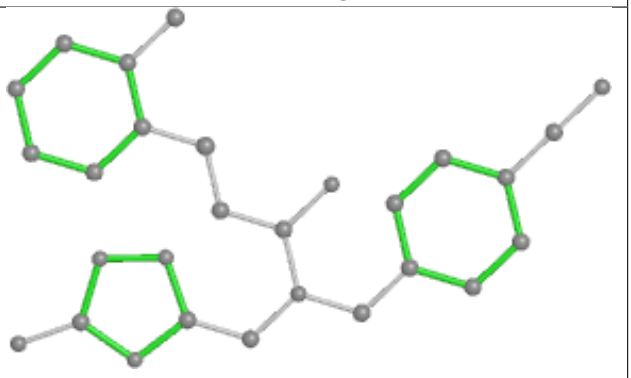

Rings

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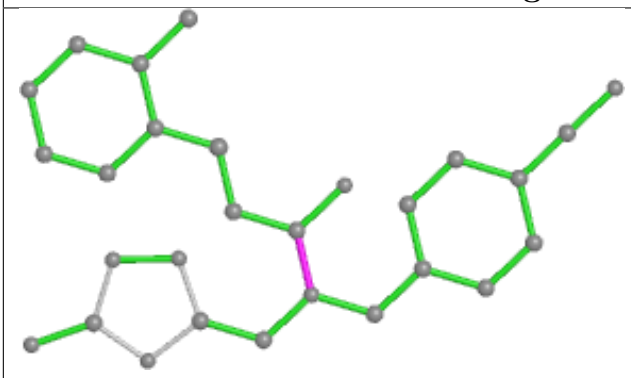

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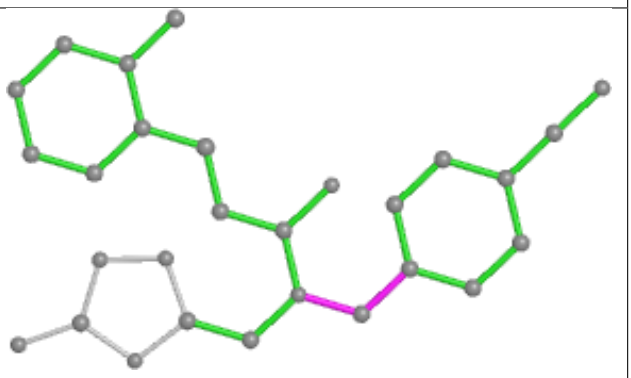

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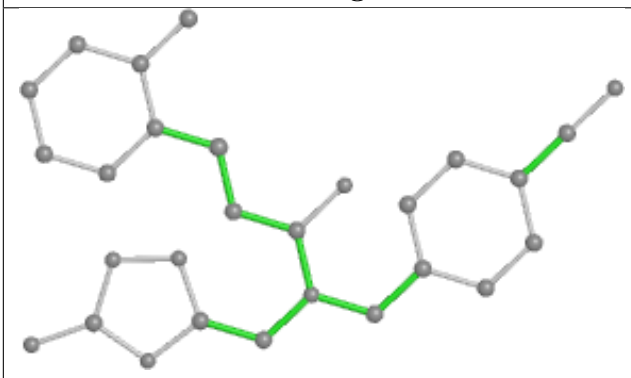

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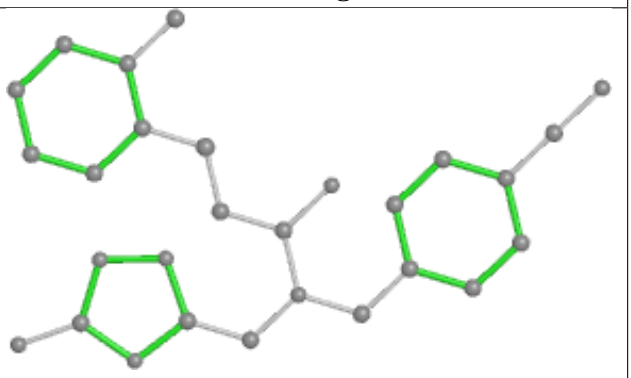
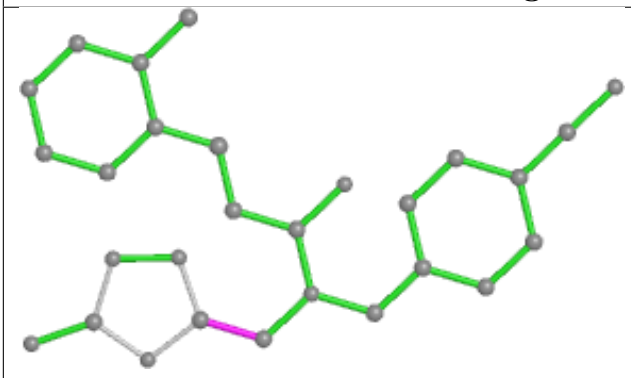


Rings

Ligand VFN T 301



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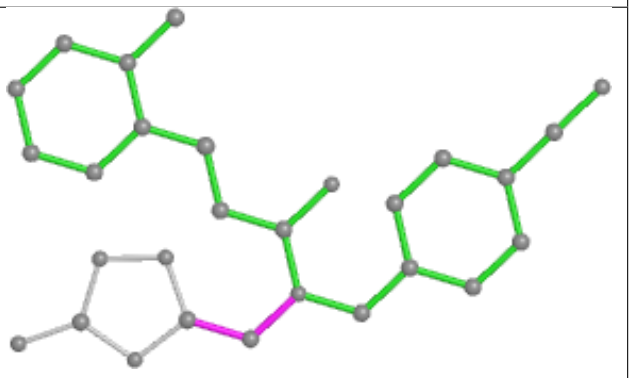
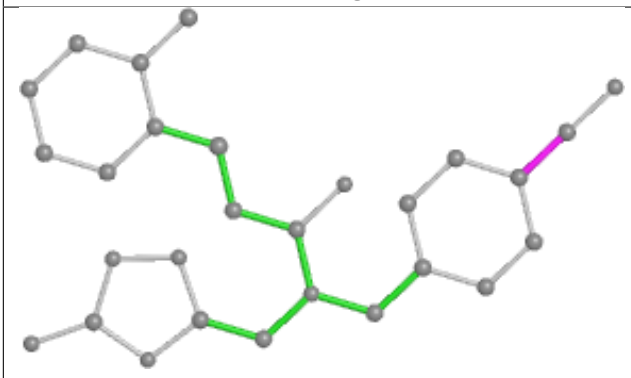


Bond angles



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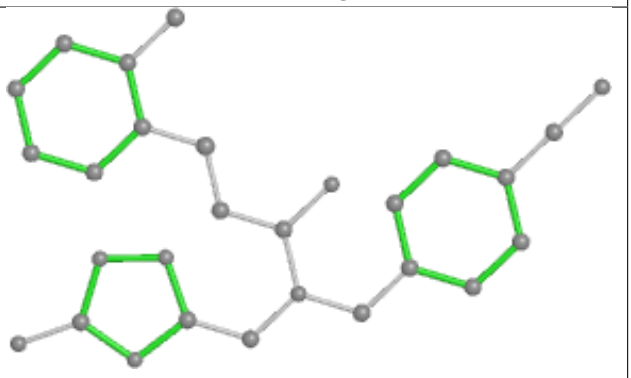

Rings

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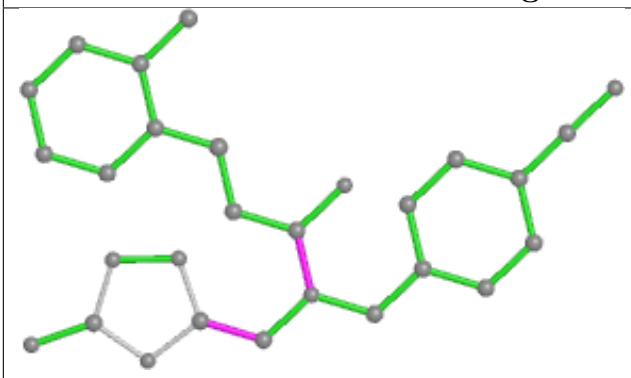

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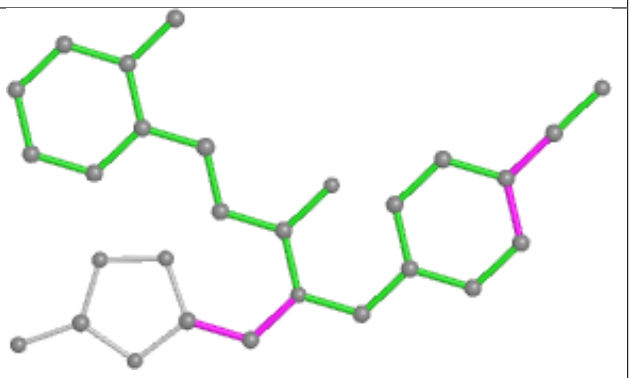
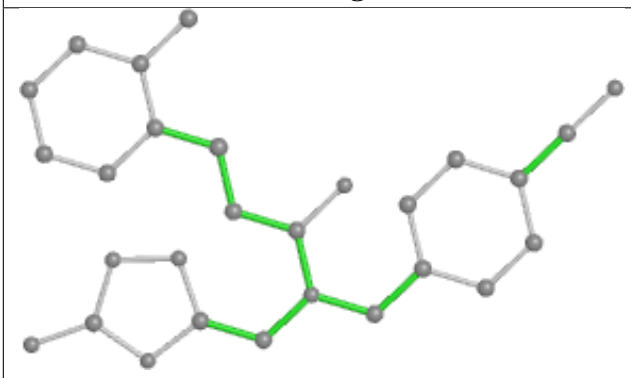


Bond angles



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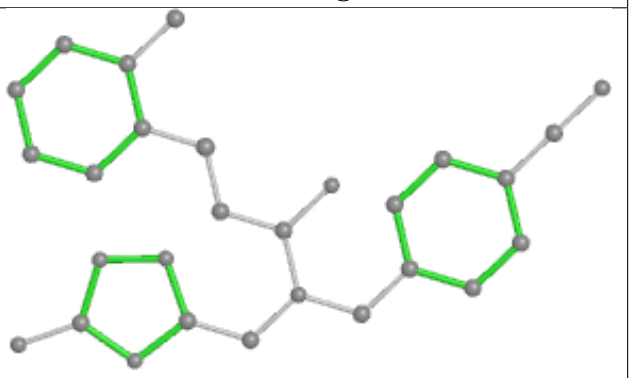
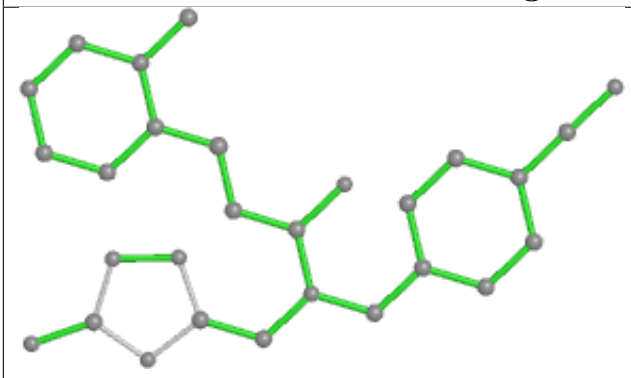


Rings

Ligand VFN B 301



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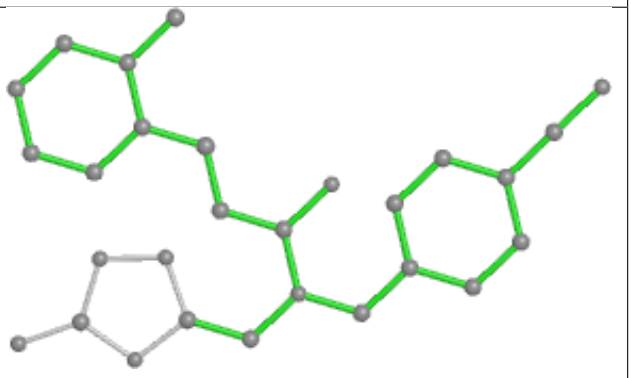

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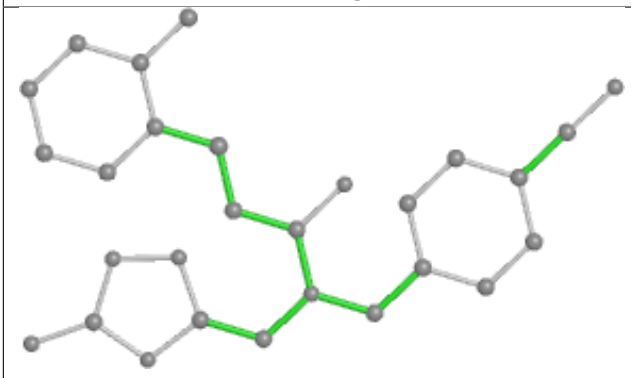

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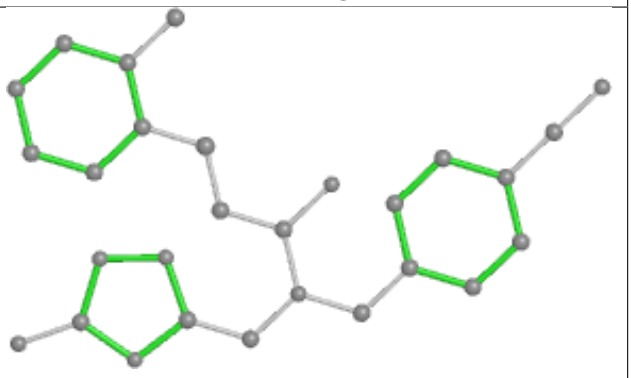

Rings

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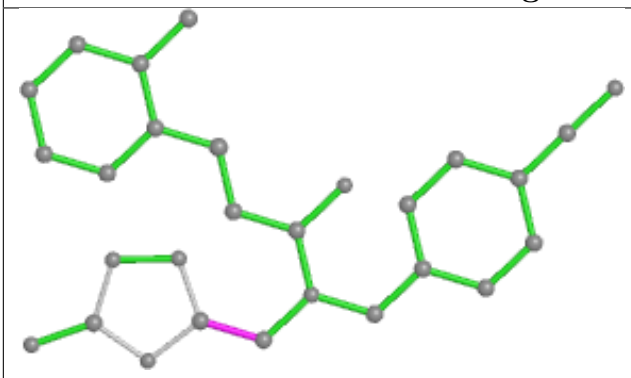

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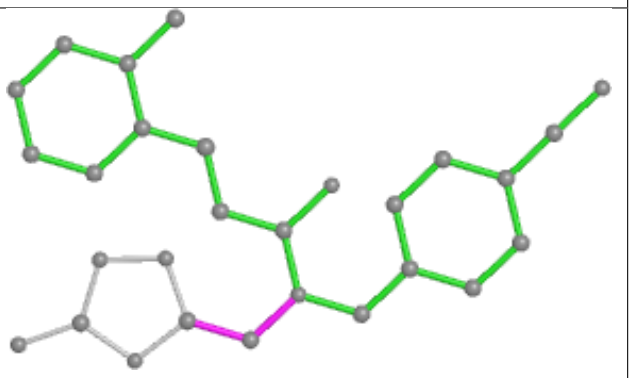

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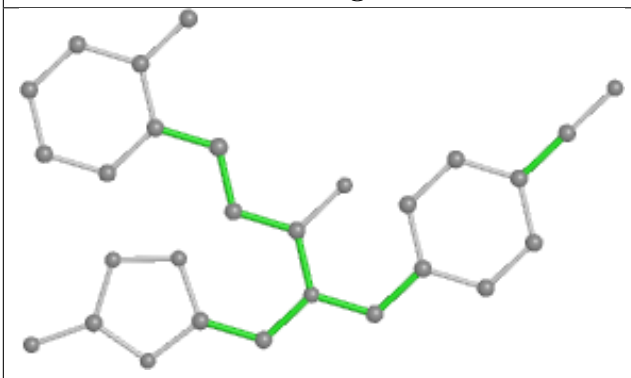

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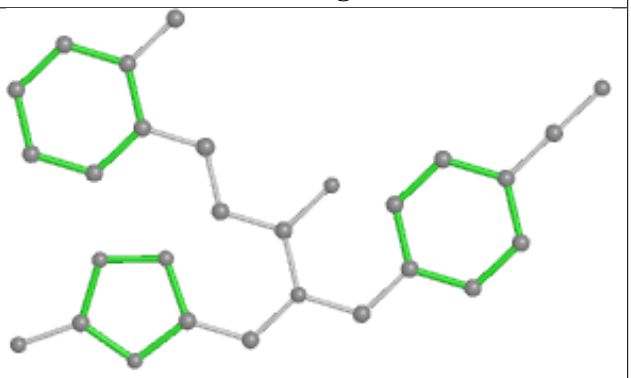
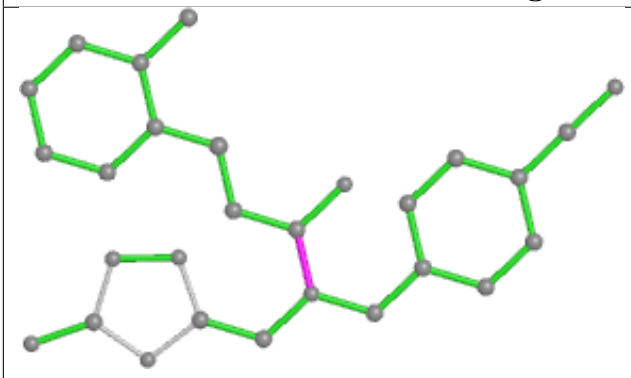


Rings

Ligand VFN 1 301



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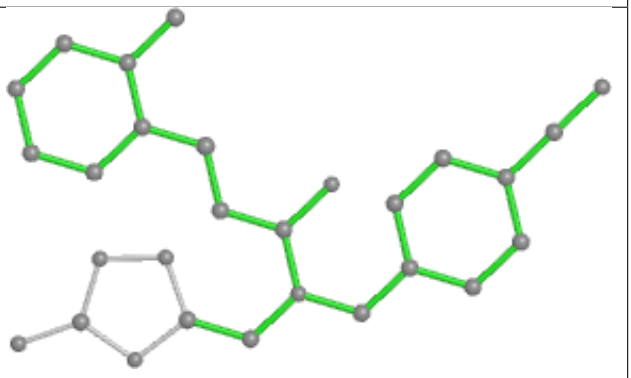

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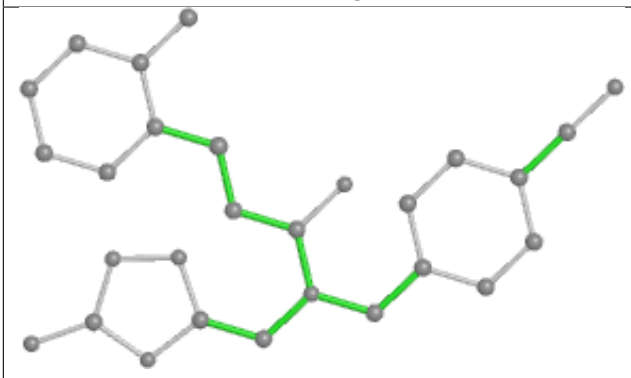

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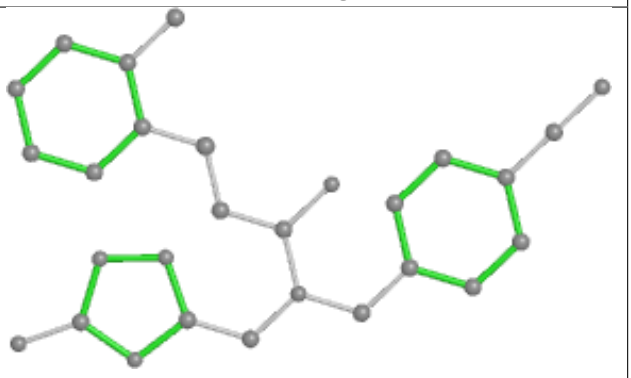
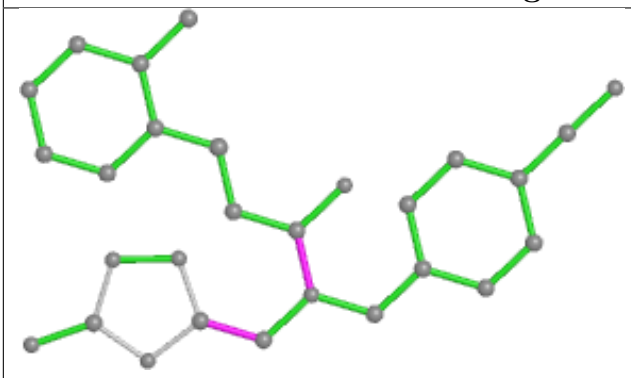


Rings

Ligand VFN P 301



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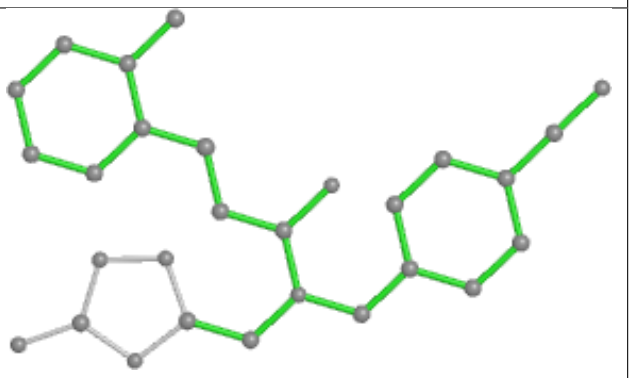

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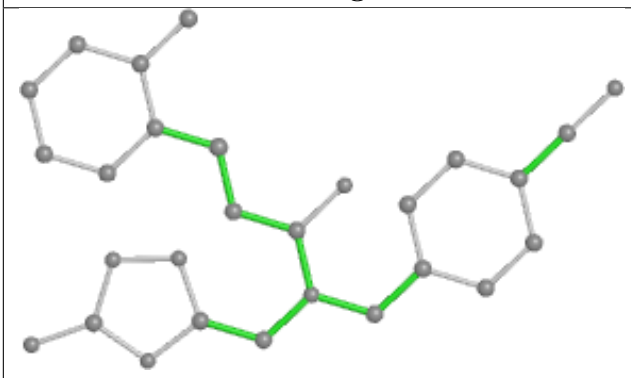

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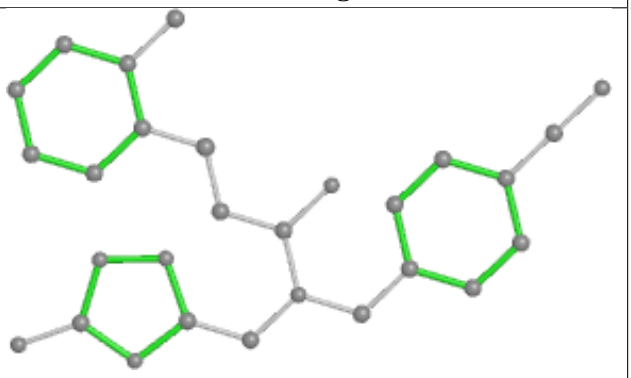
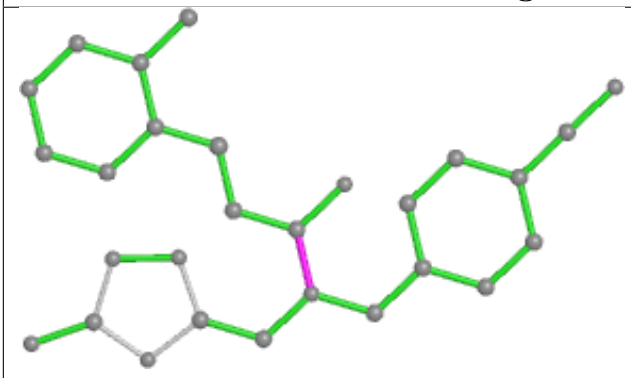


Rings

Ligand VFN W 302



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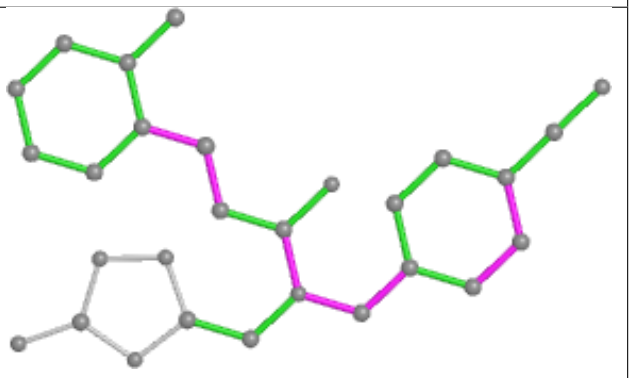

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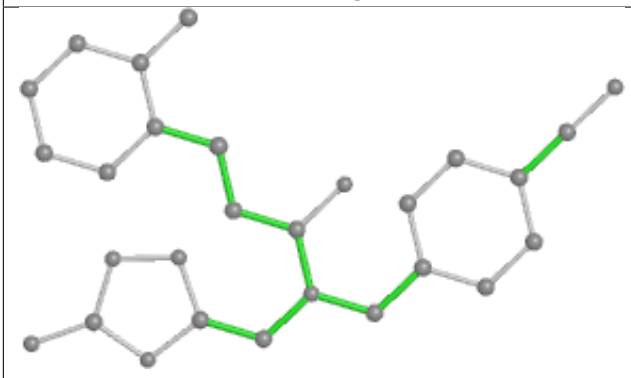

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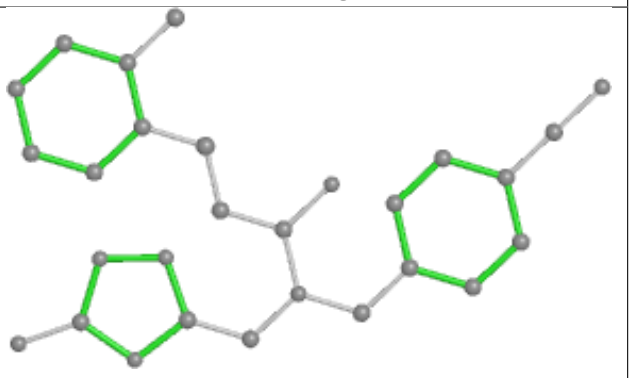
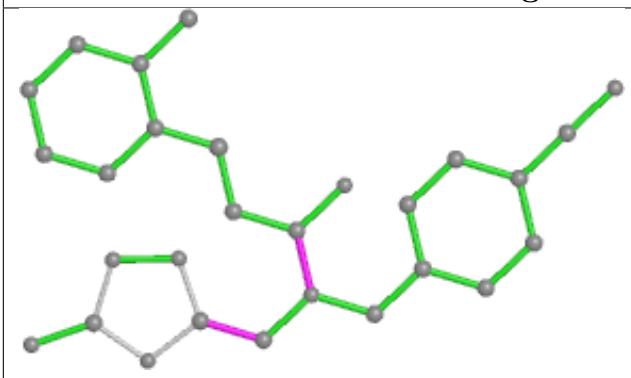


Rings

Ligand VFN H 301



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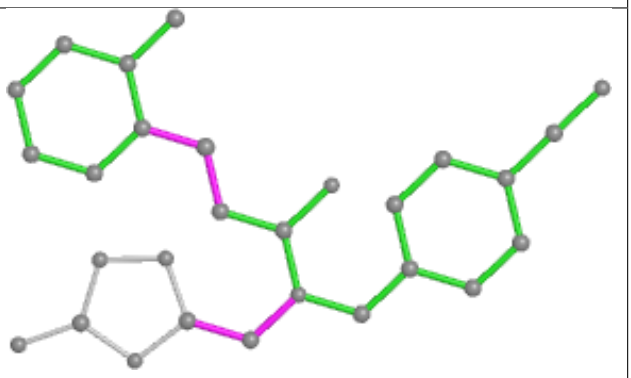

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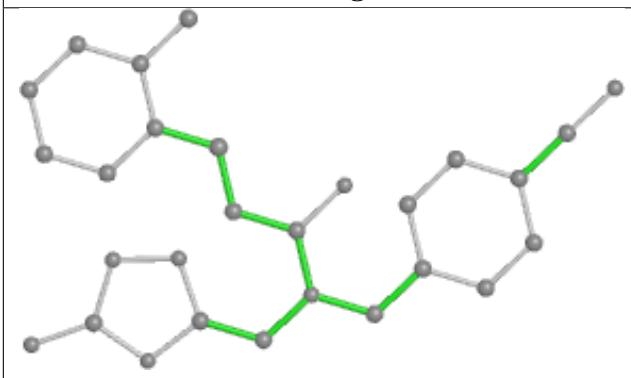

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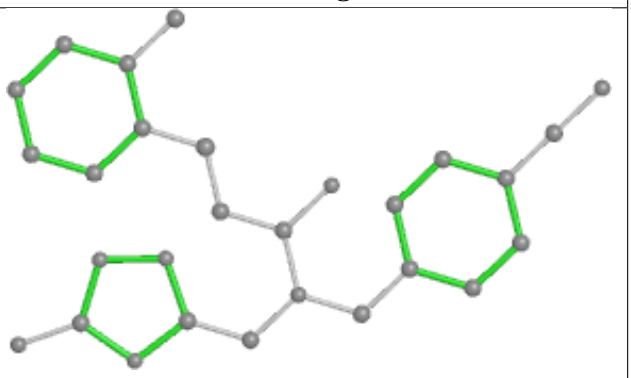
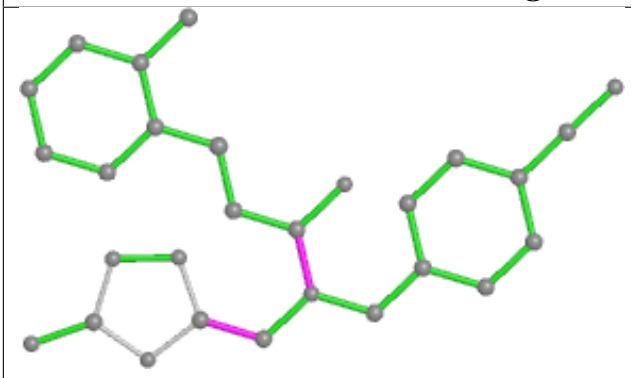


Rings

Ligand VFN F 301



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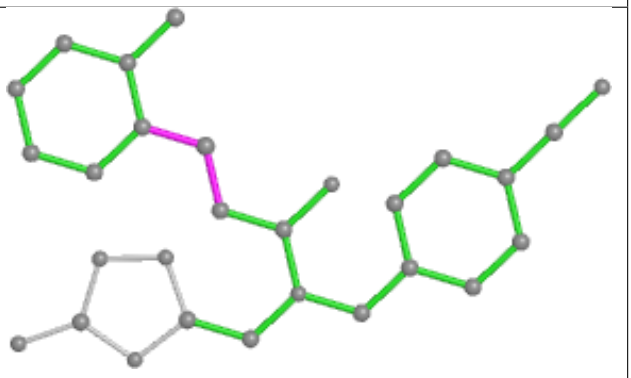

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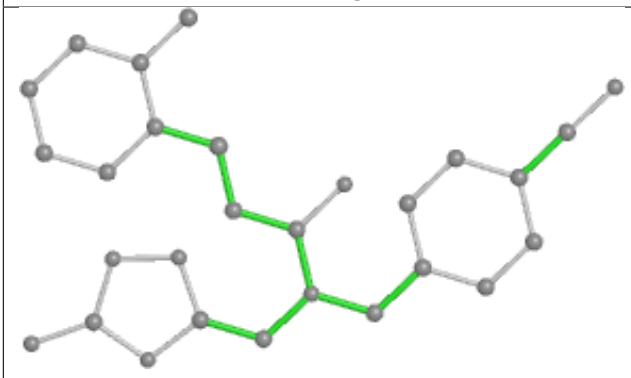

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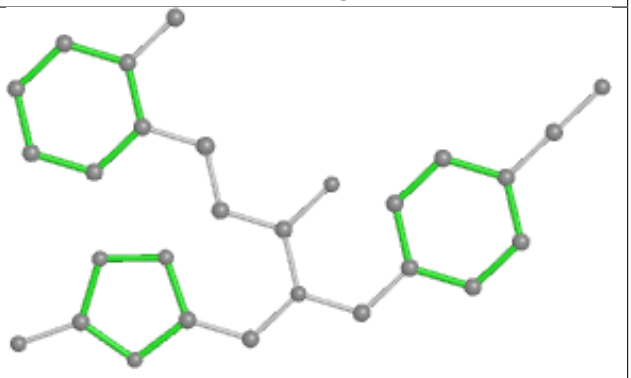
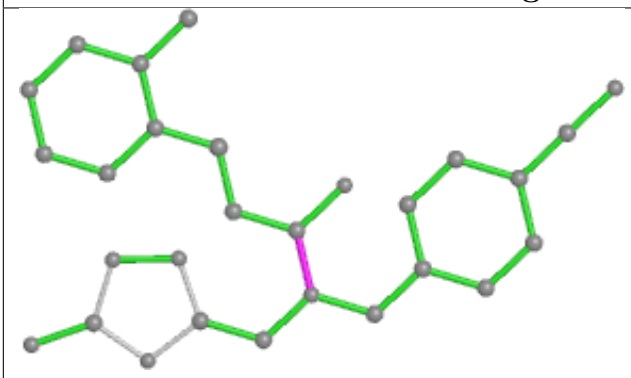


Rings

Ligand VFN O 302



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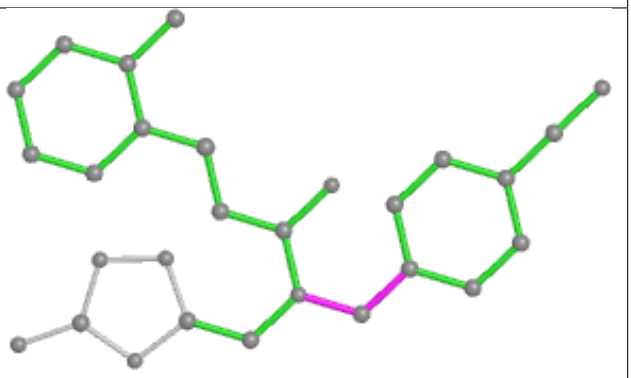
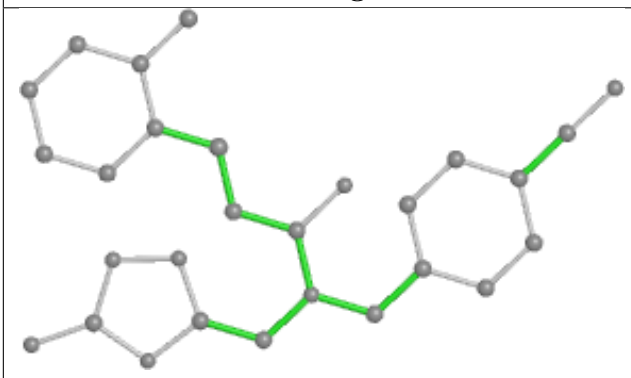
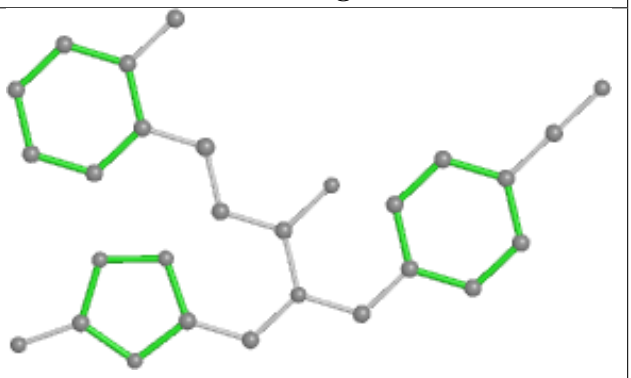


Bond angles

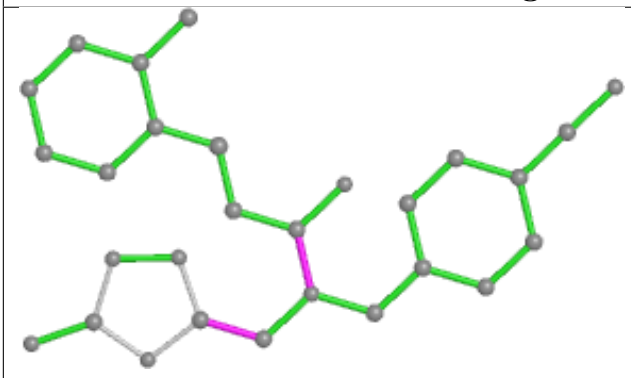


Torsions



Rings

Ligand VFN K 301



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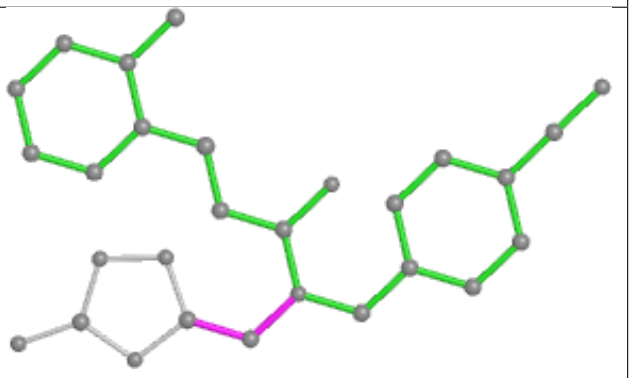
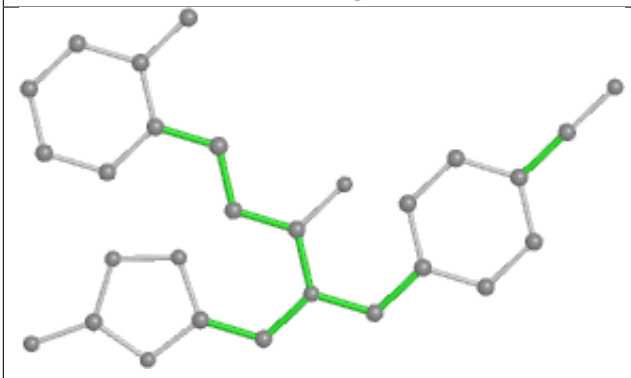


Bond angles



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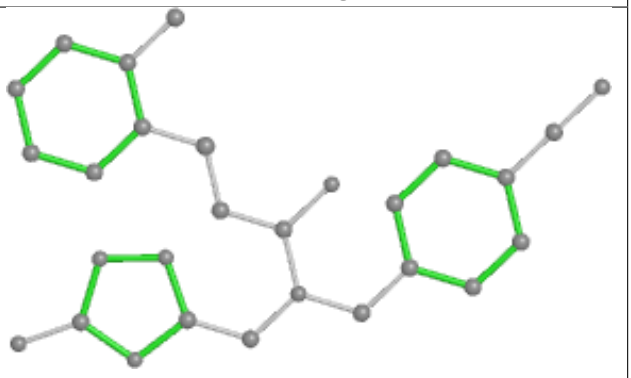

Rings

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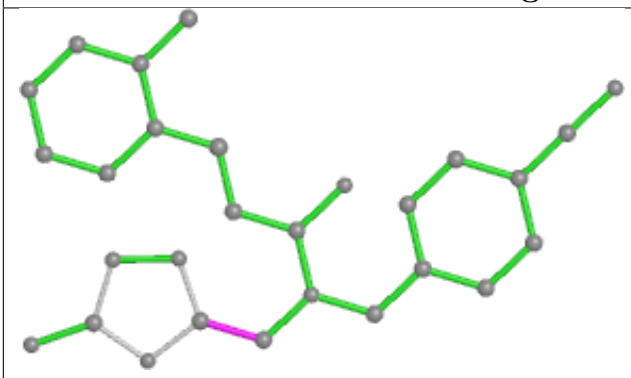

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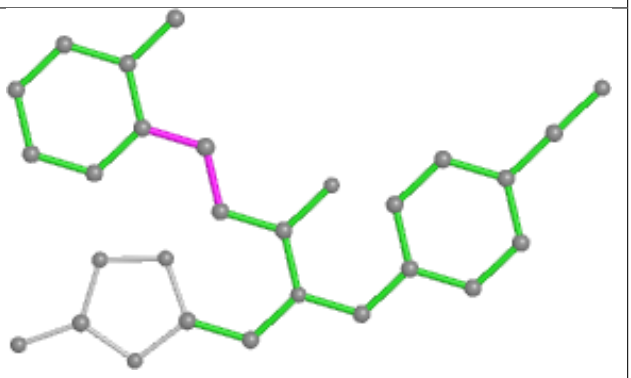
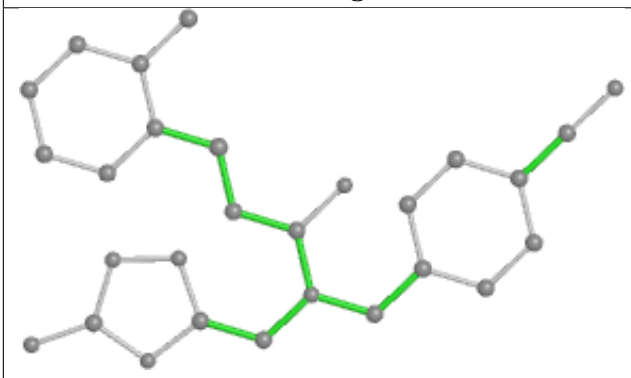


Bond angles



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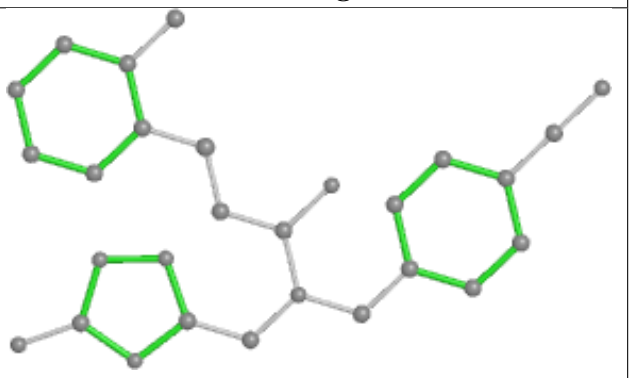
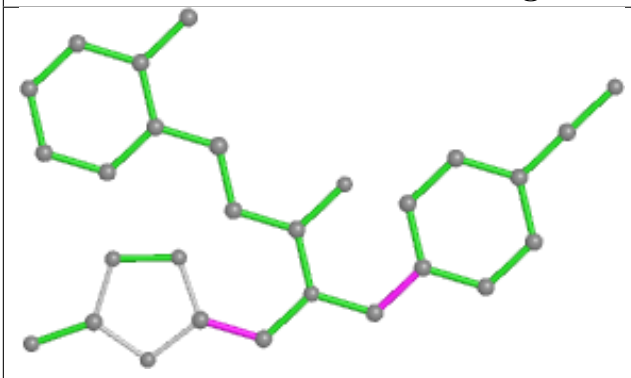


Rings

Ligand VFN A 301



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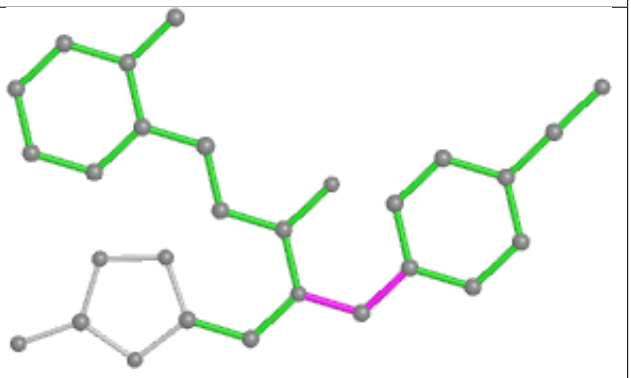

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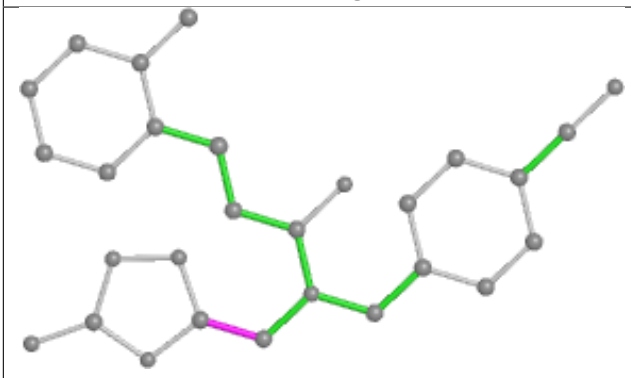
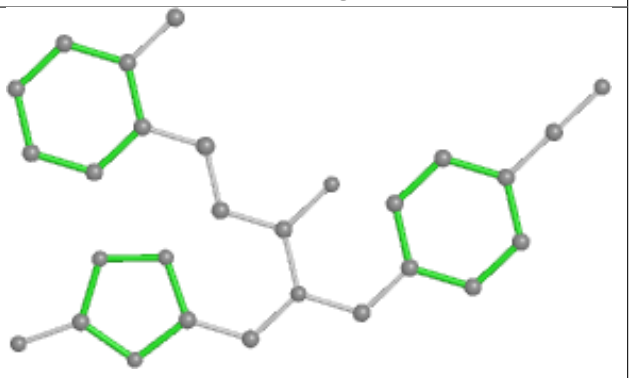
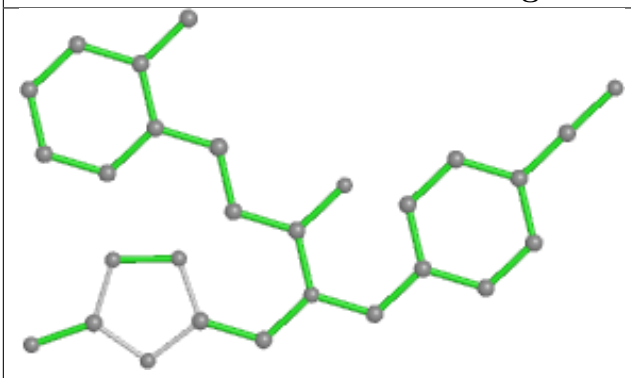


Torsions



Rings

Ligand VFN G 301



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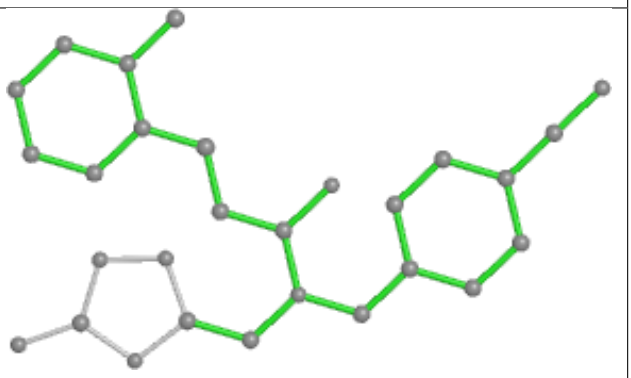

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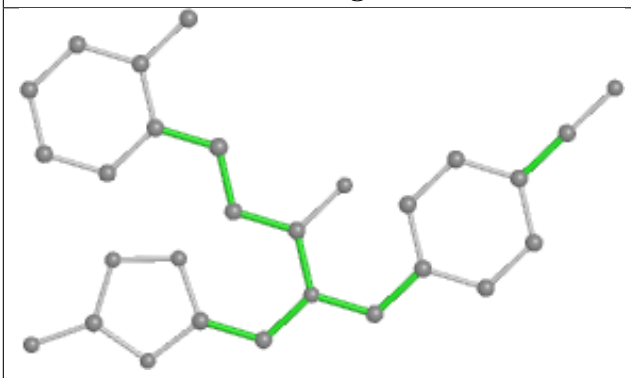

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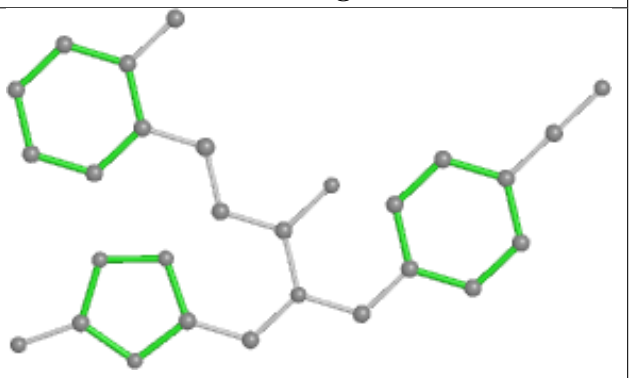
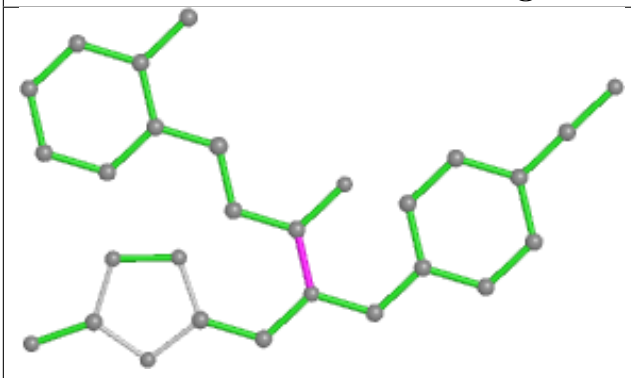


Rings

Ligand VFN W 301



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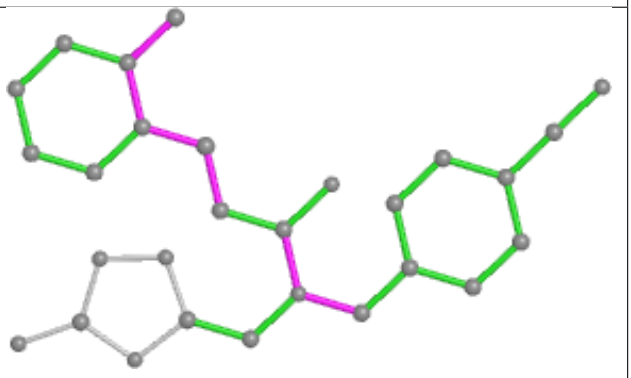

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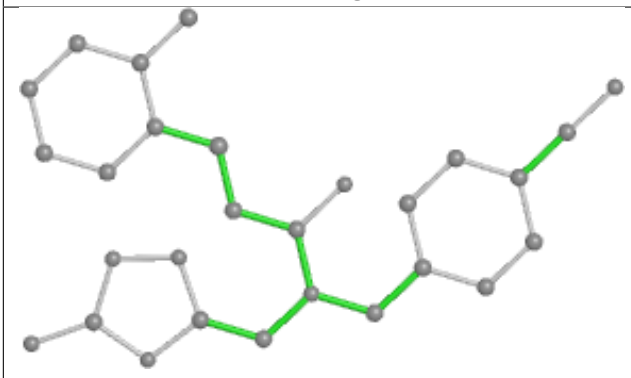

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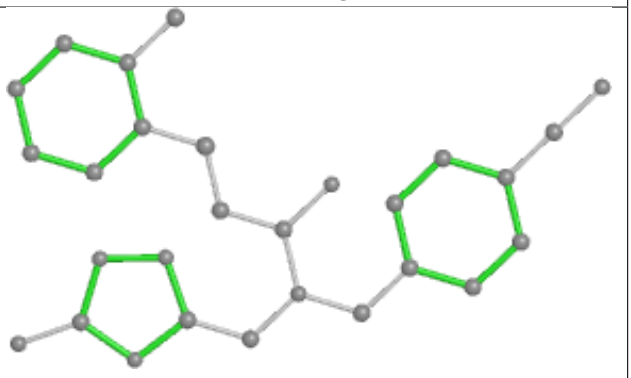
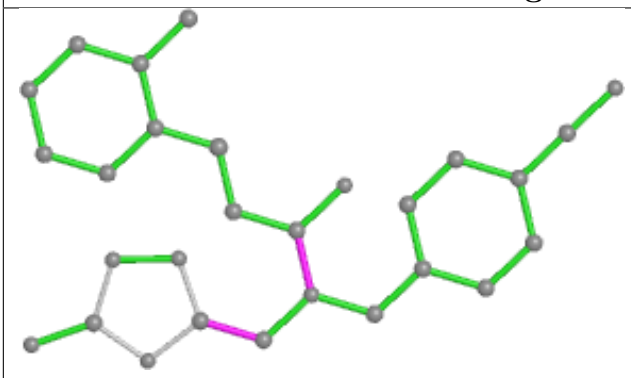


Rings

Ligand VFN L 301



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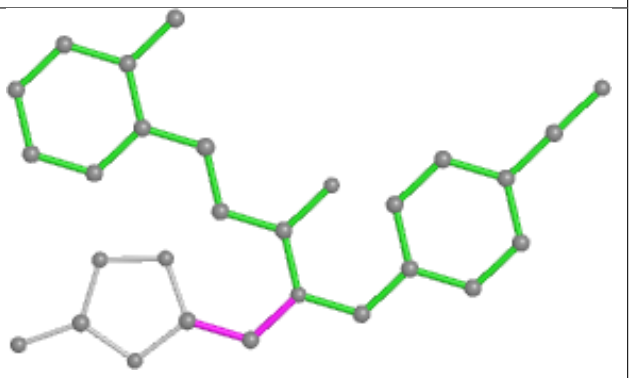

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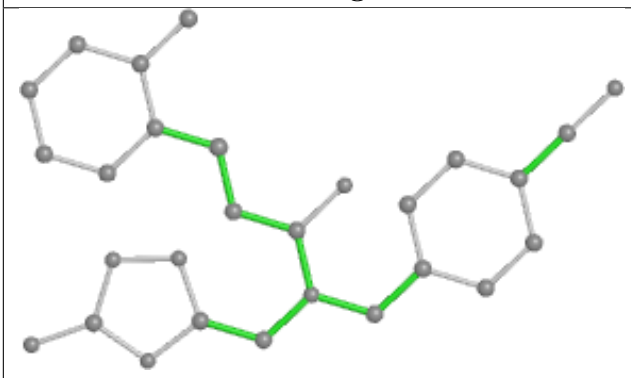

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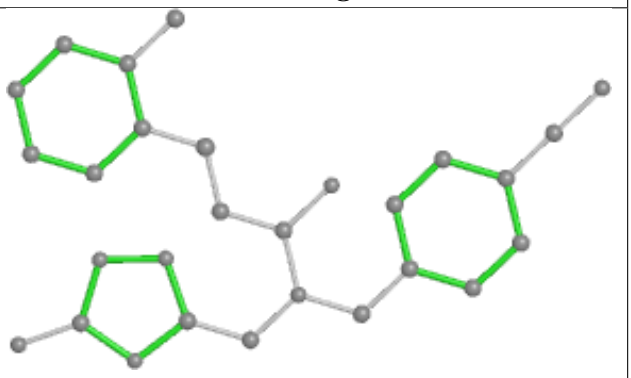

Rings

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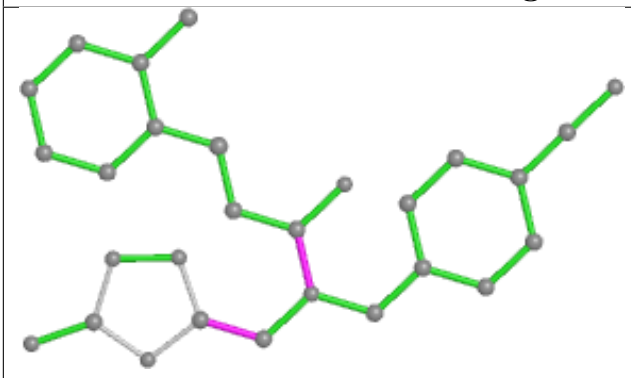

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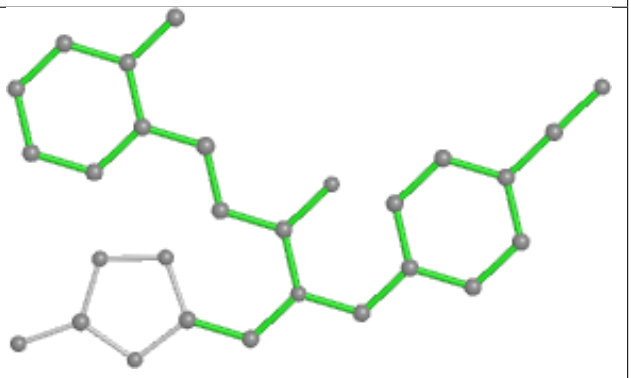

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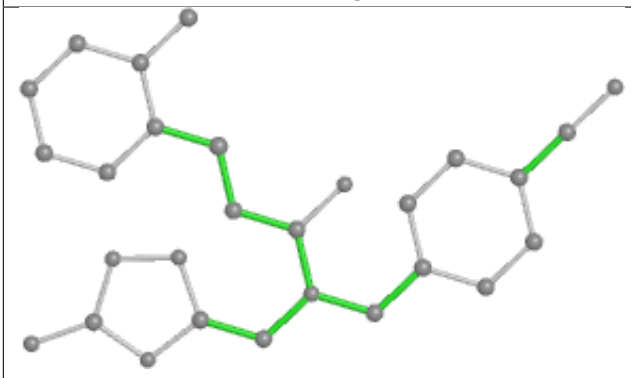

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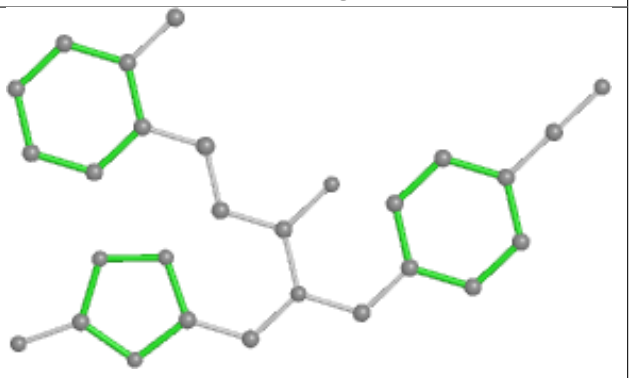

Rings

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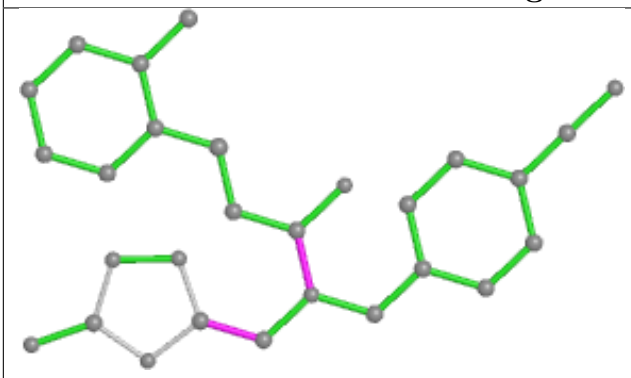

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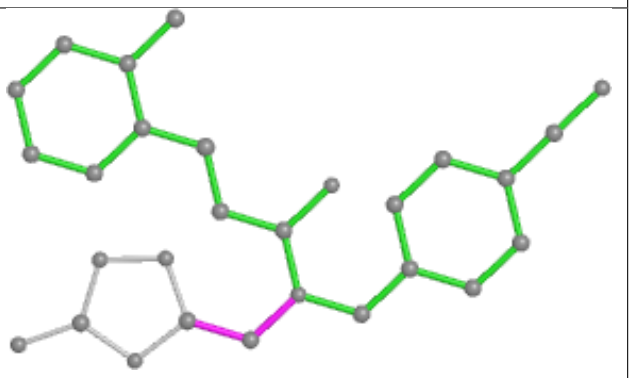

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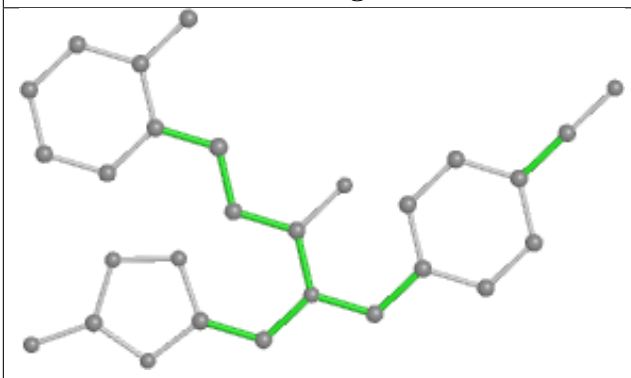

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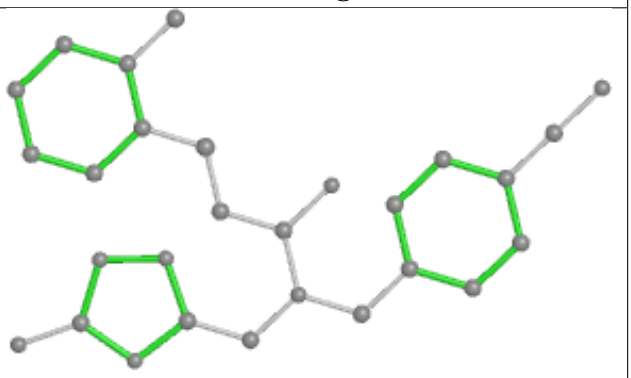

Rings

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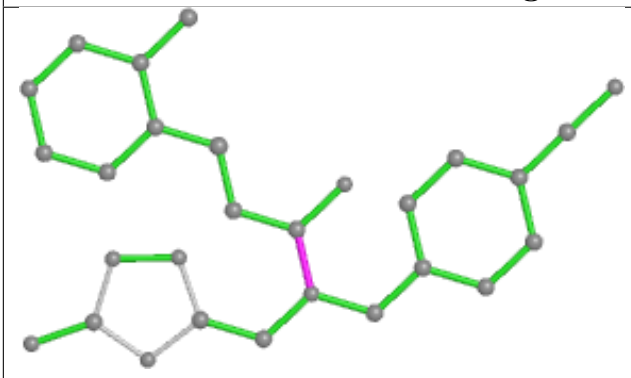

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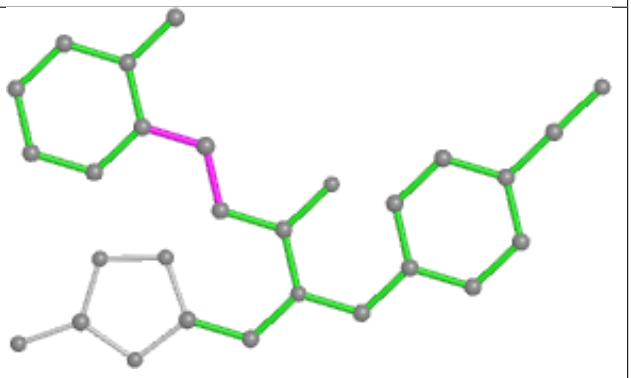

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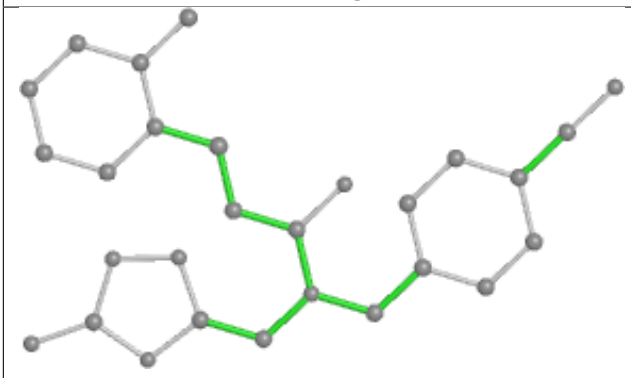

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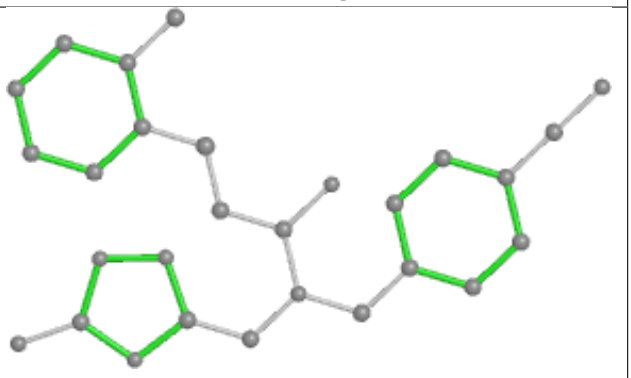

Rings

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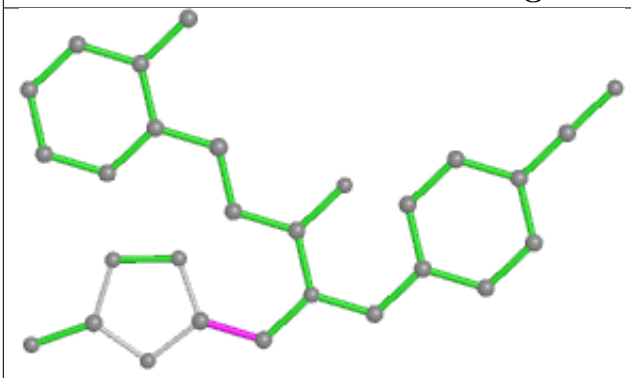

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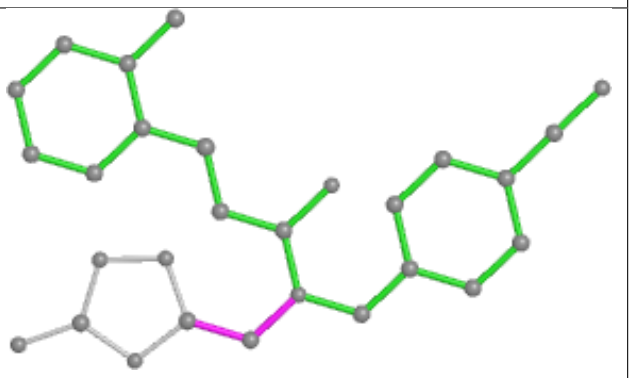

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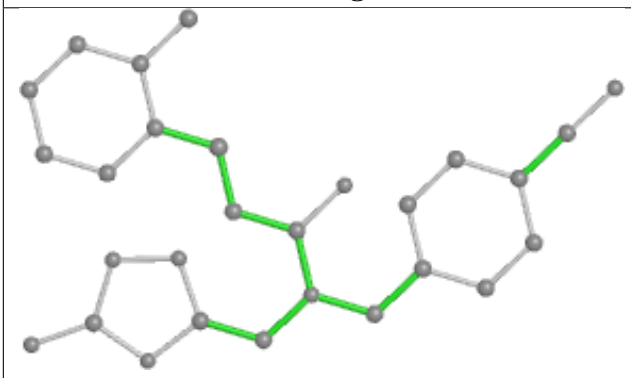

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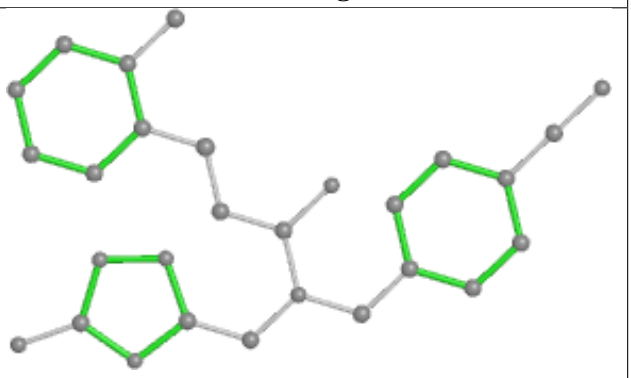
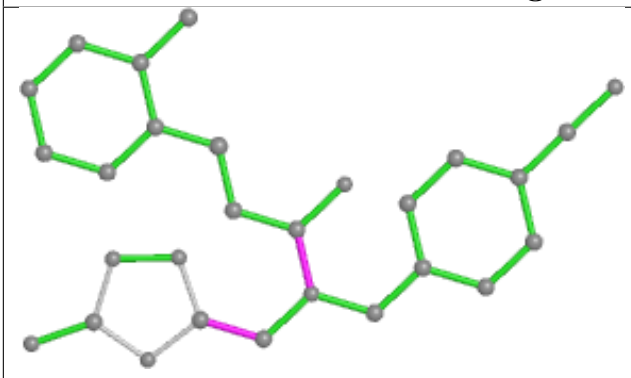


Rings

Ligand VFN 1 302



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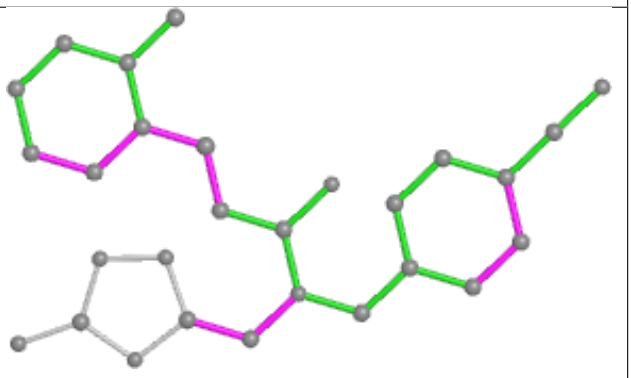

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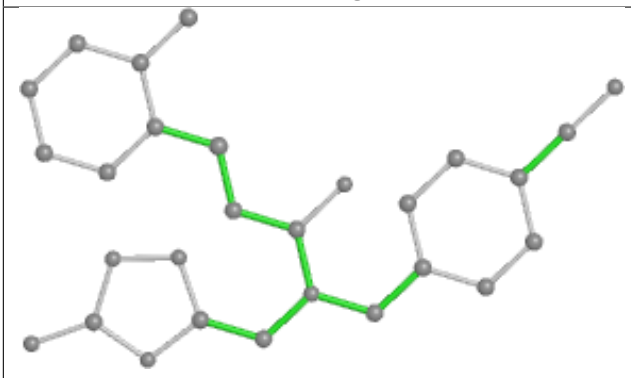

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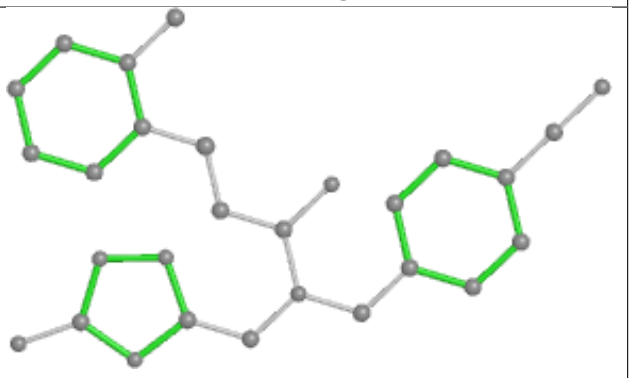
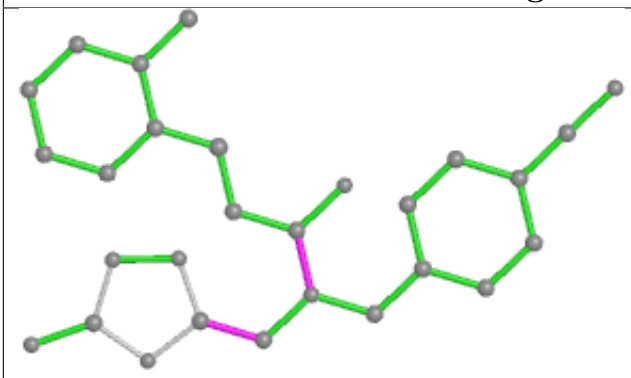


Rings

Ligand VFN 3 302



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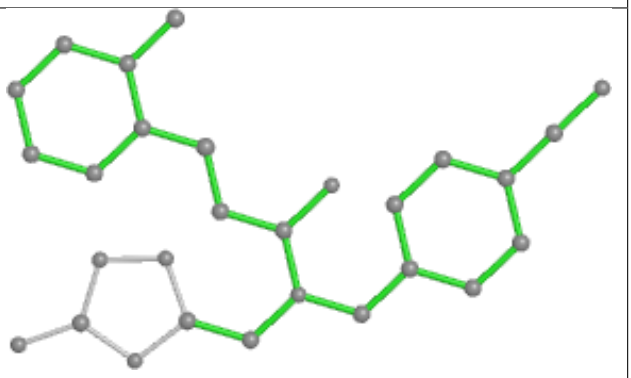

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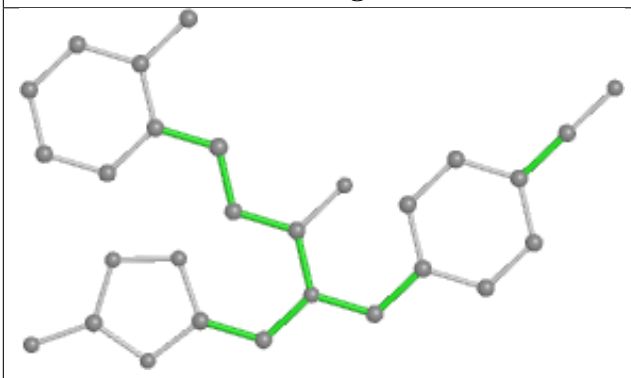

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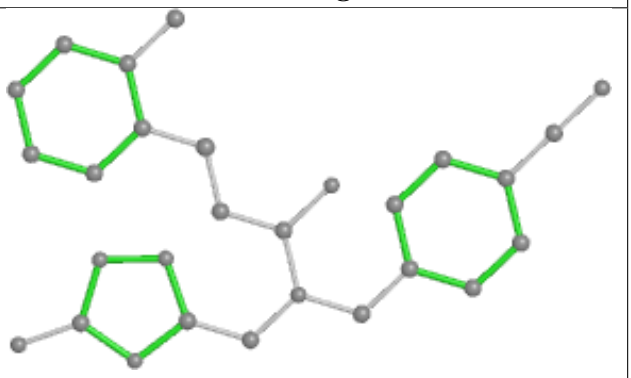
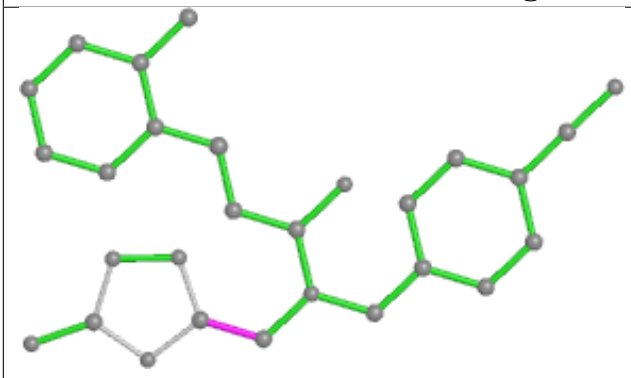


Rings

Ligand VFN A 302



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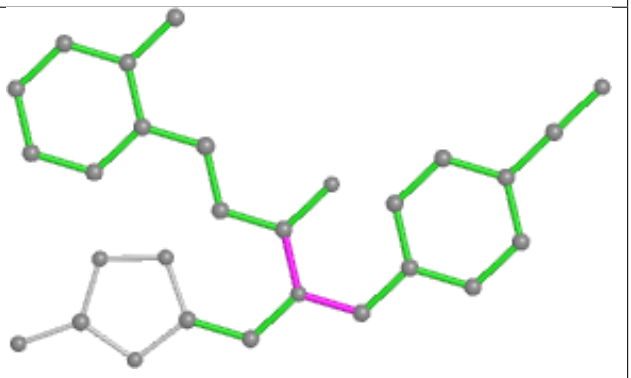

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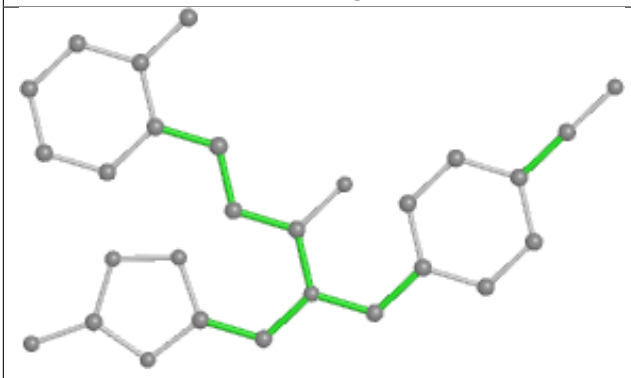

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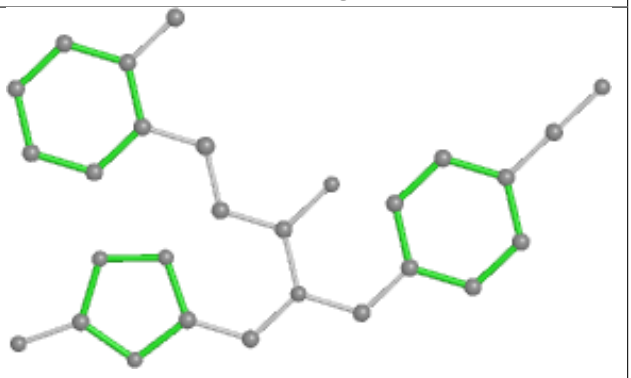
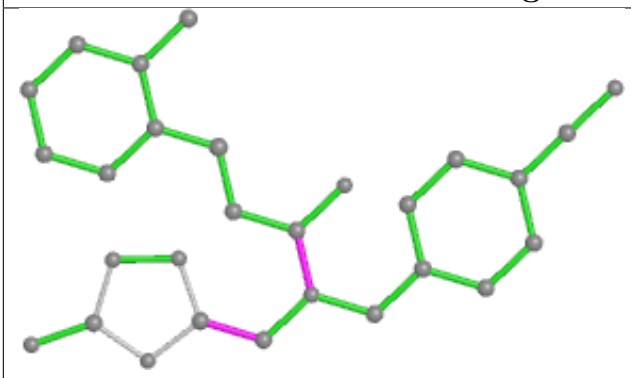


Rings

Ligand VFN R 301



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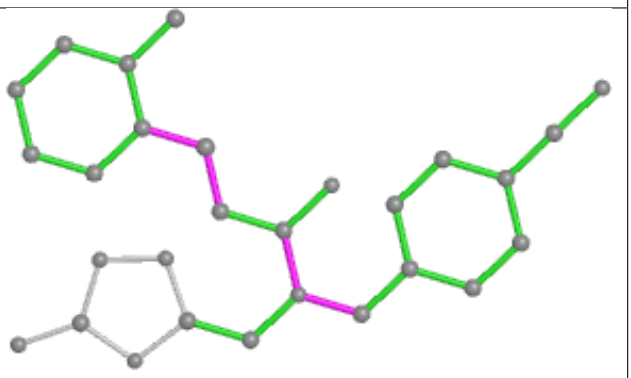

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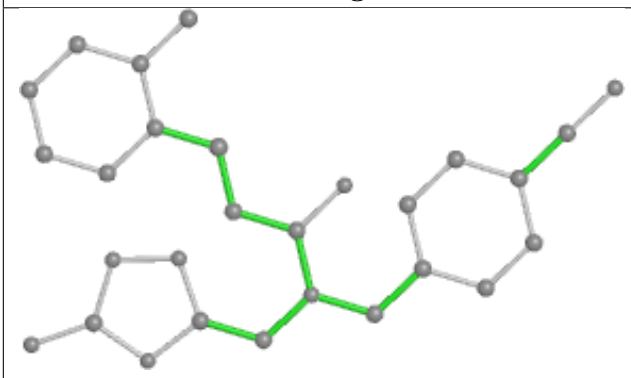

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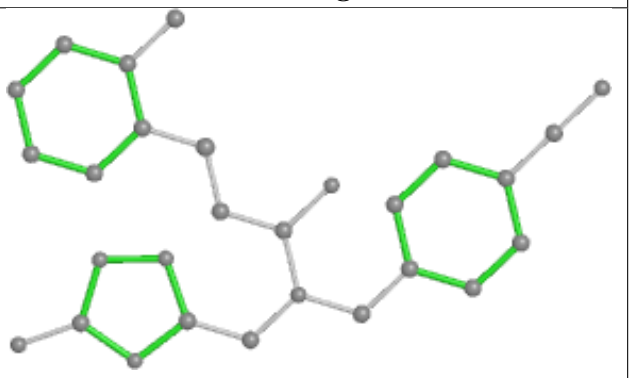
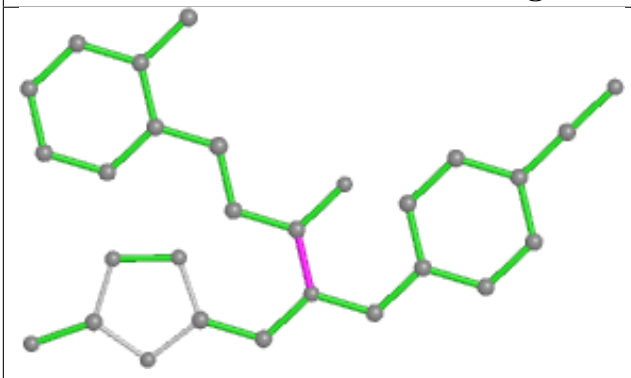


Rings

Ligand VFN 3 301



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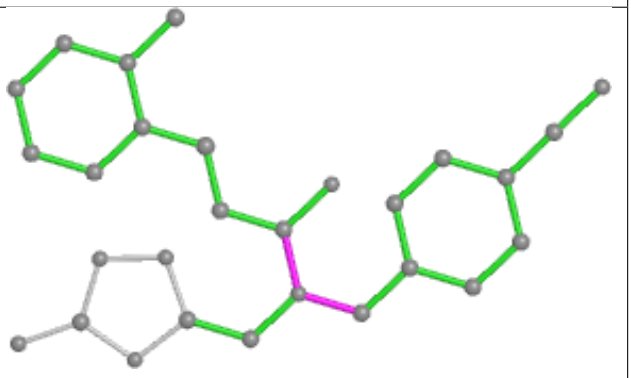

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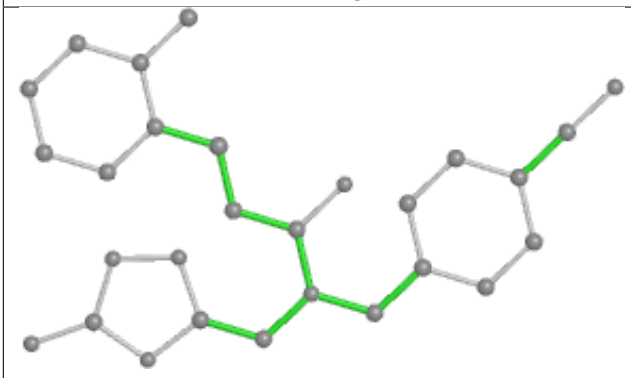

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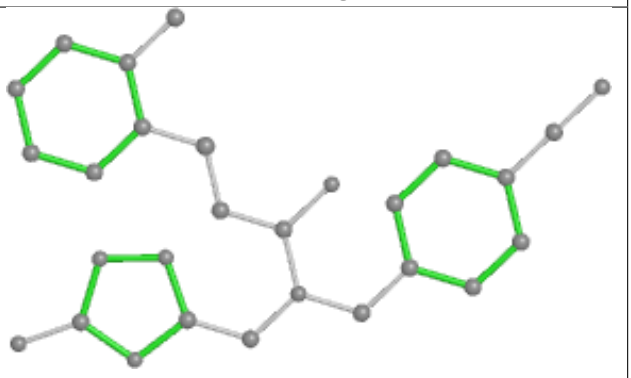
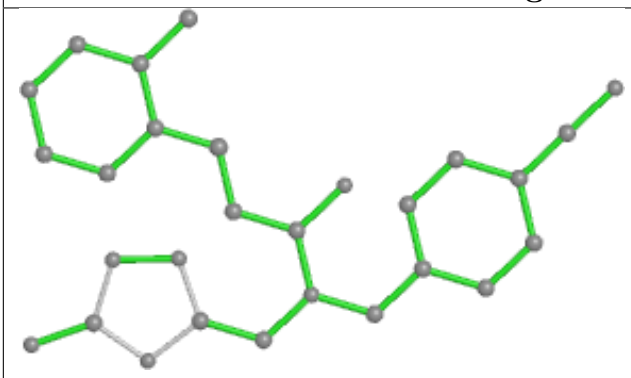


Rings

Ligand VFN S 301



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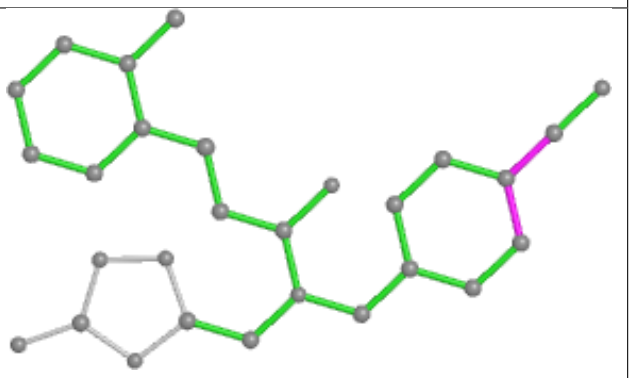
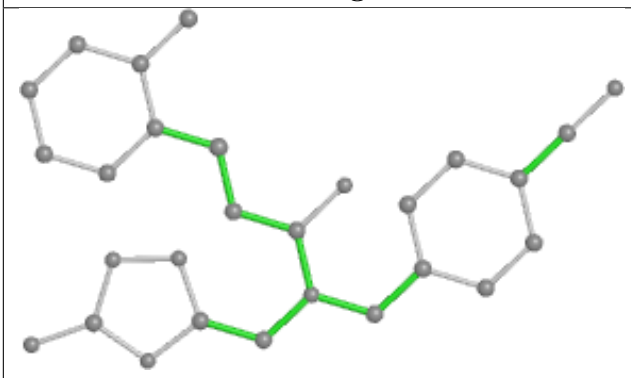
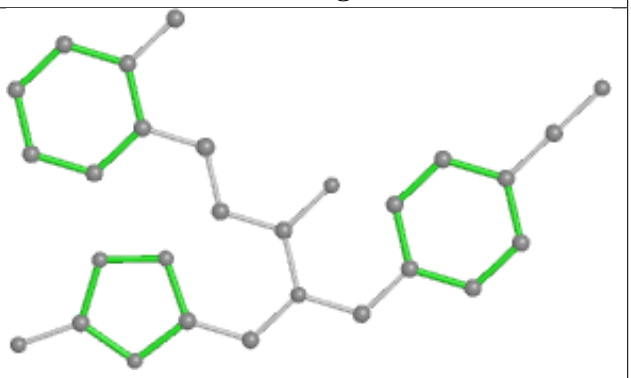


Bond angles

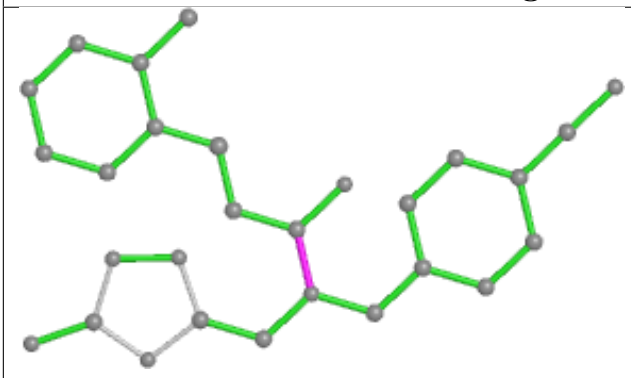


Torsions



Rings

Ligand VFN D 302



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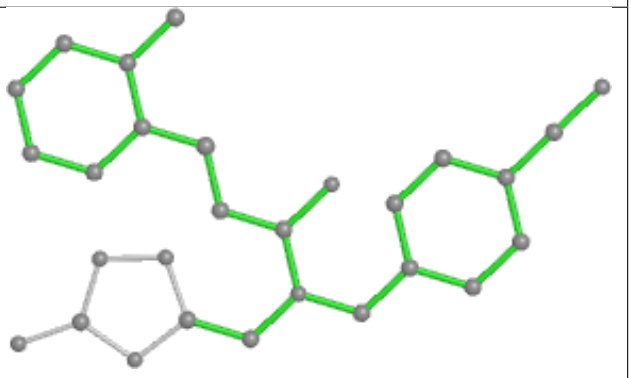

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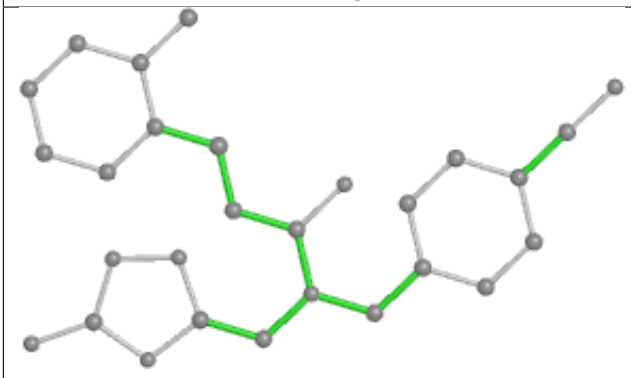
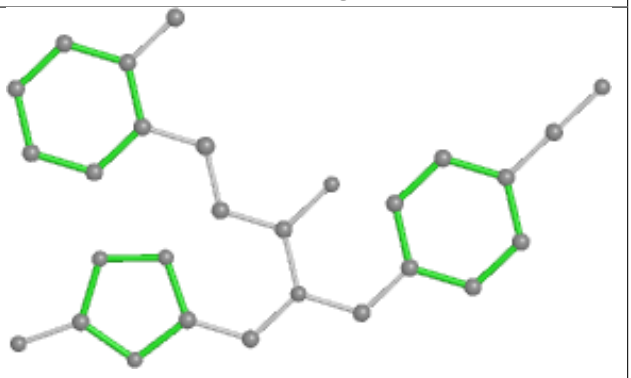


Torsions



Rings

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	1	258/261 (98%)	-0.02	0 100 100	50, 66, 87, 119	0
1	2	258/261 (98%)	0.00	2 (0%) 86 86	50, 65, 86, 122	0
1	3	258/261 (98%)	0.00	4 (1%) 72 71	47, 65, 84, 111	0
1	4	258/261 (98%)	-0.04	1 (0%) 92 93	46, 63, 82, 103	0
1	A	258/261 (98%)	-0.06	0 100 100	51, 66, 87, 104	0
1	B	258/261 (98%)	-0.03	1 (0%) 92 93	51, 65, 85, 105	0
1	C	258/261 (98%)	-0.11	0 100 100	52, 64, 85, 105	0
1	D	258/261 (98%)	-0.06	2 (0%) 86 86	47, 63, 85, 111	0
1	E	258/261 (98%)	-0.04	1 (0%) 92 93	47, 65, 83, 109	0
1	F	258/261 (98%)	-0.03	1 (0%) 92 93	51, 66, 87, 116	0
1	G	258/261 (98%)	0.08	5 (1%) 66 65	54, 73, 99, 123	0
1	H	258/261 (98%)	0.12	4 (1%) 72 71	58, 75, 102, 116	0
1	I	258/261 (98%)	0.13	5 (1%) 66 65	53, 73, 100, 124	0
1	J	258/261 (98%)	0.14	4 (1%) 72 71	51, 74, 106, 130	0
1	K	258/261 (98%)	0.08	3 (1%) 79 79	58, 76, 101, 121	0
1	L	258/261 (98%)	0.09	7 (2%) 54 50	56, 73, 100, 135	0
1	M	258/261 (98%)	0.02	1 (0%) 92 93	55, 72, 102, 125	0
1	N	258/261 (98%)	0.09	5 (1%) 66 65	55, 74, 100, 118	0
1	O	258/261 (98%)	0.04	6 (2%) 60 58	52, 72, 103, 121	0
1	P	258/261 (98%)	0.16	5 (1%) 66 65	57, 73, 100, 131	0
1	Q	258/261 (98%)	0.10	4 (1%) 72 71	58, 74, 102, 124	0
1	R	258/261 (98%)	0.13	5 (1%) 66 65	53, 71, 100, 136	0
1	S	258/261 (98%)	-0.02	3 (1%) 79 79	50, 66, 87, 112	0
1	T	258/261 (98%)	-0.07	1 (0%) 92 93	51, 66, 86, 118	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	U	258/261 (98%)	-0.09	1 (0%) 92 93	49, 64, 84, 104	0
1	V	258/261 (98%)	-0.02	1 (0%) 92 93	52, 66, 85, 109	0
1	W	258/261 (98%)	0.02	1 (0%) 92 93	45, 65, 87, 119	0
1	X	258/261 (98%)	-0.11	0 100 100	48, 63, 81, 105	0
1	Y	258/261 (98%)	0.01	2 (0%) 86 86	48, 66, 85, 116	0
1	Z	258/261 (98%)	-0.06	0 100 100	48, 66, 83, 108	0
All	All	7740/7830 (98%)	0.02	75 (0%) 82 82	45, 68, 95, 136	0

All (75) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	I	1	MET	4.6
1	J	1	MET	4.3
1	H	1	MET	4.1
1	Q	1	MET	4.0
1	P	1	MET	3.8
1	J	18	ALA	3.8
1	P	15	ARG	3.7
1	L	1	MET	3.6
1	O	1	MET	3.6
1	M	1	MET	3.5
1	N	77	PRO	3.4
1	W	1	MET	3.4
1	Y	1	MET	3.4
1	R	15	ARG	3.4
1	Q	18	ALA	3.4
1	R	3	LEU	3.4
1	P	3	LEU	3.3
1	F	1	MET	3.0
1	K	18	ALA	3.0
1	S	1	MET	2.9
1	P	14	ALA	2.8
1	G	1	MET	2.8
1	K	15	ARG	2.8
1	L	2	SER	2.7
1	N	18	ALA	2.7
1	Q	14	ALA	2.7
1	Q	15	ARG	2.7
1	J	15	ARG	2.7
1	K	13	SER	2.6

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Mol	Chain	Res	Type	RSRZ
1	R	36	GLU	2.6
1	H	15	ARG	2.6
1	S	15	ARG	2.6
1	I	3	LEU	2.6
1	D	1	MET	2.6
1	O	15	ARG	2.6
1	L	51	LYS	2.5
1	I	12	PRO	2.5
1	H	19	ASP	2.5
1	J	3	LEU	2.5
1	T	54	LYS	2.4
1	2	1	MET	2.4
1	I	10	ILE	2.4
1	3	15	ARG	2.4
1	N	1	MET	2.4
1	O	16	LEU	2.4
1	G	16	LEU	2.3
1	B	15	ARG	2.3
1	Y	18	ALA	2.3
1	U	99	VAL	2.3
1	3	19	ASP	2.3
1	4	15	ARG	2.3
1	S	35	GLY	2.2
1	O	39	VAL	2.2
1	2	15	ARG	2.2
1	R	51	LYS	2.2
1	H	20	VAL	2.2
1	N	108	GLY	2.2
1	3	1	MET	2.2
1	N	15	ARG	2.2
1	L	205	SER	2.2
1	O	20	VAL	2.1
1	P	99	VAL	2.1
1	L	3	LEU	2.1
1	I	13	SER	2.1
1	G	20	VAL	2.1
1	G	34	ILE	2.1
1	E	51	LYS	2.1
1	3	20	VAL	2.1
1	O	36	GLU	2.1
1	R	18	ALA	2.1
1	D	15	ARG	2.1

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Mol	Chain	Res	Type	RSRZ
1	V	17	ALA	2.0
1	G	79	ARG	2.0
1	L	19	ASP	2.0
1	L	77	PRO	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
3	SO4	C	302	5/5	0.90	0.22	98,99,100,100	0
2	VFN	3	302	28/28	0.94	0.24	61,72,76,76	0
2	VFN	H	302	28/28	0.95	0.21	73,77,84,85	0
2	VFN	K	301	28/28	0.95	0.23	77,90,93,93	0
2	VFN	R	301	28/28	0.95	0.21	71,75,81,82	0
2	VFN	D	302	28/28	0.95	0.23	59,66,70,72	0
2	VFN	B	301	28/28	0.96	0.20	68,72,76,77	0
2	VFN	2	301	28/28	0.96	0.20	56,65,72,77	0
2	VFN	F	301	28/28	0.96	0.19	51,62,70,75	0
2	VFN	G	301	28/28	0.96	0.20	64,73,79,83	0
2	VFN	H	301	28/28	0.96	0.19	73,77,81,84	0
2	VFN	3	301	28/28	0.96	0.21	60,65,68,69	0
2	VFN	1	302	28/28	0.96	0.21	56,65,72,75	0
2	VFN	L	301	28/28	0.96	0.20	78,81,87,87	0
2	VFN	N	301	28/28	0.96	0.19	64,72,85,86	0
2	VFN	O	301	28/28	0.96	0.22	66,74,77,80	0
2	VFN	O	302	28/28	0.96	0.20	80,84,88,89	0
2	VFN	P	301	28/28	0.96	0.19	77,83,86,88	0
2	VFN	A	301	28/28	0.96	0.19	61,66,71,72	0

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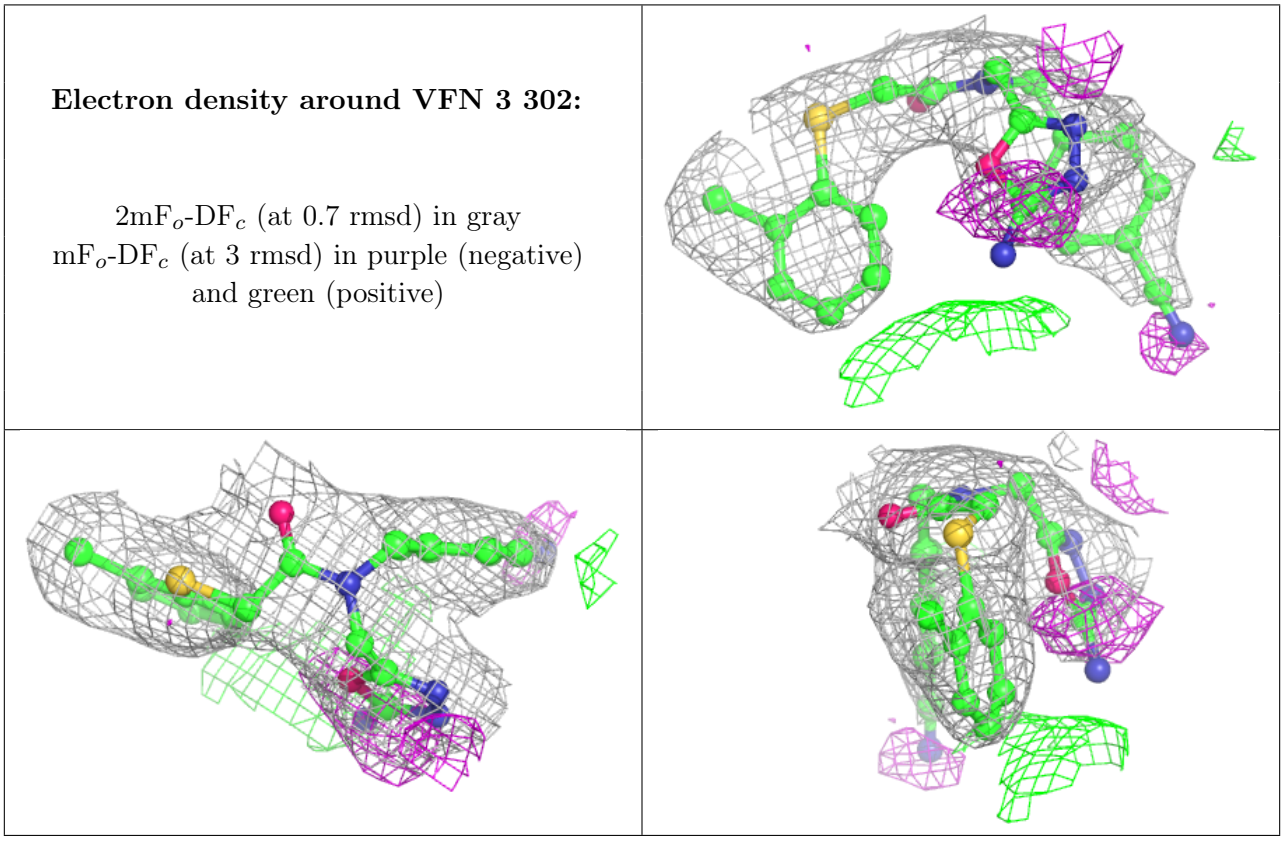
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	VFN	S	301	28/28	0.96	0.20	64,71,74,76	0
2	VFN	W	301	28/28	0.96	0.21	56,64,72,73	0
2	VFN	W	302	28/28	0.96	0.21	57,74,83,84	0
2	VFN	A	302	28/28	0.96	0.20	65,73,76,76	0
3	SO4	F	302	5/5	0.96	0.16	84,84,85,88	0
2	VFN	S	302	28/28	0.97	0.18	55,64,73,75	0
2	VFN	T	301	28/28	0.97	0.21	61,68,77,82	0
2	VFN	V	301	28/28	0.97	0.18	51,63,67,68	0
2	VFN	J	301	28/28	0.97	0.18	61,75,84,85	0
2	VFN	P	302	28/28	0.97	0.17	67,73,76,77	0
2	VFN	Z	301	28/28	0.97	0.19	60,67,78,79	0
3	SO4	C	301	5/5	0.97	0.17	98,98,99,99	0
2	VFN	D	301	28/28	0.97	0.20	57,65,73,74	0
2	VFN	1	301	28/28	0.97	0.18	54,61,67,71	0
3	SO4	G	302	5/5	0.97	0.18	99,100,100,101	0
3	SO4	H	303	5/5	0.97	0.17	92,93,93,96	0
3	SO4	J	302	5/5	0.97	0.12	83,86,87,89	0
3	SO4	O	303	5/5	0.97	0.16	85,87,87,87	0
3	SO4	U	301	5/5	0.97	0.15	80,82,83,85	0
3	SO4	W	303	5/5	0.97	0.13	91,93,93,94	0
3	SO4	X	301	5/5	0.97	0.18	90,90,91,94	0
3	SO4	Y	301	5/5	0.97	0.16	91,91,93,94	0
3	SO4	A	303	5/5	0.98	0.14	88,88,89,89	0
3	SO4	I	301	5/5	0.98	0.15	80,82,82,83	0
3	SO4	1	303	5/5	0.98	0.12	91,92,92,93	0
3	SO4	L	302	5/5	0.98	0.14	93,93,95,95	0
3	SO4	M	301	5/5	0.98	0.13	90,90,91,92	0
3	SO4	N	302	5/5	0.98	0.15	89,90,91,92	0
3	SO4	2	302	5/5	0.98	0.13	94,96,98,98	0
3	SO4	P	303	5/5	0.98	0.17	95,96,96,96	0
3	SO4	Q	301	5/5	0.98	0.12	85,85,85,87	0
3	SO4	R	302	5/5	0.98	0.13	79,82,83,84	0
3	SO4	S	303	5/5	0.98	0.16	76,76,78,79	0
3	SO4	T	302	5/5	0.98	0.13	78,78,80,82	0
3	SO4	D	303	5/5	0.98	0.14	81,83,84,84	0
3	SO4	V	302	5/5	0.98	0.13	88,90,91,91	0
3	SO4	E	301	5/5	0.98	0.14	74,76,78,79	0
3	SO4	3	303	5/5	0.98	0.16	92,92,94,94	0
3	SO4	4	301	5/5	0.98	0.15	85,86,87,89	0
3	SO4	Z	302	5/5	0.98	0.15	81,81,83,83	0
3	SO4	K	302	5/5	0.99	0.15	88,89,90,92	0
3	SO4	B	302	5/5	0.99	0.10	75,76,77,77	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.

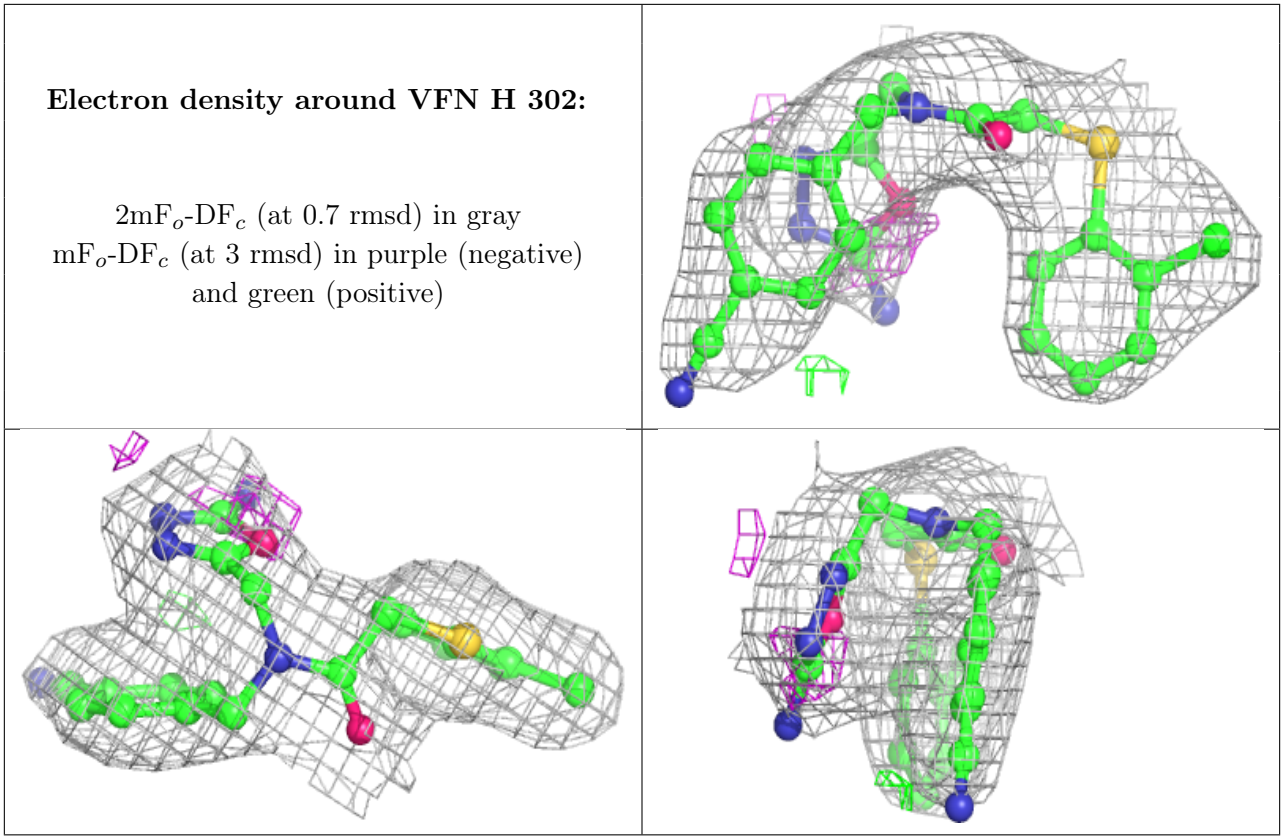
Electron density around VFN 3 302:

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



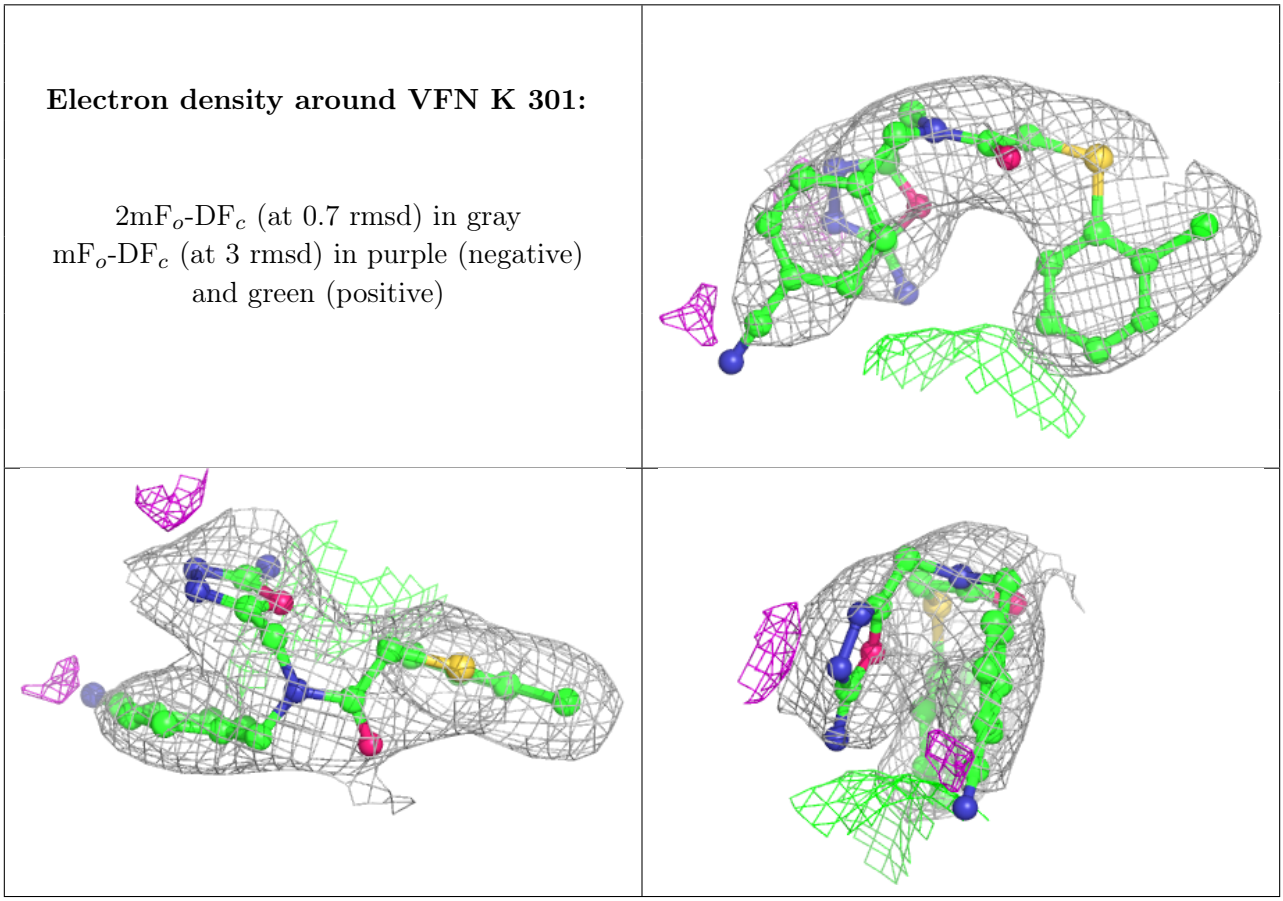
Electron density around VFN H 302:

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



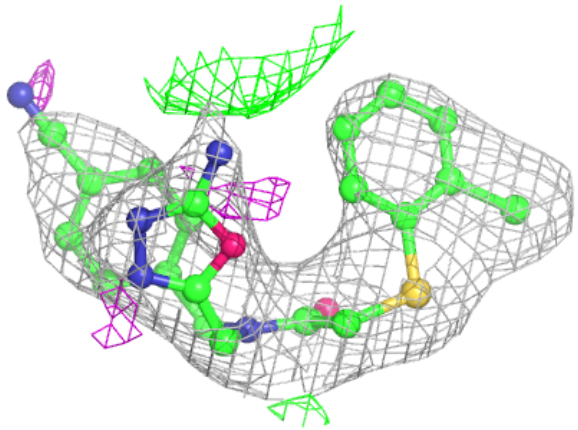
Electron density around VFN K 301:

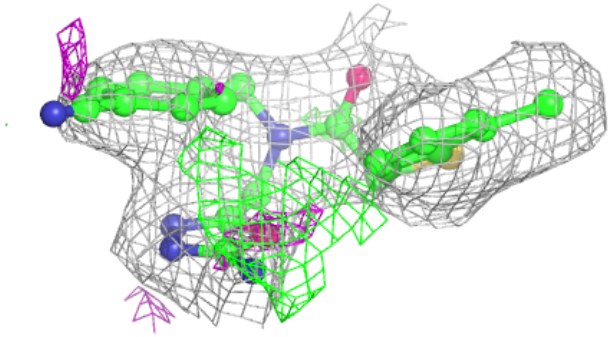
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

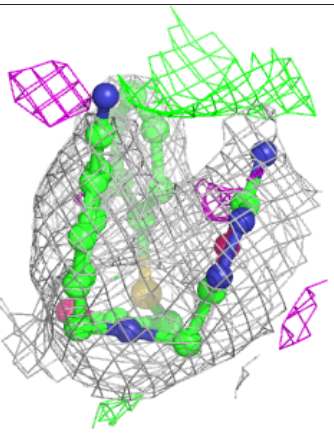


Electron density around VFN R 301:

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

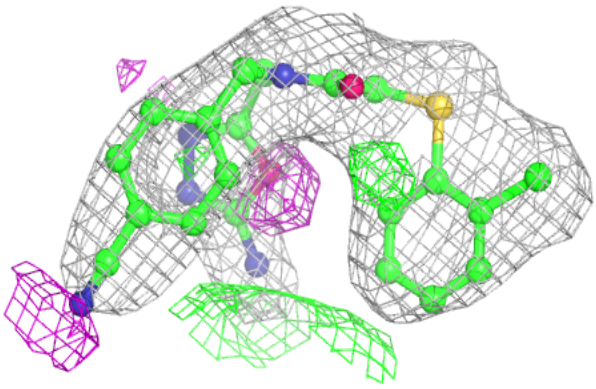


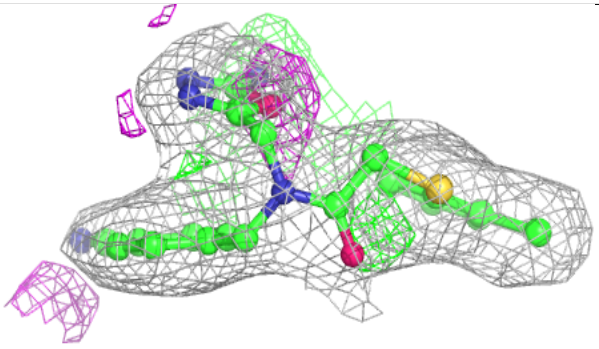


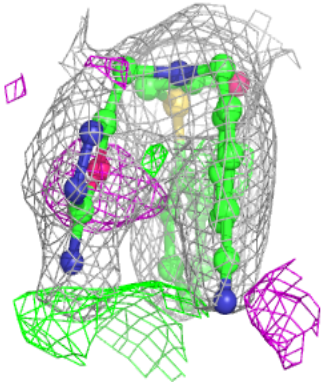


Electron density around VFN D 302:

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

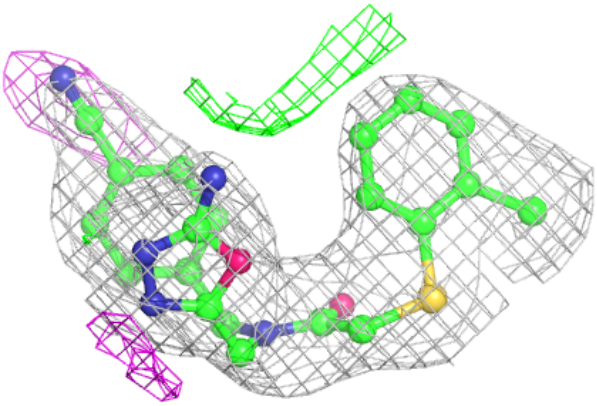


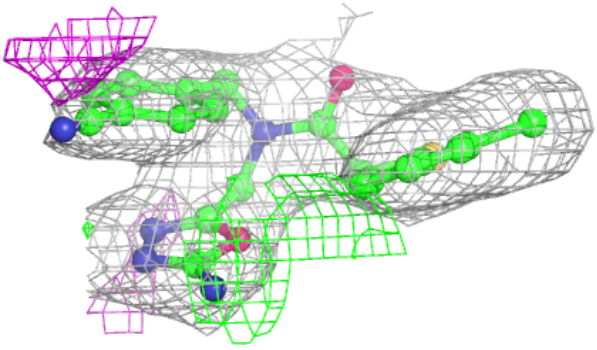


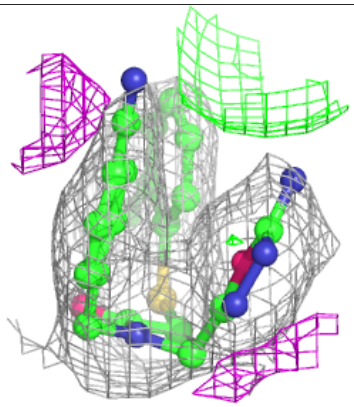


Electron density around VFN B 301:

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

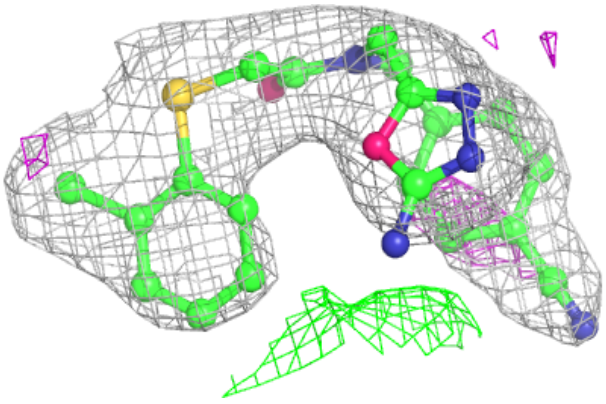


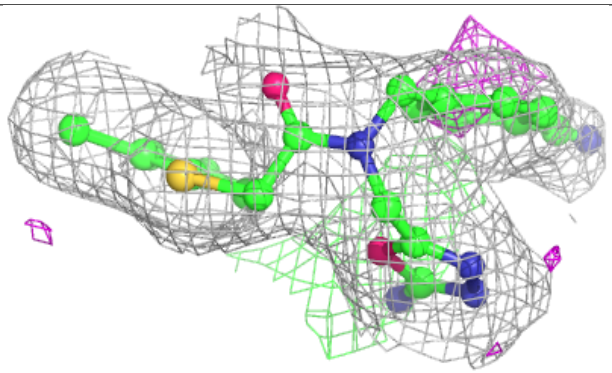


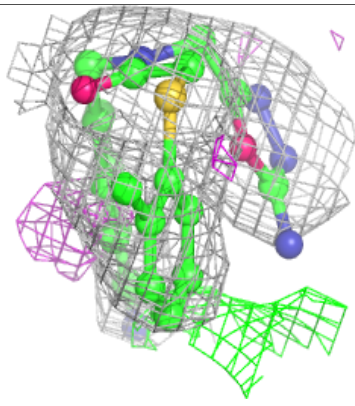


Electron density around VFN 2 301:

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

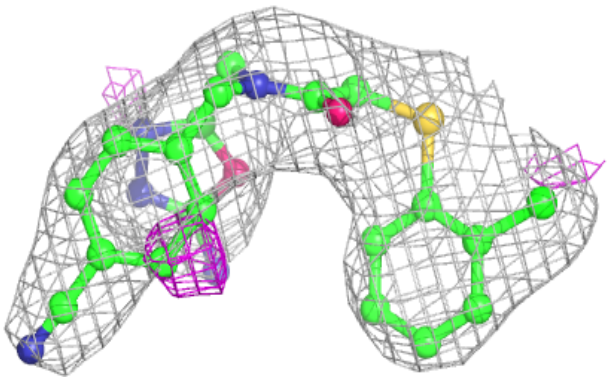


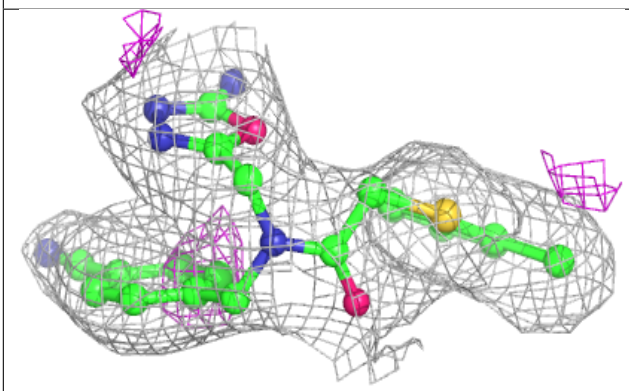


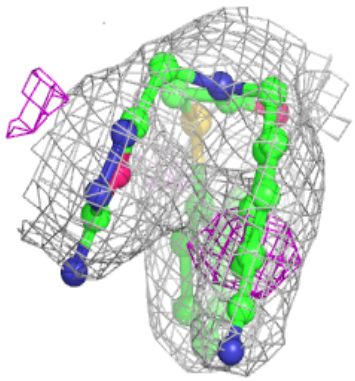


Electron density around VFN F 301:

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

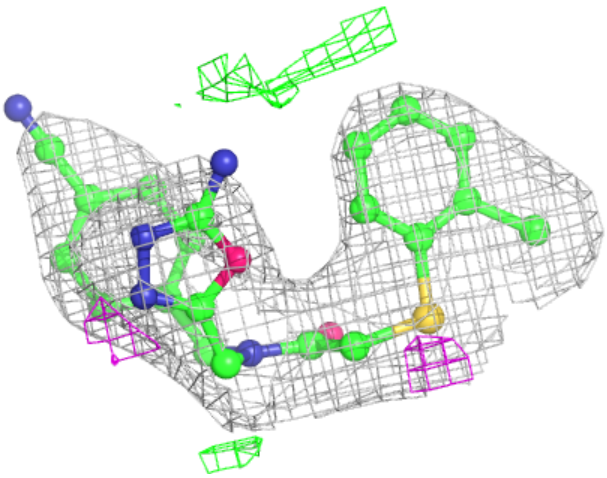


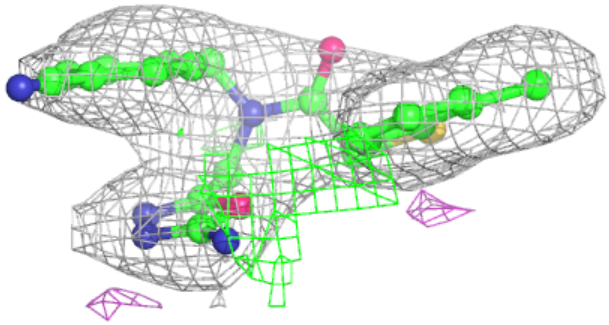


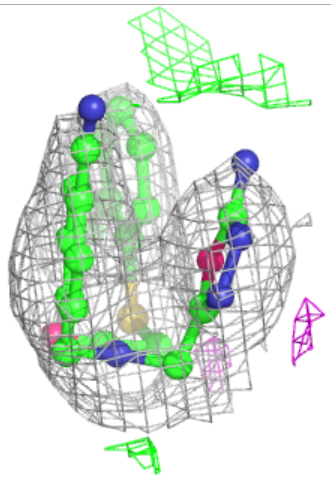


Electron density around VFN G 301:

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

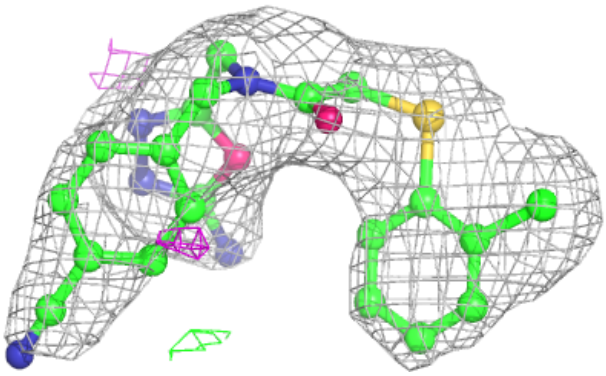


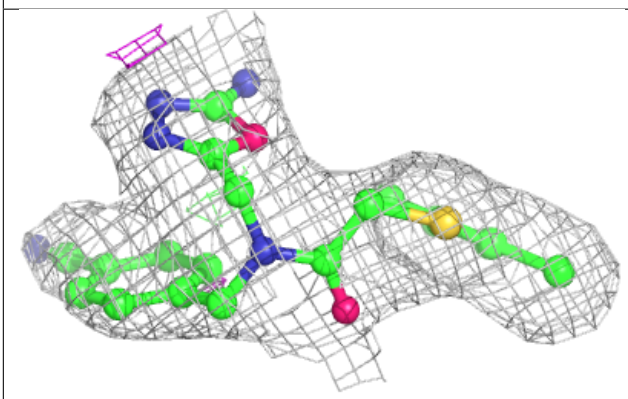


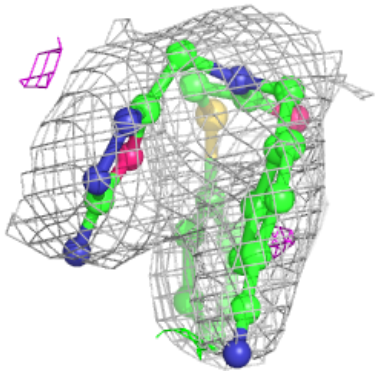


Electron density around VFN H 301:

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

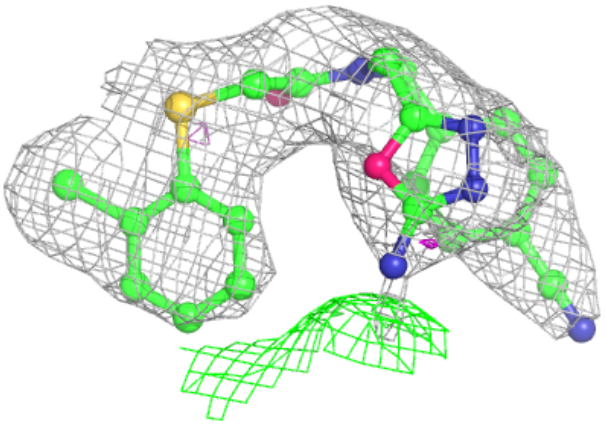


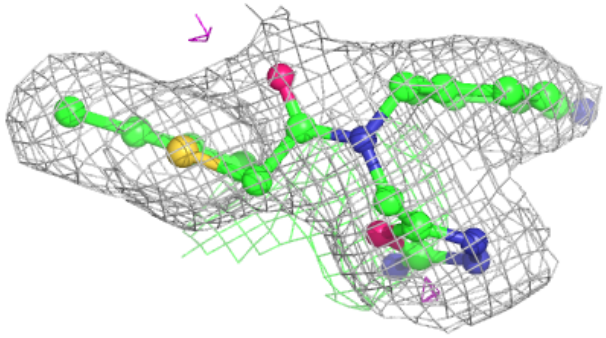


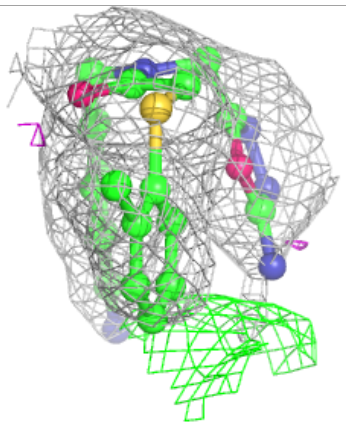


Electron density around VFN 3 301:

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

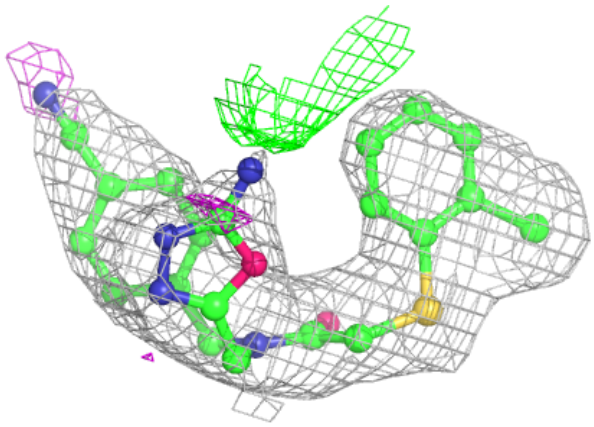


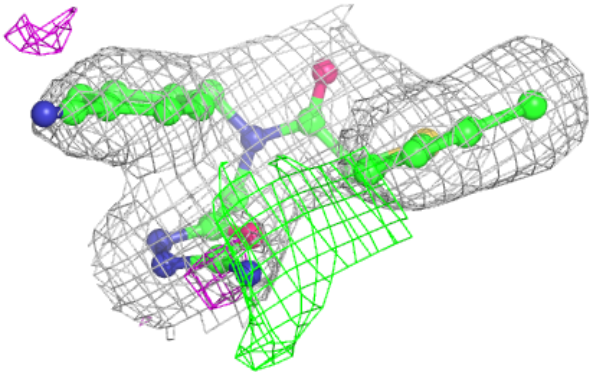


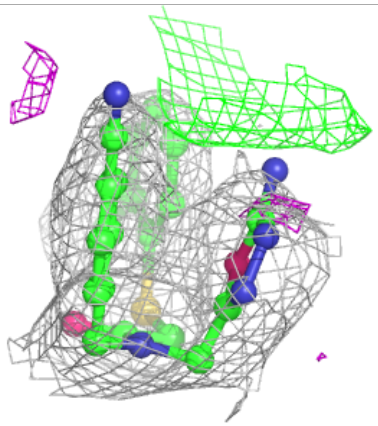


Electron density around VFN 1 302:

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

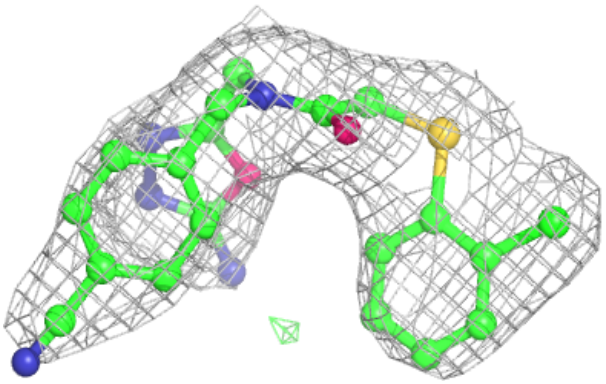


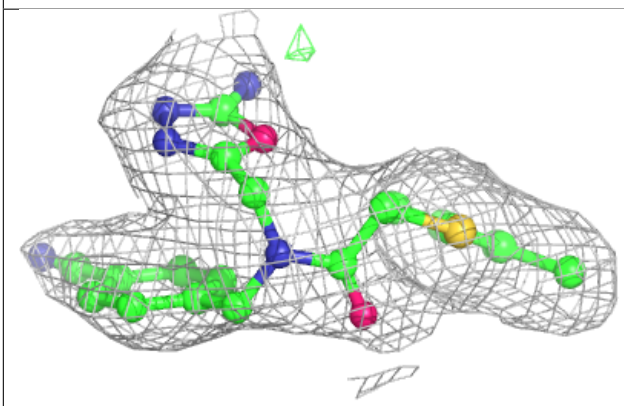


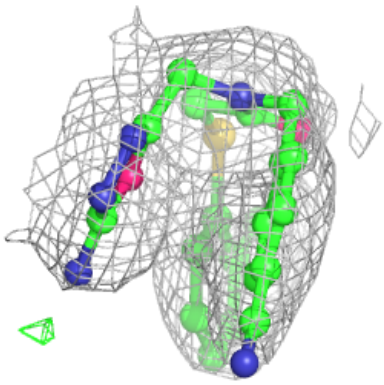


Electron density around VFN L 301:

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

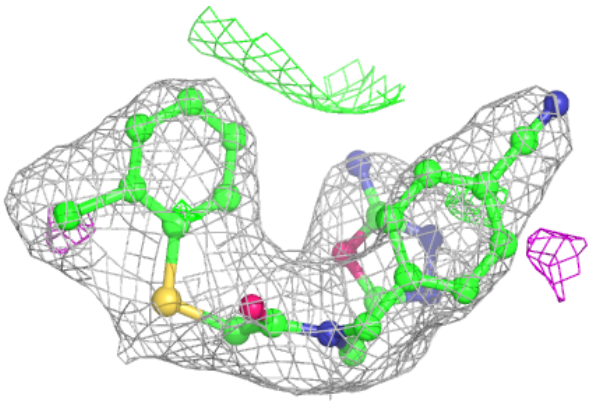


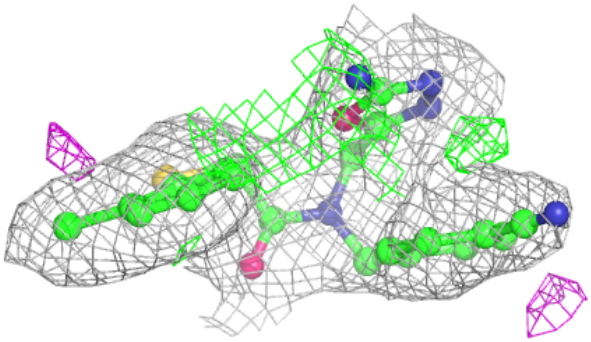


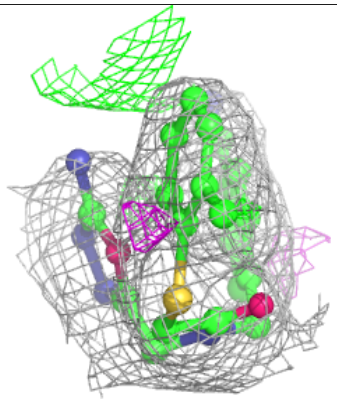


Electron density around VFN N 301:

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

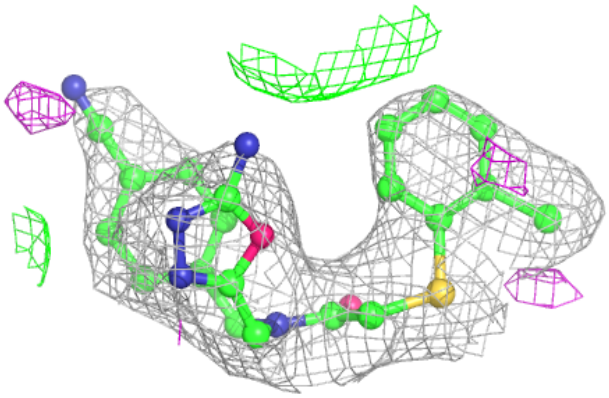


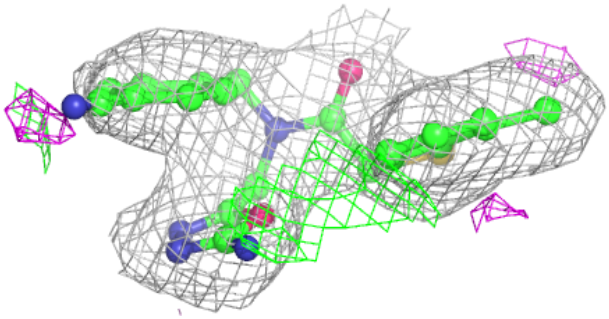


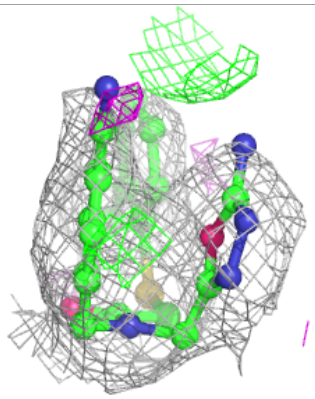


Electron density around VFN O 301:

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

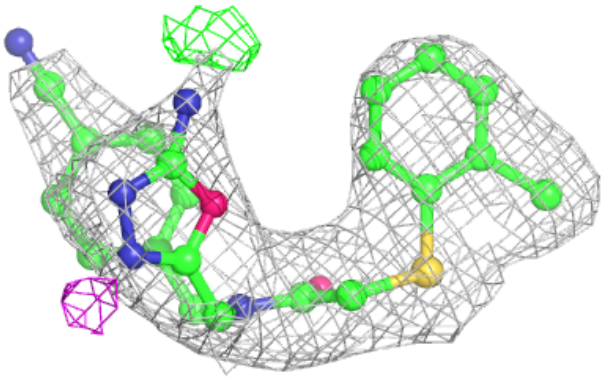


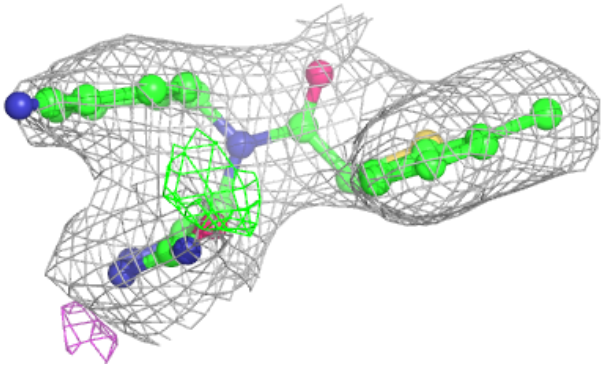


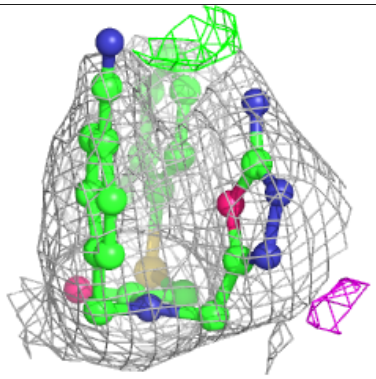


Electron density around VFN O 302:

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

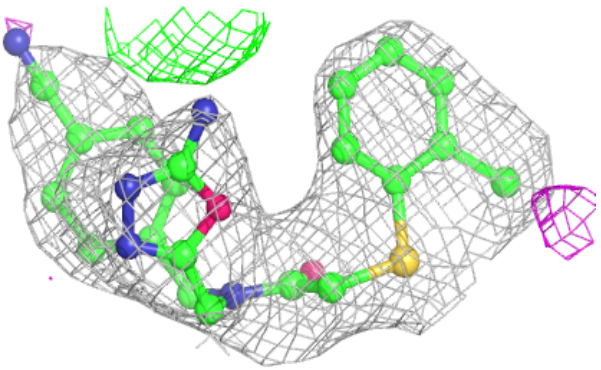


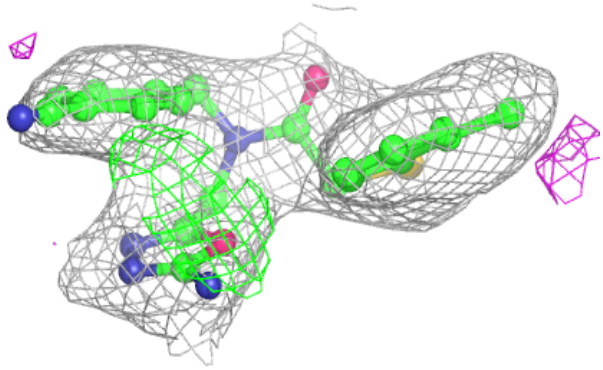


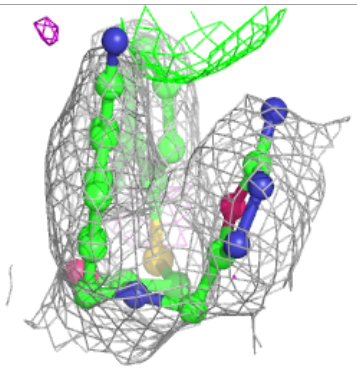


Electron density around VFN P 301:

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

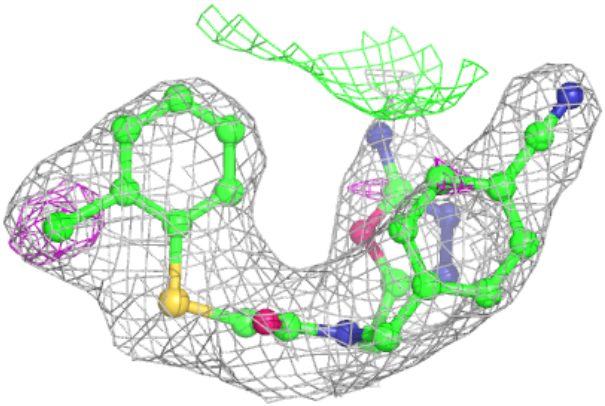


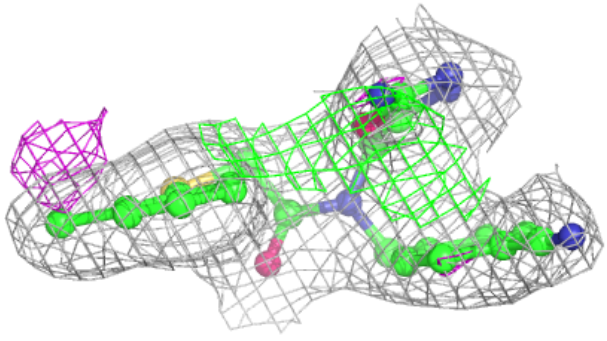


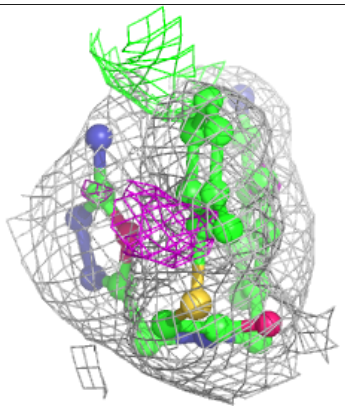


Electron density around VFN A 301:

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

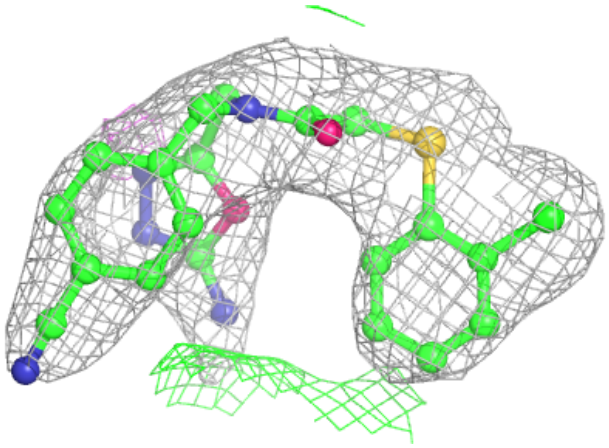


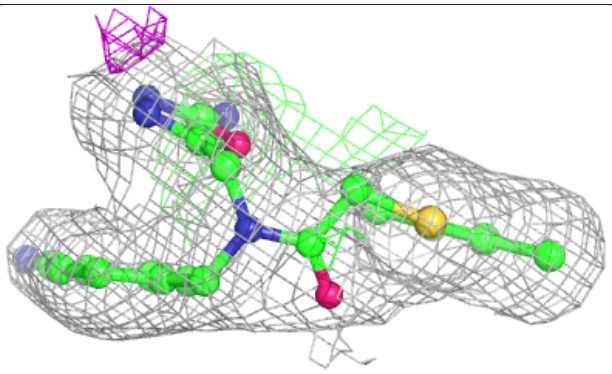


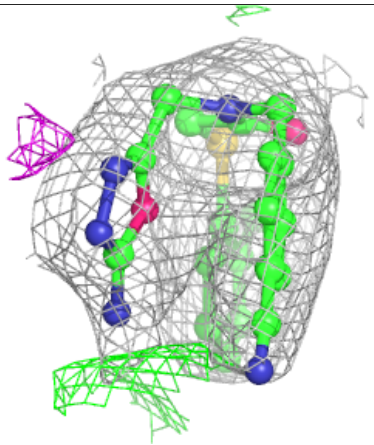


Electron density around VFN S 301:

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

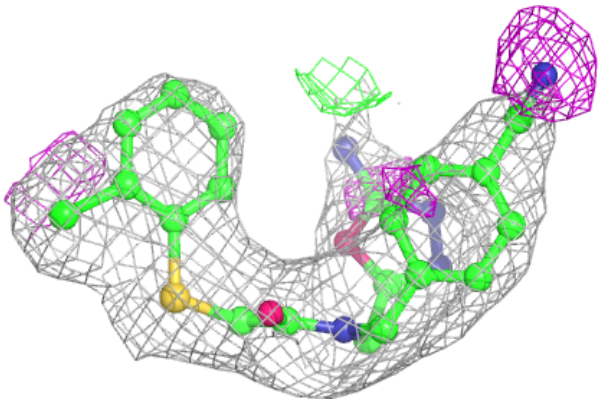


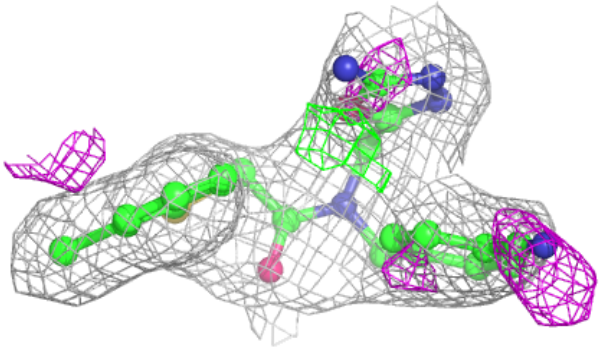


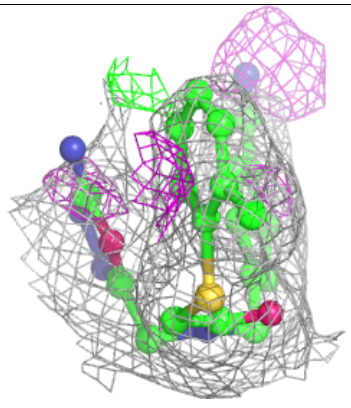


Electron density around VFN W 301:

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

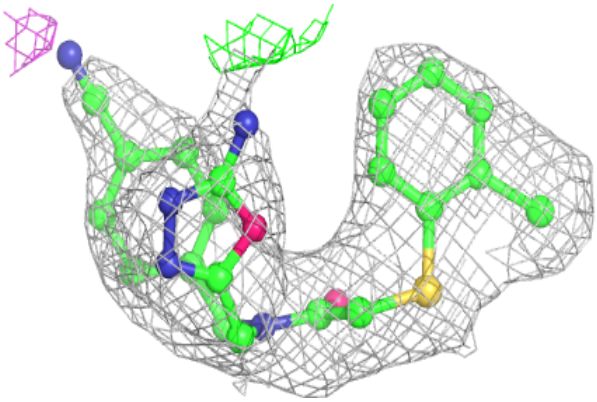


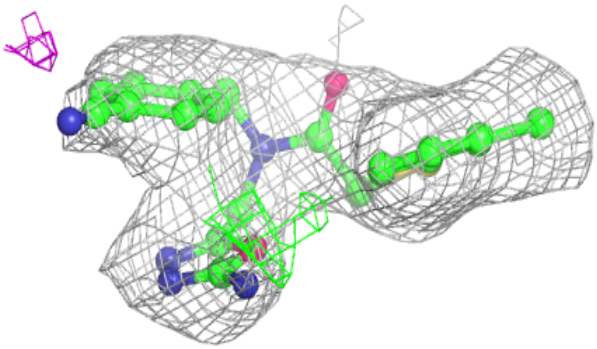


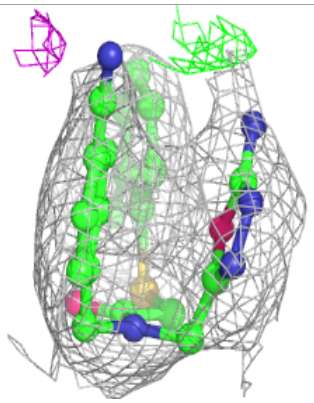


Electron density around VFN W 302:

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

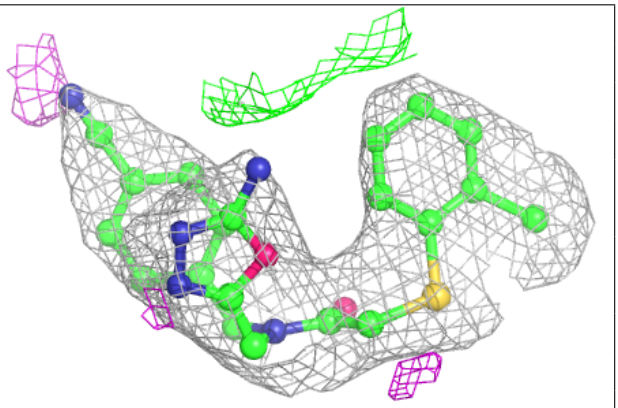


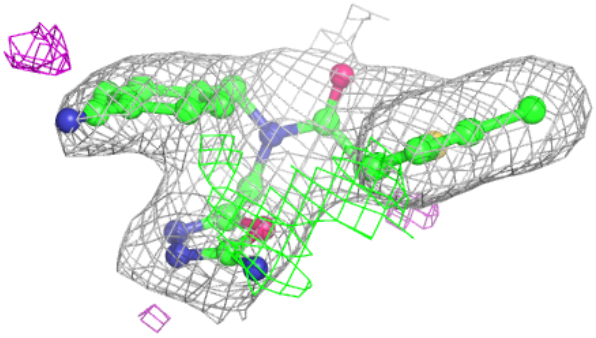


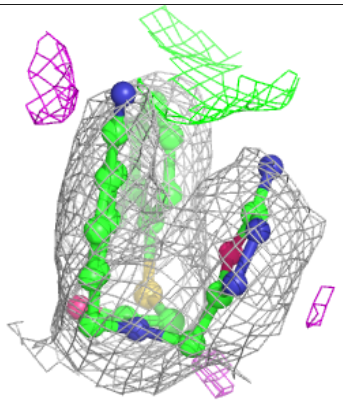


Electron density around VFN A 302:

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

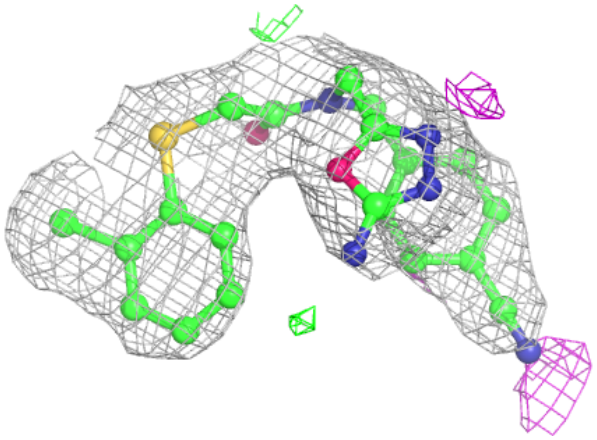


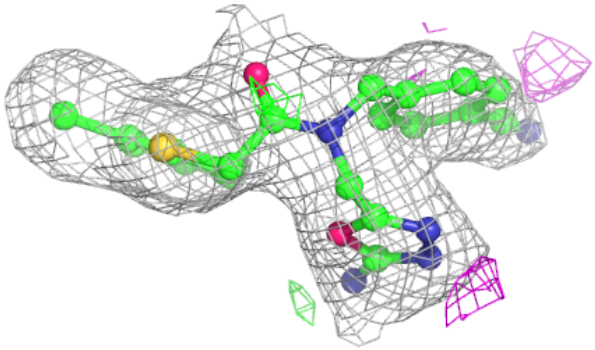


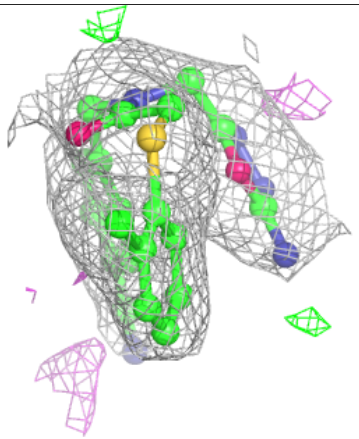


Electron density around VFN S 302:

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

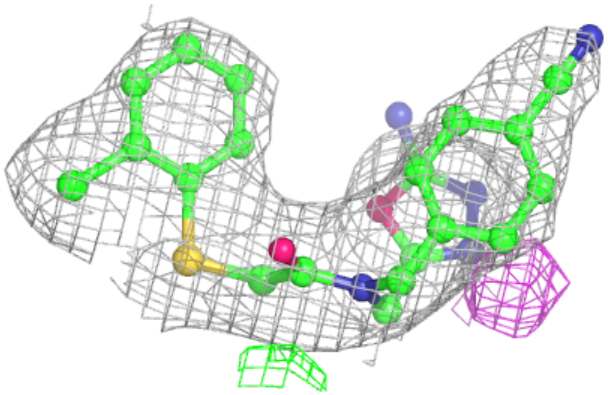


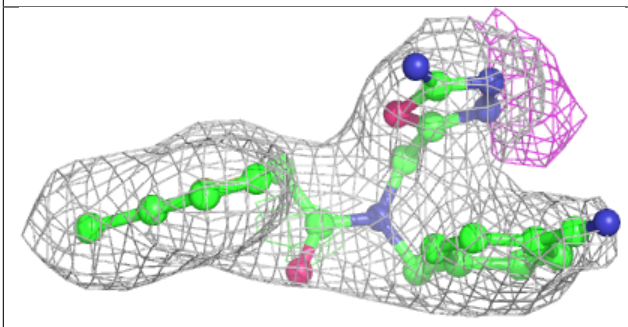


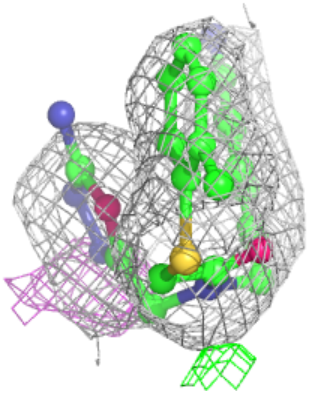


Electron density around VFN T 301:

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

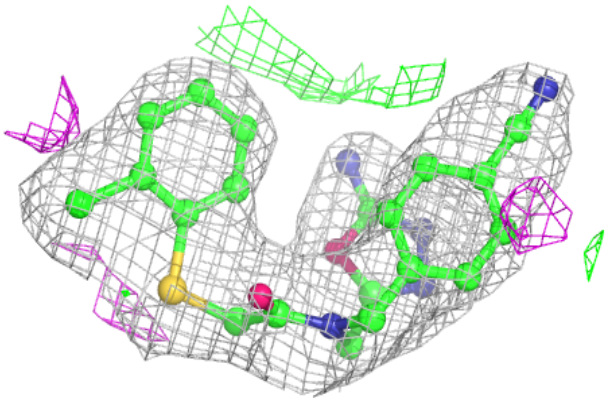


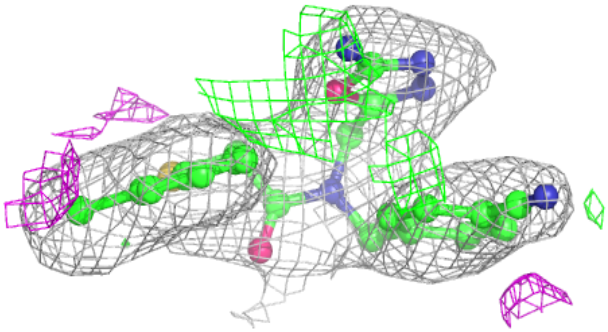


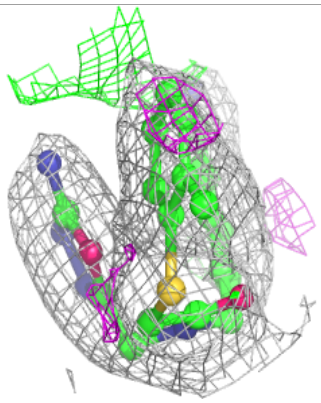


Electron density around VFN V 301:

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

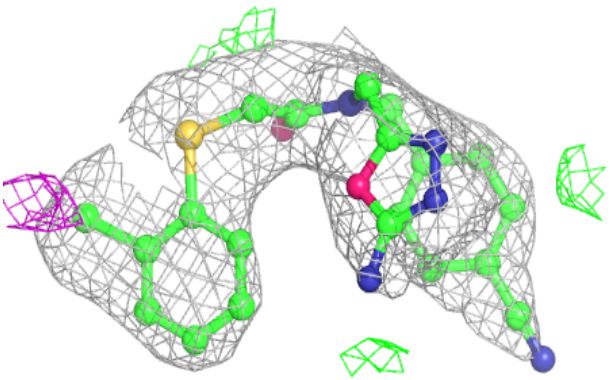


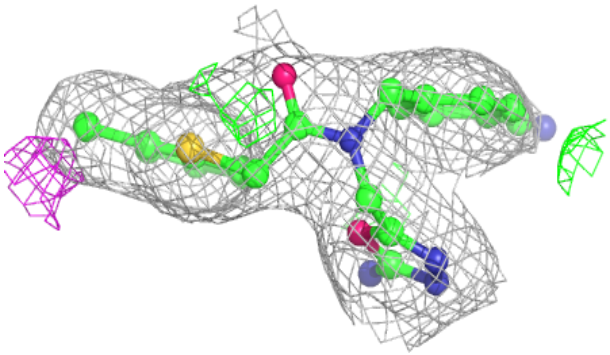


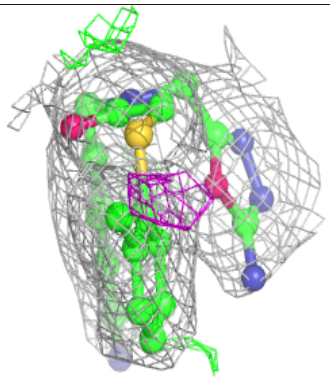


Electron density around VFN J 301:

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

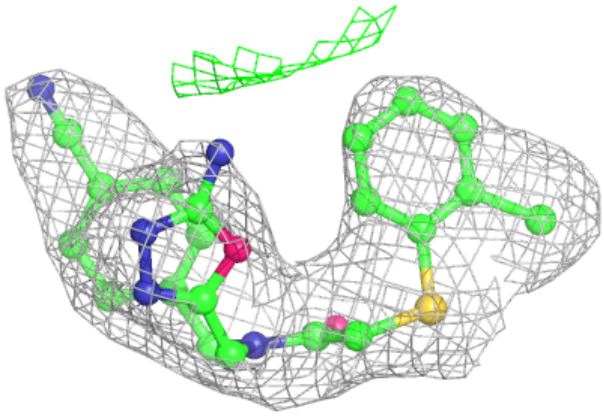


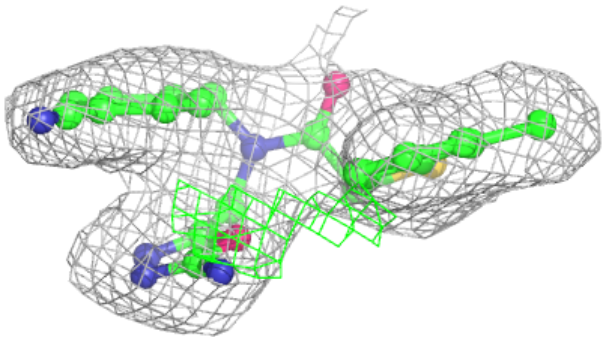


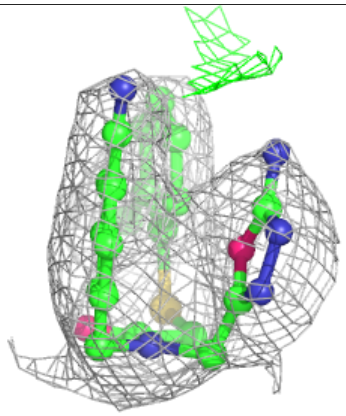


Electron density around VFN P 302:

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

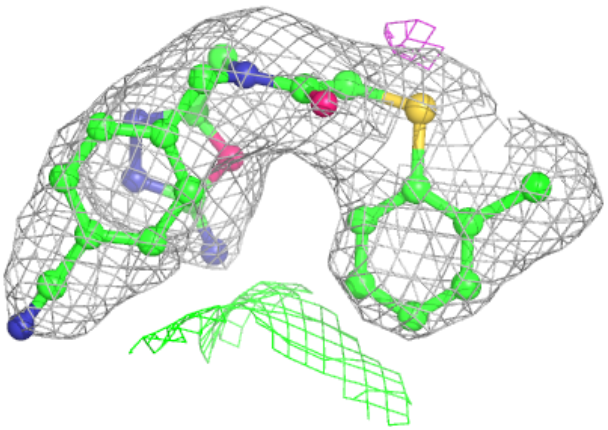


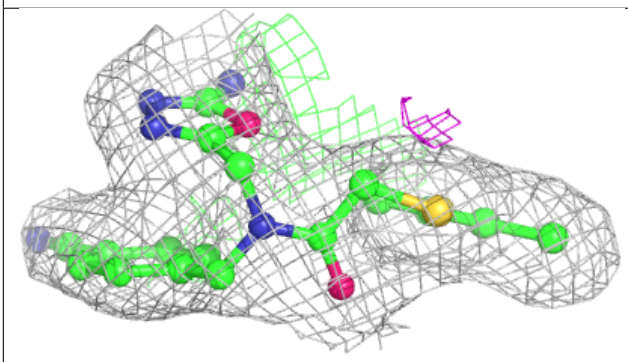


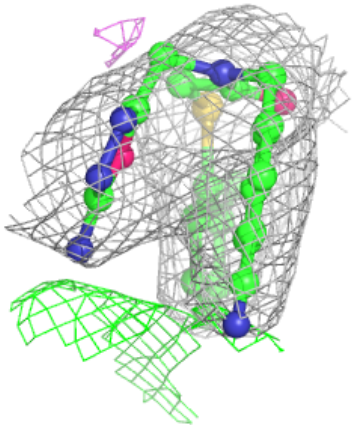


Electron density around VFN Z 301:

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

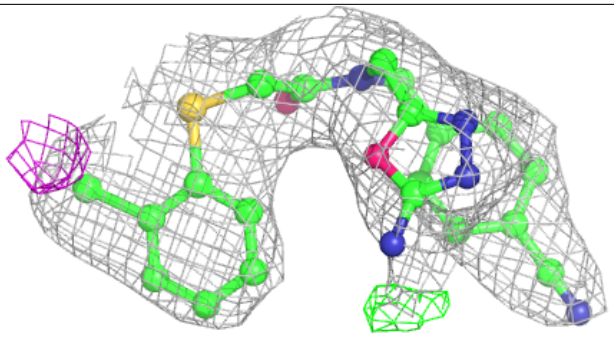


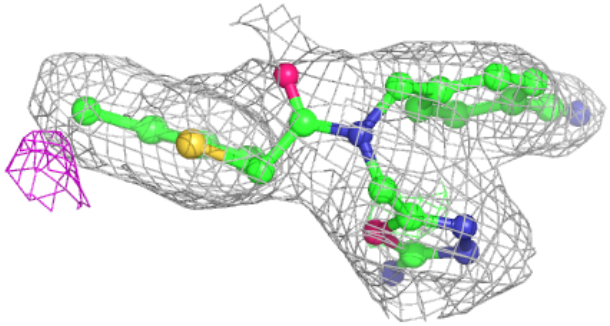


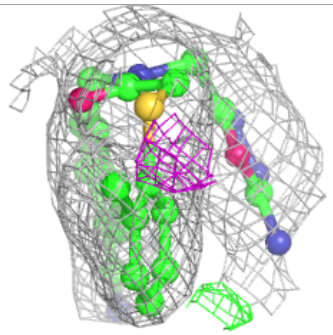


Electron density around VFN D 301:

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

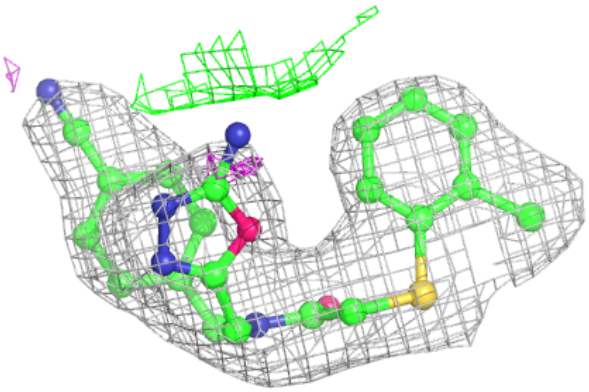


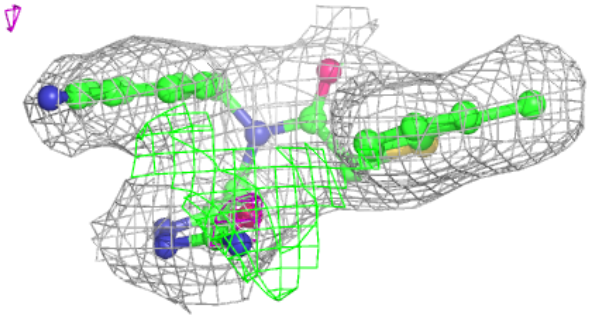


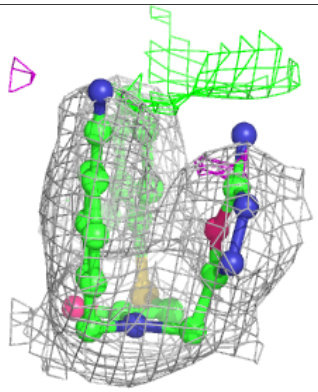


Electron density around VFN 1 301:

$2mF_o$-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.