Full wwPDB X-ray Structure Validation Report ⓘ

Oct 18, 2021 – 01:03 pm BST

PDB ID	:	7OJP
Title	:	Crystal structure of Pseudomonas aeruginosa LpxA in complex with compound 1
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	:	2.84 Å(reported)

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

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

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

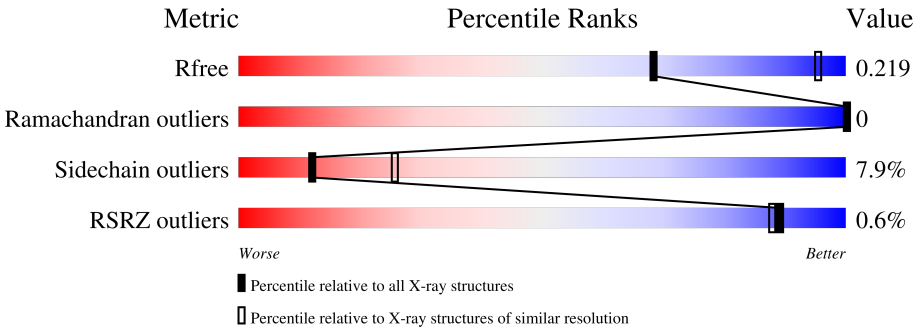
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.23.2
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0267
CCP4	:	7.1.010 (Gargrove)
Ideal geometry (proteins)	:	Engh &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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.84 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	1031 (2.86-2.82)
Ramachandran outliers	138981	1050 (2.86-2.82)
Sidechain outliers	138945	1051 (2.86-2.82)
RSRZ outliers	127900	1019 (2.86-2.82)

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

Mol	Chain	Length	Quality of chain
1	A	261	89% 6%
1	B	261	89% 6%
1	C	261	89% 6%
1	D	261	87% 8%
1	E	261	% 90% 7%
1	F	261	89% 7%

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Mol	Chain	Length	Quality of chain
1	G	261	90% 7%
1	H	261	90% 7%
1	I	261	91% 6%
1	J	261	89% 6%
1	K	261	89% 8%
1	L	261	89% 7%
1	M	261	89% 7%
1	N	261	89% 8%
1	O	261	91% 5%
1	P	261	89% 7%
1	Q	261	89% 7%
1	R	261	90% 7%
1	S	261	89% 7%
1	T	261	90% 6%
1	U	261	89% 7%
1	V	261	89% 7%
1	W	261	90% 7%
1	X	261	88% 8%
1	Y	261	90% 7%
1	Z	261	90% 6%
1	a	261	88% 8%
1	b	261	89% 5%
1	c	261	89% 6%
1	d	261	90% 8%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 60728 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Acyl-[acyl-carrier-protein]-UDP-N-acetylglucosamine O-acyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	258	Total	C	N	O	S	0	1	0
			1982	1240	367	368	7			
1	B	258	Total	C	N	O	S	0	1	0
			1982	1240	367	368	7			
1	C	257	Total	C	N	O	S	0	1	0
			1974	1235	366	367	6			
1	D	257	Total	C	N	O	S	0	1	0
			1974	1235	366	367	6			
1	E	258	Total	C	N	O	S	0	1	0
			1982	1240	367	368	7			
1	F	257	Total	C	N	O	S	0	1	0
			1974	1235	366	367	6			
1	G	258	Total	C	N	O	S	0	1	0
			1982	1240	367	368	7			
1	H	258	Total	C	N	O	S	0	1	0
			1982	1240	367	368	7			
1	I	258	Total	C	N	O	S	0	1	0
			1982	1240	367	368	7			
1	J	257	Total	C	N	O	S	0	1	0
			1974	1235	366	367	6			
1	K	258	Total	C	N	O	S	0	1	0
			1982	1240	367	368	7			
1	L	258	Total	C	N	O	S	0	1	0
			1982	1240	367	368	7			
1	M	257	Total	C	N	O	S	0	1	0
			1974	1235	366	367	6			
1	N	257	Total	C	N	O	S	0	1	0
			1974	1235	366	367	6			
1	O	257	Total	C	N	O	S	0	1	0
			1974	1235	366	367	6			
1	P	257	Total	C	N	O	S	0	1	0
			1974	1235	366	367	6			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	Q	257	Total	C	N	O	S	0	1	0
			1974	1235	366	367	6			
1	R	258	Total	C	N	O	S	0	1	0
			1982	1240	367	368	7			
1	S	258	Total	C	N	O	S	0	1	0
			1982	1240	367	368	7			
1	T	258	Total	C	N	O	S	0	1	0
			1982	1240	367	368	7			
1	U	259	Total	C	N	O	S	0	1	0
			1992	1246	370	369	7			
1	V	258	Total	C	N	O	S	0	1	0
			1982	1240	367	368	7			
1	W	258	Total	C	N	O	S	0	1	0
			1982	1240	367	368	7			
1	X	259	Total	C	N	O	S	0	2	0
			2003	1252	374	370	7			
1	Y	258	Total	C	N	O	S	0	1	0
			1982	1240	367	368	7			
1	Z	261	Total	C	N	O	S	0	1	0
			2002	1251	372	372	7			
1	a	257	Total	C	N	O	S	0	1	0
			1974	1235	366	367	6			
1	b	257	Total	C	N	O	S	0	1	0
			1974	1235	366	367	6			
1	c	257	Total	C	N	O	S	0	1	0
			1974	1235	366	367	6			
1	d	261	Total	C	N	O	S	0	1	0
			2002	1251	372	372	7			

There are 90 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
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

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Chain	Residue	Modelled	Actual	Comment	Reference
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
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

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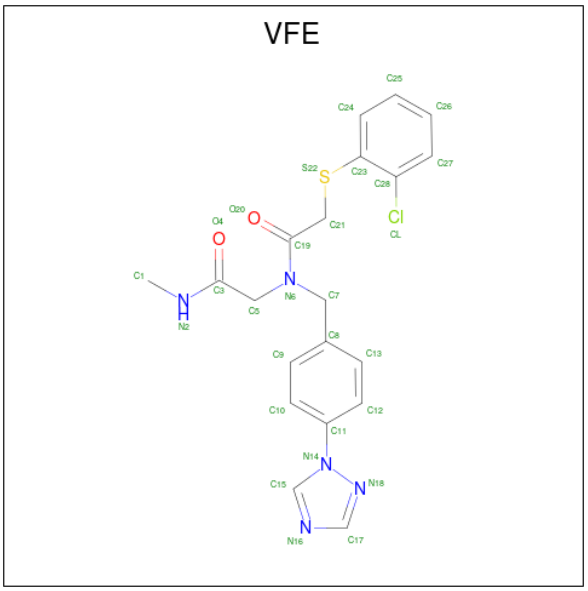
Chain	Residue	Modelled	Actual	Comment	Reference
R	0	HIS	-	expression tag	UNP A6V1E4
S	-2	GLY	-	expression tag	UNP A6V1E4
S	-1	SER	-	expression tag	UNP A6V1E4
S	0	HIS	-	expression tag	UNP A6V1E4
T	-2	GLY	-	expression tag	UNP A6V1E4
T	-1	SER	-	expression tag	UNP A6V1E4
T	0	HIS	-	expression tag	UNP A6V1E4
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
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

- Molecule 2 is 2-[2-(2-chlorophenyl)sulfanylethanoyl-[[4-(1,2,4-triazol-1-yl)phenyl]methyl]amino]-N-methyl-ethanamide (three-letter code: VFE) (formula: $C_{20}H_{20}ClN_5O_2S$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total	C	Cl	N	O	S	0	0
			29	20	1	5	2	1		
2	B	1	Total	C	Cl	N	O	S	0	0
			29	20	1	5	2	1		
2	C	1	Total	C	Cl	N	O	S	0	0
			29	20	1	5	2	1		
2	D	1	Total	C	Cl	N	O	S	0	0
			29	20	1	5	2	1		
2	E	1	Total	C	Cl	N	O	S	0	0
			29	20	1	5	2	1		
2	F	1	Total	C	Cl	N	O	S	0	0
			29	20	1	5	2	1		
2	G	1	Total	C	Cl	N	O	S	0	0
			29	20	1	5	2	1		
2	H	1	Total	C	Cl	N	O	S	0	0
			29	20	1	5	2	1		
2	I	1	Total	C	Cl	N	O	S	0	0
			29	20	1	5	2	1		
2	J	1	Total	C	Cl	N	O	S	0	0
			29	20	1	5	2	1		
2	K	1	Total	C	Cl	N	O	S	0	0
			29	20	1	5	2	1		
2	L	1	Total	C	Cl	N	O	S	0	0
			29	20	1	5	2	1		
2	M	1	Total	C	Cl	N	O	S	0	0
			29	20	1	5	2	1		
2	N	1	Total	C	Cl	N	O	S	0	0
			29	20	1	5	2	1		

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Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	O	1	Total	C	Cl	N	O	S	0	0
			29	20	1	5	2	1		
2	P	1	Total	C	Cl	N	O	S	0	0
			29	20	1	5	2	1		
2	Q	1	Total	C	Cl	N	O	S	0	0
			29	20	1	5	2	1		
2	R	1	Total	C	Cl	N	O	S	0	0
			29	20	1	5	2	1		
2	S	1	Total	C	Cl	N	O	S	0	0
			29	20	1	5	2	1		
2	T	1	Total	C	Cl	N	O	S	0	0
			29	20	1	5	2	1		
2	U	1	Total	C	Cl	N	O	S	0	0
			29	20	1	5	2	1		
2	V	1	Total	C	Cl	N	O	S	0	0
			29	20	1	5	2	1		
2	W	1	Total	C	Cl	N	O	S	0	0
			29	20	1	5	2	1		
2	X	1	Total	C	Cl	N	O	S	0	0
			29	20	1	5	2	1		
2	Y	1	Total	C	Cl	N	O	S	0	0
			29	20	1	5	2	1		
2	Z	1	Total	C	Cl	N	O	S	0	0
			29	20	1	5	2	1		
2	a	1	Total	C	Cl	N	O	S	0	0
			29	20	1	5	2	1		
2	b	1	Total	C	Cl	N	O	S	0	0
			29	20	1	5	2	1		
2	c	1	Total	C	Cl	N	O	S	0	0
			29	20	1	5	2	1		
2	d	1	Total	C	Cl	N	O	S	0	0
			29	20	1	5	2	1		

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	D	1	Total	Mg	0	0
			1	1		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	13	Total O 13 13	0	0
4	B	19	Total O 19 19	0	0
4	C	21	Total O 21 21	0	0
4	D	23	Total O 23 23	0	0
4	E	16	Total O 16 16	0	0
4	F	12	Total O 12 12	0	0
4	G	2	Total O 2 2	0	0
4	H	7	Total O 7 7	0	0
4	I	9	Total O 9 9	0	0
4	J	6	Total O 6 6	0	0
4	K	9	Total O 9 9	0	0
4	L	8	Total O 8 8	0	0
4	M	14	Total O 14 14	0	0
4	N	8	Total O 8 8	0	0
4	O	15	Total O 15 15	0	0
4	P	5	Total O 5 5	0	0
4	Q	11	Total O 11 11	0	0
4	R	10	Total O 10 10	0	0
4	S	15	Total O 15 15	0	0
4	T	17	Total O 17 17	0	0
4	U	19	Total O 19 19	0	0
4	V	13	Total O 13 13	0	0

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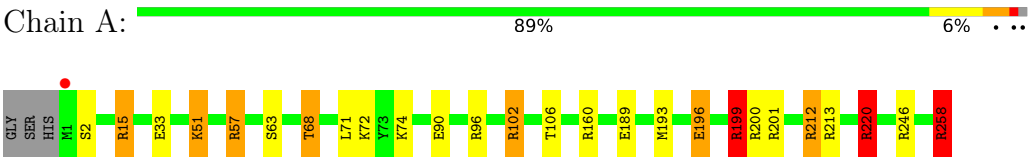
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	W	12	Total O 12 12	0	0
4	X	19	Total O 19 19	0	0
4	Y	24	Total O 24 24	0	0
4	Z	23	Total O 23 23	0	0
4	a	26	Total O 26 26	0	0
4	b	14	Total O 14 14	0	0
4	c	9	Total O 9 9	0	0
4	d	23	Total O 23 23	0	0

3 Residue-property plots (i)

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

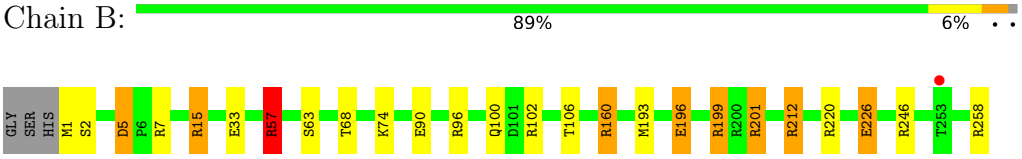
• Molecule 1: Acyl-[acyl-carrier-protein]-UDP-N-acetylglucosamine O-acyltransferase

Chain A:



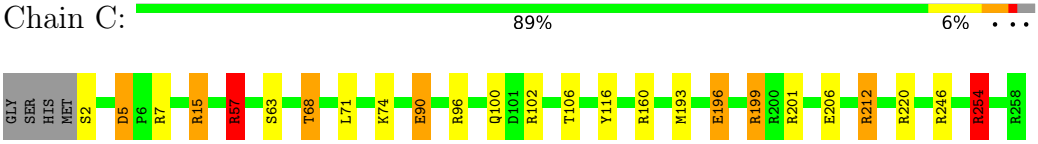
• Molecule 1: Acyl-[acyl-carrier-protein]-UDP-N-acetylglucosamine O-acyltransferase

Chain B:



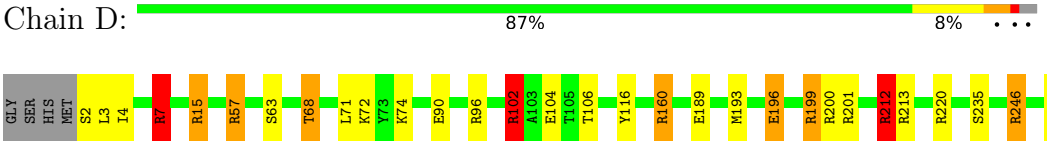
• Molecule 1: Acyl-[acyl-carrier-protein]-UDP-N-acetylglucosamine O-acyltransferase

Chain C:



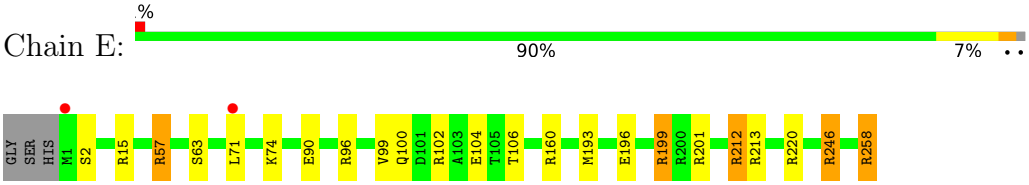
• Molecule 1: Acyl-[acyl-carrier-protein]-UDP-N-acetylglucosamine O-acyltransferase

Chain D:



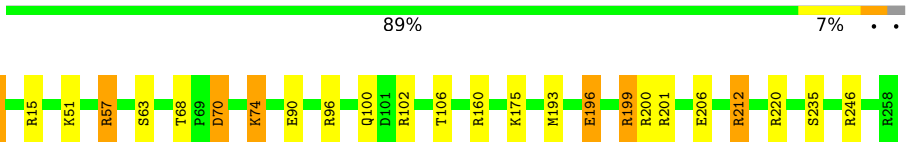
• Molecule 1: Acyl-[acyl-carrier-protein]-UDP-N-acetylglucosamine O-acyltransferase

Chain E:



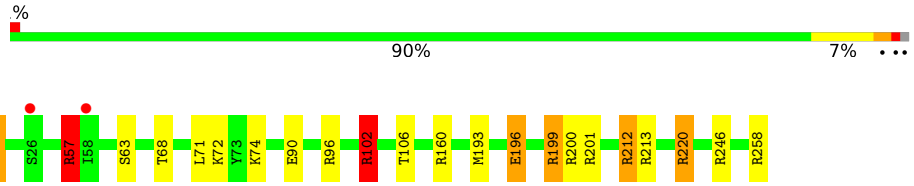
• Molecule 1: Acyl-[acyl-carrier-protein]-UDP-N-acetylglucosamine O-acyltransferase

Chain F:



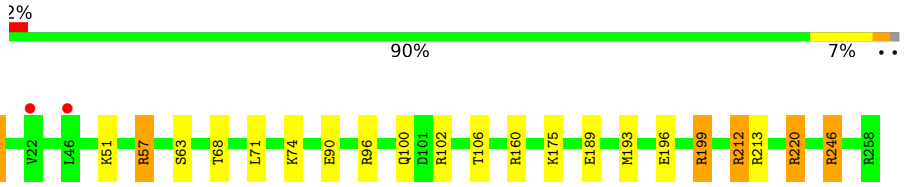
• Molecule 1: Acyl-[acyl-carrier-protein]-UDP-N-acetylglucosamine O-acyltransferase

Chain G:



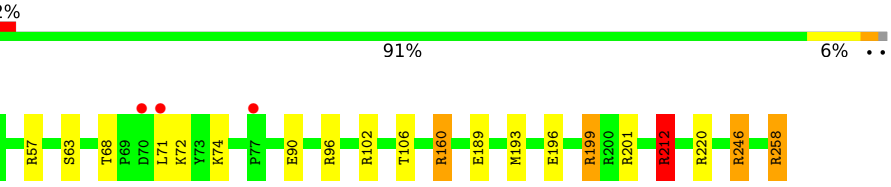
• Molecule 1: Acyl-[acyl-carrier-protein]-UDP-N-acetylglucosamine O-acyltransferase

Chain H:



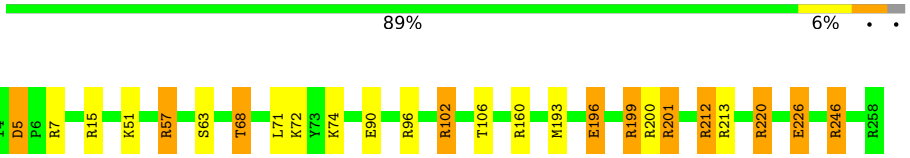
• Molecule 1: Acyl-[acyl-carrier-protein]-UDP-N-acetylglucosamine O-acyltransferase

Chain I:



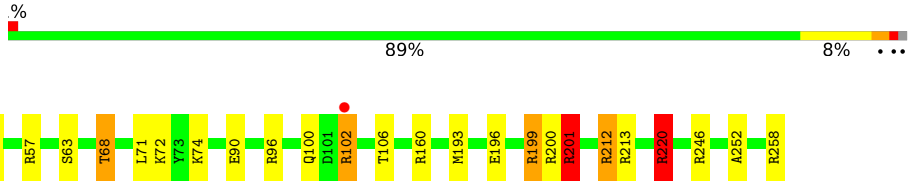
• Molecule 1: Acyl-[acyl-carrier-protein]-UDP-N-acetylglucosamine O-acyltransferase

Chain J:



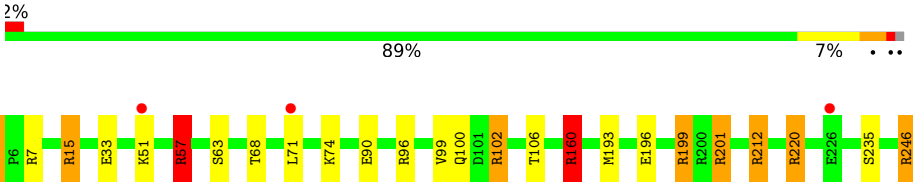
• Molecule 1: Acyl-[acyl-carrier-protein]-UDP-N-acetylglucosamine O-acyltransferase

Chain K:



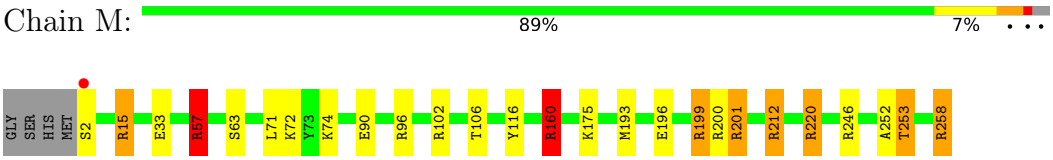
• Molecule 1: Acyl-[acyl-carrier-protein]-UDP-N-acetylglucosamine O-acyltransferase

Chain L:



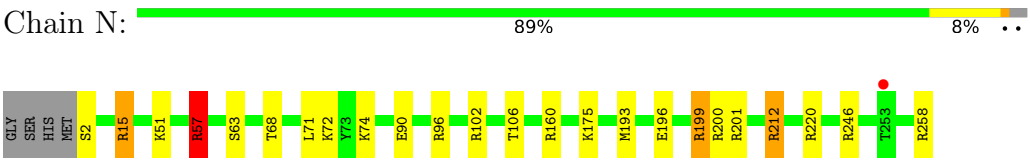
• Molecule 1: Acyl-[acyl-carrier-protein]-UDP-N-acetylglucosamine O-acyltransferase

Chain M:



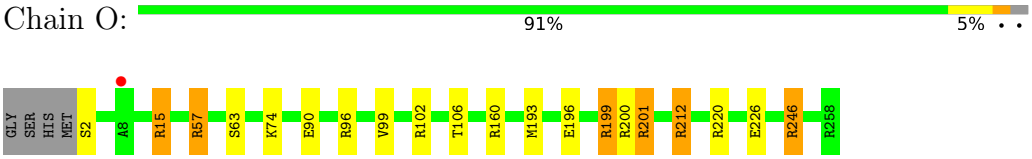
• Molecule 1: Acyl-[acyl-carrier-protein]-UDP-N-acetylglucosamine O-acyltransferase

Chain N:



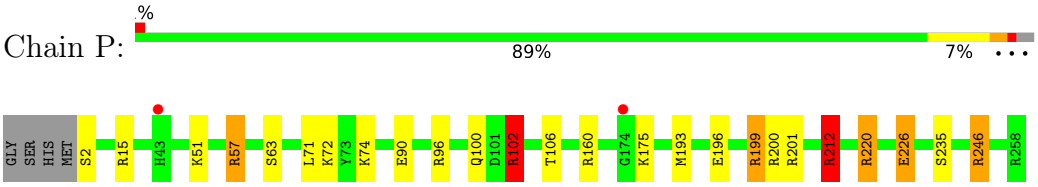
• Molecule 1: Acyl-[acyl-carrier-protein]-UDP-N-acetylglucosamine O-acyltransferase

Chain O:



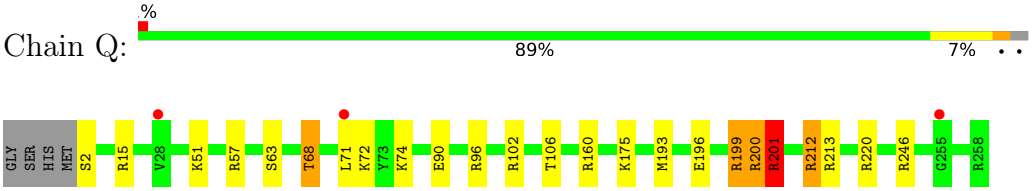
• Molecule 1: Acyl-[acyl-carrier-protein]-UDP-N-acetylglucosamine O-acyltransferase

Chain P:



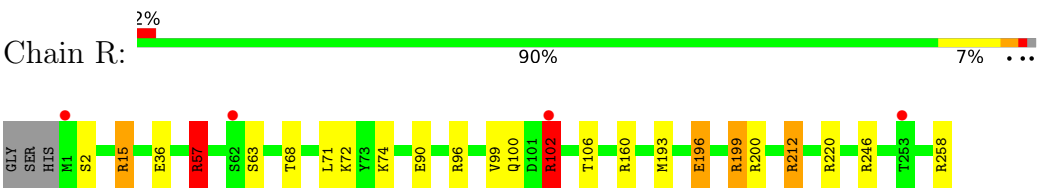
• Molecule 1: Acyl-[acyl-carrier-protein]-UDP-N-acetylglucosamine O-acyltransferase

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

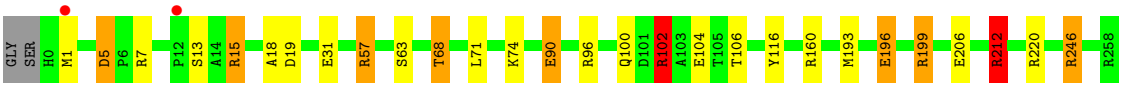
Chain S:

• 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:

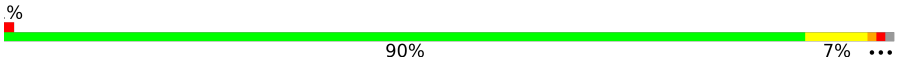


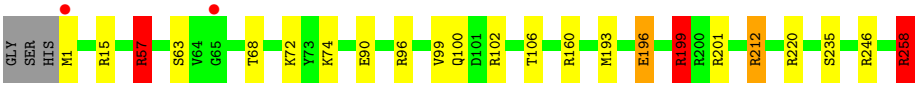
• Molecule 1: Acyl-[acyl-carrier-protein]-UDP-N-acetylglucosamine O-acyltransferase

Chain V:

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

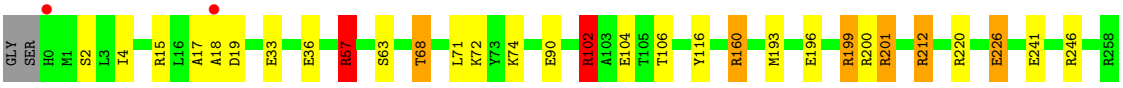
Chain W:





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

Chain X:

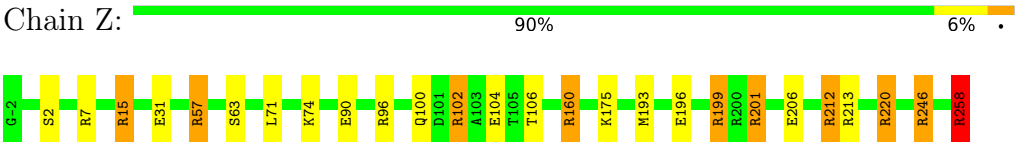


• Molecule 1: Acyl-[acyl-carrier-protein]-UDP-N-acetylglucosamine O-acyltransferase

Chain Y:

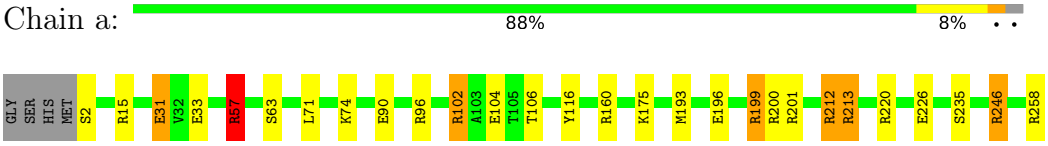
• Molecule 1: Acyl-[acyl-carrier-protein]-UDP-N-acetylglucosamine O-acyltransferase

Chain Z:



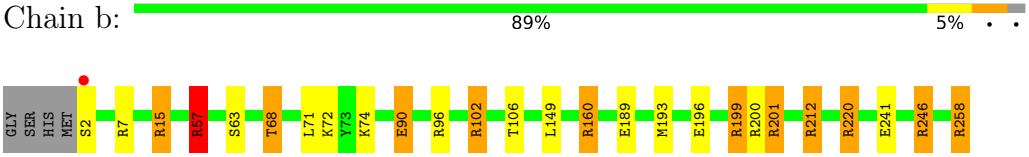
• Molecule 1: Acyl-[acyl-carrier-protein]-UDP-N-acetylglucosamine O-acyltransferase

Chain a:



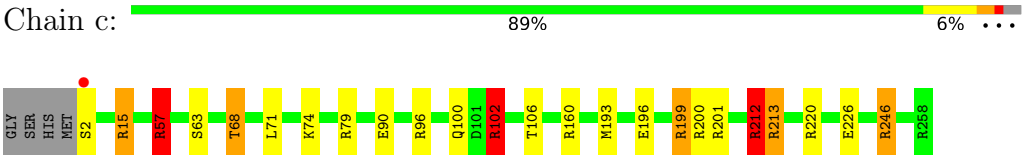
• Molecule 1: Acyl-[acyl-carrier-protein]-UDP-N-acetylglucosamine O-acyltransferase

Chain b:



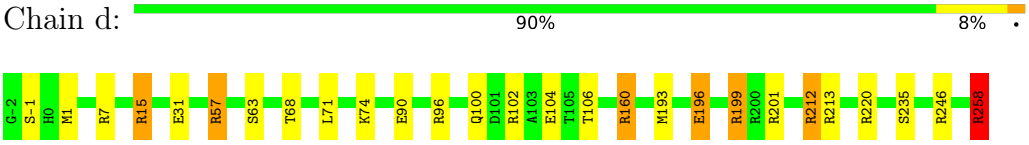
• Molecule 1: Acyl-[acyl-carrier-protein]-UDP-N-acetylglucosamine O-acyltransferase

Chain c:



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

Chain d:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	245.63Å 367.55Å 370.68Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	105.72 – 2.84 105.72 – 2.84	Depositor EDS
% Data completeness (in resolution range)	99.5 (105.72-2.84) 99.5 (105.72-2.84)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.49 (at 2.86Å)	Xtriage
Refinement program	REFMAC 5.8.0222	Depositor
R, R_{free}	0.203 , 0.216 0.206 , 0.219	Depositor DCC
R_{free} test set	19383 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å^2)	45.0	Xtriage
Anisotropy	0.393	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	(Not available) , (Not available)	EDS
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.35$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	60728	wwPDB-VP
Average B, all atoms (Å^2)	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.43% 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: MG, VFE

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	0.78	3/2027 (0.1%)	0.95	15/2748 (0.5%)
1	B	0.84	5/2027 (0.2%)	0.98	8/2748 (0.3%)
1	C	0.82	4/2019 (0.2%)	0.92	10/2738 (0.4%)
1	D	0.78	5/2019 (0.2%)	0.92	11/2738 (0.4%)
1	E	0.77	1/2027 (0.0%)	0.91	8/2748 (0.3%)
1	F	0.79	4/2019 (0.2%)	0.92	10/2738 (0.4%)
1	G	0.71	1/2027 (0.0%)	0.92	13/2748 (0.5%)
1	H	0.70	1/2027 (0.0%)	1.00	9/2748 (0.3%)
1	I	0.75	1/2027 (0.0%)	0.97	9/2748 (0.3%)
1	J	0.76	3/2019 (0.1%)	0.91	9/2738 (0.3%)
1	K	0.70	1/2027 (0.0%)	0.84	5/2748 (0.2%)
1	L	0.78	2/2027 (0.1%)	0.94	12/2748 (0.4%)
1	M	0.77	2/2019 (0.1%)	1.04	19/2738 (0.7%)
1	N	0.70	0/2019	0.86	5/2738 (0.2%)
1	O	0.70	1/2019 (0.0%)	0.88	6/2738 (0.2%)
1	P	0.73	1/2019 (0.0%)	0.92	8/2738 (0.3%)
1	Q	0.70	0/2019	0.97	10/2738 (0.4%)
1	R	0.72	1/2027 (0.0%)	0.91	7/2748 (0.3%)
1	S	0.73	0/2027	0.90	7/2748 (0.3%)
1	T	0.74	0/2027	0.90	6/2748 (0.2%)
1	U	0.90	8/2038 (0.4%)	1.05	18/2763 (0.7%)
1	V	0.74	0/2027	0.87	11/2748 (0.4%)
1	W	0.78	2/2027 (0.1%)	1.02	16/2748 (0.6%)
1	X	0.93	9/2049 (0.4%)	1.06	21/2777 (0.8%)
1	Y	0.76	2/2027 (0.1%)	0.98	14/2748 (0.5%)
1	Z	0.86	5/2048 (0.2%)	0.93	9/2776 (0.3%)
1	a	0.88	5/2019 (0.2%)	0.93	9/2738 (0.3%)
1	b	0.82	4/2019 (0.2%)	0.94	12/2738 (0.4%)
1	c	0.73	1/2019 (0.0%)	1.01	16/2738 (0.6%)
1	d	0.84	6/2048 (0.3%)	0.91	7/2776 (0.3%)
All	All	0.78	78/60789 (0.1%)	0.94	320/82420 (0.4%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	12
1	B	0	11
1	C	0	10
1	D	0	12
1	E	0	9
1	F	0	10
1	G	0	10
1	H	0	11
1	I	0	7
1	J	0	12
1	K	0	13
1	L	0	11
1	M	0	11
1	N	0	10
1	O	0	10
1	P	0	10
1	Q	0	10
1	R	0	9
1	S	0	12
1	T	0	10
1	U	0	11
1	V	0	10
1	W	0	10
1	X	0	9
1	Y	0	6
1	Z	0	11
1	a	0	12
1	b	0	11
1	c	0	10
1	d	0	10
All	All	0	310

All (78) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	a	33	GLU	CD-OE2	14.72	1.41	1.25
1	Z	206	GLU	CD-OE1	9.15	1.35	1.25
1	X	19	ASP	N-CA	9.11	1.64	1.46
1	L	33	GLU	CD-OE2	8.78	1.35	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	196	GLU	CD-OE2	-7.86	1.17	1.25
1	G	196	GLU	CD-OE2	7.85	1.34	1.25
1	U	31	GLU	CD-OE2	-7.78	1.17	1.25
1	X	104	GLU	CD-OE2	7.41	1.33	1.25
1	U	196	GLU	CD-OE2	7.31	1.33	1.25
1	J	2	SER	C-O	-7.21	1.09	1.23
1	F	196	GLU	CD-OE2	7.11	1.33	1.25
1	C	196	GLU	CD-OE1	6.94	1.33	1.25
1	a	226	GLU	CD-OE1	6.94	1.33	1.25
1	B	226	GLU	CD-OE1	6.93	1.33	1.25
1	b	189	GLU	CD-OE1	6.77	1.33	1.25
1	X	18	ALA	C-O	6.75	1.36	1.23
1	M	2	SER	C-O	-6.68	1.10	1.23
1	U	19	ASP	N-CA	6.61	1.59	1.46
1	X	33	GLU	CD-OE2	6.46	1.32	1.25
1	a	104	GLU	CD-OE2	6.42	1.32	1.25
1	J	226	GLU	CD-OE1	-6.39	1.18	1.25
1	A	33	GLU	CD-OE1	-6.33	1.18	1.25
1	U	206	GLU	CD-OE1	6.27	1.32	1.25
1	Y	206	GLU	CD-OE1	6.26	1.32	1.25
1	Z	206	GLU	CD-OE2	6.26	1.32	1.25
1	O	226	GLU	CD-OE1	6.25	1.32	1.25
1	B	33	GLU	CD-OE2	6.22	1.32	1.25
1	Z	2	SER	C-O	6.18	1.35	1.23
1	W	196	GLU	CD-OE1	6.03	1.32	1.25
1	X	36	GLU	CD-OE2	6.01	1.32	1.25
1	X	33	GLU	CD-OE1	6.01	1.32	1.25
1	U	18	ALA	C-O	5.99	1.34	1.23
1	U	13	SER	CB-OG	-5.93	1.34	1.42
1	c	226	GLU	CD-OE1	5.86	1.32	1.25
1	P	235	SER	CA-CB	-5.85	1.44	1.52
1	d	235	SER	CA-CB	-5.80	1.44	1.52
1	B	196	GLU	CD-OE2	5.79	1.32	1.25
1	B	2	SER	CB-OG	-5.75	1.34	1.42
1	F	235	SER	CA-CB	-5.69	1.44	1.52
1	d	104	GLU	CD-OE2	5.65	1.31	1.25
1	F	196	GLU	CD-OE1	5.65	1.31	1.25
1	D	235	SER	CA-CB	-5.64	1.44	1.52
1	F	206	GLU	CD-OE1	5.64	1.31	1.25
1	W	235	SER	CA-CB	-5.63	1.44	1.52
1	a	235	SER	CA-CB	-5.61	1.44	1.52
1	d	31	GLU	CD-OE2	5.59	1.31	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	M	33	GLU	CD-OE2	5.55	1.31	1.25
1	X	241	GLU	CD-OE1	5.55	1.31	1.25
1	L	235	SER	CA-CB	-5.55	1.44	1.52
1	K	201	ARG	NE-CZ	5.55	1.40	1.33
1	U	104	GLU	CD-OE2	5.53	1.31	1.25
1	d	31	GLU	CD-OE1	5.51	1.31	1.25
1	a	31	GLU	CB-CG	5.51	1.62	1.52
1	R	36	GLU	CD-OE2	5.44	1.31	1.25
1	b	201	ARG	CG-CD	5.40	1.65	1.51
1	C	5	ASP	CG-OD1	-5.38	1.12	1.25
1	Z	104	GLU	CD-OE2	5.37	1.31	1.25
1	X	2	SER	CA-CB	-5.36	1.45	1.52
1	d	196	GLU	CD-OE2	5.33	1.31	1.25
1	Z	31	GLU	CD-OE1	5.33	1.31	1.25
1	d	7	ARG	NE-CZ	-5.30	1.26	1.33
1	H	189	GLU	CD-OE1	5.29	1.31	1.25
1	D	189	GLU	CD-OE2	5.28	1.31	1.25
1	A	189	GLU	CD-OE1	5.28	1.31	1.25
1	J	196	GLU	CD-OE1	5.27	1.31	1.25
1	B	196	GLU	CD-OE1	5.26	1.31	1.25
1	D	102	ARG	CG-CD	5.26	1.65	1.51
1	E	104	GLU	CD-OE2	5.25	1.31	1.25
1	X	33	GLU	CG-CD	5.25	1.59	1.51
1	C	90	GLU	CD-OE2	5.24	1.31	1.25
1	Y	104	GLU	CD-OE2	5.22	1.31	1.25
1	I	189	GLU	CD-OE1	5.20	1.31	1.25
1	D	104	GLU	CD-OE2	5.19	1.31	1.25
1	b	90	GLU	CD-OE2	5.17	1.31	1.25
1	C	206	GLU	CD-OE1	5.15	1.31	1.25
1	b	241	GLU	CD-OE1	5.10	1.31	1.25
1	U	90	GLU	CD-OE2	5.08	1.31	1.25
1	D	196	GLU	CD-OE1	5.03	1.31	1.25

All (320) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	246	ARG	CG-CD-NE	-17.93	74.15	111.80
1	H	199	ARG	CG-CD-NE	-17.18	75.72	111.80
1	W	199	ARG	NE-CZ-NH2	17.14	128.87	120.30
1	H	199	ARG	NE-CZ-NH1	-16.52	112.04	120.30
1	Q	201	ARG	NE-CZ-NH1	-15.91	112.34	120.30
1	Y	220	ARG	NE-CZ-NH2	-15.00	112.80	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	I	246	ARG	CG-CD-NE	-13.50	83.45	111.80
1	D	102	ARG	CG-CD-NE	12.62	138.30	111.80
1	M	57[A]	ARG	NE-CZ-NH1	-12.03	114.28	120.30
1	M	57[B]	ARG	NE-CZ-NH1	-12.03	114.28	120.30
1	I	246	ARG	NE-CZ-NH2	11.17	125.89	120.30
1	F	70	ASP	CB-CG-OD2	10.93	128.14	118.30
1	a	15	ARG	NE-CZ-NH1	10.79	125.69	120.30
1	T	57[A]	ARG	CG-CD-NE	10.48	133.80	111.80
1	T	57[B]	ARG	CG-CD-NE	10.48	133.80	111.80
1	S	15	ARG	CG-CD-NE	10.24	133.31	111.80
1	Y	201	ARG	CD-NE-CZ	10.09	137.72	123.60
1	A	199	ARG	NE-CZ-NH2	-9.97	115.31	120.30
1	Q	200	ARG	NE-CZ-NH2	-9.93	115.34	120.30
1	Q	200	ARG	NE-CZ-NH1	9.66	125.13	120.30
1	U	15	ARG	NE-CZ-NH2	-9.60	115.50	120.30
1	W	199	ARG	NE-CZ-NH1	-9.44	115.58	120.30
1	M	15	ARG	NE-CZ-NH2	9.41	125.00	120.30
1	Y	160	ARG	CB-CG-CD	9.23	135.61	111.60
1	M	57[A]	ARG	NE-CZ-NH2	9.18	124.89	120.30
1	M	57[B]	ARG	NE-CZ-NH2	9.18	124.89	120.30
1	c	213	ARG	NE-CZ-NH1	-9.12	115.74	120.30
1	P	57[A]	ARG	NE-CZ-NH1	-8.95	115.82	120.30
1	P	57[B]	ARG	NE-CZ-NH1	-8.95	115.82	120.30
1	L	15	ARG	NE-CZ-NH1	8.82	124.71	120.30
1	U	57[A]	ARG	NE-CZ-NH1	8.79	124.70	120.30
1	U	57[B]	ARG	NE-CZ-NH1	8.79	124.70	120.30
1	L	57[A]	ARG	CG-CD-NE	8.71	130.10	111.80
1	L	57[B]	ARG	CG-CD-NE	8.71	130.10	111.80
1	U	7	ARG	NE-CZ-NH1	-8.70	115.95	120.30
1	c	201	ARG	NE-CZ-NH1	-8.66	115.97	120.30
1	P	57[A]	ARG	NE-CZ-NH2	8.65	124.62	120.30
1	P	57[B]	ARG	NE-CZ-NH2	8.65	124.62	120.30
1	U	102	ARG	CB-CG-CD	8.61	133.99	111.60
1	I	246	ARG	NE-CZ-NH1	-8.57	116.01	120.30
1	X	102[A]	ARG	CB-CG-CD	8.55	133.83	111.60
1	X	102[B]	ARG	CB-CG-CD	8.55	133.83	111.60
1	Y	102	ARG	CB-CG-CD	8.47	133.63	111.60
1	R	57[A]	ARG	CG-CD-NE	8.43	129.50	111.80
1	R	57[B]	ARG	CG-CD-NE	8.43	129.50	111.80
1	c	57[A]	ARG	NE-CZ-NH1	8.42	124.51	120.30
1	c	57[B]	ARG	NE-CZ-NH1	8.42	124.51	120.30
1	c	102	ARG	CB-CG-CD	8.42	133.48	111.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	c	79	ARG	NE-CZ-NH1	8.28	124.44	120.30
1	b	15	ARG	NE-CZ-NH2	8.15	124.37	120.30
1	R	196	GLU	OE1-CD-OE2	-8.12	113.55	123.30
1	F	70	ASP	CB-CG-OD1	-8.04	111.06	118.30
1	D	160	ARG	NE-CZ-NH1	7.97	124.28	120.30
1	b	201	ARG	CB-CG-CD	7.92	132.20	111.60
1	W	57[A]	ARG	CB-CG-CD	7.89	132.12	111.60
1	W	57[B]	ARG	CB-CG-CD	7.89	132.12	111.60
1	K	220	ARG	CB-CG-CD	7.88	132.09	111.60
1	X	106	THR	CA-CB-OG1	7.88	125.55	109.00
1	V	102	ARG	CB-CG-CD	7.82	131.94	111.60
1	D	106	THR	CA-CB-OG1	7.78	125.33	109.00
1	c	201	ARG	CG-CD-NE	-7.78	95.47	111.80
1	A	15	ARG	NE-CZ-NH2	-7.77	116.41	120.30
1	G	57[A]	ARG	NE-CZ-NH1	-7.69	116.45	120.30
1	G	57[B]	ARG	NE-CZ-NH1	-7.69	116.45	120.30
1	Y	160	ARG	CA-CB-CG	7.68	130.29	113.40
1	c	201	ARG	CD-NE-CZ	7.64	134.30	123.60
1	c	15	ARG	NE-CZ-NH2	7.63	124.11	120.30
1	X	57[A]	ARG	NE-CZ-NH1	-7.59	116.50	120.30
1	X	57[B]	ARG	NE-CZ-NH1	-7.59	116.50	120.30
1	X	18	ALA	C-N-CA	7.53	140.51	121.70
1	A	199	ARG	NE-CZ-NH1	7.50	124.05	120.30
1	A	201	ARG	NE-CZ-NH2	-7.50	116.55	120.30
1	D	102	ARG	NE-CZ-NH2	7.50	124.05	120.30
1	Y	220	ARG	NE-CZ-NH1	7.43	124.02	120.30
1	d	15	ARG	NE-CZ-NH2	7.42	124.01	120.30
1	b	7	ARG	NE-CZ-NH2	-7.41	116.59	120.30
1	c	79	ARG	CG-CD-NE	-7.41	96.24	111.80
1	Z	7	ARG	NE-CZ-NH2	-7.40	116.60	120.30
1	d	1	MET	CG-SD-CE	7.38	112.01	100.20
1	A	57[A]	ARG	NE-CZ-NH1	7.37	123.98	120.30
1	A	57[B]	ARG	NE-CZ-NH1	7.37	123.98	120.30
1	L	201	ARG	CB-CG-CD	7.37	130.75	111.60
1	X	15	ARG	NE-CZ-NH1	-7.37	116.62	120.30
1	U	18	ALA	C-N-CA	7.34	140.06	121.70
1	d	201	ARG	NE-CZ-NH2	-7.33	116.64	120.30
1	W	57[A]	ARG	NE-CZ-NH1	-7.32	116.64	120.30
1	W	57[B]	ARG	NE-CZ-NH1	-7.32	116.64	120.30
1	W	258	ARG	NE-CZ-NH1	-7.31	116.64	120.30
1	X	57[A]	ARG	NE-CZ-NH2	7.31	123.95	120.30
1	X	57[B]	ARG	NE-CZ-NH2	7.31	123.95	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	H	199	ARG	CD-NE-CZ	7.30	133.83	123.60
1	W	201	ARG	NE-CZ-NH2	-7.30	116.65	120.30
1	R	102	ARG	CB-CG-CD	7.29	130.55	111.60
1	E	106	THR	CA-CB-OG1	7.29	124.30	109.00
1	Z	15	ARG	NE-CZ-NH2	7.25	123.92	120.30
1	F	57[A]	ARG	NE-CZ-NH1	7.22	123.91	120.30
1	F	57[B]	ARG	NE-CZ-NH1	7.22	123.91	120.30
1	P	102	ARG	NE-CZ-NH2	-7.21	116.69	120.30
1	R	15	ARG	NE-CZ-NH2	7.19	123.90	120.30
1	U	106	THR	CA-CB-OG1	7.15	124.01	109.00
1	B	5	ASP	CB-CG-OD1	-7.14	111.87	118.30
1	C	57[A]	ARG	CB-CG-CD	7.13	130.15	111.60
1	C	57[B]	ARG	CB-CG-CD	7.13	130.15	111.60
1	X	201	ARG	CB-CG-CD	7.08	130.01	111.60
1	Q	57[A]	ARG	NE-CZ-NH1	7.07	123.84	120.30
1	Q	57[B]	ARG	NE-CZ-NH1	7.07	123.84	120.30
1	H	199	ARG	NE-CZ-NH2	-7.06	116.77	120.30
1	W	160	ARG	NE-CZ-NH2	7.04	123.82	120.30
1	Y	106	THR	CA-CB-OG1	7.03	123.76	109.00
1	Q	201	ARG	NE-CZ-NH2	7.00	123.80	120.30
1	I	212	ARG	NE-CZ-NH2	-6.99	116.80	120.30
1	E	201	ARG	CD-NE-CZ	6.97	133.35	123.60
1	b	258	ARG	CB-CG-CD	6.95	129.67	111.60
1	L	160	ARG	CB-CG-CD	6.94	129.65	111.60
1	W	57[A]	ARG	NE-CZ-NH2	6.94	123.77	120.30
1	W	57[B]	ARG	NE-CZ-NH2	6.94	123.77	120.30
1	H	220	ARG	NE-CZ-NH2	6.90	123.75	120.30
1	V	99	VAL	CA-CB-CG2	-6.90	100.56	110.90
1	U	5	ASP	CB-CG-OD1	-6.89	112.10	118.30
1	O	201	ARG	CB-CG-CD	6.83	129.35	111.60
1	S	68	THR	CA-CB-CG2	6.83	121.96	112.40
1	Z	7	ARG	NE-CZ-NH1	6.83	123.71	120.30
1	H	15	ARG	NE-CZ-NH2	6.82	123.71	120.30
1	W	99	VAL	CA-CB-CG2	-6.82	100.67	110.90
1	O	99	VAL	CA-CB-CG2	-6.81	100.68	110.90
1	Y	201	ARG	CG-CD-NE	6.81	126.11	111.80
1	E	99	VAL	CA-CB-CG2	-6.80	100.70	110.90
1	Y	68	THR	CA-CB-CG2	6.79	121.91	112.40
1	d	160	ARG	CB-CG-CD	6.79	129.25	111.60
1	d	258	ARG	NE-CZ-NH2	-6.78	116.91	120.30
1	b	68	THR	CA-CB-CG2	6.78	121.89	112.40
1	L	99	VAL	CA-CB-CG2	-6.76	100.76	110.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	a	106	THR	CA-CB-OG1	6.75	123.17	109.00
1	G	201	ARG	NE-CZ-NH2	-6.74	116.93	120.30
1	U	68	THR	CA-CB-CG2	6.73	121.83	112.40
1	b	106	THR	CA-CB-OG1	6.72	123.12	109.00
1	E	57[A]	ARG	CB-CG-CD	6.71	129.06	111.60
1	E	57[B]	ARG	CB-CG-CD	6.71	129.06	111.60
1	Y	160	ARG	CG-CD-NE	6.71	125.90	111.80
1	c	57[A]	ARG	NE-CZ-NH2	-6.71	116.95	120.30
1	c	57[B]	ARG	NE-CZ-NH2	-6.71	116.95	120.30
1	L	7	ARG	NE-CZ-NH2	-6.70	116.95	120.30
1	B	160	ARG	NE-CZ-NH2	-6.70	116.95	120.30
1	N	15	ARG	NE-CZ-NH2	6.69	123.65	120.30
1	X	15	ARG	NE-CZ-NH2	6.64	123.62	120.30
1	G	15	ARG	NE-CZ-NH2	6.62	123.61	120.30
1	M	57[A]	ARG	CD-NE-CZ	6.61	132.85	123.60
1	M	57[B]	ARG	CD-NE-CZ	6.61	132.85	123.60
1	J	2	SER	CA-C-O	-6.61	106.22	120.10
1	H	57[A]	ARG	NE-CZ-NH1	6.59	123.59	120.30
1	H	57[B]	ARG	NE-CZ-NH1	6.59	123.59	120.30
1	B	57[A]	ARG	CB-CG-CD	6.56	128.67	111.60
1	B	57[B]	ARG	CB-CG-CD	6.56	128.67	111.60
1	F	74	LYS	CA-CB-CG	6.56	127.84	113.40
1	C	7	ARG	NE-CZ-NH2	-6.56	117.02	120.30
1	R	57[A]	ARG	NE-CZ-NH1	6.53	123.57	120.30
1	R	57[B]	ARG	NE-CZ-NH1	6.53	123.57	120.30
1	G	57[A]	ARG	CB-CG-CD	6.53	128.58	111.60
1	G	57[B]	ARG	CB-CG-CD	6.53	128.58	111.60
1	D	15	ARG	NE-CZ-NH2	6.46	123.53	120.30
1	a	57[A]	ARG	NE-CZ-NH2	-6.45	117.08	120.30
1	a	57[B]	ARG	NE-CZ-NH2	-6.45	117.08	120.30
1	X	68	THR	CA-CB-CG2	6.44	121.41	112.40
1	I	57[A]	ARG	NE-CZ-NH1	6.43	123.52	120.30
1	I	57[B]	ARG	NE-CZ-NH1	6.43	123.52	120.30
1	M	57[A]	ARG	CG-CD-NE	-6.42	98.31	111.80
1	M	57[B]	ARG	CG-CD-NE	-6.42	98.31	111.80
1	Z	106	THR	CA-CB-OG1	6.42	122.48	109.00
1	J	201	ARG	NE-CZ-NH1	6.42	123.51	120.30
1	W	57[A]	ARG	CD-NE-CZ	6.42	132.58	123.60
1	W	57[B]	ARG	CD-NE-CZ	6.42	132.58	123.60
1	F	5	ASP	CB-CG-OD1	-6.41	112.54	118.30
1	J	57[A]	ARG	NE-CZ-NH1	6.38	123.49	120.30
1	J	57[B]	ARG	NE-CZ-NH1	6.38	123.49	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	T	68	THR	CA-CB-CG2	6.37	121.31	112.40
1	Z	201	ARG	CB-CG-CD	6.36	128.14	111.60
1	X	116	TYR	CB-CG-CD2	6.35	124.81	121.00
1	J	7	ARG	NE-CZ-NH1	-6.35	117.13	120.30
1	Z	201	ARG	CD-NE-CZ	6.28	132.40	123.60
1	A	258	ARG	CG-CD-NE	6.27	124.97	111.80
1	I	258	ARG	CG-CD-NE	6.27	124.96	111.80
1	C	201	ARG	CD-NE-CZ	6.25	132.35	123.60
1	M	2	SER	CA-C-O	-6.25	106.97	120.10
1	Q	201	ARG	CD-NE-CZ	6.25	132.35	123.60
1	S	57[A]	ARG	NE-CZ-NH1	6.24	123.42	120.30
1	S	57[B]	ARG	NE-CZ-NH1	6.24	123.42	120.30
1	L	102	ARG	NE-CZ-NH1	-6.24	117.18	120.30
1	T	201	ARG	CB-CG-CD	6.24	127.83	111.60
1	O	57[A]	ARG	NE-CZ-NH1	6.22	123.41	120.30
1	O	57[B]	ARG	NE-CZ-NH1	6.22	123.41	120.30
1	X	18	ALA	CA-C-N	-6.20	103.57	117.20
1	C	15	ARG	NE-CZ-NH2	6.19	123.39	120.30
1	G	57[A]	ARG	NE-CZ-NH2	6.12	123.36	120.30
1	G	57[B]	ARG	NE-CZ-NH2	6.12	123.36	120.30
1	J	226	GLU	CA-CB-CG	6.12	126.87	113.40
1	L	201	ARG	CD-NE-CZ	6.12	132.16	123.60
1	b	220	ARG	CB-CG-CD	6.08	127.42	111.60
1	P	226	GLU	CA-CB-CG	6.08	126.77	113.40
1	U	212	ARG	NE-CZ-NH1	-6.06	117.27	120.30
1	F	201	ARG	NE-CZ-NH2	-6.06	117.27	120.30
1	J	5	ASP	CB-CG-OD1	-6.05	112.85	118.30
1	U	15	ARG	CG-CD-NE	6.03	124.46	111.80
1	W	235	SER	N-CA-CB	6.01	119.52	110.50
1	Q	200	ARG	CD-NE-CZ	6.01	132.01	123.60
1	D	7	ARG	CA-CB-CG	5.99	126.57	113.40
1	C	254	ARG	CG-CD-NE	5.96	124.32	111.80
1	U	102	ARG	CG-CD-NE	5.96	124.31	111.80
1	M	201	ARG	CB-CG-CD	5.94	127.05	111.60
1	U	7	ARG	NE-CZ-NH2	5.93	123.26	120.30
1	O	15	ARG	NE-CZ-NH2	5.92	123.26	120.30
1	b	57[A]	ARG	NE-CZ-NH1	-5.88	117.36	120.30
1	b	57[B]	ARG	NE-CZ-NH1	-5.88	117.36	120.30
1	C	116	TYR	CB-CG-CD2	5.88	124.53	121.00
1	Y	102	ARG	CG-CD-NE	5.87	124.13	111.80
1	A	51	LYS	CA-CB-CG	5.87	126.30	113.40
1	Z	258	ARG	NE-CZ-NH2	-5.86	117.37	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	226	GLU	CA-CB-CG	5.85	126.27	113.40
1	V	220	ARG	CA-CB-CG	5.85	126.27	113.40
1	d	201	ARG	CD-NE-CZ	5.85	131.79	123.60
1	E	57[A]	ARG	NE-CZ-NH2	5.83	123.22	120.30
1	E	57[B]	ARG	NE-CZ-NH2	5.83	123.22	120.30
1	N	57[A]	ARG	NE-CZ-NH2	-5.80	117.40	120.30
1	N	57[B]	ARG	NE-CZ-NH2	-5.80	117.40	120.30
1	F	201	ARG	CD-NE-CZ	5.80	131.72	123.60
1	O	201	ARG	CD-NE-CZ	5.79	131.70	123.60
1	M	253	THR	OG1-CB-CG2	5.77	123.27	110.00
1	L	235	SER	N-CA-CB	5.73	119.09	110.50
1	a	201	ARG	CD-NE-CZ	5.73	131.62	123.60
1	A	74	LYS	CA-CB-CG	5.72	125.98	113.40
1	Z	102	ARG	NE-CZ-NH1	-5.72	117.44	120.30
1	U	1	MET	CG-SD-CE	5.71	109.34	100.20
1	a	116	TYR	CB-CG-CD2	5.71	124.42	121.00
1	I	160	ARG	NE-CZ-NH2	5.70	123.15	120.30
1	L	102	ARG	NE-CZ-NH2	5.68	123.14	120.30
1	B	201	ARG	CD-NE-CZ	5.64	131.49	123.60
1	A	15	ARG	NE-CZ-NH1	5.62	123.11	120.30
1	b	57[A]	ARG	CA-CB-CG	5.60	125.71	113.40
1	b	57[B]	ARG	CA-CB-CG	5.60	125.71	113.40
1	L	5	ASP	CB-CG-OD1	-5.59	113.27	118.30
1	N	201	ARG	CD-NE-CZ	5.59	131.43	123.60
1	a	235	SER	N-CA-CB	5.59	118.89	110.50
1	G	57[A]	ARG	CD-NE-CZ	5.58	131.41	123.60
1	G	57[B]	ARG	CD-NE-CZ	5.58	131.41	123.60
1	M	116	TYR	CB-CG-CD2	5.58	124.35	121.00
1	P	201	ARG	CD-NE-CZ	5.57	131.40	123.60
1	A	220	ARG	NE-CZ-NH2	5.54	123.07	120.30
1	K	201	ARG	NE-CZ-NH1	5.54	123.07	120.30
1	X	57[A]	ARG	CG-CD-NE	5.54	123.43	111.80
1	X	57[B]	ARG	CG-CD-NE	5.54	123.43	111.80
1	D	212	ARG	NE-CZ-NH1	-5.52	117.54	120.30
1	C	57[A]	ARG	CD-NE-CZ	5.51	131.32	123.60
1	C	57[B]	ARG	CD-NE-CZ	5.51	131.32	123.60
1	U	116	TYR	CB-CG-CD2	5.51	124.31	121.00
1	V	7	ARG	NE-CZ-NH2	-5.49	117.56	120.30
1	E	258	ARG	NE-CZ-NH2	-5.48	117.56	120.30
1	I	201	ARG	CD-NE-CZ	5.46	131.25	123.60
1	S	102	ARG	NE-CZ-NH2	-5.45	117.58	120.30
1	U	18	ALA	CA-C-N	-5.45	105.21	117.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	P	212	ARG	CG-CD-NE	-5.44	100.37	111.80
1	A	51	LYS	CB-CG-CD	5.44	125.74	111.60
1	H	199	ARG	NH1-CZ-NH2	5.43	125.38	119.40
1	F	200	ARG	NE-CZ-NH1	-5.42	117.59	120.30
1	T	160	ARG	NE-CZ-NH2	5.42	123.01	120.30
1	M	160	ARG	NE-CZ-NH1	5.41	123.00	120.30
1	G	201	ARG	CD-NE-CZ	5.40	131.16	123.60
1	B	201	ARG	CB-CG-CD	5.38	125.60	111.60
1	W	201	ARG	CD-NE-CZ	5.37	131.12	123.60
1	M	72	LYS	CB-CG-CD	5.36	125.53	111.60
1	D	116	TYR	CB-CG-CD2	5.34	124.20	121.00
1	K	201	ARG	CB-CG-CD	5.33	125.47	111.60
1	c	102	ARG	NE-CZ-NH1	-5.33	117.64	120.30
1	V	68	THR	OG1-CB-CG2	5.33	122.25	110.00
1	S	212	ARG	NE-CZ-NH1	-5.32	117.64	120.30
1	T	201	ARG	CD-NE-CZ	5.31	131.03	123.60
1	V	57[A]	ARG	CA-CB-CG	5.30	125.07	113.40
1	V	57[B]	ARG	CA-CB-CG	5.30	125.07	113.40
1	G	200	ARG	NE-CZ-NH1	-5.29	117.66	120.30
1	V	220	ARG	CB-CG-CD	5.28	125.33	111.60
1	V	258	ARG	CB-CG-CD	5.28	125.33	111.60
1	d	235	SER	N-CA-CB	5.24	118.36	110.50
1	X	160	ARG	NE-CZ-NH2	5.23	122.92	120.30
1	A	68	THR	OG1-CB-CG2	5.23	122.02	110.00
1	A	201	ARG	CD-NE-CZ	5.22	130.91	123.60
1	c	68	THR	OG1-CB-CG2	5.22	122.01	110.00
1	V	201	ARG	CD-NE-CZ	5.22	130.91	123.60
1	Z	160	ARG	NE-CZ-NH2	5.21	122.91	120.30
1	Q	200	ARG	CB-CG-CD	5.21	125.15	111.60
1	M	160	ARG	CB-CG-CD	5.20	125.11	111.60
1	c	212	ARG	CG-CD-NE	-5.19	100.89	111.80
1	G	102	ARG	NE-CZ-NH1	5.16	122.88	120.30
1	X	201	ARG	CD-NE-CZ	5.16	130.82	123.60
1	a	15	ARG	NH1-CZ-NH2	-5.15	113.74	119.40
1	M	258	ARG	NE-CZ-NH2	-5.14	117.73	120.30
1	J	68	THR	OG1-CB-CG2	5.13	121.80	110.00
1	F	235	SER	N-CA-CB	5.13	118.19	110.50
1	Q	68	THR	OG1-CB-CG2	5.12	121.78	110.00
1	D	235	SER	N-CA-CB	5.12	118.17	110.50
1	X	226	GLU	CA-CB-CG	5.11	124.65	113.40
1	K	68	THR	OG1-CB-CG2	5.11	121.75	110.00
1	S	201	ARG	CD-NE-CZ	5.11	130.75	123.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	J	2	SER	CA-C-N	5.11	128.43	117.20
1	C	68	THR	OG1-CB-CG2	5.10	121.74	110.00
1	U	15	ARG	CA-CB-CG	-5.10	102.18	113.40
1	D	68	THR	OG1-CB-CG2	5.09	121.71	110.00
1	M	2	SER	CA-C-N	5.09	128.40	117.20
1	a	213	ARG	NE-CZ-NH1	-5.08	117.76	120.30
1	K	102	ARG	NE-CZ-NH2	5.07	122.83	120.30
1	N	201	ARG	NE-CZ-NH2	-5.07	117.77	120.30
1	D	201	ARG	CD-NE-CZ	5.06	130.69	123.60
1	Y	102	ARG	CA-CB-CG	5.05	124.52	113.40
1	U	7	ARG	CD-NE-CZ	5.04	130.66	123.60
1	X	102[A]	ARG	NE-CZ-NH2	5.04	122.82	120.30
1	X	102[B]	ARG	NE-CZ-NH2	5.04	122.82	120.30
1	M	160	ARG	CG-CD-NE	5.04	122.39	111.80
1	A	15	ARG	CG-CD-NE	-5.04	101.23	111.80
1	Y	201	ARG	CB-CG-CD	5.04	124.69	111.60
1	Y	201	ARG	NE-CZ-NH1	-5.03	117.78	120.30
1	V	102	ARG	CA-CB-CG	5.02	124.45	113.40
1	b	258	ARG	NE-CZ-NH2	-5.00	117.80	120.30
1	c	246	ARG	NE-CZ-NH2	-5.00	117.80	120.30

There are no chirality outliers.

All (310) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	102	ARG	Sidechain
1	A	15	ARG	Sidechain
1	A	160	ARG	Sidechain
1	A	199	ARG	Sidechain
1	A	200	ARG	Sidechain
1	A	212	ARG	Sidechain
1	A	213	ARG	Sidechain
1	A	220	ARG	Sidechain
1	A	258	ARG	Sidechain
1	A	57[A]	ARG	Sidechain
1	A	57[B]	ARG	Sidechain
1	A	96	ARG	Sidechain
1	B	102	ARG	Sidechain
1	B	15	ARG	Sidechain
1	B	160	ARG	Sidechain
1	B	199	ARG	Sidechain
1	B	212	ARG	Sidechain

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Mol	Chain	Res	Type	Group
1	B	220	ARG	Sidechain
1	B	5	ASP	Sidechain
1	B	57[A]	ARG	Sidechain
1	B	57[B]	ARG	Sidechain
1	B	7	ARG	Sidechain
1	B	96	ARG	Sidechain
1	C	102	ARG	Sidechain
1	C	160	ARG	Sidechain
1	C	199	ARG	Sidechain
1	C	212	ARG	Sidechain
1	C	220	ARG	Sidechain
1	C	254	ARG	Sidechain
1	C	5	ASP	Sidechain
1	C	57[A]	ARG	Sidechain
1	C	57[B]	ARG	Sidechain
1	C	96	ARG	Sidechain
1	D	102	ARG	Sidechain
1	D	160	ARG	Sidechain
1	D	199	ARG	Sidechain
1	D	200	ARG	Sidechain
1	D	212	ARG	Sidechain
1	D	213	ARG	Sidechain
1	D	220	ARG	Sidechain
1	D	246	ARG	Sidechain
1	D	57[A]	ARG	Sidechain
1	D	57[B]	ARG	Sidechain
1	D	7	ARG	Sidechain
1	D	96	ARG	Sidechain
1	E	102	ARG	Sidechain
1	E	15	ARG	Sidechain
1	E	160	ARG	Sidechain
1	E	199	ARG	Sidechain
1	E	212	ARG	Sidechain
1	E	213	ARG	Sidechain
1	E	220	ARG	Sidechain
1	E	246	ARG	Sidechain
1	E	96	ARG	Sidechain
1	F	102	ARG	Sidechain
1	F	15	ARG	Sidechain
1	F	160	ARG	Sidechain
1	F	199	ARG	Sidechain
1	F	212	ARG	Sidechain

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Mol	Chain	Res	Type	Group
1	F	220	ARG	Sidechain
1	F	5	ASP	Sidechain
1	F	57[A]	ARG	Sidechain
1	F	57[B]	ARG	Sidechain
1	F	96	ARG	Sidechain
1	G	1	MET	Peptide
1	G	102	ARG	Sidechain
1	G	160	ARG	Sidechain
1	G	199	ARG	Sidechain
1	G	212	ARG	Sidechain
1	G	213	ARG	Sidechain
1	G	220	ARG	Sidechain
1	G	57[A]	ARG	Sidechain
1	G	57[B]	ARG	Sidechain
1	G	96	ARG	Sidechain
1	H	1	MET	Peptide
1	H	102	ARG	Sidechain
1	H	160	ARG	Sidechain
1	H	199	ARG	Sidechain
1	H	212	ARG	Sidechain
1	H	213	ARG	Sidechain
1	H	220	ARG	Sidechain
1	H	246	ARG	Sidechain
1	H	57[A]	ARG	Sidechain
1	H	57[B]	ARG	Sidechain
1	H	96	ARG	Sidechain
1	I	102	ARG	Sidechain
1	I	160	ARG	Sidechain
1	I	199	ARG	Sidechain
1	I	212	ARG	Sidechain
1	I	220	ARG	Sidechain
1	I	246	ARG	Sidechain
1	I	96	ARG	Sidechain
1	J	102	ARG	Sidechain
1	J	160	ARG	Sidechain
1	J	199	ARG	Sidechain
1	J	200	ARG	Sidechain
1	J	212	ARG	Sidechain
1	J	213	ARG	Sidechain
1	J	220	ARG	Sidechain
1	J	246	ARG	Sidechain
1	J	5	ASP	Sidechain

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Mol	Chain	Res	Type	Group
1	J	57[A]	ARG	Sidechain
1	J	57[B]	ARG	Sidechain
1	J	96	ARG	Sidechain
1	K	102	ARG	Sidechain
1	K	15	ARG	Sidechain
1	K	160	ARG	Sidechain
1	K	199	ARG	Sidechain
1	K	200	ARG	Sidechain
1	K	201	ARG	Sidechain
1	K	212	ARG	Sidechain
1	K	213	ARG	Sidechain
1	K	220	ARG	Sidechain
1	K	252	ALA	Peptide
1	K	57[A]	ARG	Sidechain
1	K	57[B]	ARG	Sidechain
1	K	96	ARG	Sidechain
1	L	102	ARG	Sidechain
1	L	15	ARG	Sidechain
1	L	160	ARG	Sidechain
1	L	199	ARG	Sidechain
1	L	212	ARG	Sidechain
1	L	220	ARG	Sidechain
1	L	246	ARG	Sidechain
1	L	5	ASP	Sidechain
1	L	57[A]	ARG	Sidechain
1	L	57[B]	ARG	Sidechain
1	L	96	ARG	Sidechain
1	M	102	ARG	Sidechain
1	M	160	ARG	Sidechain
1	M	199	ARG	Sidechain
1	M	200	ARG	Sidechain
1	M	212	ARG	Sidechain
1	M	220	ARG	Sidechain
1	M	252	ALA	Peptide
1	M	258	ARG	Sidechain
1	M	57[A]	ARG	Sidechain
1	M	57[B]	ARG	Sidechain
1	M	96	ARG	Sidechain
1	N	102	ARG	Sidechain
1	N	160	ARG	Sidechain
1	N	199	ARG	Sidechain
1	N	200	ARG	Sidechain

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Mol	Chain	Res	Type	Group
1	N	212	ARG	Sidechain
1	N	220	ARG	Sidechain
1	N	258	ARG	Sidechain
1	N	57[A]	ARG	Sidechain
1	N	57[B]	ARG	Sidechain
1	N	96	ARG	Sidechain
1	O	102	ARG	Sidechain
1	O	160	ARG	Sidechain
1	O	199	ARG	Sidechain
1	O	200	ARG	Sidechain
1	O	212	ARG	Sidechain
1	O	220	ARG	Sidechain
1	O	246	ARG	Sidechain
1	O	57[A]	ARG	Sidechain
1	O	57[B]	ARG	Sidechain
1	O	96	ARG	Sidechain
1	P	102	ARG	Sidechain
1	P	160	ARG	Sidechain
1	P	199	ARG	Sidechain
1	P	200	ARG	Sidechain
1	P	212	ARG	Sidechain
1	P	220	ARG	Sidechain
1	P	246	ARG	Sidechain
1	P	57[A]	ARG	Sidechain
1	P	57[B]	ARG	Sidechain
1	P	96	ARG	Sidechain
1	Q	102	ARG	Sidechain
1	Q	15	ARG	Sidechain
1	Q	160	ARG	Sidechain
1	Q	199	ARG	Sidechain
1	Q	200	ARG	Sidechain
1	Q	201	ARG	Sidechain
1	Q	212	ARG	Sidechain
1	Q	213	ARG	Sidechain
1	Q	220	ARG	Sidechain
1	Q	96	ARG	Sidechain
1	R	102	ARG	Sidechain
1	R	160	ARG	Sidechain
1	R	199	ARG	Sidechain
1	R	200	ARG	Sidechain
1	R	212	ARG	Sidechain
1	R	220	ARG	Sidechain

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Mol	Chain	Res	Type	Group
1	R	57[A]	ARG	Sidechain
1	R	57[B]	ARG	Sidechain
1	R	96	ARG	Sidechain
1	S	102	ARG	Sidechain
1	S	15	ARG	Sidechain
1	S	160	ARG	Sidechain
1	S	199	ARG	Sidechain
1	S	200	ARG	Sidechain
1	S	212	ARG	Sidechain
1	S	213	ARG	Sidechain
1	S	220	ARG	Sidechain
1	S	246	ARG	Sidechain
1	S	57[A]	ARG	Sidechain
1	S	57[B]	ARG	Sidechain
1	S	96	ARG	Sidechain
1	T	102	ARG	Sidechain
1	T	160	ARG	Sidechain
1	T	199	ARG	Sidechain
1	T	200	ARG	Sidechain
1	T	212	ARG	Sidechain
1	T	220	ARG	Sidechain
1	T	246	ARG	Sidechain
1	T	57[A]	ARG	Sidechain
1	T	57[B]	ARG	Sidechain
1	T	96	ARG	Sidechain
1	U	102	ARG	Sidechain
1	U	15	ARG	Sidechain
1	U	160	ARG	Sidechain
1	U	199	ARG	Sidechain
1	U	212	ARG	Sidechain
1	U	220	ARG	Sidechain
1	U	246	ARG	Sidechain
1	U	5	ASP	Sidechain
1	U	57[A]	ARG	Sidechain
1	U	57[B]	ARG	Sidechain
1	U	96	ARG	Sidechain
1	V	102	ARG	Sidechain
1	V	160	ARG	Sidechain
1	V	199	ARG	Sidechain
1	V	200	ARG	Sidechain
1	V	212	ARG	Sidechain
1	V	213	ARG	Sidechain

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Mol	Chain	Res	Type	Group
1	V	220	ARG	Sidechain
1	V	57[A]	ARG	Sidechain
1	V	57[B]	ARG	Sidechain
1	V	96	ARG	Sidechain
1	W	1	MET	Peptide
1	W	102	ARG	Sidechain
1	W	15	ARG	Sidechain
1	W	199	ARG	Sidechain
1	W	212	ARG	Sidechain
1	W	220	ARG	Sidechain
1	W	258	ARG	Sidechain
1	W	57[A]	ARG	Sidechain
1	W	57[B]	ARG	Sidechain
1	W	96	ARG	Sidechain
1	X	102[A]	ARG	Sidechain
1	X	160	ARG	Sidechain
1	X	17	ALA	Peptide
1	X	199	ARG	Sidechain
1	X	200	ARG	Sidechain
1	X	212	ARG	Sidechain
1	X	220	ARG	Sidechain
1	X	57[A]	ARG	Sidechain
1	X	57[B]	ARG	Sidechain
1	Y	102	ARG	Sidechain
1	Y	199	ARG	Sidechain
1	Y	200	ARG	Sidechain
1	Y	212	ARG	Sidechain
1	Y	220	ARG	Sidechain
1	Y	96	ARG	Sidechain
1	Z	102	ARG	Sidechain
1	Z	160	ARG	Sidechain
1	Z	199	ARG	Sidechain
1	Z	212	ARG	Sidechain
1	Z	213	ARG	Sidechain
1	Z	220	ARG	Sidechain
1	Z	246	ARG	Sidechain
1	Z	258	ARG	Sidechain
1	Z	57[A]	ARG	Sidechain
1	Z	57[B]	ARG	Sidechain
1	Z	96	ARG	Sidechain
1	a	102	ARG	Sidechain
1	a	160	ARG	Sidechain

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Mol	Chain	Res	Type	Group
1	a	199	ARG	Sidechain
1	a	200	ARG	Sidechain
1	a	212	ARG	Sidechain
1	a	213	ARG	Sidechain
1	a	220	ARG	Sidechain
1	a	246	ARG	Sidechain
1	a	258	ARG	Sidechain
1	a	57[A]	ARG	Sidechain
1	a	57[B]	ARG	Sidechain
1	a	96	ARG	Sidechain
1	b	102	ARG	Sidechain
1	b	160	ARG	Sidechain
1	b	199	ARG	Sidechain
1	b	200	ARG	Sidechain
1	b	212	ARG	Sidechain
1	b	220	ARG	Sidechain
1	b	246	ARG	Sidechain
1	b	258	ARG	Sidechain
1	b	57[A]	ARG	Sidechain
1	b	57[B]	ARG	Sidechain
1	b	96	ARG	Sidechain
1	c	102	ARG	Sidechain
1	c	160	ARG	Sidechain
1	c	199	ARG	Sidechain
1	c	200	ARG	Sidechain
1	c	212	ARG	Sidechain
1	c	213	ARG	Sidechain
1	c	220	ARG	Sidechain
1	c	57[A]	ARG	Sidechain
1	c	57[B]	ARG	Sidechain
1	c	96	ARG	Sidechain
1	d	102	ARG	Sidechain
1	d	160	ARG	Sidechain
1	d	199	ARG	Sidechain
1	d	212	ARG	Sidechain
1	d	213	ARG	Sidechain
1	d	220	ARG	Sidechain
1	d	258	ARG	Sidechain
1	d	57[A]	ARG	Sidechain
1	d	57[B]	ARG	Sidechain
1	d	96	ARG	Sidechain

5.2 Too-close contacts

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

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	257/261 (98%)	246 (96%)	11 (4%)	0	100	100
1	B	257/261 (98%)	247 (96%)	10 (4%)	0	100	100
1	C	256/261 (98%)	246 (96%)	10 (4%)	0	100	100
1	D	256/261 (98%)	246 (96%)	10 (4%)	0	100	100
1	E	257/261 (98%)	246 (96%)	11 (4%)	0	100	100
1	F	256/261 (98%)	246 (96%)	10 (4%)	0	100	100
1	G	257/261 (98%)	247 (96%)	10 (4%)	0	100	100
1	H	257/261 (98%)	246 (96%)	11 (4%)	0	100	100
1	I	257/261 (98%)	245 (95%)	12 (5%)	0	100	100
1	J	256/261 (98%)	245 (96%)	11 (4%)	0	100	100
1	K	257/261 (98%)	247 (96%)	10 (4%)	0	100	100
1	L	257/261 (98%)	246 (96%)	11 (4%)	0	100	100
1	M	256/261 (98%)	245 (96%)	11 (4%)	0	100	100
1	N	256/261 (98%)	245 (96%)	11 (4%)	0	100	100
1	O	256/261 (98%)	245 (96%)	11 (4%)	0	100	100
1	P	256/261 (98%)	245 (96%)	11 (4%)	0	100	100
1	Q	256/261 (98%)	246 (96%)	10 (4%)	0	100	100
1	R	257/261 (98%)	246 (96%)	11 (4%)	0	100	100
1	S	257/261 (98%)	247 (96%)	10 (4%)	0	100	100
1	T	257/261 (98%)	247 (96%)	10 (4%)	0	100	100
1	U	258/261 (99%)	245 (95%)	13 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	V	257/261 (98%)	248 (96%)	9 (4%)	0	100	100
1	W	257/261 (98%)	247 (96%)	10 (4%)	0	100	100
1	X	259/261 (99%)	246 (95%)	13 (5%)	0	100	100
1	Y	257/261 (98%)	247 (96%)	10 (4%)	0	100	100
1	Z	260/261 (100%)	251 (96%)	9 (4%)	0	100	100
1	a	256/261 (98%)	246 (96%)	10 (4%)	0	100	100
1	b	256/261 (98%)	244 (95%)	12 (5%)	0	100	100
1	c	256/261 (98%)	245 (96%)	11 (4%)	0	100	100
1	d	260/261 (100%)	249 (96%)	11 (4%)	0	100	100
All	All	7707/7830 (98%)	7387 (96%)	320 (4%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	207/208 (100%)	191 (92%)	16 (8%)	13	27
1	B	207/208 (100%)	190 (92%)	17 (8%)	11	24
1	C	206/208 (99%)	189 (92%)	17 (8%)	11	24
1	D	206/208 (99%)	186 (90%)	20 (10%)	8	16
1	E	207/208 (100%)	193 (93%)	14 (7%)	16	31
1	F	206/208 (99%)	191 (93%)	15 (7%)	14	29
1	G	207/208 (100%)	188 (91%)	19 (9%)	9	18
1	H	207/208 (100%)	192 (93%)	15 (7%)	14	29
1	I	207/208 (100%)	194 (94%)	13 (6%)	18	34
1	J	206/208 (99%)	188 (91%)	18 (9%)	10	21
1	K	207/208 (100%)	189 (91%)	18 (9%)	10	21
1	L	207/208 (100%)	187 (90%)	20 (10%)	8	16

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	M	206/208 (99%)	188 (91%)	18 (9%)	10 21
1	N	206/208 (99%)	188 (91%)	18 (9%)	10 21
1	O	206/208 (99%)	194 (94%)	12 (6%)	20 38
1	P	206/208 (99%)	187 (91%)	19 (9%)	9 18
1	Q	206/208 (99%)	190 (92%)	16 (8%)	12 26
1	R	207/208 (100%)	187 (90%)	20 (10%)	8 16
1	S	207/208 (100%)	189 (91%)	18 (9%)	10 21
1	T	207/208 (100%)	188 (91%)	19 (9%)	9 18
1	U	208/208 (100%)	196 (94%)	12 (6%)	20 38
1	V	207/208 (100%)	189 (91%)	18 (9%)	10 21
1	W	207/208 (100%)	192 (93%)	15 (7%)	14 29
1	X	209/208 (100%)	191 (91%)	18 (9%)	10 22
1	Y	207/208 (100%)	189 (91%)	18 (9%)	10 21
1	Z	209/208 (100%)	192 (92%)	17 (8%)	11 24
1	a	206/208 (99%)	191 (93%)	15 (7%)	14 29
1	b	206/208 (99%)	187 (91%)	19 (9%)	9 18
1	c	206/208 (99%)	189 (92%)	17 (8%)	11 24
1	d	209/208 (100%)	192 (92%)	17 (8%)	11 24
All	All	6205/6240 (99%)	5697 (92%)	508 (8%)	12 24

All (508) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	SER
1	A	51	LYS
1	A	63	SER
1	A	68	THR
1	A	71	LEU
1	A	72	LYS
1	A	90	GLU
1	A	102	ARG
1	A	106	THR
1	A	193	MET
1	A	196	GLU
1	A	199	ARG
1	A	212	ARG

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Mol	Chain	Res	Type
1	A	220	ARG
1	A	246	ARG
1	A	258	ARG
1	B	1	MET
1	B	15	ARG
1	B	57[A]	ARG
1	B	57[B]	ARG
1	B	63	SER
1	B	68	THR
1	B	74	LYS
1	B	90	GLU
1	B	100	GLN
1	B	106	THR
1	B	193	MET
1	B	196	GLU
1	B	199	ARG
1	B	201	ARG
1	B	212	ARG
1	B	226	GLU
1	B	258	ARG
1	C	2	SER
1	C	15	ARG
1	C	57[A]	ARG
1	C	57[B]	ARG
1	C	63	SER
1	C	68	THR
1	C	71	LEU
1	C	74	LYS
1	C	90	GLU
1	C	100	GLN
1	C	106	THR
1	C	193	MET
1	C	196	GLU
1	C	199	ARG
1	C	212	ARG
1	C	246	ARG
1	C	254	ARG
1	D	2	SER
1	D	3	LEU
1	D	4	ILE
1	D	7	ARG
1	D	15	ARG

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Mol	Chain	Res	Type
1	D	57[A]	ARG
1	D	57[B]	ARG
1	D	63	SER
1	D	68	THR
1	D	71	LEU
1	D	72	LYS
1	D	74	LYS
1	D	90	GLU
1	D	102	ARG
1	D	193	MET
1	D	196	GLU
1	D	199	ARG
1	D	212	ARG
1	D	246	ARG
1	D	258	ARG
1	E	2	SER
1	E	57[A]	ARG
1	E	57[B]	ARG
1	E	63	SER
1	E	71	LEU
1	E	74	LYS
1	E	90	GLU
1	E	100	GLN
1	E	193	MET
1	E	196	GLU
1	E	199	ARG
1	E	212	ARG
1	E	246	ARG
1	E	258	ARG
1	F	2	SER
1	F	51	LYS
1	F	63	SER
1	F	68	THR
1	F	70	ASP
1	F	74	LYS
1	F	90	GLU
1	F	100	GLN
1	F	106	THR
1	F	175	LYS
1	F	193	MET
1	F	196	GLU
1	F	199	ARG

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Mol	Chain	Res	Type
1	F	212	ARG
1	F	246	ARG
1	G	2	SER
1	G	15	ARG
1	G	57[A]	ARG
1	G	57[B]	ARG
1	G	63	SER
1	G	68	THR
1	G	71	LEU
1	G	72	LYS
1	G	74	LYS
1	G	90	GLU
1	G	102	ARG
1	G	106	THR
1	G	193	MET
1	G	196	GLU
1	G	199	ARG
1	G	212	ARG
1	G	220	ARG
1	G	246	ARG
1	G	258	ARG
1	H	2	SER
1	H	15	ARG
1	H	51	LYS
1	H	63	SER
1	H	68	THR
1	H	71	LEU
1	H	74	LYS
1	H	90	GLU
1	H	100	GLN
1	H	106	THR
1	H	175	LYS
1	H	193	MET
1	H	196	GLU
1	H	212	ARG
1	H	246	ARG
1	I	2	SER
1	I	63	SER
1	I	68	THR
1	I	71	LEU
1	I	72	LYS
1	I	74	LYS

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Mol	Chain	Res	Type
1	I	90	GLU
1	I	106	THR
1	I	193	MET
1	I	196	GLU
1	I	199	ARG
1	I	212	ARG
1	I	258	ARG
1	J	15	ARG
1	J	51	LYS
1	J	63	SER
1	J	68	THR
1	J	71	LEU
1	J	72	LYS
1	J	74	LYS
1	J	90	GLU
1	J	102	ARG
1	J	106	THR
1	J	193	MET
1	J	196	GLU
1	J	199	ARG
1	J	201	ARG
1	J	212	ARG
1	J	220	ARG
1	J	226	GLU
1	J	246	ARG
1	K	1	MET
1	K	2	SER
1	K	63	SER
1	K	68	THR
1	K	71	LEU
1	K	72	LYS
1	K	74	LYS
1	K	90	GLU
1	K	100	GLN
1	K	106	THR
1	K	193	MET
1	K	196	GLU
1	K	199	ARG
1	K	201	ARG
1	K	212	ARG
1	K	220	ARG
1	K	246	ARG

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Mol	Chain	Res	Type
1	K	258	ARG
1	L	2	SER
1	L	51	LYS
1	L	57[A]	ARG
1	L	57[B]	ARG
1	L	63	SER
1	L	68	THR
1	L	71	LEU
1	L	74	LYS
1	L	90	GLU
1	L	100	GLN
1	L	106	THR
1	L	160	ARG
1	L	193	MET
1	L	196	GLU
1	L	199	ARG
1	L	201	ARG
1	L	212	ARG
1	L	220	ARG
1	L	246	ARG
1	L	258	ARG
1	M	15	ARG
1	M	57[A]	ARG
1	M	57[B]	ARG
1	M	63	SER
1	M	71	LEU
1	M	74	LYS
1	M	90	GLU
1	M	106	THR
1	M	160	ARG
1	M	175	LYS
1	M	193	MET
1	M	196	GLU
1	M	199	ARG
1	M	201	ARG
1	M	212	ARG
1	M	220	ARG
1	M	246	ARG
1	M	253	THR
1	N	2	SER
1	N	15	ARG
1	N	51	LYS

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Mol	Chain	Res	Type
1	N	57[A]	ARG
1	N	57[B]	ARG
1	N	63	SER
1	N	68	THR
1	N	71	LEU
1	N	72	LYS
1	N	74	LYS
1	N	90	GLU
1	N	106	THR
1	N	175	LYS
1	N	193	MET
1	N	196	GLU
1	N	199	ARG
1	N	212	ARG
1	N	246	ARG
1	O	2	SER
1	O	15	ARG
1	O	63	SER
1	O	74	LYS
1	O	90	GLU
1	O	106	THR
1	O	193	MET
1	O	196	GLU
1	O	199	ARG
1	O	201	ARG
1	O	212	ARG
1	O	246	ARG
1	P	2	SER
1	P	15	ARG
1	P	51	LYS
1	P	63	SER
1	P	71	LEU
1	P	72	LYS
1	P	74	LYS
1	P	90	GLU
1	P	100	GLN
1	P	102	ARG
1	P	106	THR
1	P	175	LYS
1	P	193	MET
1	P	196	GLU
1	P	199	ARG

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Mol	Chain	Res	Type
1	P	212	ARG
1	P	220	ARG
1	P	226	GLU
1	P	246	ARG
1	Q	2	SER
1	Q	51	LYS
1	Q	63	SER
1	Q	68	THR
1	Q	71	LEU
1	Q	72	LYS
1	Q	74	LYS
1	Q	90	GLU
1	Q	106	THR
1	Q	175	LYS
1	Q	193	MET
1	Q	196	GLU
1	Q	199	ARG
1	Q	201	ARG
1	Q	212	ARG
1	Q	246	ARG
1	R	2	SER
1	R	15	ARG
1	R	57[A]	ARG
1	R	57[B]	ARG
1	R	63	SER
1	R	68	THR
1	R	71	LEU
1	R	72	LYS
1	R	74	LYS
1	R	90	GLU
1	R	99	VAL
1	R	100	GLN
1	R	102	ARG
1	R	106	THR
1	R	193	MET
1	R	196	GLU
1	R	199	ARG
1	R	212	ARG
1	R	246	ARG
1	R	258	ARG
1	S	1	MET
1	S	2	SER

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Mol	Chain	Res	Type
1	S	15	ARG
1	S	63	SER
1	S	68	THR
1	S	71	LEU
1	S	72	LYS
1	S	74	LYS
1	S	90	GLU
1	S	100	GLN
1	S	106	THR
1	S	193	MET
1	S	196	GLU
1	S	199	ARG
1	S	212	ARG
1	S	220	ARG
1	S	246	ARG
1	S	258	ARG
1	T	2	SER
1	T	15	ARG
1	T	57[A]	ARG
1	T	57[B]	ARG
1	T	63	SER
1	T	68	THR
1	T	71	LEU
1	T	74	LYS
1	T	90	GLU
1	T	106	THR
1	T	193	MET
1	T	196	GLU
1	T	199	ARG
1	T	201	ARG
1	T	212	ARG
1	T	213	ARG
1	T	226	GLU
1	T	246	ARG
1	T	258	ARG
1	U	63	SER
1	U	68	THR
1	U	71	LEU
1	U	74	LYS
1	U	90	GLU
1	U	100	GLN
1	U	102	ARG

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Mol	Chain	Res	Type
1	U	193	MET
1	U	196	GLU
1	U	199	ARG
1	U	212	ARG
1	U	246	ARG
1	V	1	MET
1	V	2	SER
1	V	15	ARG
1	V	57[A]	ARG
1	V	57[B]	ARG
1	V	63	SER
1	V	68	THR
1	V	71	LEU
1	V	74	LYS
1	V	90	GLU
1	V	102	ARG
1	V	106	THR
1	V	193	MET
1	V	196	GLU
1	V	199	ARG
1	V	212	ARG
1	V	246	ARG
1	V	258	ARG
1	W	57[A]	ARG
1	W	57[B]	ARG
1	W	63	SER
1	W	68	THR
1	W	72	LYS
1	W	74	LYS
1	W	90	GLU
1	W	100	GLN
1	W	106	THR
1	W	193	MET
1	W	196	GLU
1	W	199	ARG
1	W	212	ARG
1	W	246	ARG
1	W	258	ARG
1	X	4	ILE
1	X	57[A]	ARG
1	X	57[B]	ARG
1	X	63	SER

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Mol	Chain	Res	Type
1	X	68	THR
1	X	71	LEU
1	X	72	LYS
1	X	74	LYS
1	X	90	GLU
1	X	102[A]	ARG
1	X	102[B]	ARG
1	X	193	MET
1	X	196	GLU
1	X	199	ARG
1	X	201	ARG
1	X	212	ARG
1	X	226	GLU
1	X	246	ARG
1	Y	1	MET
1	Y	2	SER
1	Y	15	ARG
1	Y	63	SER
1	Y	68	THR
1	Y	71	LEU
1	Y	72	LYS
1	Y	74	LYS
1	Y	90	GLU
1	Y	102	ARG
1	Y	160	ARG
1	Y	193	MET
1	Y	196	GLU
1	Y	199	ARG
1	Y	201	ARG
1	Y	212	ARG
1	Y	246	ARG
1	Y	257	THR
1	Z	15	ARG
1	Z	57[A]	ARG
1	Z	57[B]	ARG
1	Z	63	SER
1	Z	71	LEU
1	Z	74	LYS
1	Z	90	GLU
1	Z	100	GLN
1	Z	175	LYS
1	Z	193	MET

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Mol	Chain	Res	Type
1	Z	196	GLU
1	Z	199	ARG
1	Z	201	ARG
1	Z	212	ARG
1	Z	220	ARG
1	Z	246	ARG
1	Z	258	ARG
1	a	2	SER
1	a	31	GLU
1	a	57[A]	ARG
1	a	57[B]	ARG
1	a	63	SER
1	a	71	LEU
1	a	74	LYS
1	a	90	GLU
1	a	102	ARG
1	a	175	LYS
1	a	193	MET
1	a	196	GLU
1	a	199	ARG
1	a	212	ARG
1	a	246	ARG
1	b	2	SER
1	b	15	ARG
1	b	57[A]	ARG
1	b	57[B]	ARG
1	b	63	SER
1	b	68	THR
1	b	71	LEU
1	b	72	LYS
1	b	74	LYS
1	b	90	GLU
1	b	102	ARG
1	b	149	LEU
1	b	160	ARG
1	b	193	MET
1	b	196	GLU
1	b	199	ARG
1	b	201	ARG
1	b	212	ARG
1	b	246	ARG
1	c	2	SER

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Mol	Chain	Res	Type
1	c	15	ARG
1	c	57[A]	ARG
1	c	57[B]	ARG
1	c	63	SER
1	c	68	THR
1	c	71	LEU
1	c	74	LYS
1	c	90	GLU
1	c	100	GLN
1	c	102	ARG
1	c	106	THR
1	c	193	MET
1	c	196	GLU
1	c	199	ARG
1	c	212	ARG
1	c	246	ARG
1	d	-1	SER
1	d	15	ARG
1	d	57[A]	ARG
1	d	57[B]	ARG
1	d	63	SER
1	d	68	THR
1	d	71	LEU
1	d	74	LYS
1	d	90	GLU
1	d	100	GLN
1	d	106	THR
1	d	193	MET
1	d	196	GLU
1	d	199	ARG
1	d	212	ARG
1	d	246	ARG
1	d	258	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (58) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	164	HIS
1	B	100	GLN
1	B	164	HIS
1	C	100	GLN
1	C	164	HIS

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Mol	Chain	Res	Type
1	D	156	HIS
1	D	164	HIS
1	E	100	GLN
1	E	156	HIS
1	E	164	HIS
1	F	100	GLN
1	F	164	HIS
1	G	156	HIS
1	G	164	HIS
1	H	100	GLN
1	H	156	HIS
1	H	164	HIS
1	I	156	HIS
1	I	164	HIS
1	I	209	HIS
1	J	156	HIS
1	K	100	GLN
1	K	156	HIS
1	L	100	GLN
1	L	156	HIS
1	M	43	HIS
1	N	156	HIS
1	N	164	HIS
1	O	43	HIS
1	O	164	HIS
1	P	100	GLN
1	P	156	HIS
1	P	164	HIS
1	Q	156	HIS
1	Q	164	HIS
1	R	100	GLN
1	R	164	HIS
1	S	100	GLN
1	S	157	GLN
1	S	164	HIS
1	U	21	GLN
1	U	100	GLN
1	U	164	HIS
1	V	156	HIS
1	V	164	HIS
1	W	100	GLN
1	W	156	HIS

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Mol	Chain	Res	Type
1	W	164	HIS
1	X	164	HIS
1	Y	164	HIS
1	Z	100	GLN
1	a	100	GLN
1	a	164	HIS
1	b	156	HIS
1	c	100	GLN
1	d	100	GLN
1	d	164	HIS
1	d	223	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 31 ligands modelled in this entry, 1 is monoatomic - leaving 30 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	VFE	S	1001	-	28,31,31	1.30	4 (14%)	35,41,41	1.74	10 (28%)
2	VFE	X	1001	-	28,31,31	1.81	5 (17%)	35,41,41	1.89	9 (25%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	VFE	V	1001	-	28,31,31	1.45	3 (10%)	35,41,41	1.89	8 (22%)
2	VFE	I	1001	-	28,31,31	1.50	6 (21%)	35,41,41	2.31	12 (34%)
2	VFE	E	1001	-	28,31,31	1.63	4 (14%)	35,41,41	2.69	16 (45%)
2	VFE	R	1001	-	28,31,31	1.35	3 (10%)	35,41,41	2.30	15 (42%)
2	VFE	D	1001	-	28,31,31	1.90	4 (14%)	35,41,41	2.33	13 (37%)
2	VFE	L	1001	-	28,31,31	1.48	4 (14%)	35,41,41	2.45	17 (48%)
2	VFE	U	1001	-	28,31,31	1.91	6 (21%)	35,41,41	2.14	11 (31%)
2	VFE	W	1001	-	28,31,31	1.30	5 (17%)	35,41,41	2.04	10 (28%)
2	VFE	J	1001	-	28,31,31	1.33	2 (7%)	35,41,41	1.94	11 (31%)
2	VFE	A	1001	-	28,31,31	1.70	4 (14%)	35,41,41	2.36	14 (40%)
2	VFE	B	1001	-	28,31,31	1.18	3 (10%)	35,41,41	1.41	6 (17%)
2	VFE	H	1001	-	28,31,31	1.06	2 (7%)	35,41,41	2.03	9 (25%)
2	VFE	O	1001	-	28,31,31	1.47	4 (14%)	35,41,41	1.63	6 (17%)
2	VFE	Q	1001	-	28,31,31	1.13	3 (10%)	35,41,41	2.14	11 (31%)
2	VFE	Y	1001	-	28,31,31	1.34	3 (10%)	35,41,41	1.64	9 (25%)
2	VFE	Z	1001	-	28,31,31	1.67	4 (14%)	35,41,41	2.36	13 (37%)
2	VFE	F	1001	-	28,31,31	1.20	2 (7%)	35,41,41	1.67	8 (22%)
2	VFE	T	1001	-	28,31,31	1.49	5 (17%)	35,41,41	2.35	14 (40%)
2	VFE	G	1001	-	28,31,31	1.20	2 (7%)	35,41,41	1.86	9 (25%)
2	VFE	K	1001	-	28,31,31	1.53	4 (14%)	35,41,41	1.88	10 (28%)
2	VFE	N	1001	-	28,31,31	1.24	1 (3%)	35,41,41	1.64	7 (20%)
2	VFE	a	1001	-	28,31,31	1.38	5 (17%)	35,41,41	2.17	15 (42%)
2	VFE	b	1001	-	28,31,31	1.22	3 (10%)	35,41,41	1.43	7 (20%)
2	VFE	C	1001	-	28,31,31	1.64	4 (14%)	35,41,41	2.42	13 (37%)
2	VFE	d	1001	-	28,31,31	1.31	3 (10%)	35,41,41	2.23	15 (42%)
2	VFE	P	1001	-	28,31,31	1.47	4 (14%)	35,41,41	1.42	6 (17%)
2	VFE	c	1001	-	28,31,31	1.05	2 (7%)	35,41,41	1.86	10 (28%)
2	VFE	M	1001	-	28,31,31	1.74	5 (17%)	35,41,41	2.74	13 (37%)

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	VFE	S	1001	-	-	2/23/23/23	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	VFE	X	1001	-	-	2/23/23/23	0/3/3/3
2	VFE	V	1001	-	-	4/23/23/23	0/3/3/3
2	VFE	I	1001	-	-	5/23/23/23	0/3/3/3
2	VFE	E	1001	-	-	2/23/23/23	0/3/3/3
2	VFE	R	1001	-	-	3/23/23/23	0/3/3/3
2	VFE	D	1001	-	-	2/23/23/23	0/3/3/3
2	VFE	L	1001	-	-	4/23/23/23	0/3/3/3
2	VFE	U	1001	-	-	3/23/23/23	0/3/3/3
2	VFE	W	1001	-	-	2/23/23/23	0/3/3/3
2	VFE	J	1001	-	-	2/23/23/23	0/3/3/3
2	VFE	A	1001	-	-	2/23/23/23	0/3/3/3
2	VFE	B	1001	-	-	4/23/23/23	0/3/3/3
2	VFE	H	1001	-	-	2/23/23/23	0/3/3/3
2	VFE	O	1001	-	-	4/23/23/23	0/3/3/3
2	VFE	Q	1001	-	-	2/23/23/23	0/3/3/3
2	VFE	Y	1001	-	-	3/23/23/23	0/3/3/3
2	VFE	Z	1001	-	-	4/23/23/23	0/3/3/3
2	VFE	F	1001	-	-	2/23/23/23	0/3/3/3
2	VFE	T	1001	-	-	2/23/23/23	0/3/3/3
2	VFE	G	1001	-	-	2/23/23/23	0/3/3/3
2	VFE	K	1001	-	-	4/23/23/23	0/3/3/3
2	VFE	N	1001	-	-	2/23/23/23	0/3/3/3
2	VFE	a	1001	-	-	2/23/23/23	0/3/3/3
2	VFE	b	1001	-	-	4/23/23/23	0/3/3/3
2	VFE	C	1001	-	-	4/23/23/23	0/3/3/3
2	VFE	d	1001	-	-	2/23/23/23	0/3/3/3
2	VFE	P	1001	-	-	4/23/23/23	0/3/3/3
2	VFE	c	1001	-	-	2/23/23/23	0/3/3/3
2	VFE	M	1001	-	-	2/23/23/23	0/3/3/3

All (109) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1001	VFE	C23-S22	6.11	1.86	1.77
2	K	1001	VFE	C23-S22	5.90	1.86	1.77
2	E	1001	VFE	C23-S22	5.87	1.86	1.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	1001	VFE	C27-C28	5.57	1.50	1.38
2	M	1001	VFE	C23-S22	5.57	1.85	1.77
2	C	1001	VFE	C23-S22	5.28	1.85	1.77
2	X	1001	VFE	C27-C28	-5.10	1.28	1.38
2	U	1001	VFE	C23-S22	5.09	1.84	1.77
2	V	1001	VFE	C23-S22	4.85	1.84	1.77
2	D	1001	VFE	C25-C24	4.69	1.48	1.38
2	I	1001	VFE	C23-S22	4.64	1.84	1.77
2	Z	1001	VFE	C23-S22	4.40	1.83	1.77
2	X	1001	VFE	C25-C24	-4.40	1.29	1.38
2	J	1001	VFE	C23-S22	4.37	1.83	1.77
2	P	1001	VFE	C23-S22	4.25	1.83	1.77
2	D	1001	VFE	C23-S22	4.14	1.83	1.77
2	L	1001	VFE	C19-N6	4.02	1.43	1.35
2	G	1001	VFE	C23-S22	3.90	1.83	1.77
2	U	1001	VFE	C25-C24	3.80	1.46	1.38
2	a	1001	VFE	C23-S22	3.79	1.82	1.77
2	R	1001	VFE	C23-S22	3.73	1.82	1.77
2	U	1001	VFE	C27-C28	3.64	1.46	1.38
2	U	1001	VFE	C26-C27	-3.51	1.31	1.38
2	X	1001	VFE	C5-C3	3.44	1.57	1.52
2	M	1001	VFE	C19-N6	3.41	1.42	1.35
2	L	1001	VFE	C23-S22	3.30	1.82	1.77
2	T	1001	VFE	C23-S22	3.22	1.82	1.77
2	N	1001	VFE	C5-C3	3.21	1.57	1.52
2	U	1001	VFE	C21-S22	3.20	1.88	1.80
2	O	1001	VFE	C23-S22	3.19	1.82	1.77
2	O	1001	VFE	C21-S22	3.18	1.88	1.80
2	Z	1001	VFE	C7-C8	-3.09	1.45	1.51
2	Y	1001	VFE	C5-C3	3.05	1.57	1.52
2	E	1001	VFE	C5-C3	3.03	1.57	1.52
2	T	1001	VFE	C7-C8	-3.01	1.46	1.51
2	H	1001	VFE	C23-S22	2.96	1.81	1.77
2	d	1001	VFE	O4-C3	2.93	1.29	1.23
2	W	1001	VFE	C24-C23	-2.92	1.34	1.39
2	Z	1001	VFE	C19-N6	2.92	1.41	1.35
2	F	1001	VFE	C21-C19	-2.85	1.46	1.51
2	C	1001	VFE	C24-C23	-2.85	1.34	1.39
2	Q	1001	VFE	C5-N6	2.82	1.49	1.45
2	T	1001	VFE	C7-N6	-2.79	1.42	1.46
2	A	1001	VFE	C19-N6	2.76	1.40	1.35
2	V	1001	VFE	C26-C27	-2.75	1.33	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	M	1001	VFE	C21-S22	2.74	1.87	1.80
2	P	1001	VFE	C25-C24	2.73	1.44	1.38
2	b	1001	VFE	C7-C8	-2.65	1.46	1.51
2	S	1001	VFE	C23-S22	2.65	1.81	1.77
2	M	1001	VFE	C26-C27	-2.64	1.33	1.38
2	O	1001	VFE	C19-N6	2.60	1.40	1.35
2	V	1001	VFE	C7-C8	-2.59	1.46	1.51
2	X	1001	VFE	C7-N6	-2.57	1.42	1.46
2	a	1001	VFE	C28-CL	-2.56	1.67	1.73
2	S	1001	VFE	C7-C8	-2.54	1.46	1.51
2	W	1001	VFE	C28-CL	-2.52	1.67	1.73
2	D	1001	VFE	C21-S22	2.49	1.86	1.80
2	O	1001	VFE	C5-C3	2.48	1.56	1.52
2	W	1001	VFE	C26-C27	-2.47	1.33	1.38
2	T	1001	VFE	C10-C9	-2.45	1.34	1.38
2	c	1001	VFE	C21-C19	-2.44	1.47	1.51
2	G	1001	VFE	C11-N14	-2.43	1.37	1.44
2	L	1001	VFE	C7-C8	-2.43	1.47	1.51
2	Q	1001	VFE	C23-S22	2.42	1.80	1.77
2	K	1001	VFE	C19-N6	2.36	1.40	1.35
2	b	1001	VFE	C5-C3	2.36	1.56	1.52
2	c	1001	VFE	C23-S22	2.33	1.80	1.77
2	J	1001	VFE	C25-C24	-2.32	1.34	1.38
2	W	1001	VFE	C19-N6	2.32	1.40	1.35
2	L	1001	VFE	C5-N6	2.31	1.48	1.45
2	E	1001	VFE	C28-CL	-2.30	1.68	1.73
2	a	1001	VFE	C21-S22	2.29	1.86	1.80
2	Q	1001	VFE	C19-N6	2.27	1.39	1.35
2	C	1001	VFE	C26-C27	-2.27	1.34	1.38
2	B	1001	VFE	C21-C19	-2.26	1.47	1.51
2	Y	1001	VFE	C23-S22	2.25	1.80	1.77
2	M	1001	VFE	C5-C3	2.25	1.55	1.52
2	T	1001	VFE	C19-N6	2.25	1.39	1.35
2	H	1001	VFE	C21-C19	-2.24	1.47	1.51
2	Y	1001	VFE	C19-N6	2.23	1.39	1.35
2	I	1001	VFE	C7-N6	-2.22	1.43	1.46
2	S	1001	VFE	C19-N6	2.22	1.39	1.35
2	B	1001	VFE	C11-N14	-2.22	1.37	1.44
2	I	1001	VFE	C26-C27	-2.20	1.34	1.38
2	b	1001	VFE	C21-S22	2.18	1.85	1.80
2	a	1001	VFE	C11-N14	-2.17	1.37	1.44
2	S	1001	VFE	C7-N6	-2.16	1.43	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	I	1001	VFE	C5-C3	2.15	1.55	1.52
2	d	1001	VFE	C1-N2	2.14	1.49	1.45
2	A	1001	VFE	C28-CL	-2.14	1.68	1.73
2	Z	1001	VFE	C21-S22	2.13	1.85	1.80
2	C	1001	VFE	C21-S22	2.13	1.85	1.80
2	I	1001	VFE	C11-N14	-2.12	1.38	1.44
2	K	1001	VFE	C7-C8	-2.10	1.47	1.51
2	P	1001	VFE	N18-N14	-2.09	1.33	1.38
2	F	1001	VFE	C1-N2	2.07	1.49	1.45
2	P	1001	VFE	C7-N6	-2.07	1.43	1.46
2	K	1001	VFE	C5-N6	2.06	1.48	1.45
2	A	1001	VFE	C11-N14	-2.06	1.38	1.44
2	W	1001	VFE	C5-C3	2.05	1.55	1.52
2	I	1001	VFE	C21-S22	2.04	1.85	1.80
2	U	1001	VFE	C19-N6	2.04	1.39	1.35
2	X	1001	VFE	C28-C23	-2.04	1.34	1.39
2	R	1001	VFE	C5-C3	2.03	1.55	1.52
2	d	1001	VFE	N18-N14	-2.02	1.33	1.38
2	R	1001	VFE	C7-C8	-2.02	1.47	1.51
2	B	1001	VFE	C23-S22	2.01	1.80	1.77
2	a	1001	VFE	C26-C27	-2.01	1.34	1.38
2	E	1001	VFE	C19-N6	2.00	1.39	1.35

All (327) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	M	1001	VFE	C21-S22-C23	9.06	116.51	102.61
2	Z	1001	VFE	C3-C5-N6	-7.46	95.77	113.60
2	E	1001	VFE	C21-S22-C23	6.78	113.02	102.61
2	Q	1001	VFE	C21-S22-C23	6.13	112.02	102.61
2	D	1001	VFE	C24-C23-C28	-6.09	109.43	117.52
2	T	1001	VFE	C3-C5-N6	-5.90	99.50	113.60
2	V	1001	VFE	C24-C23-C28	-5.85	109.74	117.52
2	C	1001	VFE	C23-C28-CL	-5.83	109.45	119.69
2	H	1001	VFE	C21-S22-C23	5.77	111.47	102.61
2	M	1001	VFE	N16-C15-N14	-5.68	105.91	113.30
2	R	1001	VFE	C12-C11-N14	5.55	124.00	119.15
2	L	1001	VFE	C10-C11-N14	5.38	123.86	119.15
2	A	1001	VFE	C24-C23-C28	-5.37	110.38	117.52
2	L	1001	VFE	C23-C28-CL	-5.36	110.28	119.69
2	a	1001	VFE	C3-C5-N6	-5.21	101.15	113.60
2	E	1001	VFE	C24-C23-C28	-5.20	110.60	117.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	M	1001	VFE	C23-C28-CL	-5.11	110.72	119.69
2	d	1001	VFE	C3-C5-N6	-5.09	101.44	113.60
2	E	1001	VFE	C12-C11-N14	4.99	123.51	119.15
2	A	1001	VFE	C3-C5-N6	-4.98	101.69	113.60
2	C	1001	VFE	C24-C23-S22	4.96	133.55	121.46
2	C	1001	VFE	C26-C27-C28	-4.95	111.92	119.39
2	D	1001	VFE	C3-C5-N6	-4.91	101.87	113.60
2	C	1001	VFE	C27-C28-C23	4.88	132.71	122.28
2	X	1001	VFE	O4-C3-C5	4.85	129.56	121.08
2	A	1001	VFE	N16-C15-N14	-4.85	106.99	113.30
2	S	1001	VFE	C23-C28-CL	-4.81	111.24	119.69
2	a	1001	VFE	C17-N18-N14	-4.81	99.03	102.85
2	I	1001	VFE	C8-C7-N6	4.79	120.83	113.13
2	Q	1001	VFE	C23-C28-CL	-4.70	111.44	119.69
2	J	1001	VFE	C23-C28-CL	-4.61	111.60	119.69
2	T	1001	VFE	N16-C15-N14	-4.60	107.31	113.30
2	U	1001	VFE	C17-N18-N14	-4.55	99.24	102.85
2	d	1001	VFE	C17-N18-N14	-4.55	99.24	102.85
2	I	1001	VFE	C7-N6-C19	-4.52	110.21	121.91
2	L	1001	VFE	C7-N6-C5	-4.47	108.91	116.58
2	H	1001	VFE	N16-C15-N14	-4.47	107.49	113.30
2	I	1001	VFE	C10-C11-N14	-4.46	115.25	119.15
2	a	1001	VFE	N16-C15-N14	-4.42	107.55	113.30
2	D	1001	VFE	C24-C23-S22	4.42	132.23	121.46
2	G	1001	VFE	N16-C15-N14	-4.39	107.59	113.30
2	d	1001	VFE	C21-S22-C23	-4.37	95.91	102.61
2	E	1001	VFE	C23-C28-CL	-4.35	112.06	119.69
2	C	1001	VFE	C24-C23-C28	-4.32	111.78	117.52
2	K	1001	VFE	C3-C5-N6	-4.32	103.29	113.60
2	Z	1001	VFE	C23-C28-CL	-4.30	112.14	119.69
2	O	1001	VFE	C21-S22-C23	4.29	109.19	102.61
2	N	1001	VFE	O4-C3-C5	4.25	128.51	121.08
2	J	1001	VFE	N16-C15-N14	-4.25	107.77	113.30
2	W	1001	VFE	C17-N18-N14	-4.25	99.48	102.85
2	X	1001	VFE	C17-N18-N14	-4.20	99.51	102.85
2	R	1001	VFE	C26-C27-C28	-4.14	113.14	119.39
2	K	1001	VFE	C12-C11-N14	4.11	122.74	119.15
2	T	1001	VFE	C10-C11-N14	-4.10	115.58	119.15
2	U	1001	VFE	C26-C25-C24	4.07	126.39	120.19
2	I	1001	VFE	C23-C28-CL	-4.02	112.62	119.69
2	Y	1001	VFE	C23-C28-CL	-4.01	112.65	119.69
2	U	1001	VFE	C25-C26-C27	-3.99	114.11	120.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	I	1001	VFE	N16-C15-N14	-3.99	108.11	113.30
2	c	1001	VFE	O20-C19-N6	3.98	129.78	122.05
2	W	1001	VFE	C3-C5-N6	-3.95	104.16	113.60
2	M	1001	VFE	O20-C19-N6	3.94	129.72	122.05
2	d	1001	VFE	C7-C8-C13	-3.92	113.40	120.77
2	T	1001	VFE	C13-C8-C9	3.92	124.32	118.17
2	Q	1001	VFE	O4-C3-C5	3.91	127.91	121.08
2	E	1001	VFE	C8-C7-N6	3.89	119.39	113.13
2	A	1001	VFE	C23-C28-CL	-3.86	112.91	119.69
2	M	1001	VFE	C17-N18-N14	-3.84	99.81	102.85
2	A	1001	VFE	C21-S22-C23	3.83	108.49	102.61
2	I	1001	VFE	C12-C11-N14	3.81	122.49	119.15
2	R	1001	VFE	C23-C28-CL	-3.78	113.06	119.69
2	W	1001	VFE	N16-C15-N14	-3.76	108.40	113.30
2	L	1001	VFE	C11-N14-N18	3.74	122.12	118.80
2	E	1001	VFE	C7-N6-C19	-3.74	112.21	121.91
2	V	1001	VFE	C12-C11-N14	3.73	122.42	119.15
2	c	1001	VFE	C11-N14-N18	3.73	122.11	118.80
2	G	1001	VFE	C23-C28-CL	-3.71	113.17	119.69
2	F	1001	VFE	C5-C3-N2	-3.70	110.14	116.27
2	U	1001	VFE	O4-C3-C5	3.67	127.50	121.08
2	N	1001	VFE	C23-C28-CL	-3.65	113.28	119.69
2	C	1001	VFE	C26-C25-C24	3.64	125.73	120.19
2	H	1001	VFE	C23-C28-CL	-3.62	113.32	119.69
2	Z	1001	VFE	N16-C15-N14	-3.61	108.60	113.30
2	M	1001	VFE	C24-C23-S22	3.59	130.21	121.46
2	O	1001	VFE	C11-N14-N18	3.57	121.97	118.80
2	Q	1001	VFE	C24-C23-S22	3.55	130.12	121.46
2	E	1001	VFE	O4-C3-C5	3.54	127.28	121.08
2	J	1001	VFE	C3-C5-N6	-3.54	105.15	113.60
2	U	1001	VFE	N16-C15-N14	-3.52	108.72	113.30
2	D	1001	VFE	C27-C28-C23	3.51	129.79	122.28
2	G	1001	VFE	C24-C23-C28	-3.51	112.85	117.52
2	a	1001	VFE	C8-C7-N6	-3.48	107.54	113.13
2	H	1001	VFE	C24-C23-S22	3.47	129.92	121.46
2	R	1001	VFE	C11-N14-N18	3.45	121.86	118.80
2	A	1001	VFE	C27-C28-C23	3.44	129.64	122.28
2	b	1001	VFE	N16-C15-N14	-3.44	108.82	113.30
2	S	1001	VFE	N16-C15-N14	-3.42	108.85	113.30
2	U	1001	VFE	C23-C28-CL	-3.42	113.69	119.69
2	A	1001	VFE	C5-C3-N2	-3.41	110.62	116.27
2	C	1001	VFE	C11-N14-N18	3.41	121.82	118.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	U	1001	VFE	C3-C5-N6	-3.40	105.47	113.60
2	Q	1001	VFE	N16-C15-N14	-3.40	108.87	113.30
2	S	1001	VFE	C24-C23-S22	3.40	129.74	121.46
2	F	1001	VFE	O4-C3-C5	3.39	127.01	121.08
2	M	1001	VFE	C7-N6-C5	-3.38	110.76	116.58
2	K	1001	VFE	C23-C28-CL	-3.37	113.77	119.69
2	L	1001	VFE	C7-C8-C13	-3.37	114.44	120.77
2	E	1001	VFE	C24-C23-S22	3.36	129.65	121.46
2	c	1001	VFE	C3-C5-N6	-3.36	105.58	113.60
2	I	1001	VFE	C7-C8-C9	-3.35	114.47	120.77
2	R	1001	VFE	C27-C28-C23	3.33	129.41	122.28
2	E	1001	VFE	C27-C28-C23	3.33	129.41	122.28
2	F	1001	VFE	C8-C7-N6	3.33	118.49	113.13
2	R	1001	VFE	C24-C23-C28	-3.32	113.11	117.52
2	I	1001	VFE	C24-C23-S22	3.32	129.55	121.46
2	L	1001	VFE	C12-C11-N14	-3.31	116.26	119.15
2	D	1001	VFE	C25-C26-C27	-3.30	115.16	120.19
2	E	1001	VFE	C11-N14-N18	3.27	121.71	118.80
2	K	1001	VFE	C24-C23-S22	3.27	129.43	121.46
2	U	1001	VFE	C7-N6-C19	-3.27	113.44	121.91
2	B	1001	VFE	C21-S22-C23	3.27	107.63	102.61
2	E	1001	VFE	C12-C11-C10	-3.26	116.49	121.33
2	F	1001	VFE	C23-C28-CL	-3.26	113.95	119.69
2	K	1001	VFE	C24-C23-C28	-3.25	113.20	117.52
2	Y	1001	VFE	N16-C15-N14	-3.25	109.08	113.30
2	D	1001	VFE	C23-C28-CL	-3.24	113.99	119.69
2	W	1001	VFE	C26-C25-C24	3.23	125.12	120.19
2	a	1001	VFE	C24-C23-C28	-3.23	113.23	117.52
2	M	1001	VFE	C12-C11-N14	3.23	121.98	119.15
2	c	1001	VFE	N16-C15-N14	-3.23	109.10	113.30
2	M	1001	VFE	C27-C28-CL	3.22	124.88	118.41
2	R	1001	VFE	C7-N6-C19	-3.22	113.56	121.91
2	G	1001	VFE	C24-C23-S22	3.22	129.31	121.46
2	W	1001	VFE	C23-C28-CL	-3.21	114.05	119.69
2	T	1001	VFE	O20-C19-N6	3.21	128.29	122.05
2	Z	1001	VFE	C24-C23-C28	-3.19	113.28	117.52
2	T	1001	VFE	C15-N16-C17	3.16	105.90	102.34
2	J	1001	VFE	C26-C27-C28	-3.16	114.62	119.39
2	B	1001	VFE	O4-C3-C5	3.16	126.60	121.08
2	P	1001	VFE	C17-N18-N14	-3.14	100.36	102.85
2	S	1001	VFE	C3-C5-N6	-3.11	106.17	113.60
2	a	1001	VFE	C27-C28-C23	3.09	128.90	122.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	R	1001	VFE	C24-C23-S22	3.07	128.95	121.46
2	N	1001	VFE	C11-N14-N18	3.07	121.52	118.80
2	W	1001	VFE	C11-N14-N18	3.06	121.52	118.80
2	X	1001	VFE	C12-C11-N14	3.06	121.83	119.15
2	O	1001	VFE	O4-C3-C5	3.04	126.39	121.08
2	R	1001	VFE	C3-C5-N6	-3.03	106.35	113.60
2	d	1001	VFE	C23-C28-CL	-3.03	114.37	119.69
2	d	1001	VFE	O4-C3-C5	3.03	126.38	121.08
2	L	1001	VFE	C24-C23-S22	3.02	128.83	121.46
2	T	1001	VFE	C5-N6-C19	3.02	129.38	120.69
2	T	1001	VFE	C21-S22-C23	3.02	107.25	102.61
2	C	1001	VFE	C12-C11-N14	3.02	121.79	119.15
2	Z	1001	VFE	C7-N6-C19	-3.02	114.09	121.91
2	X	1001	VFE	C21-S22-C23	3.01	107.24	102.61
2	Z	1001	VFE	C11-N14-N18	3.01	121.47	118.80
2	C	1001	VFE	C7-N6-C19	-3.01	114.12	121.91
2	P	1001	VFE	C5-N6-C19	3.00	129.31	120.69
2	S	1001	VFE	C7-N6-C19	-2.99	114.16	121.91
2	V	1001	VFE	C23-C28-CL	-2.99	114.44	119.69
2	H	1001	VFE	O20-C19-N6	2.99	127.86	122.05
2	c	1001	VFE	C23-C28-CL	-2.96	114.48	119.69
2	D	1001	VFE	C26-C25-C24	2.96	124.70	120.19
2	L	1001	VFE	C24-C23-C28	-2.95	113.59	117.52
2	M	1001	VFE	C15-N16-C17	2.95	105.67	102.34
2	M	1001	VFE	C10-C11-N14	-2.95	116.58	119.15
2	Y	1001	VFE	C11-N14-N18	2.94	121.41	118.80
2	U	1001	VFE	C24-C23-S22	2.94	128.62	121.46
2	L	1001	VFE	C5-N6-C19	2.93	129.13	120.69
2	L	1001	VFE	O4-C3-C5	-2.93	115.94	121.08
2	X	1001	VFE	C3-C5-N6	-2.93	106.60	113.60
2	Z	1001	VFE	C8-C7-N6	-2.92	108.44	113.13
2	J	1001	VFE	C24-C23-S22	2.91	128.56	121.46
2	A	1001	VFE	C24-C23-S22	2.89	128.51	121.46
2	I	1001	VFE	C5-N6-C19	2.89	128.99	120.69
2	U	1001	VFE	C24-C23-C28	-2.88	113.70	117.52
2	P	1001	VFE	C25-C26-C27	-2.85	115.85	120.19
2	Q	1001	VFE	C12-C11-N14	2.84	121.64	119.15
2	A	1001	VFE	C17-N18-N14	-2.84	100.59	102.85
2	W	1001	VFE	C8-C7-N6	2.83	117.68	113.13
2	Y	1001	VFE	O20-C19-N6	2.83	127.55	122.05
2	I	1001	VFE	C17-N18-N14	-2.83	100.61	102.85
2	X	1001	VFE	N16-C15-N14	-2.82	109.64	113.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	d	1001	VFE	C7-C8-C9	2.81	126.06	120.77
2	H	1001	VFE	C17-N18-N14	-2.81	100.62	102.85
2	K	1001	VFE	C5-N6-C19	2.80	128.75	120.69
2	L	1001	VFE	O20-C19-N6	2.80	127.49	122.05
2	F	1001	VFE	C24-C23-S22	2.77	128.21	121.46
2	K	1001	VFE	N16-C15-N14	-2.77	109.70	113.30
2	D	1001	VFE	C11-N14-N18	2.76	121.25	118.80
2	R	1001	VFE	N16-C15-N14	-2.76	109.71	113.30
2	d	1001	VFE	N16-C15-N14	-2.76	109.72	113.30
2	N	1001	VFE	N16-C15-N14	-2.76	109.72	113.30
2	d	1001	VFE	C7-N6-C5	-2.75	111.85	116.58
2	d	1001	VFE	C10-C11-N14	2.75	121.55	119.15
2	a	1001	VFE	O20-C19-C21	2.74	127.02	120.93
2	J	1001	VFE	C5-N6-C19	2.72	128.52	120.69
2	R	1001	VFE	C10-C11-N14	-2.72	116.78	119.15
2	a	1001	VFE	C7-N6-C19	-2.71	114.88	121.91
2	T	1001	VFE	C7-N6-C5	-2.71	111.93	116.58
2	B	1001	VFE	C23-C28-CL	-2.70	114.94	119.69
2	Z	1001	VFE	C12-C11-N14	2.70	121.51	119.15
2	W	1001	VFE	C7-N6-C19	-2.70	114.92	121.91
2	G	1001	VFE	C7-N6-C19	-2.69	114.95	121.91
2	G	1001	VFE	C27-C28-C23	2.68	128.01	122.28
2	E	1001	VFE	C17-N18-N14	-2.68	100.72	102.85
2	L	1001	VFE	C27-C28-C23	2.68	128.00	122.28
2	c	1001	VFE	C13-C12-C11	2.67	122.95	119.07
2	E	1001	VFE	C25-C26-C27	-2.64	116.16	120.19
2	O	1001	VFE	C3-C5-N6	-2.64	107.29	113.60
2	L	1001	VFE	C8-C7-N6	-2.64	108.89	113.13
2	b	1001	VFE	C3-C5-N6	-2.61	107.37	113.60
2	C	1001	VFE	N16-C15-N14	-2.60	109.92	113.30
2	V	1001	VFE	C27-C28-C23	2.59	127.82	122.28
2	Y	1001	VFE	C24-C23-S22	2.58	127.74	121.46
2	Z	1001	VFE	C7-N6-C5	-2.58	112.15	116.58
2	c	1001	VFE	C8-C7-N6	-2.57	109.00	113.13
2	Q	1001	VFE	C11-N14-N18	2.57	121.08	118.80
2	B	1001	VFE	C26-C25-C24	2.57	124.11	120.19
2	Z	1001	VFE	C5-N6-C19	2.57	128.07	120.69
2	X	1001	VFE	C8-C7-N6	2.56	117.24	113.13
2	D	1001	VFE	C5-N6-C19	2.55	128.04	120.69
2	Q	1001	VFE	O20-C19-N6	2.55	127.01	122.05
2	d	1001	VFE	C5-N6-C19	2.55	128.03	120.69
2	G	1001	VFE	C21-S22-C23	2.55	106.53	102.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	Y	1001	VFE	C7-N6-C5	-2.55	112.20	116.58
2	R	1001	VFE	C7-C8-C9	-2.54	115.98	120.77
2	X	1001	VFE	C11-N14-N18	2.53	121.05	118.80
2	D	1001	VFE	C8-C7-N6	2.53	117.19	113.13
2	P	1001	VFE	C26-C27-C28	2.52	123.20	119.39
2	S	1001	VFE	C27-C28-CL	2.52	123.45	118.41
2	G	1001	VFE	C5-N6-C19	2.51	127.91	120.69
2	W	1001	VFE	C27-C28-C23	2.51	127.65	122.28
2	Z	1001	VFE	C13-C8-C9	2.50	122.10	118.17
2	M	1001	VFE	C5-N6-C19	2.50	127.88	120.69
2	a	1001	VFE	C23-C28-CL	-2.50	115.30	119.69
2	I	1001	VFE	C7-C8-C13	2.49	125.45	120.77
2	Z	1001	VFE	C24-C23-S22	2.49	127.53	121.46
2	V	1001	VFE	O4-C3-C5	2.48	125.42	121.08
2	D	1001	VFE	O4-C3-C5	2.48	125.41	121.08
2	d	1001	VFE	C8-C7-N6	-2.47	109.17	113.13
2	H	1001	VFE	C25-C26-C27	-2.46	116.44	120.19
2	T	1001	VFE	C26-C27-C28	-2.46	115.67	119.39
2	C	1001	VFE	C5-N6-C19	2.45	127.74	120.69
2	b	1001	VFE	C7-N6-C19	-2.45	115.56	121.91
2	R	1001	VFE	C5-C3-N2	-2.44	112.24	116.27
2	N	1001	VFE	C24-C23-S22	2.43	127.38	121.46
2	J	1001	VFE	C24-C23-C28	-2.41	114.31	117.52
2	B	1001	VFE	N16-C15-N14	-2.40	110.18	113.30
2	b	1001	VFE	O4-C3-C5	2.40	125.27	121.08
2	Y	1001	VFE	O4-C3-C5	2.39	125.26	121.08
2	V	1001	VFE	C25-C24-C23	2.39	123.78	119.63
2	J	1001	VFE	C11-N14-N18	2.37	120.91	118.80
2	N	1001	VFE	C7-N6-C19	-2.37	115.76	121.91
2	Q	1001	VFE	C5-N6-C19	2.37	127.52	120.69
2	a	1001	VFE	C5-N6-C19	2.37	127.51	120.69
2	T	1001	VFE	C23-C28-CL	-2.37	115.53	119.69
2	D	1001	VFE	N16-C15-N14	-2.37	110.22	113.30
2	L	1001	VFE	C10-C9-C8	-2.36	117.78	121.03
2	E	1001	VFE	C9-C10-C11	2.36	122.50	119.07
2	D	1001	VFE	C12-C11-N14	2.35	121.21	119.15
2	X	1001	VFE	C24-C23-S22	2.34	127.17	121.46
2	T	1001	VFE	C11-N14-N18	2.34	120.88	118.80
2	V	1001	VFE	C24-C23-S22	2.33	127.15	121.46
2	c	1001	VFE	C24-C23-S22	2.33	127.13	121.46
2	A	1001	VFE	C25-C24-C23	2.32	123.67	119.63
2	E	1001	VFE	N16-C15-N14	-2.32	110.29	113.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	R	1001	VFE	C21-S22-C23	2.31	106.16	102.61
2	H	1001	VFE	C11-N14-N18	2.29	120.84	118.80
2	A	1001	VFE	C15-N16-C17	2.28	104.91	102.34
2	O	1001	VFE	N16-C15-N14	-2.27	110.34	113.30
2	E	1001	VFE	C26-C25-C24	2.26	123.64	120.19
2	J	1001	VFE	C7-C8-C13	-2.26	116.52	120.77
2	F	1001	VFE	C11-N14-N18	2.26	120.81	118.80
2	O	1001	VFE	C5-N6-C19	2.26	127.18	120.69
2	J	1001	VFE	C15-N16-C17	2.25	104.88	102.34
2	I	1001	VFE	C24-C23-C28	-2.25	114.53	117.52
2	a	1001	VFE	C21-S22-C23	-2.25	99.16	102.61
2	A	1001	VFE	O4-C3-C5	2.25	125.01	121.08
2	G	1001	VFE	C17-N18-N14	-2.24	101.07	102.85
2	c	1001	VFE	C5-N6-C19	2.23	127.11	120.69
2	P	1001	VFE	C12-C13-C8	-2.23	117.97	121.03
2	a	1001	VFE	C26-C25-C24	2.22	123.58	120.19
2	F	1001	VFE	N16-C15-N14	-2.22	110.42	113.30
2	R	1001	VFE	O4-C3-C5	2.22	124.95	121.08
2	T	1001	VFE	C5-C3-N2	-2.21	112.61	116.27
2	a	1001	VFE	C26-C27-C28	-2.20	116.07	119.39
2	d	1001	VFE	O20-C19-N6	2.19	126.31	122.05
2	U	1001	VFE	C21-S22-C23	2.19	105.98	102.61
2	d	1001	VFE	C26-C27-C28	-2.19	116.09	119.39
2	S	1001	VFE	C21-S22-C23	2.19	105.97	102.61
2	K	1001	VFE	C10-C11-N14	-2.18	117.25	119.15
2	T	1001	VFE	C10-C9-C8	-2.18	118.03	121.03
2	K	1001	VFE	C11-N14-N18	2.16	120.72	118.80
2	Z	1001	VFE	O20-C19-N6	2.16	126.25	122.05
2	c	1001	VFE	C10-C11-N14	2.16	121.04	119.15
2	S	1001	VFE	O4-C3-C5	2.16	124.85	121.08
2	B	1001	VFE	C12-C11-N14	2.15	121.04	119.15
2	N	1001	VFE	C5-C3-N2	-2.15	112.71	116.27
2	b	1001	VFE	C23-C28-CL	-2.15	115.91	119.69
2	Y	1001	VFE	C21-S22-C23	-2.15	99.32	102.61
2	Q	1001	VFE	C27-C28-CL	2.15	122.71	118.41
2	a	1001	VFE	O20-C19-N6	-2.14	117.87	122.05
2	J	1001	VFE	C27-C28-C23	2.13	126.83	122.28
2	L	1001	VFE	C13-C8-C9	2.12	121.50	118.17
2	S	1001	VFE	C26-C27-C28	-2.12	116.19	119.39
2	P	1001	VFE	C7-N6-C19	-2.11	116.44	121.91
2	A	1001	VFE	C8-C7-N6	2.11	116.52	113.13
2	K	1001	VFE	C7-N6-C19	-2.10	116.46	121.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	d	1001	VFE	C12-C11-N14	-2.10	117.32	119.15
2	S	1001	VFE	C5-N6-C19	2.10	126.72	120.69
2	M	1001	VFE	C8-C7-N6	2.09	116.50	113.13
2	L	1001	VFE	C26-C27-C28	-2.09	116.23	119.39
2	b	1001	VFE	C5-N6-C19	2.08	126.66	120.69
2	A	1001	VFE	C11-N14-N18	2.07	120.64	118.80
2	L	1001	VFE	N16-C15-N14	-2.07	110.60	113.30
2	V	1001	VFE	C7-N6-C19	-2.07	116.54	121.91
2	b	1001	VFE	C17-N18-N14	-2.07	101.20	102.85
2	F	1001	VFE	O20-C19-N6	2.07	126.07	122.05
2	H	1001	VFE	C27-C28-CL	2.06	122.54	118.41
2	a	1001	VFE	C24-C23-S22	2.05	126.47	121.46
2	Q	1001	VFE	C7-N6-C19	-2.05	116.61	121.91
2	C	1001	VFE	C3-C5-N6	-2.03	108.76	113.60
2	Y	1001	VFE	C27-C28-CL	2.02	122.46	118.41
2	C	1001	VFE	C12-C11-C10	-2.02	118.34	121.33
2	W	1001	VFE	C26-C27-C28	-2.01	116.36	119.39

There are no chirality outliers.

All (84) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	I	1001	VFE	C5-C3-N2-C1
2	I	1001	VFE	C3-C5-N6-C19
2	K	1001	VFE	C5-C3-N2-C1
2	L	1001	VFE	C5-C3-N2-C1
2	O	1001	VFE	C5-C3-N2-C1
2	Z	1001	VFE	C5-C3-N2-C1
2	I	1001	VFE	O4-C3-N2-C1
2	K	1001	VFE	O4-C3-N2-C1
2	c	1001	VFE	O4-C3-C5-N6
2	G	1001	VFE	N2-C3-C5-N6
2	P	1001	VFE	N2-C3-C5-N6
2	K	1001	VFE	O4-C3-C5-N6
2	P	1001	VFE	O4-C3-C5-N6
2	A	1001	VFE	N2-C3-C5-N6
2	H	1001	VFE	N2-C3-C5-N6
2	K	1001	VFE	N2-C3-C5-N6
2	Q	1001	VFE	N2-C3-C5-N6
2	R	1001	VFE	N2-C3-C5-N6
2	U	1001	VFE	N2-C3-C5-N6
2	V	1001	VFE	N2-C3-C5-N6

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Mol	Chain	Res	Type	Atoms
2	Y	1001	VFE	N2-C3-C5-N6
2	Z	1001	VFE	N2-C3-C5-N6
2	c	1001	VFE	N2-C3-C5-N6
2	G	1001	VFE	O4-C3-C5-N6
2	Z	1001	VFE	O4-C3-C5-N6
2	L	1001	VFE	O4-C3-N2-C1
2	A	1001	VFE	O4-C3-C5-N6
2	D	1001	VFE	O4-C3-C5-N6
2	H	1001	VFE	O4-C3-C5-N6
2	Q	1001	VFE	O4-C3-C5-N6
2	R	1001	VFE	O4-C3-C5-N6
2	U	1001	VFE	O4-C3-C5-N6
2	V	1001	VFE	O4-C3-C5-N6
2	Y	1001	VFE	O4-C3-C5-N6
2	B	1001	VFE	O4-C3-C5-N6
2	b	1001	VFE	O4-C3-C5-N6
2	B	1001	VFE	N2-C3-C5-N6
2	C	1001	VFE	N2-C3-C5-N6
2	D	1001	VFE	N2-C3-C5-N6
2	F	1001	VFE	N2-C3-C5-N6
2	I	1001	VFE	N2-C3-C5-N6
2	J	1001	VFE	N2-C3-C5-N6
2	M	1001	VFE	N2-C3-C5-N6
2	N	1001	VFE	N2-C3-C5-N6
2	T	1001	VFE	N2-C3-C5-N6
2	W	1001	VFE	N2-C3-C5-N6
2	a	1001	VFE	N2-C3-C5-N6
2	b	1001	VFE	N2-C3-C5-N6
2	d	1001	VFE	N2-C3-C5-N6
2	C	1001	VFE	O4-C3-C5-N6
2	M	1001	VFE	O4-C3-C5-N6
2	S	1001	VFE	O4-C3-C5-N6
2	T	1001	VFE	O4-C3-C5-N6
2	W	1001	VFE	O4-C3-C5-N6
2	O	1001	VFE	O4-C3-N2-C1
2	P	1001	VFE	O4-C3-N2-C1
2	Z	1001	VFE	O4-C3-N2-C1
2	S	1001	VFE	N2-C3-C5-N6
2	F	1001	VFE	O4-C3-C5-N6
2	N	1001	VFE	O4-C3-C5-N6
2	a	1001	VFE	O4-C3-C5-N6
2	X	1001	VFE	N2-C3-C5-N6

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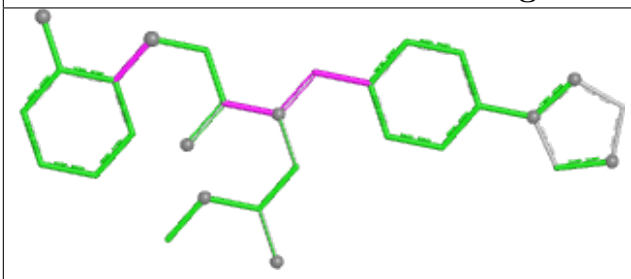
Mol	Chain	Res	Type	Atoms
2	C	1001	VFE	C5-C3-N2-C1
2	P	1001	VFE	C5-C3-N2-C1
2	R	1001	VFE	C5-C3-N2-C1
2	U	1001	VFE	C5-C3-N2-C1
2	V	1001	VFE	C5-C3-N2-C1
2	Y	1001	VFE	C5-C3-N2-C1
2	b	1001	VFE	C5-C3-N2-C1
2	I	1001	VFE	O4-C3-C5-N6
2	b	1001	VFE	O4-C3-N2-C1
2	J	1001	VFE	O4-C3-C5-N6
2	L	1001	VFE	C3-C5-N6-C7
2	d	1001	VFE	O4-C3-C5-N6
2	E	1001	VFE	N2-C3-C5-N6
2	L	1001	VFE	O4-C3-C5-N6
2	E	1001	VFE	O4-C3-C5-N6
2	O	1001	VFE	N2-C3-C5-N6
2	B	1001	VFE	O20-C19-N6-C5
2	C	1001	VFE	O4-C3-N2-C1
2	B	1001	VFE	C21-C19-N6-C5
2	X	1001	VFE	O4-C3-C5-N6
2	V	1001	VFE	O4-C3-N2-C1
2	O	1001	VFE	O4-C3-C5-N6

There are no ring outliers.

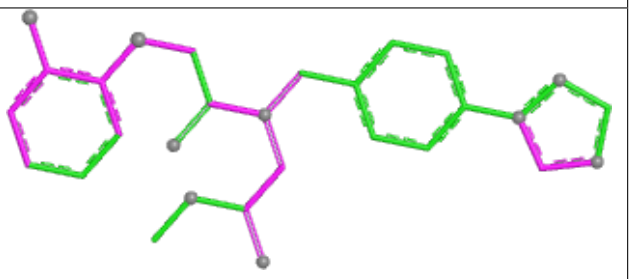
No monomer is involved in short contacts.

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

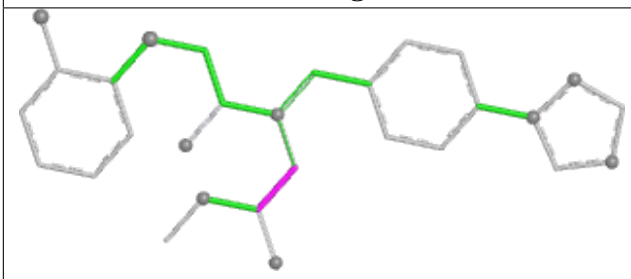
Ligand VFE S 1001



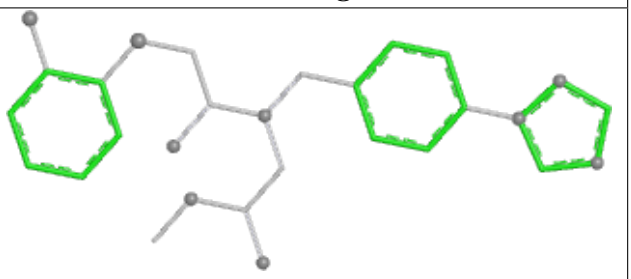
Bond lengths



Bond angles

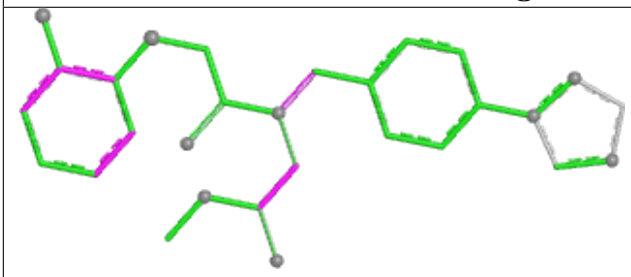


Torsions



Rings

Ligand VFE X 1001



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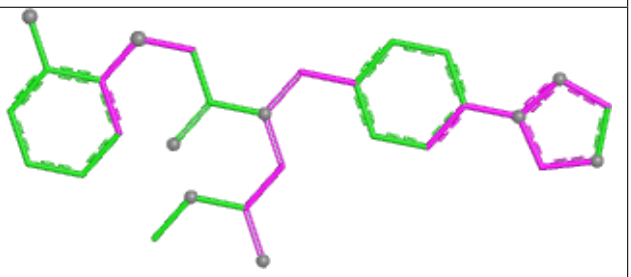

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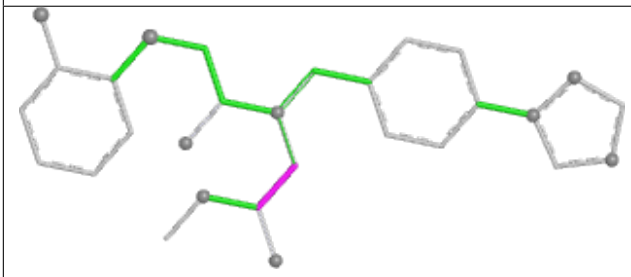

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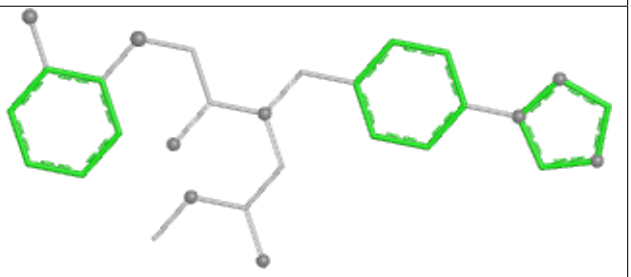
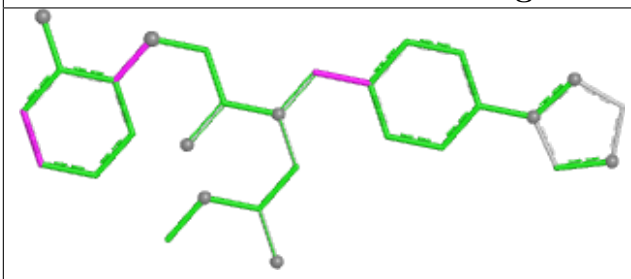


Rings

Ligand VFE V 1001



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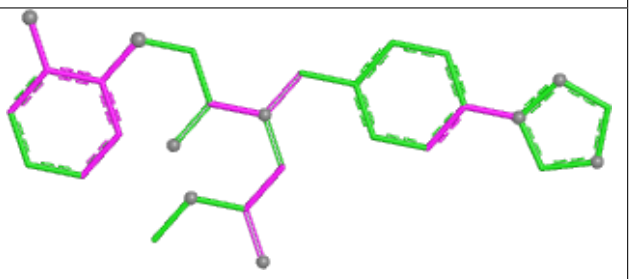

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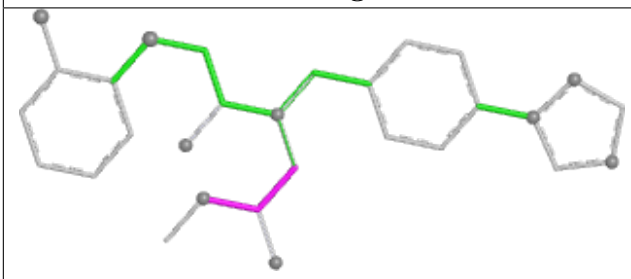

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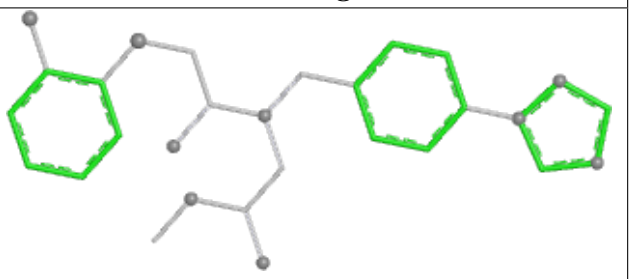
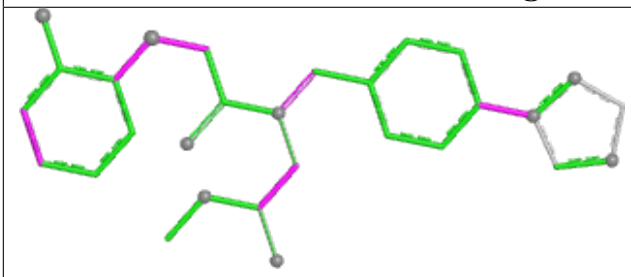


Rings

Ligand VFE I 1001



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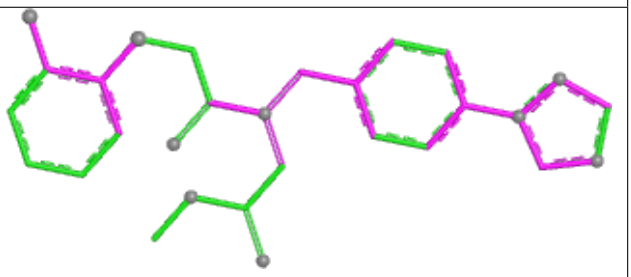

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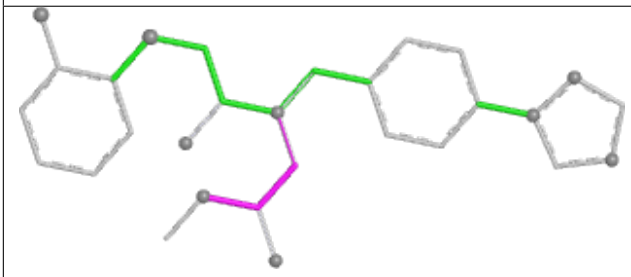

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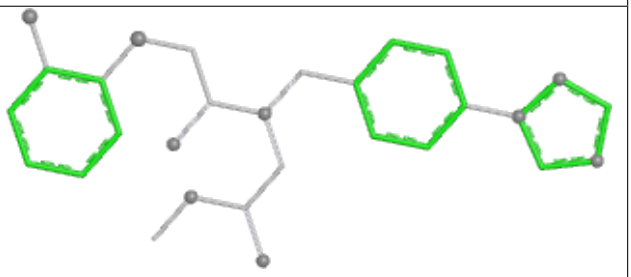

Rings

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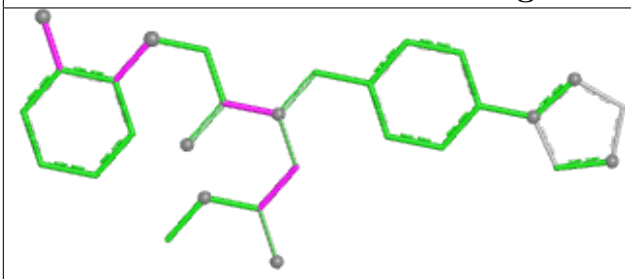

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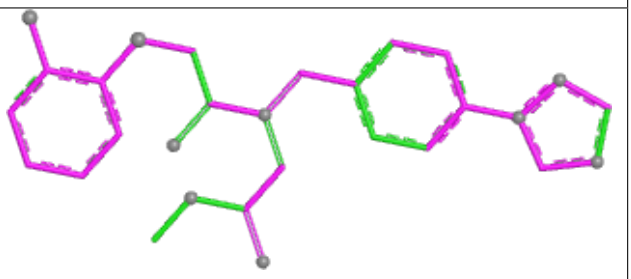

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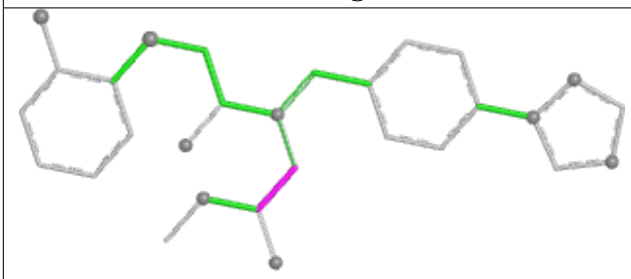

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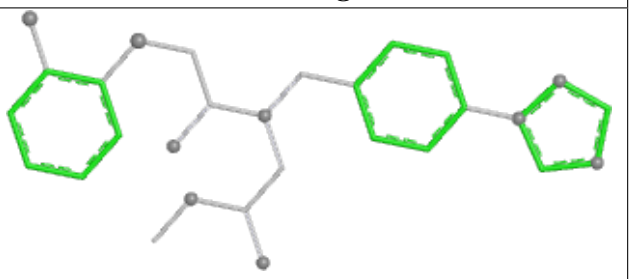
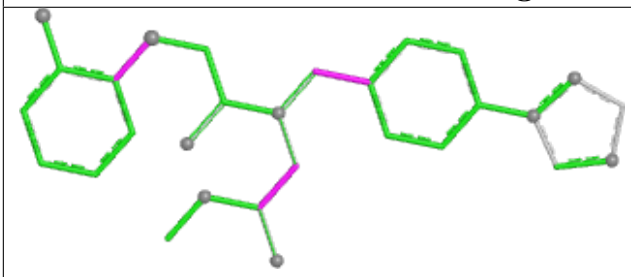


Rings

Ligand VFE R 1001



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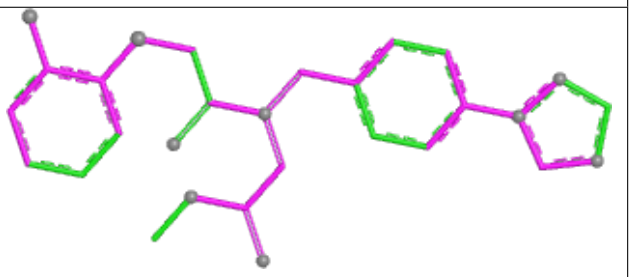

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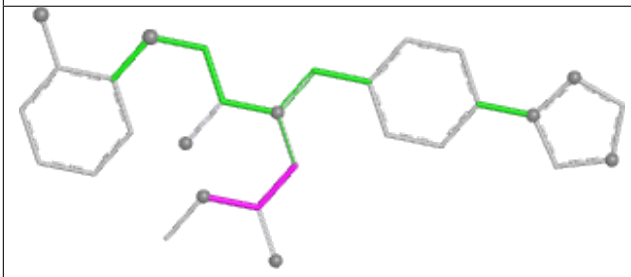

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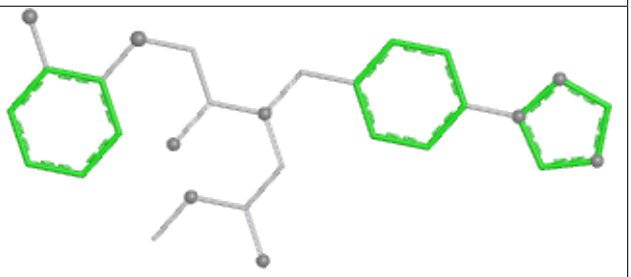

Rings

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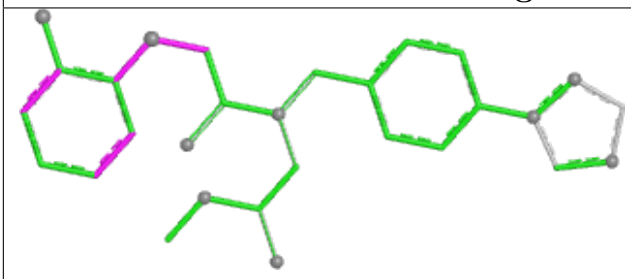
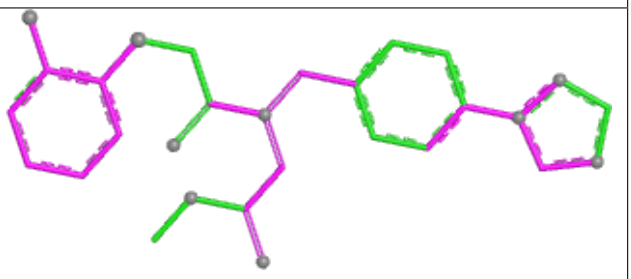
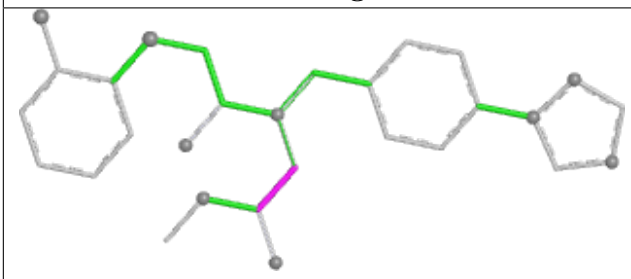
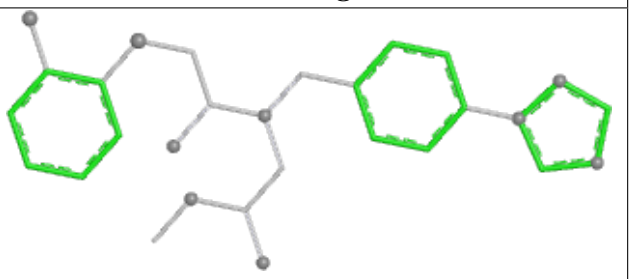
	
Bond lengths	Bond angles
	
Torsions	Rings

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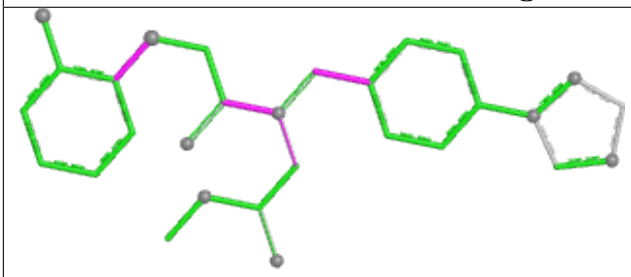
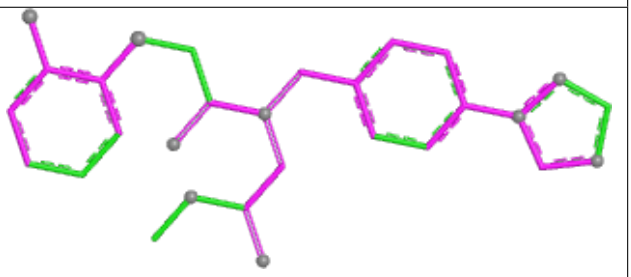
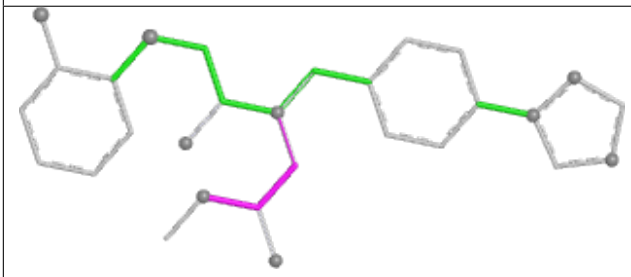
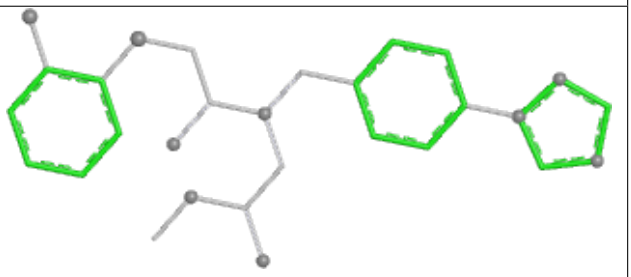
	
Bond lengths	Bond angles
	
Torsions	Rings

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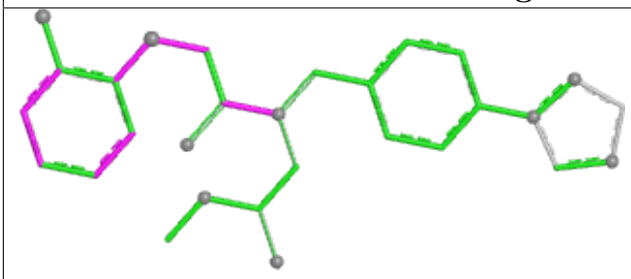

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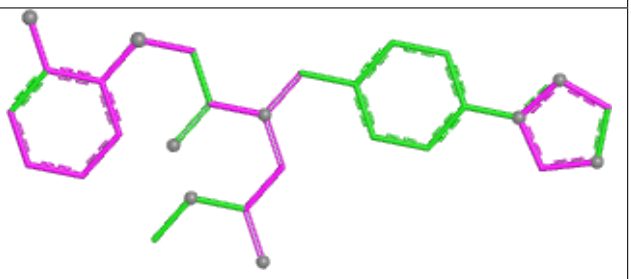

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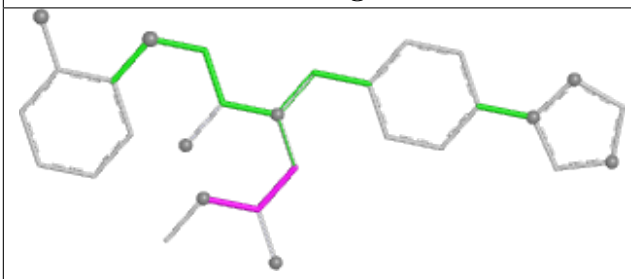

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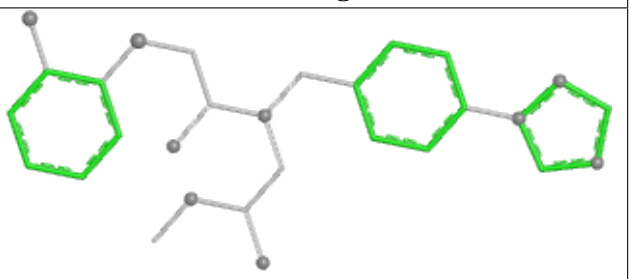
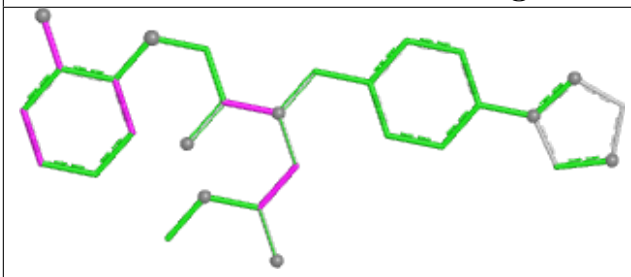


Rings

Ligand VFE W 1001



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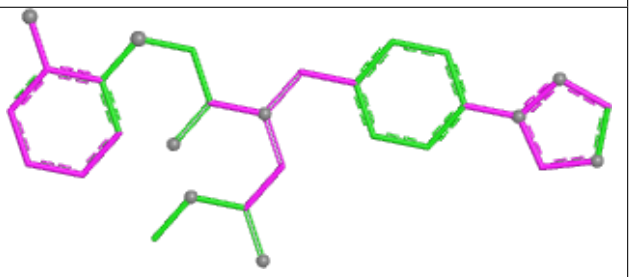

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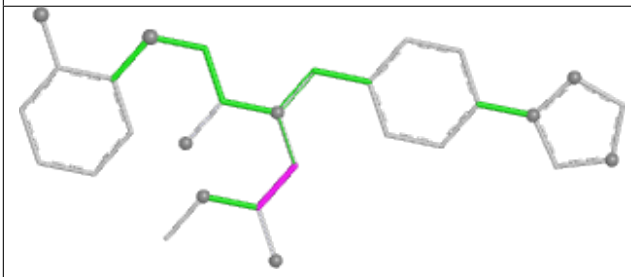

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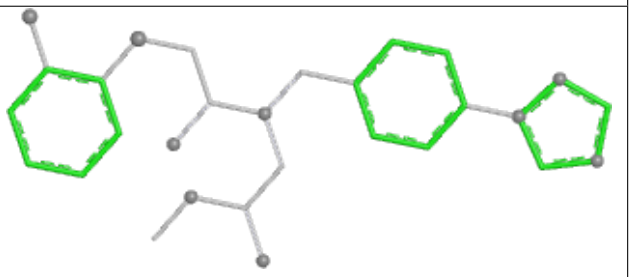
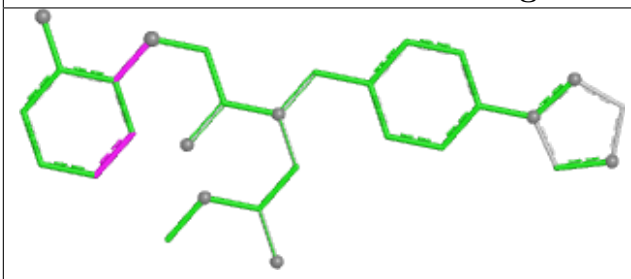
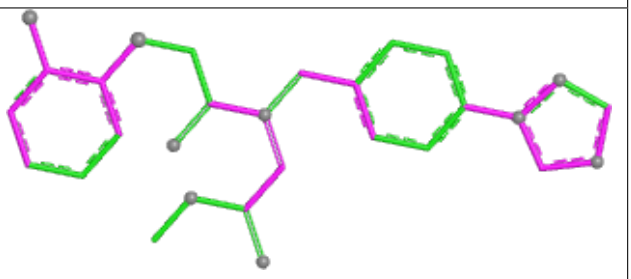
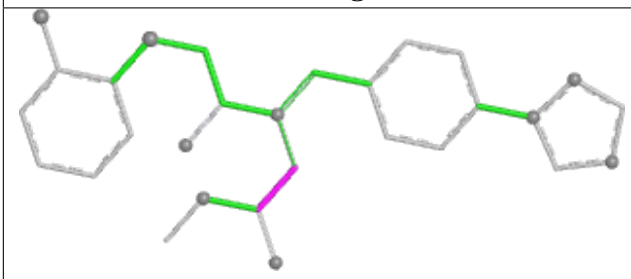
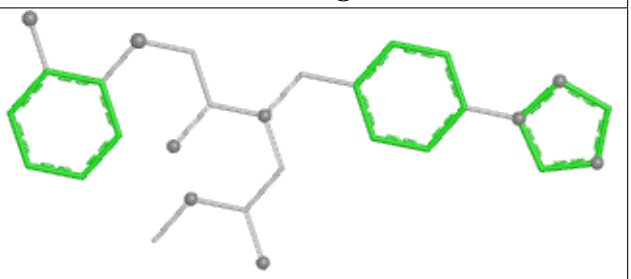


Rings

Ligand VFE J 1001	
	
Bond lengths	Bond angles
	
Torsions	Rings

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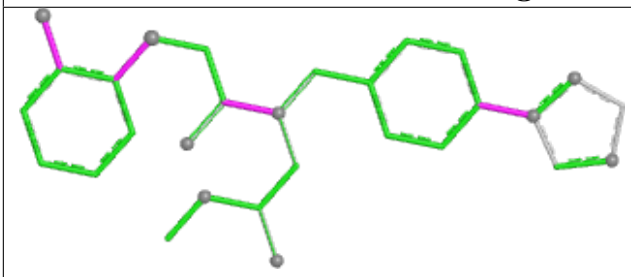
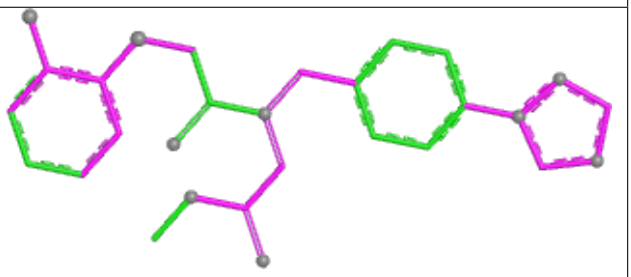
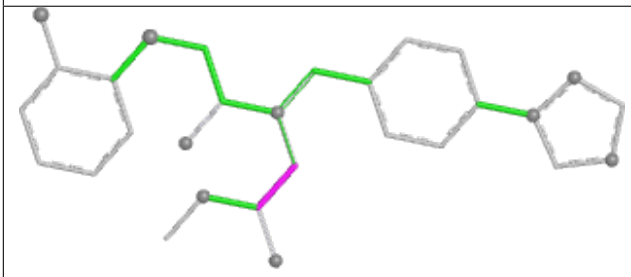
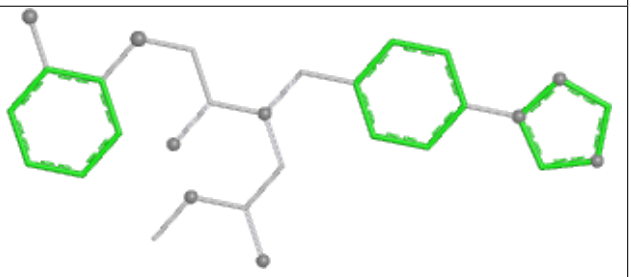
	
Bond lengths	Bond angles
	
Torsions	Rings

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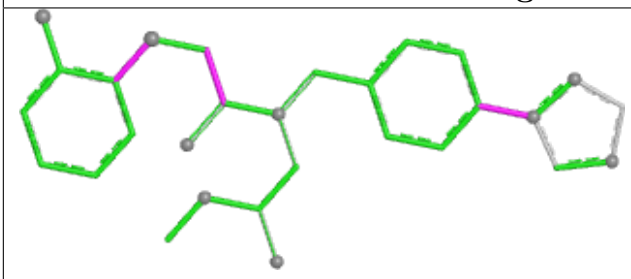
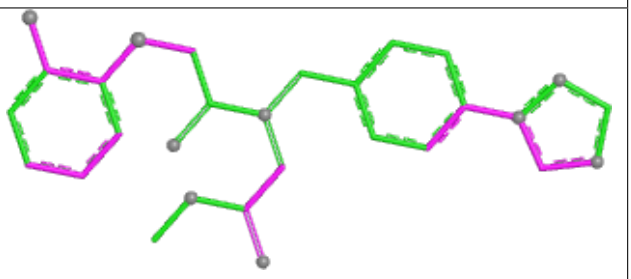
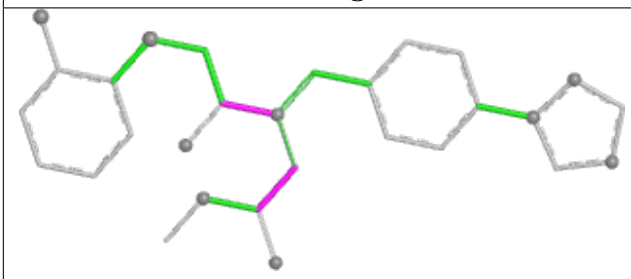
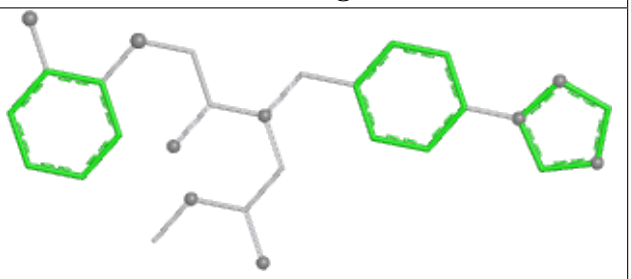
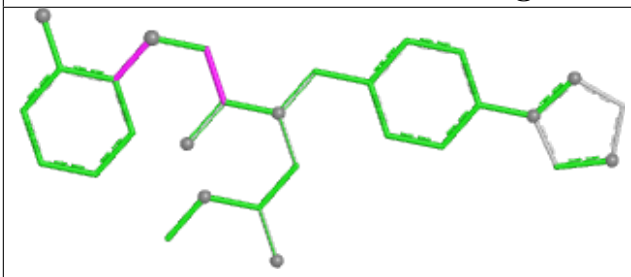
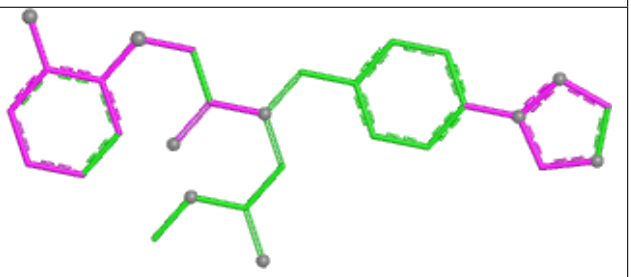
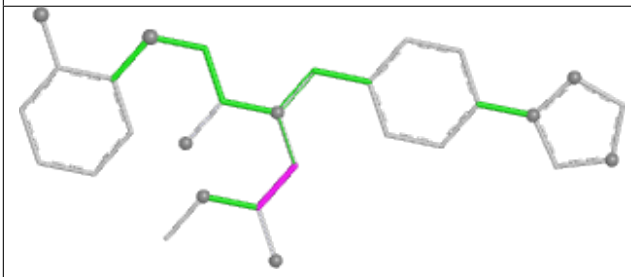
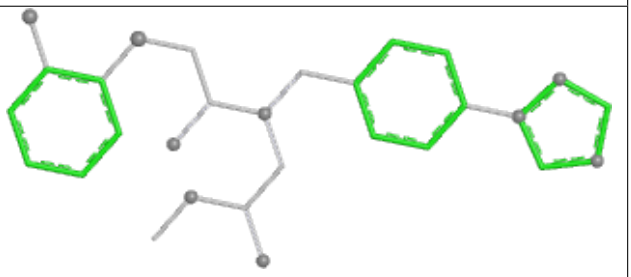
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand VFE H 1001	
 Bond lengths	 Bond angles
 Torsions	 Rings

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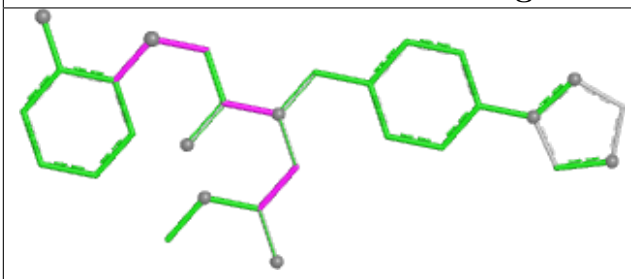
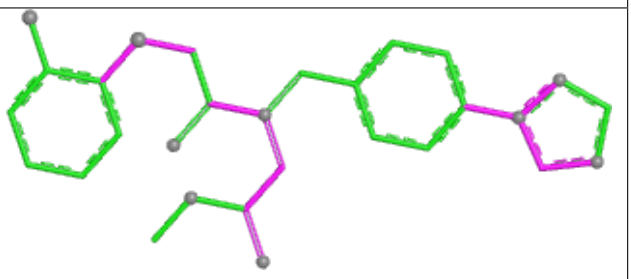
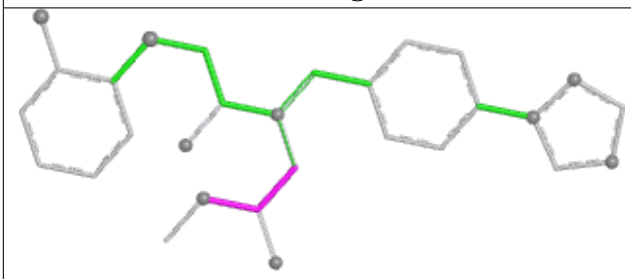
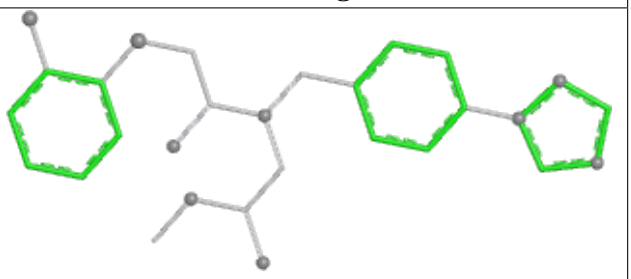
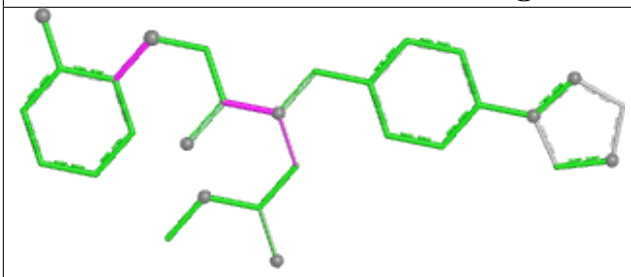
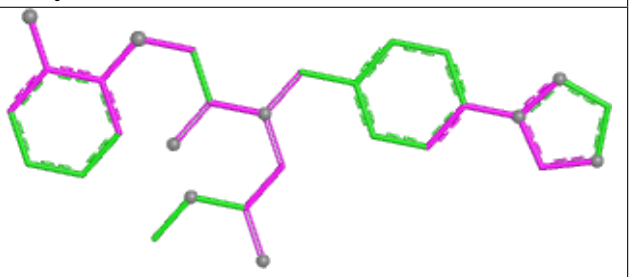
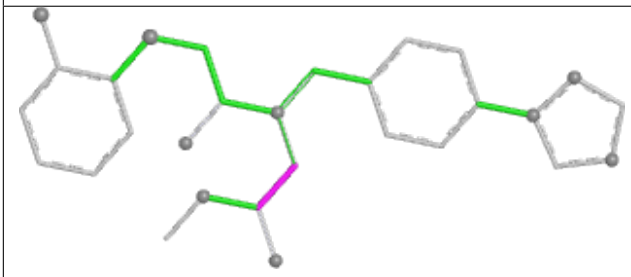
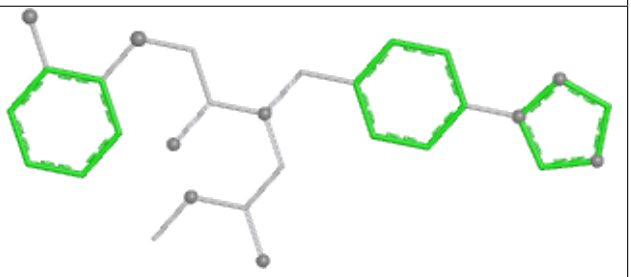
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand VFE Q 1001	
 Bond lengths	 Bond angles
 Torsions	 Rings

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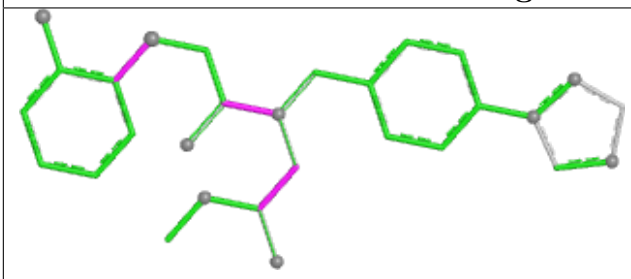
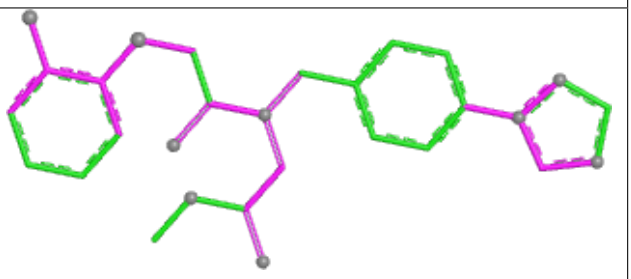
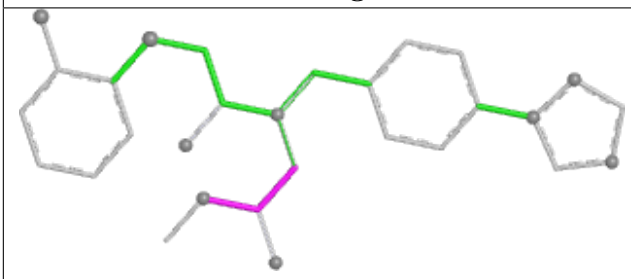
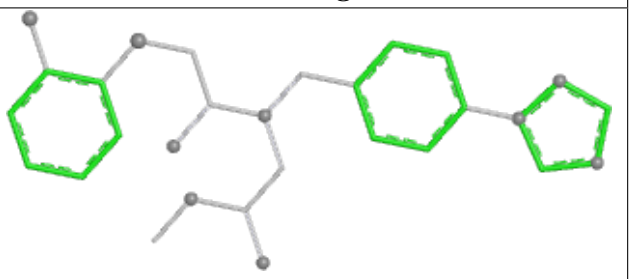
 Bond lengths	 Bond angles
 Torsions	 Rings

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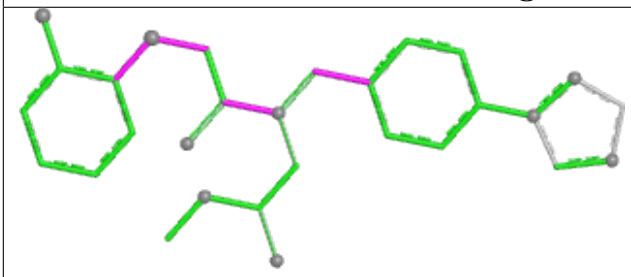
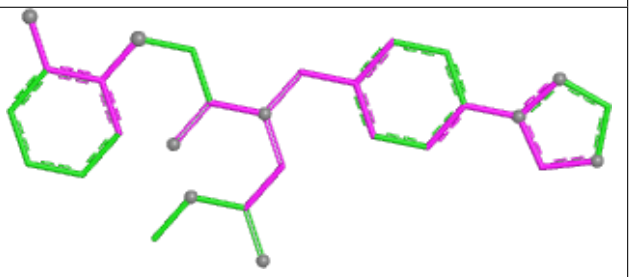
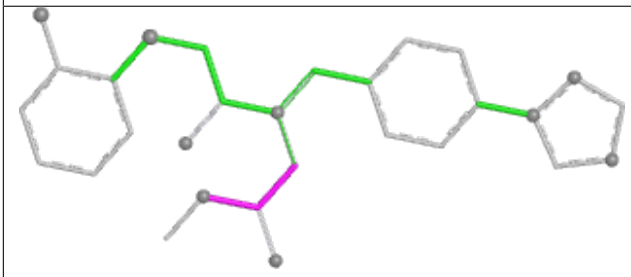
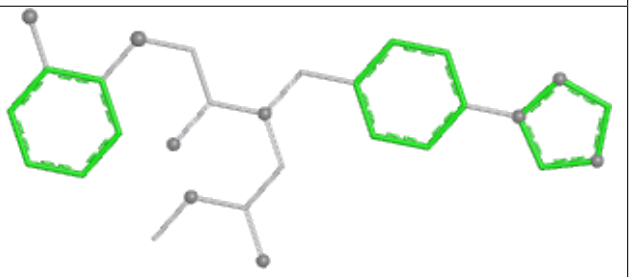
 Bond lengths	 Bond angles
 Torsions	 Rings

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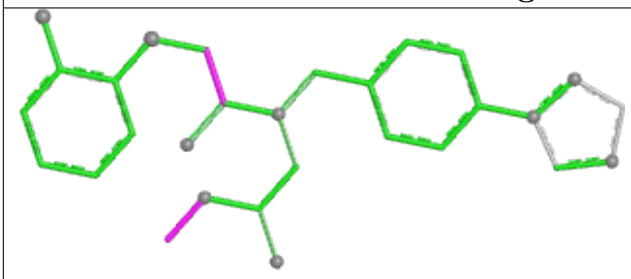
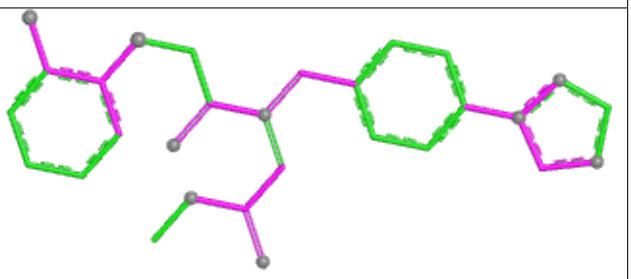
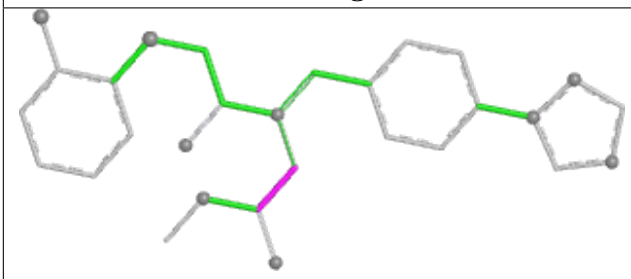
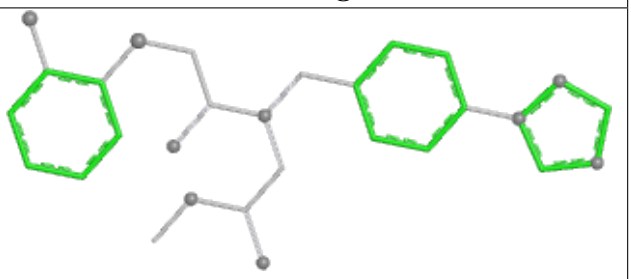
 Bond lengths	 Bond angles
 Torsions	 Rings

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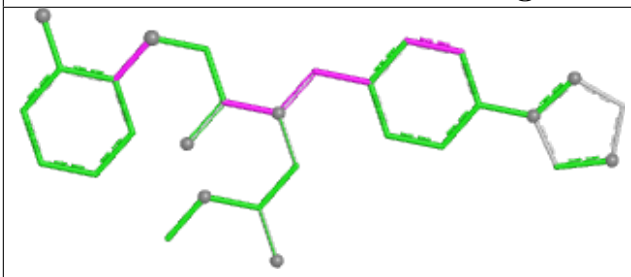
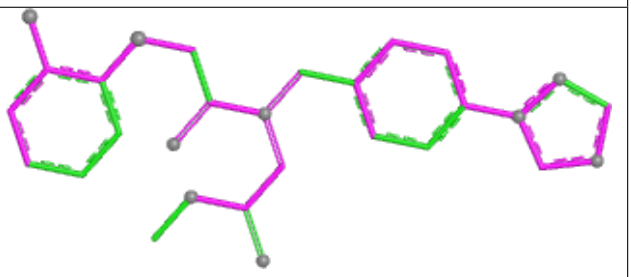
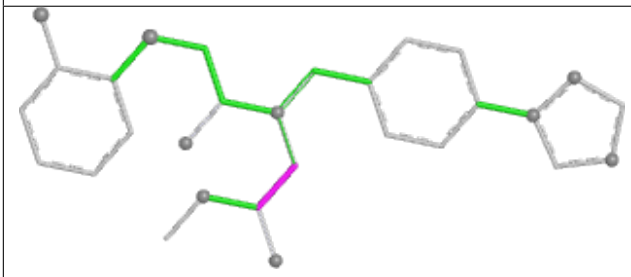
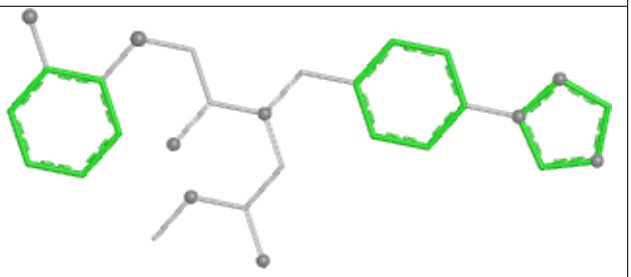
 Bond lengths	 Bond angles
 Torsions	 Rings

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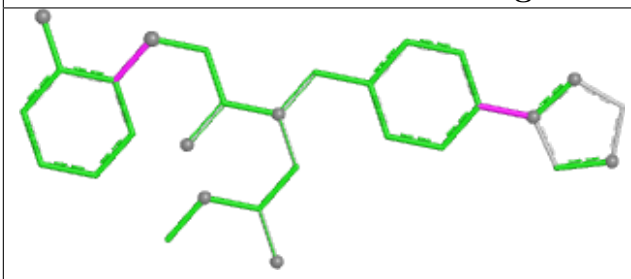	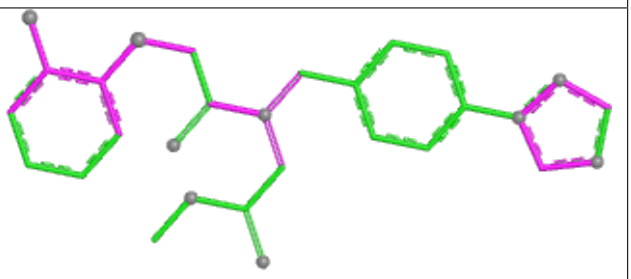
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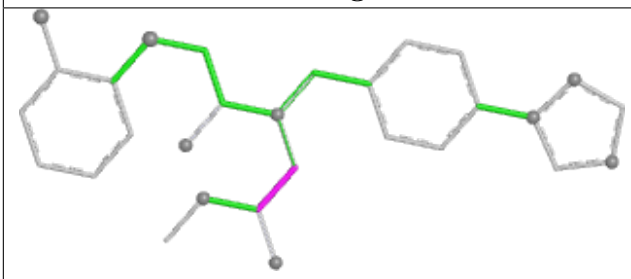	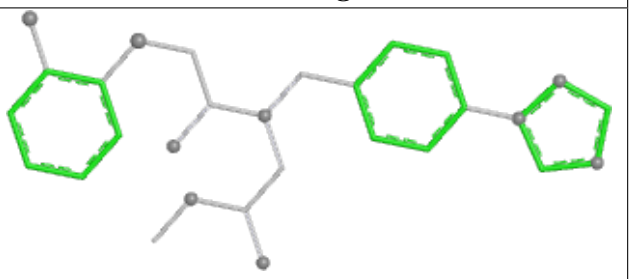
Torsions	Rings

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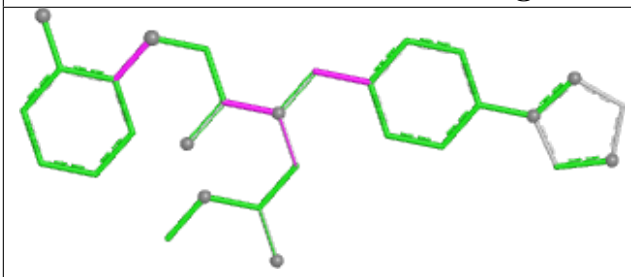	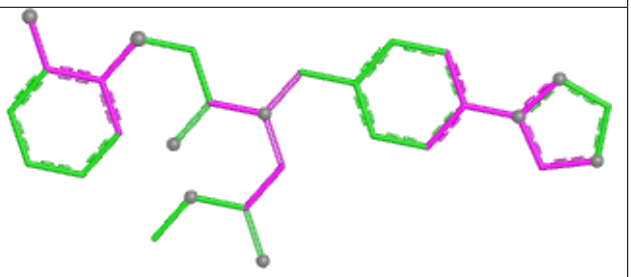
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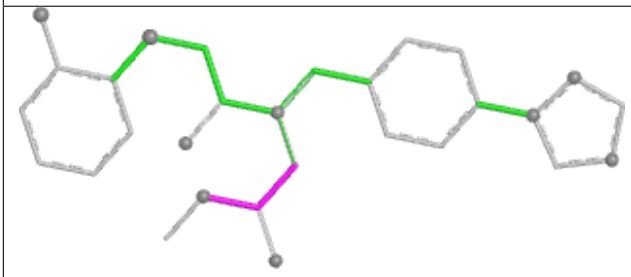	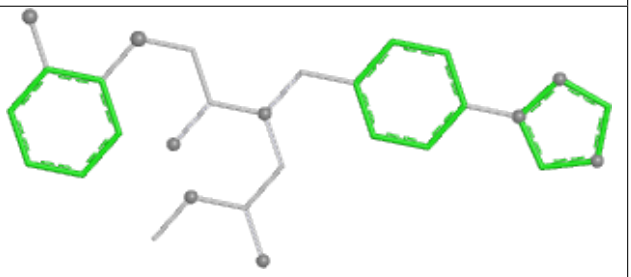
Torsions	Rings

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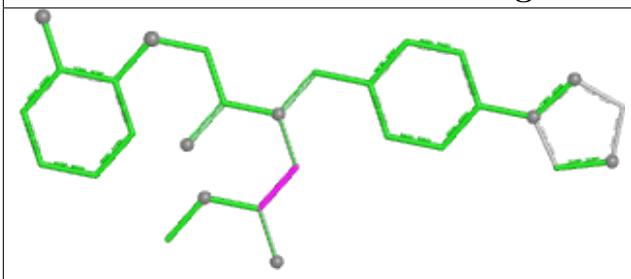

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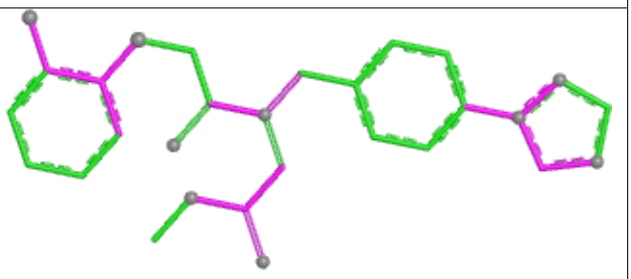

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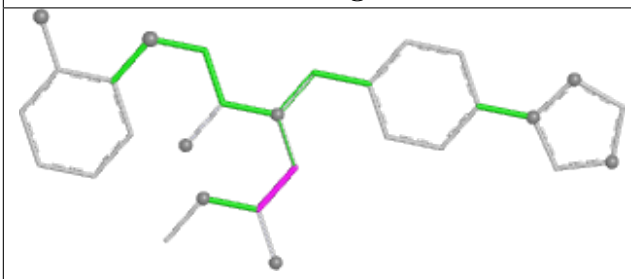

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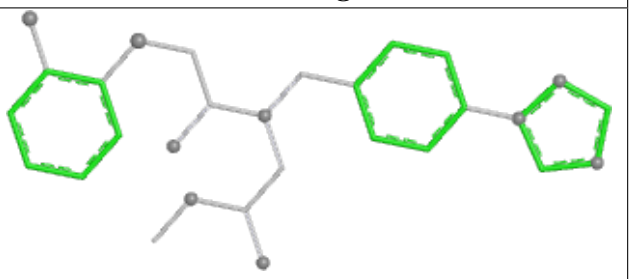

Rings

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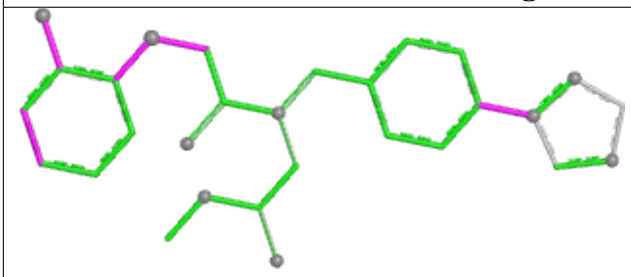

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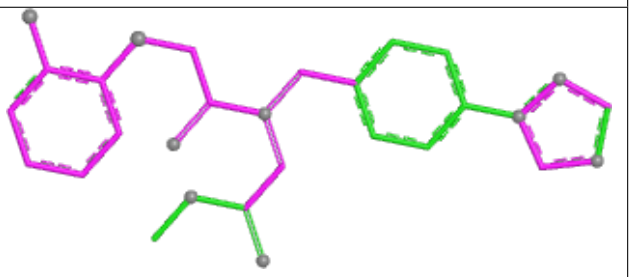

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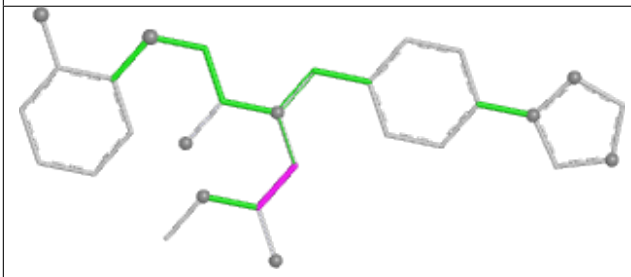

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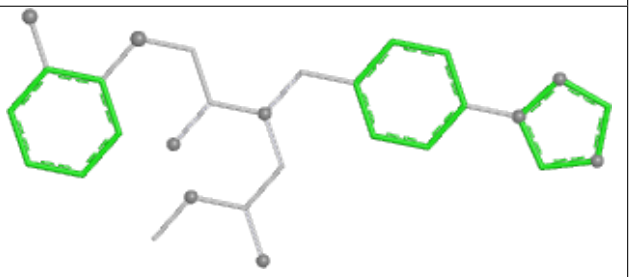

Rings

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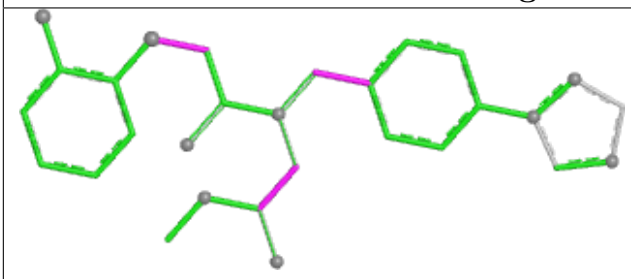
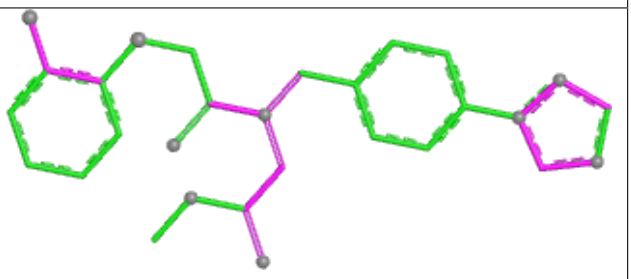
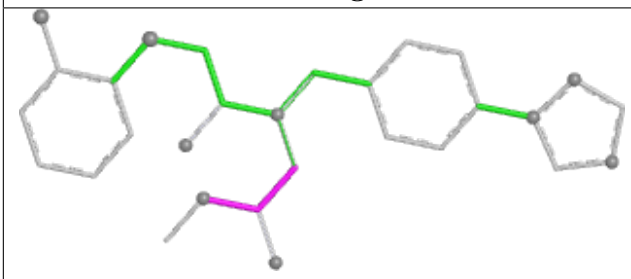
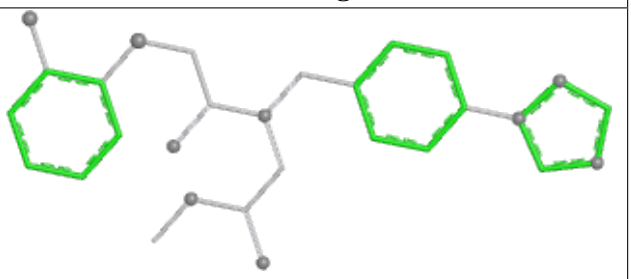
 Bond lengths	 Bond angles
 Torsions	 Rings

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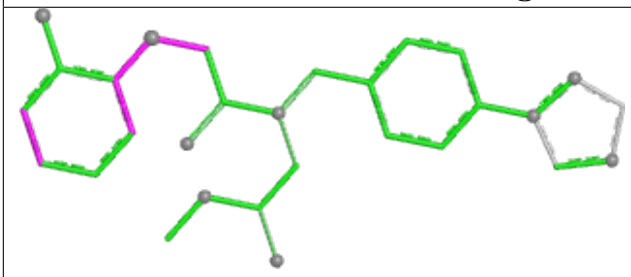
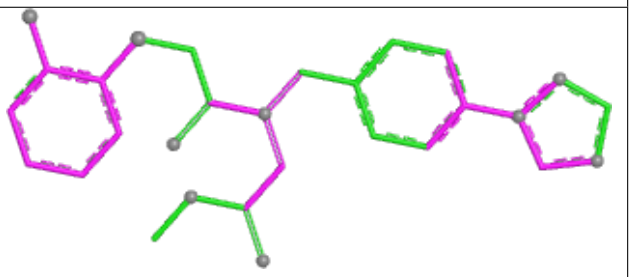
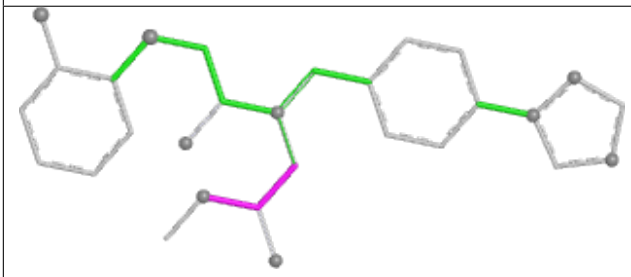
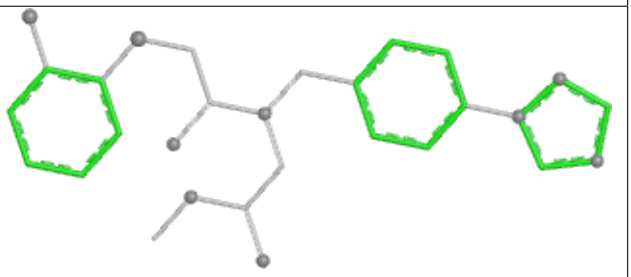
 Bond lengths	 Bond angles
 Torsions	 Rings

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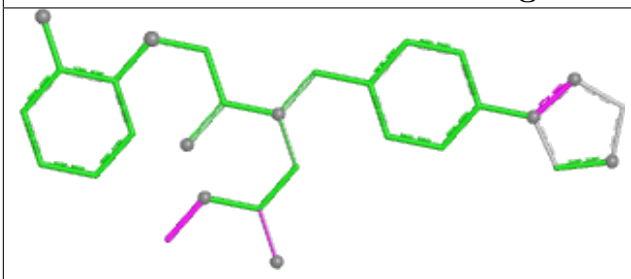
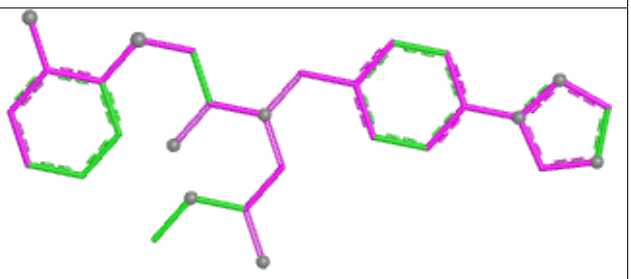
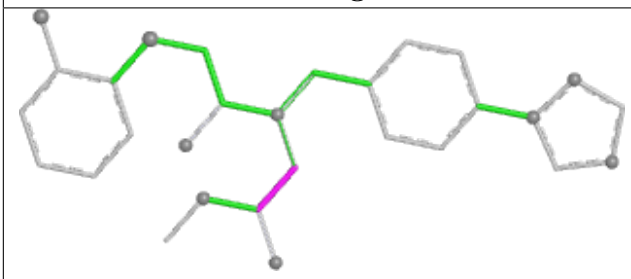
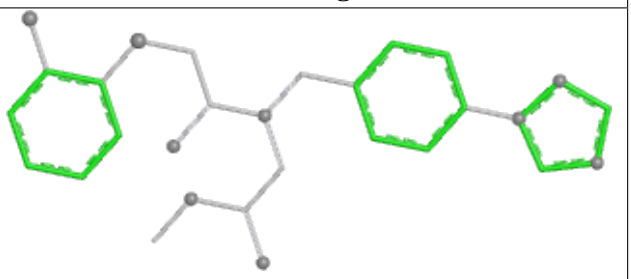
	
Bond lengths	Bond angles
	
Torsions	Rings

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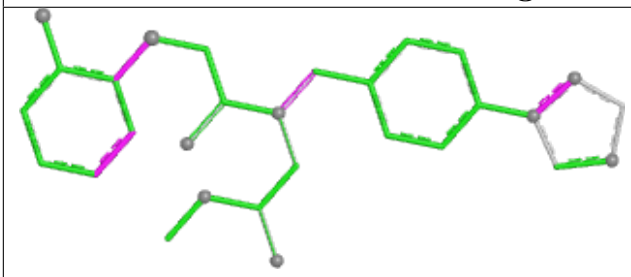
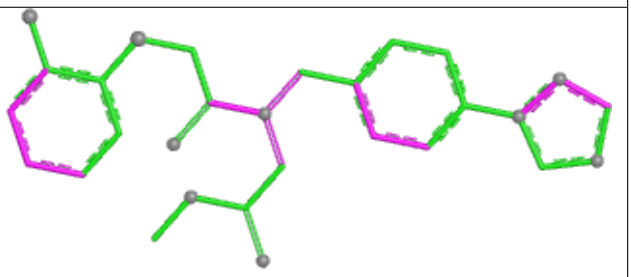
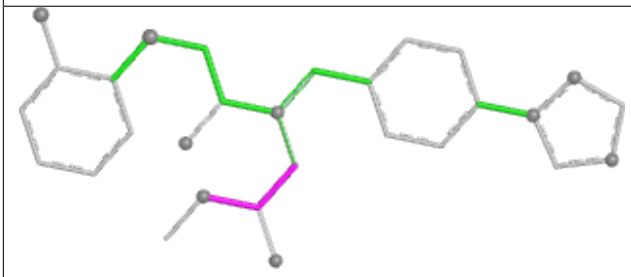
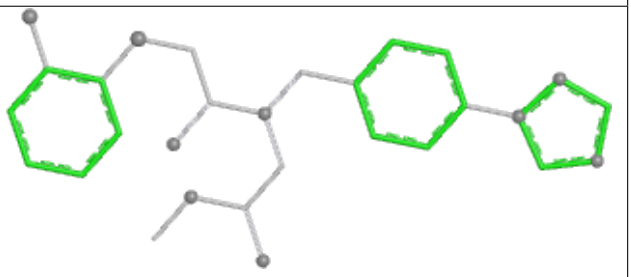
	
Bond lengths	Bond angles
	
Torsions	Rings

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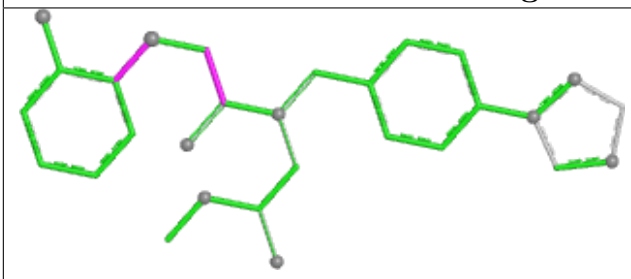
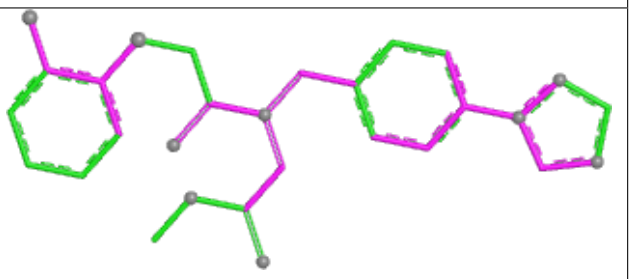
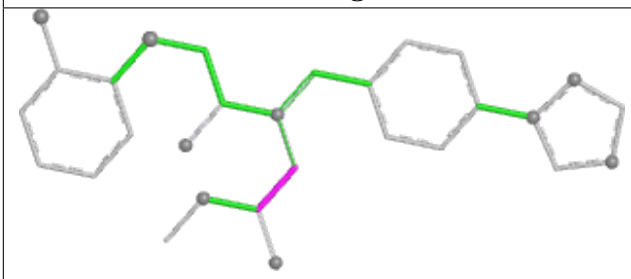
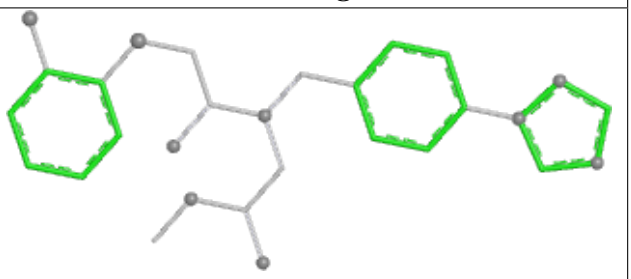
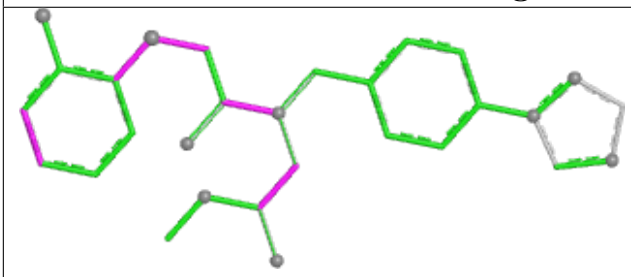
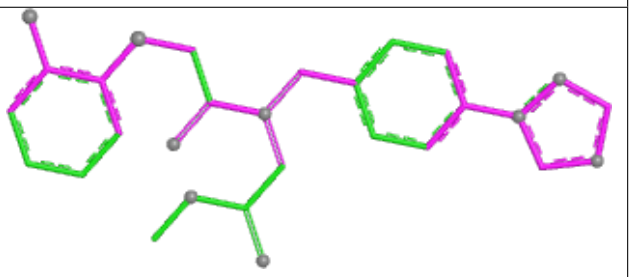
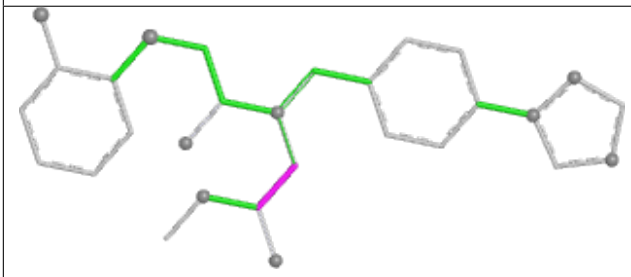
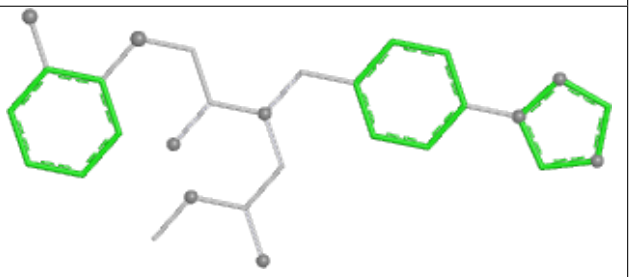
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand VFE M 1001	
 Bond lengths	 Bond angles
 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	A	258/261 (98%)	0.28	1 (0%) 92 91	33, 44, 73, 124	0
1	B	258/261 (98%)	0.32	1 (0%) 92 91	32, 43, 71, 105	0
1	C	257/261 (98%)	0.27	0 100 100	31, 42, 69, 84	0
1	D	257/261 (98%)	0.28	0 100 100	30, 42, 69, 84	0
1	E	258/261 (98%)	0.27	2 (0%) 86 85	30, 42, 69, 125	0
1	F	257/261 (98%)	0.30	0 100 100	32, 43, 70, 89	0
1	G	258/261 (98%)	0.43	3 (1%) 79 76	37, 56, 93, 136	0
1	H	258/261 (98%)	0.49	5 (1%) 66 62	39, 55, 93, 127	0
1	I	258/261 (98%)	0.51	5 (1%) 66 62	37, 54, 89, 117	0
1	J	257/261 (98%)	0.36	1 (0%) 92 91	34, 54, 87, 96	0
1	K	258/261 (98%)	0.31	2 (0%) 86 85	35, 54, 88, 140	0
1	L	258/261 (98%)	0.45	5 (1%) 66 62	37, 55, 90, 134	0
1	M	257/261 (98%)	0.30	1 (0%) 92 91	36, 51, 82, 103	0
1	N	257/261 (98%)	0.48	1 (0%) 92 91	36, 54, 88, 103	0
1	O	257/261 (98%)	0.37	1 (0%) 92 91	32, 52, 86, 98	0
1	P	257/261 (98%)	0.55	2 (0%) 86 85	38, 55, 91, 104	0
1	Q	257/261 (98%)	0.53	3 (1%) 79 76	37, 55, 91, 102	0
1	R	258/261 (98%)	0.45	4 (1%) 72 68	33, 52, 90, 122	0
1	S	258/261 (98%)	0.30	1 (0%) 92 91	32, 45, 70, 123	0
1	T	258/261 (98%)	0.43	0 100 100	34, 46, 74, 110	0
1	U	259/261 (99%)	0.29	2 (0%) 86 85	32, 43, 73, 117	0
1	V	258/261 (98%)	0.21	1 (0%) 92 91	33, 46, 73, 121	0
1	W	258/261 (98%)	0.30	2 (0%) 86 85	33, 45, 72, 107	0
1	X	259/261 (99%)	0.31	2 (0%) 86 85	32, 43, 69, 121	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	Y	258/261 (98%)	0.39	1 (0%) 92 91	31, 44, 76, 124	0
1	Z	261/261 (100%)	0.31	0 100 100	30, 42, 69, 81	0
1	a	257/261 (98%)	0.27	0 100 100	33, 44, 71, 91	0
1	b	257/261 (98%)	0.30	1 (0%) 92 91	31, 42, 69, 94	0
1	c	257/261 (98%)	0.35	1 (0%) 92 91	30, 43, 70, 87	0
1	d	261/261 (100%)	0.35	0 100 100	28, 40, 67, 81	0
All	All	7736/7830 (98%)	0.36	48 (0%) 89 88	28, 47, 81, 140	0

All (48) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	1	MET	4.9
1	H	1	MET	4.8
1	I	1	MET	4.6
1	L	1	MET	4.3
1	W	1	MET	4.3
1	G	1	MET	4.0
1	b	2	SER	3.8
1	S	1	MET	3.7
1	Q	71	LEU	3.2
1	R	1	MET	2.8
1	L	2	SER	2.7
1	A	1	MET	2.7
1	I	32	VAL	2.6
1	I	77	PRO	2.6
1	I	71	LEU	2.6
1	L	51	LYS	2.6
1	M	2	SER	2.6
1	K	1	MET	2.5
1	H	2	SER	2.4
1	X	18	ALA	2.4
1	R	62	SER	2.4
1	V	1	MET	2.4
1	U	12	PRO	2.4
1	H	46	LEU	2.4
1	Q	28	VAL	2.4
1	Y	1	MET	2.3
1	P	174	GLY	2.3
1	E	71	LEU	2.3
1	W	65	GLY	2.3

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Mol	Chain	Res	Type	RSRZ
1	X	0	HIS	2.3
1	N	253	THR	2.2
1	c	2	SER	2.2
1	L	71	LEU	2.2
1	O	8	ALA	2.2
1	P	43	HIS	2.2
1	H	15	ARG	2.1
1	K	102	ARG	2.1
1	L	226	GLU	2.1
1	G	26	SER	2.1
1	B	253	THR	2.1
1	U	1	MET	2.1
1	R	102	ARG	2.1
1	R	253	THR	2.1
1	I	70	ASP	2.1
1	H	22	VAL	2.1
1	J	3	LEU	2.0
1	Q	255	GLY	2.0
1	G	58	ILE	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	VFE	I	1001	29/29	0.91	0.29	58,63,70,80	0
2	VFE	U	1001	29/29	0.92	0.29	53,58,66,71	0
2	VFE	d	1001	29/29	0.92	0.26	44,57,66,70	0
2	VFE	M	1001	29/29	0.93	0.30	53,62,70,82	0

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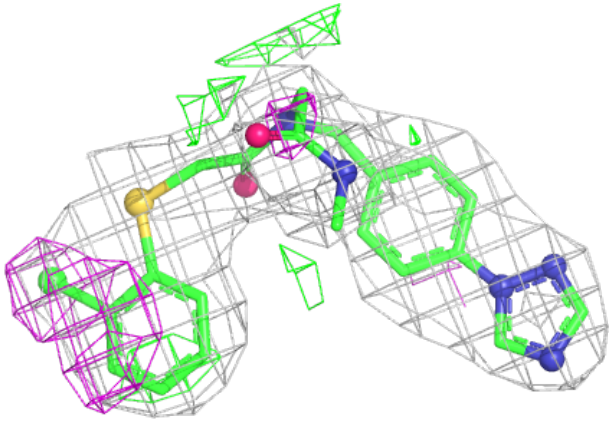
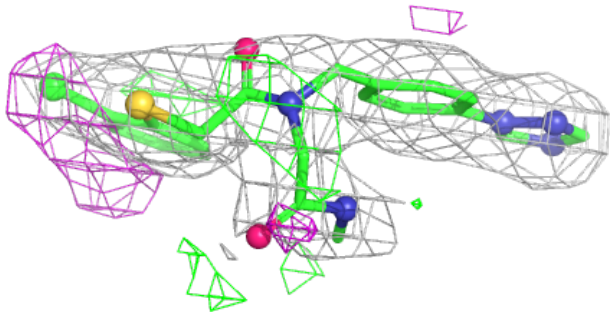
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	VFE	R	1001	29/29	0.93	0.32	52,58,80,80	0
2	VFE	J	1001	29/29	0.93	0.26	55,59,69,71	0
2	VFE	X	1001	29/29	0.93	0.26	51,57,67,72	0
2	VFE	K	1001	29/29	0.93	0.29	61,67,77,82	0
2	VFE	L	1001	29/29	0.94	0.31	59,63,73,81	0
2	VFE	G	1001	29/29	0.94	0.29	56,65,69,74	0
2	VFE	P	1001	29/29	0.94	0.34	56,60,66,77	0
2	VFE	H	1001	29/29	0.94	0.36	61,69,73,82	0
2	VFE	T	1001	29/29	0.94	0.27	47,57,69,72	0
2	VFE	A	1001	29/29	0.94	0.29	46,53,62,69	0
2	VFE	C	1001	29/29	0.94	0.29	49,56,62,81	0
2	VFE	c	1001	29/29	0.94	0.29	47,54,65,78	0
2	VFE	D	1001	29/29	0.94	0.26	47,52,65,68	0
2	VFE	B	1001	29/29	0.95	0.28	46,50,61,63	0
2	VFE	O	1001	29/29	0.95	0.29	56,63,76,78	0
2	VFE	E	1001	29/29	0.95	0.27	49,55,64,72	0
2	VFE	Y	1001	29/29	0.95	0.30	50,58,71,73	0
2	VFE	Z	1001	29/29	0.95	0.28	51,58,72,76	0
2	VFE	a	1001	29/29	0.95	0.28	51,56,67,73	0
2	VFE	b	1001	29/29	0.95	0.30	54,59,73,82	0
2	VFE	Q	1001	29/29	0.95	0.35	57,65,72,78	0
2	VFE	F	1001	29/29	0.95	0.31	46,52,65,76	0
2	VFE	W	1001	29/29	0.96	0.31	52,55,67,72	0
2	VFE	N	1001	29/29	0.96	0.30	50,57,64,73	0
2	VFE	S	1001	29/29	0.96	0.27	45,54,59,71	0
2	VFE	V	1001	29/29	0.96	0.29	49,55,60,73	0
3	MG	D	1002	1/1	0.96	0.10	58,58,58,58	0

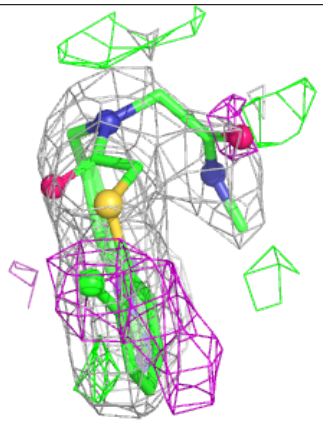
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around VFE I 1001:

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

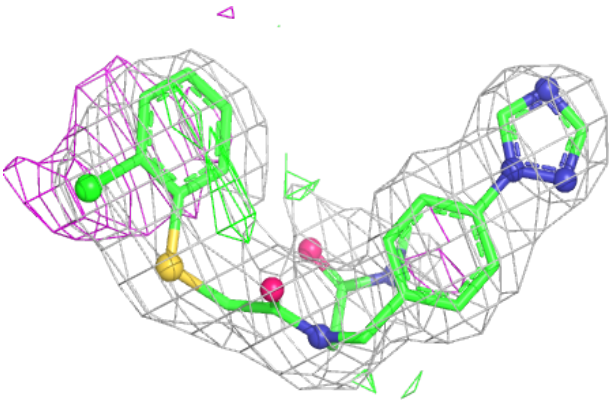


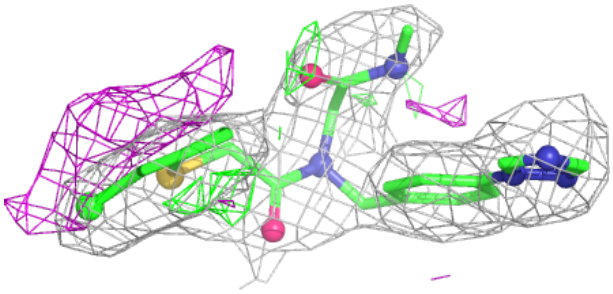


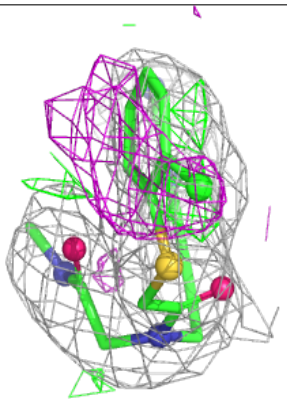


Electron density around VFE U 1001:

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

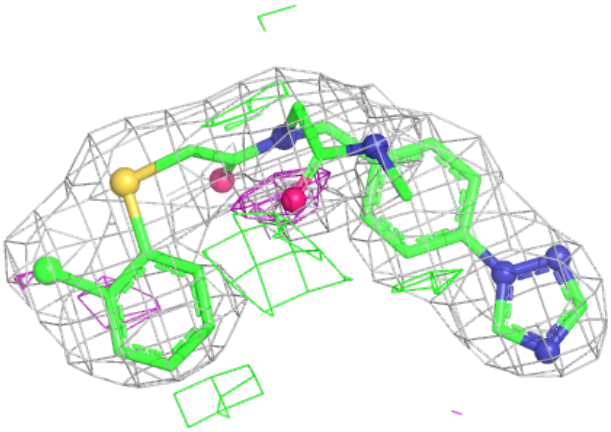


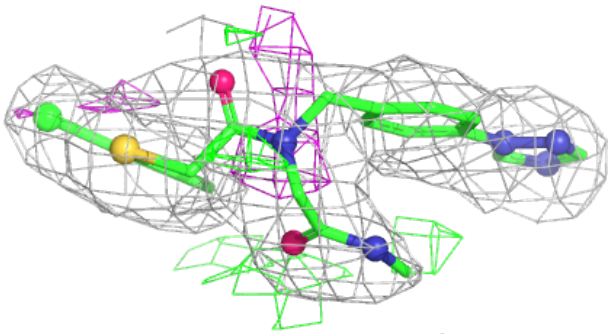


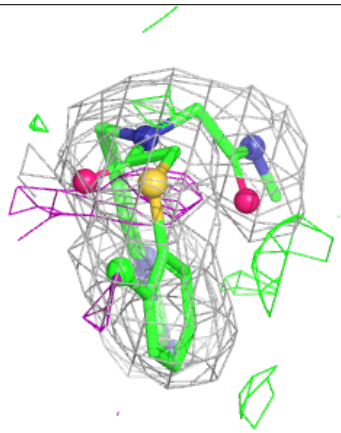


Electron density around VFE d 1001:

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

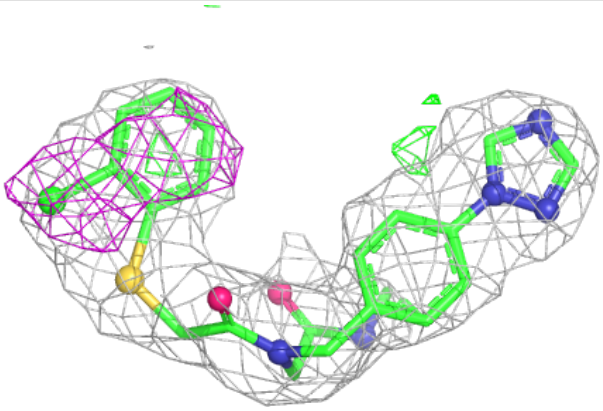


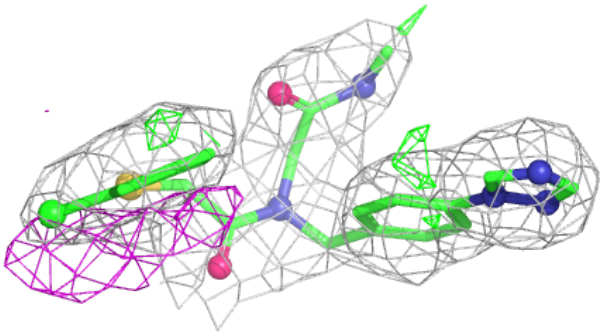


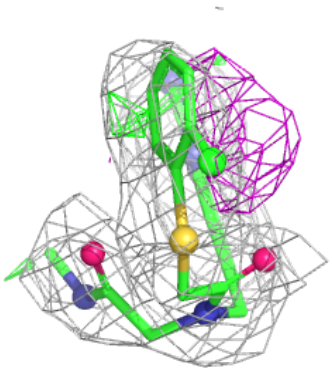


Electron density around VFE M 1001:

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

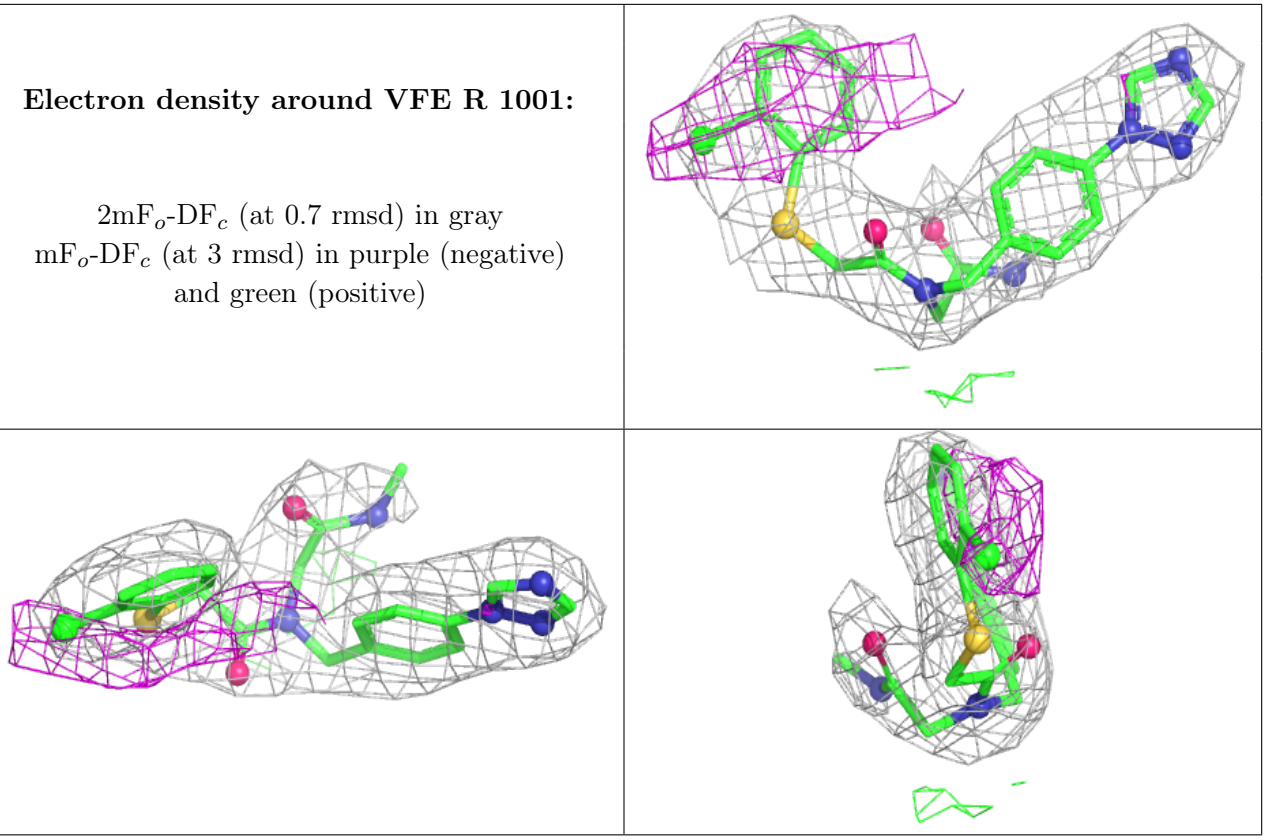






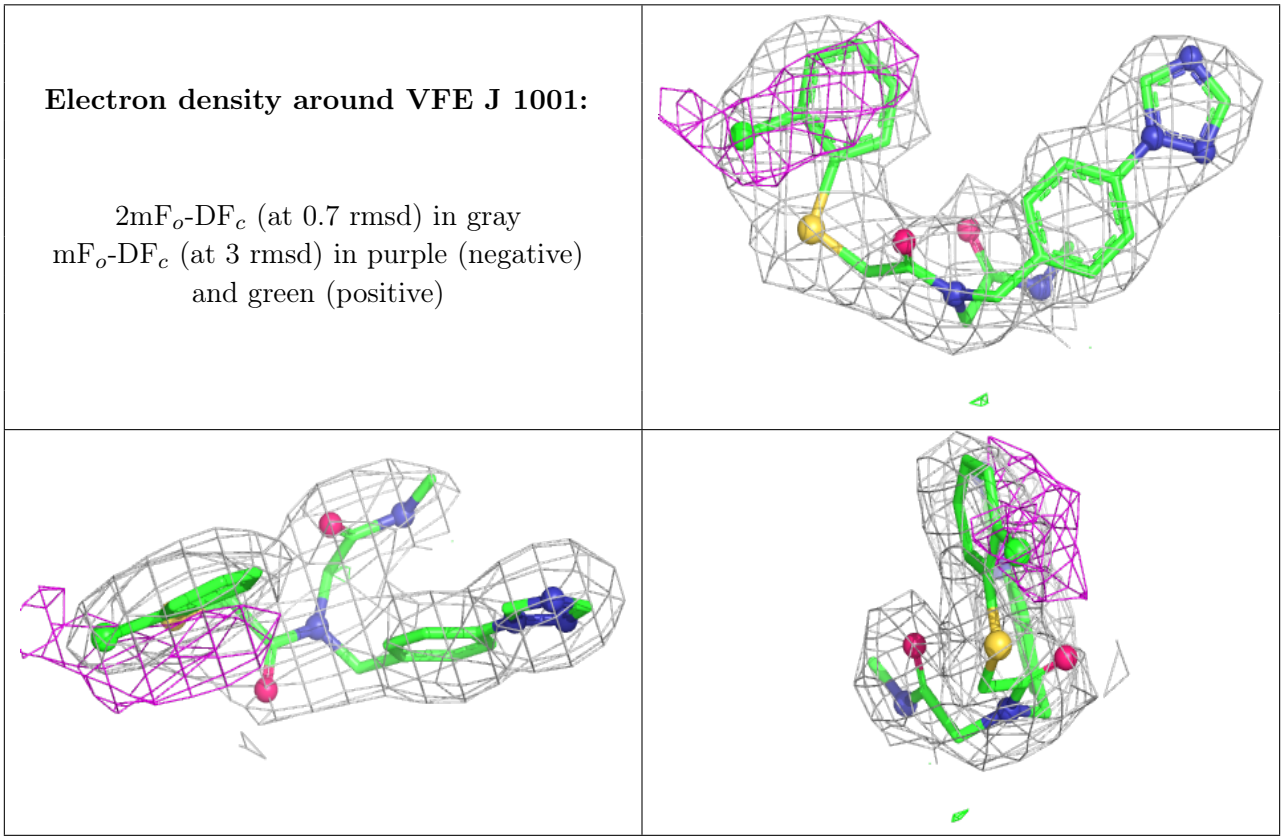
Electron density around VFE R 1001:

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



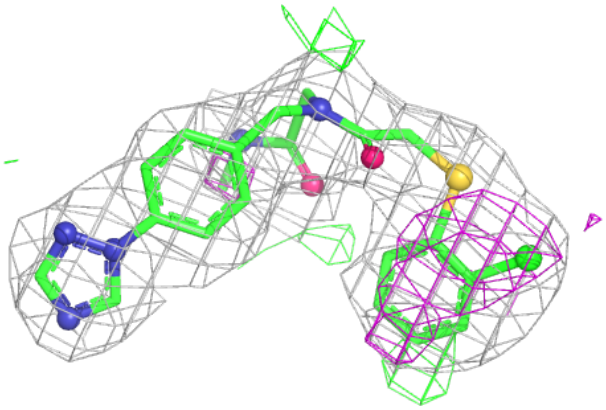
Electron density around VFE J 1001:

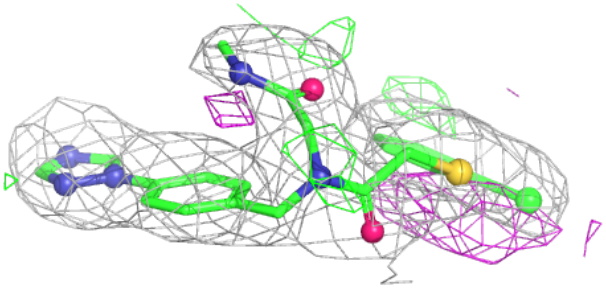
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

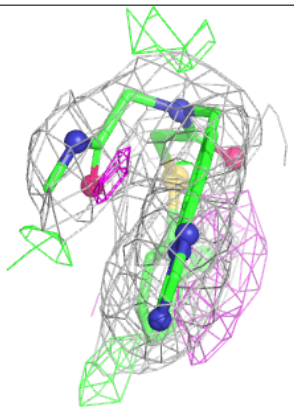


Electron density around VFE X 1001:

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

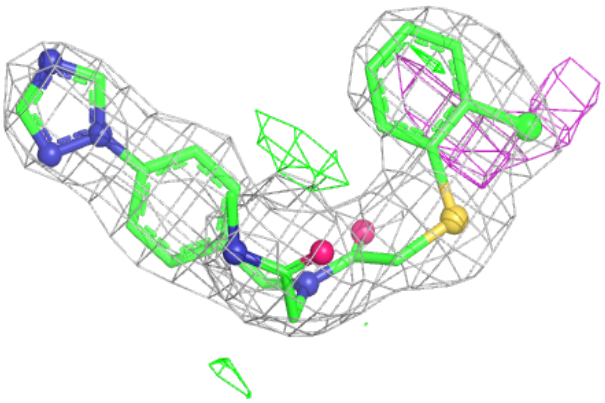


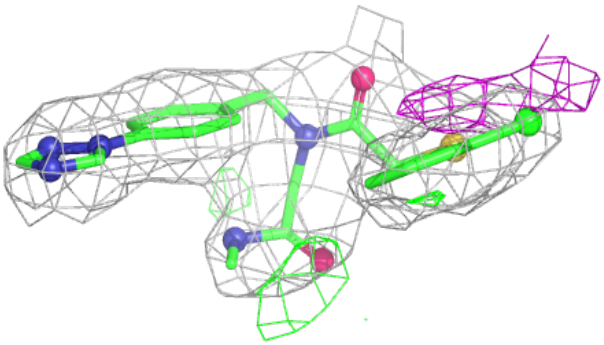


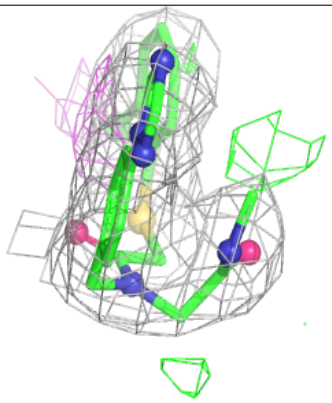


Electron density around VFE K 1001:

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

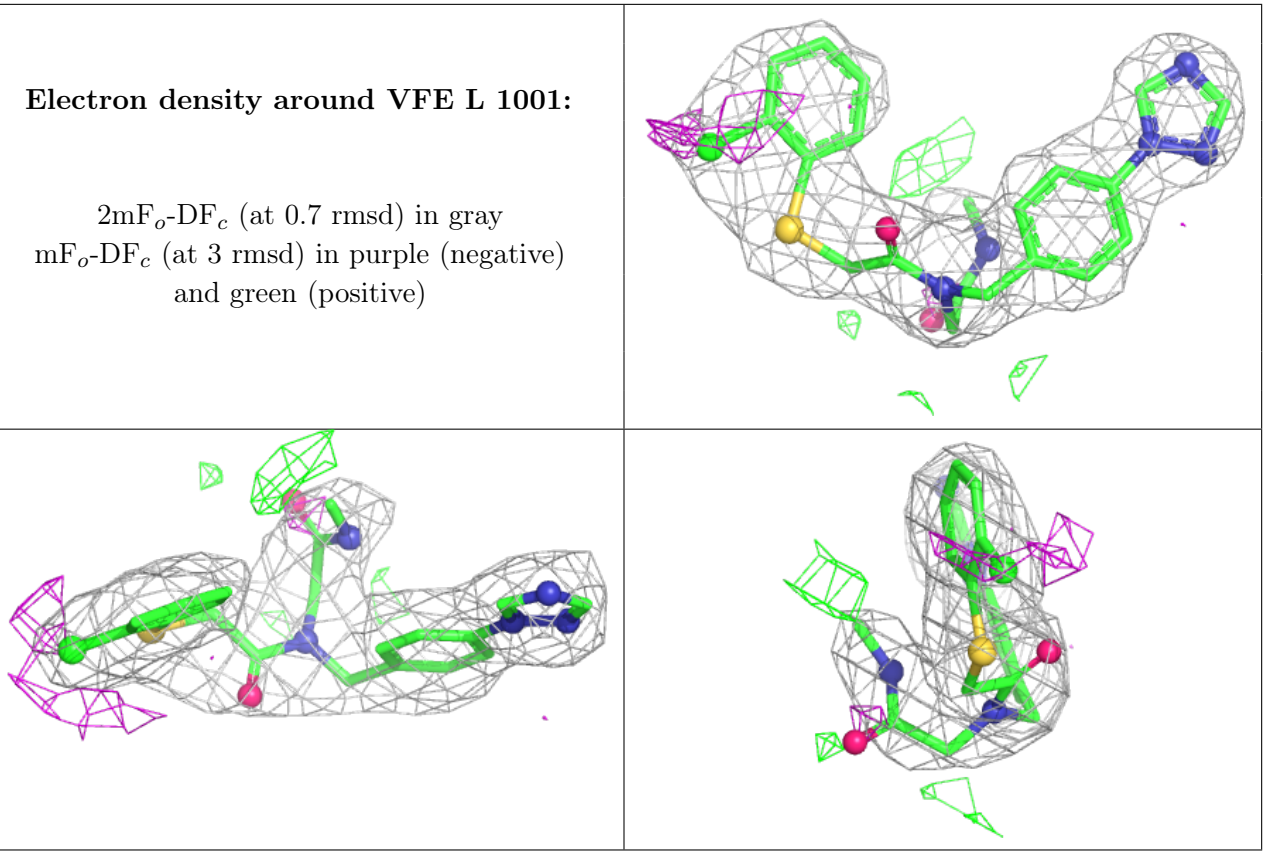






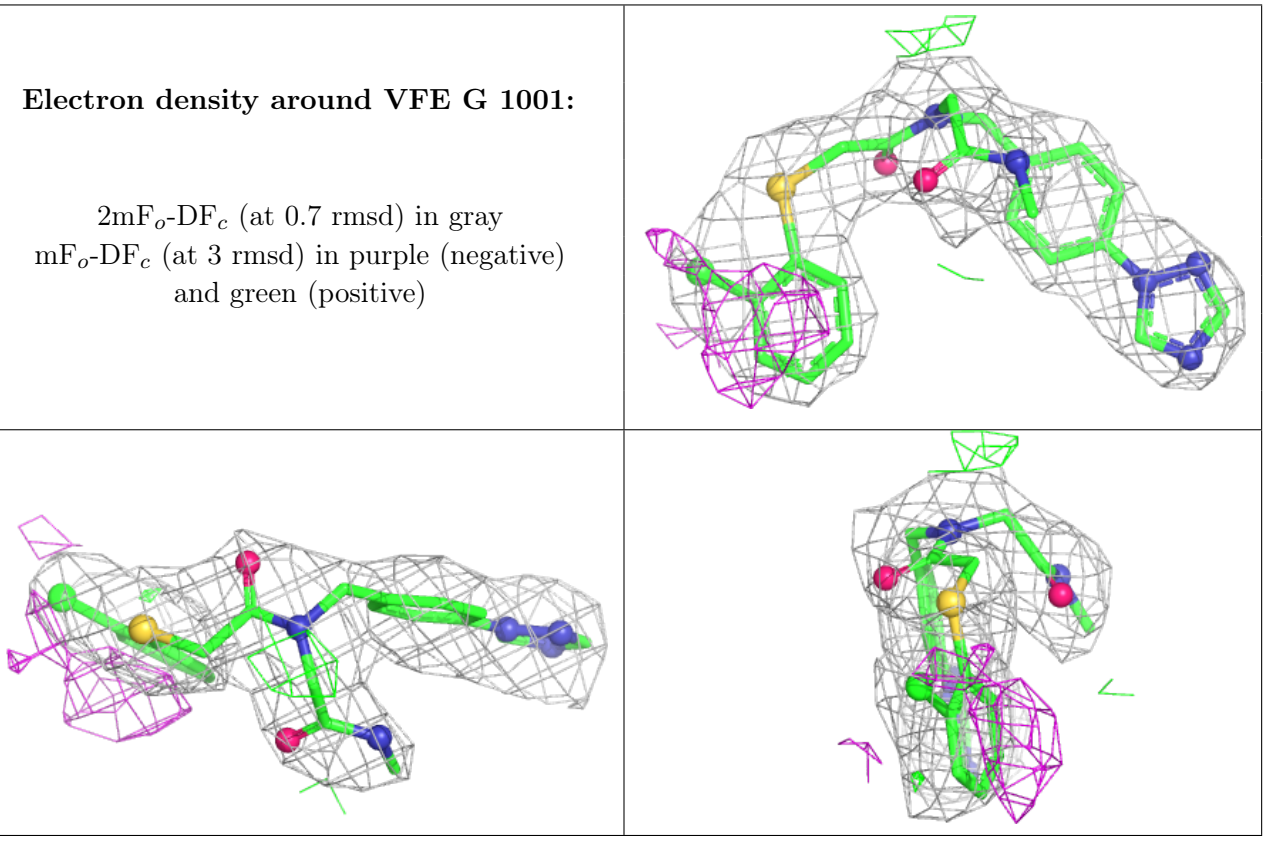
Electron density around VFE L 1001:

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



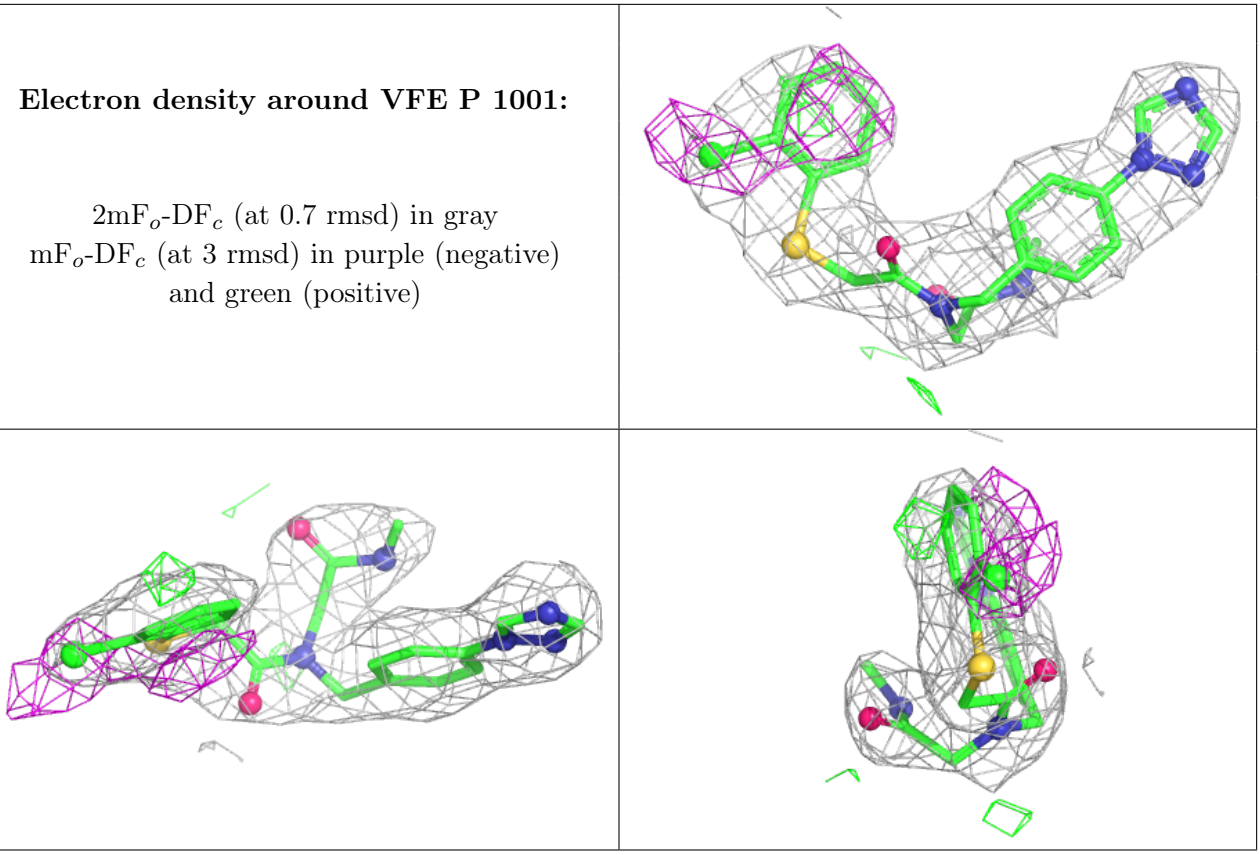
Electron density around VFE G 1001:

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



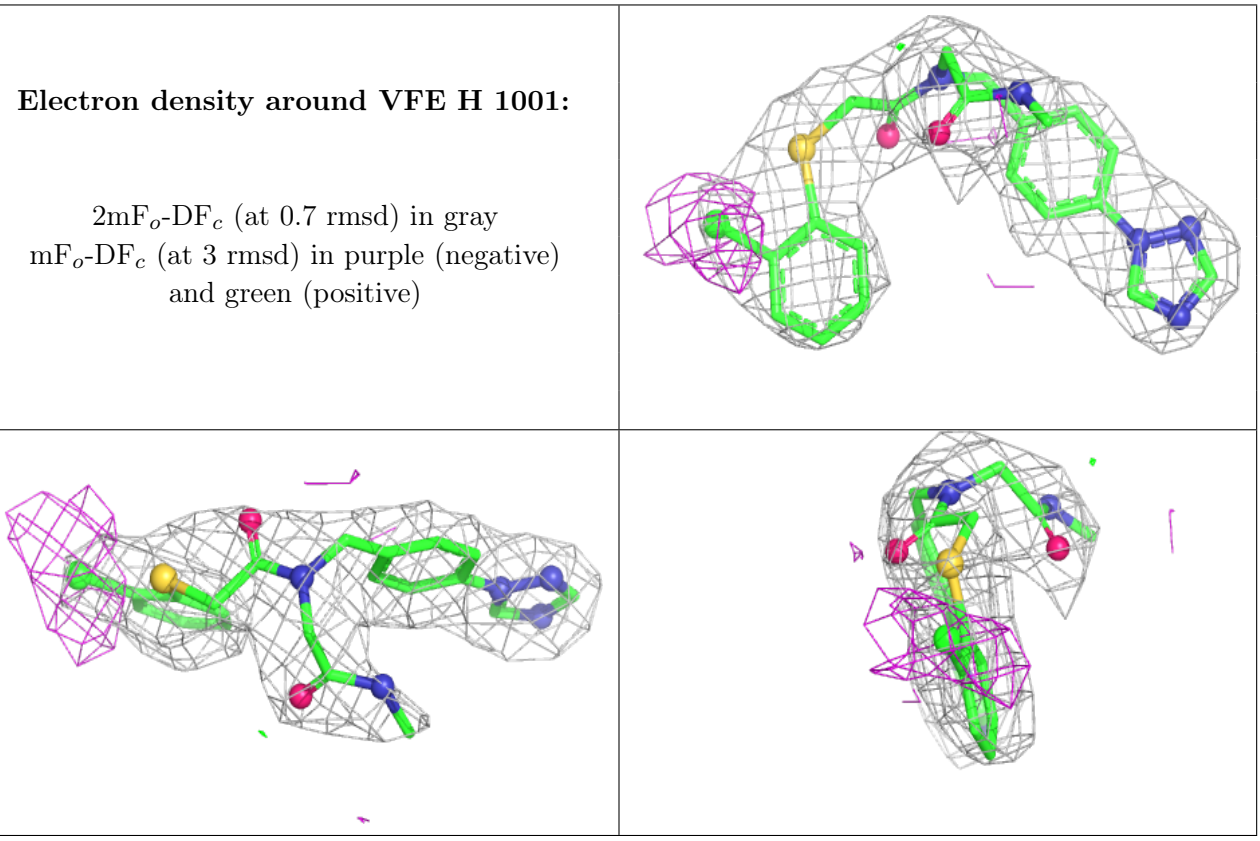
Electron density around VFE P 1001:

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



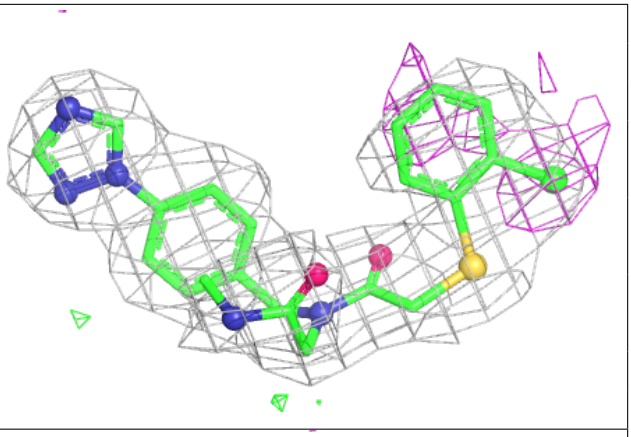
Electron density around VFE H 1001:

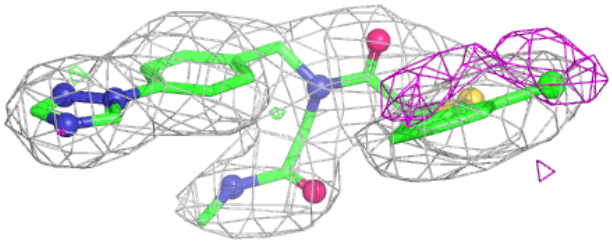
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

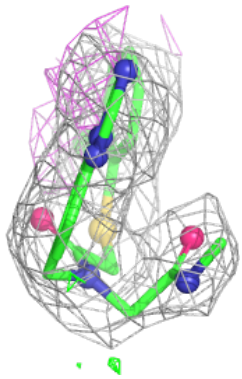


Electron density around VFE T 1001:

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

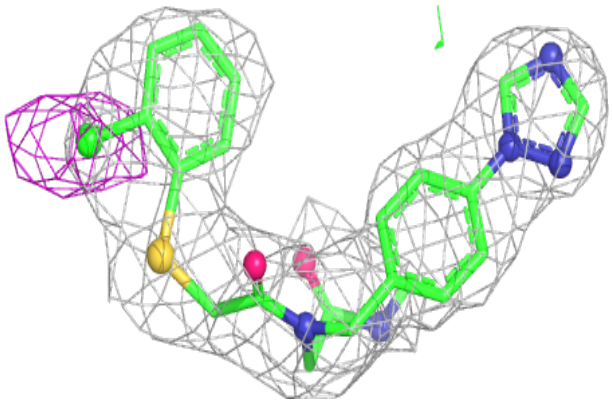


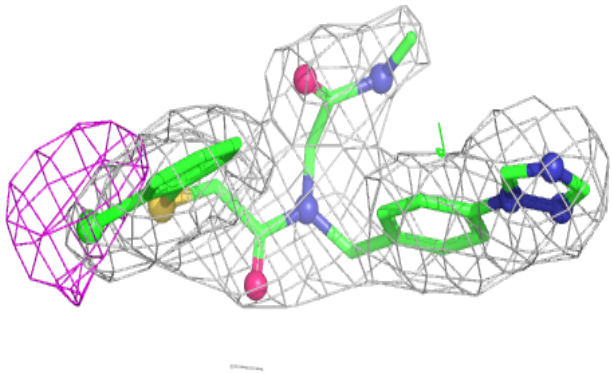


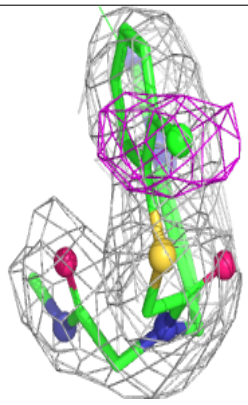


Electron density around VFE A 1001:

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

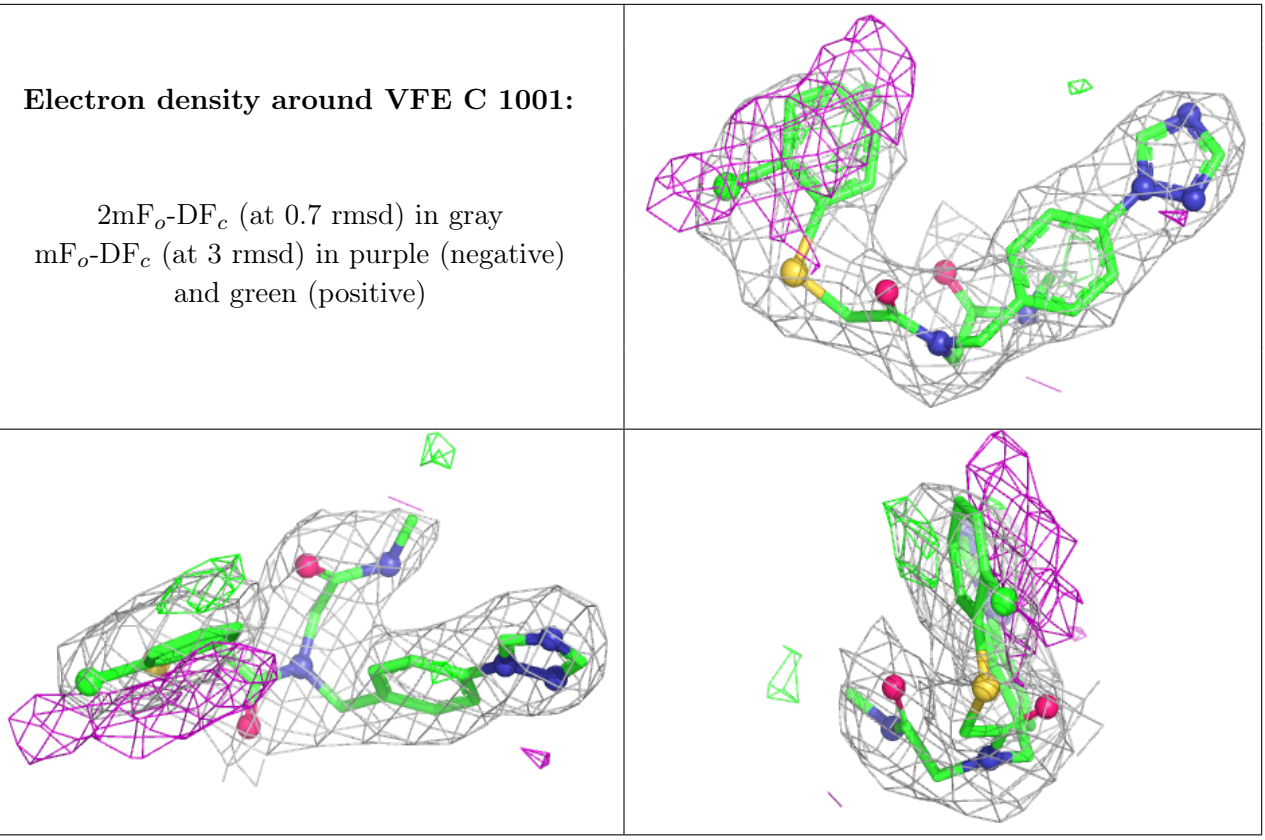






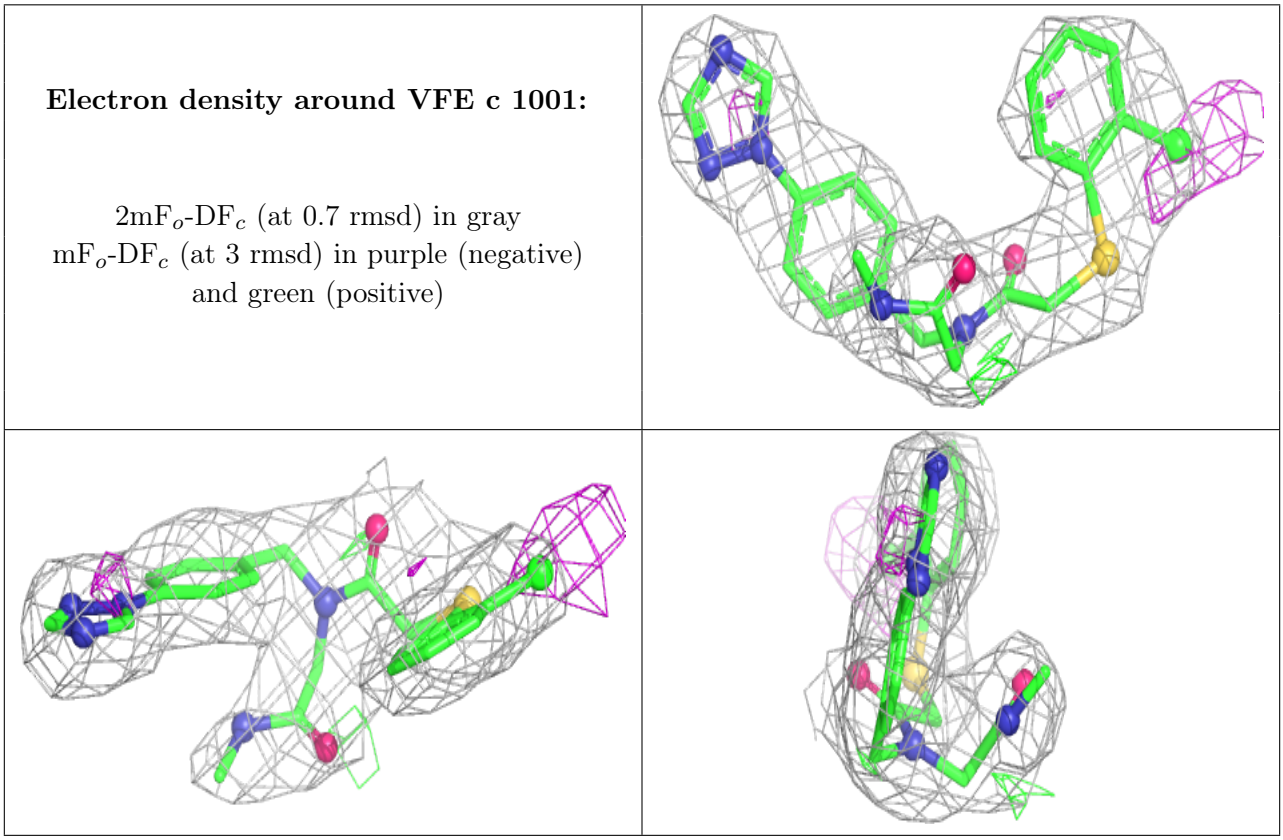
Electron density around VFE C 1001:

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



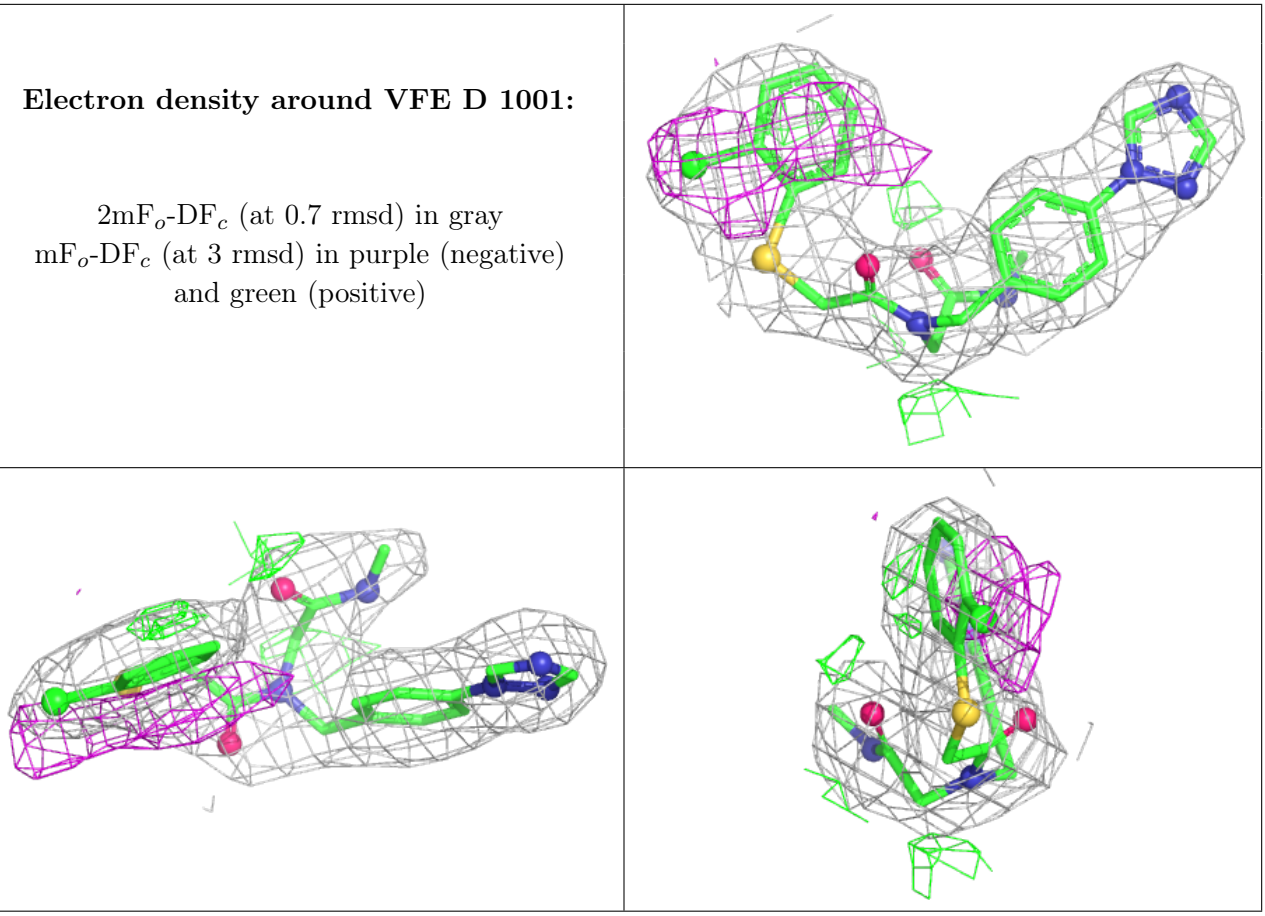
Electron density around VFE c 1001:

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



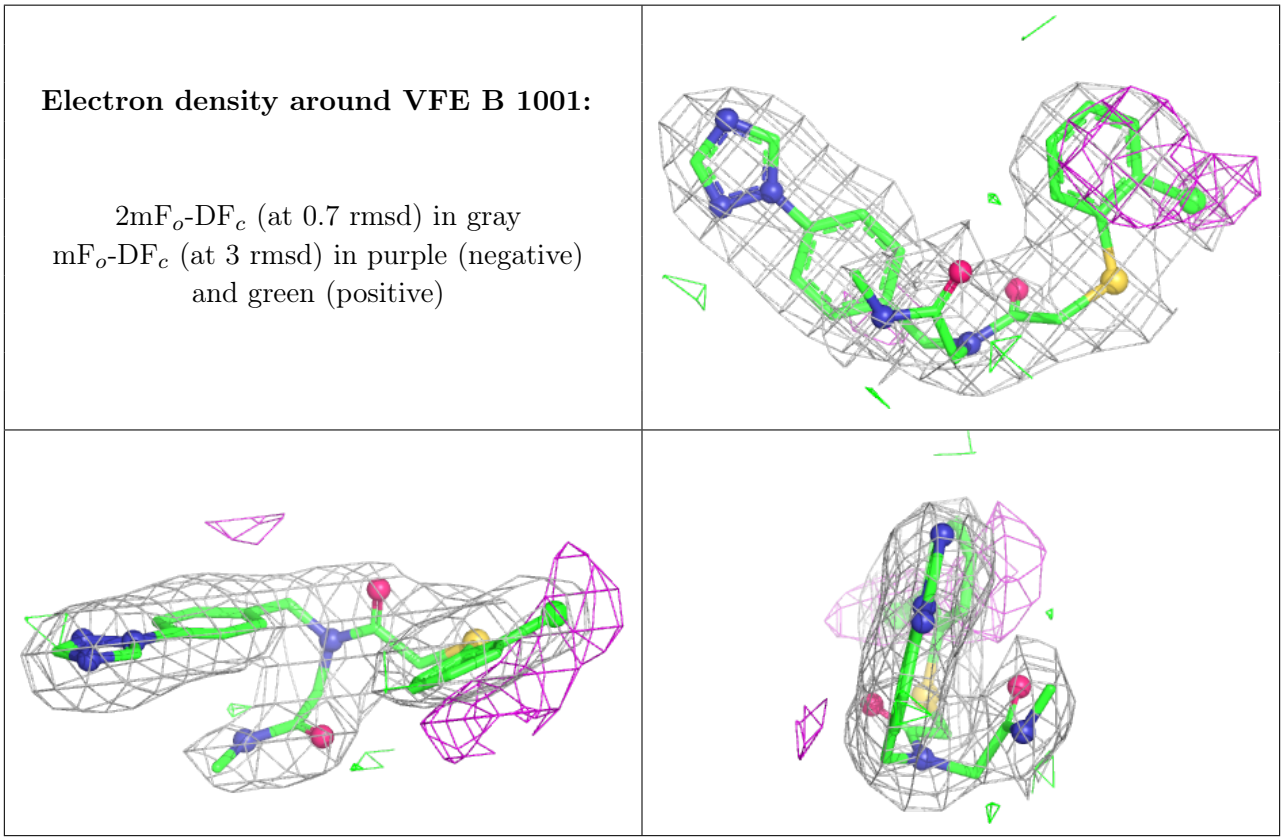
Electron density around VFE D 1001:

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



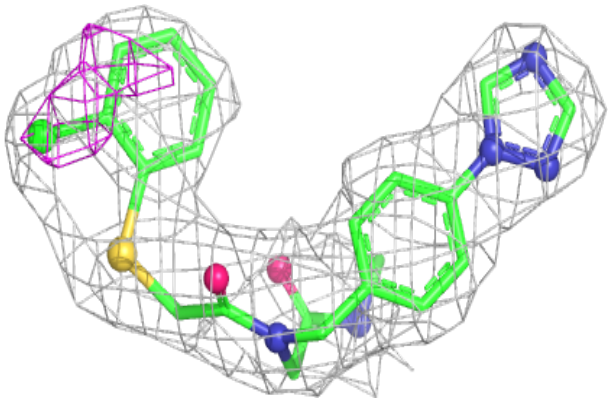
Electron density around VFE B 1001:

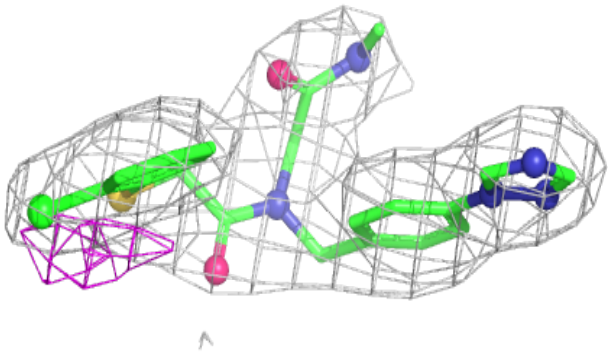
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

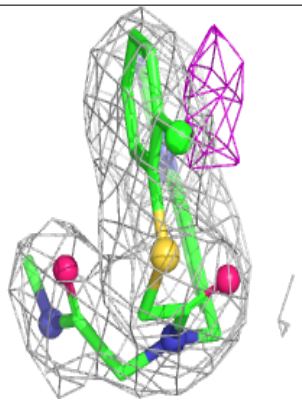


Electron density around VFE O 1001:

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

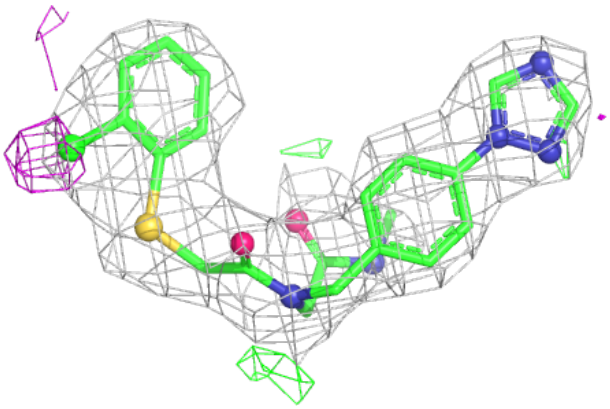


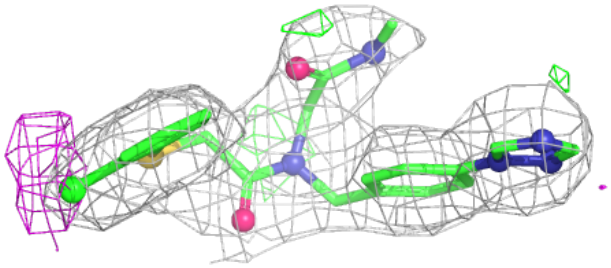


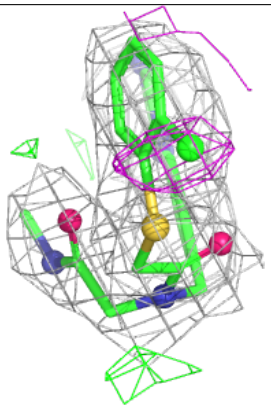


Electron density around VFE E 1001:

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

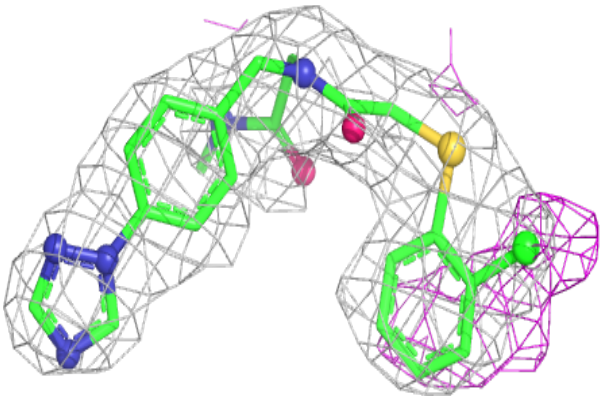


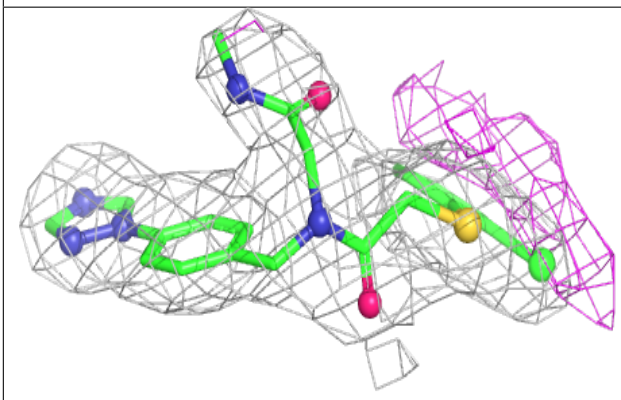


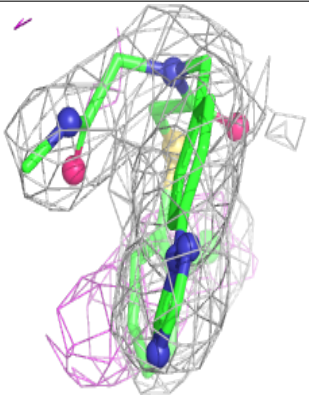


Electron density around VFE Y 1001:

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

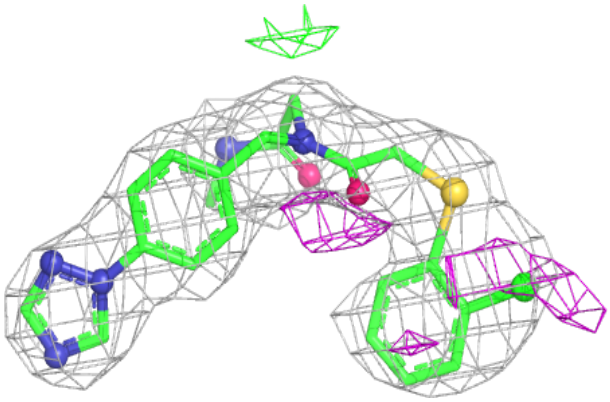


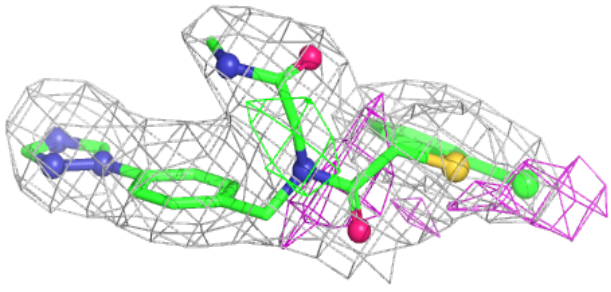


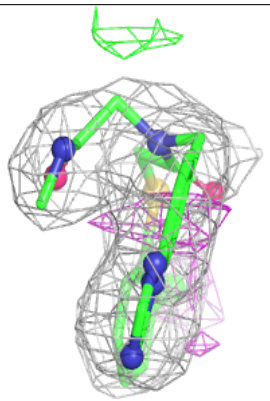


Electron density around VFE Z 1001:

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

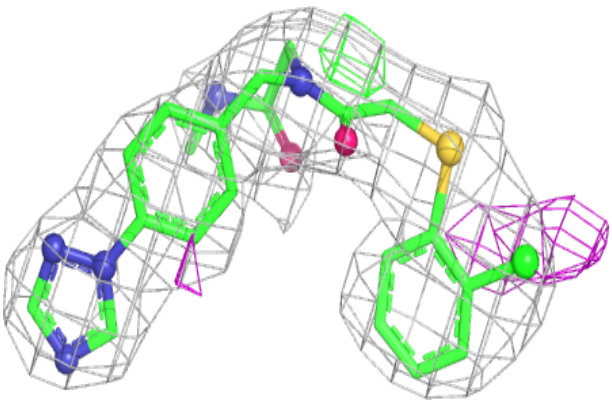


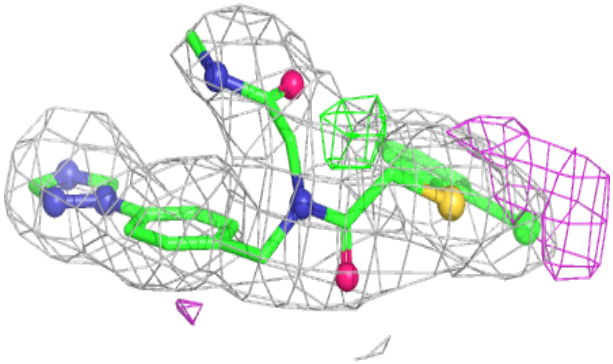


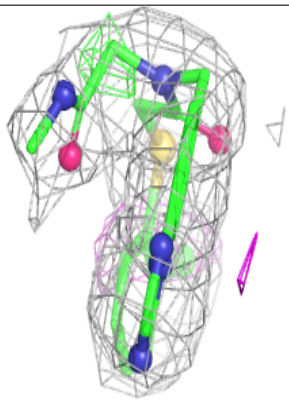


Electron density around VFE a 1001:

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

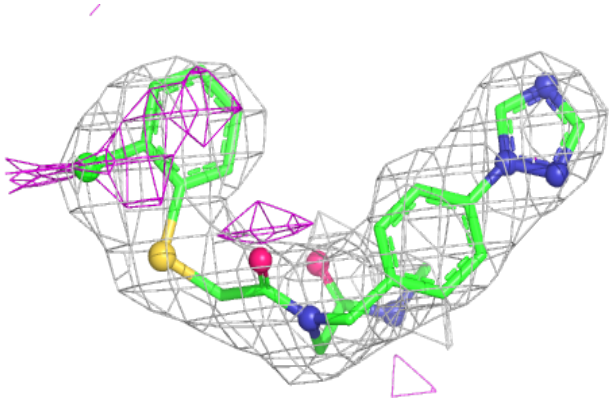


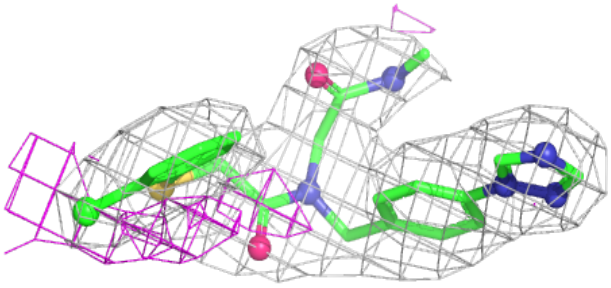


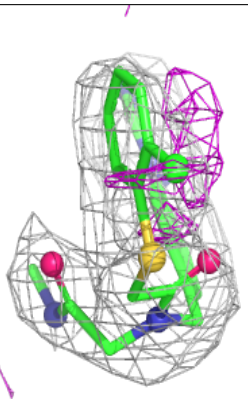


Electron density around VFE b 1001:

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

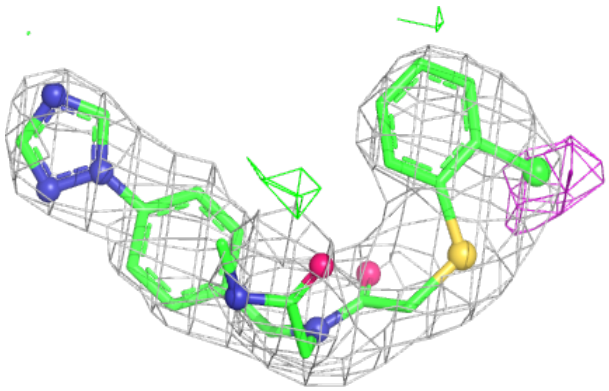


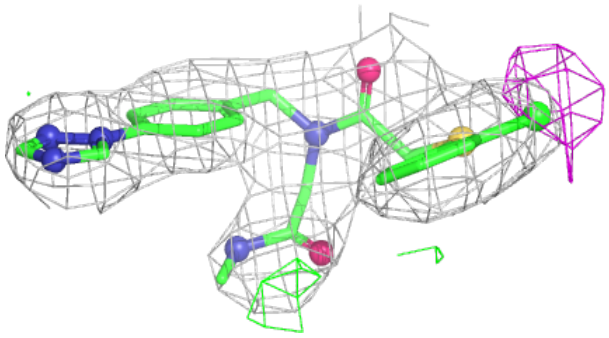


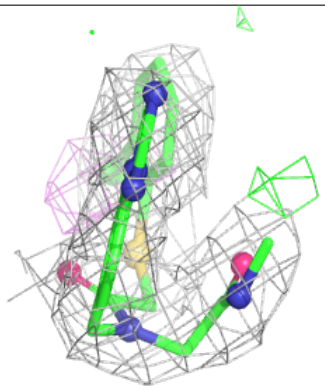


Electron density around VFE Q 1001:

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

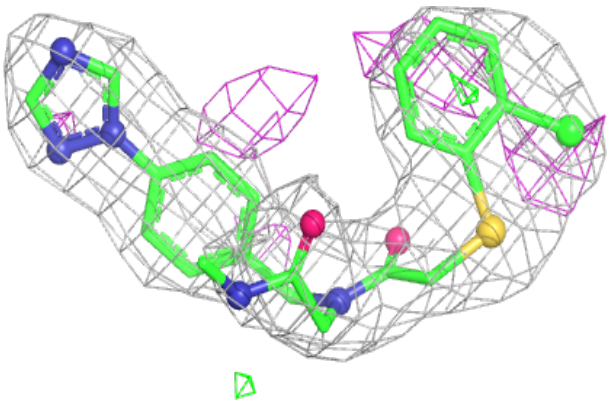


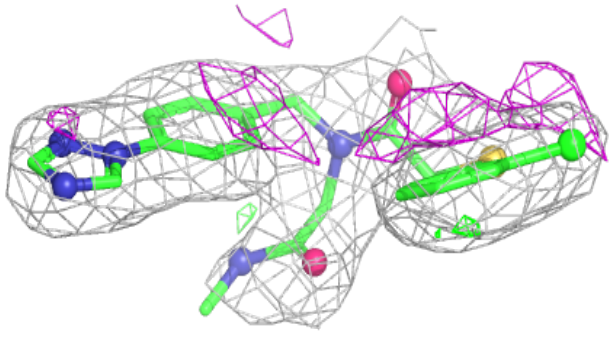


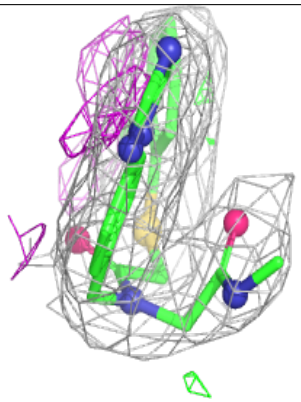


Electron density around VFE F 1001:

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

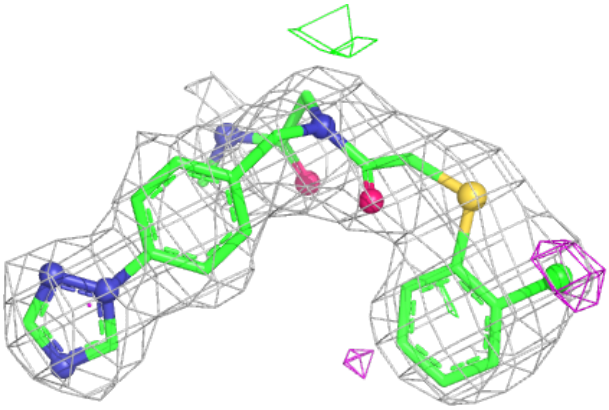


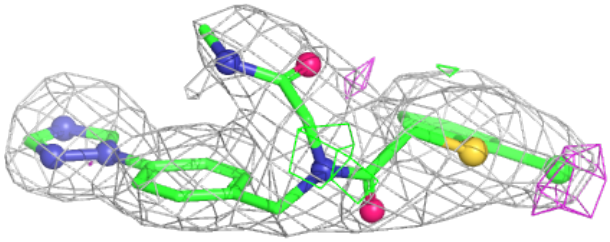


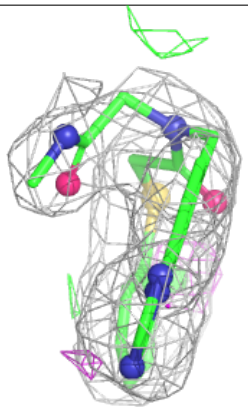


Electron density around VFE W 1001:

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

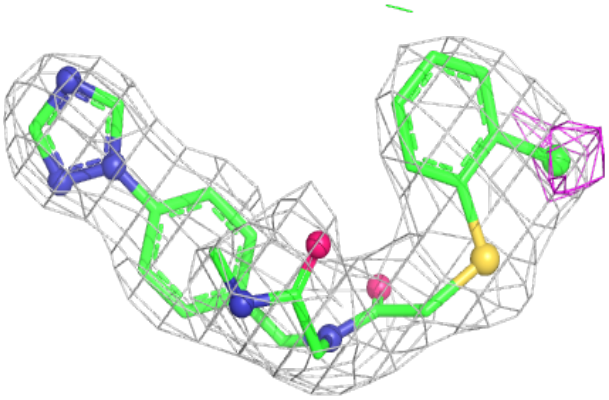


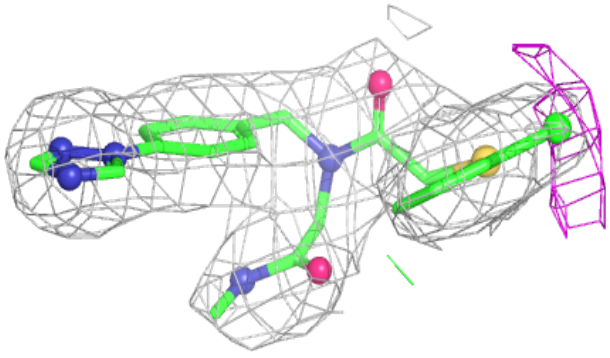


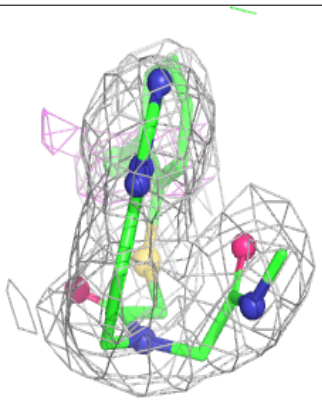


Electron density around VFE N 1001:

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

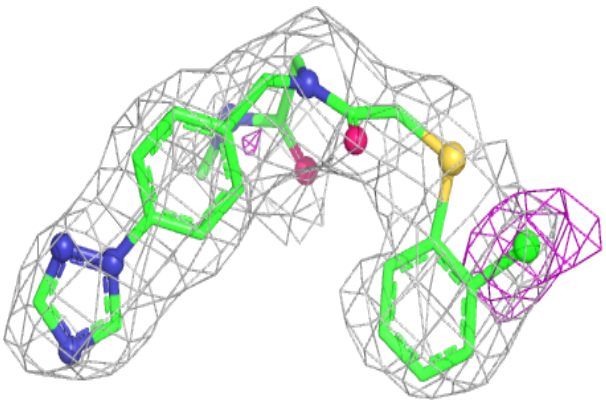


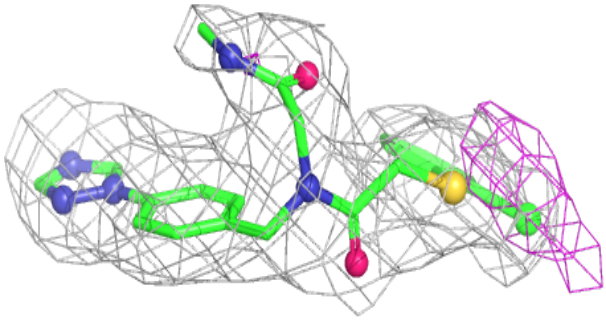


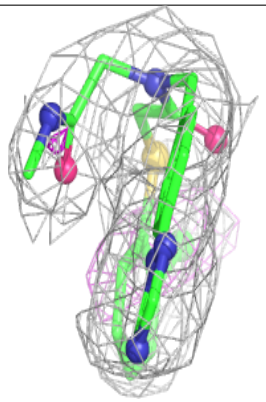


Electron density around VFE S 1001:

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

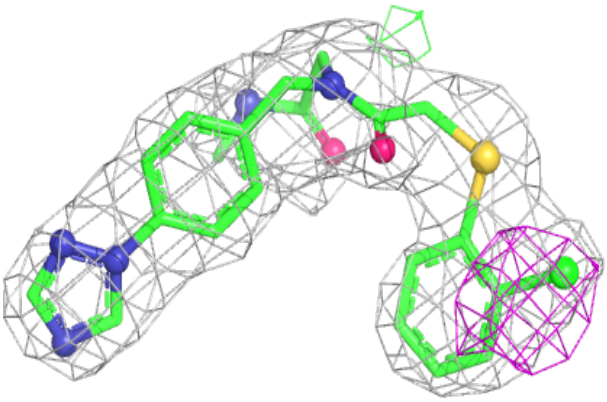


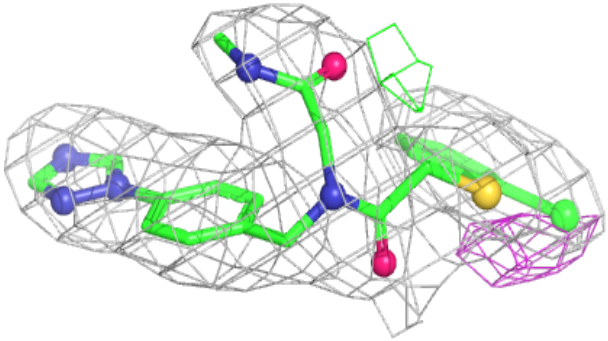


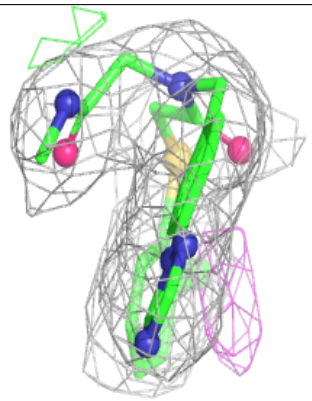


Electron density around VFE V 1001:

$2mF_o$-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.