



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 10:11 PM UTC

PDB ID : 7OK2 / pdb_00007ok2
Title : Crystal structure of Pseudomonas aeruginosa LpxA in complex with compound 3
Authors : Ryan, M.D.; Parkes, A.L.; Southey, M.; Andersen, O.A.; Zahn, M.; Barker, J.; DeJonge, B.L.M.
Deposited on : 2021-05-17
Resolution : 2.89 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

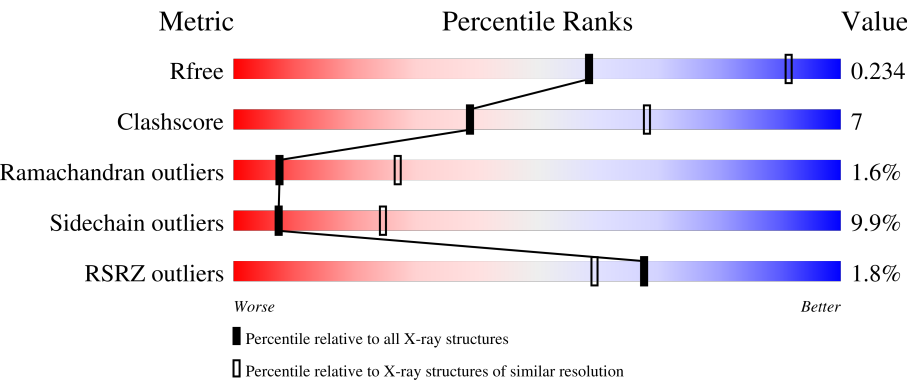
MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal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

1 Overall quality at a glance i

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

The reported resolution of this entry is 2.89 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



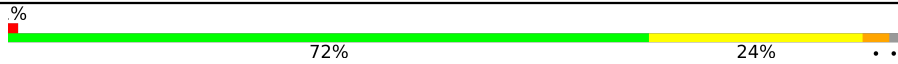
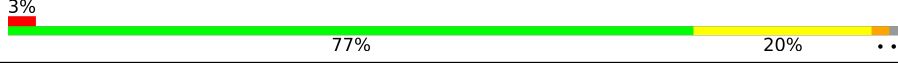
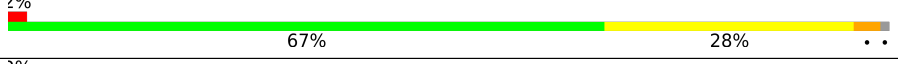
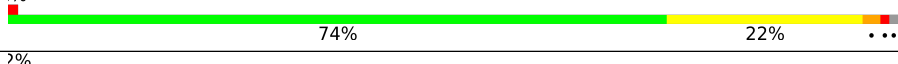
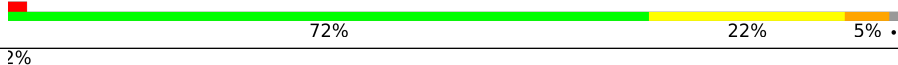
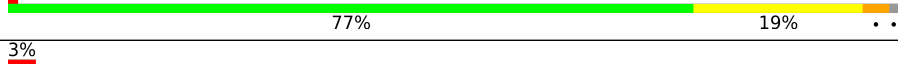
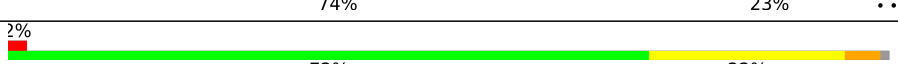
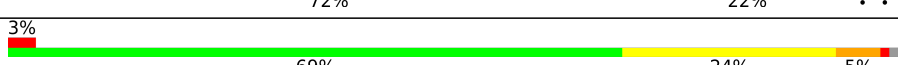
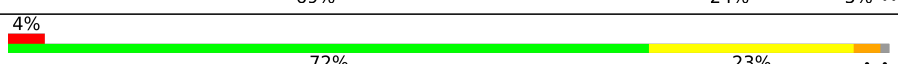
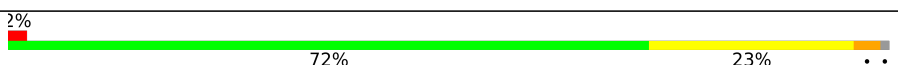
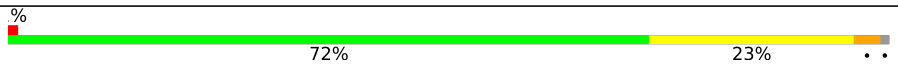
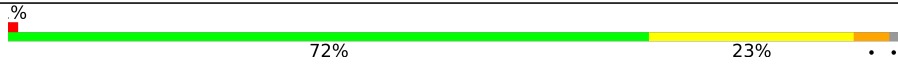
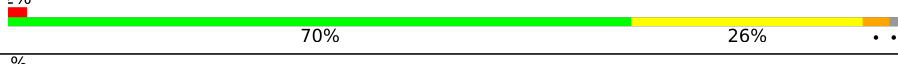
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R _{free}	180053	2481 (2.90-2.90)
Clashscore	190562	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)
RSRZ outliers	180081	2481 (2.90-2.90)

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

Mol	Chain	Length	Quality of chain
1	1	261	2% 75% 21% ..
1	2	261	2% 76% 20% ..
1	3	261	2% 69% 28% ..
1	4	261	% 77% 20% ..

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Mol	Chain	Length	Quality of chain
1	A	261	
1	B	261	
1	C	261	
1	D	261	
1	E	261	
1	F	261	
1	G	261	
1	H	261	
1	I	261	
1	J	261	
1	K	261	
1	L	261	
1	M	261	
1	N	261	
1	O	261	
1	P	261	
1	Q	261	
1	R	261	
1	S	261	
1	T	261	
1	U	261	
1	V	261	
1	W	261	
1	X	261	
1	Y	261	

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Mol	Chain	Length	Quality of chain
1	Z	261	% 74% 20% 5%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 60216 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	1	258	Total	C	N	O	S	0	0	0
			1974	1235	364	368	7			
1	2	258	Total	C	N	O	S	0	0	0
			1974	1235	364	368	7			
1	3	258	Total	C	N	O	S	0	0	0
			1974	1235	364	368	7			
1	4	258	Total	C	N	O	S	0	0	0
			1974	1235	364	368	7			
1	A	258	Total	C	N	O	S	0	0	0
			1974	1235	364	368	7			
1	B	258	Total	C	N	O	S	0	0	0
			1974	1235	364	368	7			
1	C	258	Total	C	N	O	S	0	0	0
			1974	1235	364	368	7			
1	D	258	Total	C	N	O	S	0	0	0
			1974	1235	364	368	7			
1	E	258	Total	C	N	O	S	0	0	0
			1974	1235	364	368	7			
1	F	258	Total	C	N	O	S	0	0	0
			1974	1235	364	368	7			
1	G	258	Total	C	N	O	S	0	0	0
			1974	1235	364	368	7			
1	H	258	Total	C	N	O	S	0	0	0
			1974	1235	364	368	7			
1	I	258	Total	C	N	O	S	0	0	0
			1974	1235	364	368	7			
1	J	258	Total	C	N	O	S	0	0	0
			1974	1235	364	368	7			
1	K	258	Total	C	N	O	S	0	0	0
			1974	1235	364	368	7			
1	L	258	Total	C	N	O	S	0	0	0
			1974	1235	364	368	7			

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

There are 90 discrepancies between the modelled and reference sequences:

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

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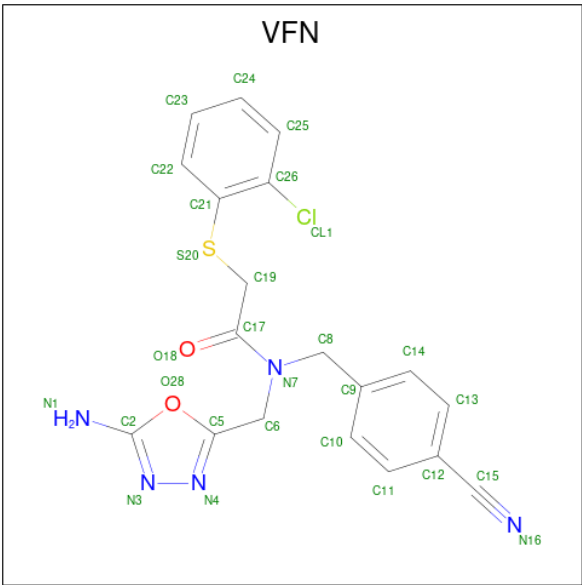
Chain	Residue	Modelled	Actual	Comment	Reference
4	0	HIS	-	expression tag	UNP A6V1E4
A	-2	GLY	-	expression tag	UNP A6V1E4
A	-1	SER	-	expression tag	UNP A6V1E4
A	0	HIS	-	expression tag	UNP A6V1E4
B	-2	GLY	-	expression tag	UNP A6V1E4
B	-1	SER	-	expression tag	UNP A6V1E4
B	0	HIS	-	expression tag	UNP A6V1E4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

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

- Molecule 2 is {N}-[(5-azanyl-1,3,4-oxadiazol-2-yl)methyl]-2-(2-chlorophenyl)sulfanyl- {N}-[(4-cyanophenyl)methyl]ethanamide (CCD ID: VFN) (formula: C₁₉H₁₆ClN₅O₂S) (labeled as "Ligand of Interest" by depositor).



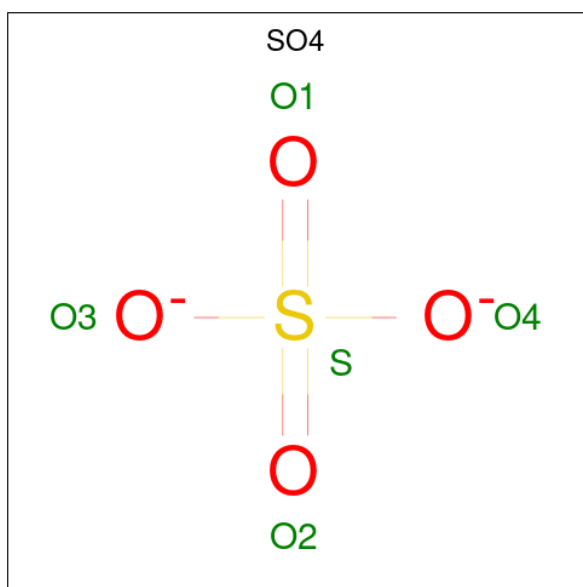
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
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2	1	1	Total 28	C 19	Cl 1	N 5	O 2	S 1	0	0
2	2	1	Total 28	C 19	Cl 1	N 5	O 2	S 1	0	0
2	3	1	Total 28	C 19	Cl 1	N 5	O 2	S 1	0	0
2	3	1	Total 28	C 19	Cl 1	N 5	O 2	S 1	0	0
2	A	1	Total 28	C 19	Cl 1	N 5	O 2	S 1	0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

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

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



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	1	1	Total	O	S	0	0
			5	4	1		
3	2	1	Total	O	S	0	0
			5	4	1		
3	3	1	Total	O	S	0	0
			5	4	1		
3	4	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	C	1	Total	O	S	0	0
			5	4	1		
3	C	1	Total	O	S	0	0
			5	4	1		
3	D	1	Total	O	S	0	0
			5	4	1		
3	E	1	Total	O	S	0	0
			5	4	1		
3	F	1	Total	O	S	0	0
			5	4	1		
3	G	1	Total	O	S	0	0
			5	4	1		
3	H	1	Total	O	S	0	0
			5	4	1		
3	I	1	Total	O	S	0	0
			5	4	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	J	1	Total	O	S	0	0
			5	4	1		
3	K	1	Total	O	S	0	0
			5	4	1		
3	L	1	Total	O	S	0	0
			5	4	1		
3	M	1	Total	O	S	0	0
			5	4	1		
3	N	1	Total	O	S	0	0
			5	4	1		
3	O	1	Total	O	S	0	0
			5	4	1		
3	P	1	Total	O	S	0	0
			5	4	1		
3	Q	1	Total	O	S	0	0
			5	4	1		
3	R	1	Total	O	S	0	0
			5	4	1		
3	S	1	Total	O	S	0	0
			5	4	1		
3	T	1	Total	O	S	0	0
			5	4	1		
3	U	1	Total	O	S	0	0
			5	4	1		
3	V	1	Total	O	S	0	0
			5	4	1		
3	W	1	Total	O	S	0	0
			5	4	1		
3	X	1	Total	O	S	0	0
			5	4	1		
3	Y	1	Total	O	S	0	0
			5	4	1		
3	Z	1	Total	O	S	0	0
			5	4	1		

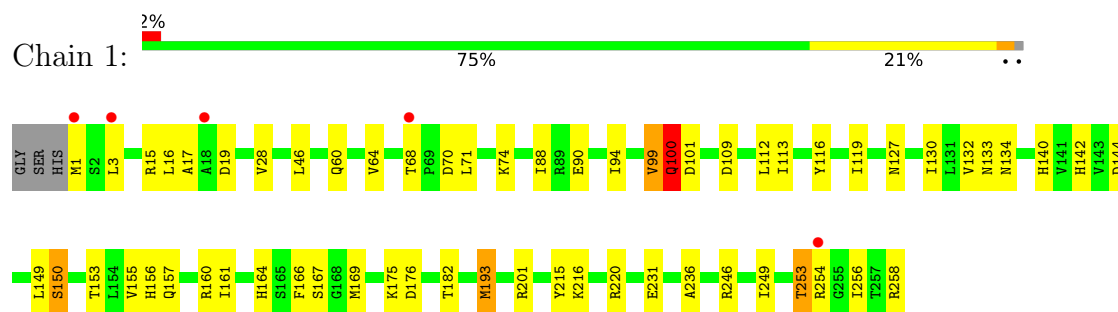
- Molecule 4 is water.

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

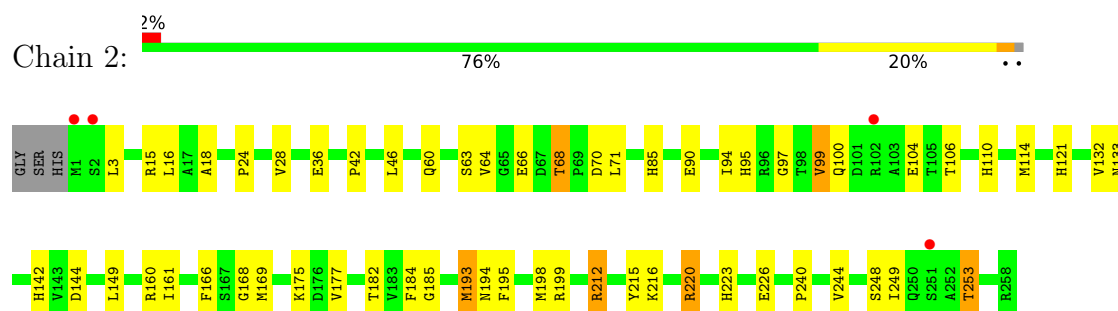
3 Residue-property plots

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

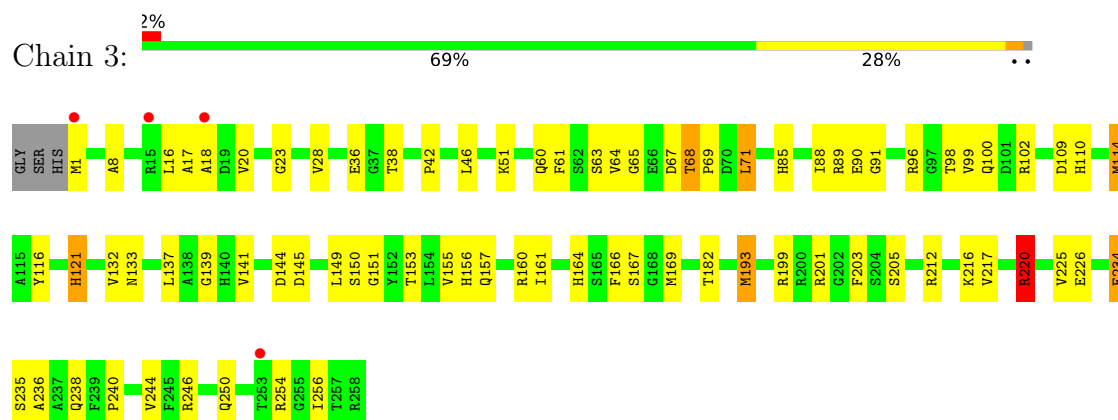
- Molecule 1: Acyl-[acyl-carrier-protein]-UDP-N-acetylglucosamine O-acyltransferase



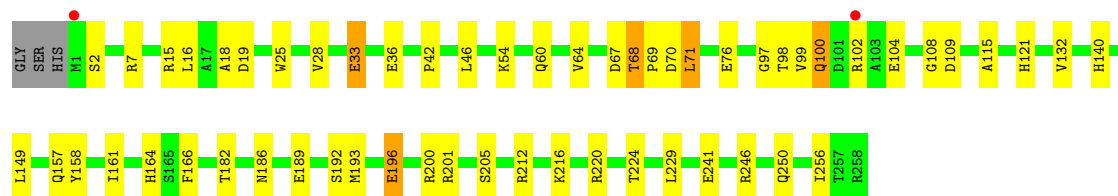
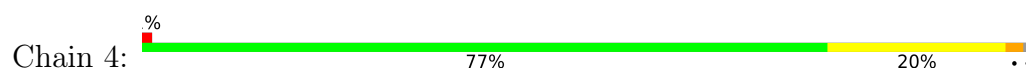
- Molecule 1: Acyl-[acyl-carrier-protein]-UDP-N-acetylglucosamine O-acyltransferase



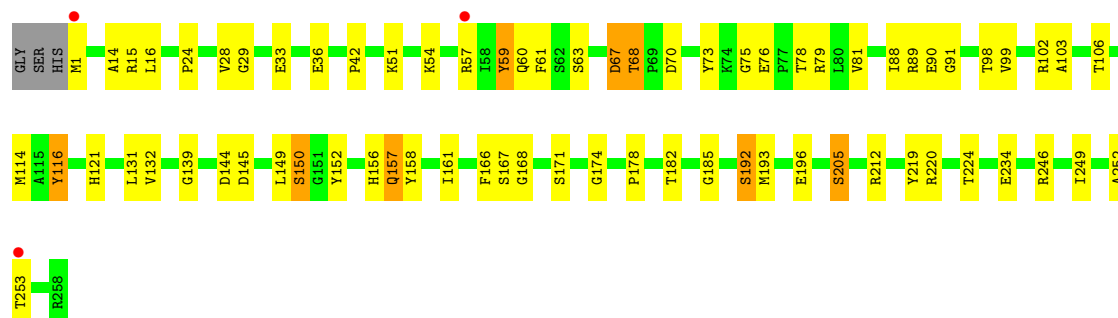
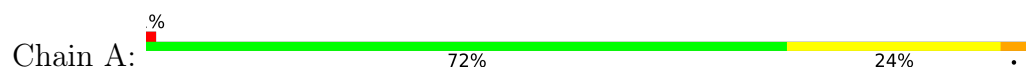
- Molecule 1: Acyl-[acyl-carrier-protein]-UDP-N-acetylglucosamine O-acyltransferase



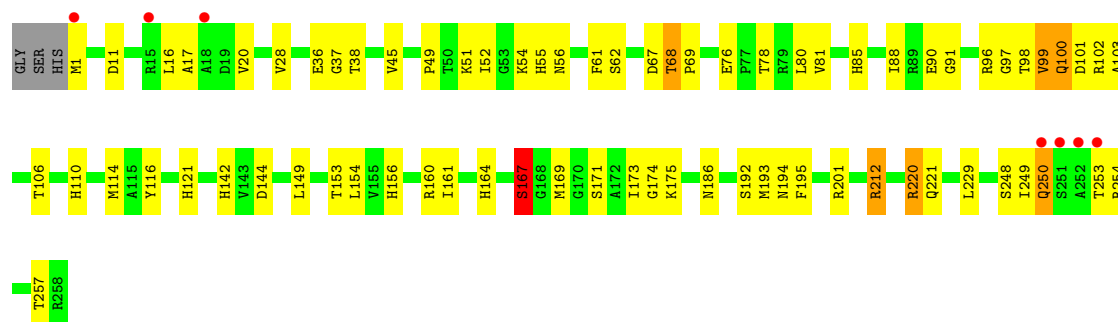
- Molecule 1: Acyl-[acyl-carrier-protein]-UDP-N-acetylglucosamine O-acyltransferase



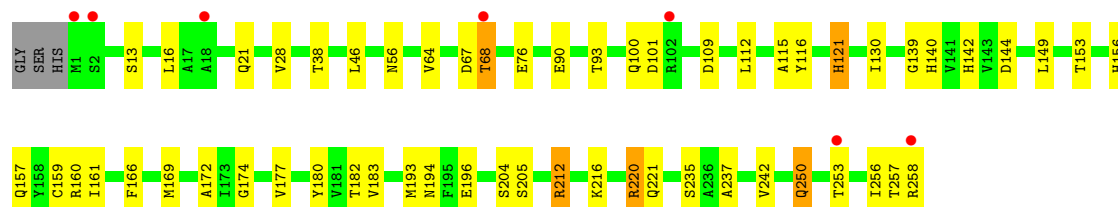
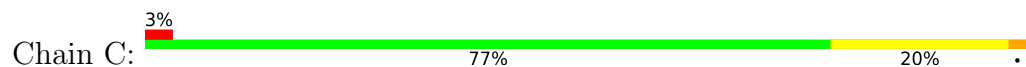
- Molecule 1: Acyl-[acyl-carrier-protein]-UDP-N-acetylglucosamine O-acyltransferase



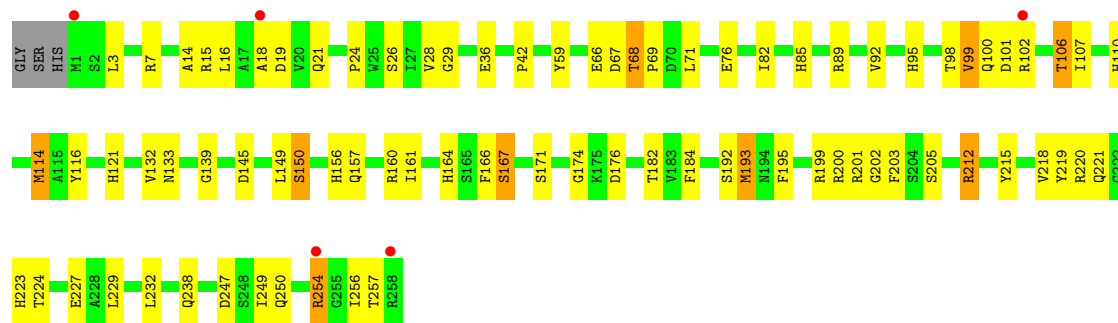
- Molecule 1: Acyl-[acyl-carrier-protein]-UDP-N-acetylglucosamine O-acyltransferase



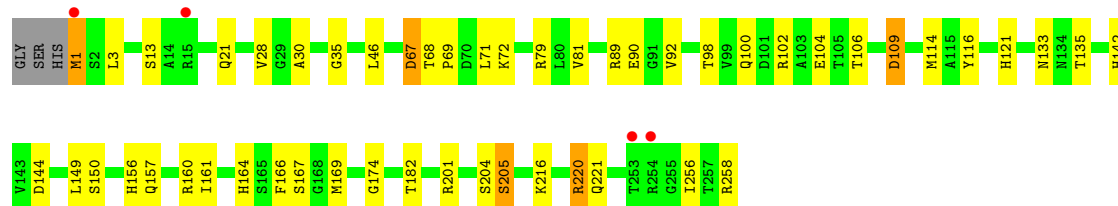
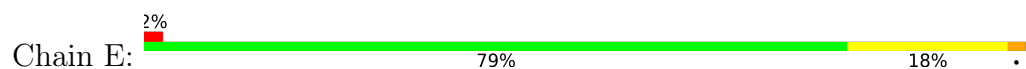
- Molecule 1: Acyl-[acyl-carrier-protein]-UDP-N-acetylglucosamine O-acyltransferase



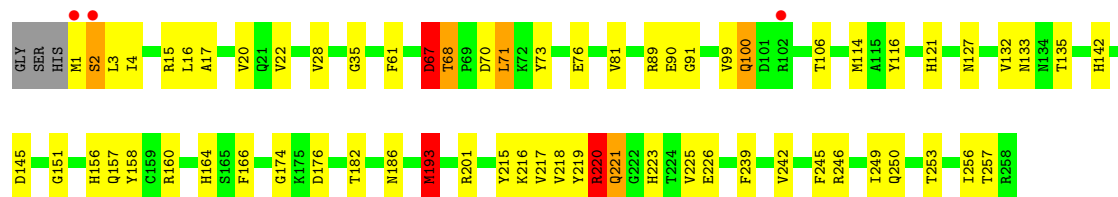
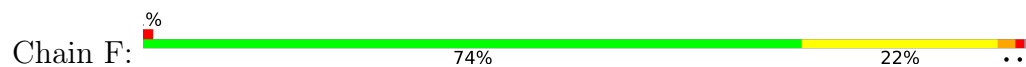
- Molecule 1: Acyl-[acyl-carrier-protein]-UDP-N-acetylglucosamine O-acyltransferase



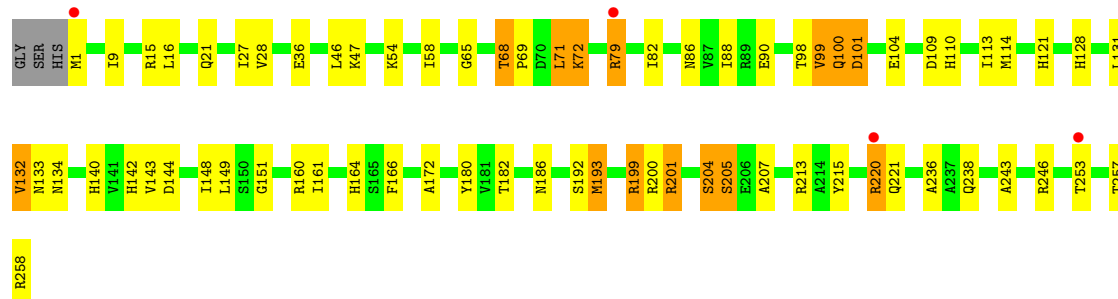
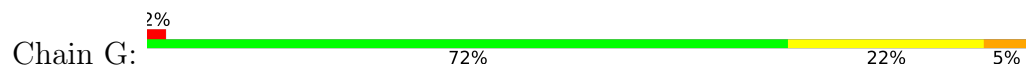
- Molecule 1: Acyl-[acyl-carrier-protein]-UDP-N-acetylglucosamine O-acyltransferase



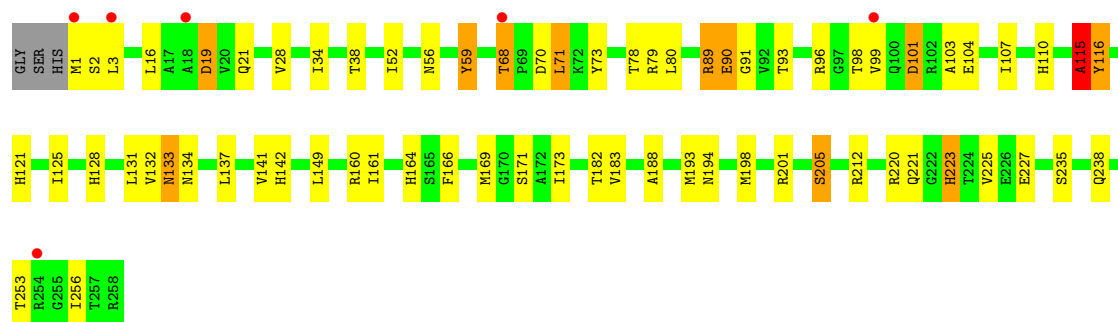
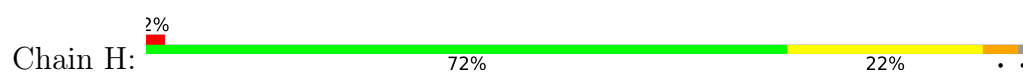
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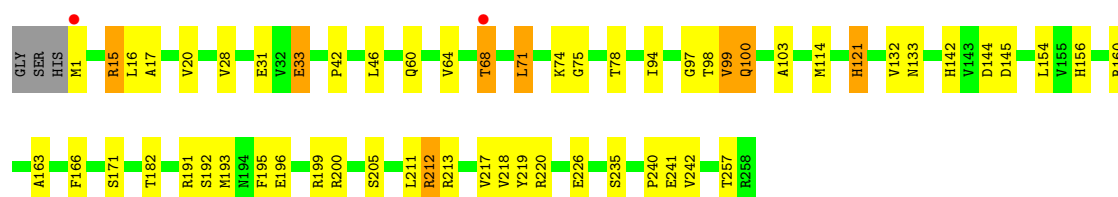
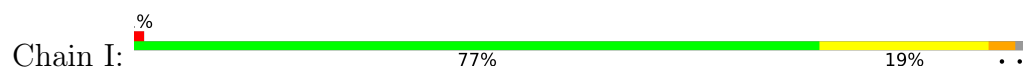
- Molecule 1: Acyl-[acyl-carrier-protein]-UDP-N-acetylglucosamine O-acyltransferase



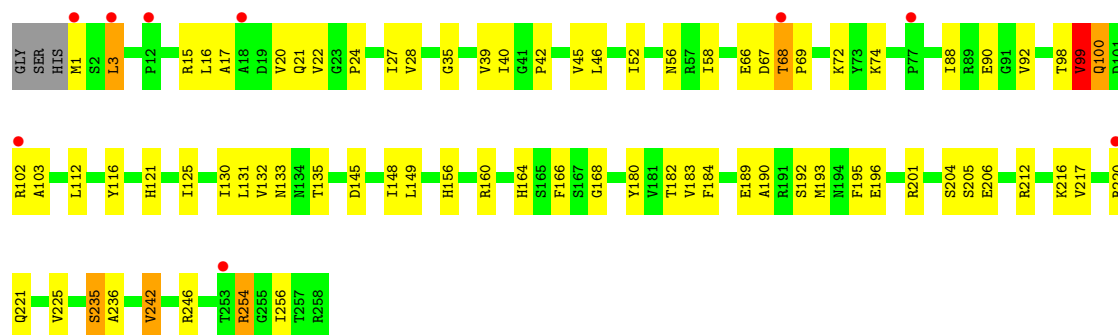
- Molecule 1: Acyl-[acyl-carrier-protein]-UDP-N-acetylglucosamine O-acyltransferase



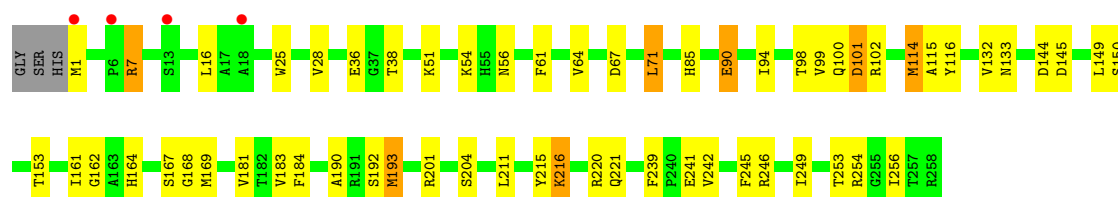
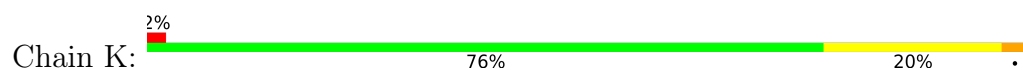
- Molecule 1: Acyl-[acyl-carrier-protein]-UDP-N-acetylglucosamine O-acyltransferase



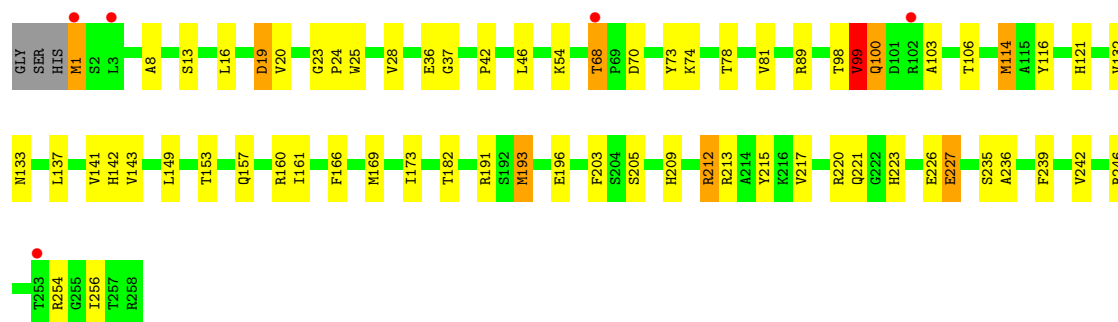
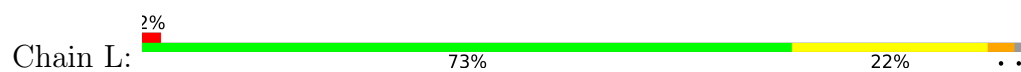
- Molecule 1: Acyl-[acyl-carrier-protein]-UDP-N-acetylglucosamine O-acyltransferase



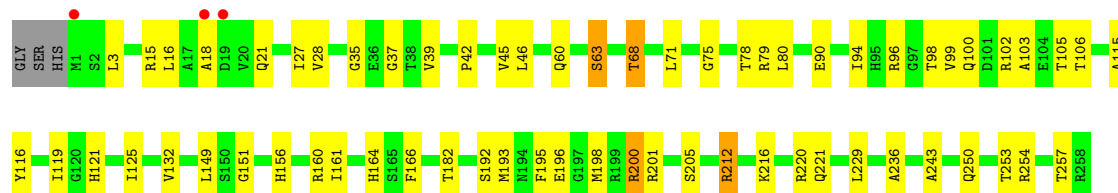
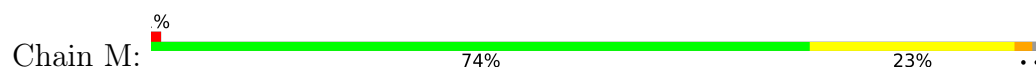
- Molecule 1: Acyl-[acyl-carrier-protein]-UDP-N-acetylglucosamine O-acyltransferase



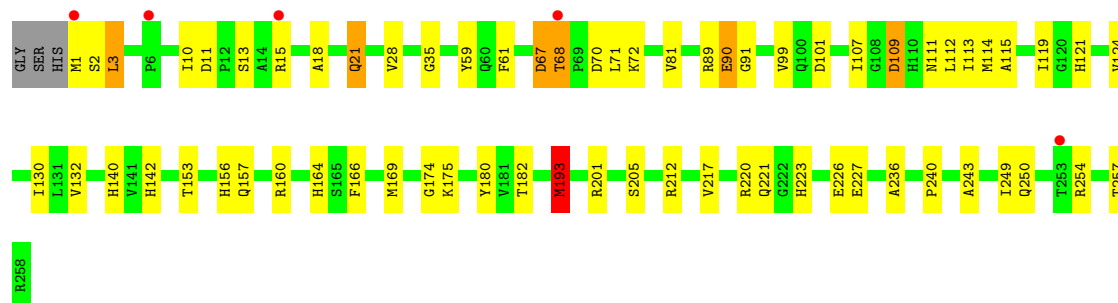
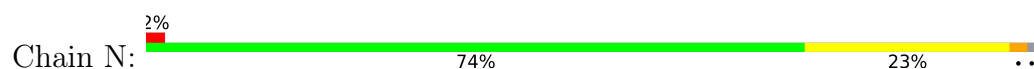
- Molecule 1: Acyl-[acyl-carrier-protein]-UDP-N-acetylglucosamine O-acyltransferase



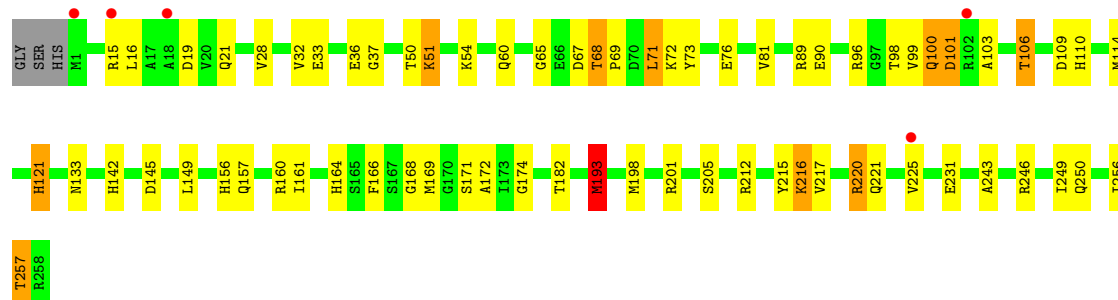
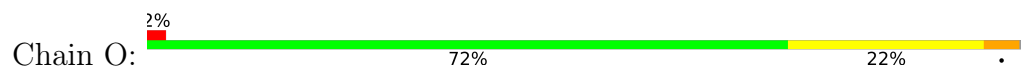
- Molecule 1: Acyl-[acyl-carrier-protein]-UDP-N-acetylglucosamine O-acyltransferase



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

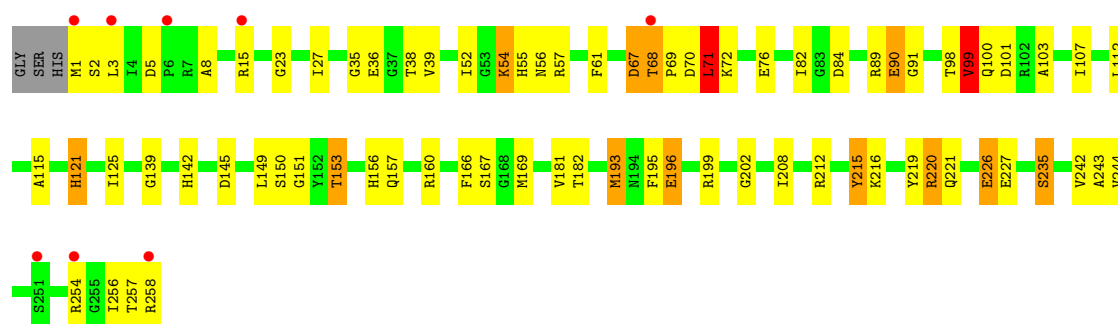


- Molecule 1: Acyl-[acyl-carrier-protein]-UDP-N-acetylglucosamine O-acyltransferase



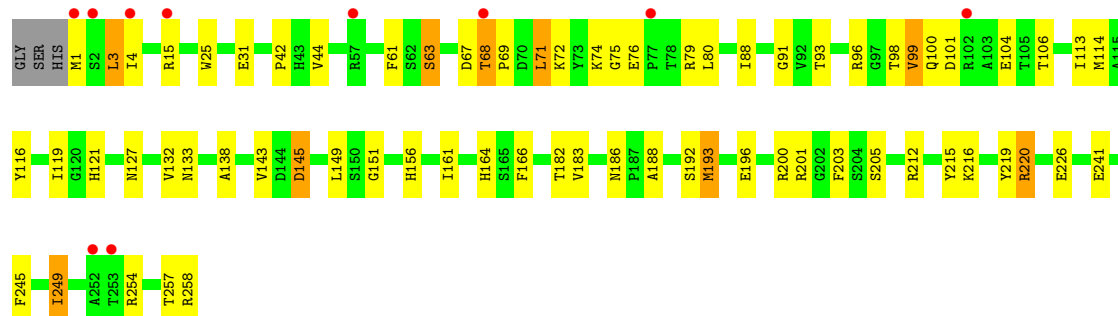
• Molecule 1: Acyl-[acyl-carrier-protein]-UDP-N-acetylglucosamine O-acyltransferase

Chain P:  3% 69% 24% 5% ..



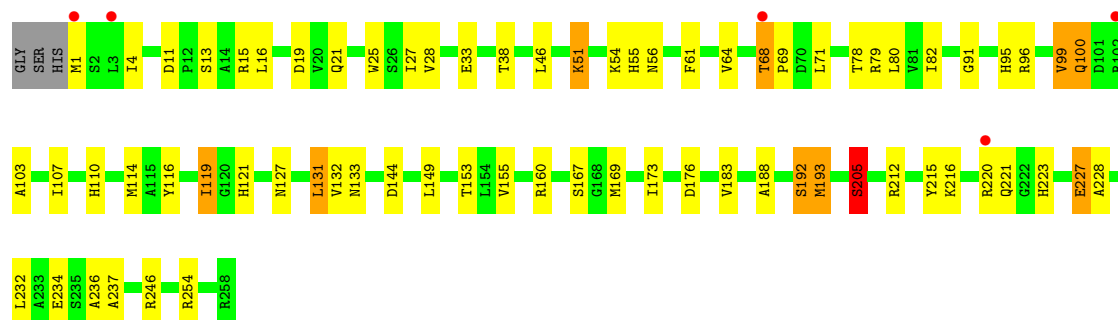
• Molecule 1: Acyl-[acyl-carrier-protein]-UDP-N-acetylglucosamine O-acyltransferase

Chain Q:  4% 72% 23% ..



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

Chain R:  2% 72% 23% ..



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

Chain S:  % 72% 23% ..

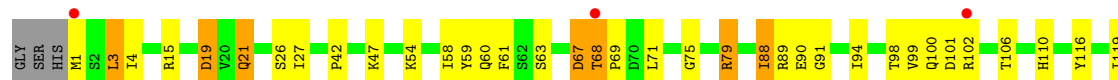




- Molecule 1: Acyl-[acyl-carrier-protein]-UDP-N-acetylglucosamine O-acyltransferase



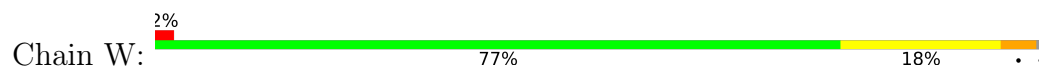
- Molecule 1: Acyl-[acyl-carrier-protein]-UDP-N-acetylglucosamine O-acyltransferase

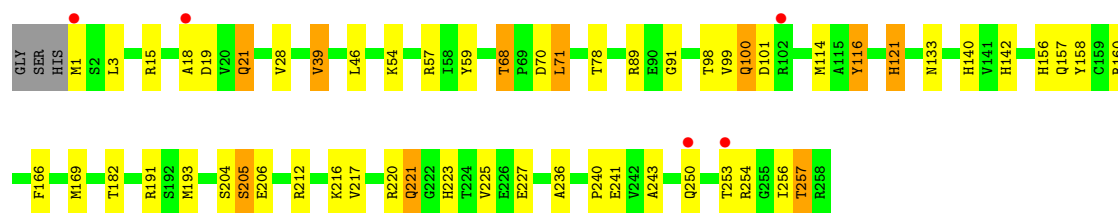


- Molecule 1: Acyl-[acyl-carrier-protein]-UDP-N-acetylglucosamine O-acyltransferase

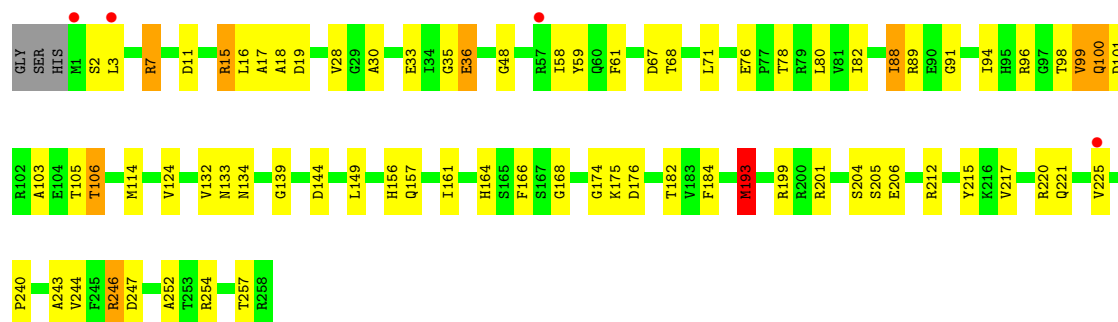


- Molecule 1: Acyl-[acyl-carrier-protein]-UDP-N-acetylglucosamine O-acyltransferase

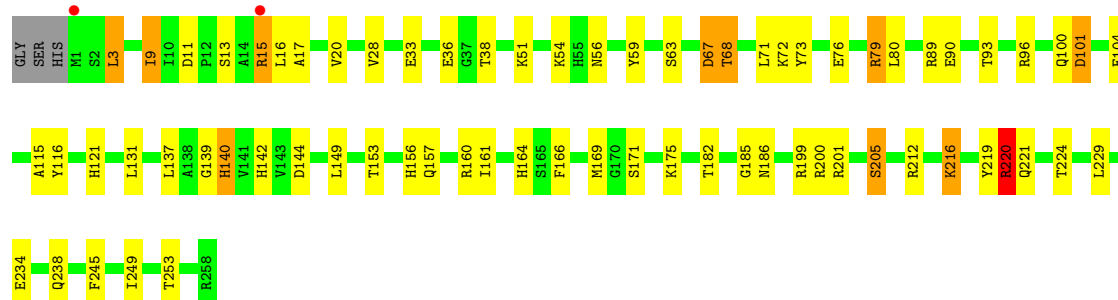




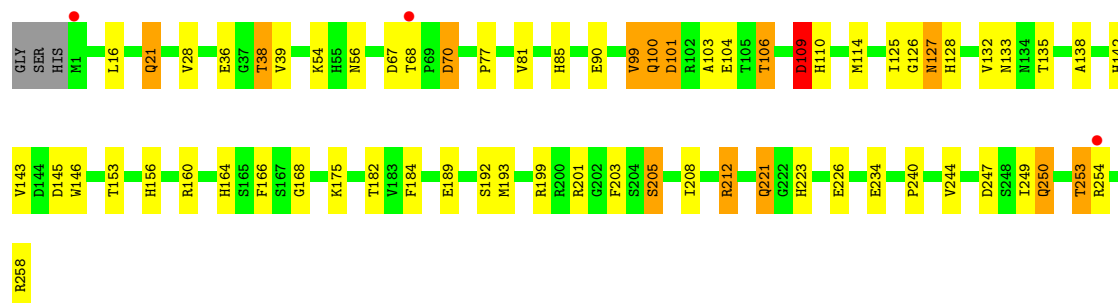
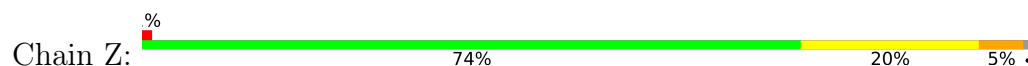
• Molecule 1: Acyl-[acyl-carrier-protein]-UDP-N-acetylglucosamine O-acyltransferase



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



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



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	247.29Å 367.65Å 372.08Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.45 – 2.89 49.45 – 2.89	Depositor EDS
% Data completeness (in resolution range)	99.8 (49.45-2.89) 99.8 (49.45-2.89)	Depositor EDS
R_{merge}	0.59	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.37 (at 2.91Å)	Xtriage
Refinement program	BUSTER 2.11.7	Depositor
R, R_{free}	0.192 , 0.231 (Not available) , 0.234	Depositor DCC
R_{free} test set	18696 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	66.5	Xtriage
Anisotropy	0.266	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 71.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.25$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	60216	wwPDB-VP
Average B, all atoms (Å ²)	71.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.37% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	1	0.95	0/2016	1.46	9/2734 (0.3%)
1	2	0.93	1/2016 (0.0%)	1.43	13/2734 (0.5%)
1	3	0.94	2/2016 (0.1%)	1.48	15/2734 (0.5%)
1	4	0.94	0/2016	1.48	12/2734 (0.4%)
1	A	0.94	0/2016	1.48	20/2734 (0.7%)
1	B	0.91	1/2016 (0.0%)	1.42	10/2734 (0.4%)
1	C	0.91	0/2016	1.44	9/2734 (0.3%)
1	D	0.97	0/2016	1.51	20/2734 (0.7%)
1	E	0.95	0/2016	1.47	11/2734 (0.4%)
1	F	0.93	2/2016 (0.1%)	1.45	12/2734 (0.4%)
1	G	0.93	1/2016 (0.0%)	1.44	14/2734 (0.5%)
1	H	0.90	0/2016	1.42	11/2734 (0.4%)
1	I	0.93	0/2016	1.43	7/2734 (0.3%)
1	J	0.95	0/2016	1.45	15/2734 (0.5%)
1	K	0.90	0/2016	1.43	7/2734 (0.3%)
1	L	0.88	0/2016	1.41	7/2734 (0.3%)
1	M	0.94	0/2016	1.42	8/2734 (0.3%)
1	N	0.90	1/2016 (0.0%)	1.44	17/2734 (0.6%)
1	O	0.91	1/2016 (0.0%)	1.48	13/2734 (0.5%)
1	P	0.90	0/2016	1.47	21/2734 (0.8%)
1	Q	0.90	0/2016	1.46	13/2734 (0.5%)
1	R	0.94	0/2016	1.48	16/2734 (0.6%)
1	S	0.93	1/2016 (0.0%)	1.46	16/2734 (0.6%)
1	T	0.93	0/2016	1.44	7/2734 (0.3%)
1	U	0.95	0/2016	1.49	12/2734 (0.4%)
1	V	0.95	0/2016	1.47	14/2734 (0.5%)
1	W	0.93	0/2016	1.47	13/2734 (0.5%)
1	X	0.97	1/2016 (0.0%)	1.50	21/2734 (0.8%)
1	Y	0.92	0/2016	1.47	14/2734 (0.5%)
1	Z	0.95	1/2016 (0.0%)	1.48	18/2734 (0.7%)
All	All	0.93	12/60480 (0.0%)	1.46	395/82020 (0.5%)

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	S	193	MET	SD-CE	-7.24	1.61	1.79
1	G	193	MET	SD-CE	-6.37	1.63	1.79
1	3	193	MET	SD-CE	-5.80	1.65	1.79
1	2	193	MET	SD-CE	-5.72	1.65	1.79
1	X	193	MET	SD-CE	-5.69	1.65	1.79
1	3	169	MET	SD-CE	-5.67	1.65	1.79
1	O	193	MET	SD-CE	-5.58	1.65	1.79
1	F	193	MET	SD-CE	-5.58	1.65	1.79
1	B	220	ARG	CA-C	5.29	1.59	1.52
1	N	193	MET	SD-CE	-5.14	1.66	1.79
1	Z	85	HIS	CA-C	5.12	1.59	1.53
1	F	76	GLU	CA-C	5.00	1.59	1.52

All (395) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	Q	241	GLU	N-CA-C	-7.97	103.68	113.41
1	F	67	ASP	CA-CB-CG	7.73	120.33	112.60
1	Z	208	ILE	N-CA-C	-7.71	103.28	110.53
1	C	205	SER	CA-C-N	7.45	130.26	120.28
1	C	205	SER	C-N-CA	7.45	130.26	120.28
1	K	101	ASP	CA-CB-CG	7.36	119.96	112.60
1	Y	71	LEU	CA-C-N	7.28	130.37	120.54
1	Y	71	LEU	C-N-CA	7.28	130.37	120.54
1	W	205	SER	CA-C-N	7.24	129.85	120.44
1	W	205	SER	C-N-CA	7.24	129.85	120.44
1	E	71	LEU	CA-C-N	7.23	129.84	120.44
1	E	71	LEU	C-N-CA	7.23	129.84	120.44
1	W	71	LEU	CA-C-N	7.21	130.28	120.54
1	W	71	LEU	C-N-CA	7.21	130.28	120.54
1	3	203	PHE	CA-CB-CG	7.09	120.89	113.80
1	P	71	LEU	CA-C-N	7.06	129.74	120.28
1	P	71	LEU	C-N-CA	7.06	129.74	120.28
1	Q	205	SER	CA-C-N	6.96	129.93	120.54
1	Q	205	SER	C-N-CA	6.96	129.93	120.54
1	Q	99	VAL	CA-C-N	6.94	131.23	120.82
1	Q	99	VAL	C-N-CA	6.94	131.23	120.82
1	G	205	SER	CA-C-N	6.91	130.10	120.29
1	G	205	SER	C-N-CA	6.91	130.10	120.29
1	T	99	VAL	CA-C-N	6.89	130.21	120.28
1	T	99	VAL	C-N-CA	6.89	130.21	120.28
1	F	71	LEU	CA-C-N	6.88	130.18	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	71	LEU	C-N-CA	6.88	130.18	120.28
1	J	217	VAL	CA-C-N	6.85	129.43	120.60
1	J	217	VAL	C-N-CA	6.85	129.43	120.60
1	G	99	VAL	CA-C-N	6.83	129.32	120.44
1	G	99	VAL	C-N-CA	6.83	129.32	120.44
1	E	67	ASP	CA-CB-CG	6.83	119.43	112.60
1	G	243	ALA	CA-C-N	6.80	129.78	120.46
1	G	243	ALA	C-N-CA	6.80	129.78	120.46
1	I	240	PRO	CA-C-N	6.80	129.28	120.44
1	I	240	PRO	C-N-CA	6.80	129.28	120.44
1	A	67	ASP	CA-CB-CG	6.71	119.31	112.60
1	R	144	ASP	CA-CB-CG	6.69	119.29	112.60
1	V	99	VAL	CA-C-N	6.66	129.87	120.28
1	V	99	VAL	C-N-CA	6.66	129.87	120.28
1	N	71	LEU	CA-C-N	6.60	129.41	120.44
1	N	71	LEU	C-N-CA	6.60	129.41	120.44
1	2	99	VAL	CA-C-N	6.59	129.10	120.28
1	2	99	VAL	C-N-CA	6.59	129.10	120.28
1	P	99	VAL	CA-C-N	6.59	129.10	120.28
1	P	99	VAL	C-N-CA	6.59	129.10	120.28
1	1	99	VAL	CA-C-N	6.58	129.10	120.28
1	1	99	VAL	C-N-CA	6.58	129.10	120.28
1	Y	101	ASP	CA-CB-CG	6.58	119.18	112.60
1	2	144	ASP	CA-CB-CG	6.55	119.15	112.60
1	R	237	ALA	CA-C-N	6.55	129.59	120.29
1	R	237	ALA	C-N-CA	6.55	129.59	120.29
1	Z	99	VAL	CA-C-N	6.52	129.34	120.54
1	Z	99	VAL	C-N-CA	6.52	129.34	120.54
1	U	19	ASP	CA-CB-CG	6.51	119.11	112.60
1	E	205	SER	CA-C-N	6.44	128.82	120.44
1	E	205	SER	C-N-CA	6.44	128.82	120.44
1	D	19	ASP	CA-CB-CG	6.44	119.04	112.60
1	R	205	SER	CA-C-N	6.41	128.77	120.44
1	R	205	SER	C-N-CA	6.41	128.77	120.44
1	P	67	ASP	CA-CB-CG	6.40	119.00	112.60
1	Q	71	LEU	CA-C-N	6.39	129.36	120.29
1	Q	71	LEU	C-N-CA	6.39	129.36	120.29
1	H	205	SER	CA-C-N	6.38	128.73	120.44
1	H	205	SER	C-N-CA	6.38	128.73	120.44
1	Q	101	ASP	CA-CB-CG	6.36	118.96	112.60
1	P	226	GLU	CA-C-N	6.32	129.26	120.29
1	P	226	GLU	C-N-CA	6.32	129.26	120.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	67	ASP	CA-CB-CG	6.30	118.91	112.60
1	Y	144	ASP	CA-CB-CG	6.30	118.90	112.60
1	R	234	GLU	CA-C-N	6.28	128.98	120.38
1	R	234	GLU	C-N-CA	6.28	128.98	120.38
1	M	205	SER	CA-C-N	6.27	128.97	120.44
1	M	205	SER	C-N-CA	6.27	128.97	120.44
1	N	109	ASP	CA-CB-CG	6.26	118.86	112.60
1	D	99	VAL	CA-C-N	6.24	129.26	120.28
1	D	99	VAL	C-N-CA	6.24	129.26	120.28
1	H	225	VAL	N-CA-C	-6.23	104.20	111.00
1	X	212	ARG	N-CA-C	-6.23	104.42	111.14
1	2	185	GLY	N-CA-C	6.20	120.85	112.17
1	A	212	ARG	N-CA-C	-6.19	104.16	111.03
1	U	67	ASP	CA-CB-CG	6.19	118.79	112.60
1	B	67	ASP	CA-CB-CG	6.17	118.77	112.60
1	A	144	ASP	CA-CB-CG	6.16	118.76	112.60
1	G	172	ALA	CA-C-N	6.15	129.34	120.98
1	G	172	ALA	C-N-CA	6.15	129.34	120.98
1	K	145	ASP	CA-CB-CG	6.14	118.74	112.60
1	C	144	ASP	CA-CB-CG	6.12	118.72	112.60
1	3	144	ASP	CA-CB-CG	6.12	118.72	112.60
1	I	205	SER	CA-C-N	6.10	128.37	120.44
1	I	205	SER	C-N-CA	6.10	128.37	120.44
1	L	203	PHE	CA-CB-CG	6.08	119.89	113.80
1	E	144	ASP	CA-CB-CG	6.08	118.68	112.60
1	T	145	ASP	CA-CB-CG	6.06	118.66	112.60
1	V	59	TYR	CA-C-N	6.05	129.43	120.90
1	V	59	TYR	C-N-CA	6.05	129.43	120.90
1	A	185	GLY	N-CA-C	6.04	120.63	112.17
1	1	176	ASP	CA-CB-CG	6.04	118.64	112.60
1	X	67	ASP	CA-CB-CG	6.03	118.63	112.60
1	P	244	VAL	CA-C-N	6.03	128.64	120.44
1	P	244	VAL	C-N-CA	6.03	128.64	120.44
1	S	185	GLY	N-CA-C	6.02	119.41	111.70
1	X	101	ASP	CA-CB-CG	6.02	118.62	112.60
1	P	212	ARG	N-CA-C	-6.01	104.80	111.36
1	4	67	ASP	CA-CB-CG	6.00	118.59	112.60
1	N	217	VAL	CA-C-N	5.99	128.19	120.70
1	N	217	VAL	C-N-CA	5.99	128.19	120.70
1	I	144	ASP	CA-CB-CG	5.98	118.58	112.60
1	D	203	PHE	CA-CB-CG	5.97	119.77	113.80
1	X	206	GLU	CA-C-N	5.94	128.52	120.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	206	GLU	C-N-CA	5.94	128.52	120.44
1	O	71	LEU	CA-C-N	5.94	129.04	120.79
1	O	71	LEU	C-N-CA	5.94	129.04	120.79
1	S	35	GLY	CA-C-N	5.93	129.26	120.90
1	S	35	GLY	C-N-CA	5.93	129.26	120.90
1	M	198	MET	N-CA-C	-5.93	104.17	111.40
1	V	247	ASP	CA-CB-CG	5.93	118.53	112.60
1	U	144	ASP	CA-CB-CG	5.92	118.52	112.60
1	3	205	SER	CA-C-N	5.92	129.31	120.31
1	3	205	SER	C-N-CA	5.92	129.31	120.31
1	E	1	MET	CA-C-N	5.92	131.12	122.77
1	E	1	MET	C-N-CA	5.92	131.12	122.77
1	W	206	GLU	CB-CG-CD	5.91	122.65	112.60
1	D	212	ARG	CA-C-N	5.90	128.19	120.28
1	D	212	ARG	C-N-CA	5.90	128.19	120.28
1	S	212	ARG	N-CA-C	-5.89	104.78	111.14
1	Z	67	ASP	CA-CB-CG	5.89	118.49	112.60
1	3	225	VAL	CA-C-N	5.88	128.43	120.44
1	3	225	VAL	C-N-CA	5.88	128.43	120.44
1	D	212	ARG	N-CA-C	-5.87	104.79	111.07
1	T	104	GLU	CA-C-N	5.86	131.25	123.05
1	T	104	GLU	C-N-CA	5.86	131.25	123.05
1	O	249	ILE	CA-C-N	5.83	128.01	120.44
1	O	249	ILE	C-N-CA	5.83	128.01	120.44
1	F	3	LEU	N-CA-C	-5.81	106.74	113.88
1	3	99	VAL	CA-C-N	5.80	129.53	120.82
1	3	99	VAL	C-N-CA	5.80	129.53	120.82
1	F	186	ASN	CA-CB-CG	5.80	118.40	112.60
1	S	99	VAL	CA-C-N	5.78	127.96	120.44
1	S	99	VAL	C-N-CA	5.78	127.96	120.44
1	1	71	LEU	CA-C-N	5.78	128.50	120.29
1	1	71	LEU	C-N-CA	5.78	128.50	120.29
1	A	205	SER	CA-C-N	5.77	128.29	120.44
1	A	205	SER	C-N-CA	5.77	128.29	120.44
1	J	242	VAL	N-CA-C	-5.76	104.90	110.72
1	A	234	GLU	CA-C-N	5.76	128.00	120.28
1	A	234	GLU	C-N-CA	5.76	128.00	120.28
1	E	109	ASP	CA-CB-CG	5.75	118.35	112.60
1	Z	77	PRO	CA-C-N	5.75	129.28	120.82
1	Z	77	PRO	C-N-CA	5.75	129.28	120.82
1	H	59	TYR	CA-C-N	5.75	129.26	120.82
1	H	59	TYR	C-N-CA	5.75	129.26	120.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	R	19	ASP	CA-CB-CG	5.74	118.34	112.60
1	P	2	SER	CA-C-N	5.72	132.47	121.54
1	P	2	SER	C-N-CA	5.72	132.47	121.54
1	D	67	ASP	CA-CB-CG	5.71	118.31	112.60
1	J	205	SER	CA-C-N	5.71	128.19	120.65
1	J	205	SER	C-N-CA	5.71	128.19	120.65
1	X	144	ASP	CA-CB-CG	5.71	118.31	112.60
1	J	99	VAL	CA-C-N	5.71	127.93	120.28
1	J	99	VAL	C-N-CA	5.71	127.93	120.28
1	J	206	GLU	CA-C-N	5.70	127.92	120.28
1	J	206	GLU	C-N-CA	5.70	127.92	120.28
1	4	224	THR	N-CA-C	-5.69	102.06	110.48
1	B	194	ASN	CA-CB-CG	5.69	118.29	112.60
1	Y	219	TYR	CA-C-N	5.68	132.39	121.54
1	Y	219	TYR	C-N-CA	5.68	132.39	121.54
1	V	35	GLY	CA-C-N	5.67	129.16	121.05
1	V	35	GLY	C-N-CA	5.67	129.16	121.05
1	1	231	GLU	CA-C-N	5.66	128.13	120.38
1	1	231	GLU	C-N-CA	5.66	128.13	120.38
1	2	226	GLU	CA-C-N	5.65	128.32	120.29
1	2	226	GLU	C-N-CA	5.65	128.32	120.29
1	Z	212	ARG	CA-C-N	5.64	128.40	120.28
1	Z	212	ARG	C-N-CA	5.64	128.40	120.28
1	H	2	SER	CA-C-N	5.63	132.30	121.54
1	H	2	SER	C-N-CA	5.63	132.30	121.54
1	M	35	GLY	CA-C-N	5.63	128.84	120.90
1	M	35	GLY	C-N-CA	5.63	128.84	120.90
1	O	145	ASP	CA-CB-CG	5.63	118.23	112.60
1	4	241	GLU	N-CA-C	-5.61	105.55	112.90
1	O	101	ASP	CA-CB-CG	5.61	118.20	112.60
1	Q	203	PHE	CA-CB-CG	5.60	119.40	113.80
1	X	2	SER	CA-C-N	5.60	128.82	120.31
1	X	2	SER	C-N-CA	5.60	128.82	120.31
1	B	248	SER	CA-C-N	5.59	129.49	120.82
1	B	248	SER	C-N-CA	5.59	129.49	120.82
1	Q	186	ASN	CA-CB-CG	5.59	118.19	112.60
1	A	145	ASP	CA-CB-CG	5.58	118.18	112.60
1	X	225	VAL	CA-C-N	5.58	128.22	120.63
1	X	225	VAL	C-N-CA	5.58	128.22	120.63
1	Z	226	GLU	CA-C-N	5.57	128.78	120.31
1	Z	226	GLU	C-N-CA	5.57	128.78	120.31
1	S	217	VAL	CA-C-N	5.56	127.57	120.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	S	217	VAL	C-N-CA	5.56	127.57	120.56
1	J	225	VAL	N-CA-C	-5.56	104.51	112.35
1	D	205	SER	CA-C-N	5.55	128.18	120.29
1	D	205	SER	C-N-CA	5.55	128.18	120.29
1	W	99	VAL	CA-C-N	5.55	127.72	120.28
1	W	99	VAL	C-N-CA	5.55	127.72	120.28
1	U	244	VAL	CA-C-N	5.54	127.98	120.44
1	U	244	VAL	C-N-CA	5.54	127.98	120.44
1	E	35	GLY	CA-C-N	5.54	132.13	121.54
1	E	35	GLY	C-N-CA	5.54	132.13	121.54
1	Z	127	ASN	CA-CB-CG	5.54	118.14	112.60
1	S	205	SER	CA-C-N	5.54	127.70	120.28
1	S	205	SER	C-N-CA	5.54	127.70	120.28
1	L	99	VAL	CA-C-N	5.52	128.71	120.31
1	L	99	VAL	C-N-CA	5.52	128.71	120.31
1	N	35	GLY	CA-C-N	5.52	128.94	121.05
1	N	35	GLY	C-N-CA	5.52	128.94	121.05
1	X	247	ASP	CA-CB-CG	5.50	118.10	112.60
1	Y	205	SER	CA-C-N	5.48	129.95	120.58
1	Y	205	SER	C-N-CA	5.48	129.95	120.58
1	N	59	TYR	CA-C-N	5.47	128.87	120.82
1	N	59	TYR	C-N-CA	5.47	128.87	120.82
1	W	225	VAL	CA-C-N	5.47	127.56	120.44
1	W	225	VAL	C-N-CA	5.47	127.56	120.44
1	S	247	ASP	CA-CB-CG	5.47	118.07	112.60
1	J	254	ARG	N-CA-C	-5.47	106.28	113.12
1	D	101	ASP	CA-CB-CG	5.46	118.06	112.60
1	A	59	TYR	CA-C-N	5.45	128.59	120.90
1	A	59	TYR	C-N-CA	5.45	128.59	120.90
1	C	194	ASN	CA-CB-CG	5.44	118.04	112.60
1	W	240	PRO	CA-C-N	5.44	127.57	120.28
1	W	240	PRO	C-N-CA	5.44	127.57	120.28
1	K	162	GLY	N-CA-C	5.44	119.53	112.25
1	R	119	ILE	CB-CA-C	5.43	116.72	111.23
1	4	19	ASP	CA-CB-CG	5.43	118.03	112.60
1	R	79	ARG	N-CA-C	5.43	118.12	110.14
1	B	144	ASP	CA-CB-CG	5.42	118.03	112.60
1	F	219	TYR	CA-C-N	5.41	131.88	121.54
1	F	219	TYR	C-N-CA	5.41	131.88	121.54
1	O	110	HIS	N-CA-C	5.40	119.45	112.86
1	K	215	TYR	CA-C-N	5.38	127.80	120.54
1	K	215	TYR	C-N-CA	5.38	127.80	120.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	157	GLN	CA-C-N	5.38	131.81	121.54
1	A	157	GLN	C-N-CA	5.38	131.81	121.54
1	J	66	GLU	CA-C-N	5.37	128.47	120.90
1	J	66	GLU	C-N-CA	5.37	128.47	120.90
1	C	172	ALA	CA-C-N	5.37	127.77	120.63
1	C	172	ALA	C-N-CA	5.37	127.77	120.63
1	I	75	GLY	CA-C-N	5.37	127.85	120.39
1	I	75	GLY	C-N-CA	5.37	127.85	120.39
1	Q	145	ASP	CA-CB-CG	5.36	117.96	112.60
1	H	115	ALA	CA-C-N	5.36	131.77	121.54
1	H	115	ALA	C-N-CA	5.36	131.77	121.54
1	4	186	ASN	CA-CB-CG	5.35	117.95	112.60
1	U	197	GLY	CA-C-N	5.35	127.39	120.44
1	U	197	GLY	C-N-CA	5.35	127.39	120.44
1	Y	224	THR	N-CA-C	-5.34	103.64	110.53
1	L	226	GLU	CA-C-N	5.34	127.44	120.28
1	L	226	GLU	C-N-CA	5.34	127.44	120.28
1	R	99	VAL	CA-C-N	5.33	127.42	120.28
1	R	99	VAL	C-N-CA	5.33	127.42	120.28
1	H	223	HIS	N-CA-C	-5.32	102.58	110.46
1	K	144	ASP	CA-CB-CG	5.32	117.92	112.60
1	G	186	ASN	CA-CB-CG	5.32	117.92	112.60
1	D	145	ASP	CA-CB-CG	5.32	117.92	112.60
1	P	215	TYR	N-CA-C	-5.31	105.13	111.03
1	D	59	TYR	CA-C-N	5.31	128.38	120.90
1	D	59	TYR	C-N-CA	5.31	128.38	120.90
1	X	243	ALA	CA-C-N	5.30	127.24	120.56
1	X	243	ALA	C-N-CA	5.30	127.24	120.56
1	F	135	THR	N-CA-C	-5.29	103.03	110.50
1	B	101	ASP	CA-CB-CG	5.29	117.89	112.60
1	M	212	ARG	N-CA-C	-5.29	105.42	111.14
1	Z	101	ASP	CA-CB-CG	5.29	117.89	112.60
1	O	109	ASP	CA-CB-CG	5.29	117.89	112.60
1	U	205	SER	CA-C-N	5.29	127.36	120.28
1	U	205	SER	C-N-CA	5.29	127.36	120.28
1	V	205	SER	CA-C-N	5.29	127.31	120.44
1	V	205	SER	C-N-CA	5.29	127.31	120.44
1	O	198	MET	N-CA-C	-5.28	105.44	111.14
1	D	167	SER	CA-C-N	5.26	126.18	120.44
1	D	167	SER	C-N-CA	5.26	126.18	120.44
1	D	249	ILE	N-CA-C	-5.26	106.00	111.58
1	A	158	TYR	CA-C-N	5.26	128.55	120.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	158	TYR	C-N-CA	5.26	128.55	120.82
1	X	35	GLY	CA-C-N	5.25	128.31	120.90
1	X	35	GLY	C-N-CA	5.25	128.31	120.90
1	P	101	ASP	CA-CB-CG	5.25	117.85	112.60
1	V	84	ASP	CA-C-N	5.24	131.55	121.54
1	V	84	ASP	C-N-CA	5.24	131.55	121.54
1	R	227	GLU	CA-C-N	5.24	127.25	120.44
1	R	227	GLU	C-N-CA	5.24	127.25	120.44
1	4	205	SER	CA-C-N	5.23	127.55	120.44
1	4	205	SER	C-N-CA	5.23	127.55	120.44
1	Y	9	ILE	N-CA-CB	5.23	118.44	111.64
1	N	205	SER	CA-C-N	5.23	127.28	120.28
1	N	205	SER	C-N-CA	5.23	127.28	120.28
1	G	199	ARG	CA-C-N	5.22	127.22	120.44
1	G	199	ARG	C-N-CA	5.22	127.22	120.44
1	4	109	ASP	CA-CB-CG	5.21	117.81	112.60
1	N	67	ASP	CA-CB-CG	5.21	117.81	112.60
1	P	145	ASP	CA-CB-CG	5.21	117.81	112.60
1	B	167	SER	CA-C-N	5.20	125.28	120.34
1	B	167	SER	C-N-CA	5.20	125.28	120.34
1	T	2	SER	CA-C-N	5.20	127.56	120.54
1	T	2	SER	C-N-CA	5.20	127.56	120.54
1	P	243	ALA	CA-C-N	5.19	127.85	120.53
1	P	243	ALA	C-N-CA	5.19	127.85	120.53
1	S	144	ASP	CA-CB-CG	5.18	117.78	112.60
1	X	99	VAL	CA-C-N	5.18	127.64	120.29
1	X	99	VAL	C-N-CA	5.18	127.64	120.29
1	Q	219	TYR	CA-C-N	5.18	131.43	121.54
1	Q	219	TYR	C-N-CA	5.18	131.43	121.54
1	2	177	VAL	N-CA-C	-5.17	102.43	107.55
1	3	114	MET	CA-C-N	5.17	129.01	121.31
1	3	114	MET	C-N-CA	5.17	129.01	121.31
1	B	250	GLN	N-CA-C	-5.16	105.73	111.36
1	D	199	ARG	CA-C-N	5.16	127.14	120.44
1	D	199	ARG	C-N-CA	5.16	127.14	120.44
1	N	72	LYS	N-CA-C	-5.15	105.57	111.14
1	B	186	ASN	CA-CB-CG	5.15	117.75	112.60
1	N	2	SER	CA-C-N	5.14	127.13	120.44
1	N	2	SER	C-N-CA	5.14	127.13	120.44
1	4	99	VAL	CA-C-N	5.14	127.89	120.38
1	4	99	VAL	C-N-CA	5.14	127.89	120.38
1	O	243	ALA	CA-C-N	5.14	127.51	120.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	O	243	ALA	C-N-CA	5.14	127.51	120.77
1	2	199	ARG	CA-C-N	5.13	127.16	120.28
1	2	199	ARG	C-N-CA	5.13	127.16	120.28
1	C	250	GLN	CA-C-N	5.13	129.36	120.58
1	C	250	GLN	C-N-CA	5.13	129.36	120.58
1	Y	79	ARG	N-CA-C	5.13	117.69	110.14
1	V	2	SER	N-CA-C	5.13	117.15	110.43
1	A	79	ARG	CA-C-N	5.12	130.96	121.94
1	A	79	ARG	C-N-CA	5.12	130.96	121.94
1	1	144	ASP	CA-CB-CG	5.12	117.72	112.60
1	U	4	ILE	CA-C-N	5.12	127.94	120.51
1	U	4	ILE	C-N-CA	5.12	127.94	120.51
1	4	140	HIS	CA-C-N	5.12	128.73	121.66
1	4	140	HIS	C-N-CA	5.12	128.73	121.66
1	2	104	GLU	CA-C-N	5.12	129.49	122.84
1	2	104	GLU	C-N-CA	5.12	129.49	122.84
1	W	101	ASP	CA-CB-CG	5.12	117.72	112.60
1	2	223	HIS	N-CA-C	-5.11	102.21	110.14
1	F	217	VAL	CA-C-N	5.11	127.00	120.56
1	F	217	VAL	C-N-CA	5.11	127.00	120.56
1	S	199	ARG	CA-C-N	5.11	127.08	120.44
1	S	199	ARG	C-N-CA	5.11	127.08	120.44
1	X	217	VAL	CA-C-N	5.11	127.00	120.56
1	X	217	VAL	C-N-CA	5.11	127.00	120.56
1	X	19	ASP	CA-CB-CG	5.10	117.70	112.60
1	Y	186	ASN	CA-CB-CG	5.10	117.70	112.60
1	X	105	THR	N-CA-C	-5.10	100.93	109.24
1	Y	229	LEU	CA-C-N	5.10	127.37	120.44
1	Y	229	LEU	C-N-CA	5.10	127.37	120.44
1	N	240	PRO	CA-C-N	5.09	127.06	120.44
1	N	240	PRO	C-N-CA	5.09	127.06	120.44
1	J	35	GLY	CA-C-N	5.09	128.33	121.05
1	J	35	GLY	C-N-CA	5.09	128.33	121.05
1	G	144	ASP	CA-CB-CG	5.09	117.69	112.60
1	R	54	LYS	CA-C-N	5.08	131.25	121.54
1	R	54	LYS	C-N-CA	5.08	131.25	121.54
1	Z	203	PHE	CA-CB-CG	5.08	118.88	113.80
1	F	35	GLY	CA-C-N	5.08	129.49	121.56
1	F	35	GLY	C-N-CA	5.08	129.49	121.56
1	H	101	ASP	CA-CB-CG	5.08	117.68	112.60
1	Z	38	THR	N-CA-C	-5.07	103.70	110.55
1	1	100	GLN	CB-CG-CD	5.07	121.22	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	K	85	HIS	N-CA-C	5.07	118.76	112.47
1	L	1	MET	CA-C-N	5.07	128.41	120.75
1	L	1	MET	C-N-CA	5.07	128.41	120.75
1	M	37	GLY	CA-C-N	5.07	128.87	121.31
1	M	37	GLY	C-N-CA	5.07	128.87	121.31
1	G	134	ASN	CA-CB-CG	5.06	117.66	112.60
1	P	54	LYS	CA-C-N	5.06	131.21	121.54
1	P	54	LYS	C-N-CA	5.06	131.21	121.54
1	U	79	ARG	N-CA-C	5.06	116.50	108.96
1	Z	109	ASP	CA-C-N	5.06	129.54	122.36
1	Z	109	ASP	C-N-CA	5.06	129.54	122.36
1	Z	205	SER	CA-C-N	5.05	127.98	120.31
1	Z	205	SER	C-N-CA	5.05	127.98	120.31
1	O	198	MET	CA-C-N	5.03	127.03	120.28
1	O	198	MET	C-N-CA	5.03	127.03	120.28
1	D	184	PHE	N-CA-C	5.03	117.02	109.23
1	V	217	VAL	CA-C-N	5.03	126.85	120.72
1	V	217	VAL	C-N-CA	5.03	126.85	120.72
1	A	88	ILE	N-CA-C	-5.02	100.03	107.51
1	A	224	THR	N-CA-C	-5.02	103.42	110.50
1	3	145	ASP	CA-CB-CG	5.02	117.62	112.60
1	3	199	ARG	CA-C-N	5.02	127.00	120.28
1	3	199	ARG	C-N-CA	5.02	127.00	120.28
1	A	252	ALA	N-CA-C	-5.02	107.71	113.88
1	2	70	ASP	CA-CB-CG	5.01	117.61	112.60
1	W	241	GLU	CB-CG-CD	5.01	121.13	112.60
1	3	217	VAL	CA-C-N	5.01	127.59	120.53
1	3	217	VAL	C-N-CA	5.01	127.59	120.53
1	G	109	ASP	CA-CB-CG	5.00	117.61	112.60
1	P	35	GLY	CA-C-N	5.00	130.63	121.97
1	P	35	GLY	C-N-CA	5.00	130.63	121.97
1	S	216	LYS	CA-C-N	5.00	126.95	120.70
1	S	216	LYS	C-N-CA	5.00	126.95	120.70

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen

atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1	1974	0	1947	25	0
1	2	1974	0	1947	23	0
1	3	1974	0	1947	38	0
1	4	1974	0	1947	22	0
1	A	1974	0	1947	25	0
1	B	1974	0	1947	34	0
1	C	1974	0	1947	22	0
1	D	1974	0	1947	37	0
1	E	1974	0	1947	20	0
1	F	1974	0	1947	37	0
1	G	1974	0	1947	33	0
1	H	1974	0	1947	29	0
1	I	1974	0	1947	24	0
1	J	1974	0	1947	38	0
1	K	1974	0	1947	25	0
1	L	1974	0	1947	35	0
1	M	1974	0	1947	29	0
1	N	1974	0	1947	22	0
1	O	1974	0	1947	35	0
1	P	1974	0	1947	37	0
1	Q	1974	0	1947	27	0
1	R	1974	0	1947	33	0
1	S	1974	0	1947	30	0
1	T	1974	0	1947	34	0
1	U	1974	0	1947	26	0
1	V	1974	0	1947	26	0
1	W	1974	0	1947	23	0
1	X	1974	0	1947	30	0
1	Y	1974	0	1947	31	0
1	Z	1974	0	1947	28	0
2	1	56	0	0	0	0
2	2	28	0	0	1	0
2	3	56	0	0	3	0
2	A	56	0	0	0	0
2	B	28	0	0	0	0
2	D	56	0	0	0	0
2	F	28	0	0	0	0
2	G	28	0	0	1	0
2	H	56	0	0	3	0
2	J	28	0	0	0	0
2	K	28	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	L	28	0	0	0	0
2	N	28	0	0	1	0
2	O	56	0	0	0	0
2	P	56	0	0	3	0
2	R	28	0	0	1	0
2	S	56	0	0	0	0
2	T	28	0	0	0	0
2	V	28	0	0	0	0
2	W	56	0	0	1	0
2	Z	28	0	0	0	0
3	1	5	0	0	0	0
3	2	5	0	0	0	0
3	3	5	0	0	0	0
3	4	5	0	0	0	0
3	A	5	0	0	0	0
3	B	5	0	0	0	0
3	C	10	0	0	0	0
3	D	5	0	0	0	0
3	E	5	0	0	0	0
3	F	5	0	0	0	0
3	G	5	0	0	0	0
3	H	5	0	0	0	0
3	I	5	0	0	0	0
3	J	5	0	0	0	0
3	K	5	0	0	0	0
3	L	5	0	0	0	0
3	M	5	0	0	0	0
3	N	5	0	0	0	0
3	O	5	0	0	0	0
3	P	5	0	0	0	0
3	Q	5	0	0	0	0
3	R	5	0	0	0	0
3	S	5	0	0	0	0
3	T	5	0	0	0	0
3	U	5	0	0	0	0
3	V	5	0	0	0	0
3	W	5	0	0	0	0
3	X	5	0	0	0	0
3	Y	5	0	0	0	0
3	Z	5	0	0	0	0
4	B	1	0	0	0	0
All	All	60216	0	58410	807	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 7.

All (807) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:68:THR:HG21	1:C:121:HIS:HD2	1.36	0.89
1:H:164:HIS:CE1	1:H:201:ARG:HG3	2.09	0.88
1:3:98:THR:HB	1:3:100:GLN:HE21	1.38	0.88
1:S:198:MET:HE2	1:S:211:LEU:HD13	1.57	0.86
1:1:249:ILE:O	1:1:253:THR:HG22	1.76	0.86
1:H:164:HIS:HE1	1:H:201:ARG:HG3	1.40	0.84
1:R:100:GLN:H	1:R:100:GLN:HE21	1.28	0.82
1:X:132:VAL:HG12	1:X:133:ASN:H	1.45	0.81
1:D:69:PRO:HG2	1:F:114:MET:HE3	1.62	0.80
1:S:164:HIS:HE1	1:S:201:ARG:HG3	1.46	0.80
1:C:68:THR:HG21	1:C:121:HIS:CD2	2.18	0.79
1:1:150:SER:HB2	1:1:167:SER:O	1.83	0.78
1:3:98:THR:HB	1:3:100:GLN:NE2	1.98	0.78
1:Z:38:THR:HG23	1:Z:56:ASN:HB2	1.66	0.77
1:F:164:HIS:CE1	1:F:201:ARG:HG3	2.20	0.77
1:T:164:HIS:HE1	1:T:201:ARG:HG3	1.51	0.76
1:F:166:PHE:HB3	1:F:182:THR:HG22	1.68	0.76
1:J:164:HIS:HE1	1:J:201:ARG:HG3	1.50	0.75
1:V:254:ARG:HH21	1:V:254:ARG:HB3	1.51	0.75
1:X:149:LEU:HD21	1:X:161:ILE:HG21	1.69	0.75
1:T:164:HIS:CE1	1:T:201:ARG:HG3	2.22	0.75
1:U:180:TYR:HB2	1:U:193:MET:HE2	1.68	0.74
1:W:100:GLN:H	1:W:100:GLN:HE21	1.36	0.74
1:D:149:LEU:HD21	1:D:161:ILE:HG21	1.71	0.73
1:R:16:LEU:HD11	1:R:28:VAL:HG11	1.70	0.72
1:E:142:HIS:HB2	1:E:160:ARG:HG2	1.72	0.72
1:Z:100:GLN:H	1:Z:100:GLN:HE21	1.38	0.72
1:O:164:HIS:HE1	1:O:201:ARG:HG3	1.54	0.72
1:4:164:HIS:CE1	1:4:201:ARG:HG3	2.24	0.72
1:A:150:SER:HB2	1:A:167:SER:O	1.90	0.72
1:V:98:THR:HB	1:V:100:GLN:HE21	1.54	0.72
1:T:201:ARG:HG2	1:T:201:ARG:HH11	1.55	0.71
1:Z:164:HIS:HE1	1:Z:201:ARG:HG3	1.56	0.71
1:J:27:ILE:HD11	1:L:25:TRP:HZ3	1.56	0.70
1:F:16:LEU:HD11	1:F:28:VAL:HG11	1.72	0.70
1:M:80:LEU:HB2	1:M:96:ARG:HG2	1.74	0.70
1:J:52:ILE:HG23	1:J:56:ASN:HD22	1.57	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Y:164:HIS:HE1	1:Y:201:ARG:HG3	1.56	0.69
1:F:164:HIS:HE1	1:F:201:ARG:HG3	1.54	0.69
1:M:21:GLN:HB2	1:M:39:VAL:HG22	1.74	0.69
1:M:254:ARG:HH11	1:Z:160:ARG:HD2	1.58	0.69
1:B:36:GLU:HB2	1:B:54:LYS:HG2	1.74	0.69
1:C:149:LEU:HD21	1:C:161:ILE:HG21	1.74	0.68
1:E:164:HIS:HE1	1:E:201:ARG:HG3	1.57	0.68
1:H:132:VAL:HG12	1:H:133:ASN:H	1.59	0.68
1:B:85:HIS:O	1:B:110:HIS:HA	1.94	0.68
1:D:166:PHE:HB3	1:D:182:THR:HG22	1.76	0.68
1:T:223:HIS:HB3	1:T:227:GLU:HB3	1.76	0.68
1:G:98:THR:HB	1:G:100:GLN:HE21	1.58	0.67
1:F:193:MET:HE3	1:F:215:TYR:HD2	1.59	0.67
1:M:80:LEU:HD11	1:M:94:ILE:HG22	1.75	0.67
1:V:24:PRO:HD2	1:V:42:PRO:HB3	1.76	0.67
1:M:63:SER:HB3	1:O:60:GLN:HE21	1.59	0.66
1:U:149:LEU:HD21	1:U:161:ILE:HG21	1.75	0.66
1:N:169:MET:HE2	1:O:156:HIS:CD2	2.31	0.66
1:D:98:THR:HB	1:D:100:GLN:NE2	2.11	0.66
1:J:130:ILE:HD12	1:J:148:ILE:HG12	1.76	0.66
1:E:13:SER:OG	1:E:30:ALA:HA	1.95	0.66
1:M:28:VAL:HG22	1:M:46:LEU:HD12	1.78	0.66
1:V:166:PHE:O	1:V:182:THR:HA	1.95	0.66
1:2:166:PHE:HB3	1:2:182:THR:HG22	1.79	0.65
1:4:164:HIS:HE1	1:4:201:ARG:HG3	1.61	0.65
1:E:201:ARG:HG2	1:E:201:ARG:HH11	1.61	0.65
1:P:166:PHE:HB3	1:P:182:THR:HG22	1.77	0.65
1:V:239:PHE:HB2	1:V:242:VAL:HG23	1.78	0.65
1:I:195:PHE:HZ	1:I:212:ARG:HG2	1.61	0.65
1:J:166:PHE:HB3	1:J:182:THR:HG22	1.78	0.65
1:V:193:MET:HE3	1:V:215:TYR:HB2	1.79	0.65
1:X:132:VAL:HG12	1:X:133:ASN:N	2.12	0.65
1:G:164:HIS:CE1	1:G:201:ARG:HG2	2.32	0.65
1:3:164:HIS:HE1	1:3:201:ARG:HG3	1.62	0.64
1:Q:193:MET:HE3	1:Q:215:TYR:HB2	1.80	0.64
1:1:100:GLN:H	1:1:100:GLN:HE21	1.46	0.64
1:4:149:LEU:HD21	1:4:161:ILE:HG21	1.79	0.64
1:S:211:LEU:HD11	1:S:241:GLU:HB3	1.80	0.63
1:3:164:HIS:CE1	1:3:201:ARG:HG3	2.33	0.63
1:J:183:VAL:HG12	1:J:190:ALA:HA	1.81	0.63
1:T:16:LEU:HD11	1:T:28:VAL:HG11	1.81	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:164:HIS:HE1	1:B:201:ARG:HG3	1.64	0.63
1:3:254:ARG:HH11	1:J:160:ARG:HD2	1.64	0.63
1:4:166:PHE:HB3	1:4:182:THR:HG22	1.79	0.63
1:A:166:PHE:HB3	1:A:182:THR:HG22	1.81	0.63
1:S:73:TYR:HB2	1:S:98:THR:HG22	1.80	0.63
1:3:166:PHE:HB3	1:3:182:THR:HG22	1.81	0.62
1:C:156:HIS:HB2	1:C:174:GLY:HA2	1.82	0.62
1:4:68:THR:HG21	1:4:121:HIS:ND1	2.15	0.62
1:O:81:VAL:HB	1:O:106:THR:HG23	1.82	0.62
1:F:132:VAL:HG12	1:F:133:ASN:H	1.65	0.62
1:G:132:VAL:HG12	1:G:133:ASN:H	1.65	0.62
1:U:94:ILE:HG12	1:U:119:ILE:HD12	1.82	0.61
1:M:80:LEU:HD12	1:M:105:THR:HB	1.82	0.61
1:R:160:ARG:HD2	1:W:254:ARG:HH11	1.64	0.61
1:Y:15:ARG:HH11	1:Y:33:GLU:HB2	1.65	0.61
1:A:68:THR:HG21	1:A:121:HIS:ND1	2.16	0.61
1:N:166:PHE:HB3	1:N:182:THR:HG22	1.82	0.60
1:G:164:HIS:HE1	1:G:201:ARG:HG2	1.64	0.60
1:T:201:ARG:HG2	1:T:201:ARG:NH1	2.16	0.60
1:E:258:ARG:HH22	1:S:225:VAL:HG22	1.67	0.60
1:J:166:PHE:O	1:J:182:THR:HA	2.01	0.60
1:T:25:TRP:HZ3	1:U:27:ILE:HD11	1.66	0.60
1:4:201:ARG:HG2	1:4:201:ARG:HH11	1.67	0.60
1:D:160:ARG:HB2	1:D:176:ASP:OD2	2.00	0.60
1:L:223:HIS:HB3	1:L:227:GLU:HB3	1.82	0.60
1:S:166:PHE:HB3	1:S:182:THR:HG22	1.84	0.60
1:3:16:LEU:HD11	1:3:28:VAL:HG11	1.84	0.60
1:G:98:THR:HB	1:G:100:GLN:NE2	2.16	0.59
1:E:164:HIS:CE1	1:E:201:ARG:HG3	2.37	0.59
1:1:236:ALA:HB1	1:1:246:ARG:NH1	2.18	0.59
1:H:142:HIS:HB2	1:H:160:ARG:HG3	1.83	0.59
1:Y:38:THR:HG23	1:Y:56:ASN:HB2	1.83	0.59
1:3:65:GLY:O	1:3:96:ARG:HD3	2.02	0.59
1:K:98:THR:HB	1:K:100:GLN:NE2	2.17	0.59
1:Z:164:HIS:CE1	1:Z:201:ARG:HG3	2.37	0.59
1:O:98:THR:HB	1:O:100:GLN:NE2	2.17	0.59
1:P:196:GLU:OE2	1:P:199:ARG:HD3	2.01	0.59
1:Q:68:THR:HG21	1:Q:121:HIS:ND1	2.17	0.59
1:V:254:ARG:HB3	1:V:254:ARG:NH2	2.17	0.59
1:X:166:PHE:O	1:X:182:THR:HA	2.03	0.59
1:1:236:ALA:HB1	1:1:246:ARG:HH11	1.68	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:195:PHE:HZ	1:B:212:ARG:HG2	1.67	0.59
1:M:166:PHE:HB3	1:M:182:THR:HG22	1.84	0.59
1:V:240:PRO:O	1:V:244:VAL:HG23	2.03	0.58
1:Q:149:LEU:HD21	1:Q:161:ILE:HG21	1.85	0.58
1:I:99:VAL:HA	1:I:103:ALA:HB2	1.85	0.58
1:O:164:HIS:CE1	1:O:201:ARG:HG3	2.37	0.58
1:3:132:VAL:HG12	1:3:133:ASN:H	1.68	0.58
1:F:1:MET:HG2	1:F:2:SER:N	2.18	0.58
1:M:16:LEU:HD11	1:M:28:VAL:HG11	1.85	0.58
1:E:28:VAL:HG22	1:E:46:LEU:HD12	1.86	0.58
1:1:28:VAL:HG22	1:1:46:LEU:HD12	1.86	0.58
1:T:17:ALA:HB3	1:T:20:VAL:HG23	1.85	0.58
1:F:239:PHE:HB2	1:F:242:VAL:HG23	1.85	0.58
1:2:149:LEU:HD21	1:2:161:ILE:HG21	1.86	0.58
1:X:166:PHE:HB3	1:X:182:THR:HG22	1.85	0.58
1:1:142:HIS:HB2	1:1:160:ARG:HG2	1.85	0.57
1:N:10:ILE:HG12	1:N:28:VAL:HB	1.86	0.57
1:T:149:LEU:HD21	1:T:161:ILE:HG21	1.85	0.57
1:C:38:THR:HG23	1:C:56:ASN:HB2	1.87	0.57
1:L:137:LEU:HD22	1:L:141:VAL:HG11	1.85	0.57
1:3:68:THR:HG21	1:3:121:HIS:ND1	2.20	0.57
1:O:16:LEU:HD11	1:O:28:VAL:HG11	1.86	0.57
1:Y:11:ASP:OD1	1:Y:13:SER:HB3	2.04	0.57
1:F:81:VAL:HB	1:F:106:THR:HG22	1.87	0.57
1:A:149:LEU:HD21	1:A:161:ILE:HG21	1.86	0.57
1:K:149:LEU:HD21	1:K:161:ILE:HG21	1.87	0.57
1:K:164:HIS:HE1	1:K:201:ARG:HG3	1.70	0.57
1:L:209:HIS:NE2	1:L:213:ARG:HD3	2.20	0.57
1:V:98:THR:HB	1:V:100:GLN:NE2	2.19	0.57
1:E:166:PHE:HB3	1:E:182:THR:HG22	1.87	0.56
1:K:249:ILE:O	1:K:253:THR:HG22	2.04	0.56
1:N:3:LEU:HB3	1:N:21:GLN:HG3	1.85	0.56
1:I:28:VAL:HG22	1:I:46:LEU:HD12	1.87	0.56
1:S:164:HIS:CE1	1:S:201:ARG:HG3	2.34	0.56
1:D:150:SER:HB2	1:D:167:SER:O	2.04	0.56
1:G:204:SER:HB2	1:G:207:ALA:H	1.70	0.56
1:J:235:SER:HB3	1:J:242:VAL:HG11	1.86	0.56
1:R:131:LEU:HG	1:R:149:LEU:HD12	1.87	0.56
1:H:194:ASN:O	1:H:198:MET:HG3	2.06	0.56
1:O:166:PHE:HB3	1:O:182:THR:HG22	1.87	0.56
1:P:71:LEU:HD22	2:P:302:VFN:N16	2.20	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:114:MET:HE2	1:D:132:VAL:HG13	1.87	0.56
1:T:166:PHE:HB3	1:T:182:THR:HG22	1.87	0.56
1:H:107:ILE:HG12	1:H:125:ILE:HD12	1.88	0.56
1:R:38:THR:HG23	1:R:56:ASN:HB2	1.86	0.56
1:R:69:PRO:HD3	1:R:95:HIS:CE1	2.41	0.56
1:V:16:LEU:HD11	1:V:28:VAL:HG11	1.88	0.56
1:L:100:GLN:H	1:L:100:GLN:HE21	1.51	0.56
1:P:98:THR:HB	1:P:100:GLN:HE21	1.71	0.56
1:Z:249:ILE:O	1:Z:253:THR:HG22	2.06	0.56
1:C:166:PHE:HB3	1:C:182:THR:HG22	1.87	0.56
1:U:156:HIS:HB2	1:U:174:GLY:HA2	1.87	0.56
1:H:91:GLY:O	1:H:116:TYR:HA	2.06	0.55
1:R:160:ARG:HD2	1:W:254:ARG:NH1	2.22	0.55
1:K:98:THR:HB	1:K:100:GLN:HE21	1.71	0.55
1:S:246:ARG:HB3	1:S:246:ARG:HH11	1.70	0.55
1:W:142:HIS:HB2	1:W:160:ARG:HG2	1.87	0.55
1:I:166:PHE:HB3	1:I:182:THR:HG22	1.88	0.55
1:L:142:HIS:HB2	1:L:160:ARG:HG2	1.88	0.55
1:Z:68:THR:HG22	1:Z:70:ASP:H	1.72	0.55
1:H:59:TYR:HB2	1:H:89:ARG:C	2.31	0.55
1:N:68:THR:HG21	1:N:121:HIS:ND1	2.21	0.55
1:X:58:ILE:HG12	1:X:88:ILE:HB	1.87	0.55
1:L:132:VAL:HG12	1:L:133:ASN:H	1.71	0.55
1:Z:104:GLU:HG2	1:Z:106:THR:HG22	1.89	0.55
1:2:114:MET:HE3	1:3:69:PRO:HG2	1.89	0.55
1:A:61:PHE:O	1:A:91:GLY:HA2	2.07	0.55
1:B:149:LEU:HD11	1:B:161:ILE:HG21	1.89	0.55
1:N:112:LEU:HD23	1:N:130:ILE:HG23	1.88	0.55
1:L:36:GLU:HB3	1:L:54:LYS:HG2	1.89	0.55
1:L:16:LEU:HD23	1:L:20:VAL:HG11	1.89	0.54
1:D:132:VAL:HG12	1:D:133:ASN:N	2.22	0.54
1:Y:166:PHE:HB3	1:Y:182:THR:HG22	1.89	0.54
1:J:180:TYR:HB2	1:J:193:MET:HE2	1.88	0.54
1:F:246:ARG:HH21	1:F:250:GLN:HE21	1.55	0.54
1:J:156:HIS:CD2	1:L:169:MET:HE2	2.43	0.54
1:O:98:THR:HB	1:O:100:GLN:HE21	1.71	0.54
1:D:156:HIS:HB2	1:D:174:GLY:HA2	1.90	0.54
1:1:101:ASP:HB2	1:1:140:HIS:CE1	2.43	0.54
1:3:149:LEU:HD23	1:3:153:THR:HG21	1.90	0.53
1:B:16:LEU:HD11	1:B:28:VAL:HG11	1.90	0.53
1:H:78:THR:HG22	1:H:103:ALA:HB1	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:149:LEU:HD21	1:H:161:ILE:HG21	1.89	0.53
1:T:84:ASP:O	1:T:109:ASP:HA	2.08	0.53
1:D:193:MET:HE3	1:D:215:TYR:HD2	1.73	0.53
1:A:16:LEU:HD11	1:A:28:VAL:HG11	1.91	0.53
1:I:142:HIS:HB2	1:I:160:ARG:HG2	1.90	0.53
1:Q:132:VAL:HG12	1:Q:133:ASN:H	1.72	0.53
1:S:156:HIS:CD2	1:U:169:MET:HE2	2.43	0.53
1:V:149:LEU:HD21	1:V:161:ILE:HG21	1.90	0.53
1:B:195:PHE:CZ	1:B:212:ARG:HG2	2.43	0.53
1:G:132:VAL:HG12	1:G:133:ASN:N	2.22	0.53
1:I:195:PHE:CZ	1:I:212:ARG:HG2	2.42	0.53
1:J:68:THR:HG21	1:J:121:HIS:HB3	1.91	0.53
1:M:98:THR:HB	1:M:100:GLN:NE2	2.24	0.53
1:O:193:MET:HE3	1:O:215:TYR:HB2	1.91	0.53
1:B:98:THR:HB	1:B:100:GLN:HE21	1.73	0.53
1:F:127:ASN:O	1:F:145:ASP:HA	2.09	0.53
1:K:132:VAL:HG12	1:K:133:ASN:H	1.74	0.53
1:W:78:THR:HG21	1:W:98:THR:HA	1.91	0.53
1:D:66:GLU:HB3	1:D:95:HIS:HD2	1.73	0.53
1:Q:98:THR:HB	1:Q:100:GLN:HE21	1.72	0.53
1:R:99:VAL:HA	1:R:103:ALA:HB2	1.91	0.53
1:2:16:LEU:HD11	1:2:28:VAL:HG11	1.91	0.53
1:4:216:LYS:HZ2	1:4:220:ARG:HH11	1.55	0.53
1:V:69:PRO:HG2	1:X:114:MET:HE3	1.91	0.53
1:F:17:ALA:HB3	1:F:20:VAL:HG23	1.90	0.53
1:H:132:VAL:HG12	1:H:133:ASN:N	2.24	0.53
1:D:229:LEU:HA	1:D:232:LEU:HD12	1.91	0.52
1:O:168:GLY:O	1:O:171:SER:HB2	2.08	0.52
1:R:100:GLN:HE21	1:R:100:GLN:N	2.04	0.52
1:V:38:THR:HG23	1:V:56:ASN:HB2	1.91	0.52
1:Z:21:GLN:HB2	1:Z:39:VAL:HG22	1.91	0.52
1:N:113:ILE:HG21	1:N:119:ILE:HD11	1.92	0.52
1:S:249:ILE:O	1:S:253:THR:HG22	2.09	0.52
1:F:249:ILE:O	1:F:253:THR:HG22	2.08	0.52
1:Z:135:THR:HG23	1:Z:153:THR:HB	1.91	0.52
1:2:85:HIS:O	1:2:110:HIS:HA	2.09	0.52
1:F:1:MET:HG2	1:F:2:SER:H	1.75	0.52
1:G:151:GLY:HA3	2:H:301:VFN:CL1	2.46	0.52
1:A:168:GLY:O	1:A:171:SER:HB2	2.09	0.52
1:L:239:PHE:HB2	1:L:242:VAL:HG23	1.91	0.52
1:3:240:PRO:O	1:3:244:VAL:HG23	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:169:MET:HE3	1:O:172:ALA:HB1	1.89	0.52
1:W:98:THR:HB	1:W:100:GLN:NE2	2.25	0.52
1:3:46:LEU:HD23	1:3:64:VAL:HB	1.92	0.52
1:J:246:ARG:HH11	1:J:246:ARG:HB3	1.74	0.52
1:A:249:ILE:O	1:A:253:THR:HG22	2.10	0.52
1:1:113:ILE:HG21	1:1:119:ILE:HD11	1.91	0.51
1:L:149:LEU:HD21	1:L:161:ILE:HG21	1.90	0.51
1:T:156:HIS:HB2	1:T:174:GLY:HA2	1.92	0.51
1:Z:110:HIS:O	1:Z:128:HIS:HA	2.10	0.51
1:1:109:ASP:O	1:1:127:ASN:HA	2.10	0.51
1:E:169:MET:HE2	1:F:156:HIS:CD2	2.45	0.51
1:P:98:THR:HB	1:P:100:GLN:NE2	2.25	0.51
1:S:193:MET:HE3	1:S:215:TYR:HD2	1.75	0.51
1:2:193:MET:HE3	1:2:215:TYR:HB2	1.92	0.51
1:V:68:THR:HG21	1:V:121:HIS:ND1	2.26	0.51
1:Z:221:GLN:HB3	1:Z:223:HIS:ND1	2.25	0.51
1:C:101:ASP:HB2	1:C:140:HIS:CE1	2.45	0.51
1:2:142:HIS:HB2	1:2:160:ARG:HG2	1.91	0.51
1:H:68:THR:HG21	1:H:121:HIS:HB3	1.91	0.51
1:R:33:GLU:HB3	1:R:51:LYS:HG2	1.93	0.51
1:S:36:GLU:HB3	1:S:54:LYS:HG2	1.93	0.51
1:G:79:ARG:HB2	1:G:104:GLU:HG3	1.93	0.51
1:J:69:PRO:HG2	1:L:114:MET:HG2	1.93	0.51
1:N:101:ASP:HB2	1:N:140:HIS:CE1	2.46	0.51
1:Q:151:GLY:HA3	2:R:301:VFN:CL1	2.47	0.51
1:Y:68:THR:HG21	1:Y:121:HIS:ND1	2.25	0.51
1:3:234:GLU:HG3	1:L:212:ARG:HG3	1.92	0.51
1:3:160:ARG:HD2	1:J:254:ARG:NH1	2.26	0.51
1:B:254:ARG:NH1	1:O:160:ARG:HD2	2.26	0.51
1:C:16:LEU:HD11	1:C:28:VAL:HG11	1.93	0.51
1:Q:25:TRP:HZ3	1:R:27:ILE:HD11	1.75	0.51
1:2:28:VAL:HG22	1:2:46:LEU:HD12	1.92	0.51
1:I:78:THR:HG22	1:I:103:ALA:HB1	1.92	0.51
1:L:81:VAL:HB	1:L:106:THR:HG22	1.93	0.51
1:R:223:HIS:HB3	1:R:227:GLU:HB2	1.92	0.51
1:U:166:PHE:HB3	1:U:182:THR:HG22	1.92	0.51
1:4:102:ARG:HE	1:4:104:GLU:HB3	1.75	0.51
1:Y:139:GLY:O	1:Y:157:GLN:HA	2.10	0.51
1:1:100:GLN:HE21	1:1:100:GLN:N	2.09	0.50
1:D:102:ARG:HH21	1:D:106:THR:HG21	1.74	0.50
1:O:149:LEU:HD21	1:O:161:ILE:HG21	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Y:149:LEU:HD21	1:Y:161:ILE:HG21	1.93	0.50
1:1:16:LEU:HD11	1:1:28:VAL:HG11	1.93	0.50
1:K:16:LEU:HD11	1:K:28:VAL:HG11	1.93	0.50
1:R:132:VAL:HG12	1:R:133:ASN:H	1.76	0.50
1:1:149:LEU:HD21	1:1:161:ILE:HG21	1.93	0.50
1:A:24:PRO:HD2	1:A:42:PRO:HB3	1.93	0.50
1:D:166:PHE:O	1:D:182:THR:HA	2.11	0.50
1:G:149:LEU:HD21	1:G:161:ILE:HG21	1.93	0.50
1:P:90:GLU:HG3	1:Q:93:THR:HG21	1.93	0.50
1:Q:166:PHE:HB3	1:Q:182:THR:HG22	1.93	0.50
1:V:254:ARG:HH21	1:V:254:ARG:CB	2.22	0.50
1:2:64:VAL:HG22	1:2:94:ILE:HD12	1.94	0.50
1:L:166:PHE:HB3	1:L:182:THR:HG22	1.92	0.50
1:Y:80:LEU:HB2	1:Y:96:ARG:HG2	1.94	0.50
1:2:249:ILE:O	1:2:253:THR:HG22	2.12	0.50
1:B:175:LYS:HB2	1:O:257:THR:HG23	1.94	0.50
1:E:201:ARG:HG2	1:E:201:ARG:NH1	2.27	0.50
1:I:16:LEU:HD11	1:I:28:VAL:HG11	1.93	0.50
1:I:42:PRO:O	1:I:60:GLN:HA	2.11	0.50
1:I:98:THR:HB	1:I:100:GLN:HE21	1.75	0.50
1:G:69:PRO:HG2	1:I:114:MET:HE3	1.93	0.50
1:H:71:LEU:HD22	2:H:301:VFN:N16	2.27	0.50
1:P:193:MET:HE3	1:P:215:TYR:HD2	1.77	0.50
1:Y:234:GLU:O	1:Y:238:GLN:HG3	2.12	0.50
1:1:164:HIS:CE1	1:1:201:ARG:HG3	2.47	0.50
1:4:46:LEU:HD23	1:4:64:VAL:HB	1.94	0.50
1:B:164:HIS:CE1	1:B:201:ARG:HG3	2.44	0.50
1:L:24:PRO:HD2	1:L:42:PRO:HB3	1.93	0.50
1:1:166:PHE:HB3	1:1:182:THR:HG22	1.94	0.49
1:S:228:ALA:O	1:S:232:LEU:HG	2.11	0.49
1:Y:249:ILE:O	1:Y:253:THR:HG22	2.12	0.49
2:2:301:VFN:C14	1:4:132:VAL:HG21	2.42	0.49
1:3:254:ARG:NH1	1:J:160:ARG:HD2	2.25	0.49
1:N:114:MET:HG2	1:O:69:PRO:HG2	1.94	0.49
1:Q:183:VAL:HB	1:Q:188:ALA:HB1	1.92	0.49
1:C:46:LEU:HD23	1:C:64:VAL:HB	1.93	0.49
1:F:246:ARG:HH21	1:F:250:GLN:NE2	2.10	0.49
1:K:38:THR:HG23	1:K:56:ASN:HB2	1.95	0.49
1:L:161:ILE:HD11	1:L:173:ILE:HG21	1.94	0.49
1:A:156:HIS:CD2	1:C:169:MET:HE2	2.48	0.49
1:E:79:ARG:HB2	1:E:104:GLU:HG3	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:142:HIS:HB2	1:O:160:ARG:HG2	1.94	0.49
1:G:9:ILE:HB	1:G:27:ILE:HG12	1.93	0.49
1:H:223:HIS:HB3	1:H:227:GLU:HB2	1.94	0.49
1:M:68:THR:HG21	1:M:121:HIS:ND1	2.27	0.49
1:Y:199:ARG:HH12	1:Y:200:ARG:CZ	2.26	0.49
1:Z:36:GLU:HB3	1:Z:54:LYS:HG2	1.94	0.49
1:F:67:ASP:HB3	1:F:73:TYR:CE2	2.48	0.49
1:V:236:ALA:HB1	1:V:246:ARG:HH11	1.78	0.49
1:4:16:LEU:HD11	1:4:28:VAL:HG11	1.94	0.49
1:G:131:LEU:HG	1:G:149:LEU:HD12	1.95	0.49
1:M:90:GLU:O	1:M:115:ALA:HA	2.13	0.49
1:J:212:ARG:HD3	1:J:216:LYS:HD2	1.94	0.49
1:P:156:HIS:CD2	1:R:169:MET:HE2	2.48	0.49
1:X:132:VAL:CG1	1:X:133:ASN:H	2.21	0.48
1:1:201:ARG:HH11	1:1:201:ARG:HG2	1.78	0.48
1:A:60:GLN:HG3	1:B:45:VAL:HG21	1.95	0.48
1:A:81:VAL:HB	1:A:106:THR:HG22	1.95	0.48
1:G:71:LEU:HD22	2:G:301:VFN:N16	2.28	0.48
1:G:193:MET:CE	1:G:215:TYR:HB2	2.43	0.48
1:K:168:GLY:HA3	1:K:184:PHE:CD2	2.49	0.48
1:E:149:LEU:HD21	1:E:161:ILE:HG21	1.95	0.48
1:F:142:HIS:HB2	1:F:160:ARG:HG2	1.93	0.48
1:M:27:ILE:HD13	1:M:45:VAL:HG22	1.95	0.48
1:W:166:PHE:HB3	1:W:182:THR:HG22	1.95	0.48
1:X:246:ARG:HB3	1:X:246:ARG:HH11	1.78	0.48
1:Z:127:ASN:O	1:Z:145:ASP:HA	2.14	0.48
1:3:132:VAL:HG12	1:3:133:ASN:N	2.28	0.48
1:4:36:GLU:HB3	1:4:54:LYS:HG2	1.96	0.48
1:B:49:PRO:HD2	1:B:78:THR:O	2.13	0.48
1:B:169:MET:HE2	1:C:156:HIS:CD2	2.49	0.48
1:J:156:HIS:HD2	1:L:169:MET:HE2	1.77	0.48
1:J:164:HIS:CE1	1:J:201:ARG:HG3	2.40	0.48
1:O:156:HIS:HB2	1:O:174:GLY:HA2	1.95	0.48
1:2:132:VAL:HG12	1:2:133:ASN:H	1.78	0.48
1:G:101:ASP:HB2	1:G:140:HIS:CE1	2.48	0.48
1:S:68:THR:HG21	1:S:121:HIS:ND1	2.29	0.48
1:H:166:PHE:HB3	1:H:182:THR:HG22	1.95	0.48
1:J:28:VAL:HG22	1:J:46:LEU:HD12	1.96	0.48
1:L:100:GLN:HE21	1:L:100:GLN:N	2.11	0.48
1:Y:79:ARG:HB2	1:Y:104:GLU:HG3	1.95	0.48
1:Z:168:GLY:HA3	1:Z:184:PHE:CD2	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:201:ARG:HH11	1:S:201:ARG:HG2	1.79	0.48
1:A:78:THR:HG22	1:A:103:ALA:HB1	1.96	0.48
1:I:235:SER:HB3	1:I:242:VAL:HG11	1.96	0.48
1:L:132:VAL:HG12	1:L:133:ASN:N	2.29	0.48
1:M:196:GLU:HB3	1:M:200:ARG:HH11	1.79	0.48
1:P:82:ILE:HG12	1:P:107:ILE:HD12	1.96	0.48
1:V:82:ILE:HG23	1:V:86:ASN:HD22	1.78	0.48
1:D:254:ARG:HH11	1:P:160:ARG:HD2	1.79	0.48
1:U:42:PRO:HD2	1:U:60:GLN:HB3	1.96	0.48
1:3:151:GLY:HA3	2:3:302:VFN:CL1	2.51	0.47
1:B:80:LEU:HB2	1:B:96:ARG:HG2	1.96	0.47
1:B:254:ARG:HH11	1:O:160:ARG:HD2	1.78	0.47
1:D:238:GLN:HB3	1:R:205:SER:HB3	1.96	0.47
1:Q:245:PHE:O	1:Q:249:ILE:HD12	2.14	0.47
1:U:3:LEU:HB3	1:U:21:GLN:HG2	1.96	0.47
1:Y:142:HIS:HB2	1:Y:160:ARG:HG3	1.96	0.47
1:Z:99:VAL:HA	1:Z:103:ALA:HB2	1.95	0.47
1:K:193:MET:HE1	1:K:245:PHE:CE1	2.48	0.47
1:S:100:GLN:H	1:S:100:GLN:HE21	1.61	0.47
1:T:150:SER:O	1:T:153:THR:HB	2.14	0.47
1:Z:166:PHE:HB3	1:Z:182:THR:HG22	1.96	0.47
1:C:212:ARG:HD3	1:C:216:LYS:HE3	1.97	0.47
1:D:114:MET:HG3	1:E:69:PRO:HG2	1.97	0.47
1:K:239:PHE:HB2	1:K:242:VAL:HG23	1.95	0.47
1:Q:113:ILE:HG21	1:Q:119:ILE:HD11	1.96	0.47
1:X:193:MET:HE3	1:X:215:TYR:HB2	1.96	0.47
1:2:166:PHE:O	1:2:182:THR:HA	2.13	0.47
1:C:180:TYR:HB2	1:C:193:MET:HE2	1.97	0.47
1:U:166:PHE:O	1:U:182:THR:HA	2.14	0.47
1:W:100:GLN:H	1:W:100:GLN:NE2	2.07	0.47
1:X:61:PHE:O	1:X:91:GLY:HA2	2.14	0.47
1:A:15:ARG:O	1:A:33:GLU:HA	2.15	0.47
1:P:169:MET:HE2	1:Q:156:HIS:CD2	2.49	0.47
1:S:69:PRO:HD3	1:S:95:HIS:CE1	2.50	0.47
1:W:91:GLY:O	1:W:116:TYR:HA	2.14	0.47
1:G:166:PHE:HB3	1:G:182:THR:HG22	1.97	0.47
1:V:166:PHE:HB3	1:V:182:THR:HG22	1.97	0.47
1:M:78:THR:HG22	1:M:103:ALA:HB1	1.97	0.47
1:M:156:HIS:CD2	1:O:169:MET:HE2	2.50	0.47
1:T:98:THR:HB	1:T:100:GLN:HE21	1.78	0.47
1:U:216:LYS:HZ2	1:U:220:ARG:HH11	1.62	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:249:ILE:O	1:U:253:THR:HG22	2.15	0.47
1:F:89:ARG:HB2	1:F:114:MET:HA	1.97	0.47
1:J:236:ALA:HB1	1:J:246:ARG:NH1	2.30	0.47
1:O:166:PHE:O	1:O:182:THR:HA	2.15	0.47
1:P:68:THR:OG1	1:P:121:HIS:HB3	2.13	0.47
1:W:169:MET:HE2	1:X:156:HIS:CD2	2.50	0.47
1:I:68:THR:HG21	1:I:121:HIS:ND1	2.29	0.47
1:T:99:VAL:HA	1:T:103:ALA:HB2	1.97	0.47
1:W:223:HIS:HB3	1:W:227:GLU:HB2	1.96	0.47
1:J:168:GLY:HA3	1:J:184:PHE:CD2	2.50	0.47
1:S:46:LEU:HD23	1:S:64:VAL:HB	1.97	0.47
1:S:80:LEU:HB2	1:S:96:ARG:HG2	1.97	0.47
1:X:15:ARG:O	1:X:33:GLU:HA	2.15	0.47
1:G:69:PRO:HG2	1:I:114:MET:HG2	1.96	0.46
1:G:199:ARG:HH21	1:G:200:ARG:HG2	1.79	0.46
1:P:39:VAL:HB	1:P:57:ARG:HD2	1.97	0.46
1:Q:127:ASN:O	1:Q:145:ASP:HA	2.15	0.46
1:J:17:ALA:HB3	1:J:20:VAL:HG23	1.96	0.46
1:F:160:ARG:HH21	1:L:254:ARG:HH12	1.62	0.46
1:F:166:PHE:O	1:F:182:THR:HA	2.15	0.46
1:O:33:GLU:HB3	1:O:51:LYS:HE2	1.97	0.46
1:O:73:TYR:HB2	1:O:98:THR:HG22	1.96	0.46
1:Q:42:PRO:O	1:Q:44:VAL:HG23	2.16	0.46
1:T:68:THR:HG21	1:T:121:HIS:ND1	2.30	0.46
1:B:52:ILE:HG23	1:B:56:ASN:HD22	1.80	0.46
1:C:166:PHE:O	1:C:182:THR:HA	2.15	0.46
1:F:100:GLN:H	1:F:100:GLN:HE21	1.62	0.46
1:G:28:VAL:HG22	1:G:46:LEU:HD12	1.96	0.46
1:R:132:VAL:HG12	1:R:133:ASN:N	2.30	0.46
1:V:94:ILE:HG12	1:V:119:ILE:HD12	1.97	0.46
1:3:150:SER:HB2	1:3:167:SER:O	2.15	0.46
1:X:16:LEU:HD11	1:X:28:VAL:HG11	1.98	0.46
1:X:80:LEU:HB2	1:X:96:ARG:HG2	1.97	0.46
1:X:88:ILE:HG12	1:X:94:ILE:HD11	1.97	0.46
1:2:169:MET:HE2	1:3:156:HIS:CD2	2.50	0.46
1:4:98:THR:HB	1:4:100:GLN:NE2	2.31	0.46
1:C:142:HIS:HB2	1:C:160:ARG:HG2	1.97	0.46
1:G:58:ILE:HG12	1:G:88:ILE:HB	1.98	0.46
1:Q:63:SER:HB2	1:Q:93:THR:HG22	1.97	0.46
1:U:61:PHE:O	1:U:91:GLY:HA2	2.16	0.46
1:2:168:GLY:HA3	1:2:184:PHE:CD2	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:24:PRO:HG2	1:D:42:PRO:HB3	1.97	0.46
1:J:131:LEU:HG	1:J:149:LEU:HD12	1.98	0.46
1:M:236:ALA:HB1	1:M:243:ALA:HA	1.97	0.46
1:P:61:PHE:O	1:P:91:GLY:HA2	2.16	0.46
1:Y:16:LEU:HD11	1:Y:28:VAL:HG11	1.98	0.46
1:F:68:THR:HG21	1:F:121:HIS:ND1	2.31	0.46
1:K:181:VAL:HG22	1:K:193:MET:HE2	1.97	0.46
1:L:68:THR:HG21	1:L:121:HIS:ND1	2.30	0.46
1:W:28:VAL:HG22	1:W:46:LEU:HD12	1.98	0.46
1:I:193:MET:HE3	1:I:215:TYR:HD1	1.81	0.46
1:K:36:GLU:HB3	1:K:54:LYS:HG2	1.98	0.46
1:O:32:VAL:HG22	1:O:50:THR:HB	1.97	0.46
1:P:36:GLU:HB3	1:P:54:LYS:HG2	1.98	0.46
1:U:98:THR:HB	1:U:100:GLN:NE2	2.31	0.46
1:B:98:THR:HB	1:B:100:GLN:NE2	2.32	0.45
1:E:156:HIS:HB2	1:E:174:GLY:HA2	1.97	0.45
1:G:36:GLU:HB3	1:G:54:LYS:HG2	1.98	0.45
1:N:236:ALA:HB1	1:N:243:ALA:HA	1.98	0.45
1:Q:164:HIS:HE1	1:Q:201:ARG:HG3	1.80	0.45
1:T:65:GLY:O	1:T:96:ARG:HG3	2.16	0.45
1:X:17:ALA:HB3	1:X:36:GLU:N	2.31	0.45
1:4:201:ARG:HG2	1:4:201:ARG:NH1	2.32	0.45
1:K:132:VAL:HG12	1:K:133:ASN:N	2.31	0.45
1:M:132:VAL:HG23	1:M:149:LEU:O	2.17	0.45
1:O:65:GLY:O	1:O:96:ARG:HG3	2.16	0.45
1:P:100:GLN:NE2	1:P:100:GLN:H	2.14	0.45
1:Q:166:PHE:O	1:Q:182:THR:HA	2.17	0.45
1:R:188:ALA:HB3	1:W:257:THR:HG21	1.97	0.45
1:S:196:GLU:O	1:S:200:ARG:HG3	2.16	0.45
1:V:169:MET:HE2	1:W:156:HIS:CD2	2.51	0.45
1:K:64:VAL:HG22	1:K:94:ILE:HD12	1.99	0.45
1:L:193:MET:HE3	1:L:215:TYR:HD2	1.80	0.45
1:R:46:LEU:HA	1:R:64:VAL:O	2.17	0.45
1:I:60:GLN:HE21	1:Y:63:SER:HB3	1.81	0.45
1:3:238:GLN:HB3	1:L:205:SER:HB2	1.98	0.45
1:4:15:ARG:CZ	1:4:33:GLU:HB2	2.47	0.45
1:G:72:LYS:HD3	1:G:98:THR:HG21	1.97	0.45
1:L:19:ASP:HB2	1:L:37:GLY:HA2	1.97	0.45
1:M:166:PHE:O	1:M:182:THR:HA	2.16	0.45
1:N:169:MET:HE2	1:O:156:HIS:HD2	1.78	0.45
1:P:107:ILE:HG12	1:P:125:ILE:HD12	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:68:THR:HG21	1:U:121:HIS:ND1	2.31	0.45
1:U:235:SER:HB3	1:U:242:VAL:HG11	1.98	0.45
1:X:78:THR:HG22	1:X:103:ALA:HB1	1.98	0.45
1:3:89:ARG:HB3	1:3:90:GLU:OE1	2.16	0.45
1:J:27:ILE:HD13	1:J:45:VAL:HG22	1.98	0.45
1:X:7:ARG:HE	1:X:7:ARG:HB2	1.24	0.45
1:Y:171:SER:HA	1:Y:185:GLY:O	2.17	0.45
1:2:24:PRO:HD2	1:2:42:PRO:HB3	1.99	0.45
1:F:61:PHE:O	1:F:91:GLY:HA2	2.17	0.45
1:G:148:ILE:HB	1:G:166:PHE:HD1	1.82	0.45
1:N:180:TYR:HB2	1:N:193:MET:HE2	1.99	0.45
1:O:100:GLN:HE21	1:O:100:GLN:H	1.65	0.45
1:D:3:LEU:HB3	1:D:21:GLN:HG2	1.98	0.45
1:G:82:ILE:HG23	1:G:86:ASN:HD22	1.82	0.45
1:P:68:THR:HG22	1:P:69:PRO:CD	2.46	0.45
1:P:235:SER:HB3	1:P:242:VAL:HG11	1.98	0.45
1:Z:109:ASP:O	1:Z:127:ASN:HA	2.17	0.45
1:D:132:VAL:HG12	1:D:133:ASN:H	1.81	0.45
1:G:68:THR:HG21	1:G:121:HIS:ND1	2.32	0.45
1:M:94:ILE:HG12	1:M:119:ILE:HD12	1.99	0.45
1:X:98:THR:HB	1:X:100:GLN:HE21	1.80	0.45
1:3:236:ALA:CB	1:3:246:ARG:HH11	2.30	0.45
1:D:82:ILE:HG12	1:D:107:ILE:HD12	1.99	0.45
1:J:3:LEU:H	1:J:3:LEU:HG	1.63	0.45
1:N:164:HIS:CE1	1:N:201:ARG:HG3	2.52	0.45
1:Y:169:MET:HE2	1:Z:156:HIS:CD2	2.52	0.45
1:D:224:THR:HG23	1:D:227:GLU:OE1	2.17	0.45
1:E:160:ARG:HD2	1:S:254:ARG:NH1	2.31	0.45
1:J:88:ILE:HG23	1:J:92:VAL:HG11	1.98	0.45
1:J:180:TYR:HB2	1:J:193:MET:CE	2.47	0.45
1:V:73:TYR:HB2	1:V:98:THR:HG22	1.99	0.45
1:B:68:THR:HG21	1:B:121:HIS:ND1	2.32	0.44
1:L:73:TYR:HB2	1:L:98:THR:HG22	1.98	0.44
1:N:160:ARG:HD2	1:Q:254:ARG:HH11	1.81	0.44
1:R:236:ALA:HB1	1:R:246:ARG:NH1	2.32	0.44
1:X:139:GLY:O	1:X:157:GLN:HA	2.17	0.44
1:Y:101:ASP:HB2	1:Y:140:HIS:HD1	1.82	0.44
1:3:17:ALA:O	1:3:20:VAL:HG23	2.17	0.44
1:L:28:VAL:HG22	1:L:46:LEU:HD12	1.99	0.44
1:V:150:SER:HB3	2:W:301:VFN:O18	2.17	0.44
1:V:164:HIS:HE1	1:V:201:ARG:HG3	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:W:39:VAL:HB	1:W:57:ARG:HD2	1.99	0.44
1:X:164:HIS:HE1	1:X:201:ARG:HG3	1.82	0.44
1:C:139:GLY:O	1:C:157:GLN:HA	2.17	0.44
1:F:221:GLN:HB3	1:F:223:HIS:CE1	2.52	0.44
1:K:7:ARG:HD2	1:K:25:TRP:HE1	1.83	0.44
1:M:42:PRO:HD2	1:M:60:GLN:HB3	1.99	0.44
1:Q:132:VAL:HG12	1:Q:133:ASN:N	2.31	0.44
1:R:61:PHE:O	1:R:91:GLY:HA2	2.18	0.44
1:R:167:SER:HB2	1:R:173:ILE:HD11	1.98	0.44
1:S:153:THR:HG23	1:S:171:SER:HB2	2.00	0.44
1:2:60:GLN:HE21	1:3:63:SER:HB3	1.83	0.44
1:2:194:ASN:O	1:2:198:MET:HG3	2.18	0.44
1:J:99:VAL:HA	1:J:103:ALA:HB2	1.98	0.44
1:K:211:LEU:HD11	1:K:241:GLU:HB3	1.99	0.44
1:Q:98:THR:HB	1:Q:100:GLN:NE2	2.33	0.44
1:3:114:MET:HE3	1:4:69:PRO:HG2	1.99	0.44
1:3:139:GLY:O	1:3:157:GLN:HA	2.17	0.44
1:J:132:VAL:HG12	1:J:133:ASN:H	1.83	0.44
1:3:155:VAL:HG11	1:3:161:ILE:HD11	2.00	0.44
1:M:151:GLY:HA3	2:N:301:VFN:CL1	2.55	0.44
1:O:216:LYS:HA	1:O:220:ARG:HB2	2.00	0.44
1:R:149:LEU:HD22	1:R:153:THR:HG21	2.00	0.44
1:S:110:HIS:O	1:S:128:HIS:HA	2.17	0.44
1:T:8:ALA:HB2	1:T:23:GLY:O	2.17	0.44
1:4:196:GLU:O	1:4:200:ARG:HG3	2.17	0.44
1:B:142:HIS:HB2	1:B:160:ARG:HG2	2.00	0.44
1:D:200:ARG:C	1:D:202:GLY:H	2.26	0.44
1:F:91:GLY:HA3	1:F:116:TYR:CE1	2.52	0.44
1:G:132:VAL:CG1	1:G:133:ASN:H	2.29	0.44
1:L:99:VAL:HA	1:L:103:ALA:HB2	2.00	0.44
1:Q:79:ARG:O	1:Q:104:GLU:HA	2.18	0.44
1:W:21:GLN:HB2	1:W:39:VAL:HG13	1.99	0.44
1:Y:245:PHE:CZ	1:Y:249:ILE:HD11	2.53	0.44
1:J:24:PRO:HD2	1:J:42:PRO:HB3	2.00	0.44
1:R:80:LEU:HB2	1:R:96:ARG:HG2	1.99	0.44
1:W:59:TYR:HB2	1:W:89:ARG:C	2.43	0.44
1:2:240:PRO:O	1:2:244:VAL:HG23	2.18	0.43
1:3:71:LEU:HD22	2:3:301:VFN:N16	2.32	0.43
1:B:36:GLU:O	1:B:54:LYS:HA	2.18	0.43
1:K:183:VAL:HG12	1:K:190:ALA:HA	1.99	0.43
1:W:221:GLN:HB3	1:W:223:HIS:ND1	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Z:16:LEU:HD11	1:Z:28:VAL:HG11	2.00	0.43
1:C:156:HIS:O	1:C:159:CYS:HB2	2.18	0.43
1:F:91:GLY:HA3	1:F:116:TYR:CD1	2.53	0.43
1:H:38:THR:HG23	1:H:56:ASN:HB2	2.01	0.43
1:L:8:ALA:HB2	1:L:23:GLY:O	2.17	0.43
1:L:89:ARG:HB2	1:L:114:MET:HA	2.00	0.43
1:W:236:ALA:O	1:W:243:ALA:HB2	2.19	0.43
1:3:85:HIS:O	1:3:110:HIS:HA	2.17	0.43
1:G:166:PHE:O	1:G:182:THR:HA	2.18	0.43
1:H:80:LEU:HB2	1:H:96:ARG:HG2	1.99	0.43
1:J:98:THR:HB	1:J:100:GLN:HE21	1.83	0.43
1:N:89:ARG:HB2	1:N:114:MET:HA	2.00	0.43
1:P:69:PRO:HG2	1:R:114:MET:HE3	1.99	0.43
1:T:98:THR:HB	1:T:100:GLN:NE2	2.33	0.43
1:2:68:THR:HG21	1:2:121:HIS:ND1	2.34	0.43
1:3:137:LEU:HD22	1:3:141:VAL:HG11	2.00	0.43
1:4:157:GLN:HB3	1:4:158:TYR:CD2	2.52	0.43
1:A:73:TYR:HB2	1:A:98:THR:HG22	2.00	0.43
1:C:177:VAL:HG22	1:C:183:VAL:HG11	1.99	0.43
1:H:90:GLU:O	1:H:115:ALA:HA	2.18	0.43
1:S:180:TYR:HB3	1:S:198:MET:HE3	2.01	0.43
1:V:115:ALA:HB3	1:V:133:ASN:ND2	2.33	0.43
1:P:89:ARG:HD3	1:Q:69:PRO:HB3	2.00	0.43
1:U:194:ASN:O	1:U:198:MET:HG3	2.17	0.43
1:X:240:PRO:O	1:X:244:VAL:HG23	2.18	0.43
1:1:132:VAL:HG12	1:1:133:ASN:H	1.84	0.43
1:D:68:THR:HG21	1:D:121:HIS:ND1	2.34	0.43
1:D:85:HIS:O	1:D:110:HIS:HA	2.18	0.43
1:L:236:ALA:HB1	1:L:246:ARG:NH1	2.34	0.43
1:M:229:LEU:HD11	1:M:253:THR:HG21	2.00	0.43
1:O:99:VAL:HA	1:O:103:ALA:HB2	2.00	0.43
1:S:201:ARG:HG2	1:S:201:ARG:NH1	2.34	0.43
1:A:99:VAL:HA	1:A:103:ALA:HB2	1.99	0.43
1:B:17:ALA:HB3	1:B:20:VAL:HG23	2.00	0.43
1:K:150:SER:HB2	1:K:167:SER:O	2.18	0.43
1:M:149:LEU:HD11	1:M:161:ILE:HG21	2.01	0.43
1:R:254:ARG:NH1	1:W:160:ARG:HD2	2.34	0.43
1:W:140:HIS:O	1:W:158:TYR:HA	2.18	0.43
1:Y:59:TYR:HB2	1:Y:89:ARG:C	2.44	0.43
1:2:195:PHE:HZ	1:2:212:ARG:HG2	1.84	0.43
1:F:132:VAL:HG12	1:F:133:ASN:N	2.32	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:17:ALA:HB3	1:I:20:VAL:HG23	2.00	0.43
1:3:61:PHE:O	1:3:91:GLY:HA2	2.19	0.43
1:3:216:LYS:HA	1:3:220:ARG:HB2	2.00	0.43
1:4:229:LEU:HD23	1:4:246:ARG:HG3	2.01	0.43
1:T:47:LYS:HD2	1:T:66:GLU:HA	2.00	0.43
1:U:180:TYR:HB2	1:U:193:MET:CE	2.45	0.43
1:D:160:ARG:HD2	1:P:254:ARG:NH1	2.34	0.43
1:E:216:LYS:HE3	1:E:220:ARG:NH1	2.34	0.43
1:F:216:LYS:HE2	1:F:220:ARG:NH1	2.34	0.43
1:P:70:ASP:HA	2:P:302:VFN:N16	2.33	0.43
1:U:101:ASP:HB2	1:U:140:HIS:CE1	2.54	0.43
1:U:139:GLY:O	1:U:157:GLN:HA	2.18	0.43
1:Y:216:LYS:HA	1:Y:220:ARG:HB2	2.00	0.43
1:Z:240:PRO:O	1:Z:244:VAL:HG23	2.18	0.43
1:1:112:LEU:HD23	1:1:130:ILE:HG23	2.00	0.42
1:H:235:SER:HA	1:H:238:GLN:OE1	2.19	0.42
1:O:89:ARG:HB3	1:O:90:GLU:OE1	2.19	0.42
1:T:28:VAL:HG22	1:T:46:LEU:HD12	1.99	0.42
1:T:90:GLU:O	1:T:115:ALA:HA	2.19	0.42
1:T:114:MET:HG3	1:U:69:PRO:HG2	2.00	0.42
1:Y:17:ALA:HB3	1:Y:20:VAL:HG23	2.01	0.42
1:A:156:HIS:HB2	1:A:174:GLY:HA2	2.01	0.42
1:D:98:THR:HB	1:D:100:GLN:HE21	1.82	0.42
1:D:195:PHE:HZ	1:D:212:ARG:HG2	1.84	0.42
1:H:73:TYR:HB2	1:H:98:THR:HG22	2.00	0.42
1:H:169:MET:HE2	1:I:156:HIS:CD2	2.53	0.42
1:J:16:LEU:HD11	1:J:28:VAL:HG11	2.00	0.42
1:O:217:VAL:HG11	1:O:231:GLU:HB3	2.00	0.42
1:P:38:THR:HG23	1:P:56:ASN:HB2	2.01	0.42
1:Q:61:PHE:O	1:Q:91:GLY:HA2	2.19	0.42
1:R:193:MET:HE3	1:R:215:TYR:HD2	1.84	0.42
1:A:14:ALA:HB2	1:A:29:GLY:O	2.19	0.42
2:H:302:VFN:N16	1:I:71:LEU:HD22	2.34	0.42
1:I:211:LEU:HD11	1:I:241:GLU:HB3	2.01	0.42
1:J:22:VAL:HA	1:J:40:ILE:HB	1.99	0.42
1:M:195:PHE:HZ	1:M:212:ARG:HG2	1.84	0.42
1:S:150:SER:HB2	1:S:168:GLY:C	2.44	0.42
1:X:106:THR:HG23	1:X:124:VAL:HG22	2.01	0.42
1:Z:142:HIS:HB2	1:Z:160:ARG:HG2	2.02	0.42
1:1:64:VAL:HG22	1:1:94:ILE:HD12	2.02	0.42
1:1:169:MET:HE2	1:Y:156:HIS:CD2	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:3:302:VFN:N16	1:4:71:LEU:HD22	2.35	0.42
1:D:14:ALA:HB2	1:D:29:GLY:O	2.19	0.42
1:H:79:ARG:HB2	1:H:104:GLU:HG3	1.99	0.42
1:H:183:VAL:HB	1:H:188:ALA:HB1	2.01	0.42
1:I:15:ARG:O	1:I:33:GLU:HA	2.20	0.42
1:U:58:ILE:HG12	1:U:88:ILE:HB	2.01	0.42
1:2:42:PRO:O	1:2:60:GLN:HA	2.19	0.42
1:A:139:GLY:O	1:A:157:GLN:HA	2.18	0.42
1:A:152:TYR:HB2	1:B:154:LEU:HD11	2.02	0.42
1:P:99:VAL:HA	1:P:103:ALA:HB2	2.00	0.42
1:R:107:ILE:HD11	1:R:119:ILE:HG21	2.01	0.42
1:S:38:THR:HG23	1:S:56:ASN:HB2	2.02	0.42
1:T:114:MET:CG	1:U:69:PRO:HG2	2.49	0.42
1:X:168:GLY:HA3	1:X:184:PHE:CD1	2.54	0.42
1:3:235:SER:HA	1:3:238:GLN:OE1	2.19	0.42
1:B:78:THR:HG22	1:B:103:ALA:HB1	2.01	0.42
1:C:235:SER:OG	1:C:242:VAL:HG11	2.20	0.42
1:F:160:ARG:HB2	1:F:176:ASP:OD2	2.19	0.42
1:G:180:TYR:HB2	1:G:193:MET:SD	2.59	0.42
1:H:34:ILE:HG12	1:H:52:ILE:HD13	2.02	0.42
1:H:137:LEU:HD22	1:H:141:VAL:HG11	1.99	0.42
1:J:132:VAL:HG12	1:J:133:ASN:N	2.35	0.42
1:N:124:VAL:HB	1:N:142:HIS:ND1	2.33	0.42
1:P:68:THR:HG22	1:P:69:PRO:HD2	2.01	0.42
1:P:150:SER:HB2	1:P:167:SER:O	2.20	0.42
1:B:149:LEU:HA	1:B:167:SER:OG	2.20	0.42
1:C:237:ALA:HB2	1:J:195:PHE:HB3	2.01	0.42
1:I:98:THR:HB	1:I:100:GLN:NE2	2.35	0.42
1:K:216:LYS:HA	1:K:220:ARG:HB2	2.01	0.42
1:Y:90:GLU:O	1:Y:115:ALA:HA	2.20	0.42
1:J:58:ILE:HG12	1:J:88:ILE:HB	2.01	0.42
1:L:236:ALA:HB1	1:L:246:ARG:HH11	1.84	0.42
1:1:201:ARG:HG2	1:1:201:ARG:NH1	2.34	0.42
1:E:68:THR:HG21	1:E:121:HIS:HB3	2.02	0.42
1:Q:143:VAL:HG13	1:Q:161:ILE:HB	2.02	0.42
1:R:228:ALA:O	1:R:232:LEU:HG	2.20	0.42
1:S:114:MET:HG2	1:T:69:PRO:HG2	2.02	0.42
1:T:168:GLY:HA3	1:T:184:PHE:CD2	2.55	0.42
1:4:42:PRO:HD2	1:4:60:GLN:HB3	2.02	0.42
1:H:110:HIS:O	1:H:128:HIS:HA	2.20	0.42
1:N:107:ILE:HG23	1:N:111:ASN:HD22	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:78:THR:HG22	1:R:103:ALA:HB1	2.01	0.42
1:T:59:TYR:HB2	1:T:89:ARG:C	2.45	0.42
1:T:169:MET:HG2	1:U:156:HIS:CE1	2.54	0.42
1:X:98:THR:HB	1:X:100:GLN:NE2	2.35	0.42
1:Z:247:ASP:HA	1:Z:250:GLN:HB3	2.02	0.42
1:3:236:ALA:HB1	1:3:246:ARG:HH11	1.85	0.41
1:A:178:PRO:HB3	1:A:249:ILE:HG13	2.01	0.41
1:B:99:VAL:HA	1:B:103:ALA:HB2	2.02	0.41
1:O:19:ASP:CG	1:O:37:GLY:H	2.28	0.41
1:P:142:HIS:HB2	1:P:160:ARG:HG2	2.02	0.41
1:P:151:GLY:HA3	2:P:301:VFN:CL1	2.57	0.41
1:S:178:PRO:HB2	1:S:181:VAL:CG2	2.50	0.41
1:F:193:MET:SD	1:F:215:TYR:HB2	2.60	0.41
1:K:114:MET:HB2	1:K:132:VAL:HA	2.02	0.41
1:O:68:THR:HG21	1:O:121:HIS:ND1	2.34	0.41
1:S:68:THR:HB	1:S:70:ASP:H	1.84	0.41
1:4:7:ARG:HD2	1:4:25:TRP:NE1	2.35	0.41
1:C:112:LEU:HD23	1:C:130:ILE:HG23	2.02	0.41
1:I:145:ASP:O	1:I:163:ALA:HA	2.20	0.41
1:M:164:HIS:CE1	1:M:201:ARG:HG3	2.56	0.41
1:Q:196:GLU:O	1:Q:200:ARG:HG3	2.20	0.41
1:B:61:PHE:O	1:B:91:GLY:HA2	2.19	0.41
1:B:156:HIS:HB2	1:B:174:GLY:HA2	2.02	0.41
1:I:166:PHE:O	1:I:182:THR:HA	2.20	0.41
1:T:100:GLN:NE2	1:T:100:GLN:H	2.19	0.41
1:T:114:MET:HB2	1:T:132:VAL:HA	2.02	0.41
1:3:42:PRO:HD2	1:3:60:GLN:HB3	2.01	0.41
1:B:167:SER:HB3	1:B:173:ILE:HD11	2.02	0.41
1:D:16:LEU:HD11	1:D:28:VAL:HG11	2.03	0.41
1:D:223:HIS:HB3	1:D:227:GLU:HB2	2.03	0.41
1:E:150:SER:HB2	1:E:167:SER:O	2.20	0.41
1:F:4:ILE:HG23	1:F:22:VAL:HB	2.03	0.41
1:K:7:ARG:HD2	1:K:25:TRP:NE1	2.36	0.41
1:K:71:LEU:HD22	2:K:301:VFN:N16	2.34	0.41
1:V:90:GLU:O	1:V:115:ALA:HA	2.19	0.41
1:X:30:ALA:O	1:X:48:GLY:HA3	2.21	0.41
1:Z:145:ASP:HB3	1:Z:146:TRP:CD1	2.55	0.41
1:1:90:GLU:HG3	1:Y:93:THR:HG21	2.03	0.41
1:2:132:VAL:HG12	1:2:133:ASN:N	2.35	0.41
1:3:8:ALA:HB2	1:3:23:GLY:O	2.20	0.41
1:D:164:HIS:HE1	1:D:201:ARG:HG3	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:157:GLN:HB3	1:F:158:TYR:CD2	2.56	0.41
1:F:218:VAL:HG21	1:F:245:PHE:CE2	2.56	0.41
1:N:156:HIS:HB2	1:N:174:GLY:HA2	2.03	0.41
1:2:66:GLU:HB3	1:2:95:HIS:HD2	1.84	0.41
1:B:229:LEU:HD21	1:B:249:ILE:HG22	2.02	0.41
1:H:132:VAL:CG1	1:H:133:ASN:H	2.30	0.41
1:P:27:ILE:HD11	1:R:25:TRP:HZ3	1.85	0.41
1:R:183:VAL:HB	1:R:188:ALA:HB1	2.02	0.41
1:Y:164:HIS:CE1	1:Y:201:ARG:HG3	2.43	0.41
1:D:66:GLU:HB3	1:D:95:HIS:CD2	2.55	0.41
1:F:133:ASN:O	1:F:151:GLY:HA2	2.20	0.41
1:F:156:HIS:HD2	1:F:174:GLY:HA2	1.85	0.41
1:M:250:GLN:HA	1:M:253:THR:HG22	2.02	0.41
1:P:149:LEU:HD22	1:P:153:THR:HG21	2.03	0.41
1:Y:3:LEU:H	1:Y:3:LEU:HG	1.50	0.41
1:Y:36:GLU:HB2	1:Y:54:LYS:HG2	2.02	0.41
1:A:114:MET:HE3	1:B:69:PRO:HG2	2.02	0.41
1:G:110:HIS:O	1:G:128:HIS:HA	2.20	0.41
1:H:16:LEU:HD11	1:H:28:VAL:HG11	2.03	0.41
1:J:216:LYS:NZ	1:J:220:ARG:HH11	2.19	0.41
1:K:90:GLU:O	1:K:115:ALA:HA	2.21	0.41
1:M:160:ARG:HD2	1:Z:254:ARG:HH11	1.85	0.41
1:P:195:PHE:HD1	1:P:208:ILE:HG23	1.86	0.41
1:T:112:LEU:HD23	1:T:130:ILE:HG23	2.03	0.41
1:X:156:HIS:HB2	1:X:174:GLY:HA2	2.03	0.41
1:Y:67:ASP:HB3	1:Y:73:TYR:CE2	2.56	0.41
1:D:139:GLY:O	1:D:157:GLN:HA	2.21	0.41
1:G:47:LYS:HB3	1:G:65:GLY:O	2.21	0.41
1:M:254:ARG:NH1	1:Z:160:ARG:HD2	2.32	0.41
1:N:61:PHE:O	1:N:91:GLY:HA2	2.21	0.41
1:N:223:HIS:HD2	1:N:227:GLU:HB3	1.85	0.41
1:R:160:ARG:HB2	1:R:176:ASP:OD2	2.21	0.41
1:W:157:GLN:HB3	1:W:158:TYR:CD2	2.55	0.41
1:B:54:LYS:HB3	1:B:55:HIS:CD2	2.56	0.40
1:D:247:ASP:HA	1:D:250:GLN:HB3	2.03	0.40
1:A:59:TYR:HB2	1:A:89:ARG:C	2.46	0.40
1:B:81:VAL:HB	1:B:106:THR:HG22	2.03	0.40
1:C:160:ARG:HD2	1:K:254:ARG:HH11	1.86	0.40
1:D:89:ARG:O	1:D:92:VAL:HG23	2.21	0.40
1:E:89:ARG:O	1:E:92:VAL:HG23	2.21	0.40
1:G:236:ALA:HB1	1:G:246:ARG:HH11	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:64:VAL:HG13	1:I:94:ILE:HB	2.02	0.40
1:L:166:PHE:O	1:L:182:THR:HA	2.21	0.40
1:N:90:GLU:O	1:N:115:ALA:HA	2.20	0.40
1:P:52:ILE:HG23	1:P:56:ASN:HD22	1.86	0.40
1:R:68:THR:HG21	1:R:121:HIS:HB3	2.03	0.40
1:T:56:ASN:OD1	1:T:86:ASN:HB2	2.22	0.40
1:Z:125:ILE:HG12	1:Z:143:VAL:HB	2.03	0.40
1:G:142:HIS:HB2	1:G:160:ARG:HG2	2.03	0.40
1:O:36:GLU:HB3	1:O:54:LYS:HG2	2.02	0.40
1:V:178:PRO:HG2	1:V:219:TYR:OH	2.22	0.40
1:X:164:HIS:CE1	1:X:201:ARG:HG3	2.56	0.40
1:Y:131:LEU:HD21	1:Y:137:LEU:HD11	2.03	0.40
1:B:249:ILE:O	1:B:253:THR:HG22	2.21	0.40
1:D:219:TYR:HE1	1:P:258:ARG:HB3	1.86	0.40
1:L:78:THR:HG22	1:L:103:ALA:HB1	2.03	0.40
1:O:246:ARG:HH21	1:O:250:GLN:HE21	1.68	0.40
1:P:139:GLY:O	1:P:157:GLN:HA	2.21	0.40
1:P:166:PHE:O	1:P:182:THR:HA	2.20	0.40
1:T:100:GLN:HE21	1:T:100:GLN:H	1.68	0.40
1:U:59:TYR:HB2	1:U:89:ARG:C	2.47	0.40
1:W:68:THR:HG21	1:W:121:HIS:HB3	2.03	0.40
1:Z:132:VAL:HG12	1:Z:133:ASN:N	2.37	0.40
1:I:216:LYS:HA	1:I:220:ARG:HB2	2.04	0.40
1:A:36:GLU:HB3	1:A:54:LYS:HG2	2.03	0.40
1:A:91:GLY:O	1:A:116:TYR:HA	2.22	0.40
1:E:98:THR:HB	1:E:100:GLN:HE21	1.86	0.40
1:H:166:PHE:O	1:H:182:THR:HA	2.21	0.40
1:I:132:VAL:HG12	1:I:133:ASN:H	1.87	0.40
1:P:8:ALA:HB2	1:P:23:GLY:O	2.21	0.40
1:Q:80:LEU:HB2	1:Q:96:ARG:HG2	2.04	0.40
1:T:169:MET:HE2	1:U:156:HIS:CD2	2.56	0.40
1:X:59:TYR:HB2	1:X:89:ARG:C	2.46	0.40

There are no symmetry-related clashes.

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	1	256/261 (98%)	225 (88%)	28 (11%)	3 (1%)	10	34
1	2	256/261 (98%)	224 (88%)	28 (11%)	4 (2%)	7	27
1	3	256/261 (98%)	220 (86%)	31 (12%)	5 (2%)	6	22
1	4	256/261 (98%)	218 (85%)	32 (12%)	6 (2%)	5	19
1	A	256/261 (98%)	229 (90%)	22 (9%)	5 (2%)	6	22
1	B	256/261 (98%)	222 (87%)	29 (11%)	5 (2%)	6	22
1	C	256/261 (98%)	224 (88%)	28 (11%)	4 (2%)	7	27
1	D	256/261 (98%)	221 (86%)	33 (13%)	2 (1%)	16	44
1	E	256/261 (98%)	223 (87%)	29 (11%)	4 (2%)	7	27
1	F	256/261 (98%)	230 (90%)	24 (9%)	2 (1%)	16	44
1	G	256/261 (98%)	225 (88%)	27 (10%)	4 (2%)	7	27
1	H	256/261 (98%)	227 (89%)	22 (9%)	7 (3%)	4	16
1	I	256/261 (98%)	226 (88%)	25 (10%)	5 (2%)	6	22
1	J	256/261 (98%)	219 (86%)	35 (14%)	2 (1%)	16	44
1	K	256/261 (98%)	218 (85%)	34 (13%)	4 (2%)	7	27
1	L	256/261 (98%)	229 (90%)	26 (10%)	1 (0%)	30	59
1	M	256/261 (98%)	225 (88%)	26 (10%)	5 (2%)	6	22
1	N	256/261 (98%)	228 (89%)	26 (10%)	2 (1%)	16	44
1	O	256/261 (98%)	223 (87%)	30 (12%)	3 (1%)	10	34
1	P	256/261 (98%)	223 (87%)	26 (10%)	7 (3%)	4	16
1	Q	256/261 (98%)	218 (85%)	31 (12%)	7 (3%)	4	16
1	R	256/261 (98%)	223 (87%)	28 (11%)	5 (2%)	6	22
1	S	256/261 (98%)	231 (90%)	20 (8%)	5 (2%)	6	22
1	T	256/261 (98%)	223 (87%)	31 (12%)	2 (1%)	16	44
1	U	256/261 (98%)	219 (86%)	31 (12%)	6 (2%)	5	19
1	V	256/261 (98%)	225 (88%)	26 (10%)	5 (2%)	6	22
1	W	256/261 (98%)	224 (88%)	28 (11%)	4 (2%)	7	27
1	X	256/261 (98%)	226 (88%)	27 (10%)	3 (1%)	10	34
1	Y	256/261 (98%)	228 (89%)	26 (10%)	2 (1%)	16	44

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	Z	256/261 (98%)	223 (87%)	29 (11%)	4 (2%)	7	27
All	All	7680/7830 (98%)	6719 (88%)	838 (11%)	123 (2%)	7	27

All (123) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	2	18	ALA
1	3	18	ALA
1	3	220	ARG
1	C	220	ARG
1	D	18	ALA
1	H	3	LEU
1	I	121	HIS
1	M	3	LEU
1	M	18	ALA
1	N	18	ALA
1	P	3	LEU
1	Q	3	LEU
1	Q	138	ALA
1	Q	220	ARG
1	U	220	ARG
1	V	18	ALA
1	V	85	HIS
1	X	18	ALA
1	Y	116	TYR
1	2	71	LEU
1	2	220	ARG
1	3	38	THR
1	4	18	ALA
1	A	220	ARG
1	B	116	TYR
1	C	116	TYR
1	C	121	HIS
1	E	3	LEU
1	F	220	ARG
1	H	116	TYR
1	M	75	GLY
1	M	220	ARG
1	O	133	ASN
1	P	55	HIS
1	P	220	ARG
1	Q	116	TYR

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Mol	Chain	Res	Type
1	R	220	ARG
1	S	121	HIS
1	S	220	ARG
1	T	121	HIS
1	U	133	ASN
1	W	133	ASN
1	X	252	ALA
1	Y	220	ARG
1	1	17	ALA
1	1	116	TYR
1	4	115	ALA
1	B	220	ARG
1	E	116	TYR
1	E	220	ARG
1	H	19	ASP
1	H	101	ASP
1	H	134	ASN
1	I	192	SER
1	J	116	TYR
1	N	254	ARG
1	O	101	ASP
1	P	121	HIS
1	R	116	TYR
1	U	75	GLY
1	U	110	HIS
1	U	116	TYR
1	V	121	HIS
1	V	233	ALA
1	W	18	ALA
1	W	116	TYR
1	X	134	ASN
1	1	134	ASN
1	3	116	TYR
1	3	121	HIS
1	4	192	SER
1	A	116	TYR
1	B	97	GLY
1	E	133	ASN
1	G	220	ARG
1	H	115	ALA
1	J	145	ASP
1	K	61	PHE

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Mol	Chain	Res	Type
1	K	101	ASP
1	K	116	TYR
1	L	116	TYR
1	M	116	TYR
1	O	121	HIS
1	P	219	TYR
1	Q	192	SER
1	R	192	SER
1	S	133	ASN
1	S	233	ALA
1	W	121	HIS
1	Z	101	ASP
1	Z	138	ALA
1	Z	192	SER
1	A	219	TYR
1	B	37	GLY
1	B	192	SER
1	D	116	TYR
1	F	2	SER
1	G	101	ASP
1	H	89	ARG
1	K	192	SER
1	P	202	GLY
1	R	110	HIS
1	T	116	TYR
1	U	192	SER
1	A	75	GLY
1	A	192	SER
1	C	115	ALA
1	G	192	SER
1	I	219	TYR
1	P	115	ALA
1	R	55	HIS
1	S	75	GLY
1	I	97	GLY
1	Z	126	GLY
1	4	108	GLY
1	G	132	VAL
1	I	218	VAL
1	Q	75	GLY
1	V	53	GLY
1	2	97	GLY

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Mol	Chain	Res	Type
1	Q	76	GLU
1	4	76	GLU
1	4	97	GLY

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	1	206/208 (99%)	185 (90%)	21 (10%)	7	23
1	2	206/208 (99%)	191 (93%)	15 (7%)	13	38
1	3	206/208 (99%)	190 (92%)	16 (8%)	11	35
1	4	206/208 (99%)	194 (94%)	12 (6%)	18	49
1	A	206/208 (99%)	188 (91%)	18 (9%)	9	30
1	B	206/208 (99%)	185 (90%)	21 (10%)	7	23
1	C	206/208 (99%)	187 (91%)	19 (9%)	8	27
1	D	206/208 (99%)	186 (90%)	20 (10%)	8	25
1	E	206/208 (99%)	190 (92%)	16 (8%)	11	35
1	F	206/208 (99%)	191 (93%)	15 (7%)	13	38
1	G	206/208 (99%)	182 (88%)	24 (12%)	5	17
1	H	206/208 (99%)	186 (90%)	20 (10%)	8	25
1	I	206/208 (99%)	184 (89%)	22 (11%)	6	22
1	J	206/208 (99%)	183 (89%)	23 (11%)	6	19
1	K	206/208 (99%)	189 (92%)	17 (8%)	10	32
1	L	206/208 (99%)	184 (89%)	22 (11%)	6	22
1	M	206/208 (99%)	191 (93%)	15 (7%)	13	38
1	N	206/208 (99%)	181 (88%)	25 (12%)	5	16
1	O	206/208 (99%)	185 (90%)	21 (10%)	7	23
1	P	206/208 (99%)	182 (88%)	24 (12%)	5	17
1	Q	206/208 (99%)	183 (89%)	23 (11%)	6	19

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	R	206/208 (99%)	186 (90%)	20 (10%)	8	25
1	S	206/208 (99%)	187 (91%)	19 (9%)	8	27
1	T	206/208 (99%)	179 (87%)	27 (13%)	4	13
1	U	206/208 (99%)	180 (87%)	26 (13%)	4	14
1	V	206/208 (99%)	180 (87%)	26 (13%)	4	14
1	W	206/208 (99%)	181 (88%)	25 (12%)	5	16
1	X	206/208 (99%)	182 (88%)	24 (12%)	5	17
1	Y	206/208 (99%)	189 (92%)	17 (8%)	10	32
1	Z	206/208 (99%)	187 (91%)	19 (9%)	8	27
All	All	6180/6240 (99%)	5568 (90%)	612 (10%)	7	24

All (612) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	1	1	MET
1	1	3	LEU
1	1	15	ARG
1	1	19	ASP
1	1	68	THR
1	1	70	ASP
1	1	74	LYS
1	1	88	ILE
1	1	99	VAL
1	1	100	GLN
1	1	150	SER
1	1	153	THR
1	1	155	VAL
1	1	156	HIS
1	1	157	GLN
1	1	175	LYS
1	1	193	MET
1	1	253	THR
1	1	254	ARG
1	1	256	ILE
1	1	258	ARG
1	2	3	LEU
1	2	15	ARG
1	2	36	GLU
1	2	63	SER

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Mol	Chain	Res	Type
1	2	68	THR
1	2	90	GLU
1	2	99	VAL
1	2	100	GLN
1	2	106	THR
1	2	175	LYS
1	2	212	ARG
1	2	216	LYS
1	2	220	ARG
1	2	248	SER
1	2	253	THR
1	3	1	MET
1	3	36	GLU
1	3	51	LYS
1	3	67	ASP
1	3	68	THR
1	3	71	LEU
1	3	88	ILE
1	3	102	ARG
1	3	109	ASP
1	3	193	MET
1	3	212	ARG
1	3	220	ARG
1	3	226	GLU
1	3	234	GLU
1	3	250	GLN
1	3	256	ILE
1	4	2	SER
1	4	33	GLU
1	4	68	THR
1	4	70	ASP
1	4	71	LEU
1	4	100	GLN
1	4	189	GLU
1	4	193	MET
1	4	196	GLU
1	4	212	ARG
1	4	250	GLN
1	4	256	ILE
1	A	1	MET
1	A	51	LYS
1	A	57	ARG

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Mol	Chain	Res	Type
1	A	63	SER
1	A	67	ASP
1	A	68	THR
1	A	70	ASP
1	A	76	GLU
1	A	90	GLU
1	A	102	ARG
1	A	131	LEU
1	A	132	VAL
1	A	150	SER
1	A	192	SER
1	A	193	MET
1	A	196	GLU
1	A	205	SER
1	A	246	ARG
1	B	1	MET
1	B	11	ASP
1	B	38	THR
1	B	51	LYS
1	B	62	SER
1	B	68	THR
1	B	76	GLU
1	B	88	ILE
1	B	90	GLU
1	B	99	VAL
1	B	100	GLN
1	B	102	ARG
1	B	114	MET
1	B	153	THR
1	B	167	SER
1	B	171	SER
1	B	193	MET
1	B	212	ARG
1	B	221	GLN
1	B	250	GLN
1	B	257	THR
1	C	13	SER
1	C	21	GLN
1	C	68	THR
1	C	76	GLU
1	C	90	GLU
1	C	93	THR

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Mol	Chain	Res	Type
1	C	100	GLN
1	C	109	ASP
1	C	153	THR
1	C	196	GLU
1	C	204	SER
1	C	212	ARG
1	C	220	ARG
1	C	221	GLN
1	C	250	GLN
1	C	253	THR
1	C	256	ILE
1	C	257	THR
1	C	258	ARG
1	D	7	ARG
1	D	15	ARG
1	D	26	SER
1	D	36	GLU
1	D	68	THR
1	D	71	LEU
1	D	76	GLU
1	D	99	VAL
1	D	106	THR
1	D	114	MET
1	D	150	SER
1	D	171	SER
1	D	192	SER
1	D	193	MET
1	D	218	VAL
1	D	220	ARG
1	D	221	GLN
1	D	254	ARG
1	D	256	ILE
1	D	257	THR
1	E	1	MET
1	E	21	GLN
1	E	67	ASP
1	E	72	LYS
1	E	81	VAL
1	E	90	GLU
1	E	102	ARG
1	E	106	THR
1	E	109	ASP

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Mol	Chain	Res	Type
1	E	114	MET
1	E	135	THR
1	E	157	GLN
1	E	204	SER
1	E	205	SER
1	E	221	GLN
1	E	256	ILE
1	F	15	ARG
1	F	67	ASP
1	F	68	THR
1	F	70	ASP
1	F	71	LEU
1	F	90	GLU
1	F	99	VAL
1	F	100	GLN
1	F	193	MET
1	F	220	ARG
1	F	221	GLN
1	F	225	VAL
1	F	226	GLU
1	F	256	ILE
1	F	257	THR
1	G	1	MET
1	G	15	ARG
1	G	16	LEU
1	G	21	GLN
1	G	68	THR
1	G	71	LEU
1	G	72	LYS
1	G	79	ARG
1	G	90	GLU
1	G	99	VAL
1	G	100	GLN
1	G	113	ILE
1	G	114	MET
1	G	143	VAL
1	G	201	ARG
1	G	204	SER
1	G	205	SER
1	G	213	ARG
1	G	220	ARG
1	G	221	GLN

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Mol	Chain	Res	Type
1	G	238	GLN
1	G	253	THR
1	G	257	THR
1	G	258	ARG
1	H	1	MET
1	H	19	ASP
1	H	21	GLN
1	H	68	THR
1	H	70	ASP
1	H	71	LEU
1	H	90	GLU
1	H	93	THR
1	H	99	VAL
1	H	131	LEU
1	H	133	ASN
1	H	171	SER
1	H	173	ILE
1	H	193	MET
1	H	205	SER
1	H	212	ARG
1	H	220	ARG
1	H	221	GLN
1	H	253	THR
1	H	256	ILE
1	I	1	MET
1	I	15	ARG
1	I	31	GLU
1	I	33	GLU
1	I	68	THR
1	I	71	LEU
1	I	74	LYS
1	I	99	VAL
1	I	100	GLN
1	I	154	LEU
1	I	171	SER
1	I	191	ARG
1	I	193	MET
1	I	196	GLU
1	I	199	ARG
1	I	200	ARG
1	I	212	ARG
1	I	213	ARG

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Mol	Chain	Res	Type
1	I	217	VAL
1	I	220	ARG
1	I	226	GLU
1	I	257	THR
1	J	1	MET
1	J	3	LEU
1	J	15	ARG
1	J	21	GLN
1	J	39	VAL
1	J	67	ASP
1	J	68	THR
1	J	72	LYS
1	J	74	LYS
1	J	90	GLU
1	J	99	VAL
1	J	100	GLN
1	J	102	ARG
1	J	112	LEU
1	J	125	ILE
1	J	135	THR
1	J	189	GLU
1	J	192	SER
1	J	196	GLU
1	J	204	SER
1	J	221	GLN
1	J	235	SER
1	J	256	ILE
1	K	1	MET
1	K	7	ARG
1	K	51	LYS
1	K	67	ASP
1	K	71	LEU
1	K	90	GLU
1	K	99	VAL
1	K	102	ARG
1	K	114	MET
1	K	153	THR
1	K	169	MET
1	K	193	MET
1	K	204	SER
1	K	216	LYS
1	K	221	GLN

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Mol	Chain	Res	Type
1	K	246	ARG
1	K	256	ILE
1	L	1	MET
1	L	13	SER
1	L	19	ASP
1	L	68	THR
1	L	70	ASP
1	L	74	LYS
1	L	99	VAL
1	L	100	GLN
1	L	114	MET
1	L	143	VAL
1	L	153	THR
1	L	157	GLN
1	L	191	ARG
1	L	193	MET
1	L	196	GLU
1	L	212	ARG
1	L	217	VAL
1	L	220	ARG
1	L	221	GLN
1	L	227	GLU
1	L	235	SER
1	L	256	ILE
1	M	15	ARG
1	M	63	SER
1	M	68	THR
1	M	71	LEU
1	M	79	ARG
1	M	99	VAL
1	M	102	ARG
1	M	106	THR
1	M	125	ILE
1	M	192	SER
1	M	193	MET
1	M	200	ARG
1	M	216	LYS
1	M	221	GLN
1	M	257	THR
1	N	1	MET
1	N	3	LEU
1	N	11	ASP

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Mol	Chain	Res	Type
1	N	13	SER
1	N	15	ARG
1	N	21	GLN
1	N	67	ASP
1	N	68	THR
1	N	70	ASP
1	N	81	VAL
1	N	90	GLU
1	N	99	VAL
1	N	109	ASP
1	N	132	VAL
1	N	153	THR
1	N	157	GLN
1	N	175	LYS
1	N	193	MET
1	N	212	ARG
1	N	220	ARG
1	N	221	GLN
1	N	226	GLU
1	N	249	ILE
1	N	250	GLN
1	N	257	THR
1	O	15	ARG
1	O	21	GLN
1	O	51	LYS
1	O	67	ASP
1	O	68	THR
1	O	71	LEU
1	O	72	LYS
1	O	76	GLU
1	O	100	GLN
1	O	106	THR
1	O	114	MET
1	O	157	GLN
1	O	193	MET
1	O	205	SER
1	O	212	ARG
1	O	216	LYS
1	O	220	ARG
1	O	221	GLN
1	O	225	VAL
1	O	256	ILE

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Mol	Chain	Res	Type
1	O	257	THR
1	P	1	MET
1	P	5	ASP
1	P	15	ARG
1	P	67	ASP
1	P	68	THR
1	P	71	LEU
1	P	72	LYS
1	P	76	GLU
1	P	84	ASP
1	P	90	GLU
1	P	99	VAL
1	P	112	LEU
1	P	153	THR
1	P	181	VAL
1	P	193	MET
1	P	196	GLU
1	P	216	LYS
1	P	220	ARG
1	P	221	GLN
1	P	226	GLU
1	P	227	GLU
1	P	235	SER
1	P	256	ILE
1	P	257	THR
1	Q	1	MET
1	Q	3	LEU
1	Q	4	ILE
1	Q	15	ARG
1	Q	31	GLU
1	Q	63	SER
1	Q	67	ASP
1	Q	68	THR
1	Q	71	LEU
1	Q	72	LYS
1	Q	74	LYS
1	Q	88	ILE
1	Q	99	VAL
1	Q	106	THR
1	Q	114	MET
1	Q	193	MET
1	Q	212	ARG

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Mol	Chain	Res	Type
1	Q	216	LYS
1	Q	220	ARG
1	Q	226	GLU
1	Q	249	ILE
1	Q	257	THR
1	Q	258	ARG
1	R	1	MET
1	R	4	ILE
1	R	11	ASP
1	R	13	SER
1	R	15	ARG
1	R	21	GLN
1	R	51	LYS
1	R	68	THR
1	R	71	LEU
1	R	82	ILE
1	R	100	GLN
1	R	127	ASN
1	R	131	LEU
1	R	155	VAL
1	R	192	SER
1	R	193	MET
1	R	205	SER
1	R	212	ARG
1	R	216	LYS
1	R	221	GLN
1	S	21	GLN
1	S	54	LYS
1	S	68	THR
1	S	71	LEU
1	S	72	LYS
1	S	74	LYS
1	S	81	VAL
1	S	90	GLU
1	S	99	VAL
1	S	100	GLN
1	S	106	THR
1	S	125	ILE
1	S	175	LYS
1	S	193	MET
1	S	220	ARG
1	S	221	GLN

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Mol	Chain	Res	Type
1	S	246	ARG
1	S	249	ILE
1	S	257	THR
1	T	1	MET
1	T	7	ARG
1	T	47	LYS
1	T	66	GLU
1	T	67	ASP
1	T	68	THR
1	T	71	LEU
1	T	76	GLU
1	T	88	ILE
1	T	100	GLN
1	T	102	ARG
1	T	106	THR
1	T	112	LEU
1	T	114	MET
1	T	123	SER
1	T	153	THR
1	T	157	GLN
1	T	193	MET
1	T	212	ARG
1	T	213	ARG
1	T	216	LYS
1	T	221	GLN
1	T	227	GLU
1	T	254	ARG
1	T	256	ILE
1	T	257	THR
1	T	258	ARG
1	U	1	MET
1	U	3	LEU
1	U	15	ARG
1	U	19	ASP
1	U	21	GLN
1	U	26	SER
1	U	47	LYS
1	U	54	LYS
1	U	63	SER
1	U	67	ASP
1	U	68	THR
1	U	71	LEU

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Mol	Chain	Res	Type
1	U	79	ARG
1	U	88	ILE
1	U	90	GLU
1	U	99	VAL
1	U	102	ARG
1	U	106	THR
1	U	196	GLU
1	U	199	ARG
1	U	212	ARG
1	U	221	GLN
1	U	224	THR
1	U	225	VAL
1	U	257	THR
1	U	258	ARG
1	V	1	MET
1	V	3	LEU
1	V	4	ILE
1	V	10	ILE
1	V	13	SER
1	V	45	VAL
1	V	54	LYS
1	V	67	ASP
1	V	68	THR
1	V	74	LYS
1	V	81	VAL
1	V	90	GLU
1	V	99	VAL
1	V	100	GLN
1	V	102	ARG
1	V	114	MET
1	V	135	THR
1	V	167	SER
1	V	192	SER
1	V	193	MET
1	V	205	SER
1	V	220	ARG
1	V	226	GLU
1	V	253	THR
1	V	256	ILE
1	V	258	ARG
1	W	1	MET
1	W	3	LEU

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Mol	Chain	Res	Type
1	W	15	ARG
1	W	19	ASP
1	W	21	GLN
1	W	39	VAL
1	W	54	LYS
1	W	68	THR
1	W	70	ASP
1	W	71	LEU
1	W	100	GLN
1	W	114	MET
1	W	191	ARG
1	W	193	MET
1	W	204	SER
1	W	205	SER
1	W	212	ARG
1	W	216	LYS
1	W	217	VAL
1	W	220	ARG
1	W	221	GLN
1	W	250	GLN
1	W	253	THR
1	W	256	ILE
1	W	257	THR
1	X	3	LEU
1	X	7	ARG
1	X	11	ASP
1	X	15	ARG
1	X	36	GLU
1	X	68	THR
1	X	71	LEU
1	X	76	GLU
1	X	82	ILE
1	X	88	ILE
1	X	99	VAL
1	X	100	GLN
1	X	106	THR
1	X	175	LYS
1	X	176	ASP
1	X	193	MET
1	X	199	ARG
1	X	204	SER
1	X	205	SER

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Mol	Chain	Res	Type
1	X	220	ARG
1	X	221	GLN
1	X	246	ARG
1	X	254	ARG
1	X	257	THR
1	Y	3	LEU
1	Y	9	ILE
1	Y	15	ARG
1	Y	51	LYS
1	Y	67	ASP
1	Y	68	THR
1	Y	72	LYS
1	Y	76	GLU
1	Y	100	GLN
1	Y	140	HIS
1	Y	153	THR
1	Y	175	LYS
1	Y	205	SER
1	Y	212	ARG
1	Y	216	LYS
1	Y	220	ARG
1	Y	221	GLN
1	Z	21	GLN
1	Z	70	ASP
1	Z	81	VAL
1	Z	90	GLU
1	Z	100	GLN
1	Z	106	THR
1	Z	109	ASP
1	Z	114	MET
1	Z	175	LYS
1	Z	189	GLU
1	Z	193	MET
1	Z	199	ARG
1	Z	205	SER
1	Z	212	ARG
1	Z	221	GLN
1	Z	234	GLU
1	Z	250	GLN
1	Z	253	THR
1	Z	258	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (188)

such sidechains are listed below:

Mol	Chain	Res	Type
1	1	55	HIS
1	1	95	HIS
1	1	100	GLN
1	1	110	HIS
1	1	118	HIS
1	1	157	GLN
1	1	164	HIS
1	1	250	GLN
1	2	95	HIS
1	2	100	GLN
1	2	110	HIS
1	2	128	HIS
1	2	134	ASN
1	2	142	HIS
1	2	157	GLN
1	2	164	HIS
1	2	221	GLN
1	2	223	HIS
1	2	250	GLN
1	3	95	HIS
1	3	100	GLN
1	3	110	HIS
1	3	118	HIS
1	3	128	HIS
1	3	134	ASN
1	3	142	HIS
1	3	164	HIS
1	3	186	ASN
1	3	221	GLN
1	3	223	HIS
1	4	85	HIS
1	4	95	HIS
1	4	100	GLN
1	4	110	HIS
1	4	118	HIS
1	4	128	HIS
1	4	156	HIS
1	4	164	HIS
1	4	209	HIS
1	4	223	HIS
1	A	134	ASN
1	A	142	HIS

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Mol	Chain	Res	Type
1	A	156	HIS
1	A	164	HIS
1	B	55	HIS
1	B	95	HIS
1	B	100	GLN
1	B	142	HIS
1	B	156	HIS
1	B	164	HIS
1	B	250	GLN
1	C	85	HIS
1	C	100	GLN
1	C	134	ASN
1	C	194	ASN
1	D	55	HIS
1	D	95	HIS
1	D	118	HIS
1	D	128	HIS
1	D	186	ASN
1	D	194	ASN
1	E	95	HIS
1	E	100	GLN
1	E	118	HIS
1	E	128	HIS
1	E	133	ASN
1	E	134	ASN
1	E	164	HIS
1	E	221	GLN
1	E	223	HIS
1	F	100	GLN
1	F	156	HIS
1	F	157	GLN
1	F	164	HIS
1	F	223	HIS
1	F	250	GLN
1	G	100	GLN
1	G	140	HIS
1	G	164	HIS
1	G	250	GLN
1	H	60	GLN
1	H	100	GLN
1	H	110	HIS
1	H	118	HIS

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Mol	Chain	Res	Type
1	H	134	ASN
1	H	164	HIS
1	H	221	GLN
1	H	223	HIS
1	I	100	GLN
1	I	110	HIS
1	J	56	ASN
1	J	85	HIS
1	J	100	GLN
1	J	118	HIS
1	J	164	HIS
1	J	238	GLN
1	K	55	HIS
1	K	100	GLN
1	K	110	HIS
1	K	118	HIS
1	K	128	HIS
1	K	164	HIS
1	K	250	GLN
1	L	85	HIS
1	L	95	HIS
1	L	100	GLN
1	L	110	HIS
1	L	157	GLN
1	L	186	ASN
1	M	95	HIS
1	M	100	GLN
1	M	118	HIS
1	M	156	HIS
1	N	128	HIS
1	N	134	ASN
1	N	157	GLN
1	N	164	HIS
1	N	223	HIS
1	O	55	HIS
1	O	100	GLN
1	O	157	GLN
1	O	164	HIS
1	O	194	ASN
1	O	250	GLN
1	P	100	GLN
1	P	110	HIS

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Mol	Chain	Res	Type
1	P	118	HIS
1	P	157	GLN
1	P	164	HIS
1	P	194	ASN
1	P	250	GLN
1	Q	100	GLN
1	Q	110	HIS
1	Q	142	HIS
1	Q	157	GLN
1	Q	164	HIS
1	R	100	GLN
1	R	110	HIS
1	R	118	HIS
1	R	128	HIS
1	R	133	ASN
1	R	156	HIS
1	R	186	ASN
1	R	223	HIS
1	S	21	GLN
1	S	100	GLN
1	S	156	HIS
1	S	164	HIS
1	S	250	GLN
1	T	100	GLN
1	T	118	HIS
1	T	128	HIS
1	T	157	GLN
1	T	164	HIS
1	U	21	GLN
1	U	110	HIS
1	U	186	ASN
1	V	100	GLN
1	V	110	HIS
1	V	133	ASN
1	V	142	HIS
1	V	164	HIS
1	V	221	GLN
1	V	223	HIS
1	W	100	GLN
1	W	118	HIS
1	W	156	HIS
1	W	157	GLN

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Mol	Chain	Res	Type
1	W	164	HIS
1	W	209	HIS
1	W	223	HIS
1	X	100	GLN
1	X	128	HIS
1	X	164	HIS
1	X	186	ASN
1	X	209	HIS
1	X	250	GLN
1	Y	118	HIS
1	Y	128	HIS
1	Y	133	ASN
1	Y	164	HIS
1	Z	55	HIS
1	Z	100	GLN
1	Z	110	HIS
1	Z	127	ASN
1	Z	128	HIS
1	Z	164	HIS
1	Z	238	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

61 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond

length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
3	SO4	R	302	-	4,4,4	0.31	0	6,6,6	0.29	0
2	VFN	W	302	-	30,30,30	1.06	2 (6%)	34,40,40	1.99	8 (23%)
3	SO4	K	302	-	4,4,4	0.26	0	6,6,6	0.09	0
2	VFN	V	301	-	30,30,30	1.06	3 (10%)	34,40,40	1.18	1 (2%)
2	VFN	3	302	-	30,30,30	1.09	3 (10%)	34,40,40	1.19	3 (8%)
2	VFN	P	302	-	30,30,30	1.01	2 (6%)	34,40,40	1.27	3 (8%)
2	VFN	H	302	-	30,30,30	1.04	3 (10%)	34,40,40	1.32	3 (8%)
3	SO4	1	303	-	4,4,4	0.25	0	6,6,6	0.11	0
3	SO4	L	302	-	4,4,4	0.18	0	6,6,6	0.20	0
3	SO4	C	302	-	4,4,4	0.33	0	6,6,6	0.19	0
3	SO4	N	302	-	4,4,4	0.30	0	6,6,6	0.26	0
3	SO4	I	301	-	4,4,4	0.29	0	6,6,6	0.15	0
2	VFN	A	301	-	30,30,30	0.99	1 (3%)	34,40,40	1.09	3 (8%)
3	SO4	Z	302	-	4,4,4	0.24	0	6,6,6	0.19	0
2	VFN	1	301	-	30,30,30	1.04	2 (6%)	34,40,40	1.13	1 (2%)
3	SO4	H	303	-	4,4,4	0.27	0	6,6,6	0.20	0
3	SO4	X	301	-	4,4,4	0.35	0	6,6,6	0.14	0
2	VFN	L	301	-	30,30,30	0.99	2 (6%)	34,40,40	1.03	2 (5%)
2	VFN	K	301	-	30,30,30	1.09	2 (6%)	34,40,40	1.38	4 (11%)
3	SO4	Q	301	-	4,4,4	0.25	0	6,6,6	0.22	0
2	VFN	G	301	-	30,30,30	1.09	2 (6%)	34,40,40	1.07	1 (2%)
2	VFN	H	301	-	30,30,30	1.04	2 (6%)	34,40,40	1.24	3 (8%)
3	SO4	O	303	-	4,4,4	0.30	0	6,6,6	0.09	0
2	VFN	O	302	-	30,30,30	1.02	2 (6%)	34,40,40	1.14	4 (11%)
3	SO4	T	302	-	4,4,4	0.27	0	6,6,6	0.26	0
3	SO4	Y	301	-	4,4,4	0.30	0	6,6,6	0.18	0
3	SO4	C	301	-	4,4,4	0.21	0	6,6,6	0.17	0
2	VFN	N	301	-	30,30,30	0.97	2 (6%)	34,40,40	1.02	3 (8%)
2	VFN	R	301	-	30,30,30	1.12	3 (10%)	34,40,40	1.19	4 (11%)
3	SO4	W	303	-	4,4,4	0.34	0	6,6,6	0.14	0
2	VFN	2	301	-	30,30,30	1.00	2 (6%)	34,40,40	1.19	2 (5%)
2	VFN	O	301	-	30,30,30	1.01	2 (6%)	34,40,40	1.16	2 (5%)
2	VFN	B	301	-	30,30,30	1.04	2 (6%)	34,40,40	0.98	1 (2%)
2	VFN	D	302	-	30,30,30	0.96	2 (6%)	34,40,40	1.26	3 (8%)
3	SO4	4	301	-	4,4,4	0.18	0	6,6,6	0.23	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	VFN	W	301	-	30,30,30	1.18	3 (10%)	34,40,40	1.80	7 (20%)
3	SO4	D	303	-	4,4,4	0.35	0	6,6,6	0.26	0
3	SO4	P	303	-	4,4,4	0.36	0	6,6,6	0.10	0
3	SO4	S	303	-	4,4,4	0.29	0	6,6,6	0.24	0
3	SO4	F	302	-	4,4,4	0.36	0	6,6,6	0.17	0
2	VFN	D	301	-	30,30,30	1.05	2 (6%)	34,40,40	1.14	2 (5%)
2	VFN	A	302	-	30,30,30	1.03	2 (6%)	34,40,40	1.31	4 (11%)
2	VFN	S	302	-	30,30,30	1.07	2 (6%)	34,40,40	0.95	1 (2%)
2	VFN	F	301	-	30,30,30	1.10	2 (6%)	34,40,40	1.38	2 (5%)
2	VFN	J	301	-	30,30,30	1.07	1 (3%)	34,40,40	1.01	1 (2%)
2	VFN	S	301	-	30,30,30	0.99	3 (10%)	34,40,40	1.17	3 (8%)
3	SO4	3	303	-	4,4,4	0.27	0	6,6,6	0.17	0
3	SO4	B	302	-	4,4,4	0.34	0	6,6,6	0.25	0
3	SO4	A	303	-	4,4,4	0.30	0	6,6,6	0.18	0
3	SO4	G	302	-	4,4,4	0.32	0	6,6,6	0.17	0
3	SO4	J	302	-	4,4,4	0.38	0	6,6,6	0.21	0
3	SO4	M	301	-	4,4,4	0.25	0	6,6,6	0.18	0
3	SO4	U	301	-	4,4,4	0.20	0	6,6,6	0.29	0
3	SO4	2	302	-	4,4,4	0.36	0	6,6,6	0.24	0
2	VFN	P	301	-	30,30,30	1.03	2 (6%)	34,40,40	1.09	1 (2%)
3	SO4	V	302	-	4,4,4	0.22	0	6,6,6	0.19	0
2	VFN	Z	301	-	30,30,30	1.02	1 (3%)	34,40,40	1.10	2 (5%)
2	VFN	3	301	-	30,30,30	1.05	2 (6%)	34,40,40	1.01	2 (5%)
2	VFN	1	302	-	30,30,30	1.18	4 (13%)	34,40,40	1.90	7 (20%)
2	VFN	T	301	-	30,30,30	1.01	1 (3%)	34,40,40	1.15	3 (8%)
3	SO4	E	301	-	4,4,4	0.29	0	6,6,6	0.10	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	VFN	W	302	-	-	0/19/19/19	0/3/3/3
2	VFN	V	301	-	-	0/19/19/19	0/3/3/3
2	VFN	3	302	-	-	0/19/19/19	0/3/3/3
2	VFN	P	302	-	-	0/19/19/19	0/3/3/3
2	VFN	H	302	-	-	0/19/19/19	0/3/3/3
2	VFN	A	301	-	-	1/19/19/19	0/3/3/3
2	VFN	1	301	-	-	1/19/19/19	0/3/3/3

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

All (64) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	R	301	VFN	C5-N4	2.84	1.32	1.28
2	F	301	VFN	C5-N4	2.83	1.32	1.28
2	G	301	VFN	C5-N4	2.82	1.32	1.28
2	K	301	VFN	C5-N4	2.79	1.32	1.28
2	B	301	VFN	C5-N4	2.76	1.32	1.28
2	P	302	VFN	C5-N4	2.75	1.32	1.28
2	D	301	VFN	C5-N4	2.74	1.32	1.28
2	N	301	VFN	C5-N4	2.72	1.32	1.28
2	3	302	VFN	C17-N7	2.70	1.40	1.35
2	O	301	VFN	C5-N4	2.69	1.32	1.28
2	W	301	VFN	C2-N3	2.68	1.32	1.30
2	O	302	VFN	C17-N7	2.66	1.40	1.35
2	S	302	VFN	C17-N7	2.64	1.40	1.35
2	W	301	VFN	C5-N4	2.63	1.31	1.28
2	S	301	VFN	C5-N4	2.62	1.31	1.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	302	VFN	C5-N4	2.62	1.31	1.28
2	3	301	VFN	C5-N4	2.60	1.31	1.28
2	3	302	VFN	C5-N4	2.60	1.31	1.28
2	1	301	VFN	C5-N4	2.60	1.31	1.28
2	1	302	VFN	C2-N3	2.59	1.32	1.30
2	1	302	VFN	C17-N7	2.58	1.40	1.35
2	Z	301	VFN	C5-N4	2.55	1.31	1.28
2	W	302	VFN	C5-N4	2.53	1.31	1.28
2	3	301	VFN	C17-N7	2.52	1.40	1.35
2	J	301	VFN	C5-N4	2.52	1.31	1.28
2	S	302	VFN	C5-N4	2.49	1.31	1.28
2	2	301	VFN	C5-N4	2.49	1.31	1.28
2	V	301	VFN	C5-N4	2.48	1.31	1.28
2	T	301	VFN	C5-N4	2.46	1.31	1.28
2	P	301	VFN	C17-N7	2.45	1.39	1.35
2	P	301	VFN	C5-N4	2.44	1.31	1.28
2	D	302	VFN	C5-N4	2.44	1.31	1.28
2	O	301	VFN	C17-N7	2.43	1.39	1.35
2	L	301	VFN	C5-N4	2.43	1.31	1.28
2	L	301	VFN	C17-N7	2.42	1.39	1.35
2	K	301	VFN	C17-N7	2.38	1.39	1.35
2	A	301	VFN	C5-N4	2.36	1.31	1.28
2	O	302	VFN	C5-N4	2.34	1.31	1.28
2	D	302	VFN	C17-N7	2.34	1.39	1.35
2	H	302	VFN	C5-N4	2.34	1.31	1.28
2	W	302	VFN	C17-N7	2.33	1.39	1.35
2	1	302	VFN	C5-N4	2.33	1.31	1.28
2	H	301	VFN	C5-N4	2.32	1.31	1.28
2	H	302	VFN	C17-N7	2.29	1.39	1.35
2	A	302	VFN	C2-N3	2.26	1.32	1.30
2	R	301	VFN	C2-N3	2.26	1.32	1.30
2	W	301	VFN	C17-N7	2.25	1.39	1.35
2	D	301	VFN	C17-N7	2.24	1.39	1.35
2	F	301	VFN	C17-N7	2.23	1.39	1.35
2	3	302	VFN	C2-N3	2.21	1.32	1.30
2	R	301	VFN	C17-N7	2.18	1.39	1.35
2	1	301	VFN	C17-N7	2.18	1.39	1.35
2	V	301	VFN	C2-N3	2.17	1.32	1.30
2	H	301	VFN	C17-N7	2.16	1.39	1.35
2	P	302	VFN	C17-N7	2.14	1.39	1.35
2	S	301	VFN	C2-N3	2.12	1.32	1.30
2	G	301	VFN	C17-N7	2.12	1.39	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	V	301	VFN	C17-N7	2.11	1.39	1.35
2	N	301	VFN	C17-N7	2.08	1.39	1.35
2	B	301	VFN	C17-N7	2.07	1.39	1.35
2	H	302	VFN	C2-N3	2.06	1.32	1.30
2	S	301	VFN	C17-N7	2.03	1.39	1.35
2	2	301	VFN	C17-N7	2.03	1.39	1.35
2	1	302	VFN	C6-C5	-2.00	1.47	1.49

All (86) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	W	302	VFN	C2-N3-N4	6.85	107.24	105.58
2	1	302	VFN	C2-N3-N4	6.46	107.14	105.58
2	W	302	VFN	O28-C2-N3	-5.66	111.44	112.71
2	W	301	VFN	N1-C2-N3	5.20	132.89	129.35
2	F	301	VFN	O28-C2-N3	5.10	113.87	112.71
2	3	302	VFN	C2-N3-N4	4.79	106.74	105.58
2	1	302	VFN	N1-C2-N3	4.30	132.28	129.35
2	W	301	VFN	O28-C2-N3	-4.18	111.77	112.71
2	1	302	VFN	O28-C2-N3	-4.16	111.77	112.71
2	1	301	VFN	C2-N3-N4	4.12	106.58	105.58
2	K	301	VFN	N1-C2-N3	4.03	132.10	129.35
2	A	302	VFN	N1-C2-N3	4.02	132.09	129.35
2	W	301	VFN	C2-N3-N4	3.97	106.54	105.58
2	2	301	VFN	O28-C2-N3	3.87	113.59	112.71
2	H	301	VFN	C2-N3-N4	3.86	106.51	105.58
2	D	302	VFN	C2-N3-N4	3.77	106.49	105.58
2	G	301	VFN	O28-C2-N3	3.76	113.56	112.71
2	T	301	VFN	O28-C2-N3	3.67	113.55	112.71
2	V	301	VFN	C2-N3-N4	3.66	106.47	105.58
2	O	301	VFN	O28-C2-N3	3.66	113.54	112.71
2	A	302	VFN	C2-N3-N4	3.60	106.45	105.58
2	F	301	VFN	C19-S20-C21	3.47	108.21	102.27
2	H	302	VFN	C2-N3-N4	3.19	106.35	105.58
2	P	302	VFN	O28-C2-N3	3.17	113.43	112.71
2	S	301	VFN	N1-C2-N3	3.12	131.48	129.35
2	D	301	VFN	C2-N3-N4	3.11	106.33	105.58
2	A	301	VFN	C2-N3-N4	3.10	106.33	105.58
2	K	301	VFN	O28-C2-N1	-3.07	114.64	117.66
2	H	301	VFN	N1-C2-N3	3.05	131.43	129.35
2	D	302	VFN	N1-C2-N3	3.00	131.40	129.35
2	R	301	VFN	N1-C2-N3	2.97	131.37	129.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	301	VFN	C9-C8-N7	-2.92	108.56	113.15
2	H	302	VFN	C13-C12-C15	-2.88	115.28	119.97
2	H	302	VFN	N1-C2-N3	2.82	131.27	129.35
2	O	302	VFN	N1-C2-N3	2.81	131.27	129.35
2	W	302	VFN	N1-C2-N3	2.75	131.23	129.35
2	L	301	VFN	C2-N3-N4	2.69	106.23	105.58
2	H	301	VFN	C19-S20-C21	2.69	106.87	102.27
2	W	302	VFN	C19-S20-C21	2.60	106.72	102.27
2	2	301	VFN	C9-C8-N7	-2.54	109.16	113.15
2	D	302	VFN	O28-C2-N3	-2.52	112.14	112.71
2	N	301	VFN	N1-C2-N3	2.50	131.06	129.35
2	B	301	VFN	O28-C2-N3	2.50	113.28	112.71
2	O	302	VFN	O28-C2-N3	-2.48	112.15	112.71
2	K	301	VFN	C2-N3-N4	2.48	106.18	105.58
2	O	301	VFN	C19-S20-C21	2.47	106.51	102.27
2	A	302	VFN	O28-C2-N1	-2.47	115.23	117.66
2	Z	301	VFN	O28-C2-N3	2.44	113.27	112.71
2	D	301	VFN	N1-C2-N3	2.43	131.01	129.35
2	K	301	VFN	O28-C2-N3	2.40	113.26	112.71
2	R	301	VFN	C19-S20-C21	2.39	106.36	102.27
2	W	301	VFN	O28-C2-N1	-2.37	115.33	117.66
2	3	302	VFN	C5-N4-N3	-2.36	104.96	106.25
2	P	301	VFN	C2-N3-N4	2.36	106.15	105.58
2	W	301	VFN	C19-S20-C21	2.36	106.31	102.27
2	1	302	VFN	C19-S20-C21	2.35	106.29	102.27
2	N	301	VFN	O28-C2-N3	2.33	113.24	112.71
2	O	302	VFN	C2-N3-N4	2.33	106.14	105.58
2	P	302	VFN	C9-C8-N7	-2.30	109.54	113.15
2	W	301	VFN	C21-C26-CL1	2.28	123.67	119.72
2	W	301	VFN	C8-N7-C17	-2.25	115.81	121.78
2	W	302	VFN	C14-C13-C12	-2.24	117.49	120.35
2	S	302	VFN	C2-N3-N4	2.23	106.12	105.58
2	W	302	VFN	C9-C8-N7	-2.23	109.65	113.15
2	W	302	VFN	C8-N7-C6	2.22	120.32	116.65
2	L	301	VFN	N1-C2-N3	2.19	130.85	129.35
2	1	302	VFN	C14-C13-C12	-2.19	117.55	120.35
2	3	302	VFN	O28-C5-N4	2.15	114.47	112.75
2	Z	301	VFN	N1-C2-N3	2.15	130.82	129.35
2	O	302	VFN	C9-C8-N7	-2.14	109.80	113.15
2	1	302	VFN	C23-C22-C21	2.13	123.14	119.57
2	A	302	VFN	C8-N7-C17	-2.11	116.17	121.78
2	R	301	VFN	C8-N7-C6	2.11	120.14	116.65

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	1	302	VFN	C5-N4-N3	-2.11	105.10	106.25
2	W	302	VFN	C8-N7-C17	-2.09	116.22	121.78
2	3	301	VFN	C8-N7-C17	-2.09	116.23	121.78
2	R	301	VFN	C8-N7-C17	-2.08	116.25	121.78
2	S	301	VFN	C13-C12-C15	-2.07	116.59	119.97
2	J	301	VFN	N1-C2-N3	2.03	130.74	129.35
2	3	301	VFN	C9-C8-N7	-2.03	109.96	113.15
2	T	301	VFN	C14-C9-C10	2.03	121.25	118.23
2	S	301	VFN	O28-C2-N1	-2.03	115.67	117.66
2	A	301	VFN	C17-C19-S20	-2.02	105.49	112.07
2	P	302	VFN	N1-C2-N3	2.02	130.73	129.35
2	T	301	VFN	C11-C10-C9	-2.02	118.35	121.00
2	N	301	VFN	C19-S20-C21	2.01	105.71	102.27

There are no chirality outliers.

All (5) torsion outliers are listed below:

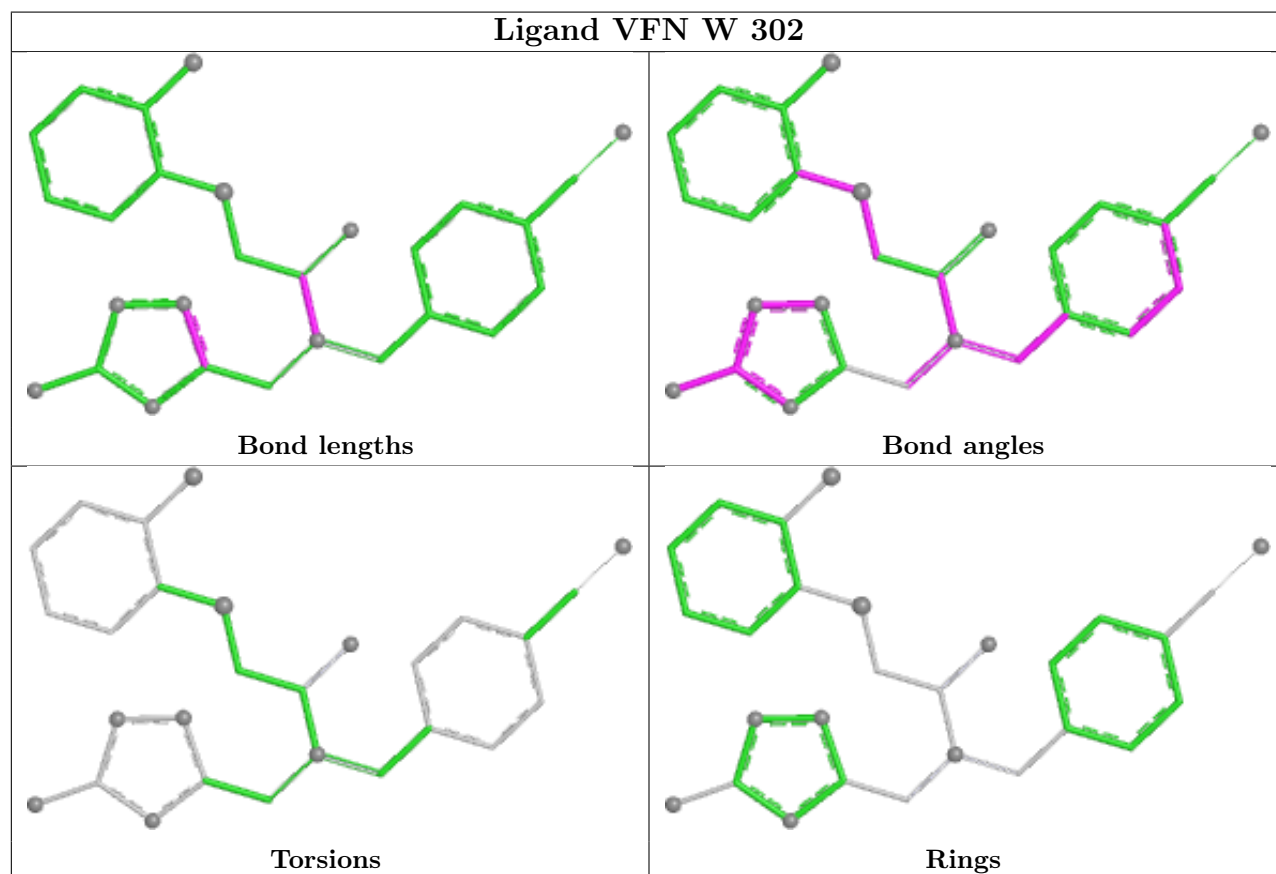
Mol	Chain	Res	Type	Atoms
2	A	301	VFN	N4-C5-C6-N7
2	2	301	VFN	C11-C12-C15-N16
2	1	301	VFN	C11-C12-C15-N16
2	3	301	VFN	C11-C12-C15-N16
2	T	301	VFN	C11-C12-C15-N16

There are no ring outliers.

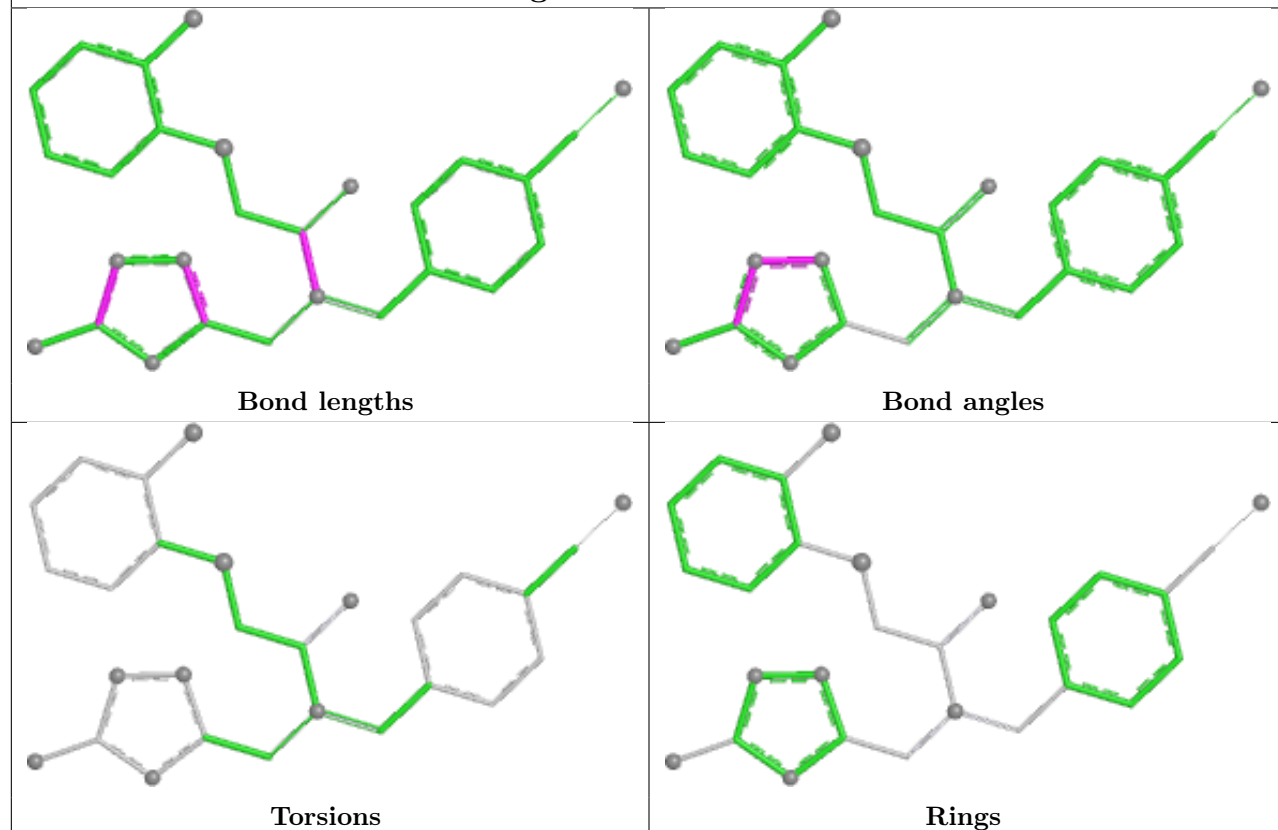
12 monomers are involved in 15 short contacts:

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

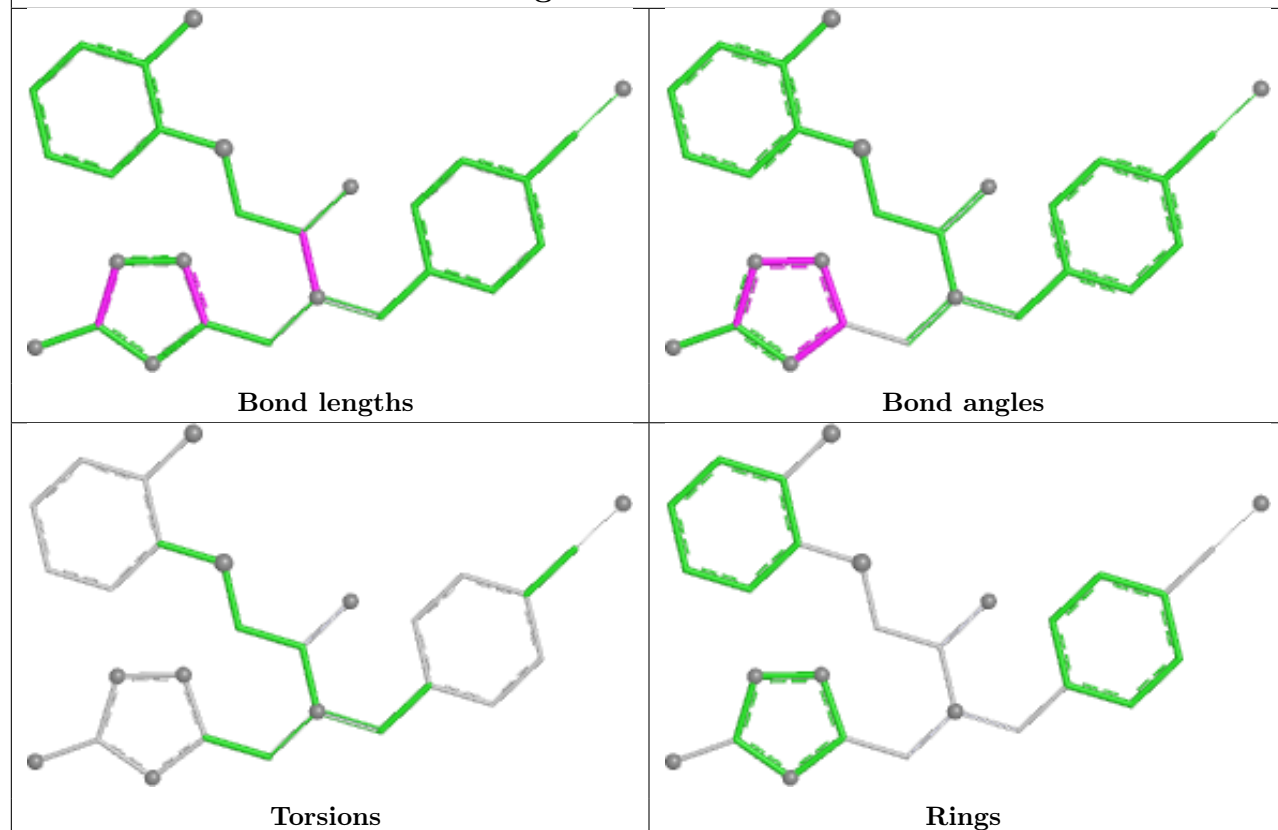
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



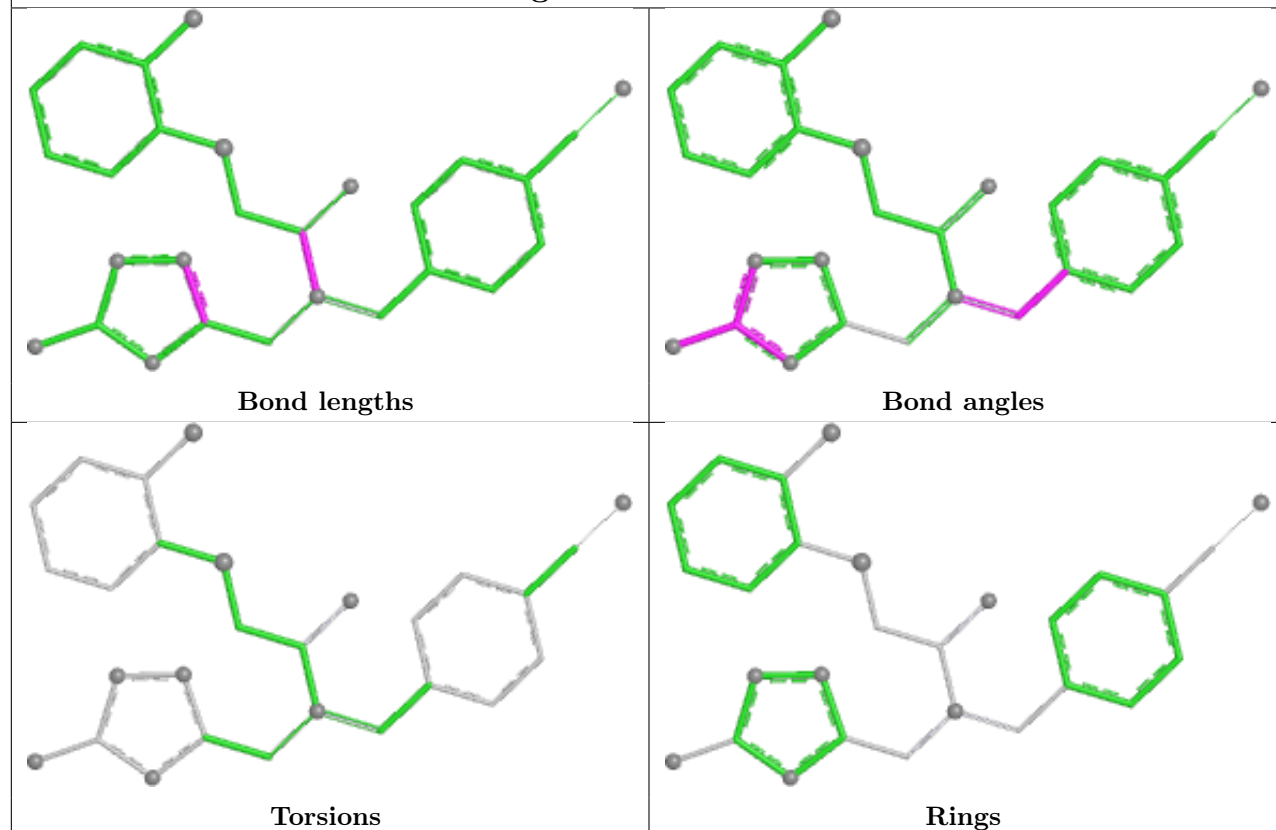
Ligand VFN V 301



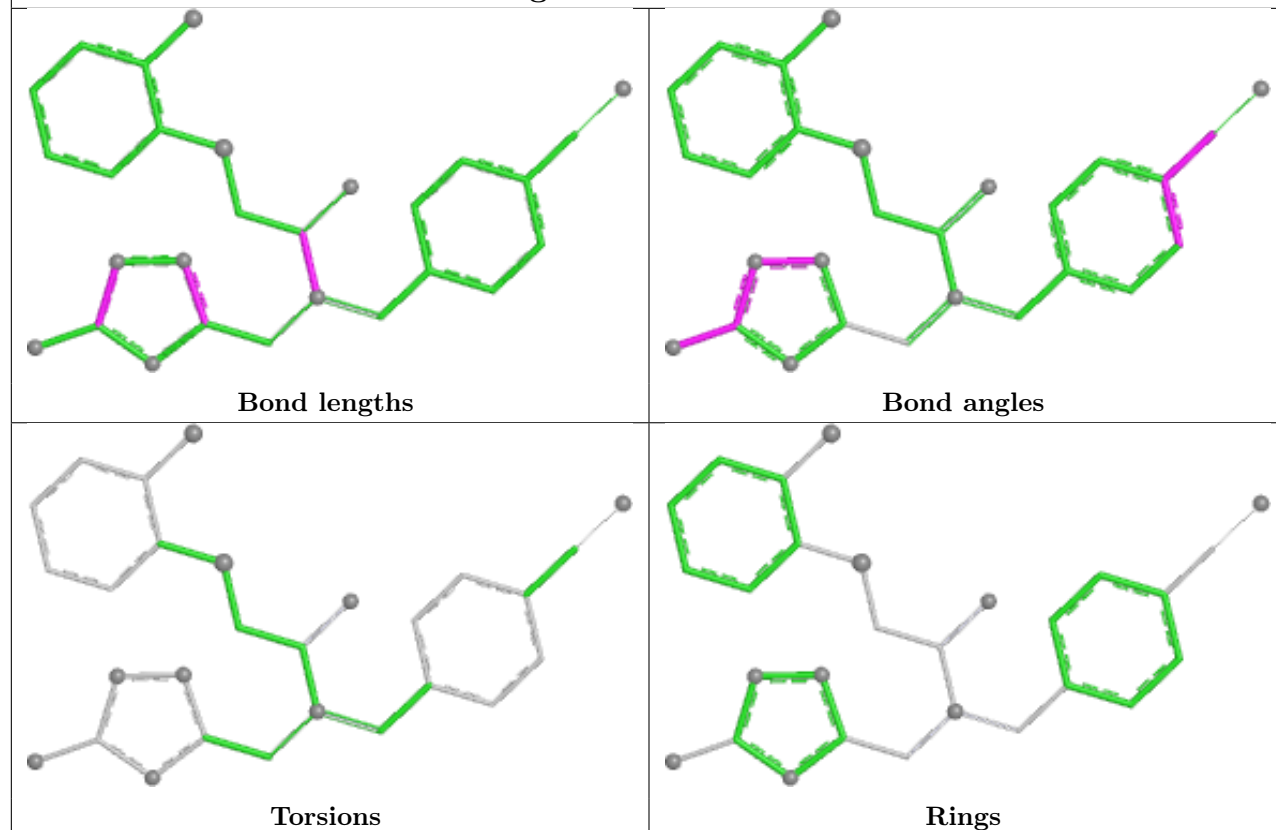
Ligand VFN 3 302



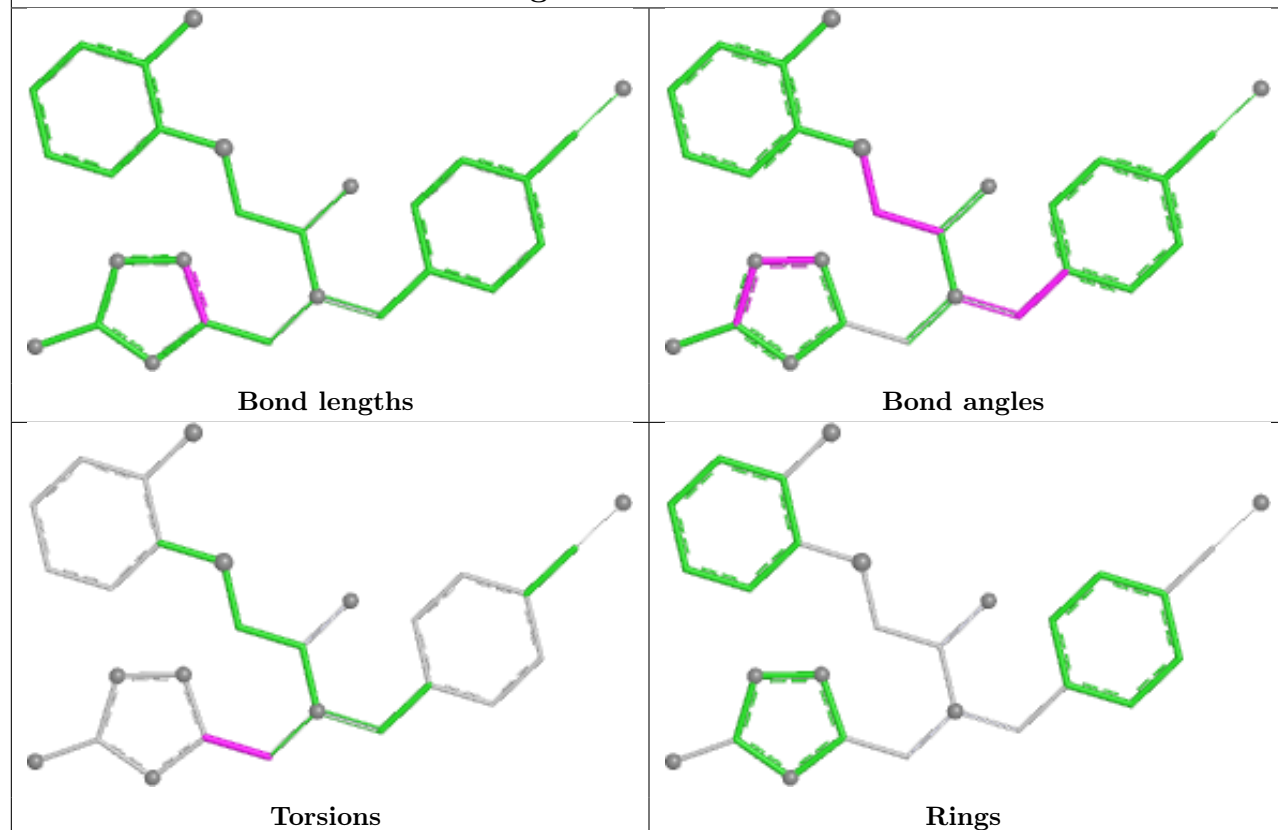
Ligand VFN P 302



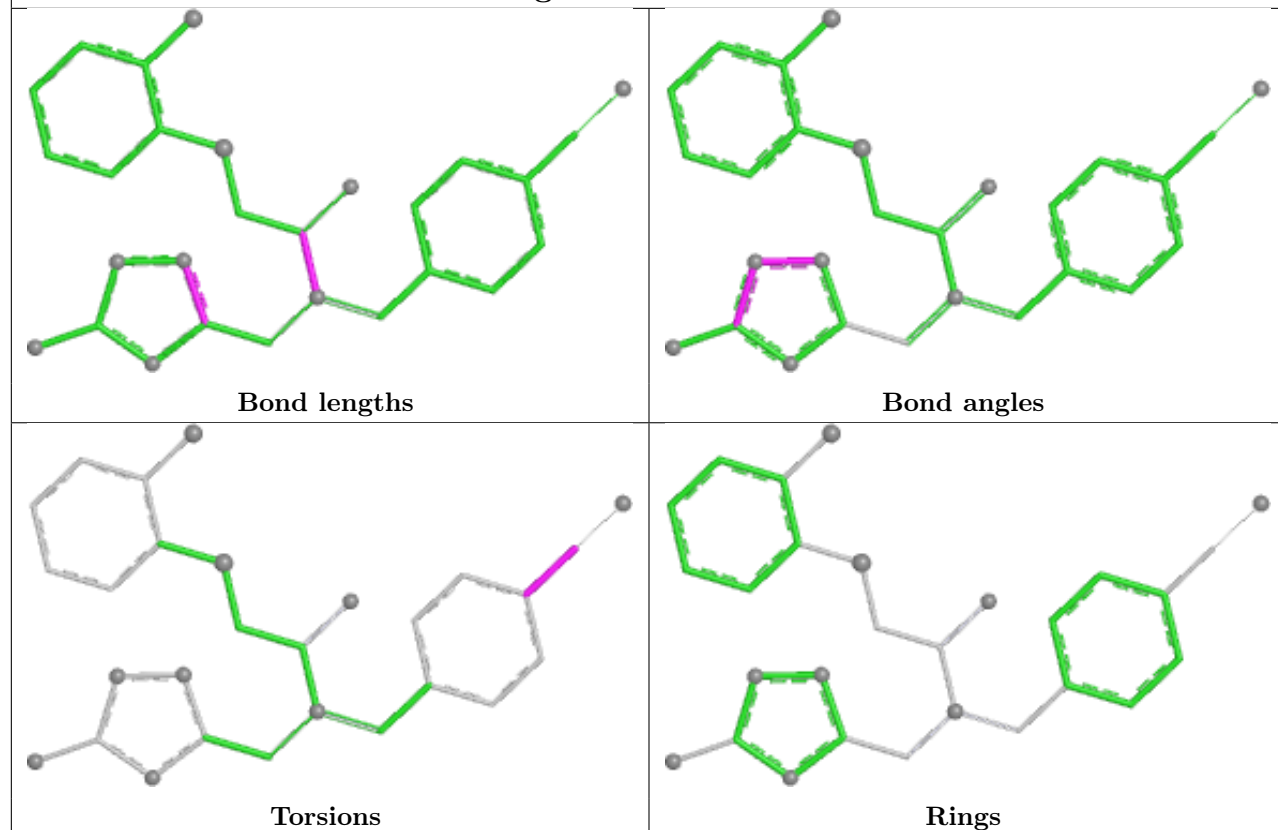
Ligand VFN H 302



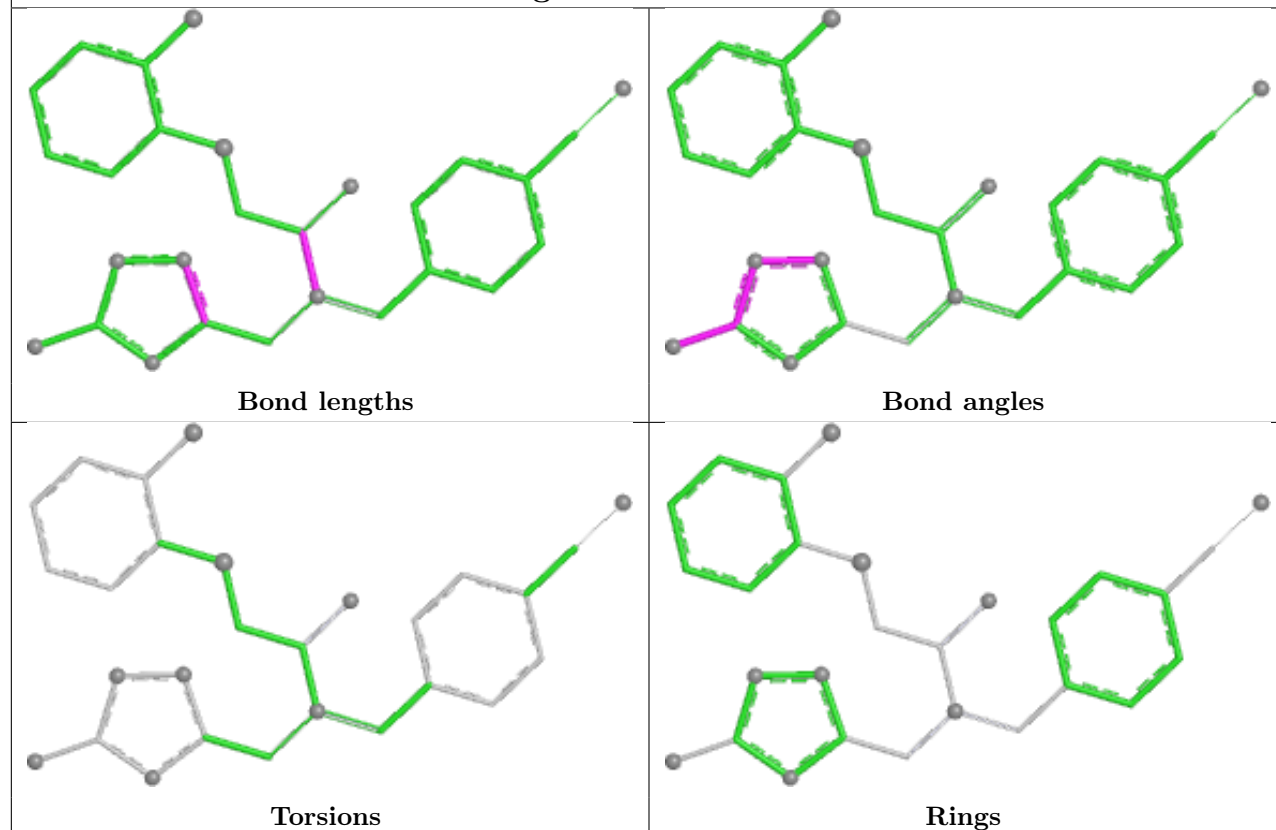
Ligand VFN A 301



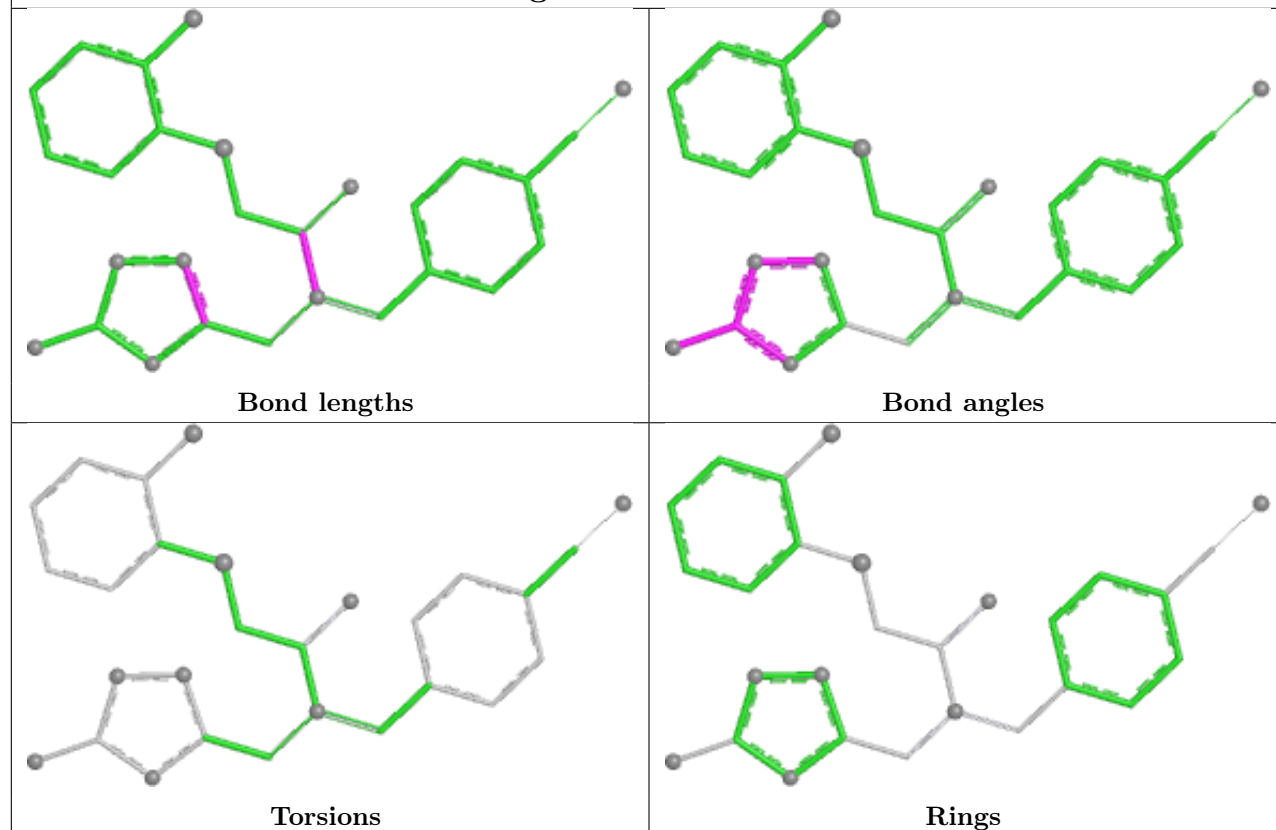
Ligand VFN 1 301

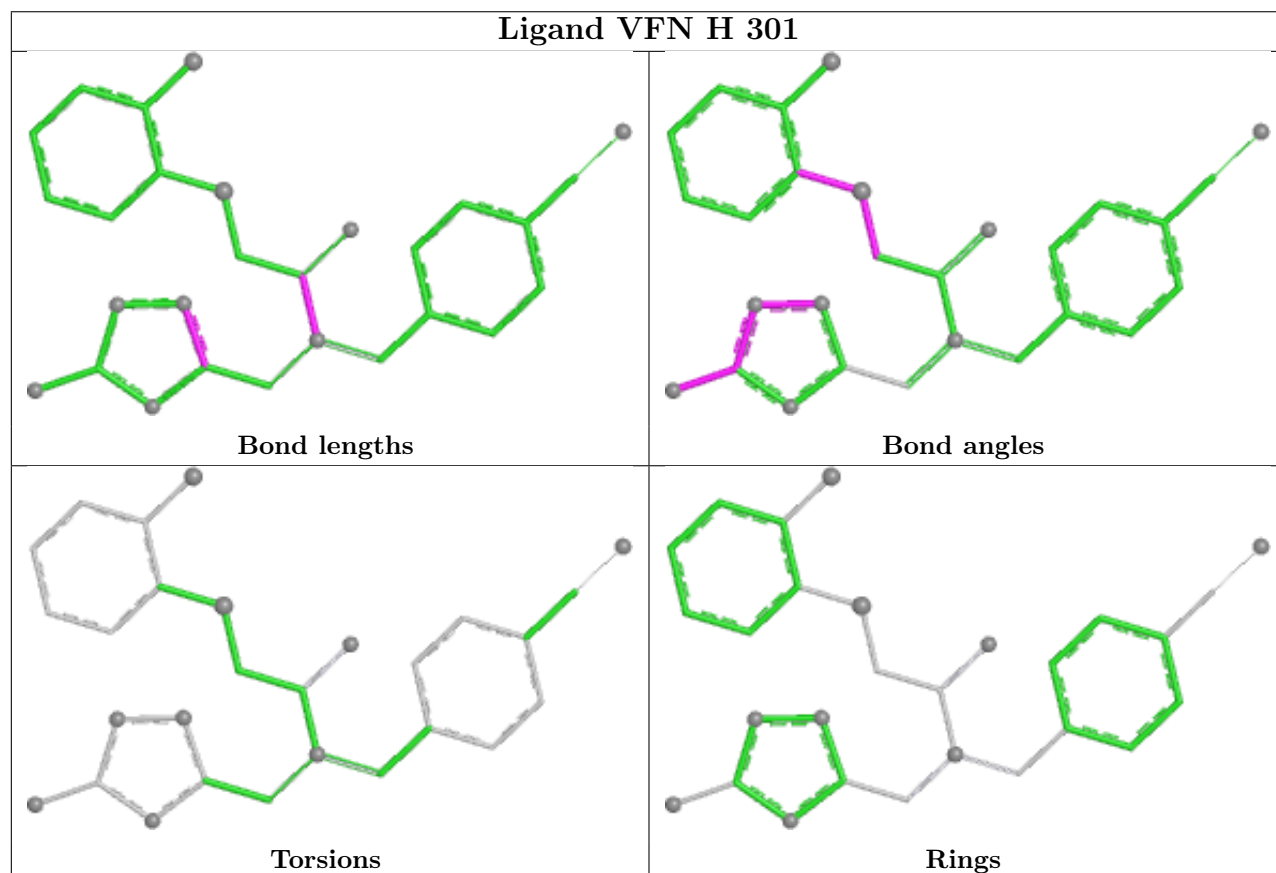
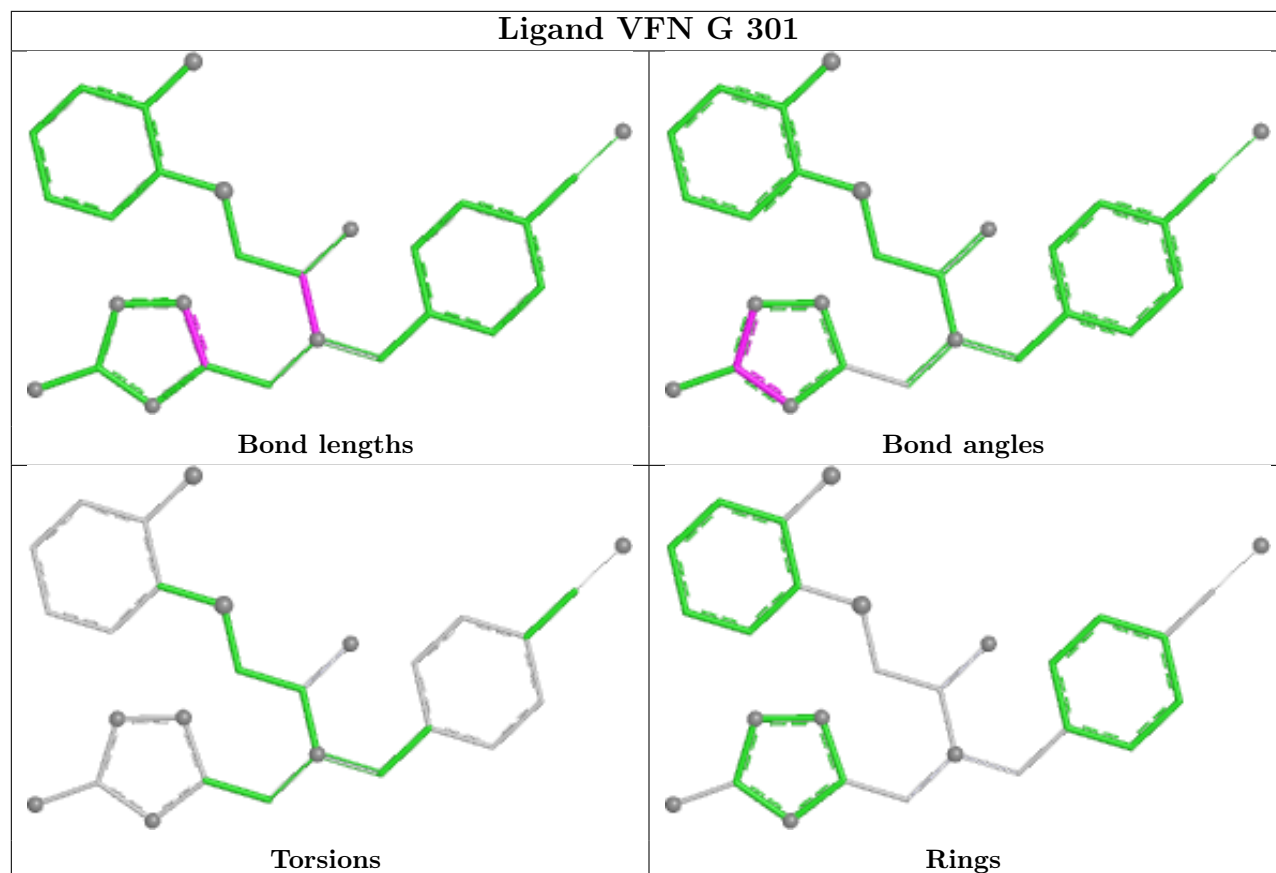


Ligand VFN L 301

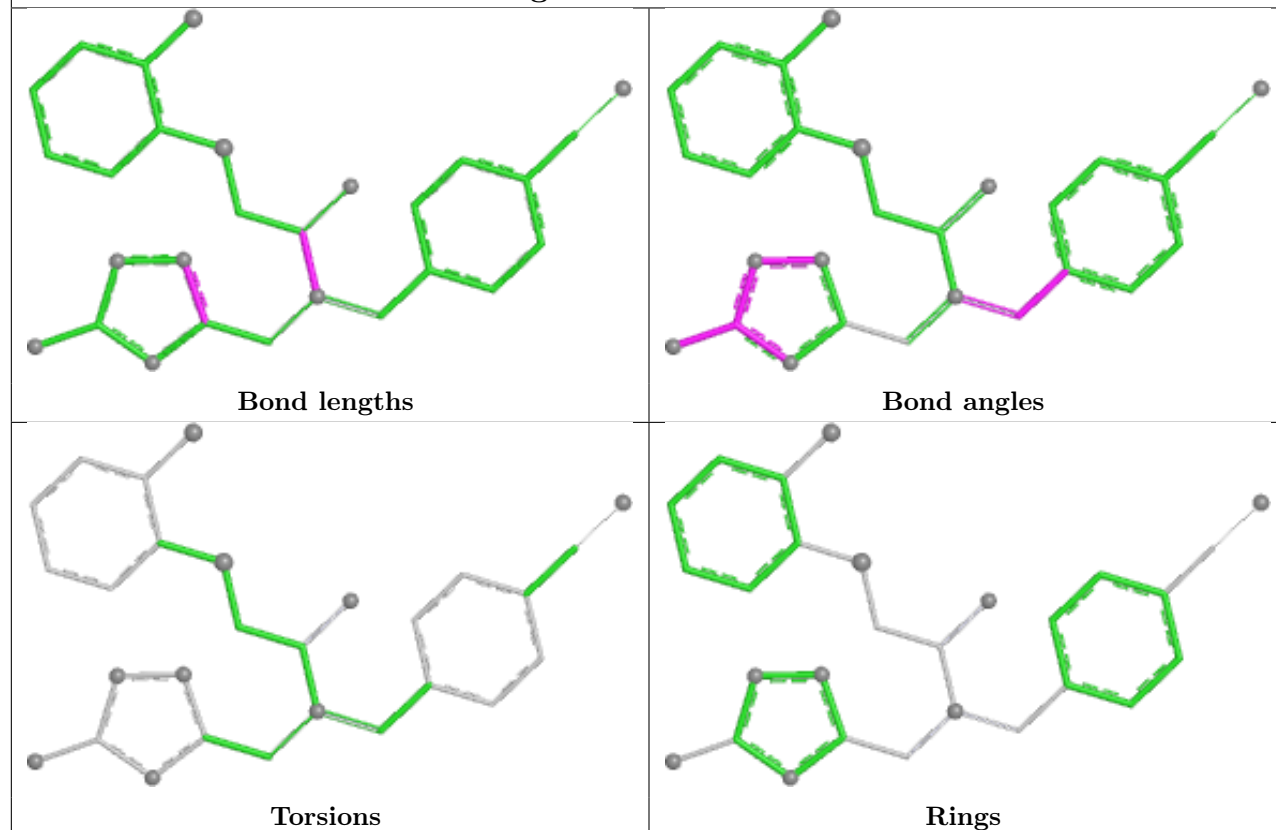


Ligand VFN K 301

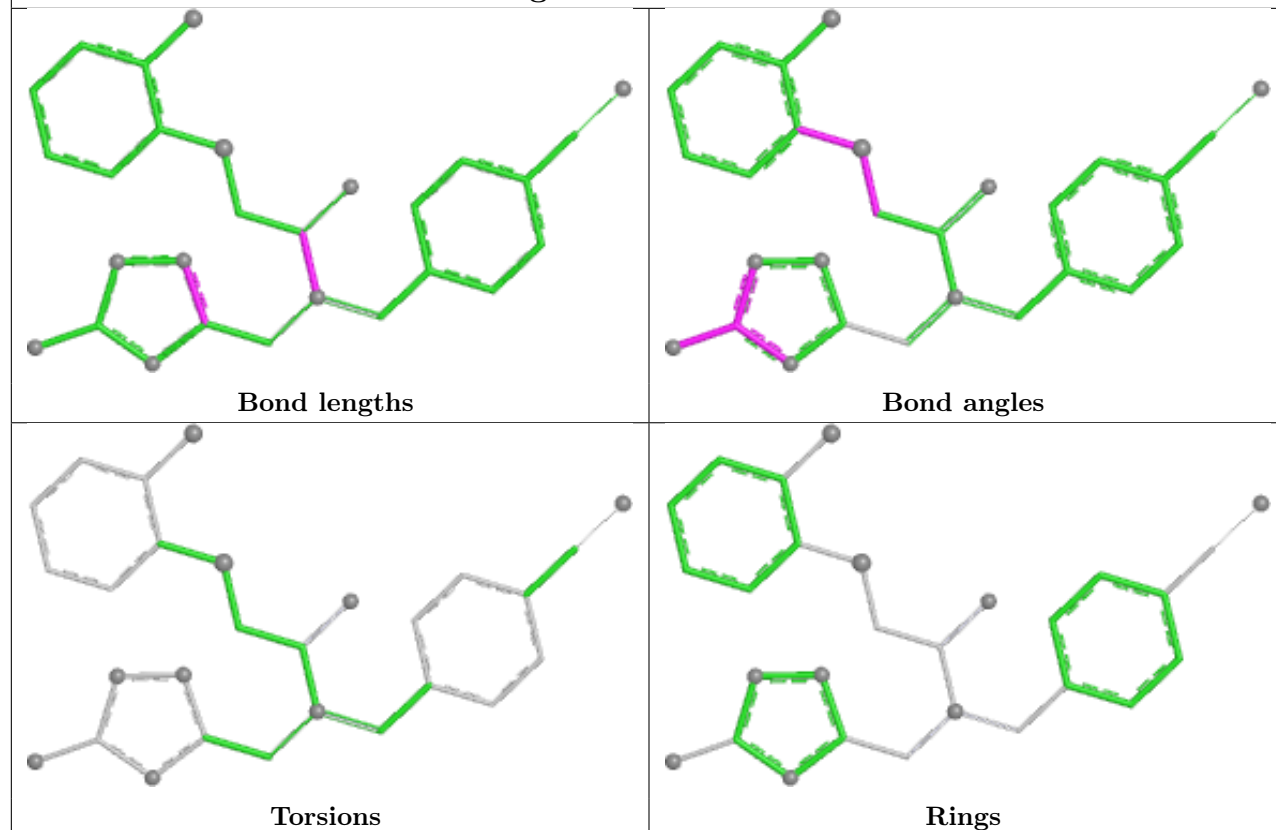




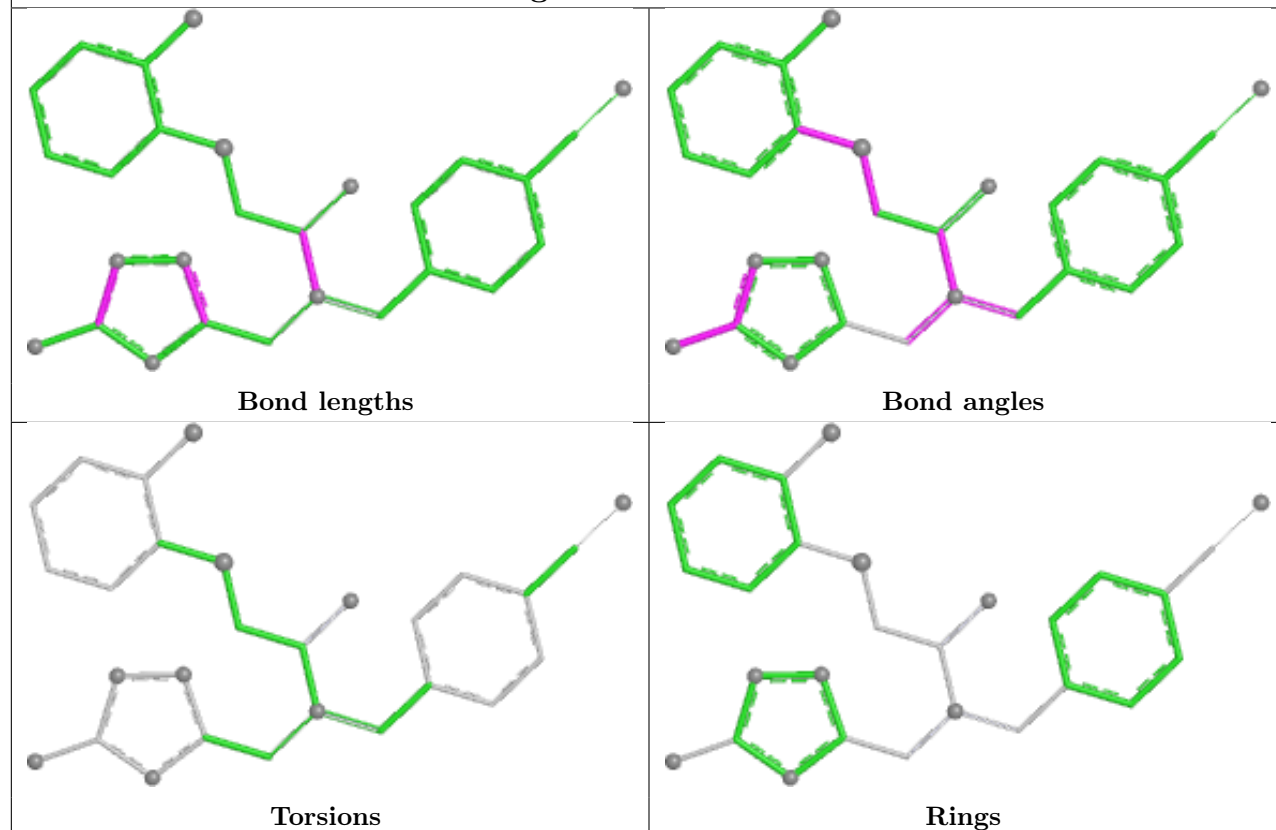
Ligand VFN O 302



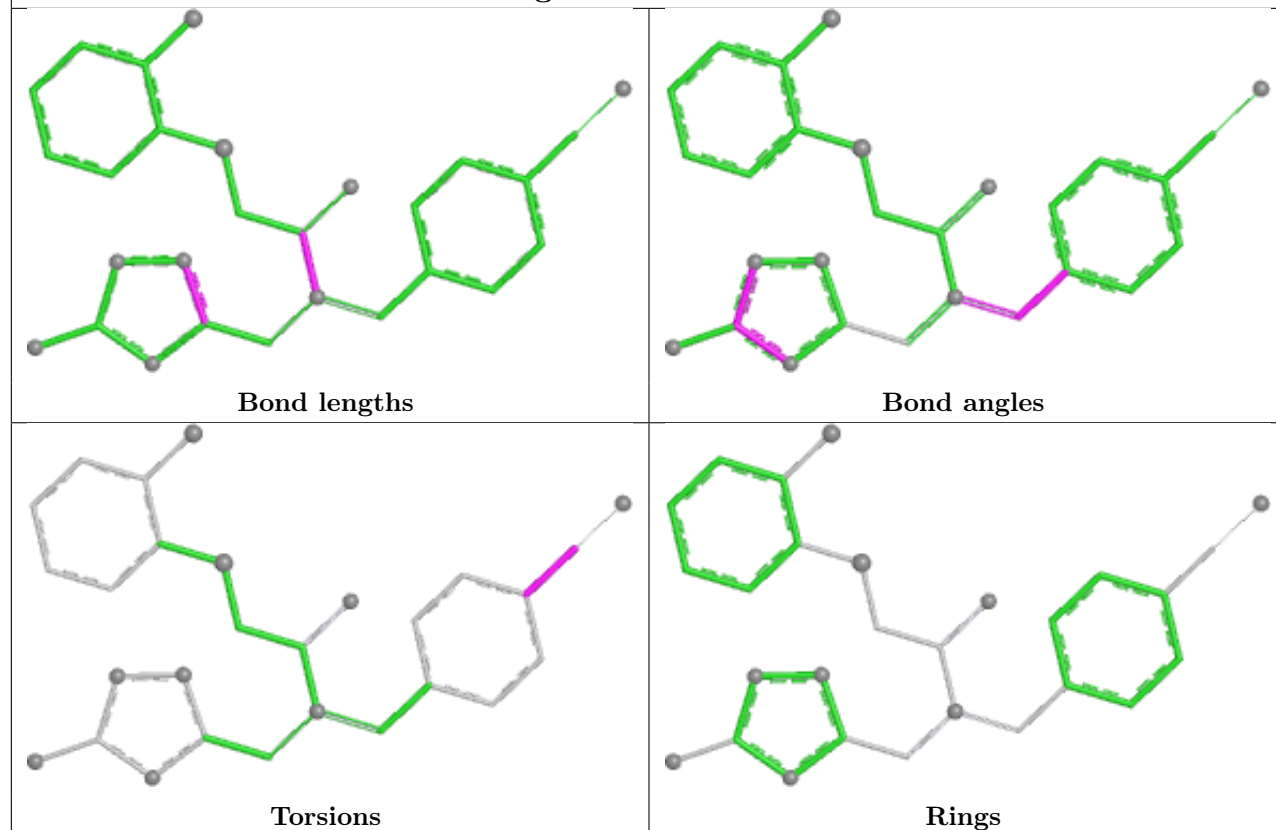
Ligand VFN N 301



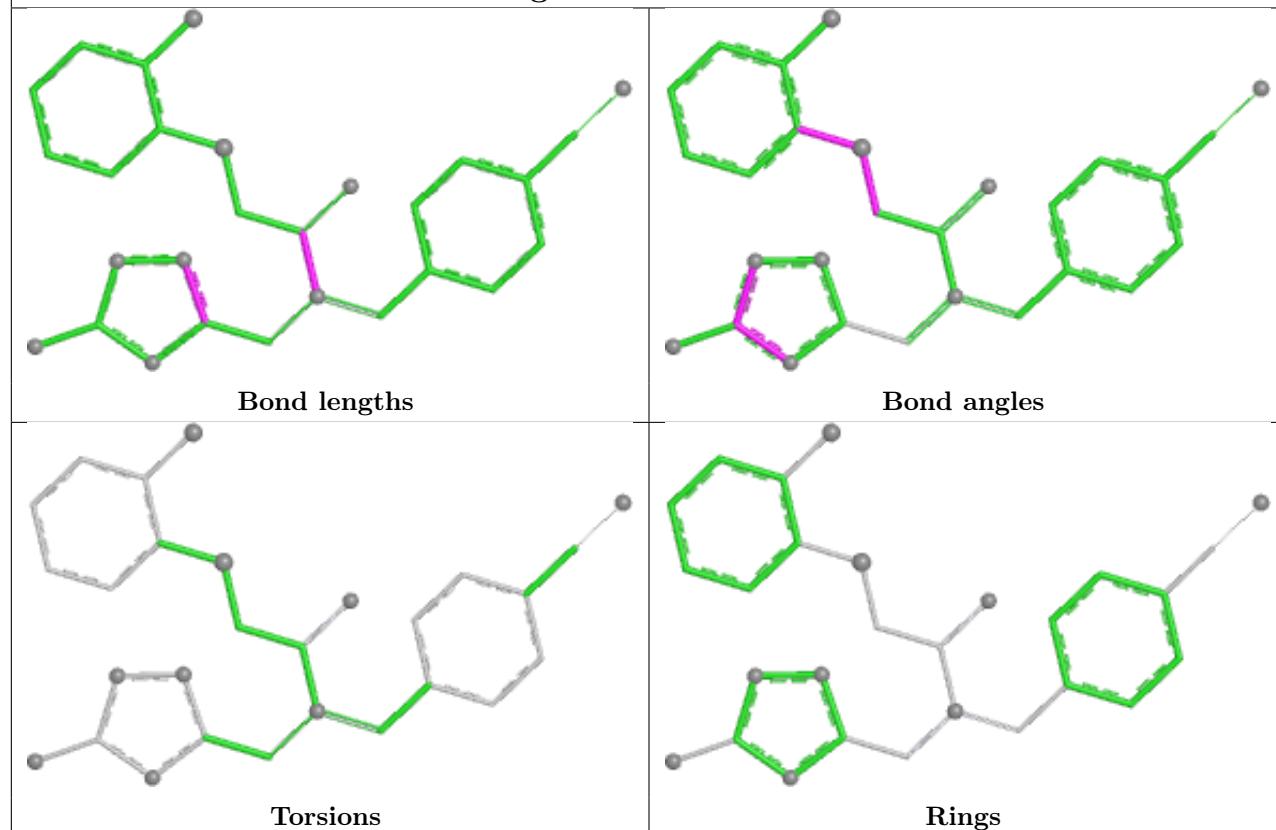
Ligand VFN R 301



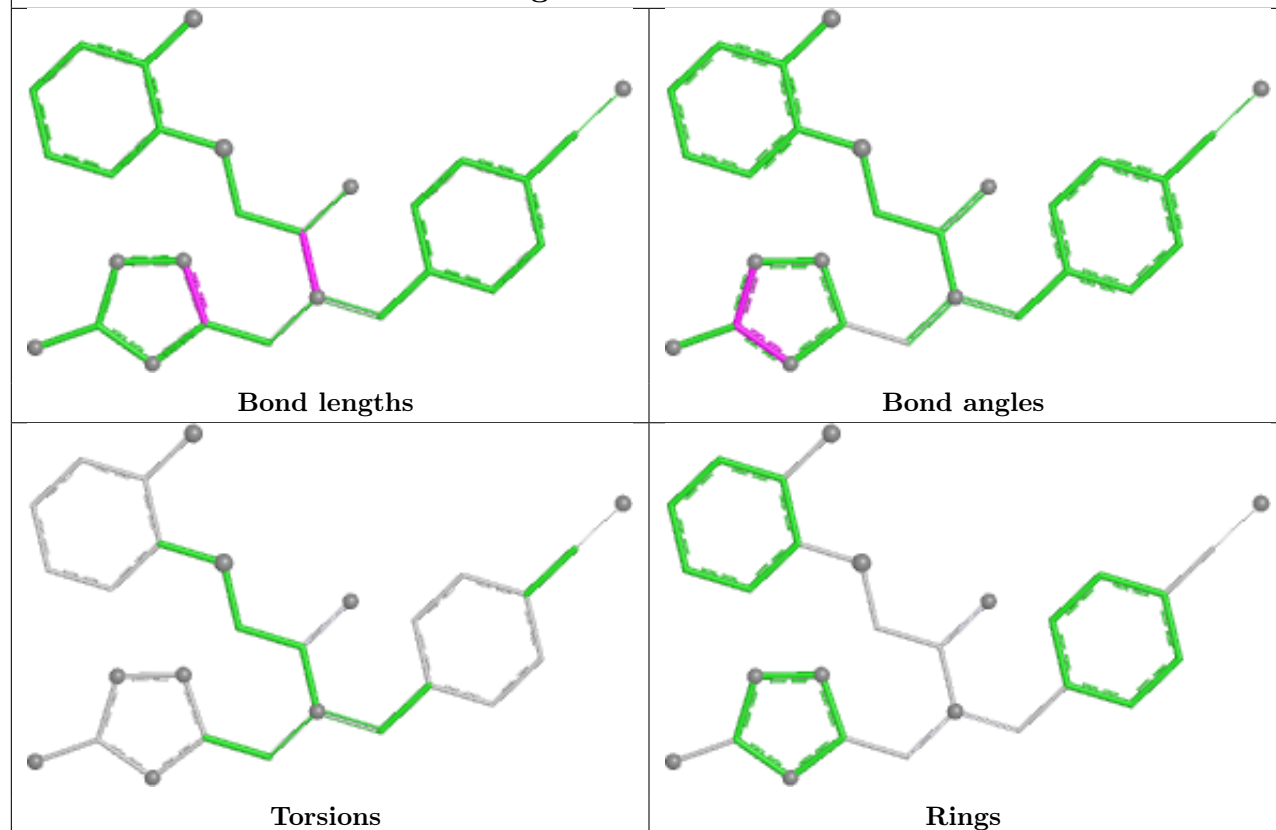
Ligand VFN 2 301

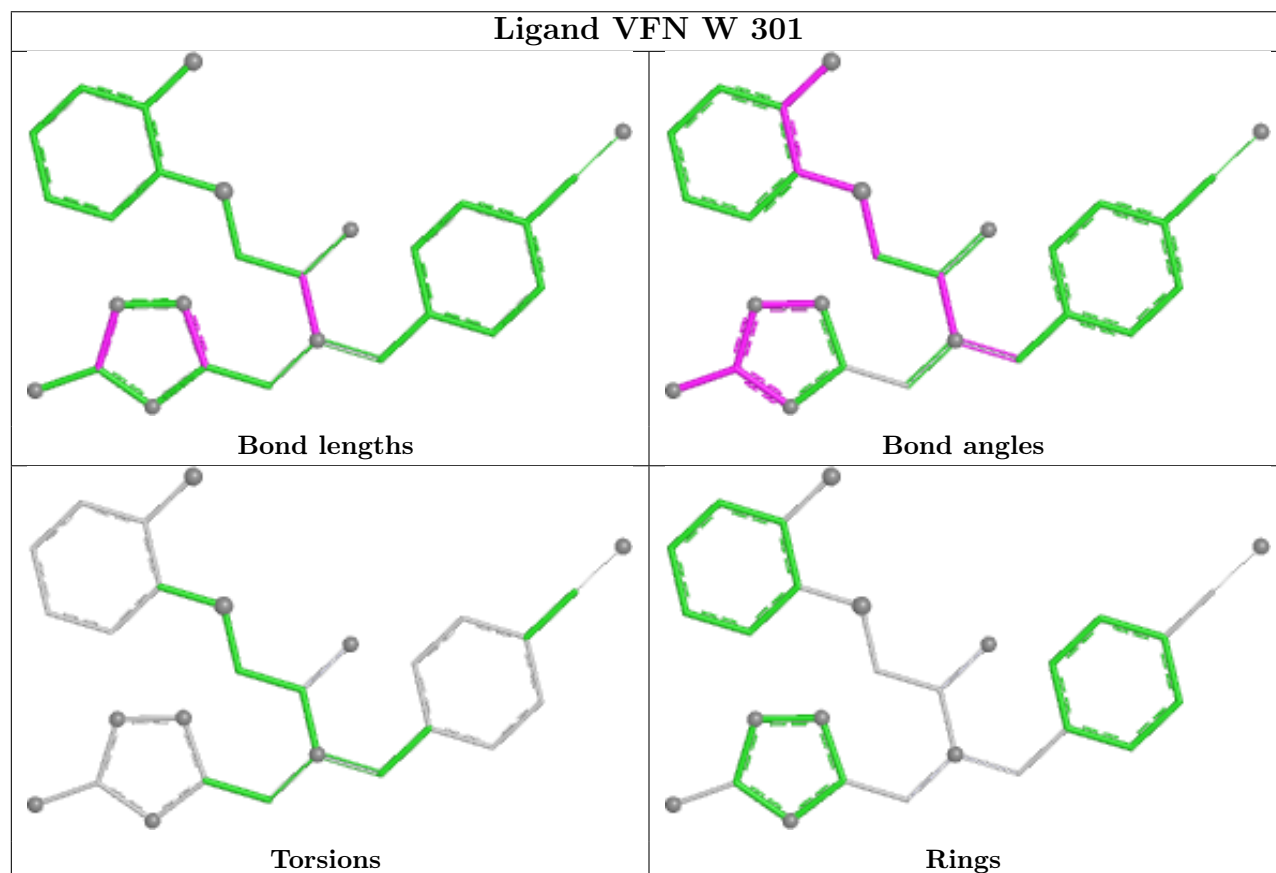
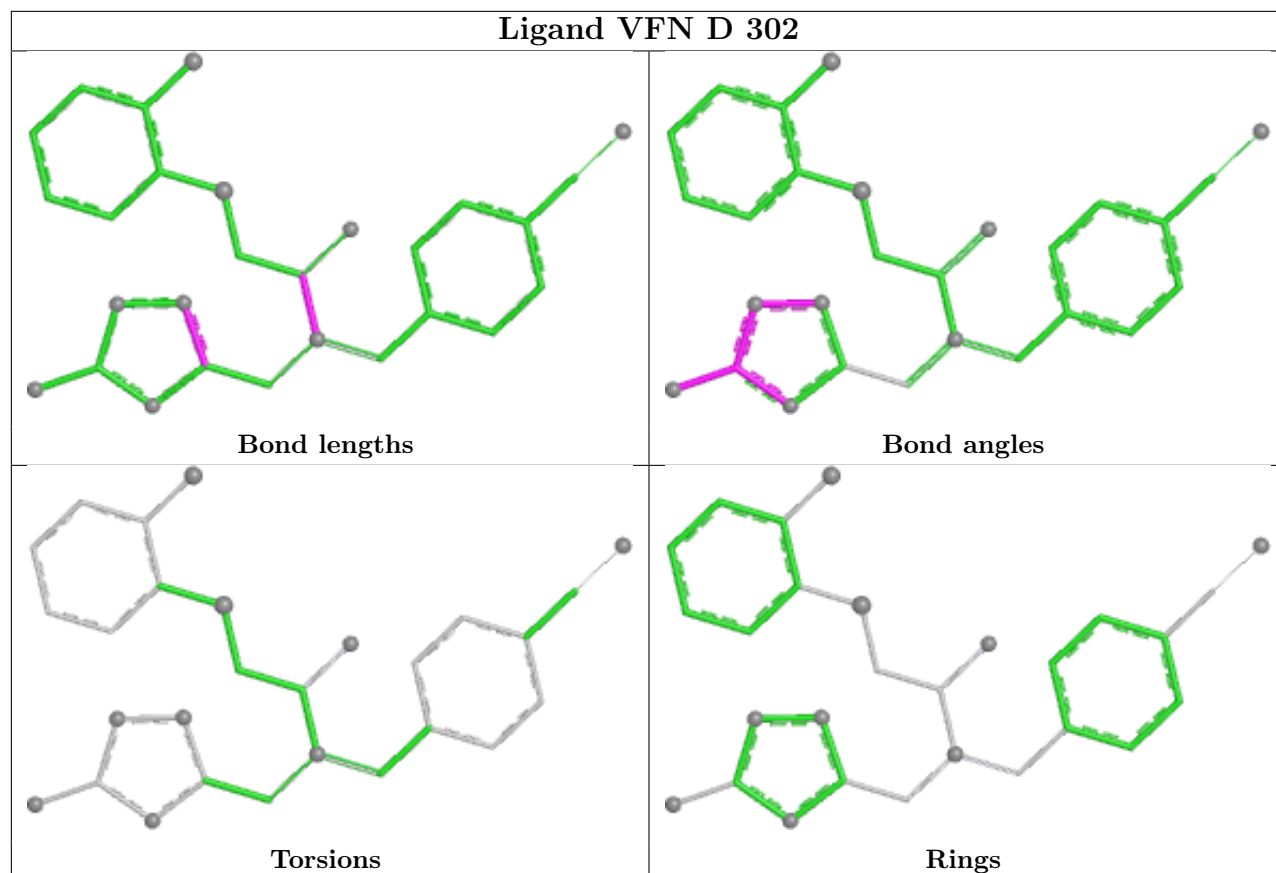


Ligand VFN O 301

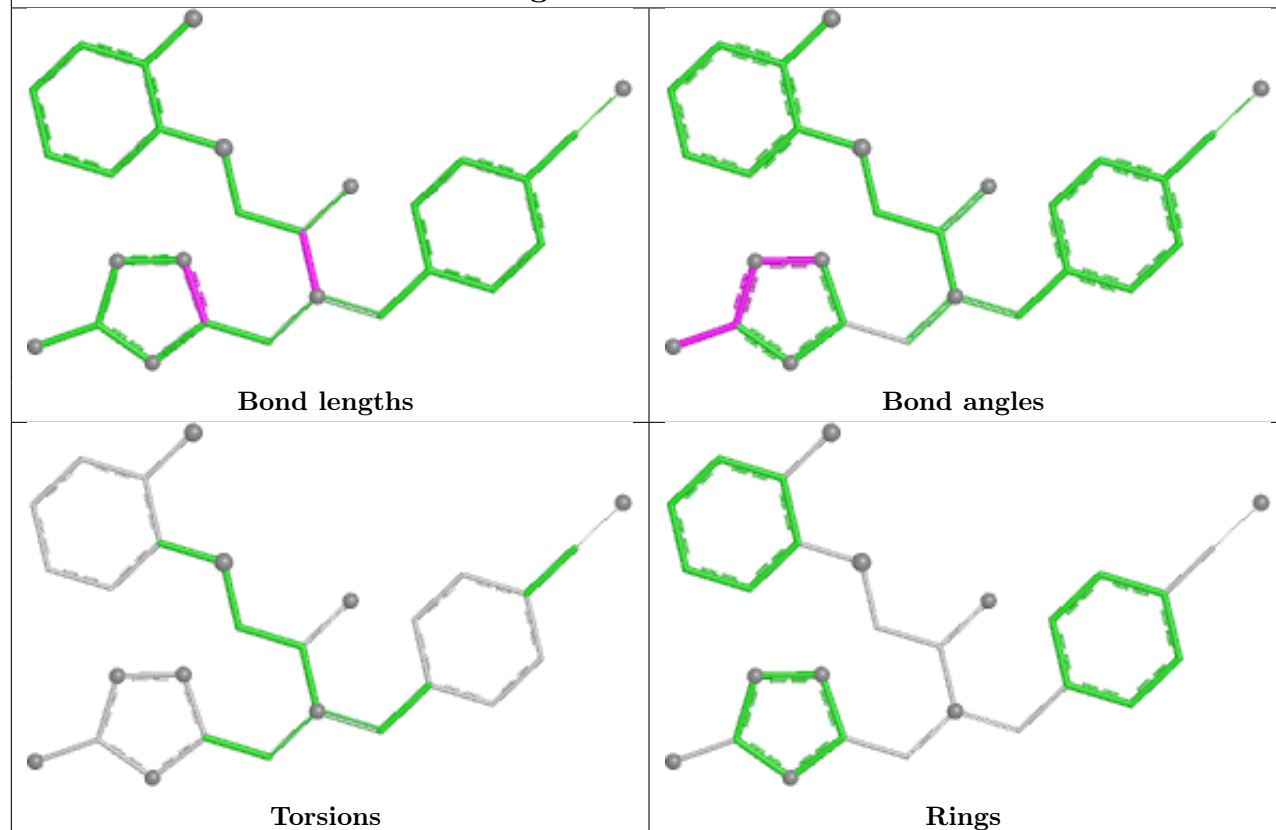


Ligand VFN B 301

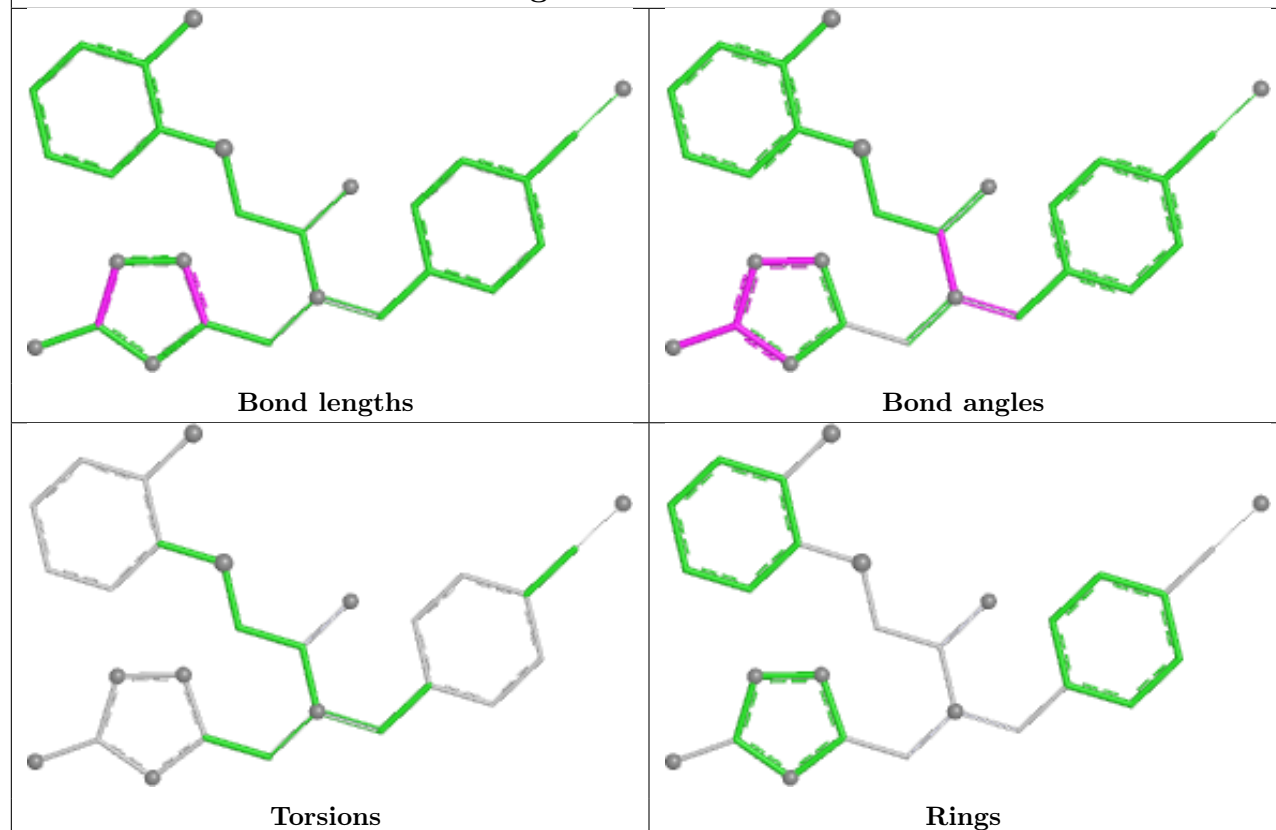




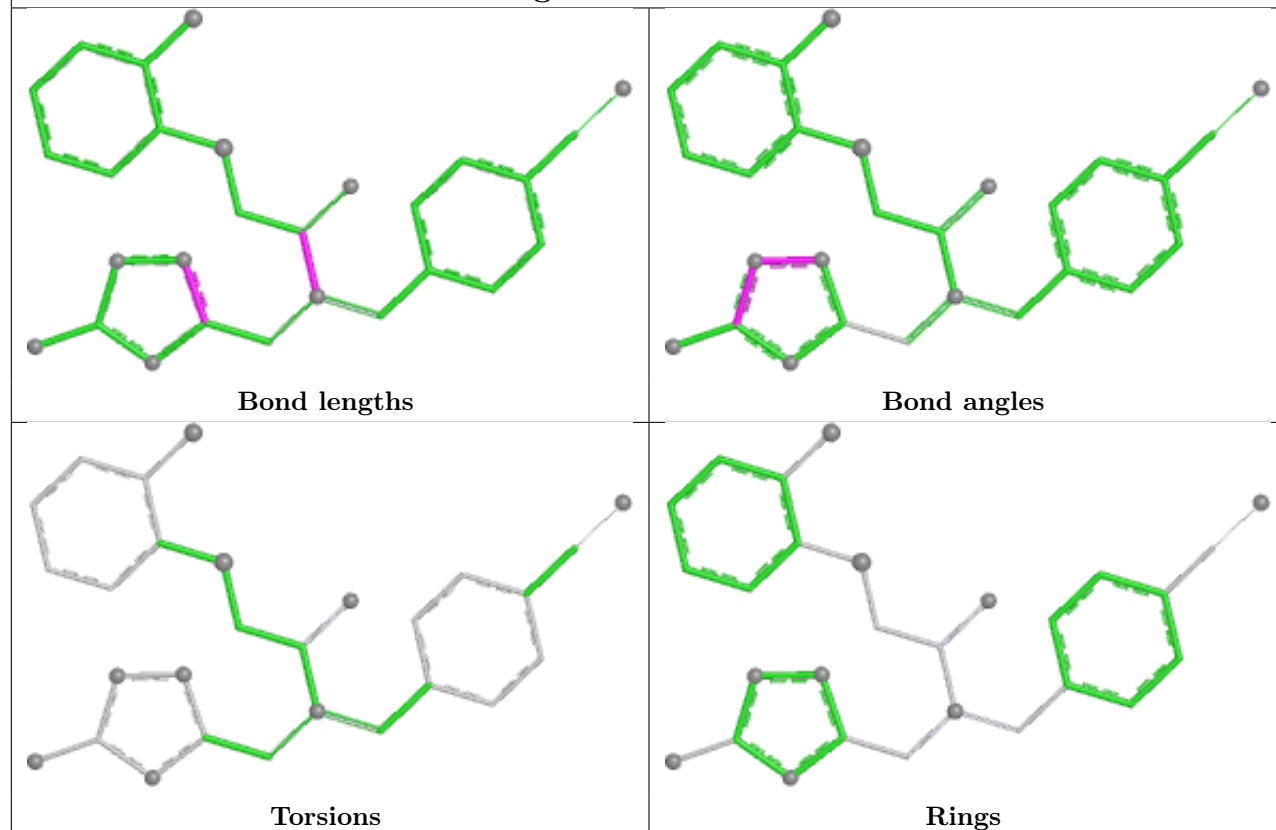
Ligand VFN D 301



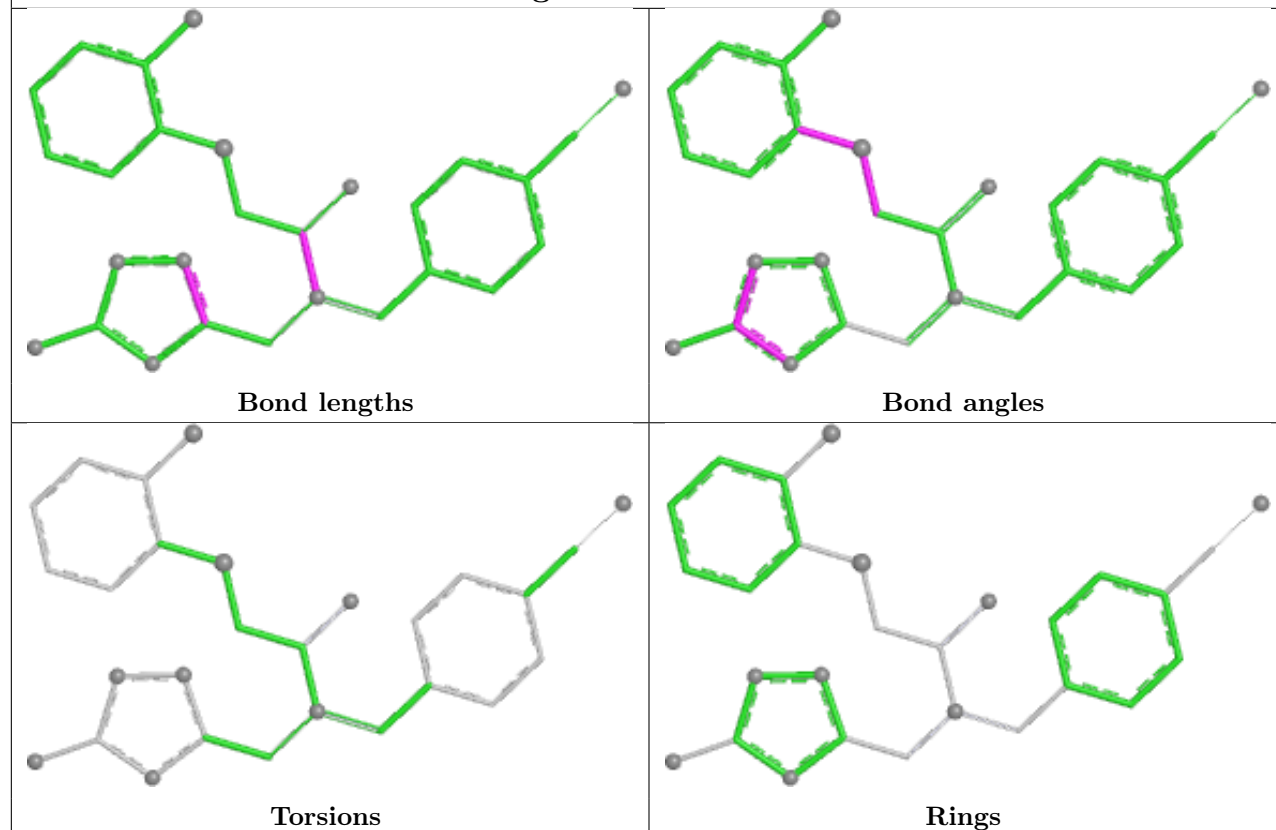
Ligand VFN A 302



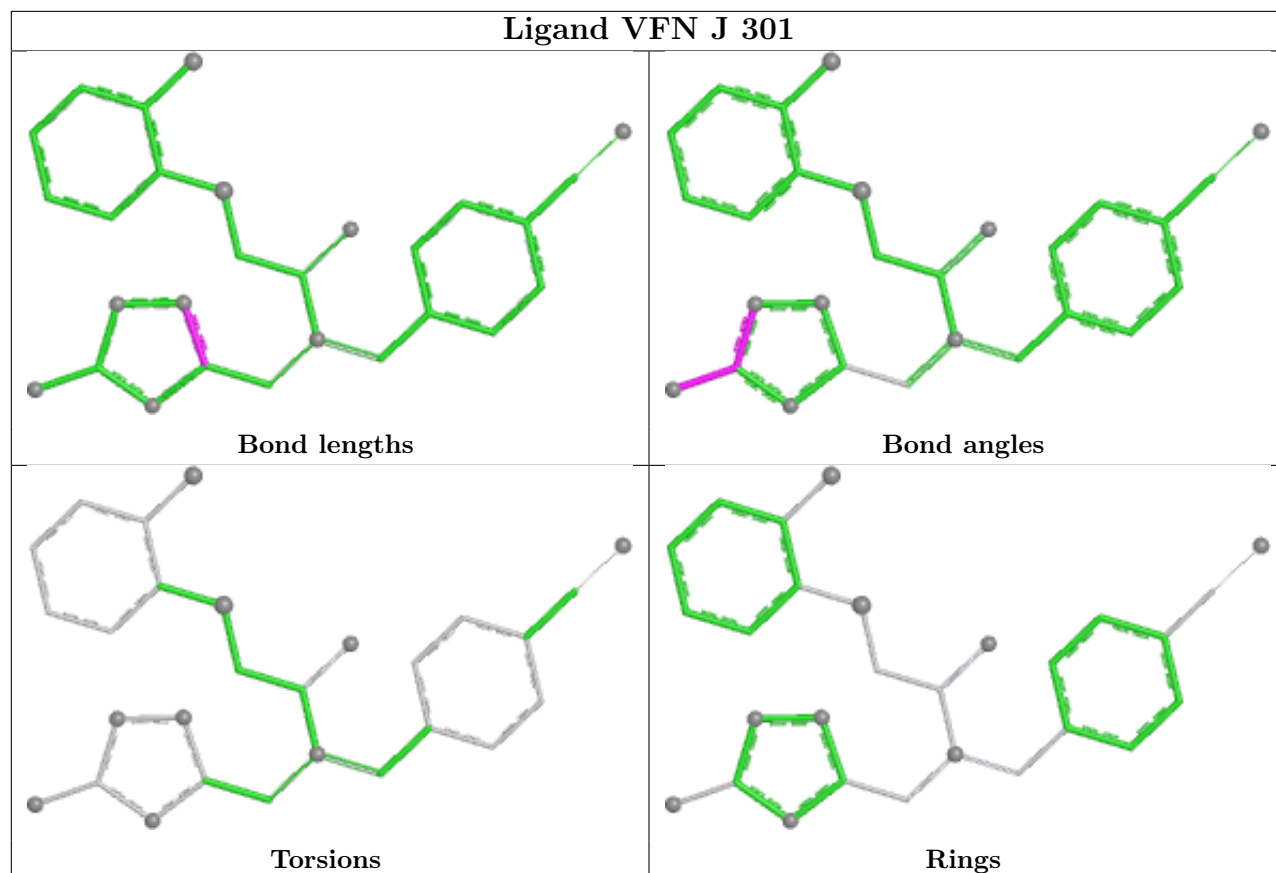
Ligand VFN S 302



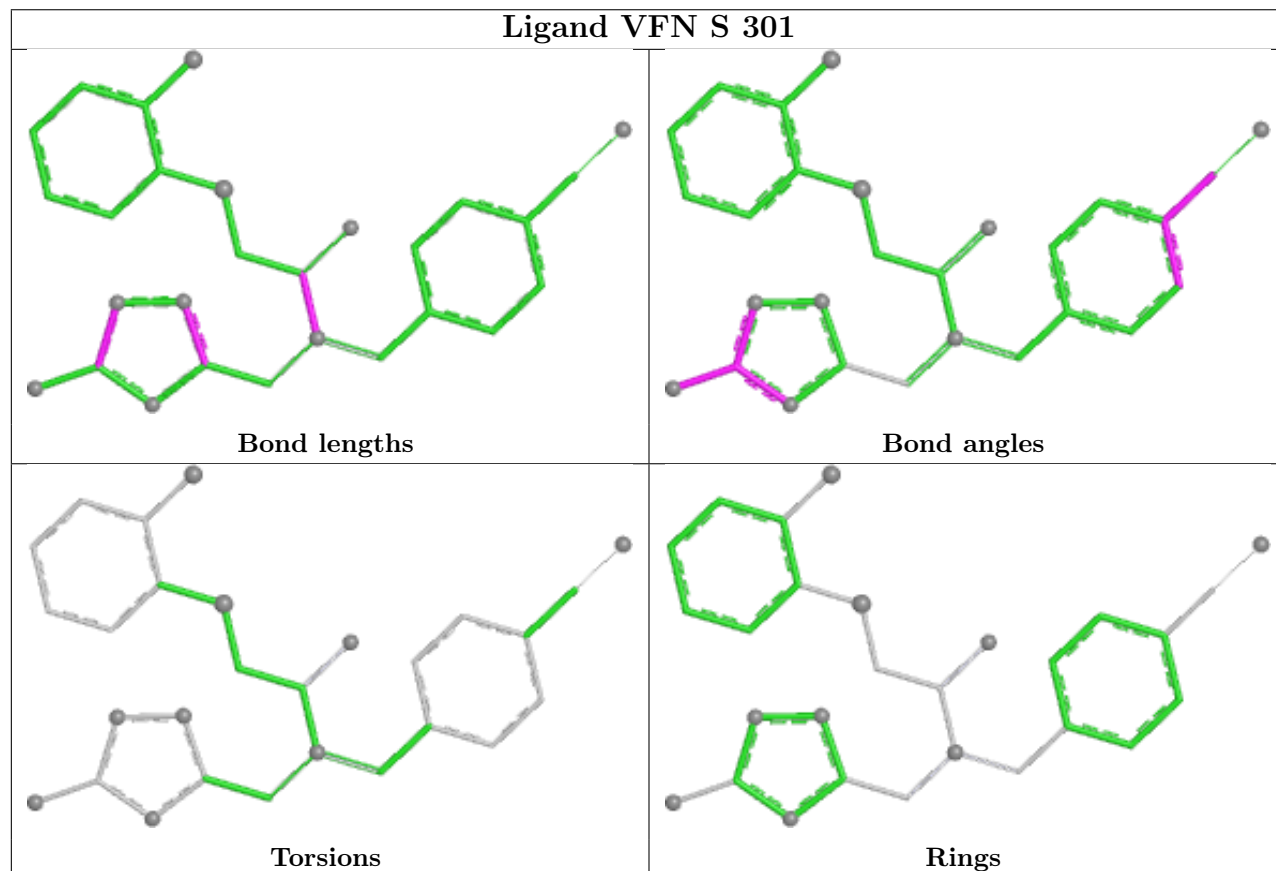
Ligand VFN F 301



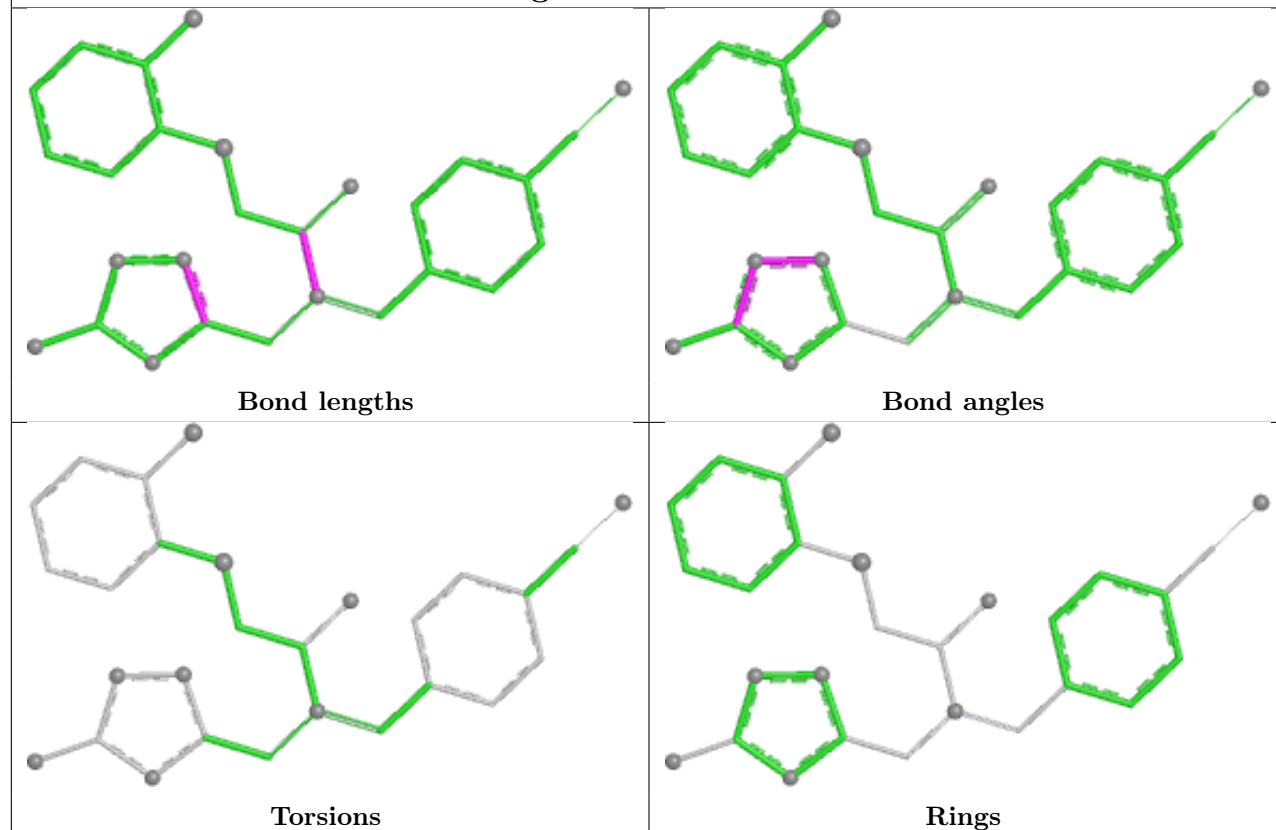
Ligand VFN J 301



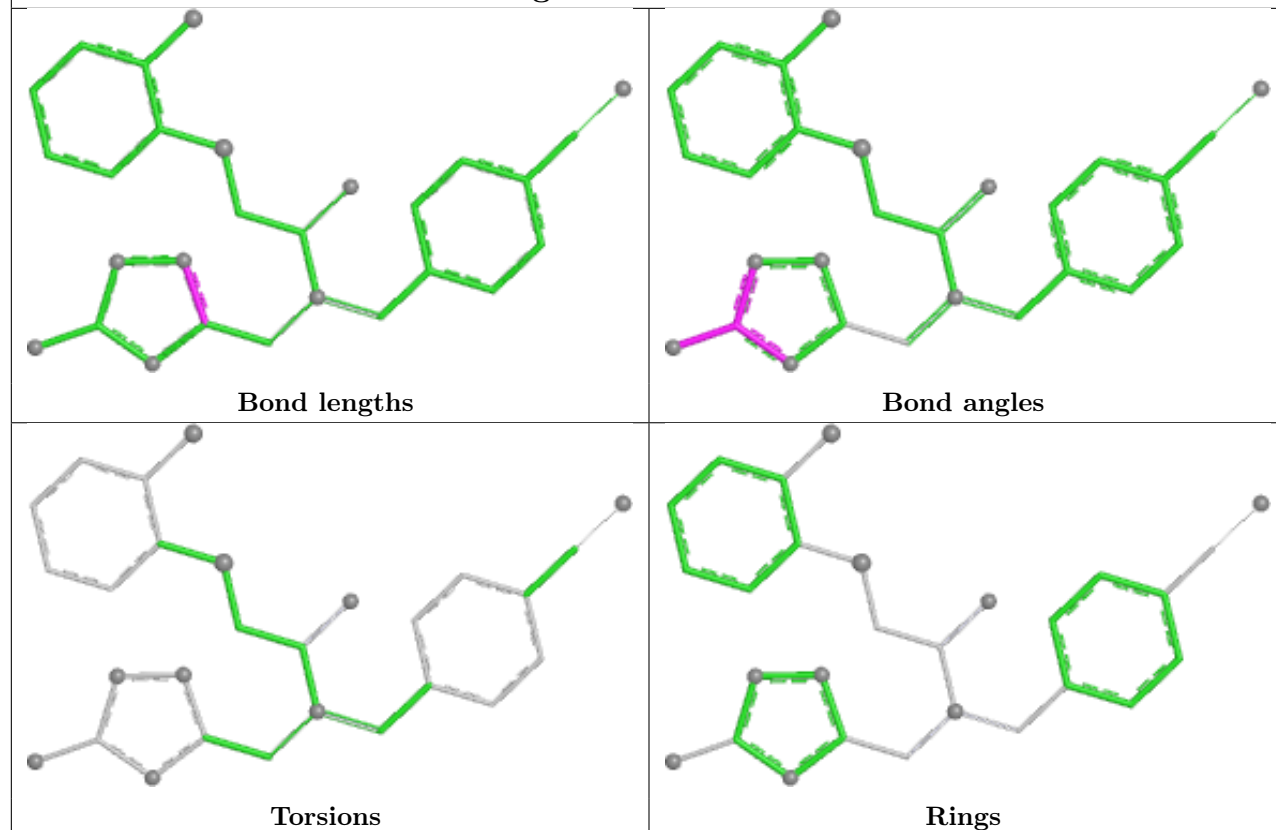
Ligand VFN S 301



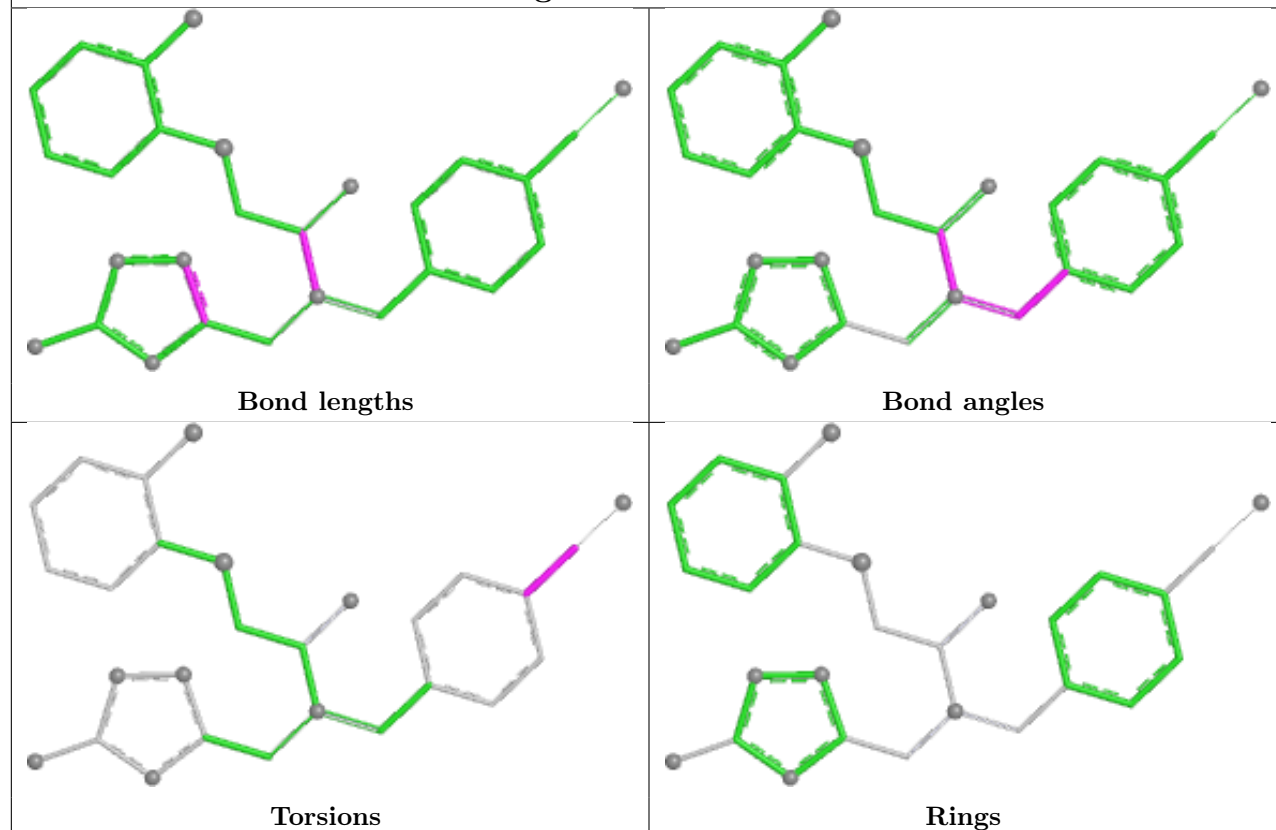
Ligand VFN P 301



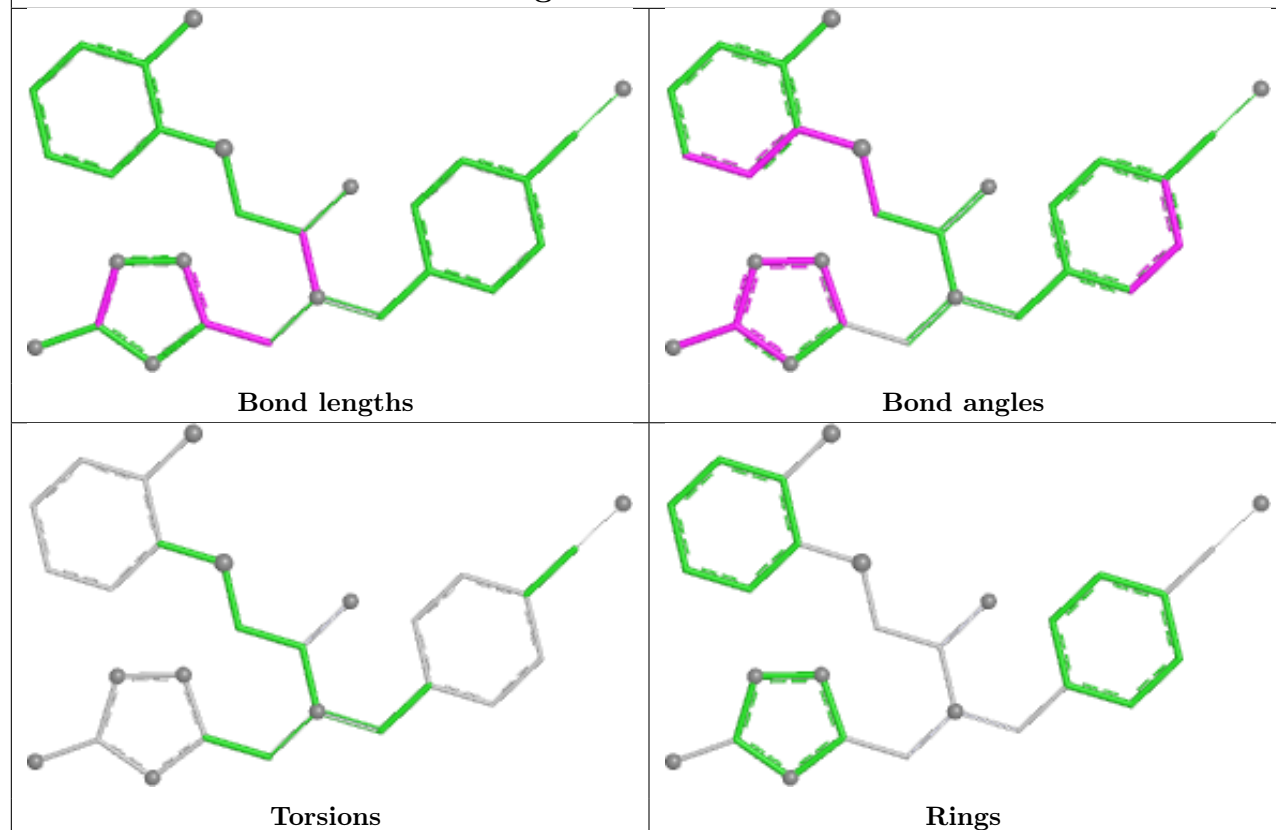
Ligand VFN Z 301

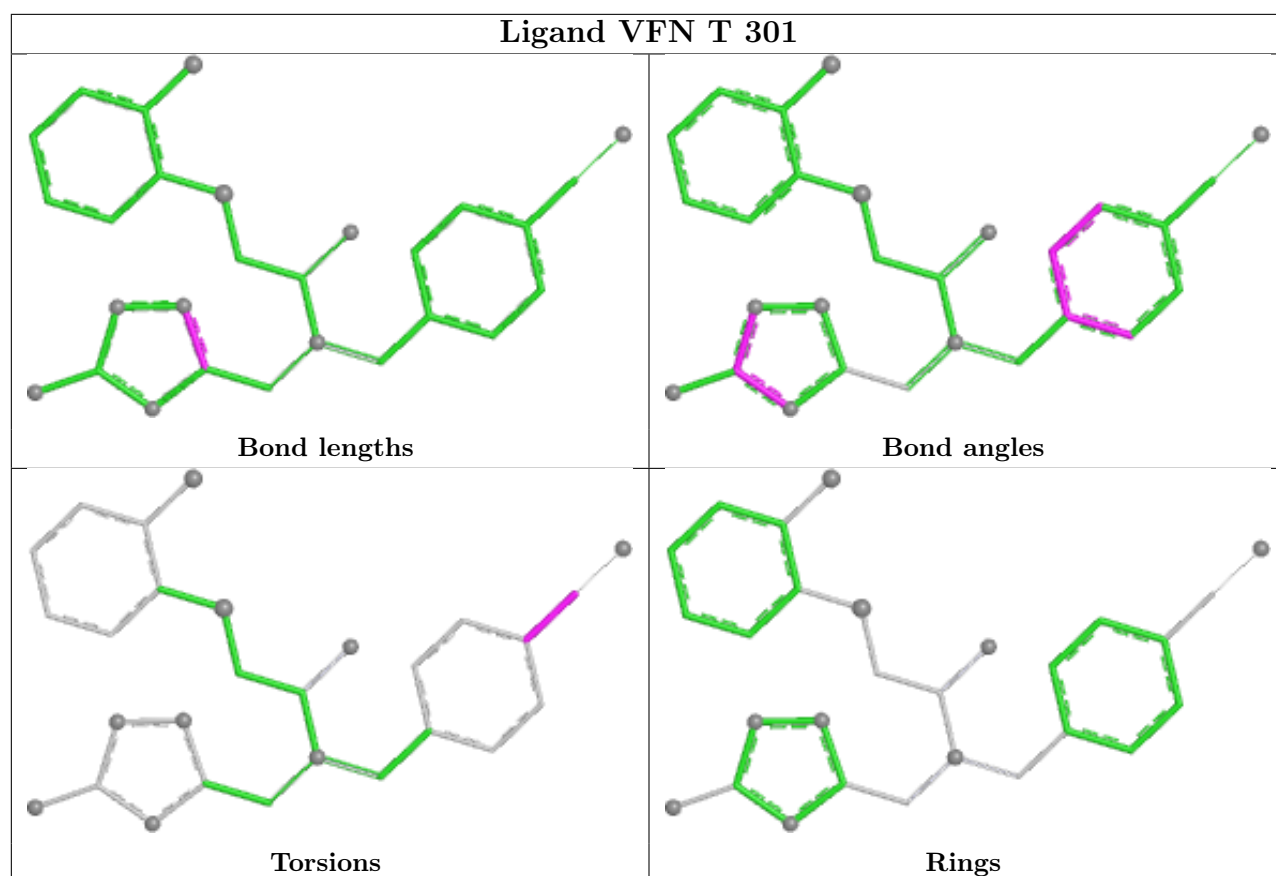


Ligand VFN 3 301



Ligand VFN 1 302





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	1	258/261 (98%)	-0.02	5 (1%) 66 58	50, 66, 87, 119	0
1	2	258/261 (98%)	-0.02	4 (1%) 70 62	50, 65, 86, 122	0
1	3	258/261 (98%)	-0.11	4 (1%) 70 62	47, 65, 84, 111	0
1	4	258/261 (98%)	-0.15	2 (0%) 82 77	46, 63, 82, 103	0
1	A	258/261 (98%)	0.02	3 (1%) 76 69	51, 66, 87, 104	0
1	B	258/261 (98%)	-0.00	7 (2%) 56 47	51, 65, 85, 105	0
1	C	258/261 (98%)	0.03	7 (2%) 56 47	52, 64, 85, 105	0
1	D	258/261 (98%)	-0.02	5 (1%) 66 58	47, 63, 85, 111	0
1	E	258/261 (98%)	-0.02	4 (1%) 70 62	47, 65, 83, 109	0
1	F	258/261 (98%)	0.02	3 (1%) 76 69	51, 66, 87, 116	0
1	G	258/261 (98%)	0.19	4 (1%) 70 62	54, 73, 99, 123	0
1	H	258/261 (98%)	0.22	6 (2%) 61 52	58, 75, 102, 116	0
1	I	258/261 (98%)	0.18	2 (0%) 82 77	53, 73, 100, 124	0
1	J	258/261 (98%)	0.14	9 (3%) 47 38	51, 74, 106, 130	0
1	K	258/261 (98%)	0.20	4 (1%) 70 62	58, 76, 101, 121	0
1	L	258/261 (98%)	0.17	5 (1%) 66 58	56, 73, 100, 135	0
1	M	258/261 (98%)	0.11	3 (1%) 76 69	55, 72, 102, 125	0
1	N	258/261 (98%)	0.12	5 (1%) 66 58	55, 74, 100, 118	0
1	O	258/261 (98%)	0.13	5 (1%) 66 58	52, 72, 103, 121	0
1	P	258/261 (98%)	0.19	8 (3%) 51 42	57, 73, 100, 131	0
1	Q	258/261 (98%)	0.20	10 (3%) 43 35	58, 74, 102, 124	0
1	R	258/261 (98%)	0.05	5 (1%) 66 58	53, 71, 100, 136	0
1	S	258/261 (98%)	-0.05	3 (1%) 76 69	50, 66, 87, 112	0
1	T	258/261 (98%)	-0.02	3 (1%) 76 69	51, 66, 86, 118	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	U	258/261 (98%)	0.00	6 (2%) 61 52	49, 64, 84, 104	0
1	V	258/261 (98%)	-0.01	3 (1%) 76 69	52, 66, 85, 109	0
1	W	258/261 (98%)	-0.03	5 (1%) 66 58	45, 65, 87, 119	0
1	X	258/261 (98%)	-0.06	4 (1%) 70 62	48, 63, 81, 105	0
1	Y	258/261 (98%)	-0.06	2 (0%) 82 77	48, 66, 85, 116	0
1	Z	258/261 (98%)	-0.02	3 (1%) 76 69	48, 66, 83, 108	0
All	All	7740/7830 (98%)	0.05	139 (1%) 67 59	45, 68, 95, 136	0

All (139) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	1	MET	4.9
1	W	1	MET	4.7
1	3	1	MET	4.7
1	D	1	MET	4.6
1	Q	253	THR	4.6
1	B	1	MET	4.3
1	N	253	THR	4.2
1	P	1	MET	4.2
1	Q	1	MET	4.2
1	L	1	MET	4.1
1	R	1	MET	4.1
1	T	1	MET	4.0
1	C	1	MET	4.0
1	G	1	MET	3.9
1	M	1	MET	3.8
1	Y	1	MET	3.8
1	1	1	MET	3.8
1	F	1	MET	3.8
1	I	1	MET	3.7
1	H	1	MET	3.6
1	K	1	MET	3.6
1	A	1	MET	3.6
1	O	1	MET	3.6
1	R	68	THR	3.5
1	H	3	LEU	3.5
1	J	68	THR	3.5
1	K	18	ALA	3.5
1	P	68	THR	3.5
1	F	102	ARG	3.4

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Mol	Chain	Res	Type	RSRZ
1	2	1	MET	3.4
1	S	1	MET	3.4
1	E	253	THR	3.3
1	V	1	MET	3.3
1	Z	1	MET	3.3
1	E	15	ARG	3.3
1	L	102	ARG	3.2
1	T	2	SER	3.2
1	B	253	THR	3.1
1	U	253	THR	3.1
1	I	68	THR	3.1
1	N	68	THR	3.0
1	B	251	SER	2.9
1	L	68	THR	2.9
1	P	258	ARG	2.9
1	C	18	ALA	2.8
1	J	1	MET	2.8
1	Y	15	ARG	2.8
1	M	18	ALA	2.8
1	Z	68	THR	2.8
1	4	1	MET	2.7
1	N	1	MET	2.7
1	J	18	ALA	2.7
1	J	253	THR	2.7
1	Q	15	ARG	2.7
1	B	15	ARG	2.7
1	T	253	THR	2.7
1	U	1	MET	2.6
1	Q	57	ARG	2.6
1	2	2	SER	2.6
1	O	102	ARG	2.6
1	2	102	ARG	2.5
1	P	251	SER	2.5
1	1	18	ALA	2.5
1	D	18	ALA	2.5
1	G	79	ARG	2.5
1	P	254	ARG	2.5
1	P	3	LEU	2.5
1	X	1	MET	2.5
1	H	254	ARG	2.5
1	G	253	THR	2.5
1	P	6	PRO	2.4

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Mol	Chain	Res	Type	RSRZ
1	4	102	ARG	2.4
1	U	226	GLU	2.4
1	L	3	LEU	2.4
1	J	12	PRO	2.4
1	P	15	ARG	2.4
1	C	68	THR	2.4
1	O	18	ALA	2.4
1	J	3	LEU	2.4
1	Q	252	ALA	2.4
1	B	18	ALA	2.3
1	Q	2	SER	2.3
1	A	57	ARG	2.3
1	W	250	GLN	2.3
1	V	4	ILE	2.3
1	K	13	SER	2.3
1	Q	77	PRO	2.3
1	B	250	GLN	2.2
1	X	225	VAL	2.2
1	1	254	ARG	2.2
1	R	102	ARG	2.2
1	U	258	ARG	2.2
1	O	225	VAL	2.2
1	C	102	ARG	2.2
1	C	258	ARG	2.2
1	D	258	ARG	2.2
1	E	254	ARG	2.2
1	J	220	ARG	2.2
1	Q	102	ARG	2.2
1	J	77	PRO	2.2
1	3	253	THR	2.2
1	A	253	THR	2.2
1	C	253	THR	2.2
1	C	2	SER	2.2
1	R	3	LEU	2.2
1	X	57	ARG	2.2
1	H	99	VAL	2.2
1	M	19	ASP	2.2
1	H	68	THR	2.2
1	Q	68	THR	2.2
1	D	102	ARG	2.1
1	1	68	THR	2.1
1	1	3	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
1	3	15	ARG	2.1
1	S	102	ARG	2.1
1	J	102	ARG	2.1
1	F	2	SER	2.1
1	U	68	THR	2.1
1	V	254	ARG	2.1
1	W	102	ARG	2.1
1	B	252	ALA	2.1
1	G	220	ARG	2.1
1	R	220	ARG	2.1
1	U	102	ARG	2.1
1	Q	4	ILE	2.1
1	D	254	ARG	2.0
1	N	15	ARG	2.0
1	O	15	ARG	2.0
1	L	253	THR	2.0
1	W	253	THR	2.0
1	S	74	LYS	2.0
1	2	251	SER	2.0
1	K	6	PRO	2.0
1	N	6	PRO	2.0
1	X	3	LEU	2.0
1	Z	254	ARG	2.0
1	3	18	ALA	2.0
1	H	18	ALA	2.0
1	W	18	ALA	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 oligosaccharides 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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	SO4	L	302	5/5	0.87	0.16	93,93,95,95	0
3	SO4	F	302	5/5	0.91	0.13	84,84,85,88	0
3	SO4	C	302	5/5	0.92	0.14	98,99,100,100	0
3	SO4	T	302	5/5	0.92	0.10	78,78,80,82	0
3	SO4	A	303	5/5	0.93	0.12	88,88,89,89	0
3	SO4	H	303	5/5	0.93	0.11	92,93,93,96	0
3	SO4	C	301	5/5	0.93	0.12	98,98,99,99	0
3	SO4	M	301	5/5	0.93	0.11	90,90,91,92	0
3	SO4	Q	301	5/5	0.93	0.13	85,85,85,87	0
3	SO4	1	303	5/5	0.93	0.11	91,92,92,93	0
3	SO4	3	303	5/5	0.94	0.16	92,92,94,94	0
2	VFN	D	302	28/28	0.94	0.14	59,66,70,72	0
3	SO4	N	302	5/5	0.94	0.11	89,90,91,92	0
3	SO4	P	303	5/5	0.94	0.09	95,96,96,96	0
3	SO4	G	302	5/5	0.94	0.09	99,100,100,101	0
2	VFN	3	302	28/28	0.94	0.13	61,72,76,76	0
3	SO4	Y	301	5/5	0.94	0.13	91,91,93,94	0
3	SO4	Z	302	5/5	0.94	0.12	81,81,83,83	0
2	VFN	W	301	28/28	0.95	0.12	56,64,72,73	0
2	VFN	A	301	28/28	0.95	0.10	61,66,71,72	0
3	SO4	2	302	5/5	0.95	0.12	94,96,98,98	0
2	VFN	H	302	28/28	0.95	0.13	73,77,84,85	0
2	VFN	J	301	28/28	0.95	0.12	61,75,84,85	0
2	VFN	K	301	28/28	0.95	0.12	77,90,93,93	0
3	SO4	R	302	5/5	0.95	0.11	79,82,83,84	0
2	VFN	P	301	28/28	0.95	0.11	77,83,86,88	0
3	SO4	V	302	5/5	0.95	0.12	88,90,91,91	0
3	SO4	W	303	5/5	0.95	0.12	91,93,93,94	0
2	VFN	R	301	28/28	0.95	0.11	71,75,81,82	0
2	VFN	S	301	28/28	0.95	0.11	64,71,74,76	0
3	SO4	B	302	5/5	0.96	0.10	75,76,77,77	0
2	VFN	L	301	28/28	0.96	0.11	78,81,87,87	0
2	VFN	N	301	28/28	0.96	0.11	64,72,85,86	0
2	VFN	O	301	28/28	0.96	0.11	66,74,77,80	0
2	VFN	O	302	28/28	0.96	0.11	80,84,88,89	0
2	VFN	A	302	28/28	0.96	0.10	65,73,76,76	0
3	SO4	I	301	5/5	0.96	0.09	80,82,82,83	0
3	SO4	J	302	5/5	0.96	0.12	83,86,87,89	0
3	SO4	K	302	5/5	0.96	0.08	88,89,90,92	0
2	VFN	P	302	28/28	0.96	0.10	67,73,76,77	0
2	VFN	B	301	28/28	0.96	0.10	68,72,76,77	0
2	VFN	2	301	28/28	0.96	0.10	56,65,72,77	0
3	SO4	O	303	5/5	0.96	0.08	85,87,87,87	0

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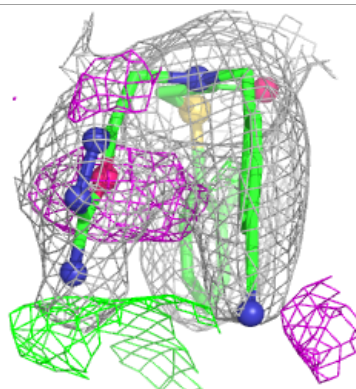
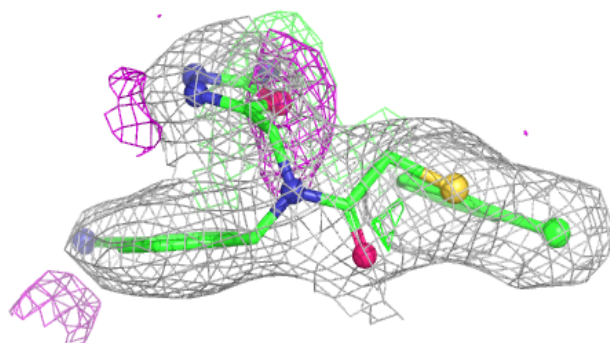
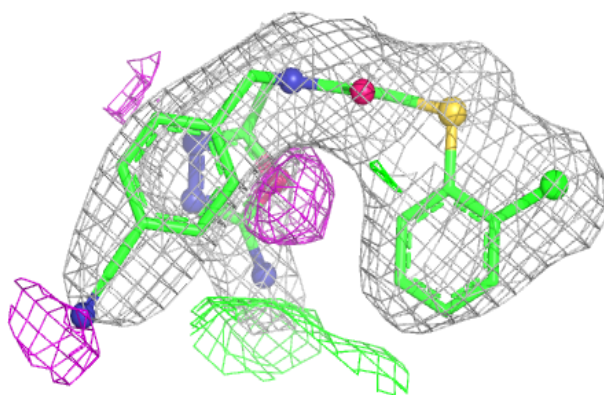
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	VFN	V	301	28/28	0.96	0.09	51,63,67,68	0
2	VFN	F	301	28/28	0.96	0.09	51,62,70,75	0
2	VFN	Z	301	28/28	0.96	0.10	60,67,78,79	0
2	VFN	G	301	28/28	0.96	0.11	64,73,79,83	0
3	SO4	U	301	5/5	0.96	0.14	80,82,83,85	0
2	VFN	3	301	28/28	0.96	0.10	60,65,68,69	0
2	VFN	1	301	28/28	0.96	0.09	54,61,67,71	0
3	SO4	4	301	5/5	0.96	0.09	85,86,87,89	0
2	VFN	1	302	28/28	0.96	0.10	56,65,72,75	0
3	SO4	D	303	5/5	0.97	0.10	81,83,84,84	0
3	SO4	E	301	5/5	0.97	0.10	74,76,78,79	0
2	VFN	W	302	28/28	0.97	0.10	57,74,83,84	0
2	VFN	S	302	28/28	0.97	0.09	55,64,73,75	0
2	VFN	T	301	28/28	0.97	0.08	61,68,77,82	0
3	SO4	X	301	5/5	0.97	0.09	90,90,91,94	0
2	VFN	H	301	28/28	0.97	0.10	73,77,81,84	0
2	VFN	D	301	28/28	0.97	0.09	57,65,73,74	0
3	SO4	S	303	5/5	0.98	0.08	76,76,78,79	0

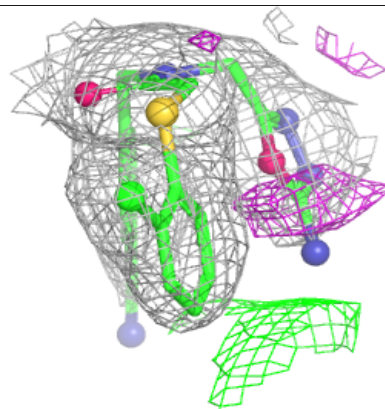
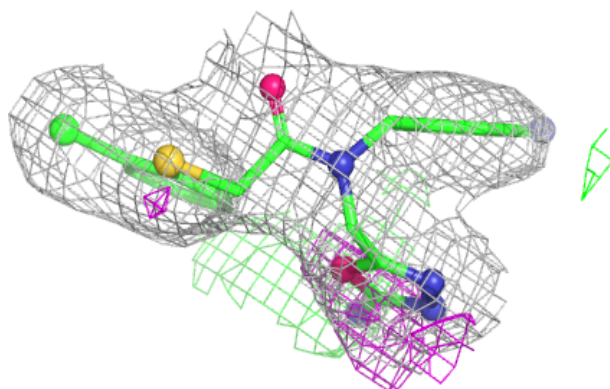
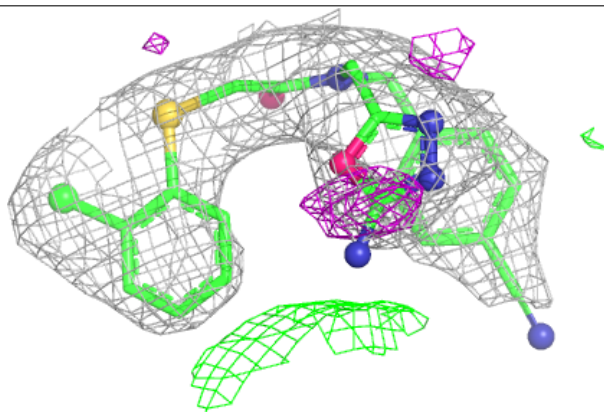
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around VFN D 302:

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

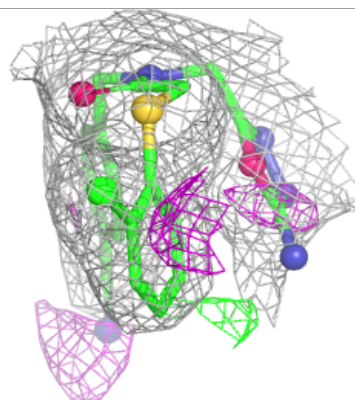
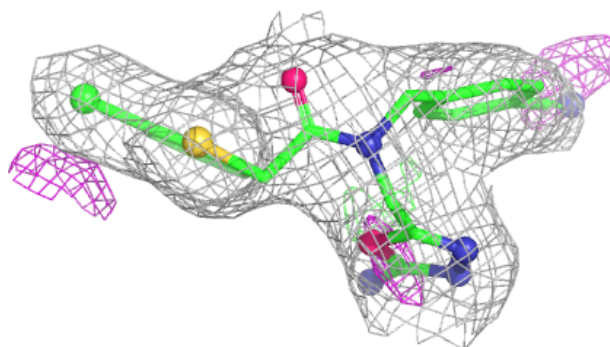
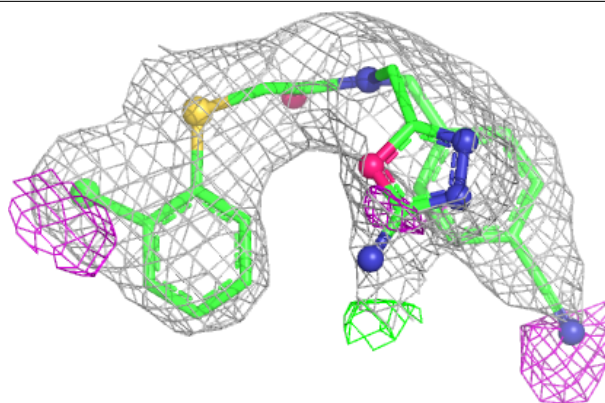
**Electron density around VFN 3 302:**

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

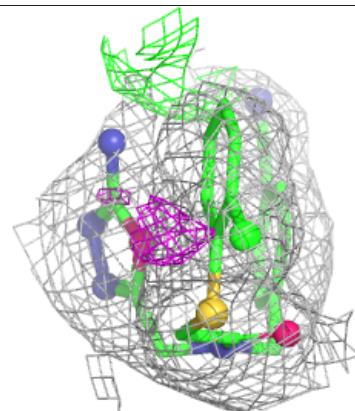
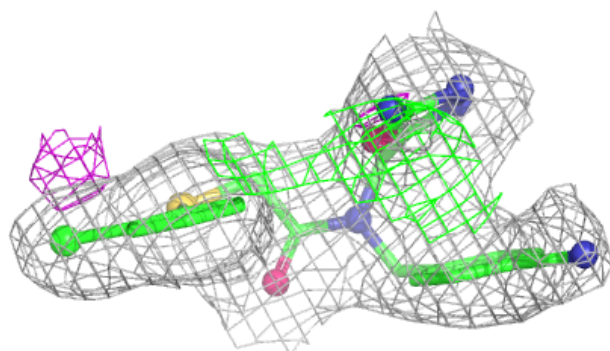
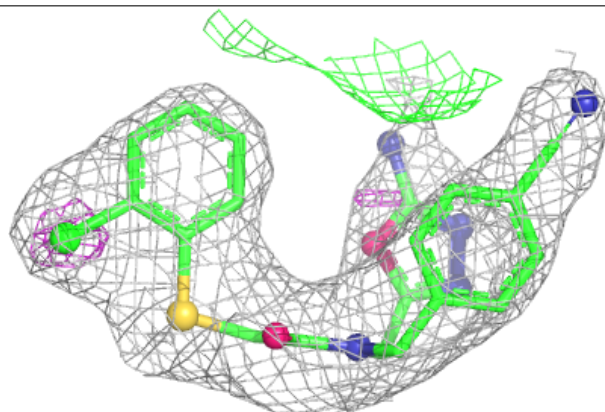


Electron density around VFN W 301:

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

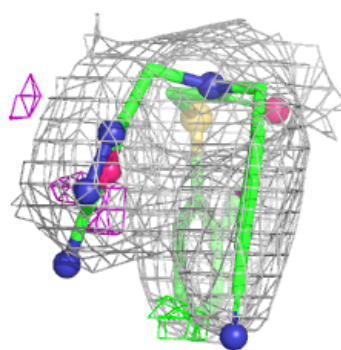
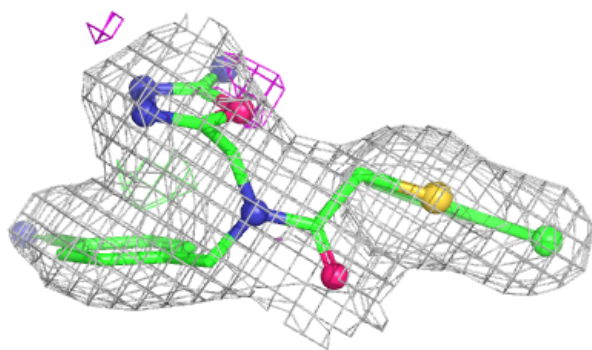
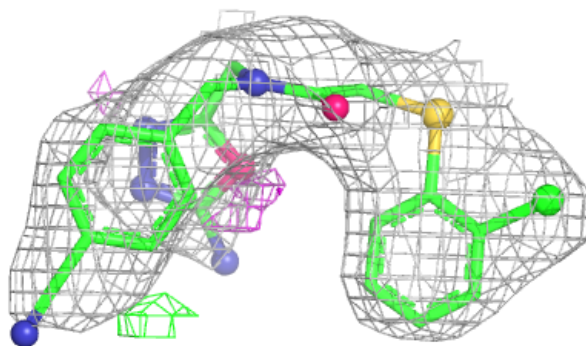
**Electron density around VFN A 301:**

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

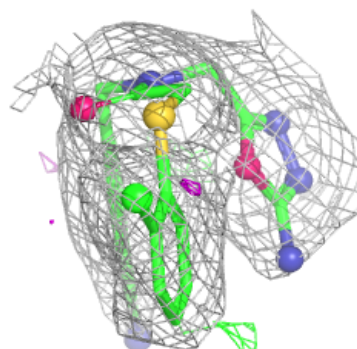
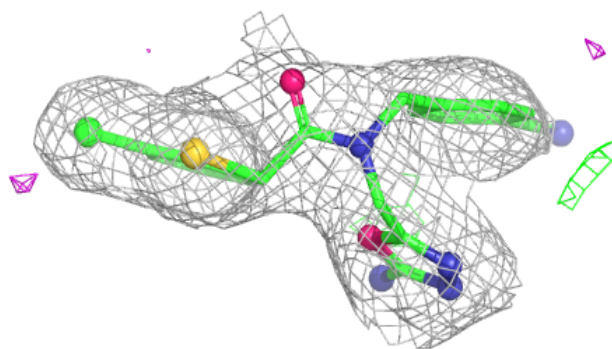
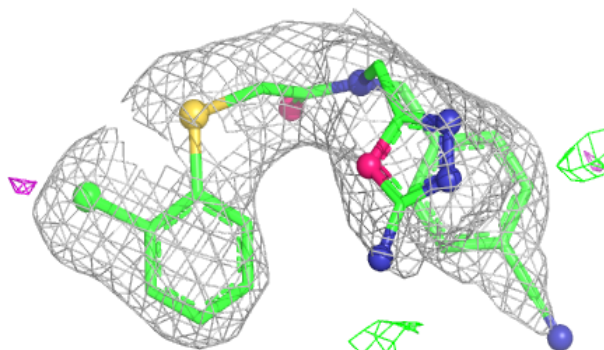


Electron density around VFN H 302:

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

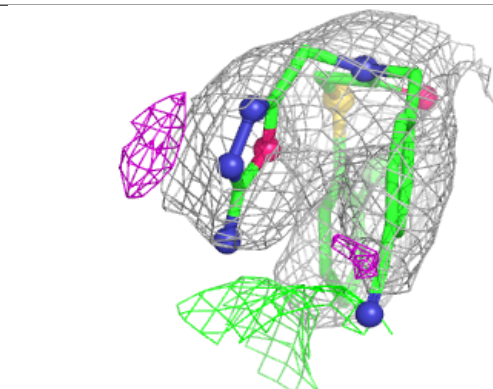
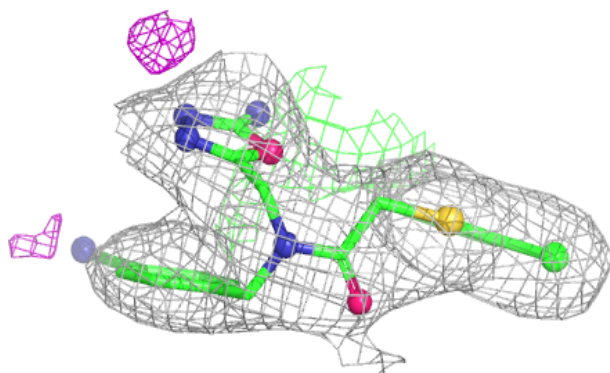
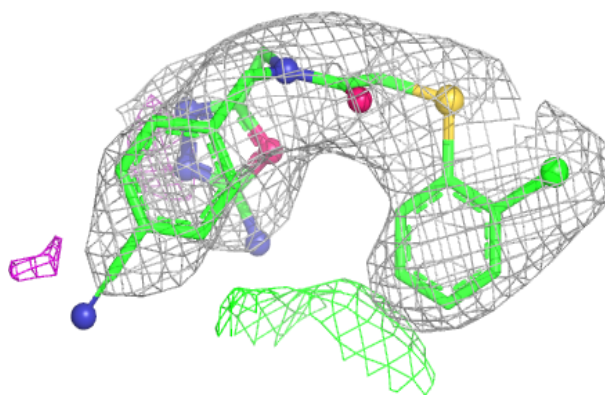
**Electron density around VFN J 301:**

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

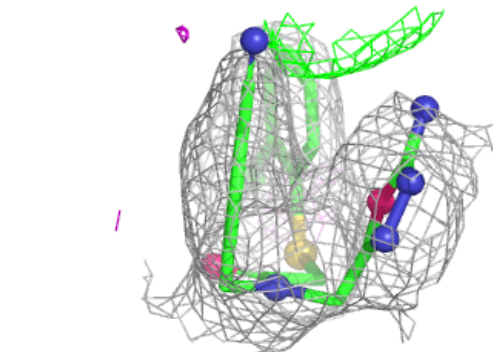
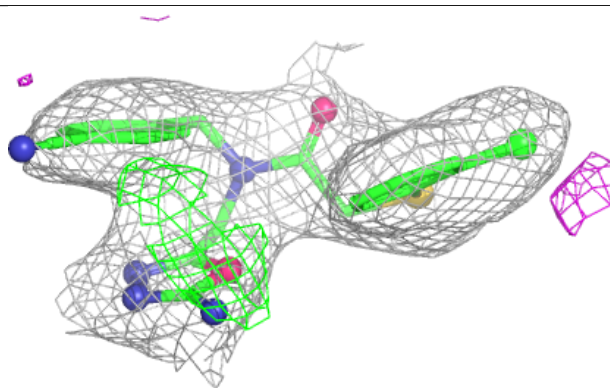
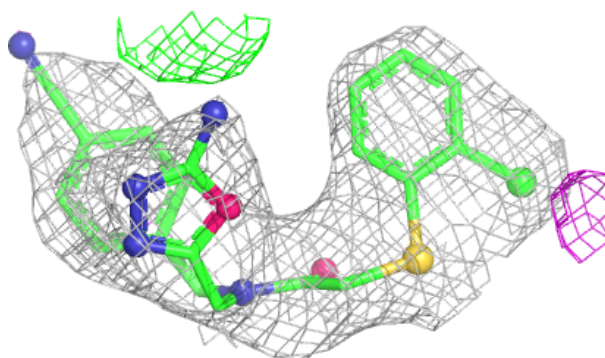


Electron density around VFN K 301:

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

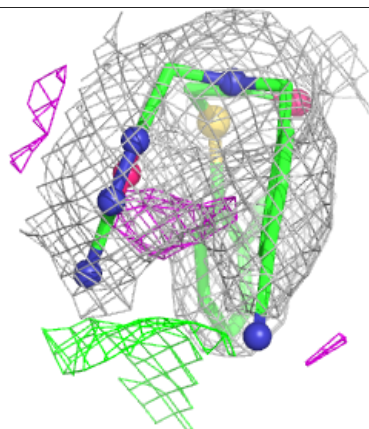
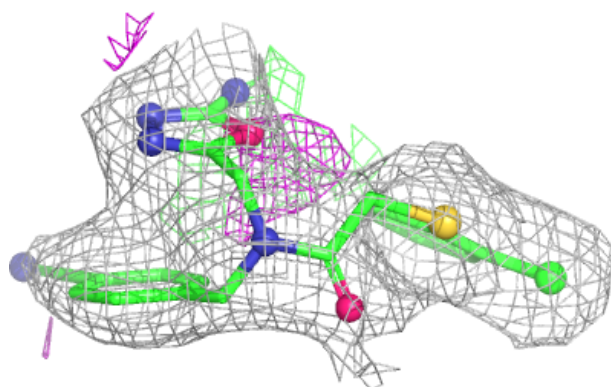
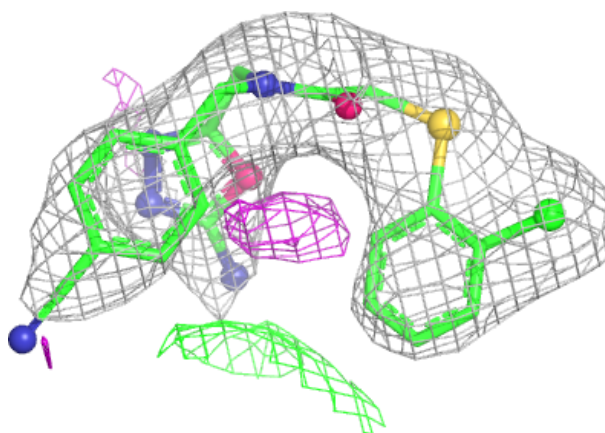
**Electron density around VFN P 301:**

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



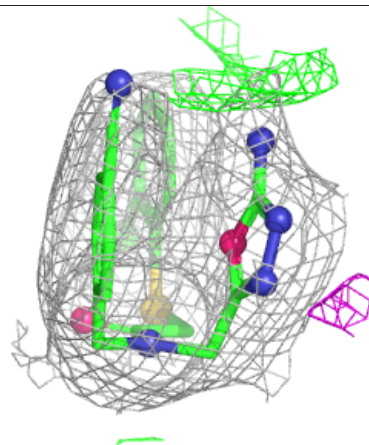
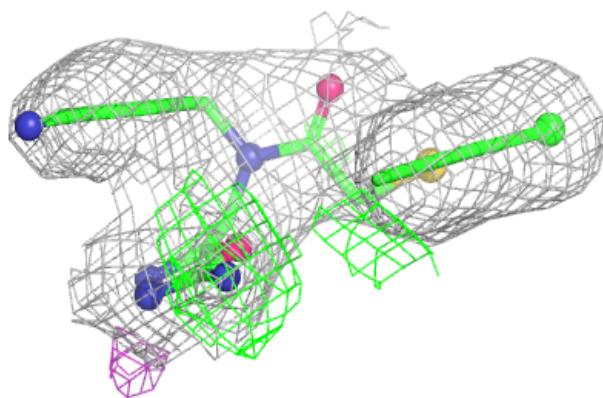
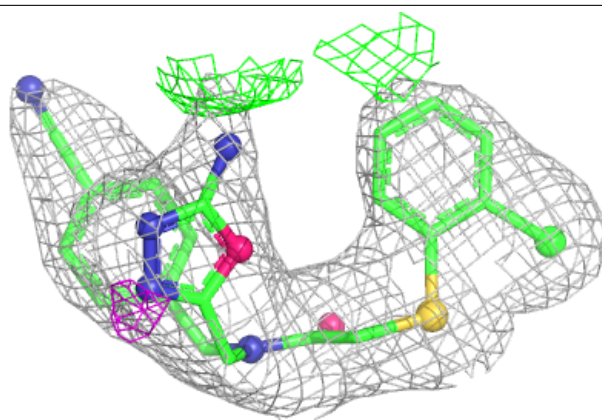
Electron density around VFN R 301:

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



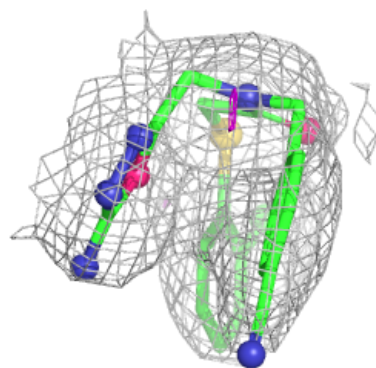
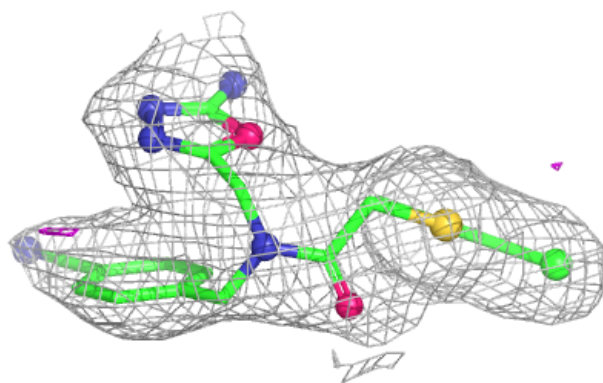
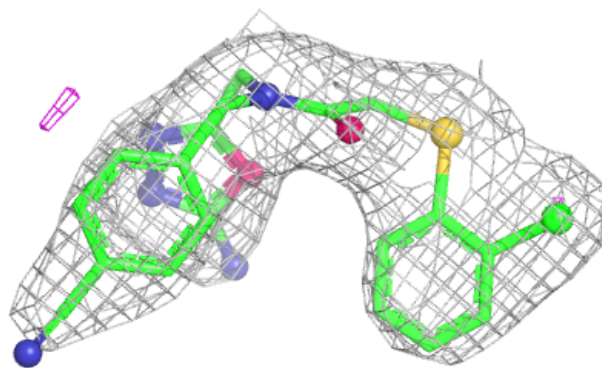
Electron density around VFN S 301:

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

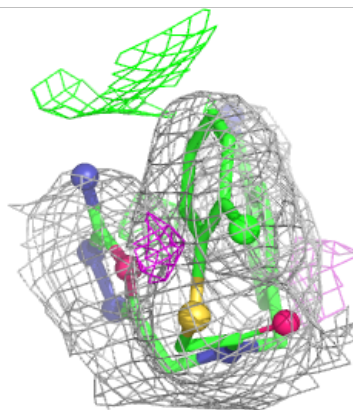
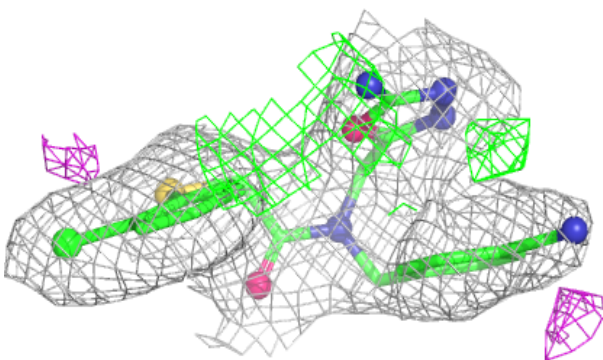
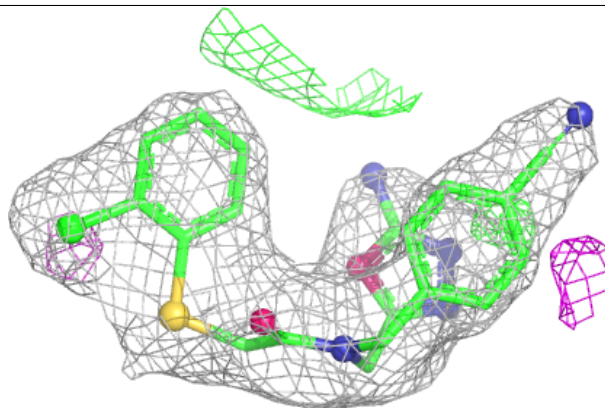


Electron density around VFN L 301:

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

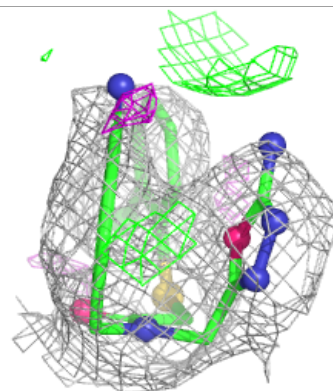
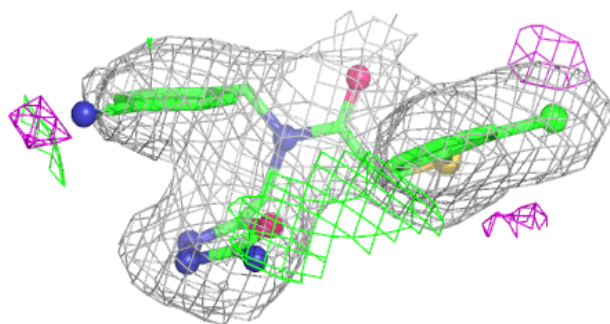
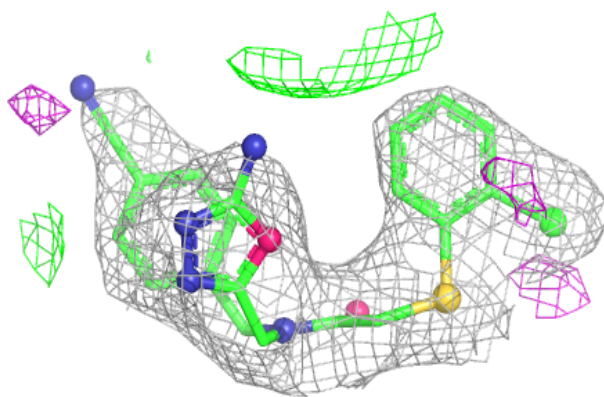
**Electron density around VFN N 301:**

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and green (positive)

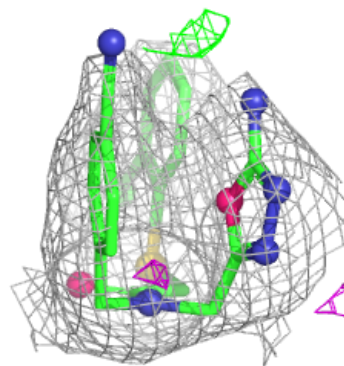
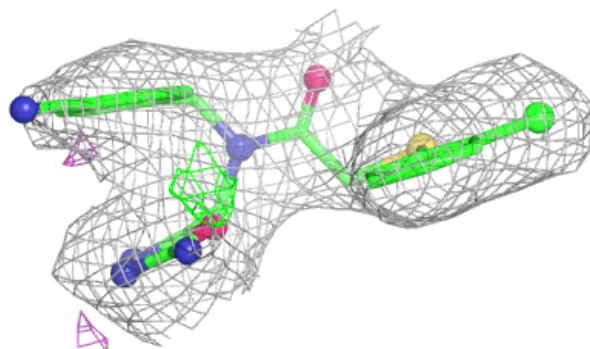
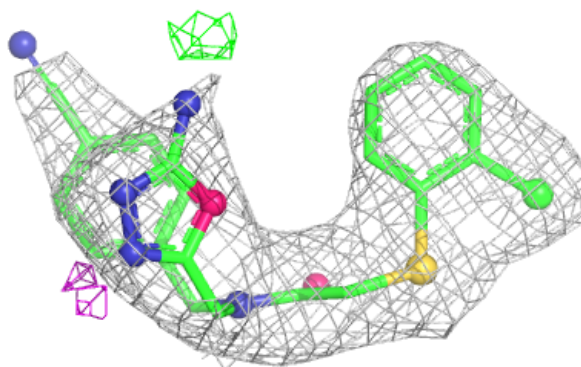


Electron density around VFN O 301:

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and green (positive)

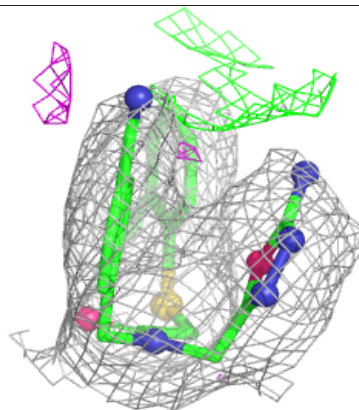
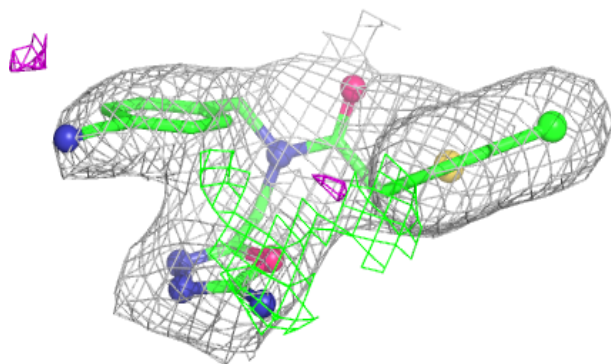
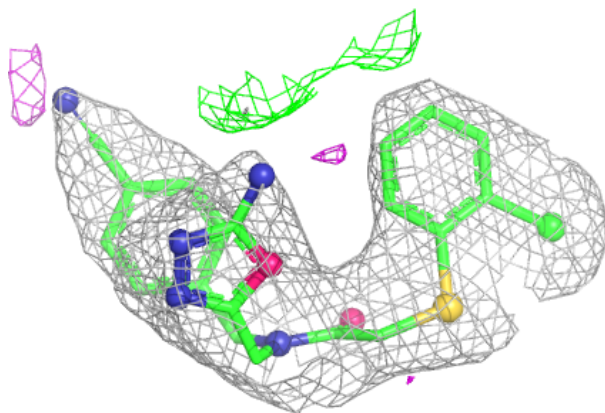
**Electron density around VFN O 302:**

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and green (positive)

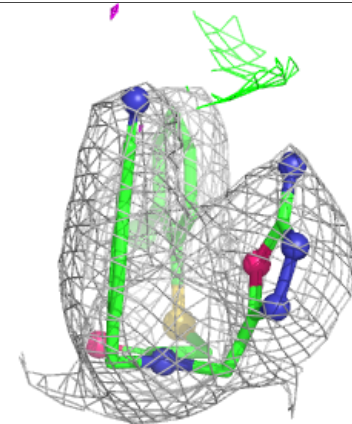
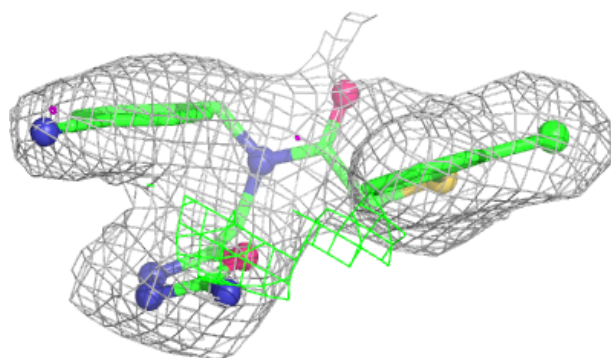
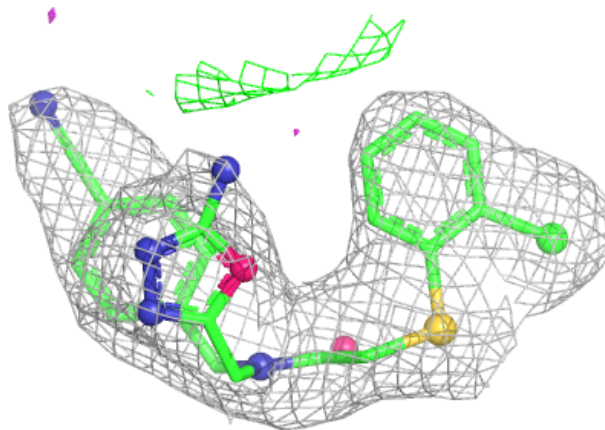


Electron density around VFN A 302:

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

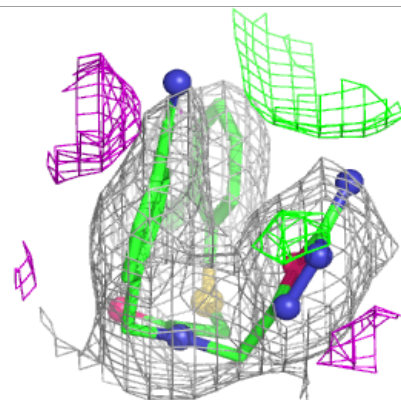
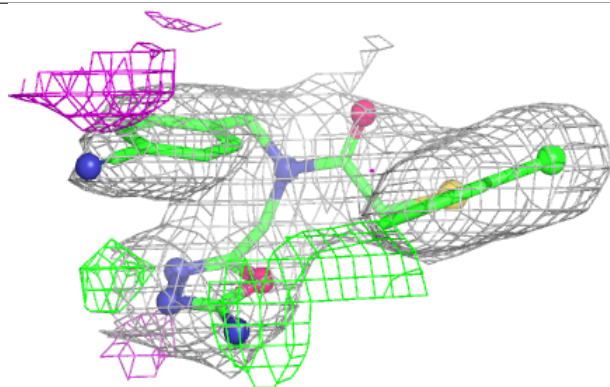
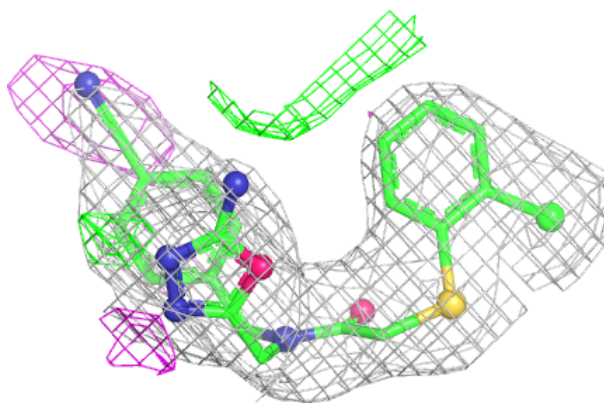
**Electron density around VFN P 302:**

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and green (positive)

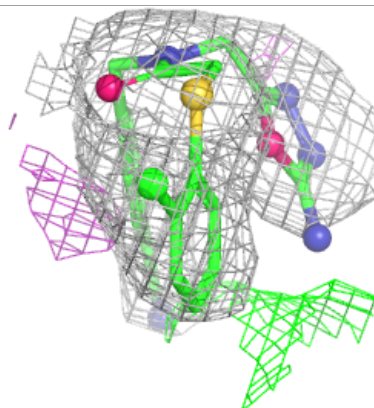
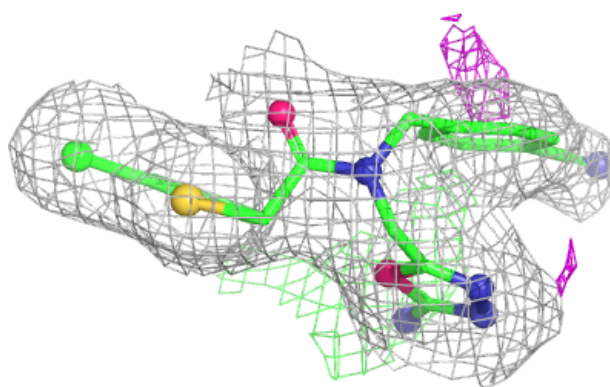
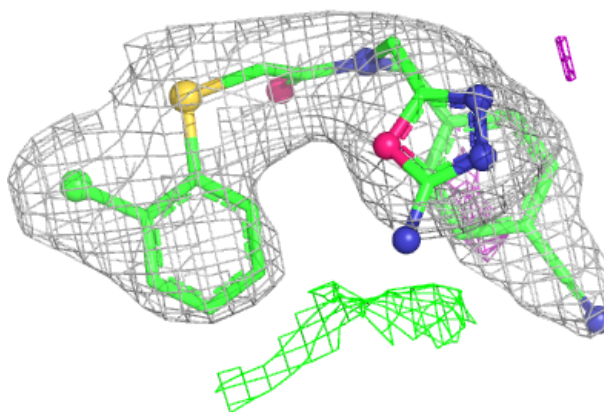


Electron density around VFN B 301:

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

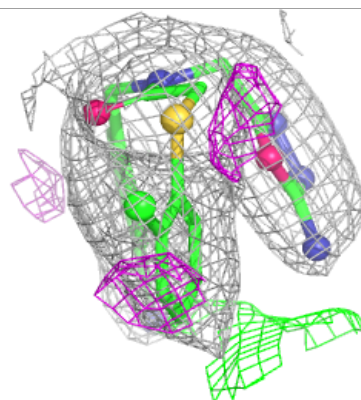
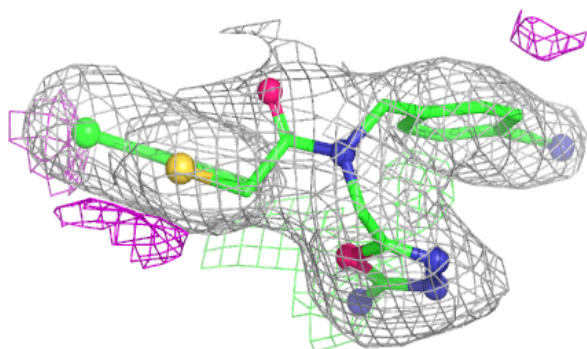
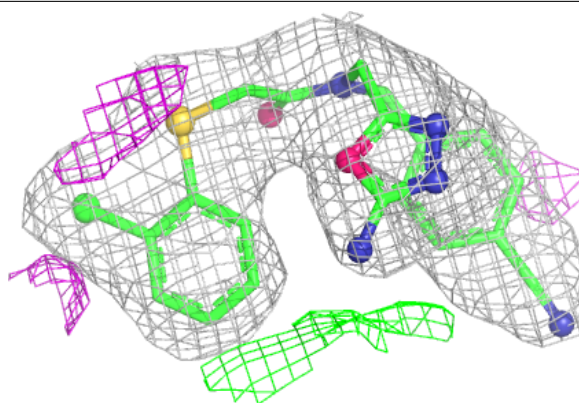
**Electron density around VFN 2 301:**

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

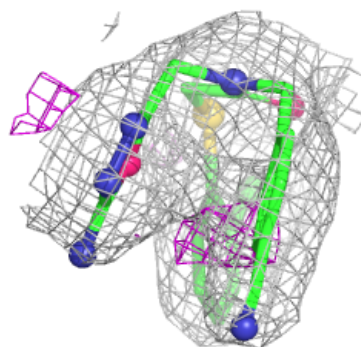
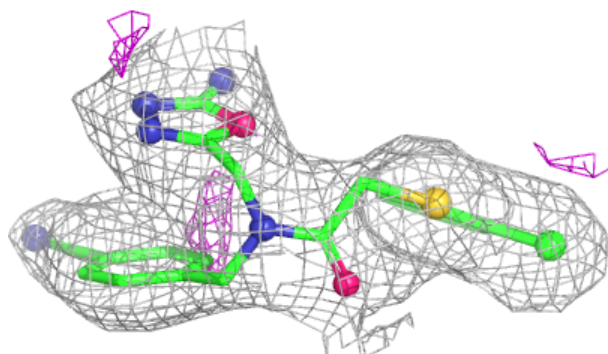
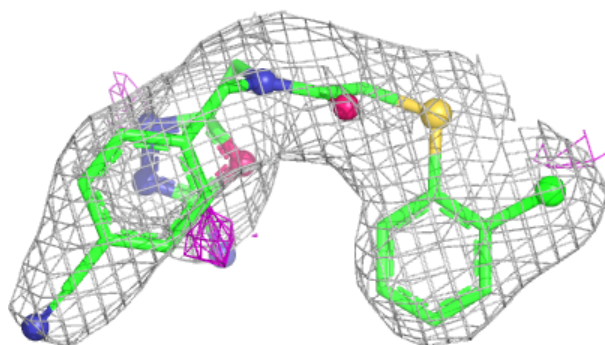


Electron density around VFN V 301:

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

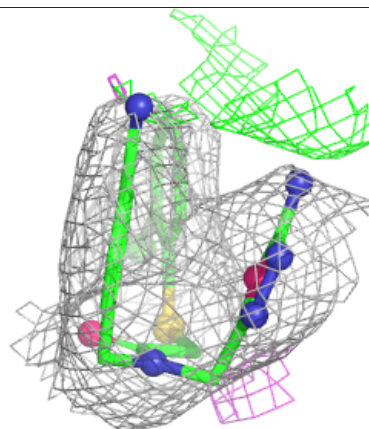
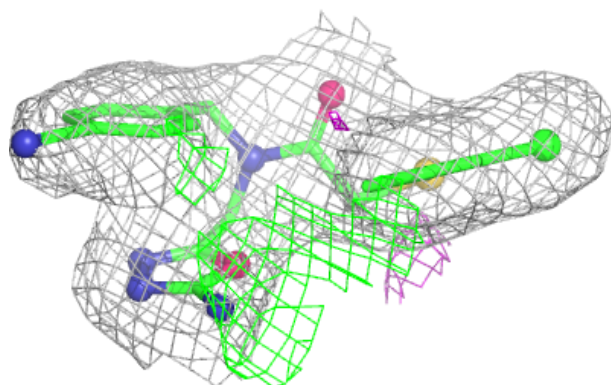
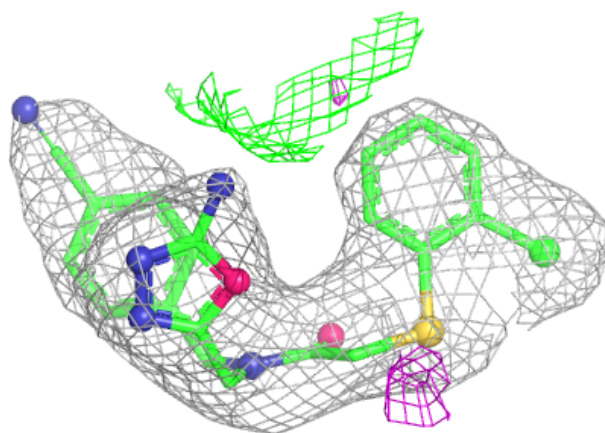
**Electron density around VFN F 301:**

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



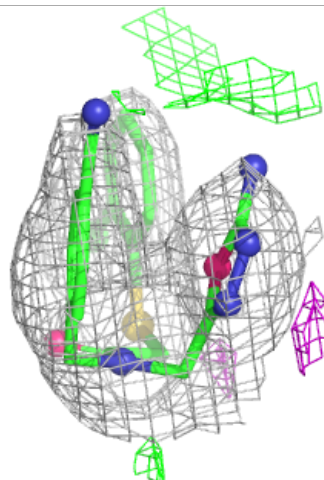
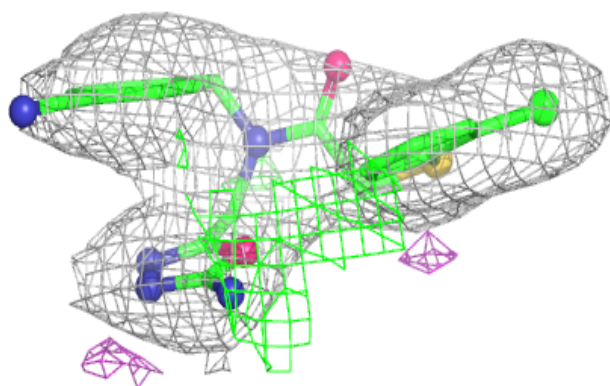
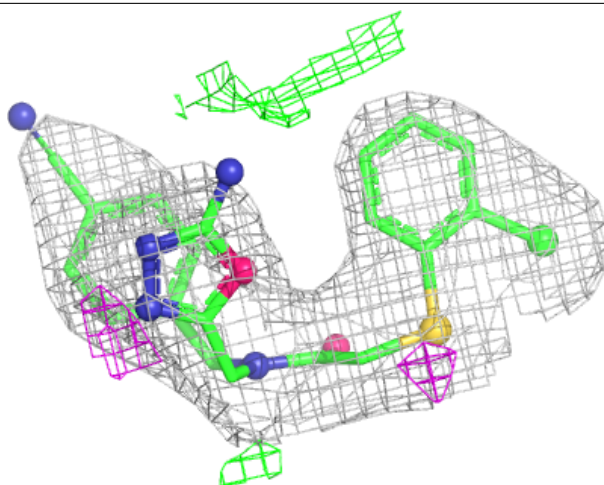
Electron density around VFN Z 301:

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



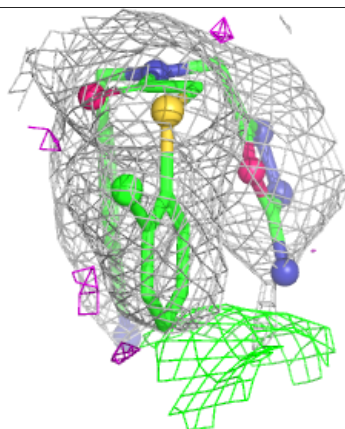
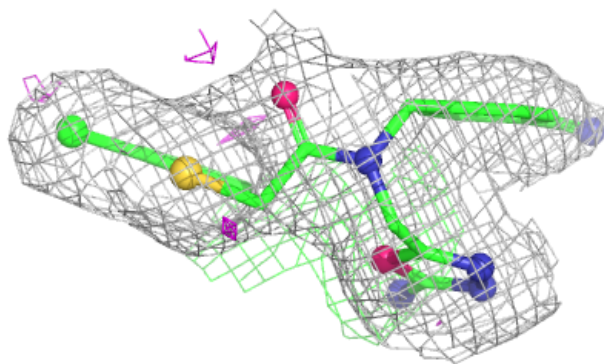
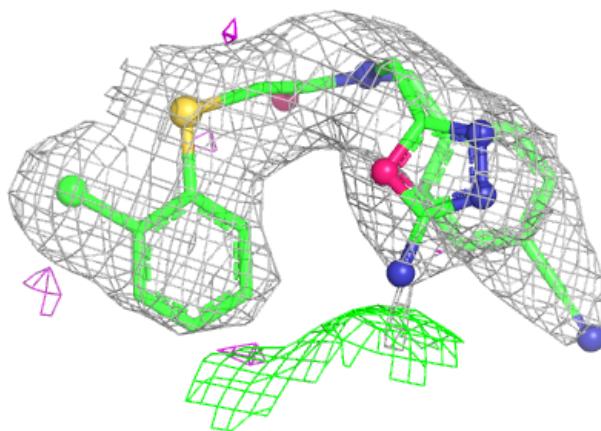
Electron density around VFN G 301:

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

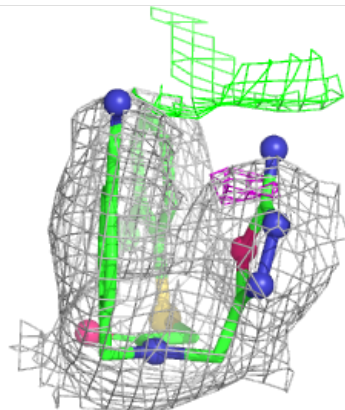
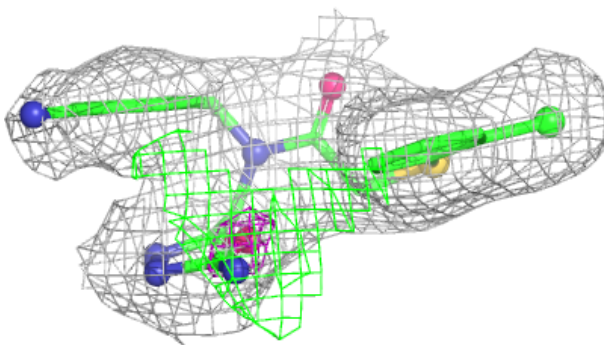
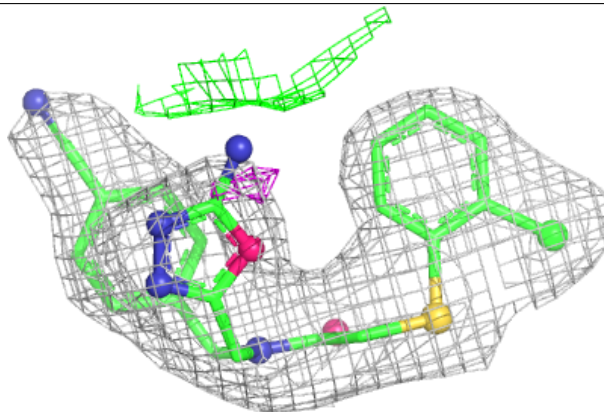


Electron density around VFN 3 301:

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

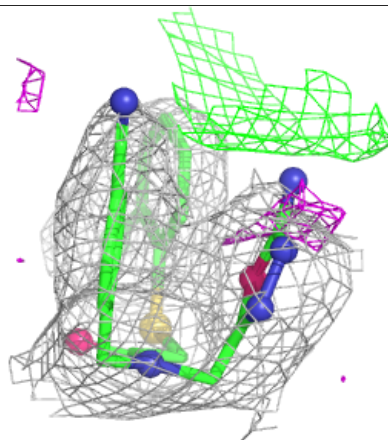
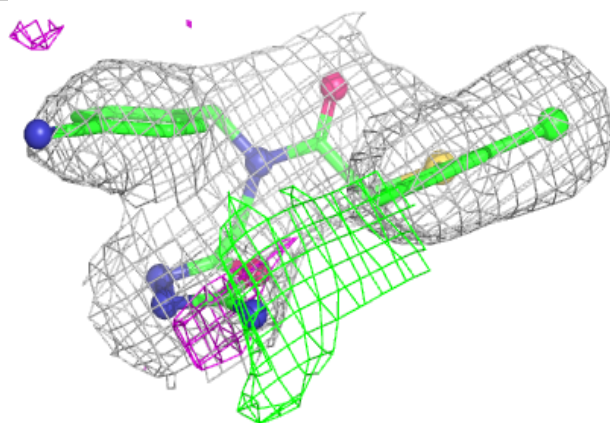
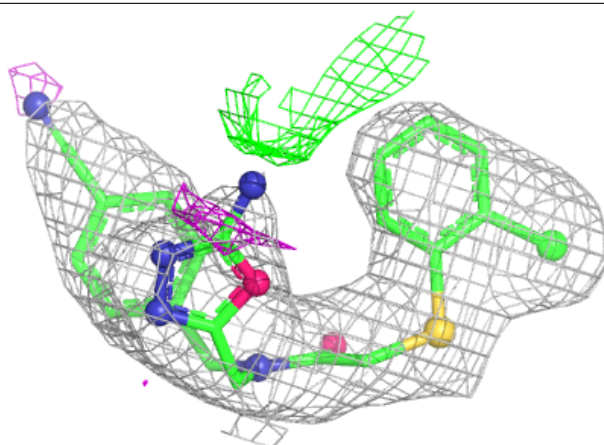
**Electron density around VFN 1 301:**

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

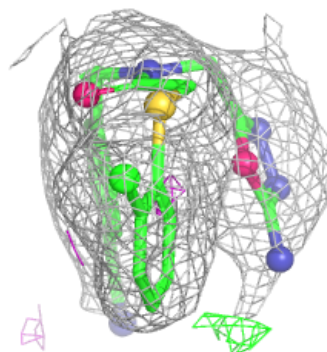
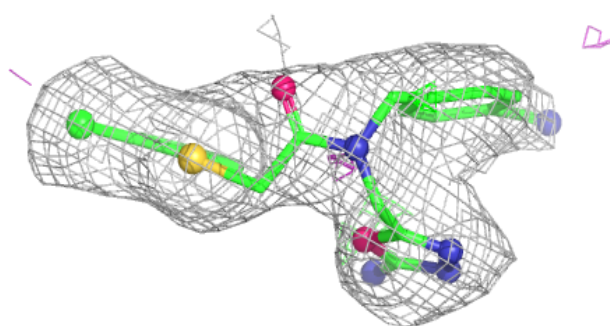
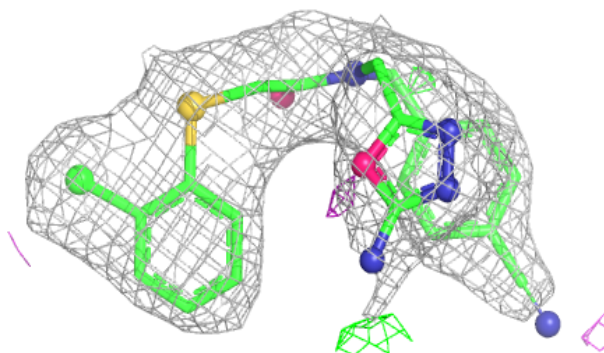


Electron density around VFN 1 302:

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

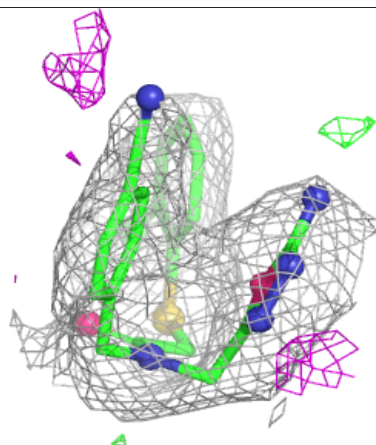
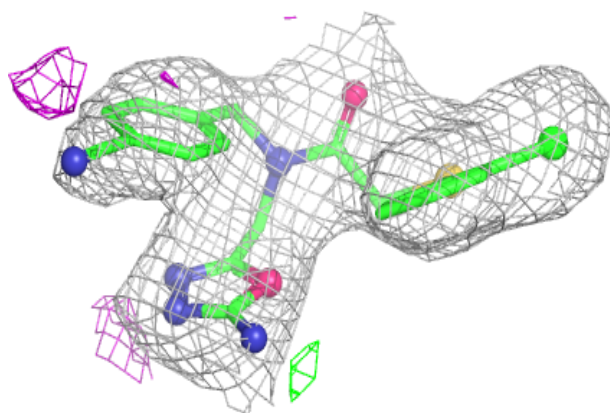
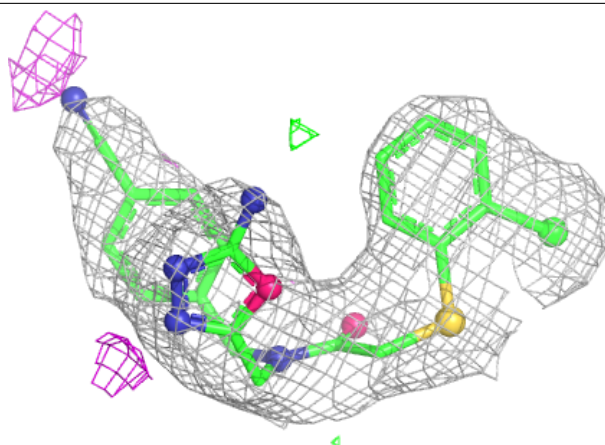
**Electron density around VFN W 302:**

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

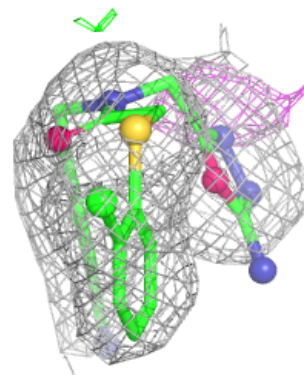
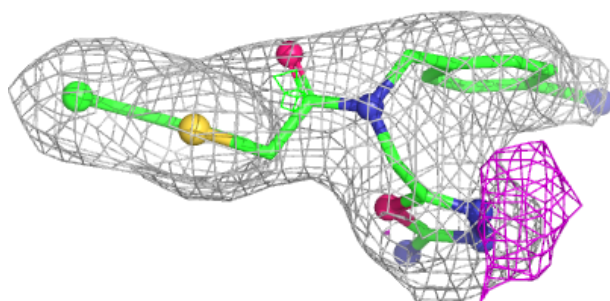
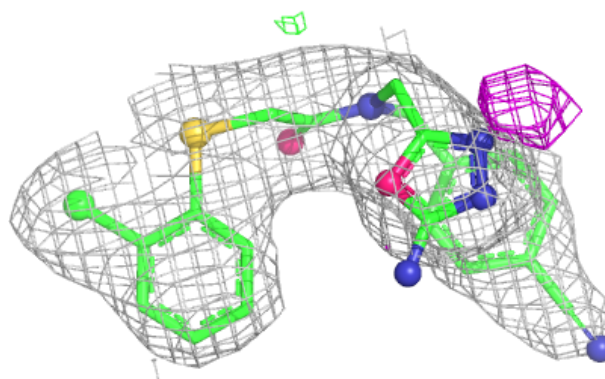


Electron density around VFN S 302:

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

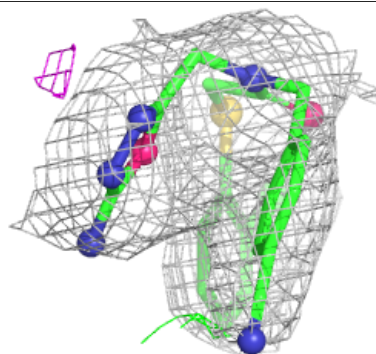
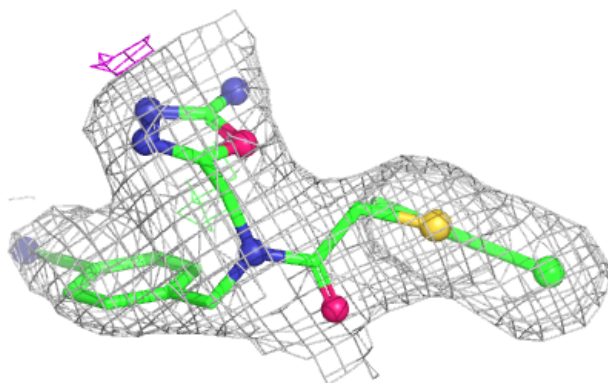
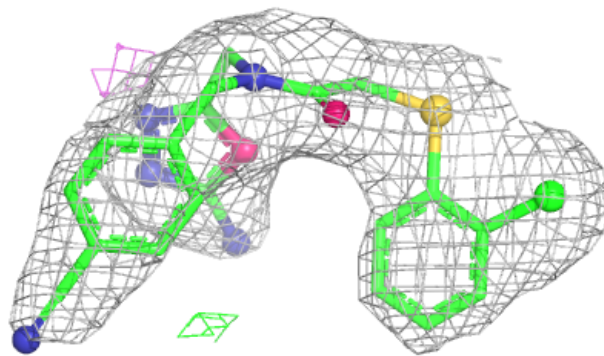
**Electron density around VFN T 301:**

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

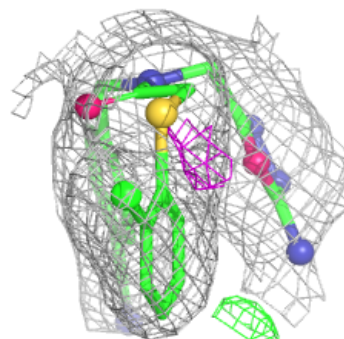
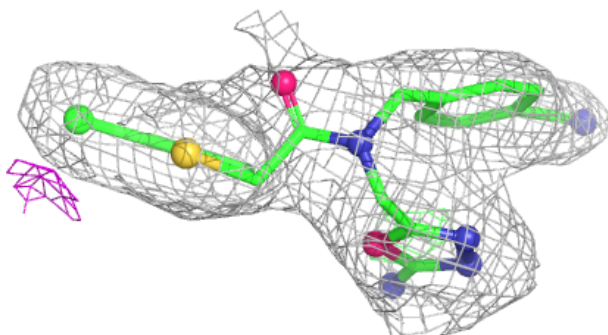
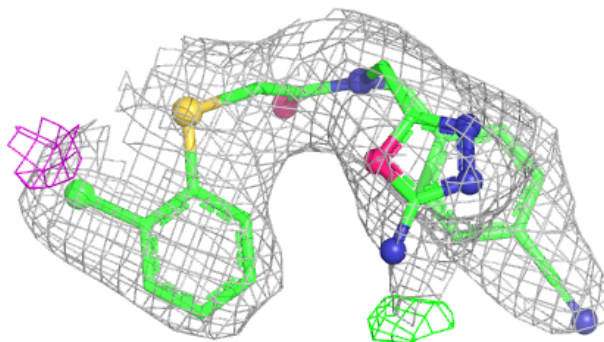


Electron density around VFN H 301:

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

**Electron density around VFN D 301:**

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



6.5 Other polymers [i](#)

There are no such residues in this entry.