wwPDB X-ray Structure Validation Summary Report (i)

Nov 30, 2023 – 12:34 pm GMT

PDB ID	:	8OLL
Title	:	Staphylococcus aureus ClpP in complex with the natural product beta-lactone inhibitor Cystargolide A at 2.7 A resolution
Authors	:	Illigmann, A.; Vielberg, M.-T.; Lakemeyer, M.; Wolf, F.; Staudt, N.; Dema, T.; Stange, P.; Malik, I.; Grond, S.; Sieber, S.A.; Groll, M.; Kaysser, L.; Broetz-Oesterhelt, H.
Deposited on	:	2023-03-30
Resolution	:	2.70 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) 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 (1)) were used in the production of this report:

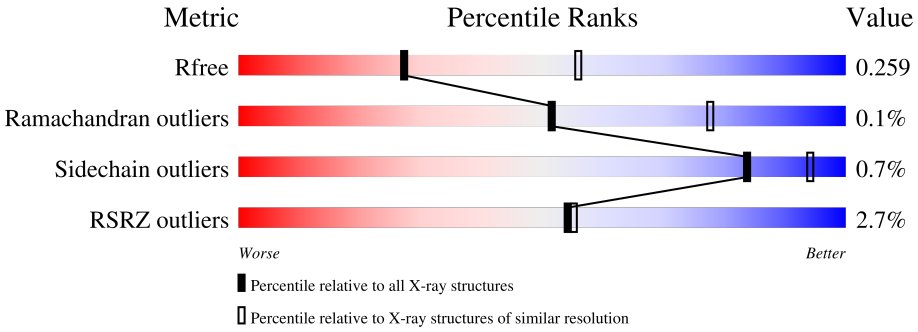
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.70 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	2808 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)

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

Mol	Chain	Length	Quality of chain
1	A	203	2% 94% 5%
1	B	203	% 93% 6%
1	C	203	2% 92% • 7%
1	D	203	3% 93% 7%
1	E	203	3% 86% 14%
1	F	203	% 87% • 12%

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Mol	Chain	Length	Quality of chain
1	G	203	2% 90% 9%
1	H	203	2% 93% 7%
1	I	203	2% 93% 7%
1	J	203	92% 7%
1	K	203	92% 8%
1	L	203	91% 8%
1	M	203	% 90% 10%
1	N	203	2% 91% 9%
1	O	203	4% 90% 10%
1	P	203	3% 88% 10%
1	Q	203	2% 91% 9%
1	R	203	2% 88% 10%
1	S	203	4% 87% 10%
1	T	203	3% 89% 10%
1	U	203	3% 89% 10%
1	V	203	4% 88% 12%
1	W	203	6% 91% 9%
1	X	203	4% 91% 9%
1	Y	203	% 89% 10%
1	Z	203	4% 89% 11%
1	a	203	89% 10%
1	b	203	2% 90% 10%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 40791 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 ATP-dependent Clp protease proteolytic subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	192	Total	C	N	O	S	0	0	0
			1484	931	255	292	6			
1	B	190	Total	C	N	O	S	0	0	0
			1466	922	249	288	7			
1	C	188	Total	C	N	O	S	0	0	0
			1454	915	247	286	6			
1	D	188	Total	C	N	O	S	0	0	0
			1450	913	246	285	6			
1	E	175	Total	C	N	O	S	0	0	0
			1351	851	230	264	6			
1	F	179	Total	C	N	O	S	0	0	0
			1382	871	234	271	6			
1	G	184	Total	C	N	O	S	0	0	0
			1422	896	242	278	6			
1	H	189	Total	C	N	O	S	0	0	0
			1457	917	247	287	6			
1	I	188	Total	C	N	O	S	0	0	0
			1450	914	245	285	6			
1	J	189	Total	C	N	O	S	0	0	0
			1458	917	248	287	6			
1	K	187	Total	C	N	O	S	0	0	0
			1441	908	245	282	6			
1	L	186	Total	C	N	O	S	0	0	0
			1433	904	241	282	6			
1	M	182	Total	C	N	O	S	0	0	0
			1405	888	237	274	6			
1	N	184	Total	C	N	O	S	0	0	0
			1422	896	242	278	6			
1	O	183	Total	C	N	O	S	0	0	0
			1411	890	238	277	6			
1	P	183	Total	C	N	O	S	0	0	0
			1414	893	238	277	6			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	Q	184	Total	C	N	O	S	0	0	0
			1419	896	239	278	6			
1	R	182	Total	C	N	O	S	0	0	0
			1402	885	237	274	6			
1	S	182	Total	C	N	O	S	0	0	0
			1406	887	237	276	6			
1	T	183	Total	C	N	O	S	0	0	0
			1411	890	238	277	6			
1	U	183	Total	C	N	O	S	0	0	0
			1411	890	238	277	6			
1	V	179	Total	C	N	O	S	0	0	0
			1378	869	234	269	6			
1	W	184	Total	C	N	O	S	0	0	0
			1419	896	239	278	6			
1	X	184	Total	C	N	O	S	0	0	0
			1419	896	239	278	6			
1	Y	182	Total	C	N	O	S	0	0	0
			1402	885	237	274	6			
1	Z	181	Total	C	N	O	S	0	0	0
			1397	882	236	273	6			
1	a	182	Total	C	N	O	S	0	0	0
			1406	887	237	276	6			
1	b	183	Total	C	N	O	S	0	0	0
			1410	891	238	275	6			

There are 224 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	196	TRP	-	expression tag	UNP Q6GIM3
A	197	SER	-	expression tag	UNP Q6GIM3
A	198	HIS	-	expression tag	UNP Q6GIM3
A	199	PRO	-	expression tag	UNP Q6GIM3
A	200	GLN	-	expression tag	UNP Q6GIM3
A	201	PHE	-	expression tag	UNP Q6GIM3
A	202	GLU	-	expression tag	UNP Q6GIM3
A	203	LYS	-	expression tag	UNP Q6GIM3
B	196	TRP	-	expression tag	UNP Q6GIM3
B	197	SER	-	expression tag	UNP Q6GIM3
B	198	HIS	-	expression tag	UNP Q6GIM3
B	199	PRO	-	expression tag	UNP Q6GIM3
B	200	GLN	-	expression tag	UNP Q6GIM3
B	201	PHE	-	expression tag	UNP Q6GIM3
B	202	GLU	-	expression tag	UNP Q6GIM3

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Chain	Residue	Modelled	Actual	Comment	Reference
B	203	LYS	-	expression tag	UNP Q6GIM3
C	196	TRP	-	expression tag	UNP Q6GIM3
C	197	SER	-	expression tag	UNP Q6GIM3
C	198	HIS	-	expression tag	UNP Q6GIM3
C	199	PRO	-	expression tag	UNP Q6GIM3
C	200	GLN	-	expression tag	UNP Q6GIM3
C	201	PHE	-	expression tag	UNP Q6GIM3
C	202	GLU	-	expression tag	UNP Q6GIM3
C	203	LYS	-	expression tag	UNP Q6GIM3
D	196	TRP	-	expression tag	UNP Q6GIM3
D	197	SER	-	expression tag	UNP Q6GIM3
D	198	HIS	-	expression tag	UNP Q6GIM3
D	199	PRO	-	expression tag	UNP Q6GIM3
D	200	GLN	-	expression tag	UNP Q6GIM3
D	201	PHE	-	expression tag	UNP Q6GIM3
D	202	GLU	-	expression tag	UNP Q6GIM3
D	203	LYS	-	expression tag	UNP Q6GIM3
E	196	TRP	-	expression tag	UNP Q6GIM3
E	197	SER	-	expression tag	UNP Q6GIM3
E	198	HIS	-	expression tag	UNP Q6GIM3
E	199	PRO	-	expression tag	UNP Q6GIM3
E	200	GLN	-	expression tag	UNP Q6GIM3
E	201	PHE	-	expression tag	UNP Q6GIM3
E	202	GLU	-	expression tag	UNP Q6GIM3
E	203	LYS	-	expression tag	UNP Q6GIM3
F	196	TRP	-	expression tag	UNP Q6GIM3
F	197	SER	-	expression tag	UNP Q6GIM3
F	198	HIS	-	expression tag	UNP Q6GIM3
F	199	PRO	-	expression tag	UNP Q6GIM3
F	200	GLN	-	expression tag	UNP Q6GIM3
F	201	PHE	-	expression tag	UNP Q6GIM3
F	202	GLU	-	expression tag	UNP Q6GIM3
F	203	LYS	-	expression tag	UNP Q6GIM3
G	196	TRP	-	expression tag	UNP Q6GIM3
G	197	SER	-	expression tag	UNP Q6GIM3
G	198	HIS	-	expression tag	UNP Q6GIM3
G	199	PRO	-	expression tag	UNP Q6GIM3
G	200	GLN	-	expression tag	UNP Q6GIM3
G	201	PHE	-	expression tag	UNP Q6GIM3
G	202	GLU	-	expression tag	UNP Q6GIM3
G	203	LYS	-	expression tag	UNP Q6GIM3
H	196	TRP	-	expression tag	UNP Q6GIM3

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Chain	Residue	Modelled	Actual	Comment	Reference
H	197	SER	-	expression tag	UNP Q6GIM3
H	198	HIS	-	expression tag	UNP Q6GIM3
H	199	PRO	-	expression tag	UNP Q6GIM3
H	200	GLN	-	expression tag	UNP Q6GIM3
H	201	PHE	-	expression tag	UNP Q6GIM3
H	202	GLU	-	expression tag	UNP Q6GIM3
H	203	LYS	-	expression tag	UNP Q6GIM3
I	196	TRP	-	expression tag	UNP Q6GIM3
I	197	SER	-	expression tag	UNP Q6GIM3
I	198	HIS	-	expression tag	UNP Q6GIM3
I	199	PRO	-	expression tag	UNP Q6GIM3
I	200	GLN	-	expression tag	UNP Q6GIM3
I	201	PHE	-	expression tag	UNP Q6GIM3
I	202	GLU	-	expression tag	UNP Q6GIM3
I	203	LYS	-	expression tag	UNP Q6GIM3
J	196	TRP	-	expression tag	UNP Q6GIM3
J	197	SER	-	expression tag	UNP Q6GIM3
J	198	HIS	-	expression tag	UNP Q6GIM3
J	199	PRO	-	expression tag	UNP Q6GIM3
J	200	GLN	-	expression tag	UNP Q6GIM3
J	201	PHE	-	expression tag	UNP Q6GIM3
J	202	GLU	-	expression tag	UNP Q6GIM3
J	203	LYS	-	expression tag	UNP Q6GIM3
K	196	TRP	-	expression tag	UNP Q6GIM3
K	197	SER	-	expression tag	UNP Q6GIM3
K	198	HIS	-	expression tag	UNP Q6GIM3
K	199	PRO	-	expression tag	UNP Q6GIM3
K	200	GLN	-	expression tag	UNP Q6GIM3
K	201	PHE	-	expression tag	UNP Q6GIM3
K	202	GLU	-	expression tag	UNP Q6GIM3
K	203	LYS	-	expression tag	UNP Q6GIM3
L	196	TRP	-	expression tag	UNP Q6GIM3
L	197	SER	-	expression tag	UNP Q6GIM3
L	198	HIS	-	expression tag	UNP Q6GIM3
L	199	PRO	-	expression tag	UNP Q6GIM3
L	200	GLN	-	expression tag	UNP Q6GIM3
L	201	PHE	-	expression tag	UNP Q6GIM3
L	202	GLU	-	expression tag	UNP Q6GIM3
L	203	LYS	-	expression tag	UNP Q6GIM3
M	196	TRP	-	expression tag	UNP Q6GIM3
M	197	SER	-	expression tag	UNP Q6GIM3
M	198	HIS	-	expression tag	UNP Q6GIM3

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Chain	Residue	Modelled	Actual	Comment	Reference
M	199	PRO	-	expression tag	UNP Q6GIM3
M	200	GLN	-	expression tag	UNP Q6GIM3
M	201	PHE	-	expression tag	UNP Q6GIM3
M	202	GLU	-	expression tag	UNP Q6GIM3
M	203	LYS	-	expression tag	UNP Q6GIM3
N	196	TRP	-	expression tag	UNP Q6GIM3
N	197	SER	-	expression tag	UNP Q6GIM3
N	198	HIS	-	expression tag	UNP Q6GIM3
N	199	PRO	-	expression tag	UNP Q6GIM3
N	200	GLN	-	expression tag	UNP Q6GIM3
N	201	PHE	-	expression tag	UNP Q6GIM3
N	202	GLU	-	expression tag	UNP Q6GIM3
N	203	LYS	-	expression tag	UNP Q6GIM3
O	196	TRP	-	expression tag	UNP Q6GIM3
O	197	SER	-	expression tag	UNP Q6GIM3
O	198	HIS	-	expression tag	UNP Q6GIM3
O	199	PRO	-	expression tag	UNP Q6GIM3
O	200	GLN	-	expression tag	UNP Q6GIM3
O	201	PHE	-	expression tag	UNP Q6GIM3
O	202	GLU	-	expression tag	UNP Q6GIM3
O	203	LYS	-	expression tag	UNP Q6GIM3
P	196	TRP	-	expression tag	UNP Q6GIM3
P	197	SER	-	expression tag	UNP Q6GIM3
P	198	HIS	-	expression tag	UNP Q6GIM3
P	199	PRO	-	expression tag	UNP Q6GIM3
P	200	GLN	-	expression tag	UNP Q6GIM3
P	201	PHE	-	expression tag	UNP Q6GIM3
P	202	GLU	-	expression tag	UNP Q6GIM3
P	203	LYS	-	expression tag	UNP Q6GIM3
Q	196	TRP	-	expression tag	UNP Q6GIM3
Q	197	SER	-	expression tag	UNP Q6GIM3
Q	198	HIS	-	expression tag	UNP Q6GIM3
Q	199	PRO	-	expression tag	UNP Q6GIM3
Q	200	GLN	-	expression tag	UNP Q6GIM3
Q	201	PHE	-	expression tag	UNP Q6GIM3
Q	202	GLU	-	expression tag	UNP Q6GIM3
Q	203	LYS	-	expression tag	UNP Q6GIM3
R	196	TRP	-	expression tag	UNP Q6GIM3
R	197	SER	-	expression tag	UNP Q6GIM3
R	198	HIS	-	expression tag	UNP Q6GIM3
R	199	PRO	-	expression tag	UNP Q6GIM3
R	200	GLN	-	expression tag	UNP Q6GIM3

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Chain	Residue	Modelled	Actual	Comment	Reference
R	201	PHE	-	expression tag	UNP Q6GIM3
R	202	GLU	-	expression tag	UNP Q6GIM3
R	203	LYS	-	expression tag	UNP Q6GIM3
S	196	TRP	-	expression tag	UNP Q6GIM3
S	197	SER	-	expression tag	UNP Q6GIM3
S	198	HIS	-	expression tag	UNP Q6GIM3
S	199	PRO	-	expression tag	UNP Q6GIM3
S	200	GLN	-	expression tag	UNP Q6GIM3
S	201	PHE	-	expression tag	UNP Q6GIM3
S	202	GLU	-	expression tag	UNP Q6GIM3
S	203	LYS	-	expression tag	UNP Q6GIM3
T	196	TRP	-	expression tag	UNP Q6GIM3
T	197	SER	-	expression tag	UNP Q6GIM3
T	198	HIS	-	expression tag	UNP Q6GIM3
T	199	PRO	-	expression tag	UNP Q6GIM3
T	200	GLN	-	expression tag	UNP Q6GIM3
T	201	PHE	-	expression tag	UNP Q6GIM3
T	202	GLU	-	expression tag	UNP Q6GIM3
T	203	LYS	-	expression tag	UNP Q6GIM3
U	196	TRP	-	expression tag	UNP Q6GIM3
U	197	SER	-	expression tag	UNP Q6GIM3
U	198	HIS	-	expression tag	UNP Q6GIM3
U	199	PRO	-	expression tag	UNP Q6GIM3
U	200	GLN	-	expression tag	UNP Q6GIM3
U	201	PHE	-	expression tag	UNP Q6GIM3
U	202	GLU	-	expression tag	UNP Q6GIM3
U	203	LYS	-	expression tag	UNP Q6GIM3
V	196	TRP	-	expression tag	UNP Q6GIM3
V	197	SER	-	expression tag	UNP Q6GIM3
V	198	HIS	-	expression tag	UNP Q6GIM3
V	199	PRO	-	expression tag	UNP Q6GIM3
V	200	GLN	-	expression tag	UNP Q6GIM3
V	201	PHE	-	expression tag	UNP Q6GIM3
V	202	GLU	-	expression tag	UNP Q6GIM3
V	203	LYS	-	expression tag	UNP Q6GIM3
W	196	TRP	-	expression tag	UNP Q6GIM3
W	197	SER	-	expression tag	UNP Q6GIM3
W	198	HIS	-	expression tag	UNP Q6GIM3
W	199	PRO	-	expression tag	UNP Q6GIM3
W	200	GLN	-	expression tag	UNP Q6GIM3
W	201	PHE	-	expression tag	UNP Q6GIM3
W	202	GLU	-	expression tag	UNP Q6GIM3

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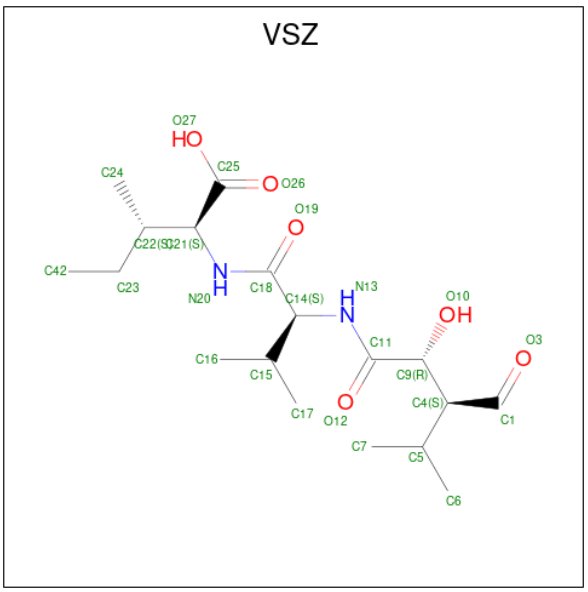
Chain	Residue	Modelled	Actual	Comment	Reference
W	203	LYS	-	expression tag	UNP Q6GIM3
X	196	TRP	-	expression tag	UNP Q6GIM3
X	197	SER	-	expression tag	UNP Q6GIM3
X	198	HIS	-	expression tag	UNP Q6GIM3
X	199	PRO	-	expression tag	UNP Q6GIM3
X	200	GLN	-	expression tag	UNP Q6GIM3
X	201	PHE	-	expression tag	UNP Q6GIM3
X	202	GLU	-	expression tag	UNP Q6GIM3
X	203	LYS	-	expression tag	UNP Q6GIM3
Y	196	TRP	-	expression tag	UNP Q6GIM3
Y	197	SER	-	expression tag	UNP Q6GIM3
Y	198	HIS	-	expression tag	UNP Q6GIM3
Y	199	PRO	-	expression tag	UNP Q6GIM3
Y	200	GLN	-	expression tag	UNP Q6GIM3
Y	201	PHE	-	expression tag	UNP Q6GIM3
Y	202	GLU	-	expression tag	UNP Q6GIM3
Y	203	LYS	-	expression tag	UNP Q6GIM3
Z	196	TRP	-	expression tag	UNP Q6GIM3
Z	197	SER	-	expression tag	UNP Q6GIM3
Z	198	HIS	-	expression tag	UNP Q6GIM3
Z	199	PRO	-	expression tag	UNP Q6GIM3
Z	200	GLN	-	expression tag	UNP Q6GIM3
Z	201	PHE	-	expression tag	UNP Q6GIM3
Z	202	GLU	-	expression tag	UNP Q6GIM3
Z	203	LYS	-	expression tag	UNP Q6GIM3
a	196	TRP	-	expression tag	UNP Q6GIM3
a	197	SER	-	expression tag	UNP Q6GIM3
a	198	HIS	-	expression tag	UNP Q6GIM3
a	199	PRO	-	expression tag	UNP Q6GIM3
a	200	GLN	-	expression tag	UNP Q6GIM3
a	201	PHE	-	expression tag	UNP Q6GIM3
a	202	GLU	-	expression tag	UNP Q6GIM3
a	203	LYS	-	expression tag	UNP Q6GIM3
b	196	TRP	-	expression tag	UNP Q6GIM3
b	197	SER	-	expression tag	UNP Q6GIM3
b	198	HIS	-	expression tag	UNP Q6GIM3
b	199	PRO	-	expression tag	UNP Q6GIM3
b	200	GLN	-	expression tag	UNP Q6GIM3
b	201	PHE	-	expression tag	UNP Q6GIM3
b	202	GLU	-	expression tag	UNP Q6GIM3
b	203	LYS	-	expression tag	UNP Q6GIM3

- Molecule 2 is Cystargolide A (bound) (three-letter code: VSZ) (formula: $C_{18}H_{32}N_2O_6$) (la-

beled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C N O 26 18 2 6	0	0
2	B	1	Total C N O 26 18 2 6	0	0
2	C	1	Total C N O 26 18 2 6	0	0
2	D	1	Total C N O 26 18 2 6	0	0
2	E	1	Total C N O 26 18 2 6	0	0
2	F	1	Total C N O 26 18 2 6	0	0
2	G	1	Total C N O 26 18 2 6	0	0
2	H	1	Total C N O 26 18 2 6	0	0
2	I	1	Total C N O 26 18 2 6	0	0
2	J	1	Total C N O 26 18 2 6	0	0
2	K	1	Total C N O 26 18 2 6	0	0
2	L	1	Total C N O 26 18 2 6	0	0
2	M	1	Total C N O 26 18 2 6	0	0

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	N	1	Total	C	N	O	0	0
			26	18	2	6		
2	O	1	Total	C	N	O	0	0
			26	18	2	6		
2	P	1	Total	C	N	O	0	0
			26	18	2	6		
2	Q	1	Total	C	N	O	0	0
			26	18	2	6		
2	R	1	Total	C	N	O	0	0
			26	18	2	6		
2	S	1	Total	C	N	O	0	0
			26	18	2	6		
2	T	1	Total	C	N	O	0	0
			26	18	2	6		
2	U	1	Total	C	N	O	0	0
			26	18	2	6		
2	V	1	Total	C	N	O	0	0
			26	18	2	6		
2	W	1	Total	C	N	O	0	0
			26	18	2	6		
2	X	1	Total	C	N	O	0	0
			26	18	2	6		
2	Y	1	Total	C	N	O	0	0
			26	18	2	6		
2	Z	1	Total	C	N	O	0	0
			26	18	2	6		
2	a	1	Total	C	N	O	0	0
			26	18	2	6		
2	b	1	Total	C	N	O	0	0
			26	18	2	6		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	14	Total	O	0	0
			14	14		
3	B	18	Total	O	0	0
			18	18		
3	C	9	Total	O	0	0
			9	9		
3	D	10	Total	O	0	0
			10	10		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	E	8	Total O 8 8	0	0
3	F	6	Total O 6 6	0	0
3	G	8	Total O 8 8	0	0
3	H	11	Total O 11 11	0	0
3	I	16	Total O 16 16	0	0
3	J	21	Total O 21 21	0	0
3	K	22	Total O 22 22	0	0
3	L	17	Total O 17 17	0	0
3	M	15	Total O 15 15	0	0
3	N	13	Total O 13 13	0	0
3	O	2	Total O 2 2	0	0
3	P	10	Total O 10 10	0	0
3	Q	3	Total O 3 3	0	0
3	R	7	Total O 7 7	0	0
3	S	5	Total O 5 5	0	0
3	T	7	Total O 7 7	0	0
3	U	12	Total O 12 12	0	0
3	V	9	Total O 9 9	0	0
3	W	5	Total O 5 5	0	0
3	X	7	Total O 7 7	0	0
3	Y	4	Total O 4 4	0	0

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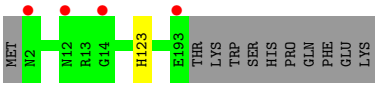
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	Z	4	Total O 4 4	0	0
3	a	9	Total O 9 9	0	0
3	b	11	Total O 11 11	0	0

3 Residue-property plots (i)

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

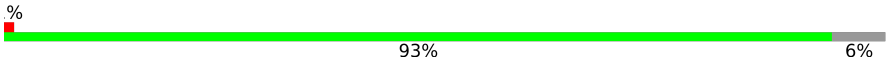
• Molecule 1: ATP-dependent Clp protease proteolytic subunit

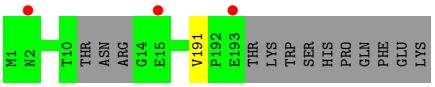
Chain A:



• Molecule 1: ATP-dependent Clp protease proteolytic subunit

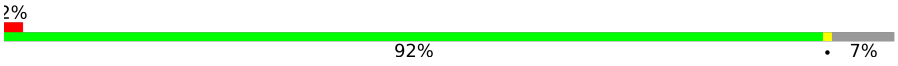
Chain B:

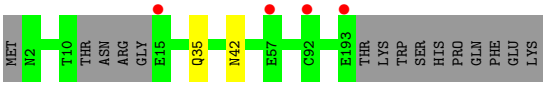




• Molecule 1: ATP-dependent Clp protease proteolytic subunit

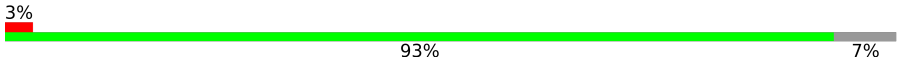
Chain C:

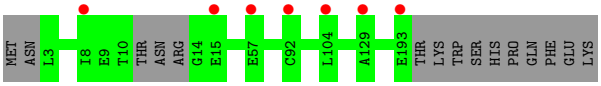




• Molecule 1: ATP-dependent Clp protease proteolytic subunit

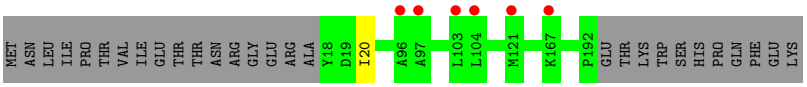
Chain D:





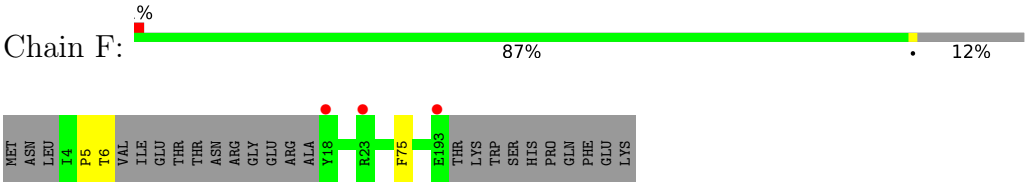
• Molecule 1: ATP-dependent Clp protease proteolytic subunit

Chain E:



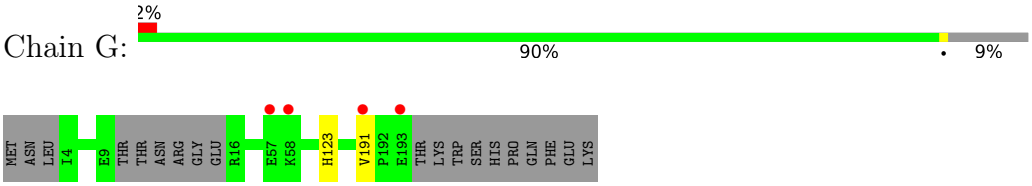
• Molecule 1: ATP-dependent Clp protease proteolytic subunit

Chain F:



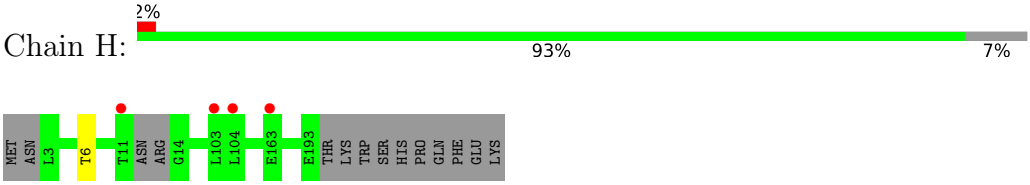
• Molecule 1: ATP-dependent Clp protease proteolytic subunit

Chain G:



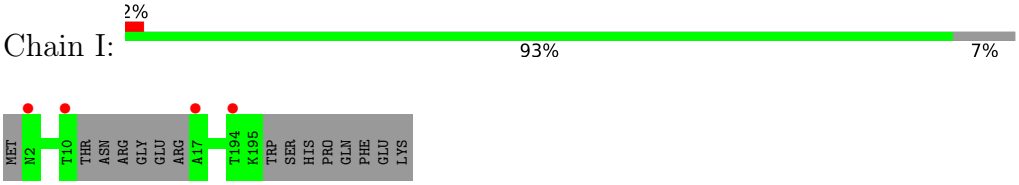
• Molecule 1: ATP-dependent Clp protease proteolytic subunit

Chain H:



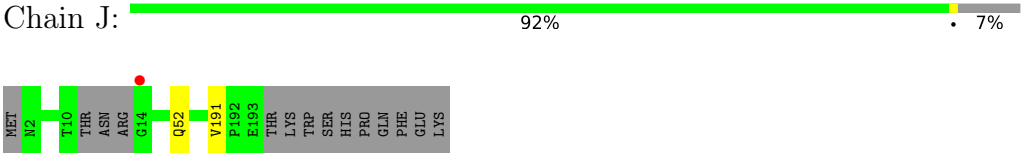
• Molecule 1: ATP-dependent Clp protease proteolytic subunit

Chain I:



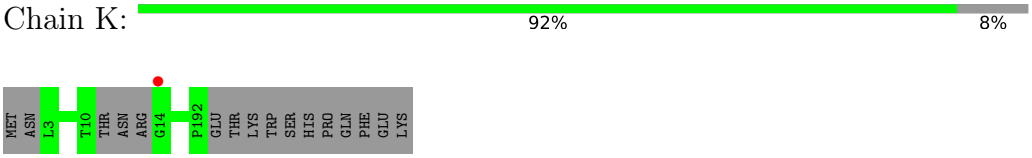
• Molecule 1: ATP-dependent Clp protease proteolytic subunit

Chain J:



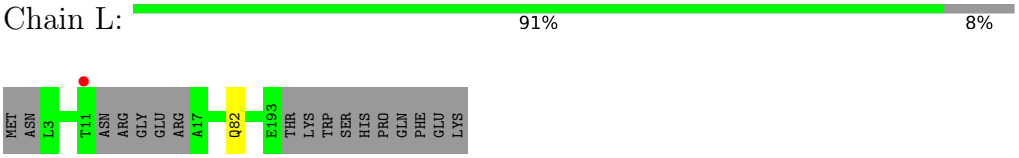
• Molecule 1: ATP-dependent Clp protease proteolytic subunit

Chain K:



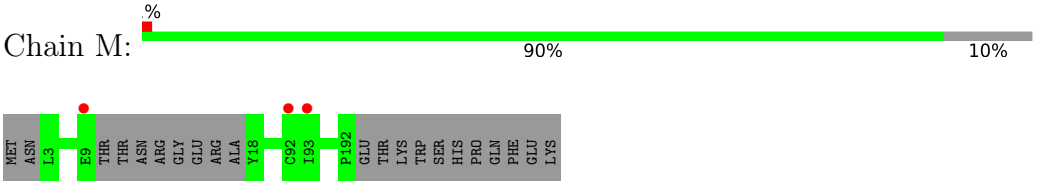
• Molecule 1: ATP-dependent Clp protease proteolytic subunit

Chain L:



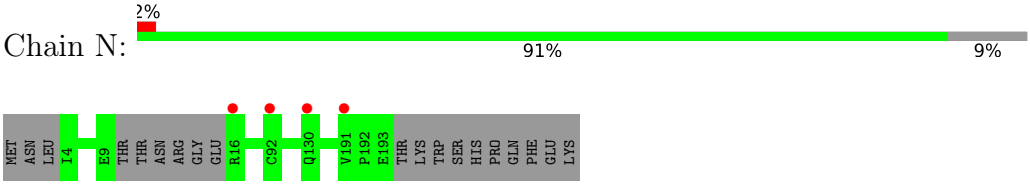
• Molecule 1: ATP-dependent Clp protease proteolytic subunit

Chain M:



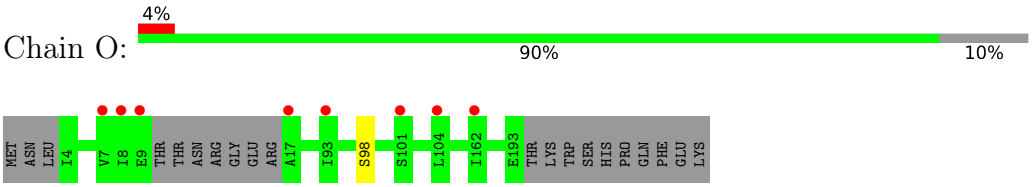
• Molecule 1: ATP-dependent Clp protease proteolytic subunit

Chain N:



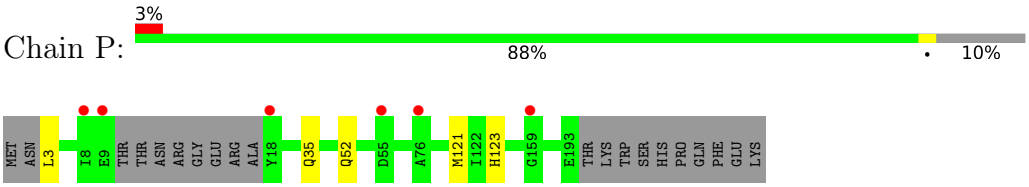
• Molecule 1: ATP-dependent Clp protease proteolytic subunit

Chain O:



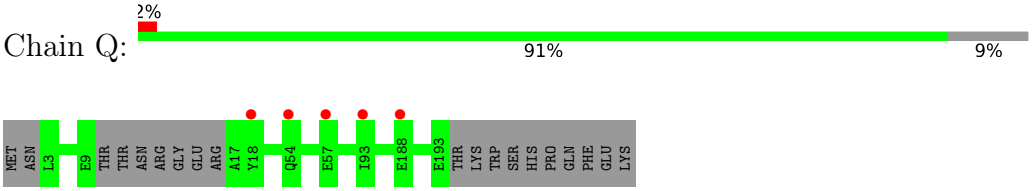
• Molecule 1: ATP-dependent Clp protease proteolytic subunit

Chain P:



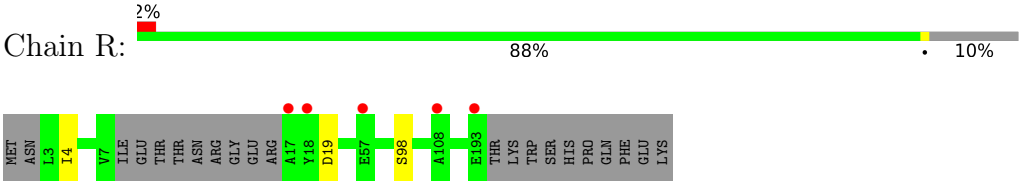
• Molecule 1: ATP-dependent Clp protease proteolytic subunit

Chain Q:



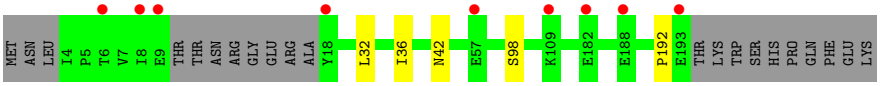
• Molecule 1: ATP-dependent Clp protease proteolytic subunit

Chain R:

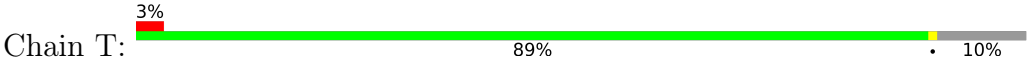


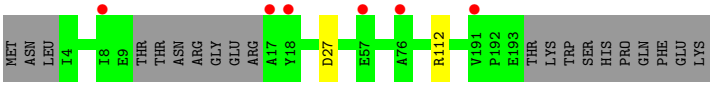
• Molecule 1: ATP-dependent Clp protease proteolytic subunit

Chain S:

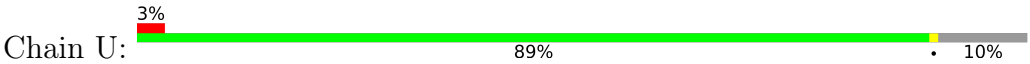


• Molecule 1: ATP-dependent Clp protease proteolytic subunit

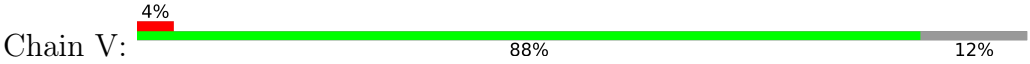


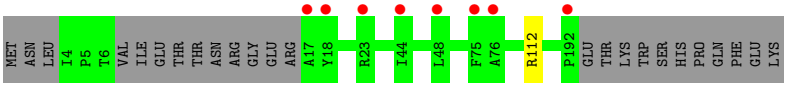


• Molecule 1: ATP-dependent Clp protease proteolytic subunit

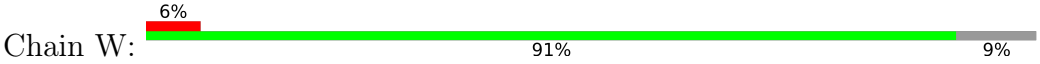


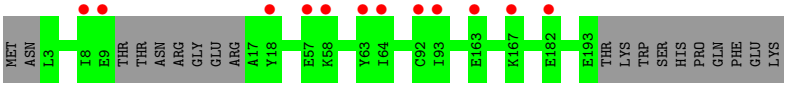
• Molecule 1: ATP-dependent Clp protease proteolytic subunit



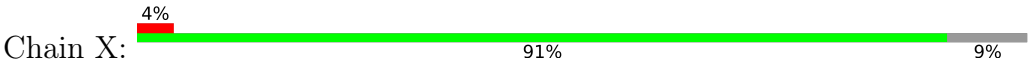


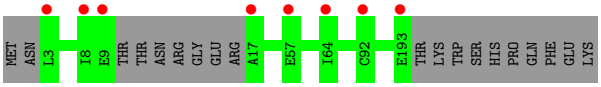
• Molecule 1: ATP-dependent Clp protease proteolytic subunit



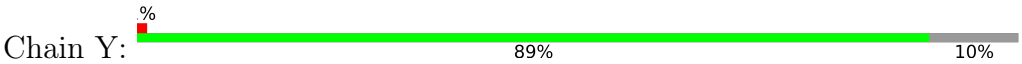


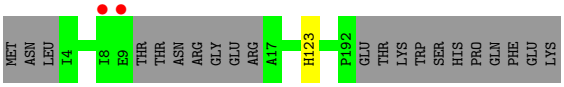
• Molecule 1: ATP-dependent Clp protease proteolytic subunit





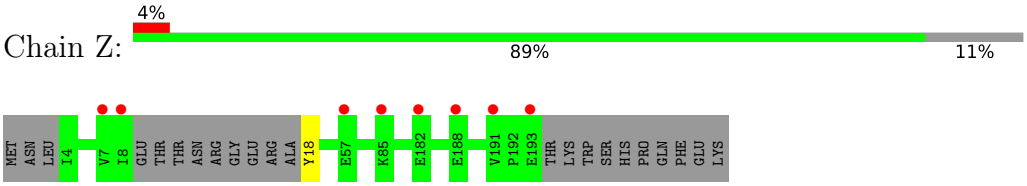
• Molecule 1: ATP-dependent Clp protease proteolytic subunit





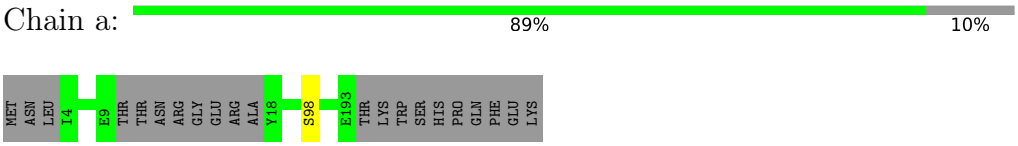
• Molecule 1: ATP-dependent Clp protease proteolytic subunit

Chain Z:



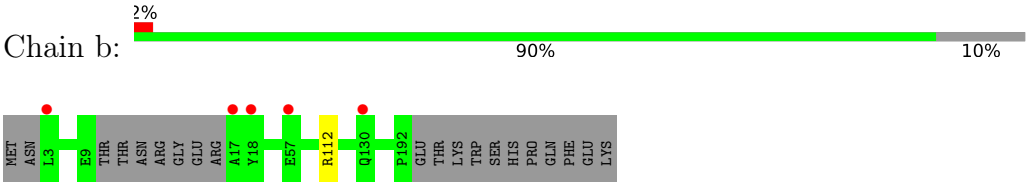
• Molecule 1: ATP-dependent Clp protease proteolytic subunit

Chain a:



• Molecule 1: ATP-dependent Clp protease proteolytic subunit

Chain b:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	96.41Å 109.73Å 173.61Å 110.09° 89.44° 108.80°	Depositor
Resolution (Å)	30.00 – 2.70 29.90 – 2.70	Depositor EDS
% Data completeness (in resolution range)	91.0 (30.00-2.70) 91.1 (29.90-2.70)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.50 (at 2.68Å)	Xtriage
Refinement program	REFMAC 5.8.0158	Depositor
R, R_{free}	0.224 , 0.258 0.226 , 0.259	Depositor DCC
R_{free} test set	7862 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	72.2	Xtriage
Anisotropy	0.378	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 40.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.52$, $< L^2 > = 0.35$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	40791	wwPDB-VP
Average B, all atoms (Å^2)	84.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.45% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	A	0.42	0/1503	0.57	0/2030
1	B	0.38	0/1484	0.59	0/2002
1	C	0.38	0/1472	0.59	0/1987
1	D	0.35	0/1468	0.57	0/1981
1	E	0.36	0/1369	0.58	0/1847
1	F	0.41	0/1400	0.58	0/1889
1	G	0.39	0/1440	0.58	0/1943
1	H	0.37	0/1475	0.55	0/1991
1	I	0.35	0/1468	0.55	0/1982
1	J	0.36	0/1476	0.59	0/1992
1	K	0.36	0/1459	0.56	0/1969
1	L	0.35	0/1451	0.54	0/1960
1	M	0.35	0/1423	0.53	0/1921
1	N	0.36	0/1440	0.55	0/1943
1	O	0.37	0/1429	0.58	1/1929 (0.1%)
1	P	0.38	0/1432	0.58	0/1933
1	Q	0.38	0/1437	0.53	0/1940
1	R	0.39	0/1420	0.58	1/1917 (0.1%)
1	S	0.42	0/1424	0.59	1/1922 (0.1%)
1	T	0.38	0/1429	0.53	0/1929
1	U	0.37	0/1429	0.56	1/1929 (0.1%)
1	V	0.38	0/1396	0.52	0/1884
1	W	0.38	0/1437	0.53	0/1940
1	X	0.41	0/1437	0.55	0/1940
1	Y	0.43	0/1420	0.55	0/1917
1	Z	0.39	0/1415	0.55	0/1910
1	a	0.38	0/1424	0.55	1/1922 (0.1%)
1	b	0.38	0/1428	0.53	0/1928
All	All	0.38	0/40285	0.56	5/54377 (0.0%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	R	98	SER	CB-CA-C	-6.48	97.79	110.10
1	U	98	SER	CB-CA-C	6.32	122.11	110.10
1	S	98	SER	CB-CA-C	6.24	121.95	110.10
1	O	98	SER	CB-CA-C	5.68	120.89	110.10
1	a	98	SER	CB-CA-C	5.55	120.65	110.10

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	190/203 (94%)	186 (98%)	4 (2%)	0	100	100
1	B	186/203 (92%)	178 (96%)	8 (4%)	0	100	100
1	C	184/203 (91%)	178 (97%)	6 (3%)	0	100	100
1	D	184/203 (91%)	180 (98%)	4 (2%)	0	100	100
1	E	173/203 (85%)	170 (98%)	3 (2%)	0	100	100
1	F	175/203 (86%)	170 (97%)	4 (2%)	1 (1%)	25	50
1	G	180/203 (89%)	176 (98%)	4 (2%)	0	100	100
1	H	185/203 (91%)	183 (99%)	2 (1%)	0	100	100
1	I	184/203 (91%)	178 (97%)	6 (3%)	0	100	100
1	J	185/203 (91%)	182 (98%)	3 (2%)	0	100	100
1	K	183/203 (90%)	177 (97%)	6 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	L	182/203 (90%)	177 (97%)	5 (3%)	0	100	100
1	M	178/203 (88%)	175 (98%)	3 (2%)	0	100	100
1	N	180/203 (89%)	178 (99%)	2 (1%)	0	100	100
1	O	179/203 (88%)	175 (98%)	4 (2%)	0	100	100
1	P	179/203 (88%)	177 (99%)	2 (1%)	0	100	100
1	Q	180/203 (89%)	173 (96%)	7 (4%)	0	100	100
1	R	178/203 (88%)	171 (96%)	7 (4%)	0	100	100
1	S	178/203 (88%)	173 (97%)	4 (2%)	1 (1%)	25	50
1	T	179/203 (88%)	172 (96%)	7 (4%)	0	100	100
1	U	179/203 (88%)	175 (98%)	3 (2%)	1 (1%)	25	50
1	V	175/203 (86%)	171 (98%)	4 (2%)	0	100	100
1	W	180/203 (89%)	173 (96%)	7 (4%)	0	100	100
1	X	180/203 (89%)	175 (97%)	5 (3%)	0	100	100
1	Y	178/203 (88%)	173 (97%)	5 (3%)	0	100	100
1	Z	177/203 (87%)	173 (98%)	4 (2%)	0	100	100
1	a	178/203 (88%)	174 (98%)	4 (2%)	0	100	100
1	b	179/203 (88%)	173 (97%)	6 (3%)	0	100	100
All	All	5048/5684 (89%)	4916 (97%)	129 (3%)	3 (0%)	51	78

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	S	192	PRO
1	F	5	PRO
1	U	192	PRO

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	160/171 (94%)	159 (99%)	1 (1%)	86 95
1	B	158/171 (92%)	157 (99%)	1 (1%)	86 95
1	C	157/171 (92%)	155 (99%)	2 (1%)	69 87
1	D	156/171 (91%)	156 (100%)	0	100 100
1	E	145/171 (85%)	144 (99%)	1 (1%)	84 94
1	F	149/171 (87%)	147 (99%)	2 (1%)	69 87
1	G	153/171 (90%)	151 (99%)	2 (1%)	69 87
1	H	157/171 (92%)	156 (99%)	1 (1%)	86 95
1	I	157/171 (92%)	157 (100%)	0	100 100
1	J	157/171 (92%)	155 (99%)	2 (1%)	69 87
1	K	155/171 (91%)	155 (100%)	0	100 100
1	L	155/171 (91%)	154 (99%)	1 (1%)	86 95
1	M	152/171 (89%)	152 (100%)	0	100 100
1	N	153/171 (90%)	153 (100%)	0	100 100
1	O	152/171 (89%)	152 (100%)	0	100 100
1	P	153/171 (90%)	148 (97%)	5 (3%)	38 67
1	Q	153/171 (90%)	153 (100%)	0	100 100
1	R	151/171 (88%)	149 (99%)	2 (1%)	69 87
1	S	152/171 (89%)	149 (98%)	3 (2%)	55 81
1	T	152/171 (89%)	150 (99%)	2 (1%)	69 87
1	U	152/171 (89%)	151 (99%)	1 (1%)	84 94
1	V	148/171 (86%)	147 (99%)	1 (1%)	84 94
1	W	153/171 (90%)	153 (100%)	0	100 100
1	X	153/171 (90%)	153 (100%)	0	100 100
1	Y	151/171 (88%)	150 (99%)	1 (1%)	84 94
1	Z	151/171 (88%)	150 (99%)	1 (1%)	84 94
1	a	152/171 (89%)	152 (100%)	0	100 100
1	b	152/171 (89%)	151 (99%)	1 (1%)	84 94
All	All	4289/4788 (90%)	4259 (99%)	30 (1%)	84 94

5 of 30 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	P	35	GLN
1	Y	123	HIS
1	P	123	HIS
1	b	112	ARG
1	T	112	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 14 such sidechains are listed below:

Mol	Chain	Res	Type
1	O	42	ASN
1	O	47	GLN
1	Y	173	ASN
1	S	123	HIS
1	X	42	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

28 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	$\#\|Z\|>2$
2	VSZ	U	301	1	25,25,25	1.66	4 (16%)	30,34,34	1.13	2 (6%)
2	VSZ	V	301	1	25,25,25	0.96	1 (4%)	30,34,34	1.00	1 (3%)
2	VSZ	G	301	1	25,25,25	1.32	3 (12%)	30,34,34	1.30	4 (13%)
2	VSZ	B	301	1	25,25,25	1.45	2 (8%)	30,34,34	1.39	4 (13%)
2	VSZ	H	301	1	25,25,25	1.37	2 (8%)	30,34,34	1.32	3 (10%)
2	VSZ	Z	301	1	25,25,25	1.46	2 (8%)	30,34,34	1.12	2 (6%)
2	VSZ	b	301	1	25,25,25	0.94	1 (4%)	30,34,34	1.47	4 (13%)
2	VSZ	a	301	1	25,25,25	1.50	2 (8%)	30,34,34	1.05	2 (6%)
2	VSZ	F	301	1	25,25,25	1.22	2 (8%)	30,34,34	1.27	4 (13%)
2	VSZ	I	301	1	25,25,25	1.28	2 (8%)	30,34,34	1.12	2 (6%)
2	VSZ	W	301	1	25,25,25	1.22	1 (4%)	30,34,34	1.17	3 (10%)
2	VSZ	Y	301	1	25,25,25	1.33	2 (8%)	30,34,34	1.39	4 (13%)
2	VSZ	M	301	1	25,25,25	1.42	2 (8%)	30,34,34	1.22	2 (6%)
2	VSZ	L	301	1	25,25,25	1.29	1 (4%)	30,34,34	1.30	4 (13%)
2	VSZ	R	301	1	25,25,25	1.22	2 (8%)	30,34,34	1.52	6 (20%)
2	VSZ	O	301	1	25,25,25	1.13	2 (8%)	30,34,34	0.86	1 (3%)
2	VSZ	P	301	1	25,25,25	0.97	1 (4%)	30,34,34	1.00	1 (3%)
2	VSZ	J	301	1	25,25,25	0.98	1 (4%)	30,34,34	1.22	4 (13%)
2	VSZ	N	301	1	25,25,25	1.44	3 (12%)	30,34,34	1.15	3 (10%)
2	VSZ	X	301	1	25,25,25	1.26	1 (4%)	30,34,34	1.57	5 (16%)
2	VSZ	T	301	1	25,25,25	1.19	1 (4%)	30,34,34	1.04	0
2	VSZ	S	301	1	25,25,25	1.26	1 (4%)	30,34,34	0.91	0
2	VSZ	E	301	1	25,25,25	1.60	4 (16%)	30,34,34	1.43	3 (10%)
2	VSZ	C	301	1	25,25,25	1.35	2 (8%)	30,34,34	1.41	5 (16%)
2	VSZ	D	301	1	25,25,25	1.06	2 (8%)	30,34,34	1.25	3 (10%)
2	VSZ	K	301	1	25,25,25	1.29	2 (8%)	30,34,34	1.36	4 (13%)
2	VSZ	A	301	1	25,25,25	1.25	3 (12%)	30,34,34	1.39	3 (10%)
2	VSZ	Q	301	1	25,25,25	1.48	3 (12%)	30,34,34	1.19	3 (10%)

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	VSZ	U	301	1	-	3/40/40/40	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	VSZ	V	301	1	-	7/40/40/40	-
2	VSZ	G	301	1	-	6/40/40/40	-
2	VSZ	B	301	1	-	5/40/40/40	-
2	VSZ	H	301	1	-	9/40/40/40	-
2	VSZ	Z	301	1	-	7/40/40/40	-
2	VSZ	b	301	1	-	6/40/40/40	-
2	VSZ	a	301	1	-	8/40/40/40	-
2	VSZ	F	301	1	-	9/40/40/40	-
2	VSZ	I	301	1	-	7/40/40/40	-
2	VSZ	W	301	1	-	4/40/40/40	-
2	VSZ	Y	301	1	-	6/40/40/40	-
2	VSZ	M	301	1	-	3/40/40/40	-
2	VSZ	L	301	1	-	6/40/40/40	-
2	VSZ	R	301	1	-	8/40/40/40	-
2	VSZ	O	301	1	-	6/40/40/40	-
2	VSZ	P	301	1	-	4/40/40/40	-
2	VSZ	J	301	1	-	2/40/40/40	-
2	VSZ	N	301	1	-	7/40/40/40	-
2	VSZ	X	301	1	-	4/40/40/40	-
2	VSZ	T	301	1	-	8/40/40/40	-
2	VSZ	S	301	1	-	2/40/40/40	-
2	VSZ	E	301	1	-	7/40/40/40	-
2	VSZ	C	301	1	-	2/40/40/40	-
2	VSZ	D	301	1	-	3/40/40/40	-
2	VSZ	K	301	1	-	6/40/40/40	-
2	VSZ	A	301	1	-	7/40/40/40	-
2	VSZ	Q	301	1	-	4/40/40/40	-

The worst 5 of 55 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	U	301	VSZ	C4-C9	-5.90	1.48	1.54
2	E	301	VSZ	C4-C9	-5.61	1.49	1.54
2	Q	301	VSZ	C4-C9	-5.58	1.49	1.54
2	B	301	VSZ	C4-C9	-5.39	1.49	1.54
2	Z	301	VSZ	C4-C9	-5.29	1.49	1.54

The worst 5 of 82 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	b	301	VSZ	C9-C4-C1	-5.41	99.44	110.65
2	A	301	VSZ	C15-C14-C18	-4.23	100.80	111.38
2	H	301	VSZ	C15-C14-C18	-4.14	101.02	111.38
2	C	301	VSZ	C9-C4-C1	-3.79	102.80	110.65
2	Y	301	VSZ	O10-C9-C4	-3.70	102.25	109.28

There are no chirality outliers.

5 of 156 torsion outliers are listed below:

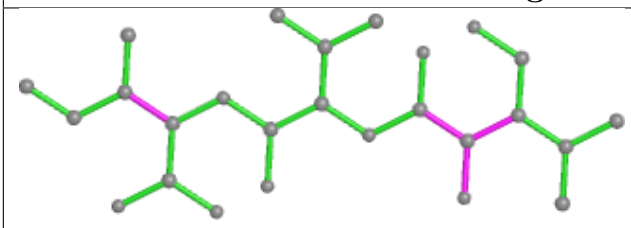
Mol	Chain	Res	Type	Atoms
2	A	301	VSZ	C9-C4-C5-C6
2	A	301	VSZ	C1-C4-C5-C6
2	A	301	VSZ	C1-C4-C5-C7
2	B	301	VSZ	N13-C11-C9-O10
2	D	301	VSZ	O3-C1-C4-C5

There are no ring outliers.

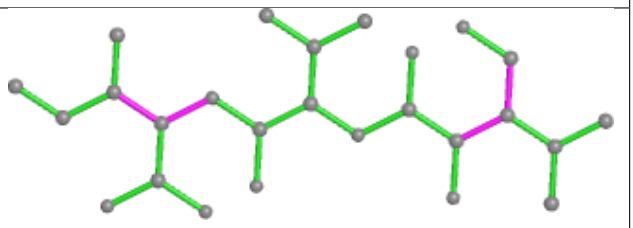
No monomer is involved in short contacts.

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

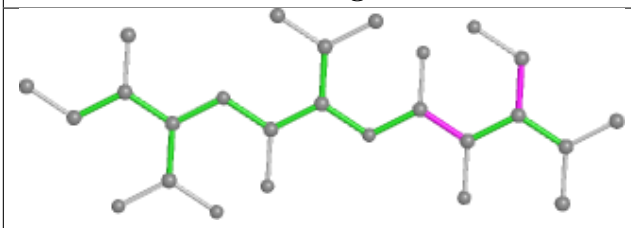
Ligand VSZ U 301



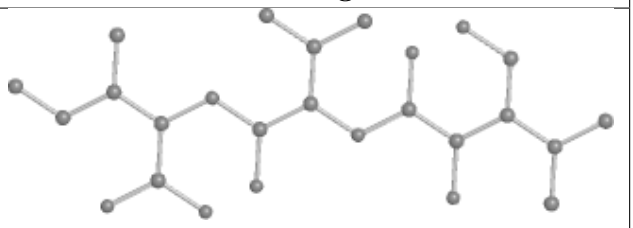
Bond lengths



Bond angles

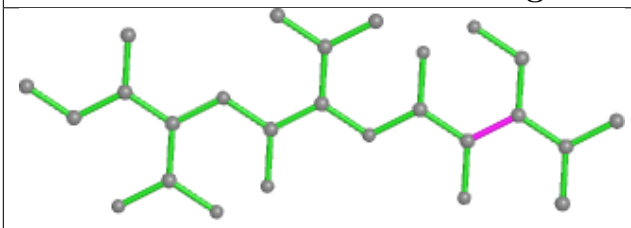


Torsions



Rings

Ligand VSZ V 301



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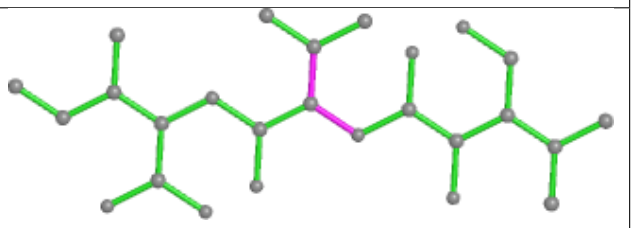

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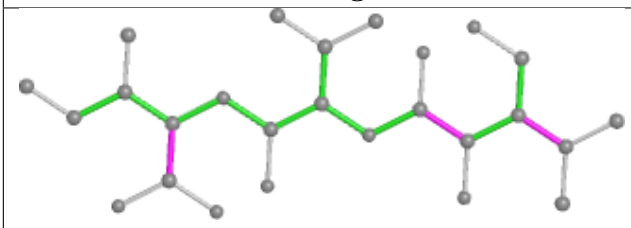

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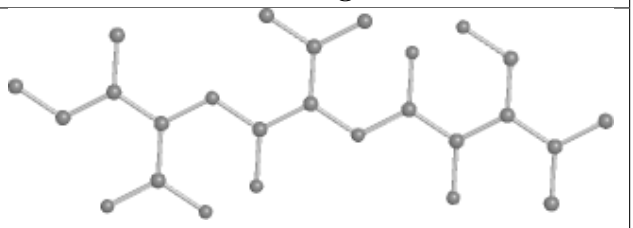
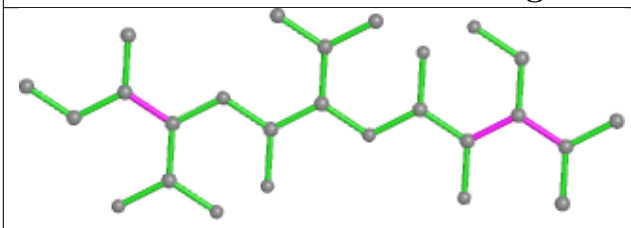


Rings

Ligand VSZ G 301



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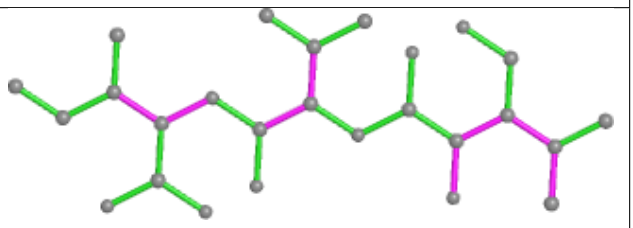
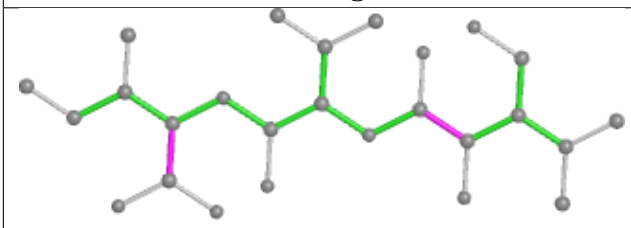
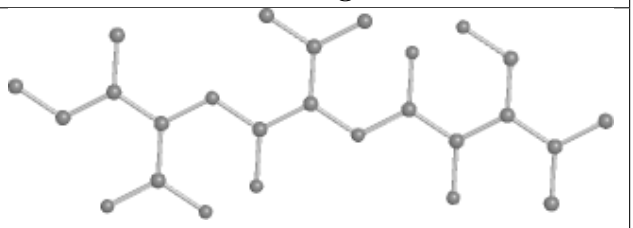


Bond angles

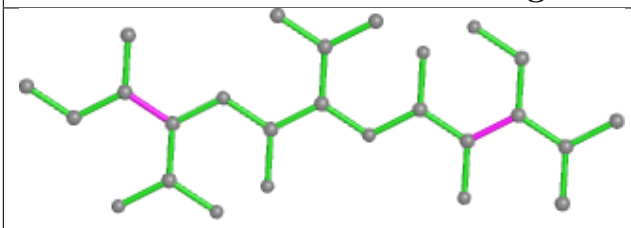


Torsions

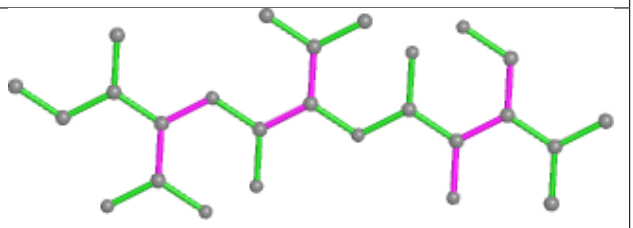


Rings

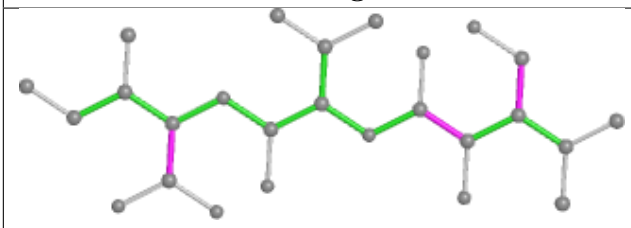
Ligand VSZ B 301



Bond lengths



Bond angles



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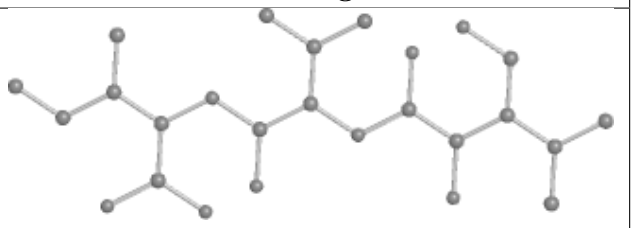
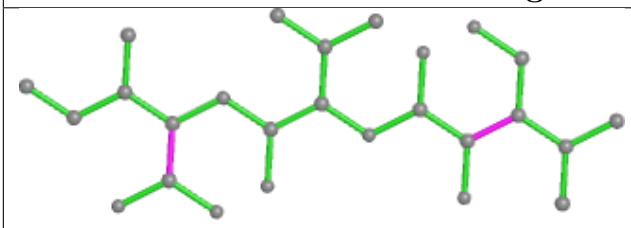
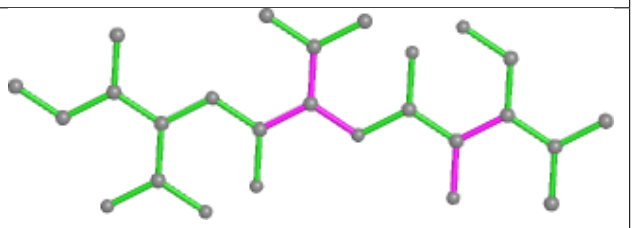


Rings

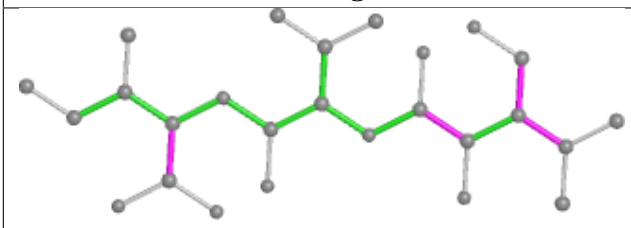
Ligand VSZ H 301



Bond lengths



Bond angles



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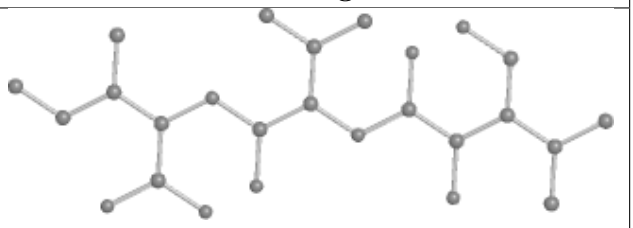
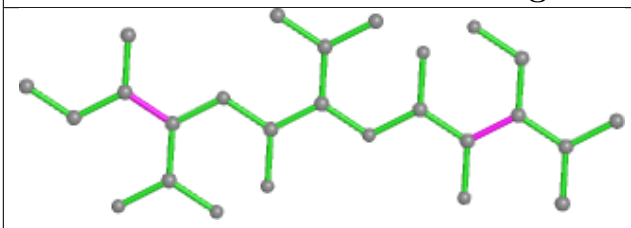
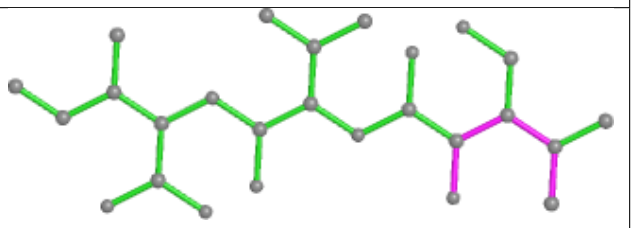


Rings

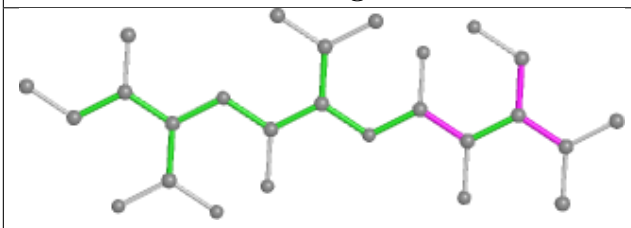
Ligand VSZ Z 301



Bond lengths



Bond angles



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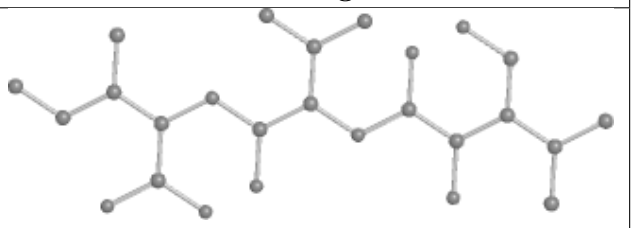

Rings

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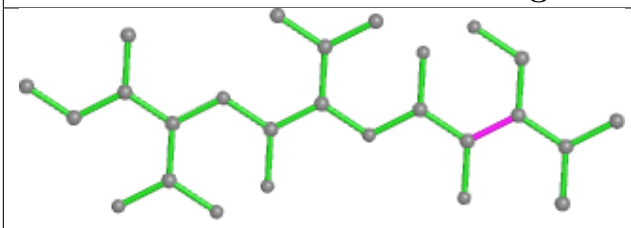

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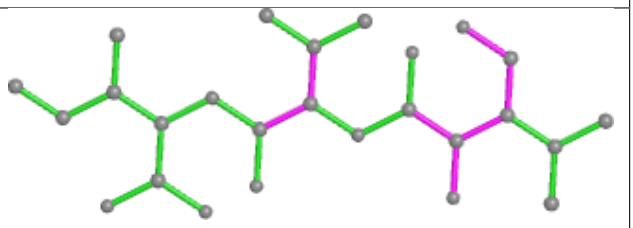

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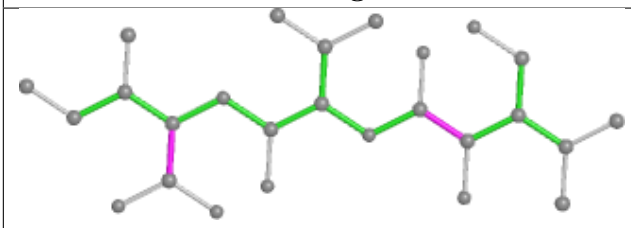

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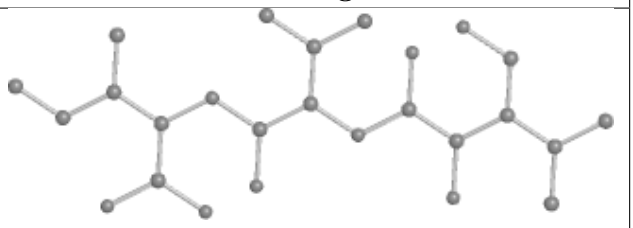

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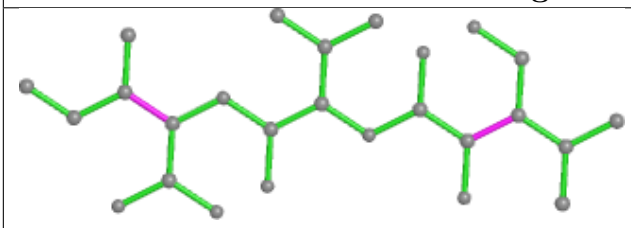

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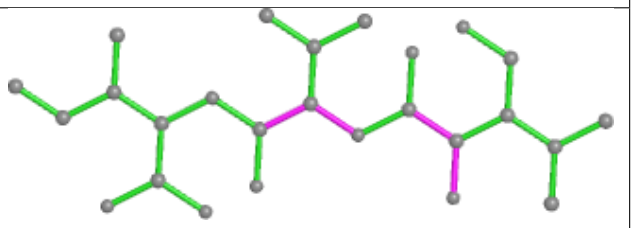

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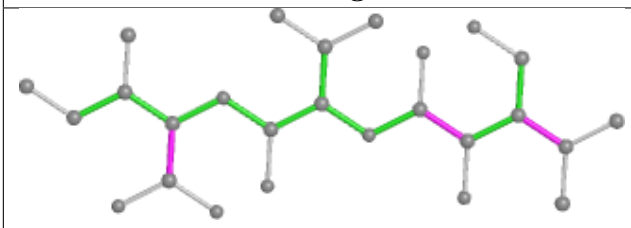

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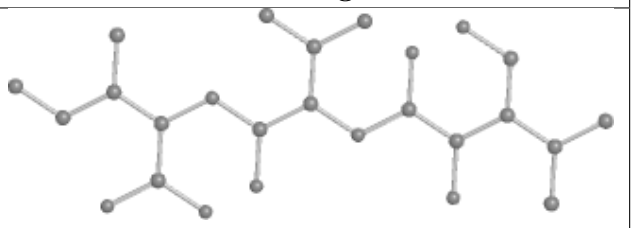

Rings

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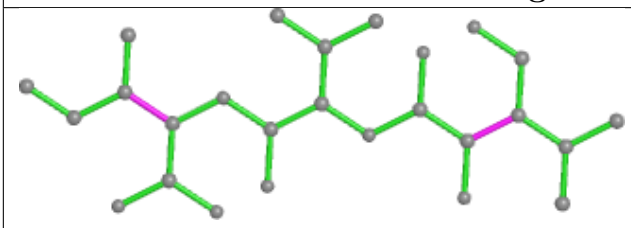

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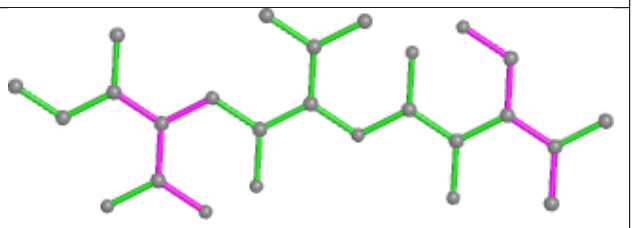

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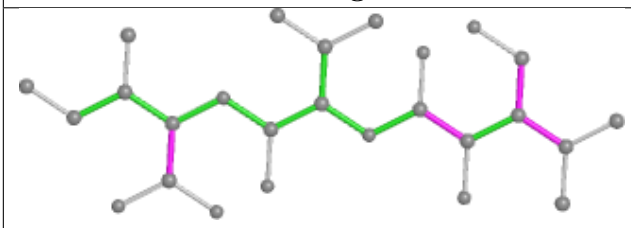

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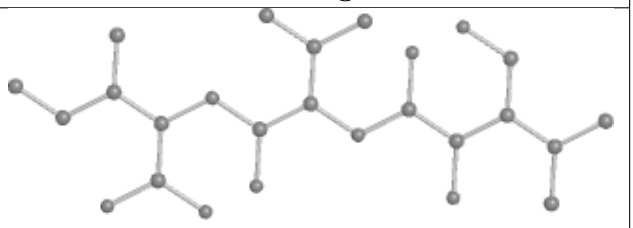

Rings

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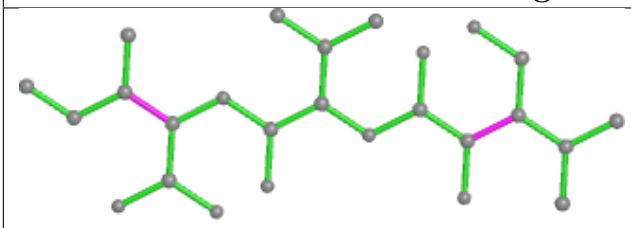

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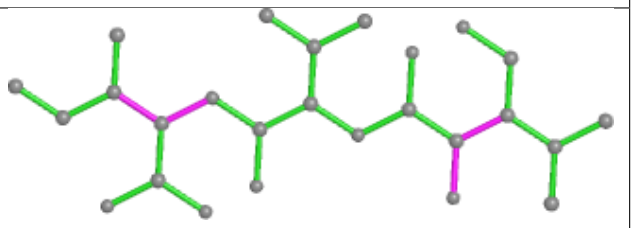

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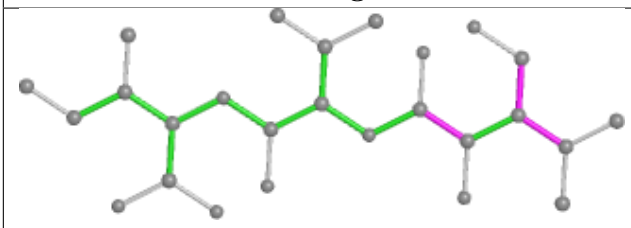

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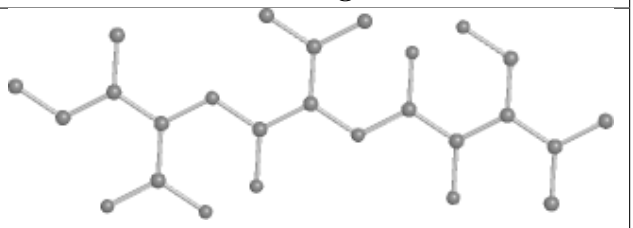

Rings

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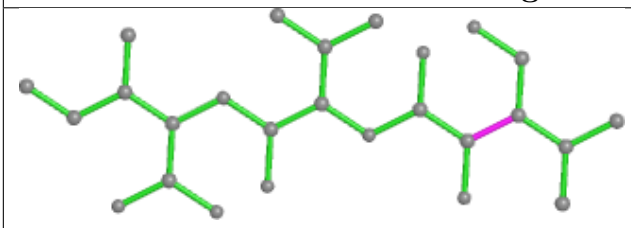

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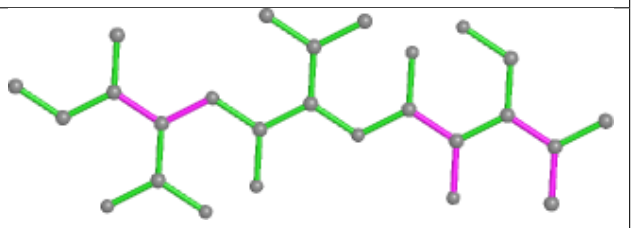

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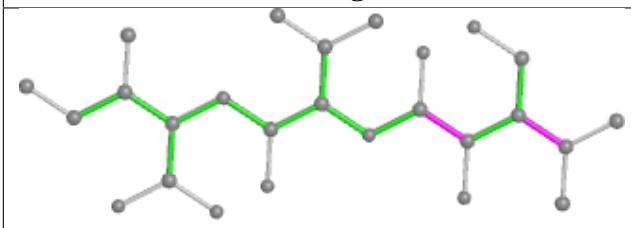

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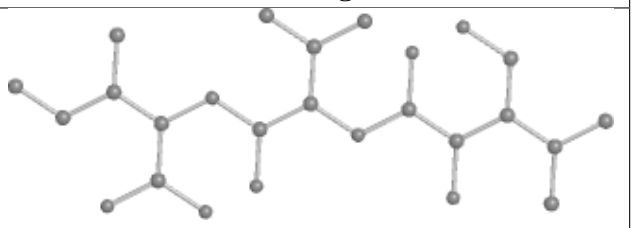

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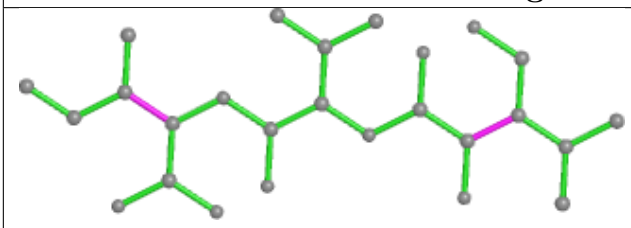

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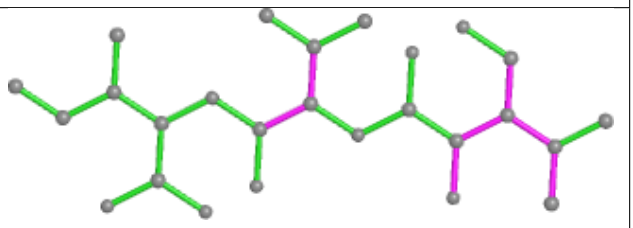

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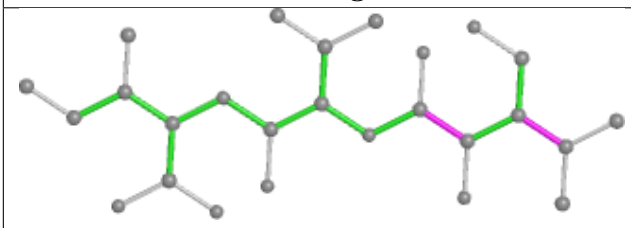

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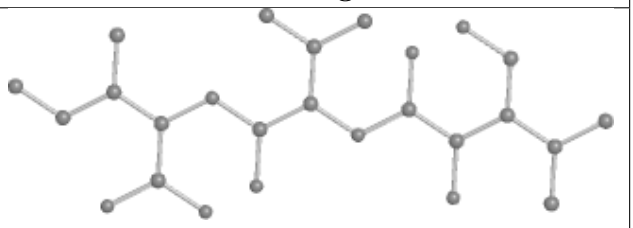

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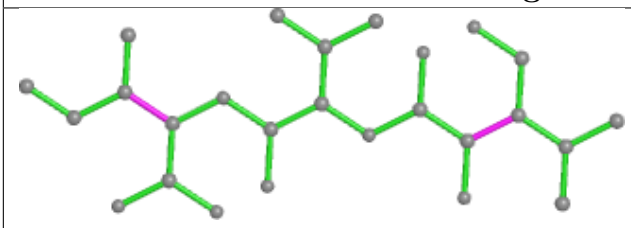

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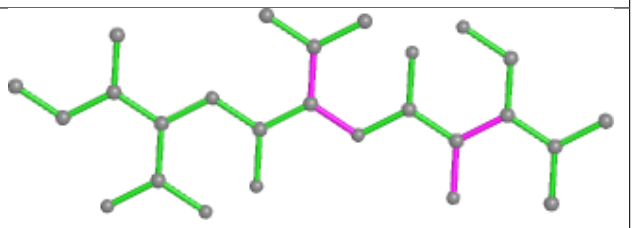

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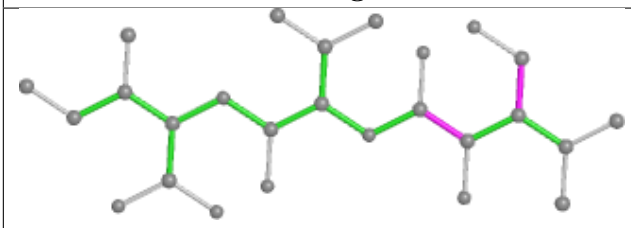

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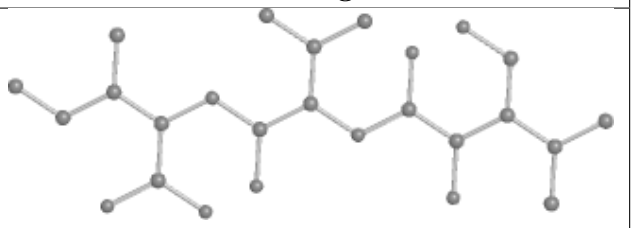

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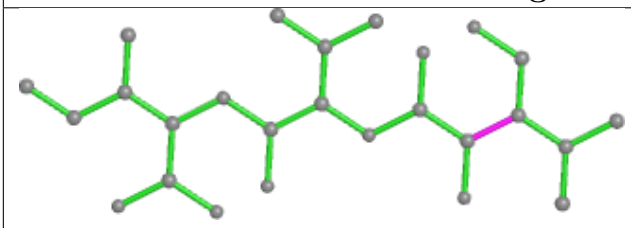

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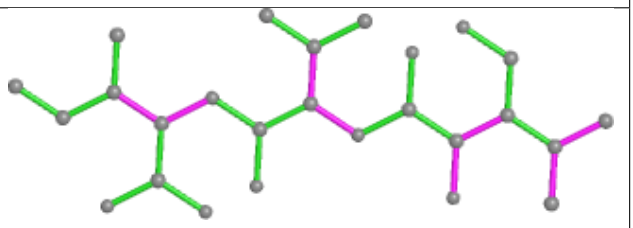

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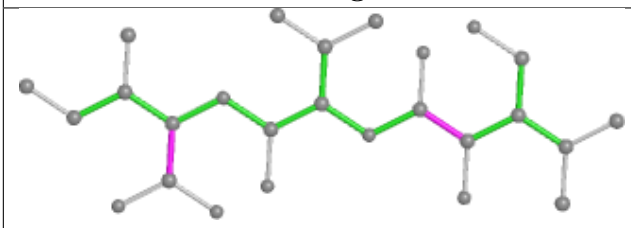

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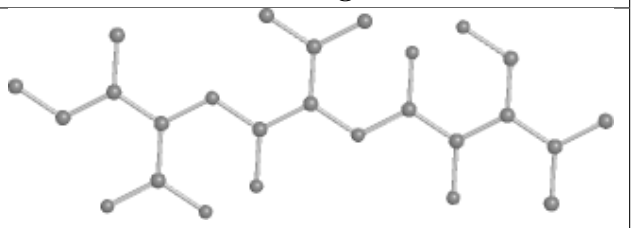

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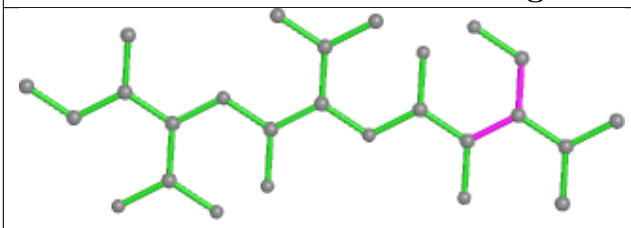

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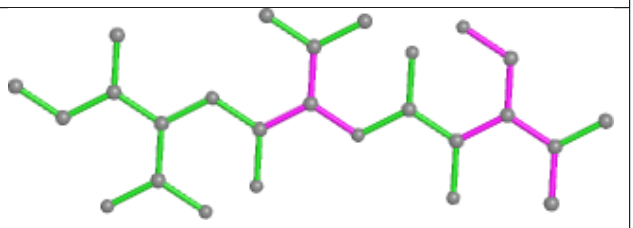

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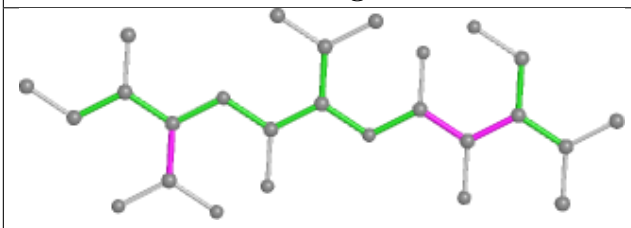

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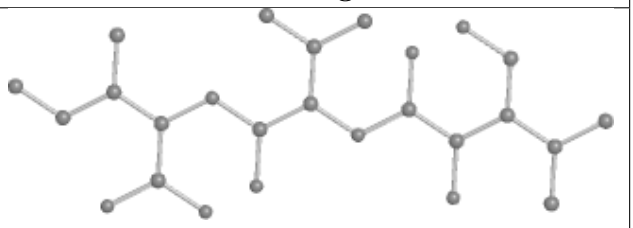

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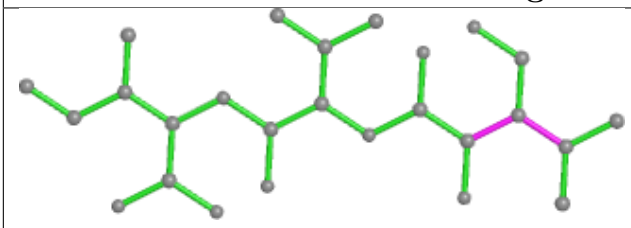

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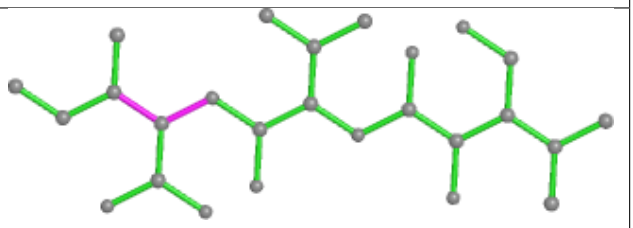

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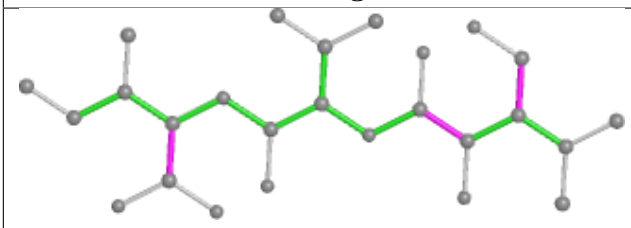

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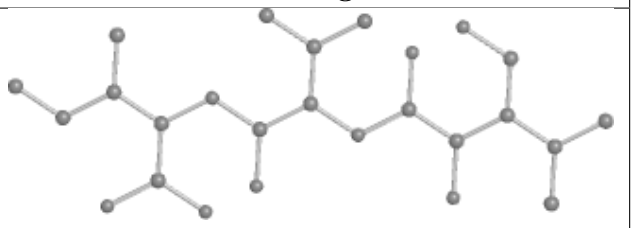

Rings

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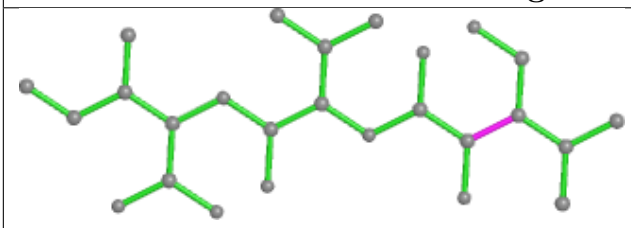

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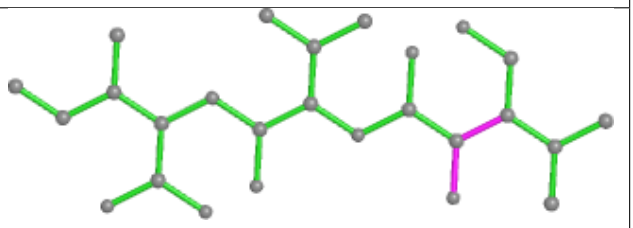

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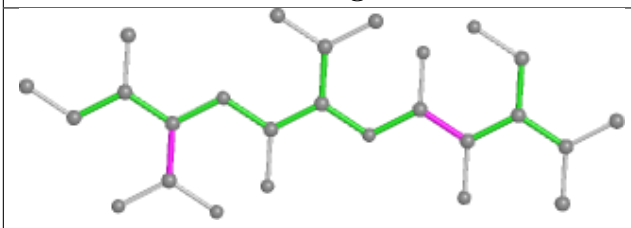

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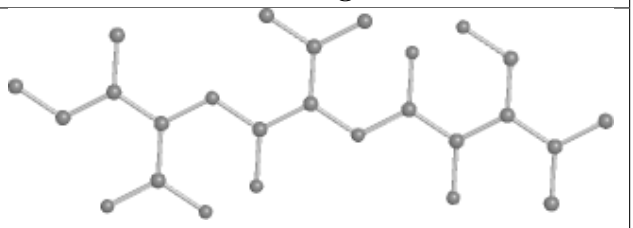

Rings

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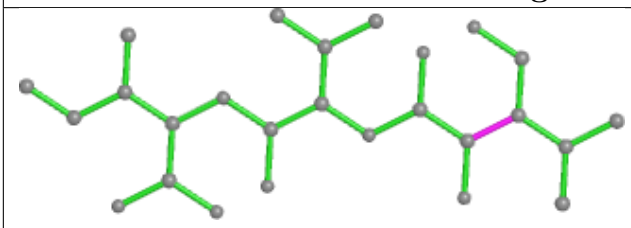

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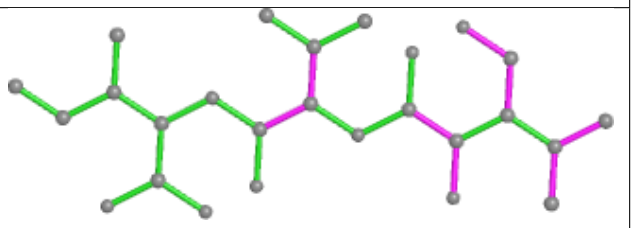

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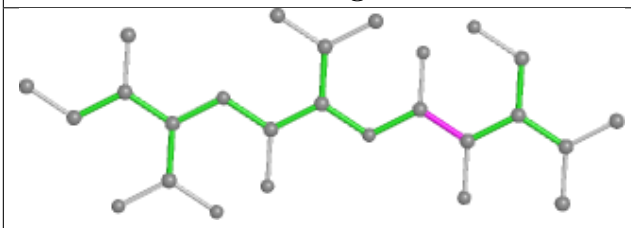

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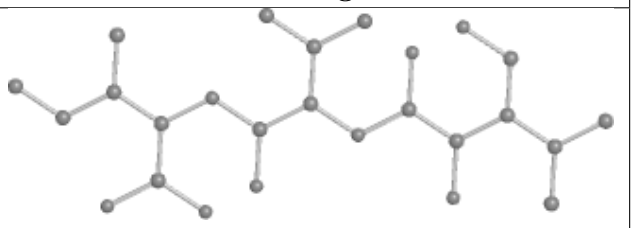

Rings

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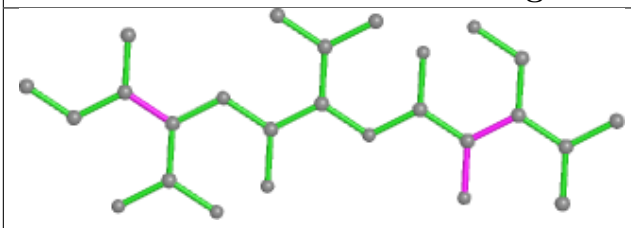

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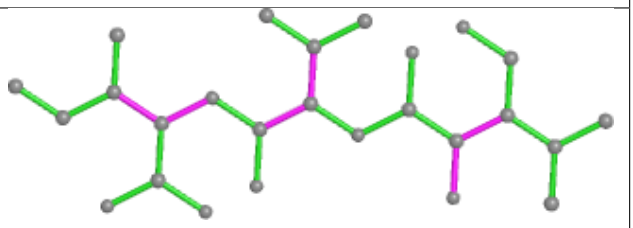

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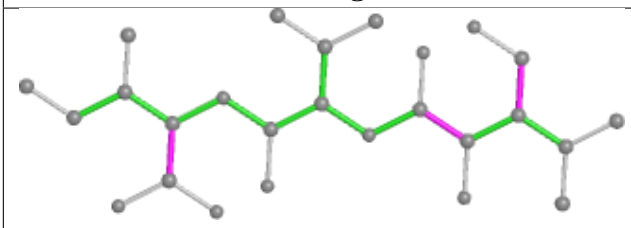

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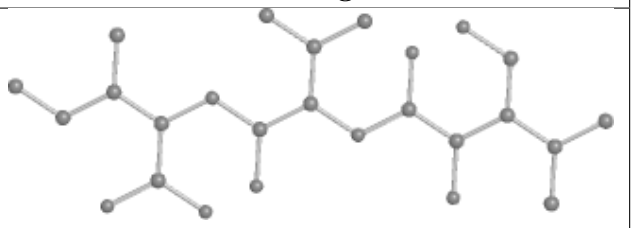

Rings

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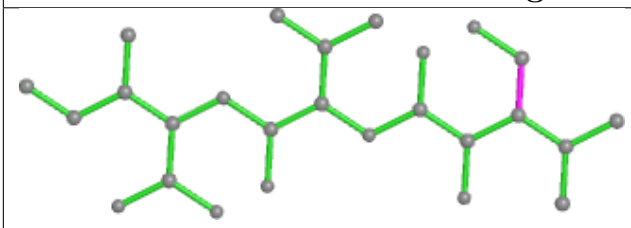

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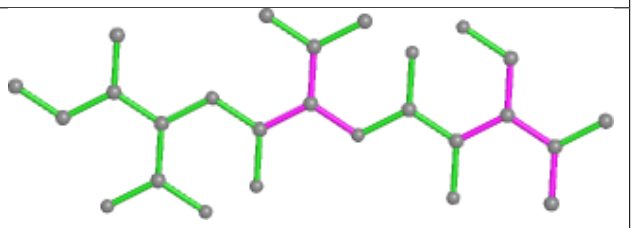

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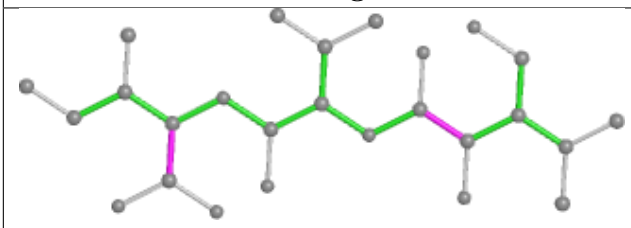

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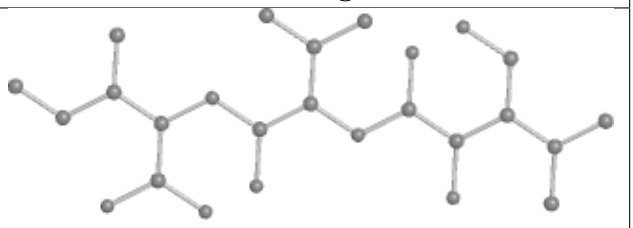
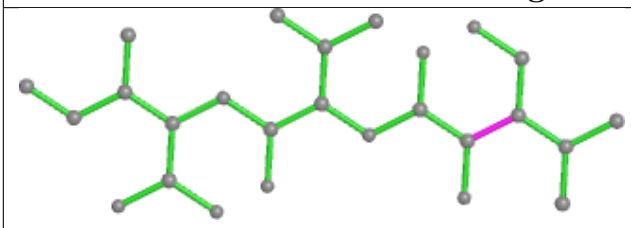
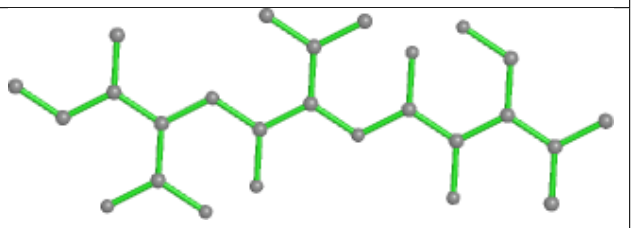


Rings

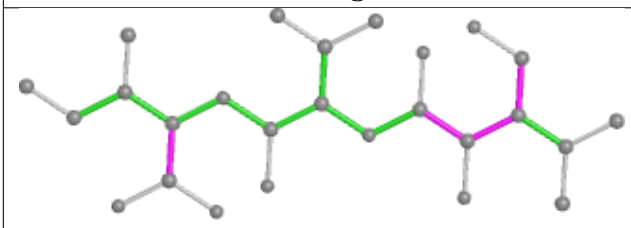
Ligand VSZ T 301



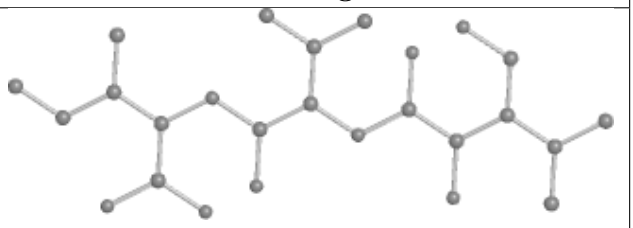
Bond lengths



Bond angles

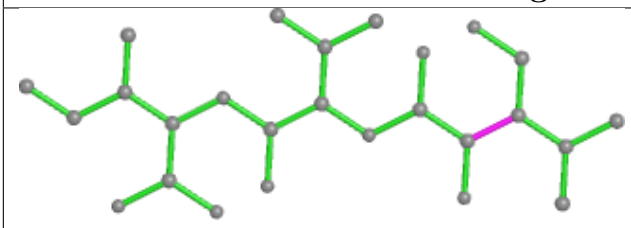


Torsions

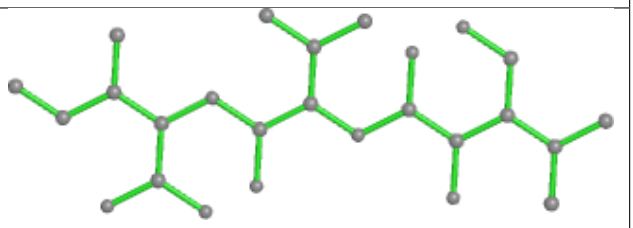


Rings

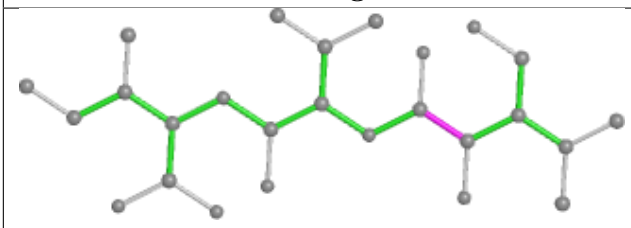
Ligand VSZ S 301



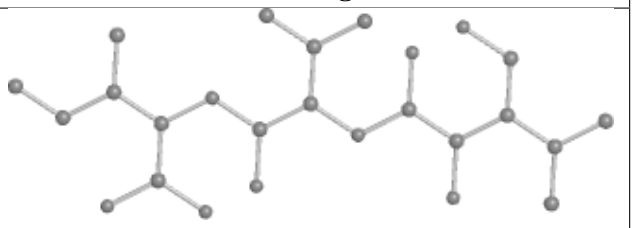
Bond lengths



Bond angles

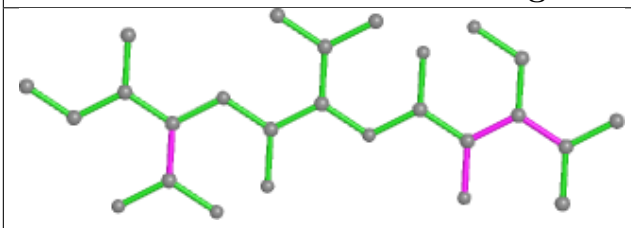


Torsions

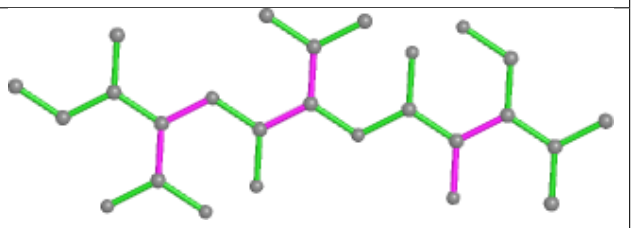


Rings

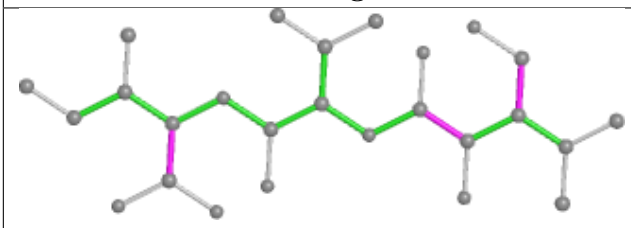
Ligand VSZ E 301



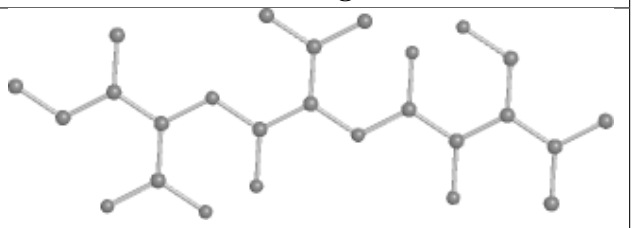
Bond lengths



Bond angles

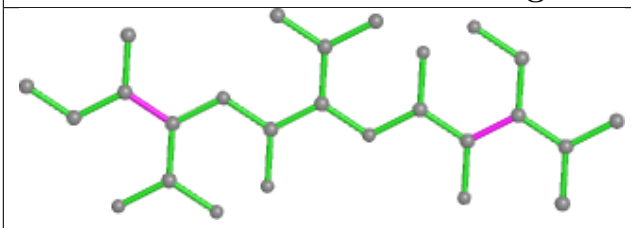


Torsions

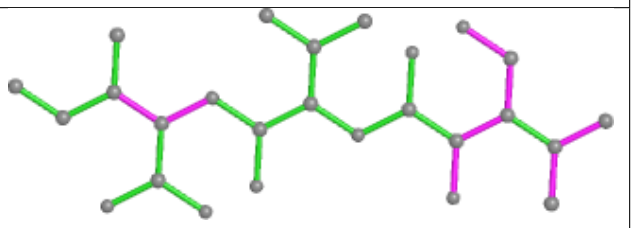


Rings

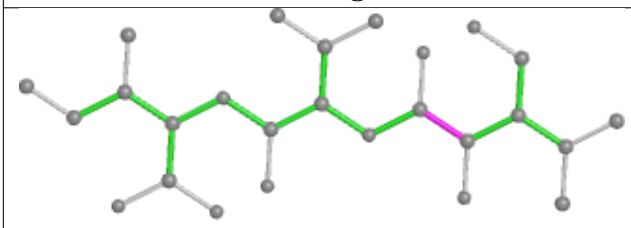
Ligand VSZ C 301



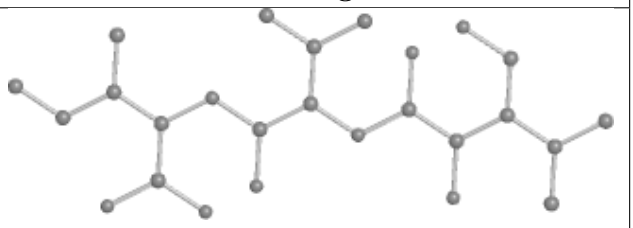
Bond lengths



Bond angles

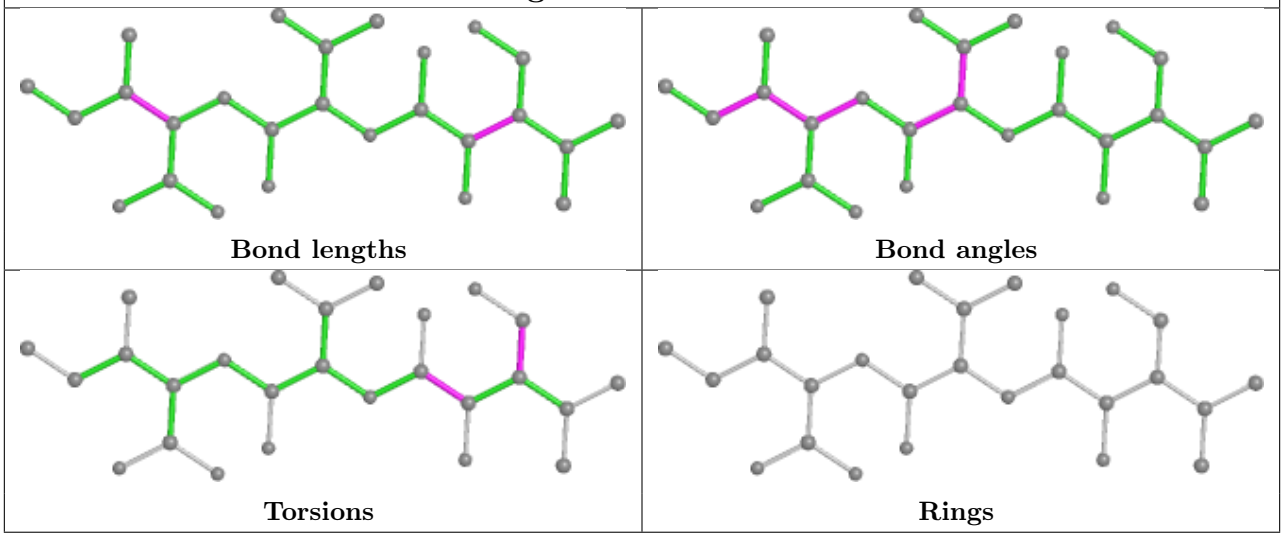


Torsions

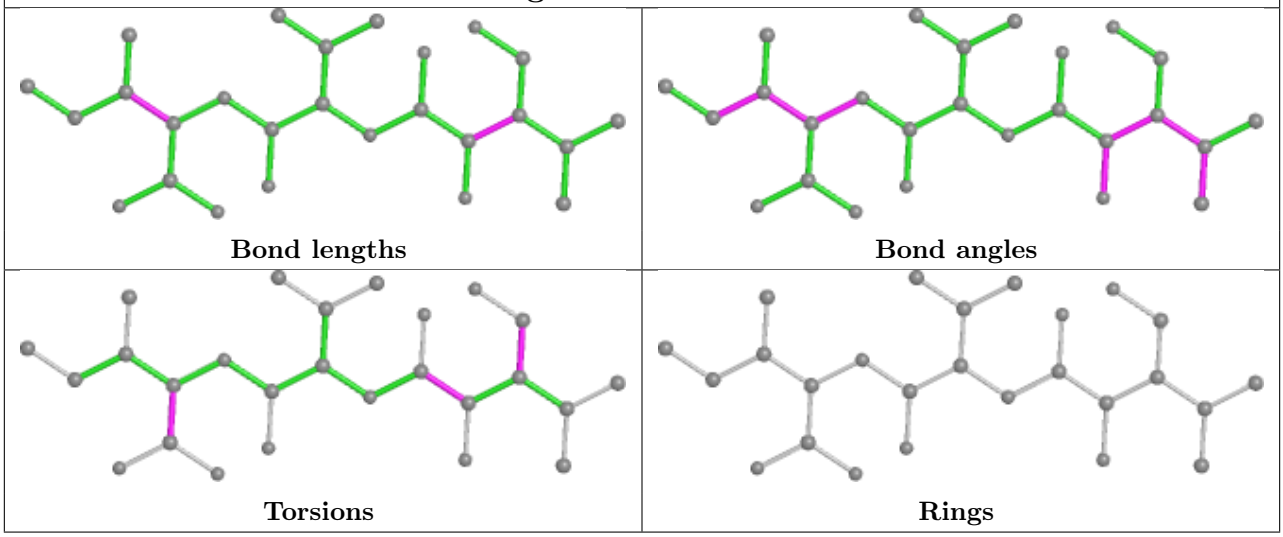


Rings

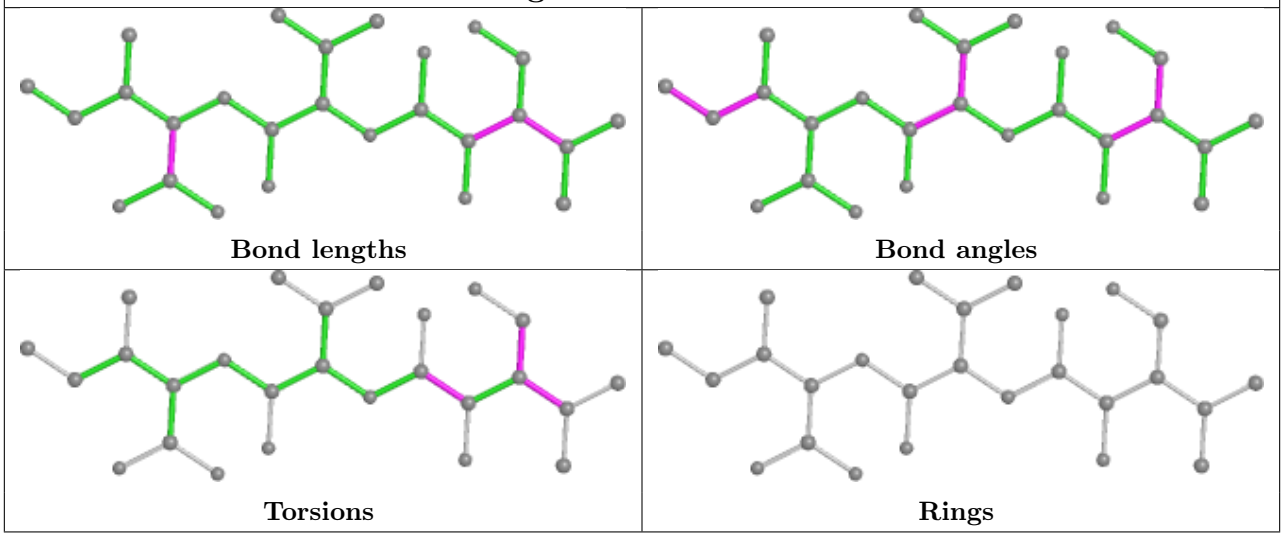
Ligand VSZ D 301



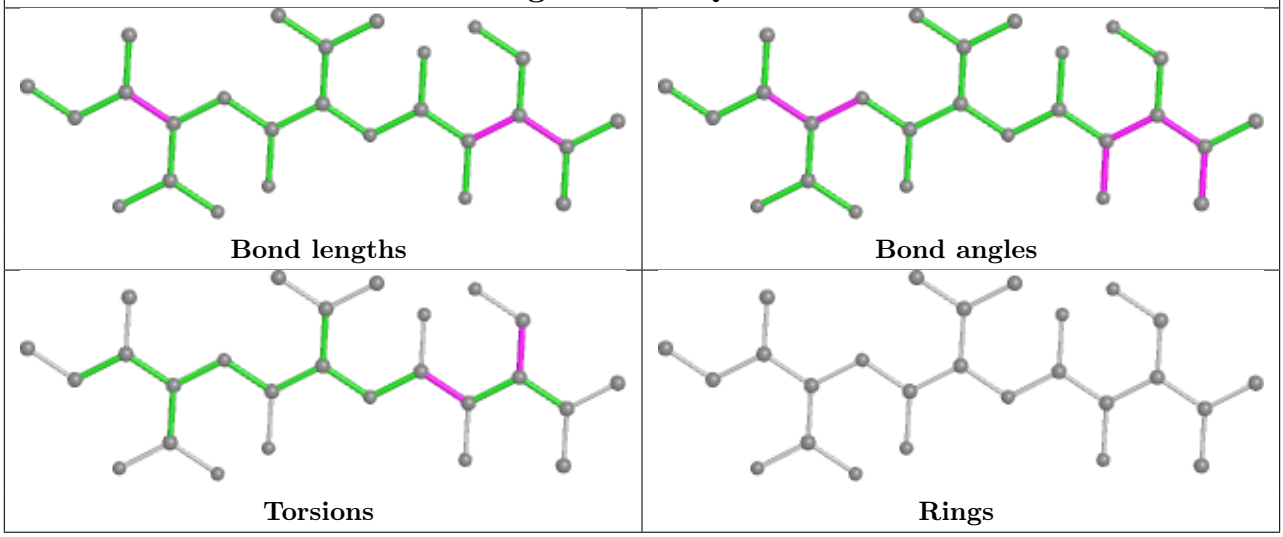
Ligand VSZ K 301



Ligand VSZ A 301



Ligand VSZ Q 301



5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	192/203 (94%)	-0.16	4 (2%)	63	65	54, 68, 100, 111	0
1	B	190/203 (93%)	-0.22	3 (1%)	72	74	50, 66, 99, 126	0
1	C	188/203 (92%)	-0.05	4 (2%)	63	65	58, 75, 99, 108	0
1	D	188/203 (92%)	0.06	7 (3%)	41	41	66, 82, 103, 114	0
1	E	175/203 (86%)	0.16	6 (3%)	45	45	73, 87, 104, 117	0
1	F	179/203 (88%)	0.02	3 (1%)	70	72	69, 91, 112, 137	0
1	G	184/203 (90%)	-0.15	4 (2%)	62	63	61, 85, 105, 132	0
1	H	189/203 (93%)	-0.04	4 (2%)	63	65	59, 75, 91, 107	0
1	I	188/203 (92%)	-0.22	4 (2%)	63	65	60, 72, 94, 104	0
1	J	189/203 (93%)	-0.31	1 (0%)	91	92	52, 68, 92, 109	0
1	K	187/203 (92%)	-0.20	1 (0%)	91	92	52, 66, 90, 111	0
1	L	186/203 (91%)	-0.16	1 (0%)	91	92	51, 69, 95, 114	0
1	M	182/203 (89%)	-0.13	3 (1%)	72	74	63, 77, 91, 122	0
1	N	184/203 (90%)	-0.04	4 (2%)	62	63	62, 77, 90, 110	0
1	O	183/203 (90%)	0.26	8 (4%)	34	33	70, 91, 112, 140	0
1	P	183/203 (90%)	-0.10	6 (3%)	46	46	67, 83, 109, 129	0
1	Q	184/203 (90%)	0.17	5 (2%)	54	55	72, 89, 114, 125	0
1	R	182/203 (89%)	0.16	5 (2%)	54	55	83, 105, 121, 140	0
1	S	182/203 (89%)	0.18	9 (4%)	29	28	75, 96, 118, 142	0
1	T	183/203 (90%)	0.04	6 (3%)	46	46	62, 82, 110, 129	0
1	U	183/203 (90%)	0.09	6 (3%)	46	46	63, 80, 109, 128	0
1	V	179/203 (88%)	0.24	8 (4%)	33	31	80, 102, 125, 134	0
1	W	184/203 (90%)	0.31	12 (6%)	18	17	80, 101, 125, 142	0
1	X	184/203 (90%)	0.02	8 (4%)	35	33	69, 84, 113, 126	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	Y	182/203 (89%)	0.02	2 (1%) 80 82	73, 86, 100, 119	0
1	Z	181/203 (89%)	0.07	8 (4%) 34 33	72, 89, 111, 124	0
1	a	182/203 (89%)	-0.07	0 100 100	67, 85, 115, 133	0
1	b	183/203 (90%)	0.11	5 (2%) 54 55	72, 86, 111, 126	0
All	All	5156/5684 (90%)	0.00	137 (2%) 54 55	50, 83, 113, 142	0

The worst 5 of 137 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	O	17	ALA	6.3
1	V	18	TYR	6.2
1	U	8	ILE	6.0
1	V	17	ALA	5.7
1	O	7	VAL	5.2

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	VSZ	Y	301	26/26	0.83	0.22	81,85,93,94	0
2	VSZ	X	301	26/26	0.87	0.26	81,82,87,88	0
2	VSZ	O	301	26/26	0.88	0.17	78,81,90,92	0
2	VSZ	R	301	26/26	0.88	0.25	96,99,104,105	0
2	VSZ	b	301	26/26	0.88	0.23	83,85,94,95	0
2	VSZ	Z	301	26/26	0.90	0.20	81,85,90,92	0
2	VSZ	S	301	26/26	0.91	0.19	87,89,92,92	0

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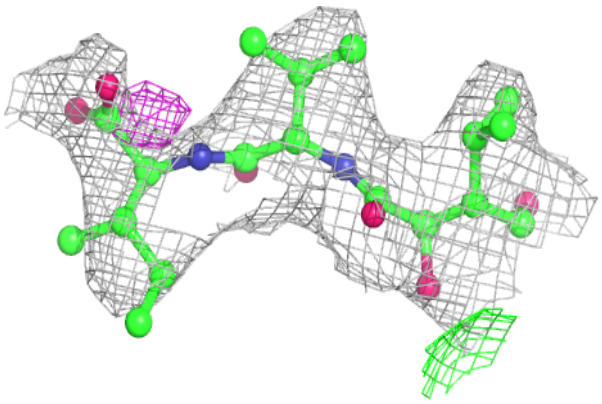
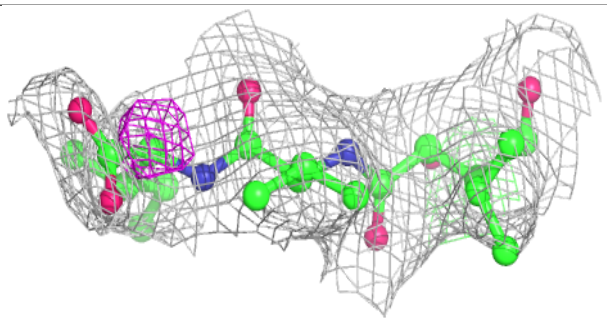
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	VSZ	V	301	26/26	0.91	0.22	87,90,94,95	0
2	VSZ	N	301	26/26	0.91	0.18	74,76,82,83	0
2	VSZ	D	301	26/26	0.92	0.21	68,70,76,77	0
2	VSZ	E	301	26/26	0.92	0.21	82,84,91,91	0
2	VSZ	L	301	26/26	0.92	0.19	59,62,72,73	0
2	VSZ	A	301	26/26	0.93	0.19	63,67,73,74	0
2	VSZ	W	301	26/26	0.93	0.17	85,88,91,93	0
2	VSZ	F	301	26/26	0.93	0.16	80,82,85,86	0
2	VSZ	G	301	26/26	0.93	0.24	76,78,79,80	0
2	VSZ	I	301	26/26	0.93	0.18	67,69,73,74	0
2	VSZ	K	301	26/26	0.93	0.15	60,62,68,70	0
2	VSZ	U	301	26/26	0.94	0.21	69,73,81,82	0
2	VSZ	C	301	26/26	0.94	0.16	62,66,72,73	0
2	VSZ	P	301	26/26	0.94	0.16	72,74,76,77	0
2	VSZ	Q	301	26/26	0.94	0.22	79,82,88,88	0
2	VSZ	M	301	26/26	0.94	0.20	70,74,81,81	0
2	VSZ	H	301	26/26	0.94	0.17	69,72,75,76	0
2	VSZ	a	301	26/26	0.94	0.21	77,79,84,86	0
2	VSZ	T	301	26/26	0.94	0.14	69,71,77,79	0
2	VSZ	B	301	26/26	0.96	0.17	61,63,69,69	0
2	VSZ	J	301	26/26	0.96	0.12	58,60,62,62	0

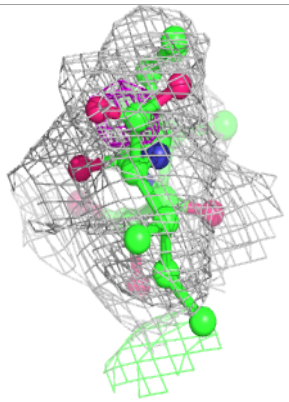
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around VSZ Y 301:

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

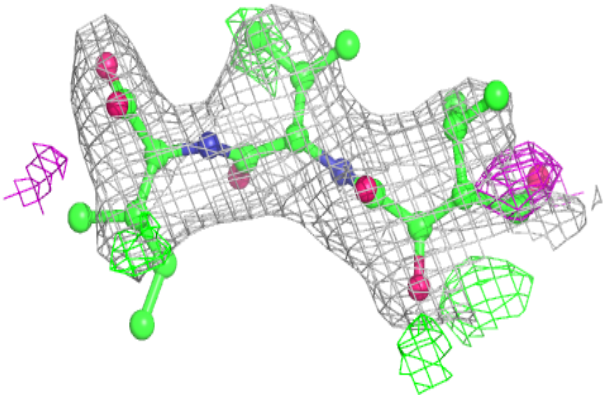


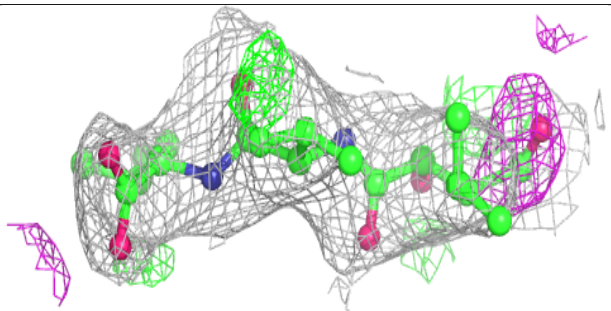


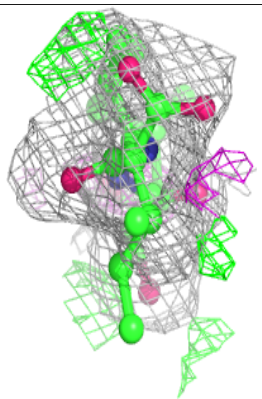


Electron density around VSZ X 301:

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

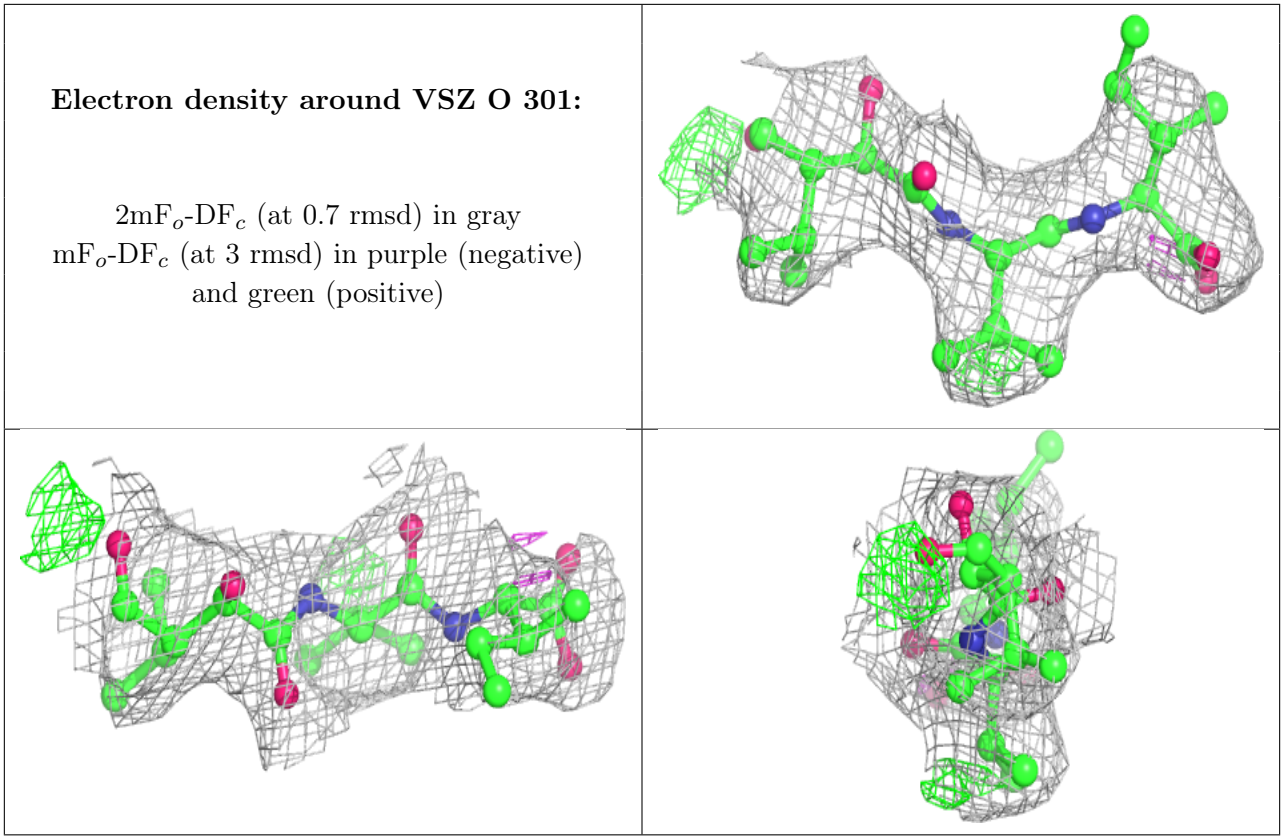






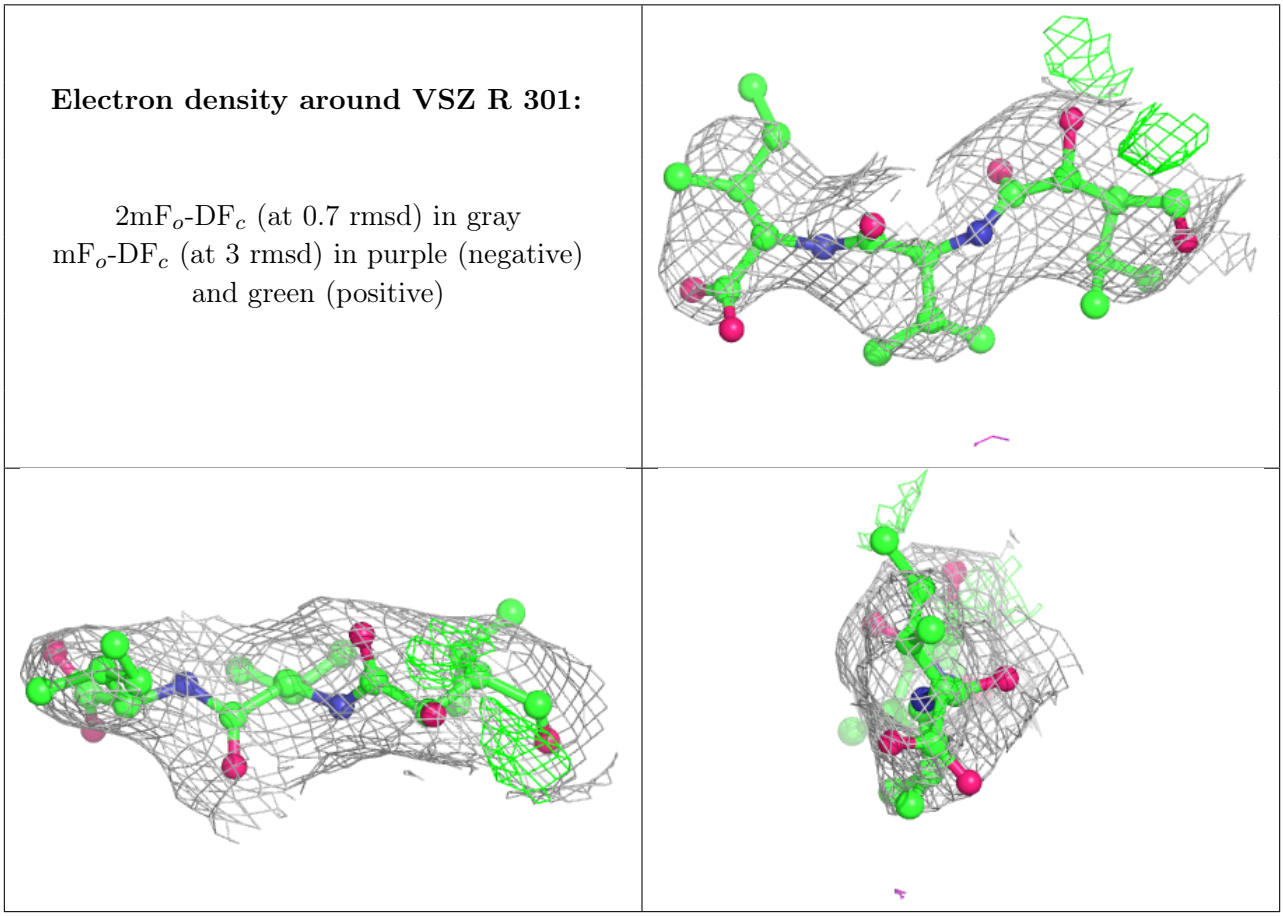
Electron density around VSZ O 301:

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



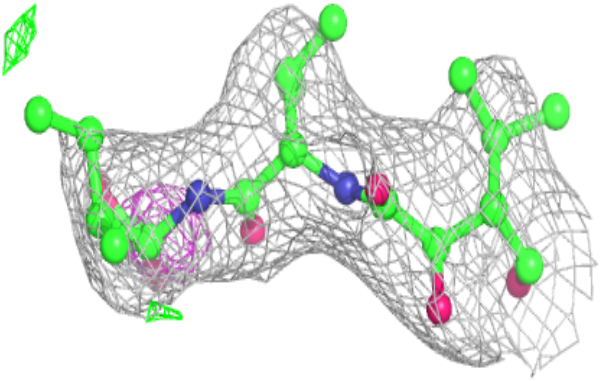
Electron density around VSZ R 301:

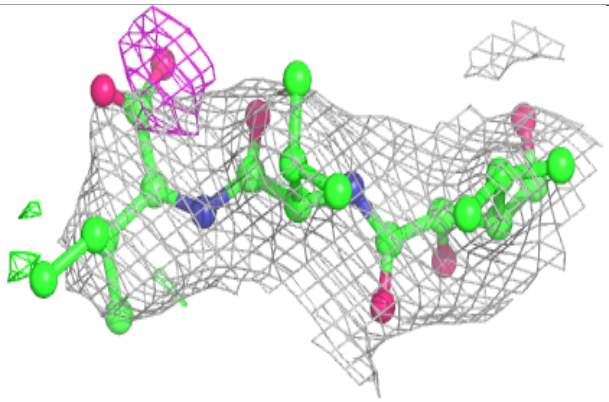
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

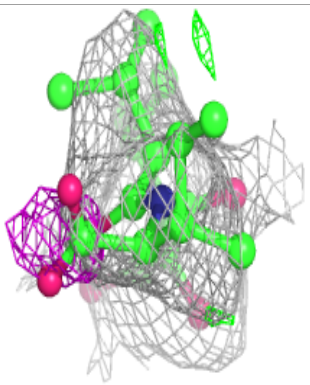


Electron density around VSZ b 301:

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

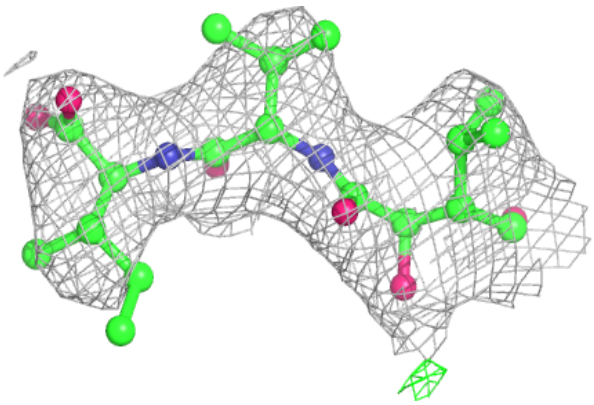


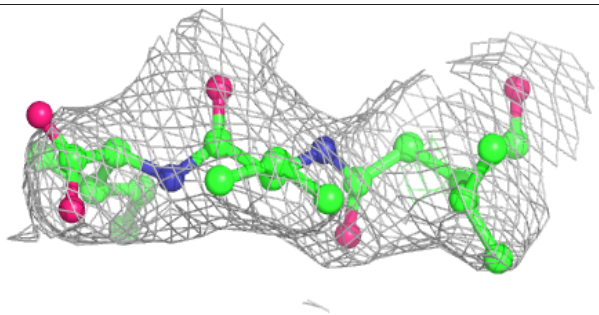


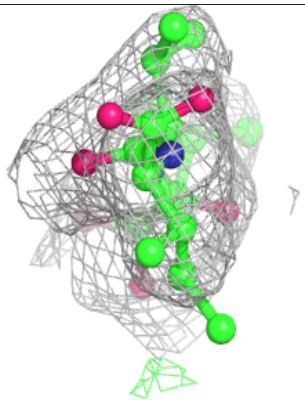


Electron density around VSZ Z 301:

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

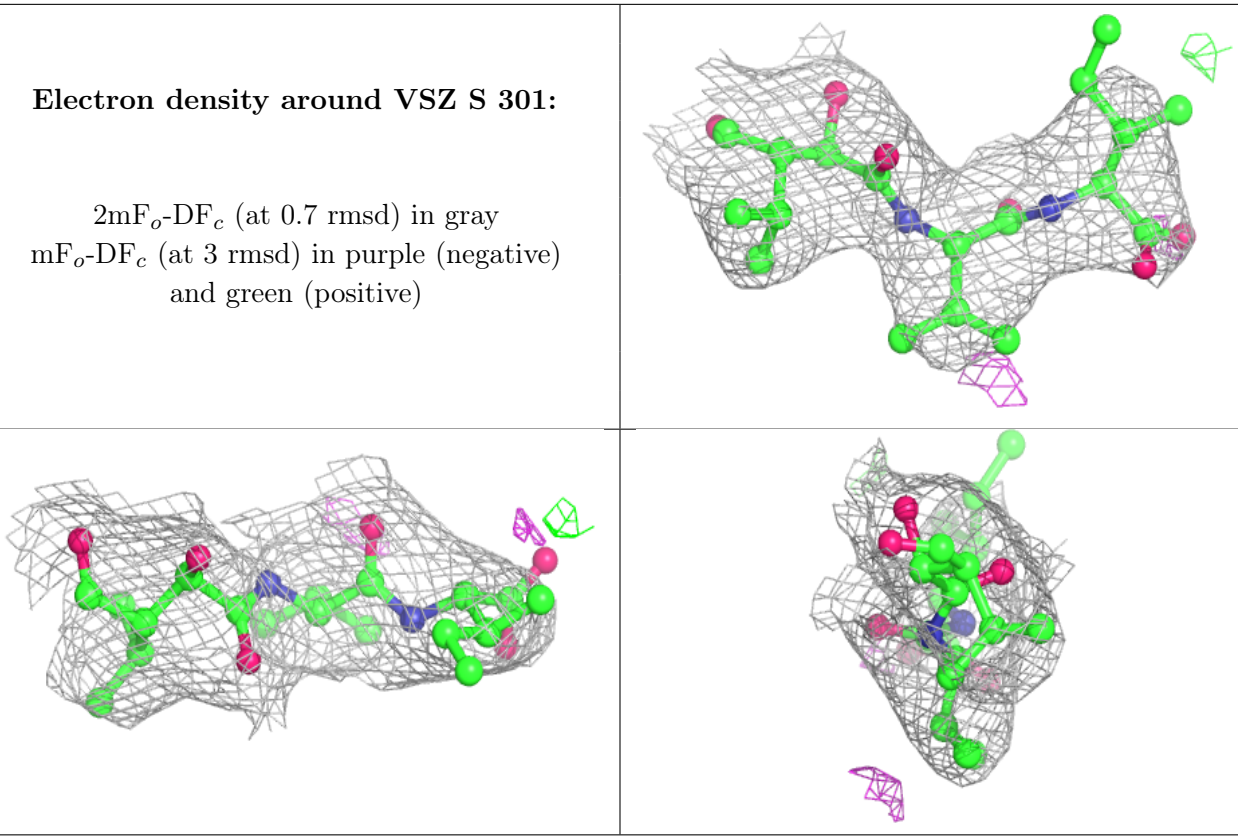






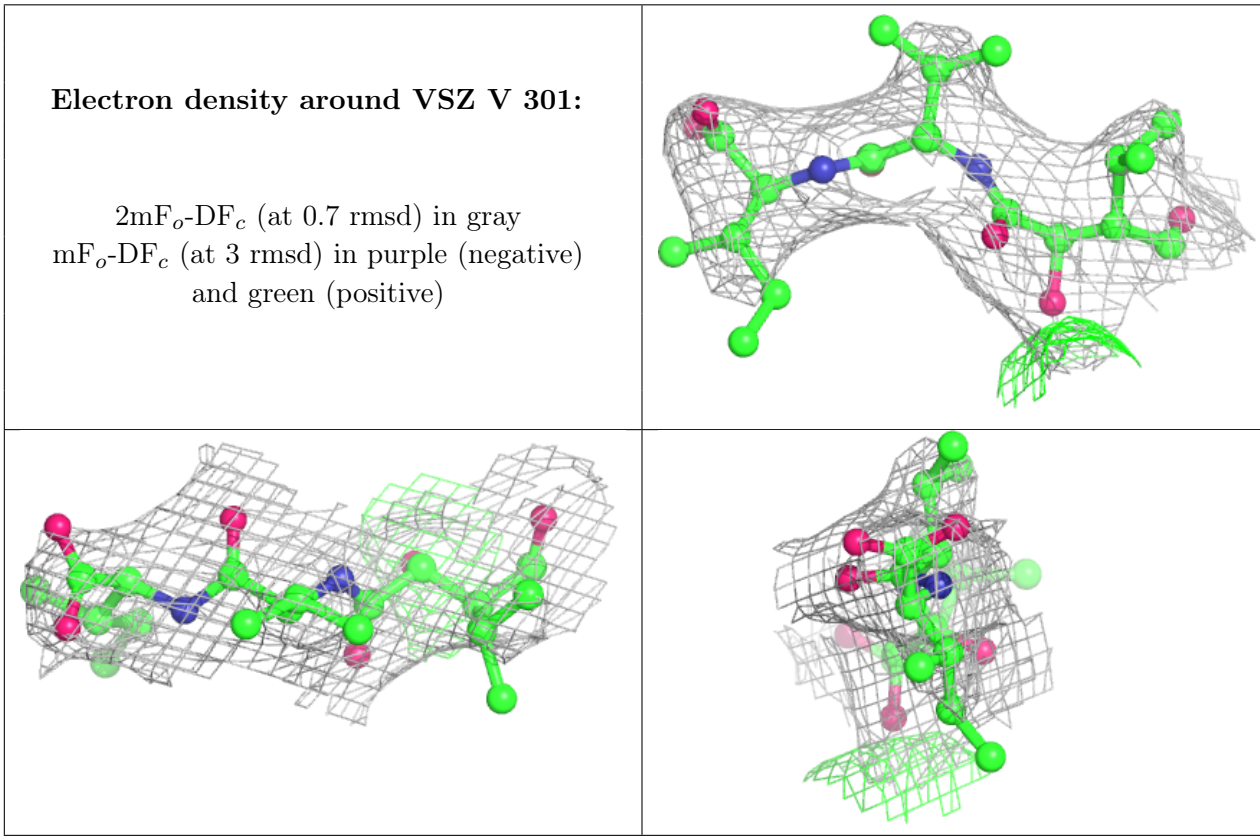
Electron density around VSZ S 301:

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



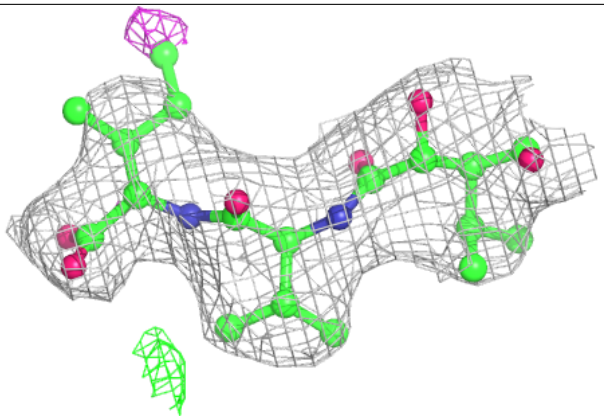
Electron density around VSZ V 301:

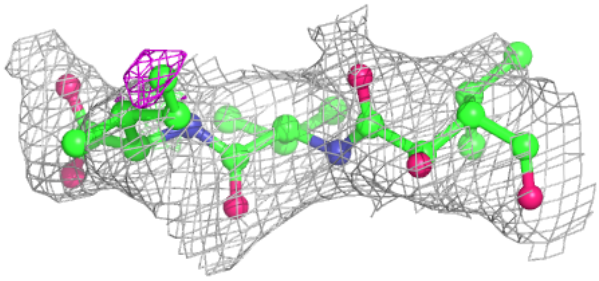
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

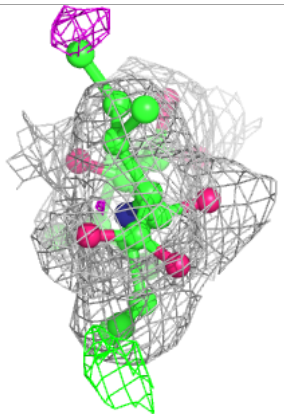


Electron density around VSZ N 301:

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

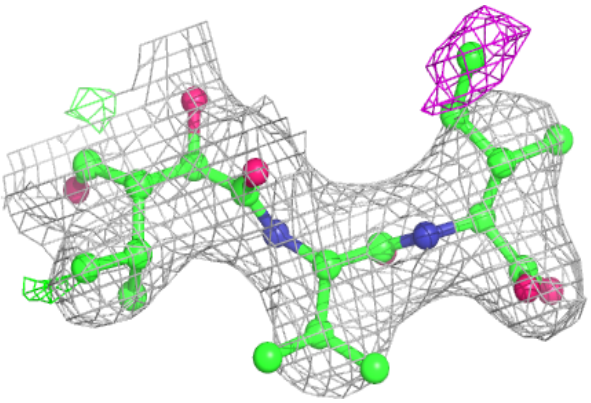


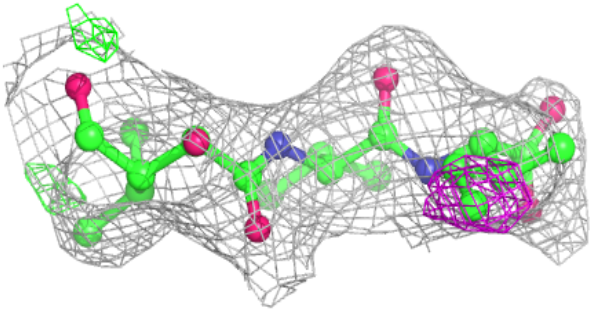


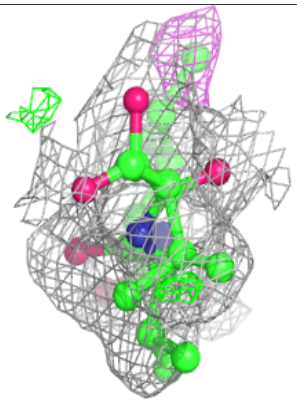


Electron density around VSZ D 301:

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

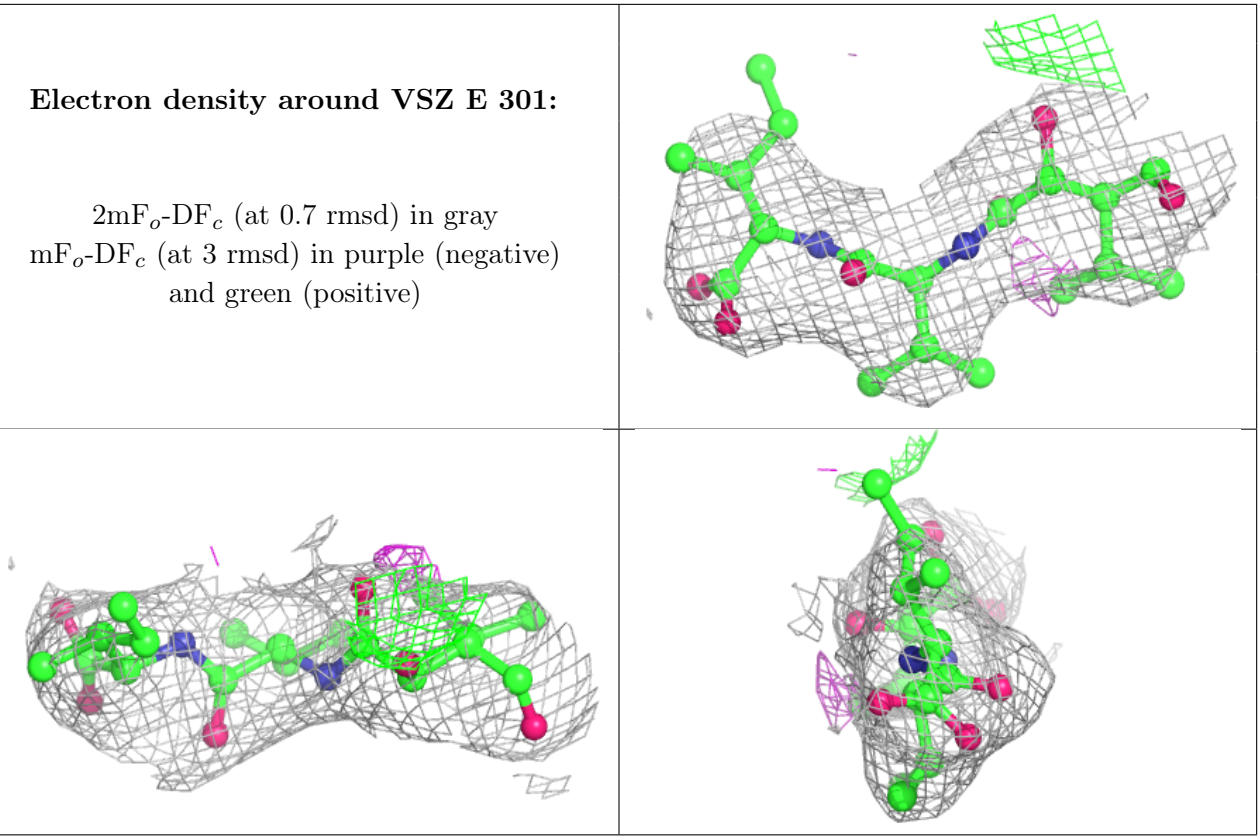






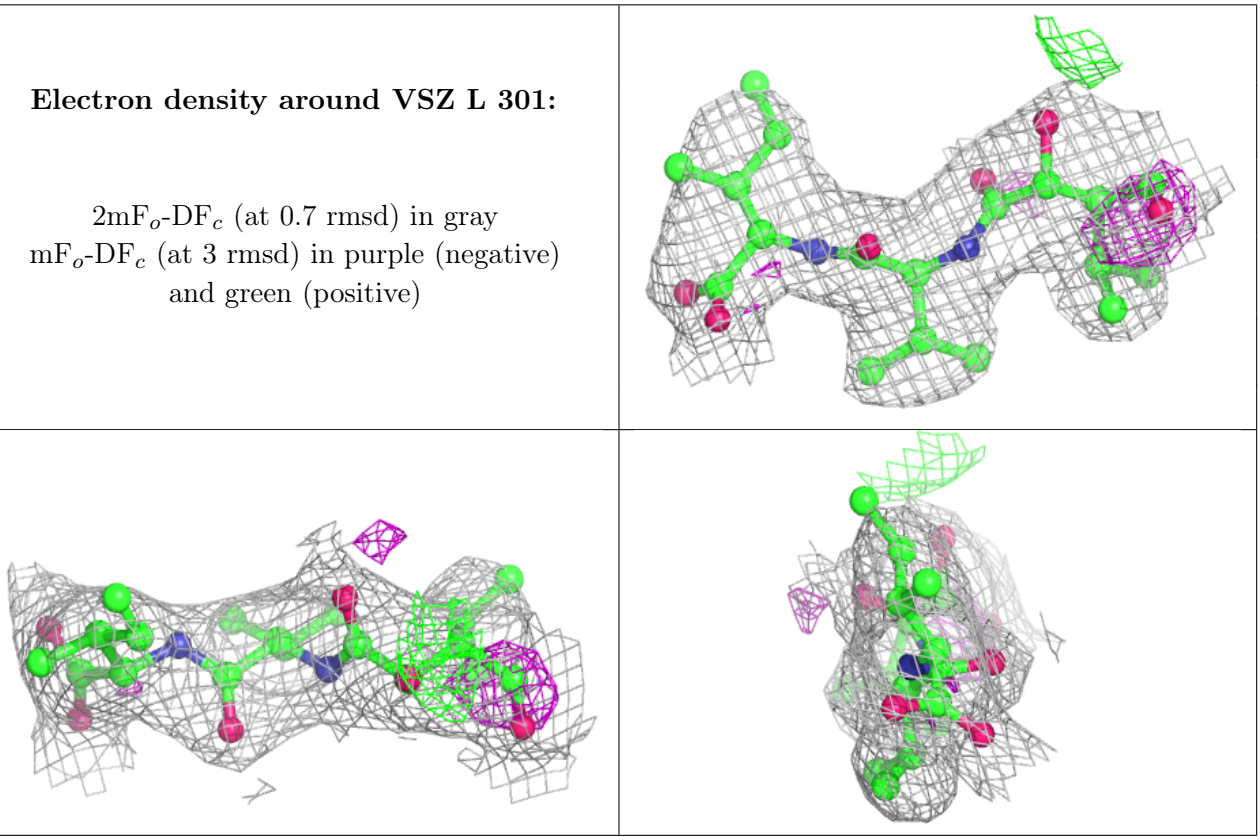
Electron density around VSZ E 301:

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



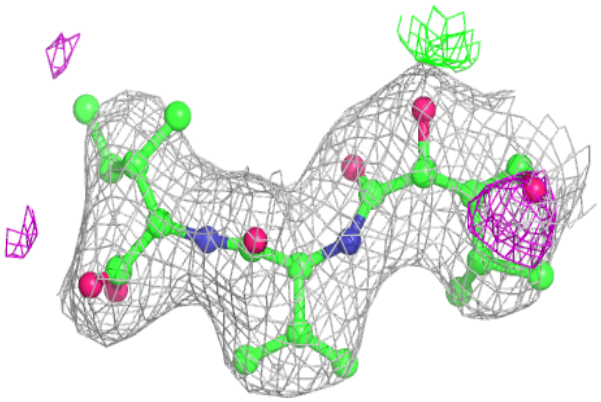
Electron density around VSZ L 301:

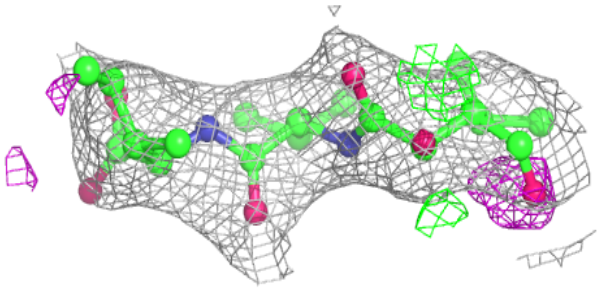
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

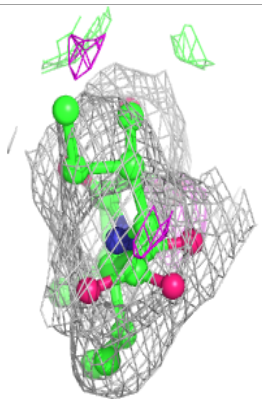


Electron density around VSZ A 301:

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

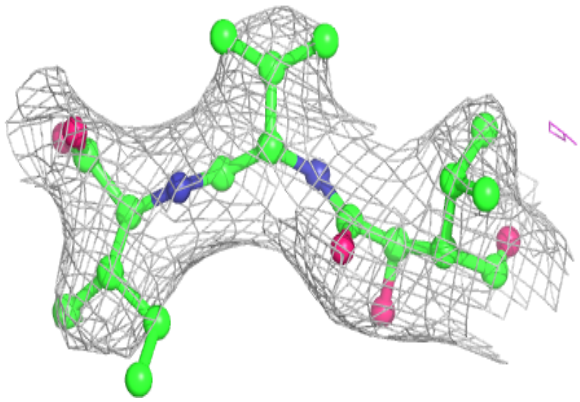


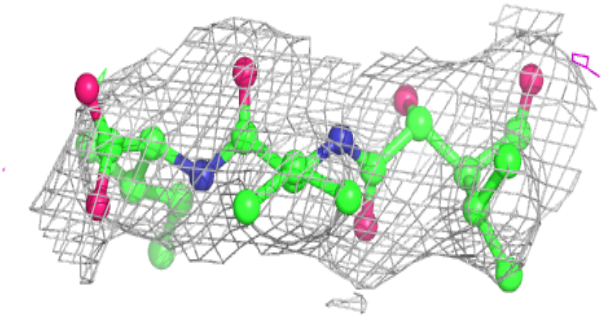


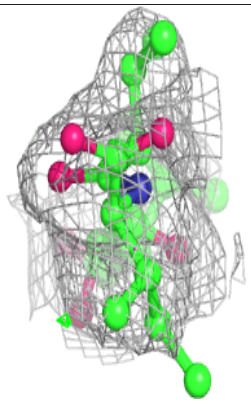


Electron density around VSZ W 301:

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

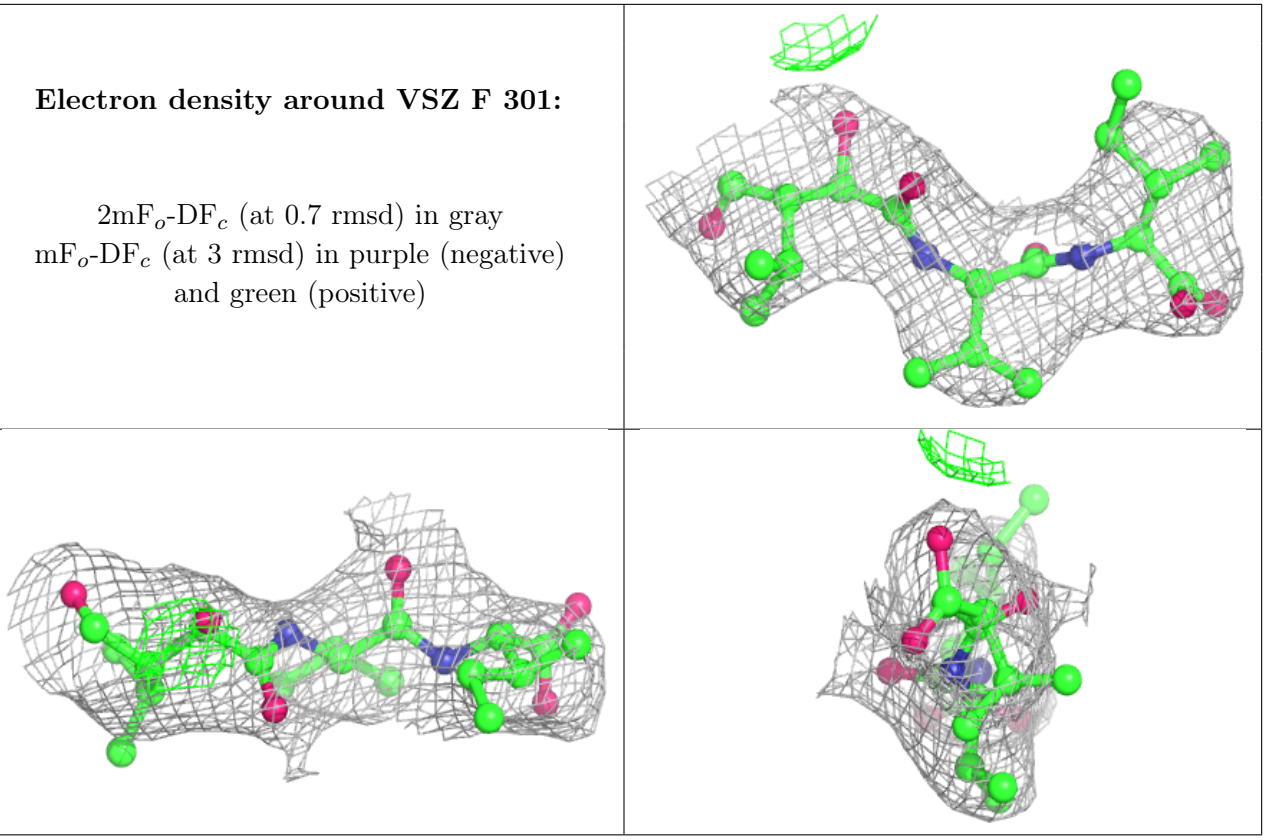






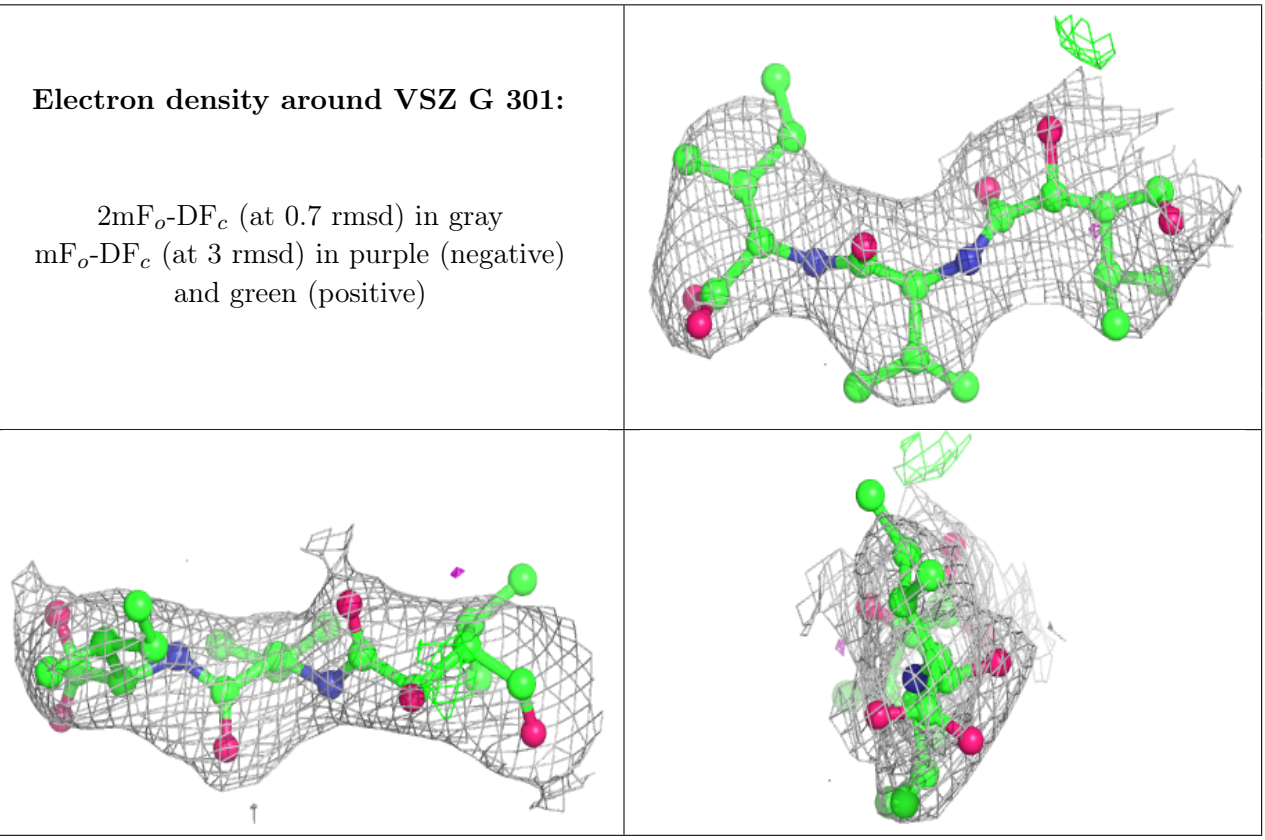
Electron density around VSZ F 301:

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



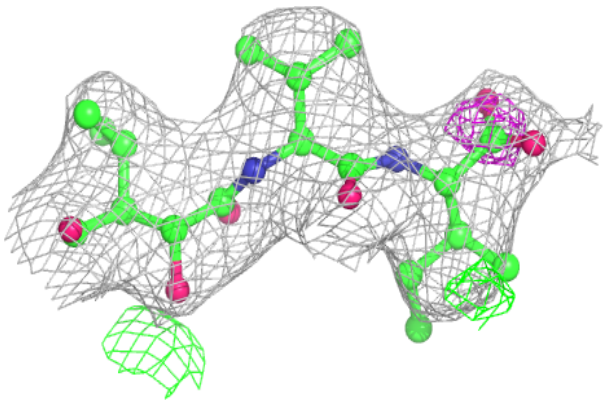
Electron density around VSZ G 301:

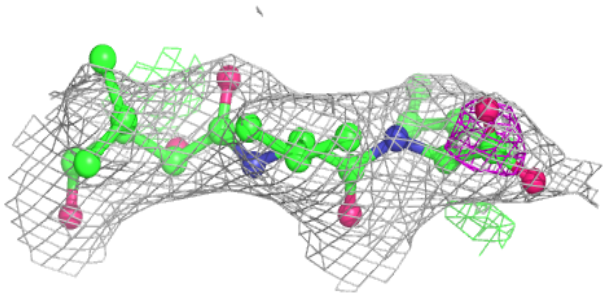
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

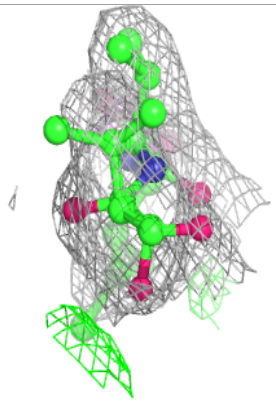


Electron density around VSZ I 301:

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

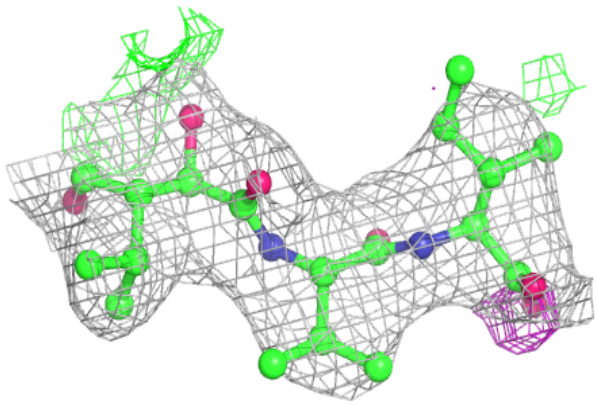


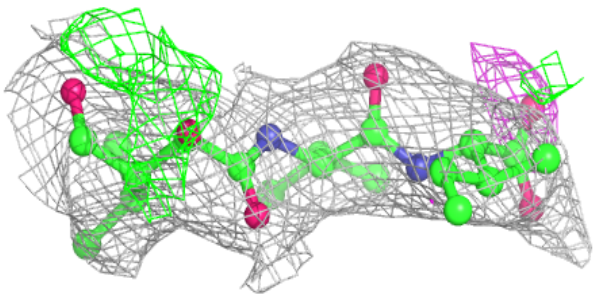


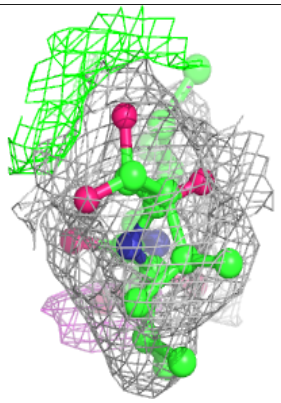


Electron density around VSZ K 301:

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

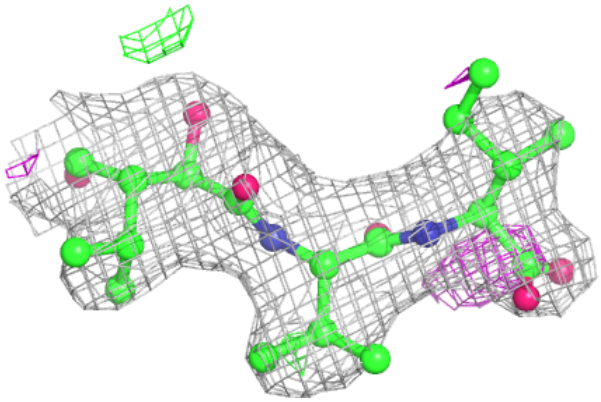


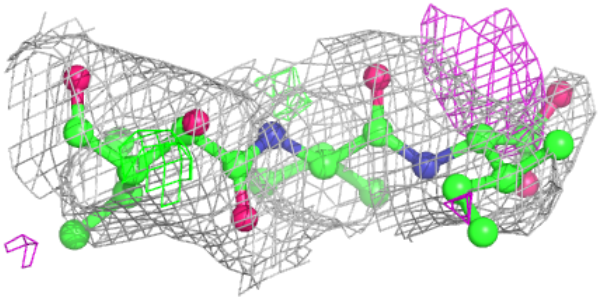


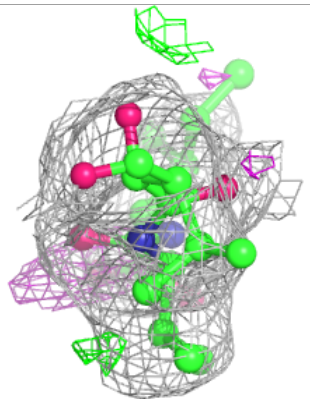


Electron density around VSZ U 301:

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

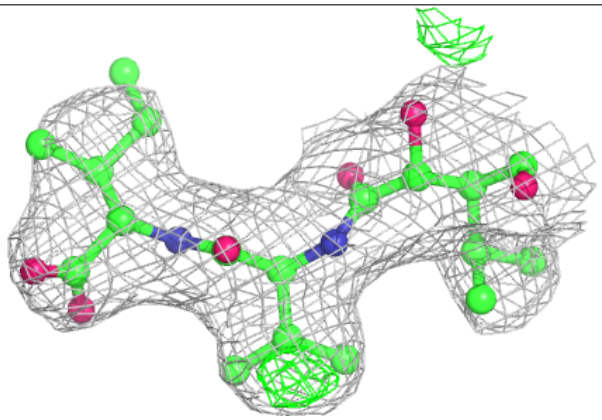


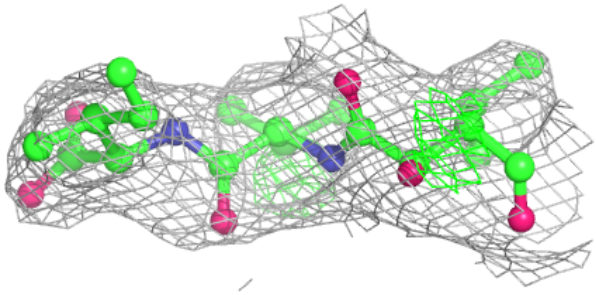


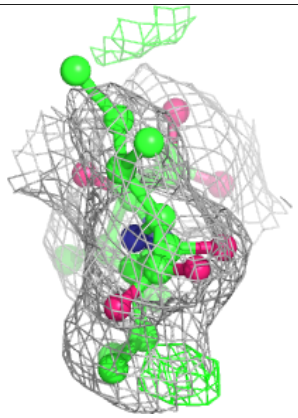


Electron density around VSZ C 301:

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

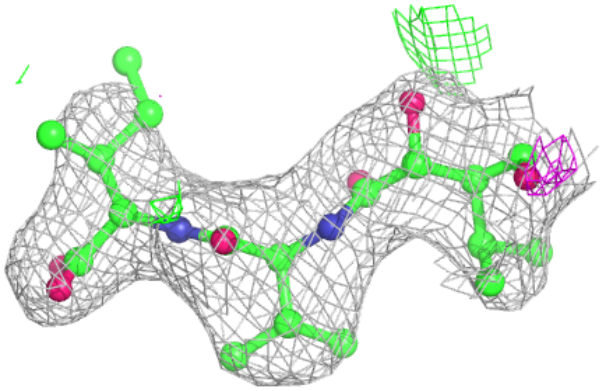


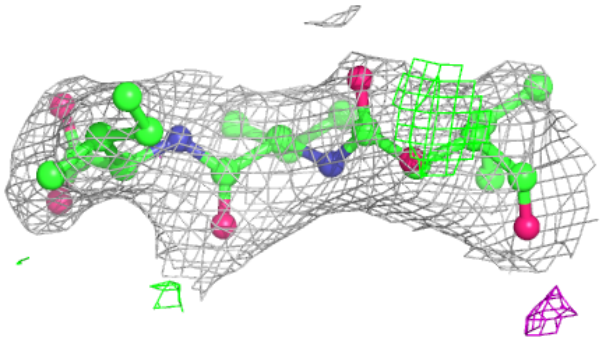


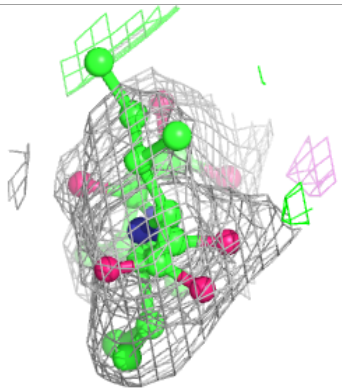


Electron density around VSZ P 301:

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

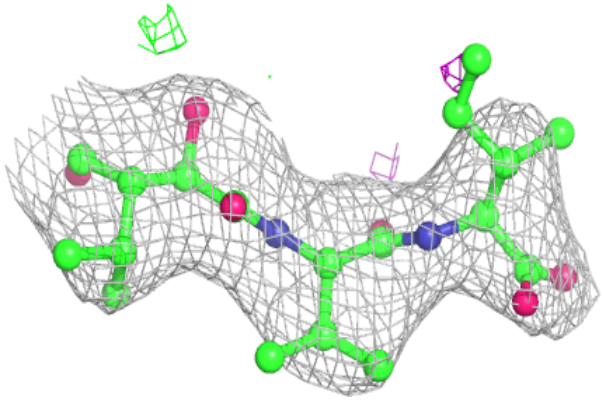


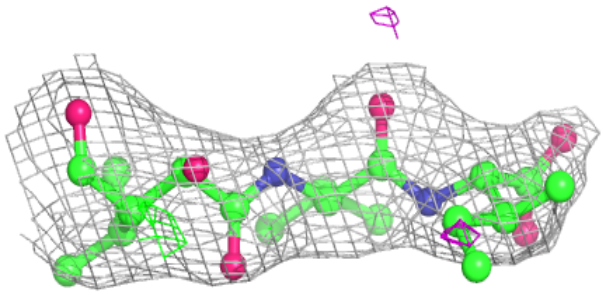


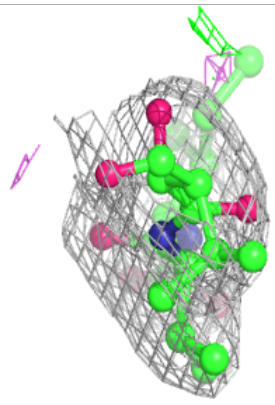


Electron density around VSZ Q 301:

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

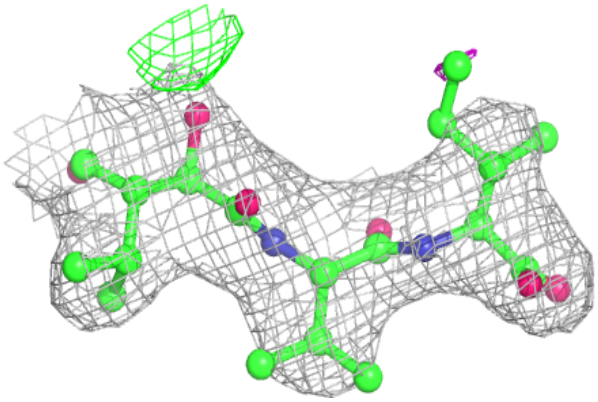


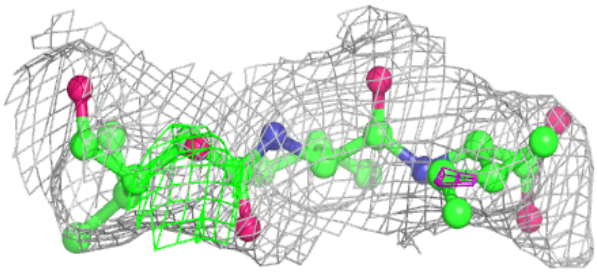


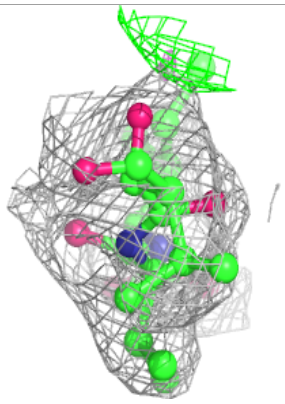


Electron density around VSZ M 301:

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

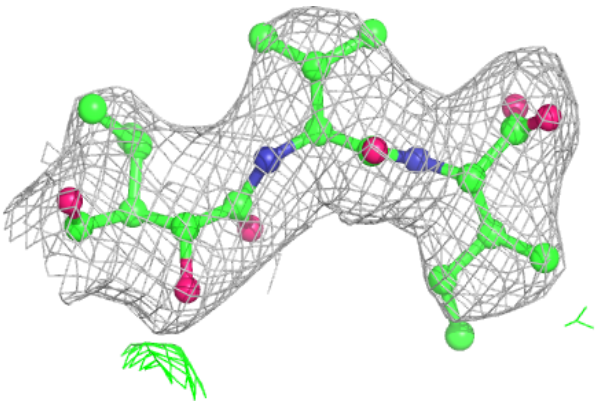


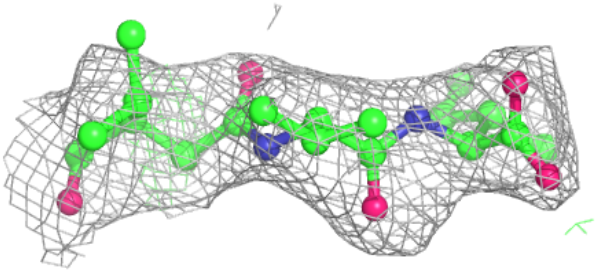


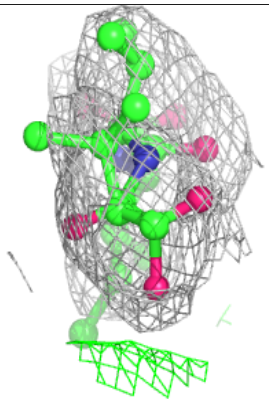


Electron density around VSZ H 301:

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

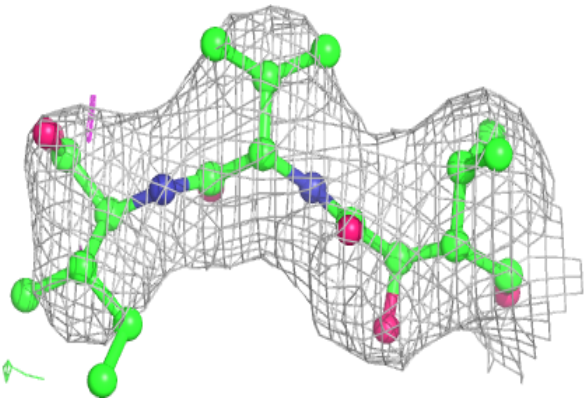


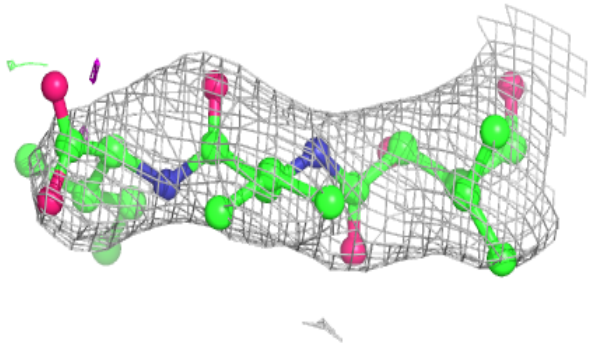


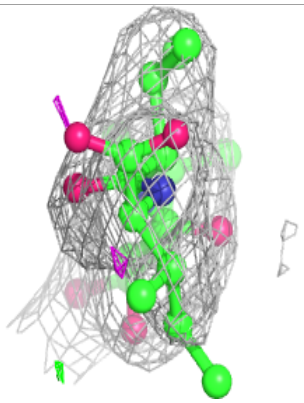


Electron density around VSZ a 301:

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

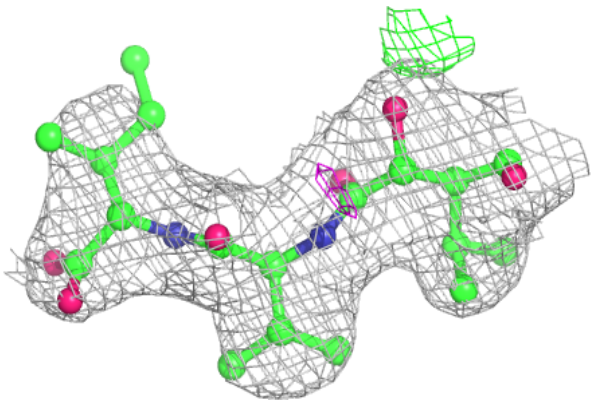


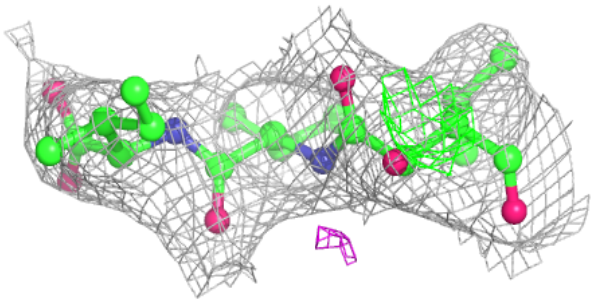


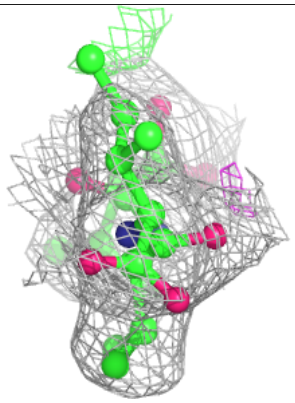


Electron density around VSZ T 301:

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

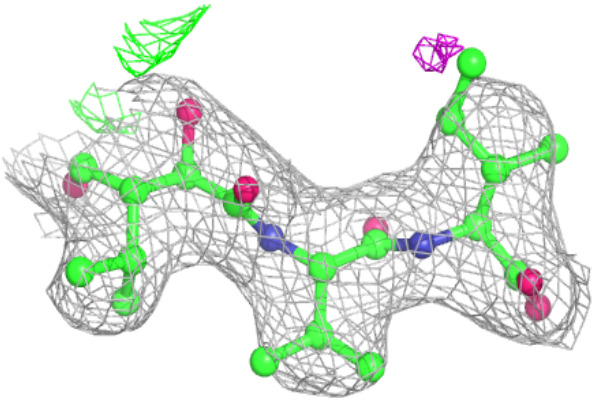


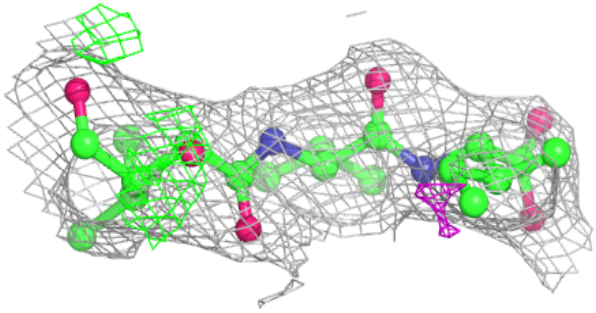


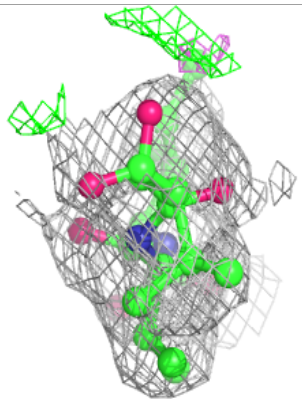


Electron density around VSZ B 301:

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

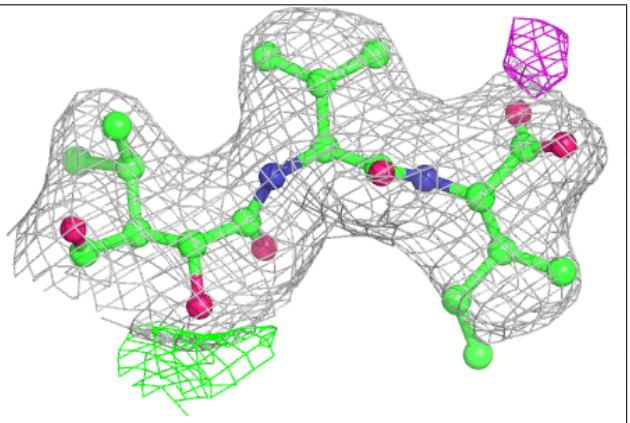


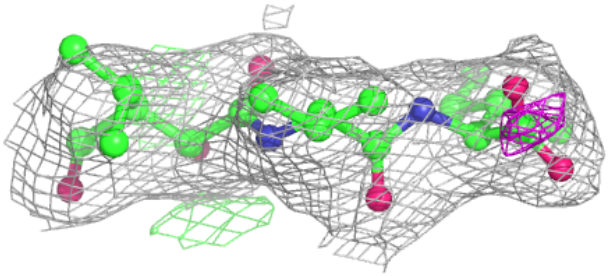


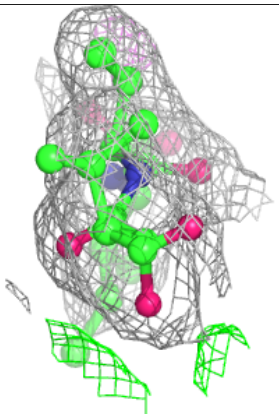


Electron density around VSZ J 301:

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







6.5 Other polymers (i)

There are no such residues in this entry.