



# Full wwPDB X-ray Structure Validation Report ⓘ

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

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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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)  
Xtrriage (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

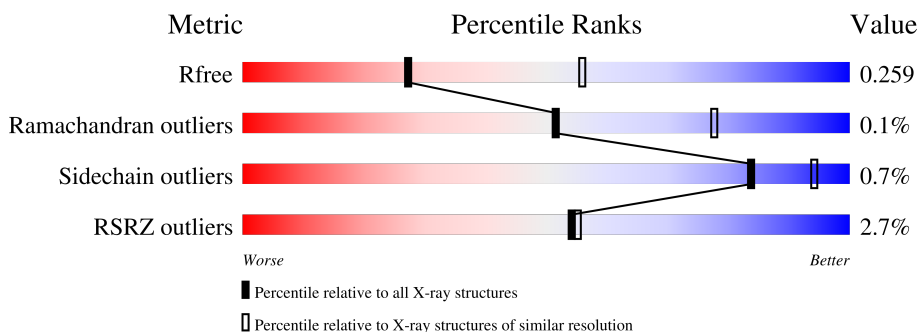
# 1 Overall quality at a glance

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	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	90% 2% 9%
1	H	203	93% 2% 7%
1	I	203	93% 2% 7%
1	J	203	92% 2% 7%
1	K	203	92% 2% 8%
1	L	203	91% 2% 8%
1	M	203	90% 2% 10%
1	N	203	91% 2% 9%
1	O	203	90% 4% 10%
1	P	203	88% 3% 10%
1	Q	203	91% 2% 9%
1	R	203	88% 2% 10%
1	S	203	87% 4% 10%
1	T	203	89% 3% 10%
1	U	203	89% 3% 10%
1	V	203	88% 4% 12%
1	W	203	91% 6% 9%
1	X	203	91% 4% 9%
1	Y	203	89% 2% 10%
1	Z	203	89% 4% 11%
1	a	203	89% 2% 10%
1	b	203	90% 2% 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
			Total	C	N	O	S			
1	A	192	1484	931	255	292	6	0	0	0
1	B	190	1466	922	249	288	7	0	0	0
1	C	188	1454	915	247	286	6	0	0	0
1	D	188	1450	913	246	285	6	0	0	0
1	E	175	1351	851	230	264	6	0	0	0
1	F	179	1382	871	234	271	6	0	0	0
1	G	184	1422	896	242	278	6	0	0	0
1	H	189	1457	917	247	287	6	0	0	0
1	I	188	1450	914	245	285	6	0	0	0
1	J	189	1458	917	248	287	6	0	0	0
1	K	187	1441	908	245	282	6	0	0	0
1	L	186	1433	904	241	282	6	0	0	0
1	M	182	1405	888	237	274	6	0	0	0
1	N	184	1422	896	242	278	6	0	0	0
1	O	183	1411	890	238	277	6	0	0	0
1	P	183	1414	893	238	277	6	0	0	0

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

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

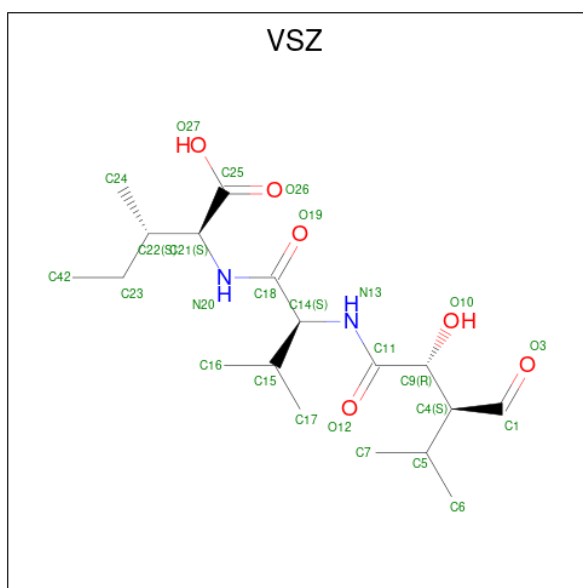
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Chain	Residue	Modelled	Actual	Comment	Reference
W	203	LYS	-	expression tag	UNP Q6GIM3
X	196	TRP	-	expression tag	UNP Q6GIM3
X	197	SER	-	expression tag	UNP Q6GIM3
X	198	HIS	-	expression tag	UNP Q6GIM3
X	199	PRO	-	expression tag	UNP Q6GIM3
X	200	GLN	-	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<sub>18</sub>H<sub>32</sub>N<sub>2</sub>O<sub>6</sub>) (la-

beled as "Ligand of Interest" by depositor).



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

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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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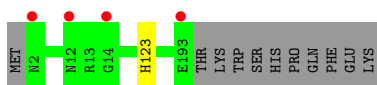
*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Residues</b>	<b>Atoms</b>	<b>ZeroOcc</b>	<b>AltConf</b>
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

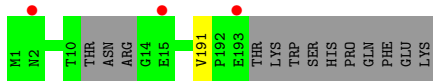
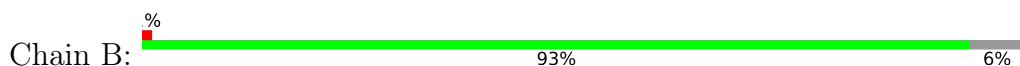
### 3 Residue-property plots [i](#)

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.

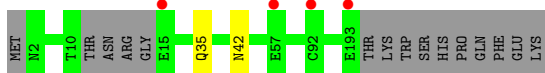
- Molecule 1: ATP-dependent Clp protease proteolytic subunit



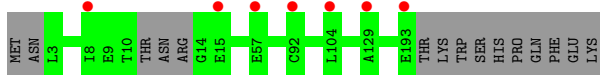
- Molecule 1: ATP-dependent Clp protease proteolytic subunit



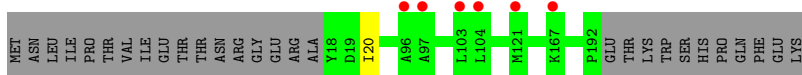
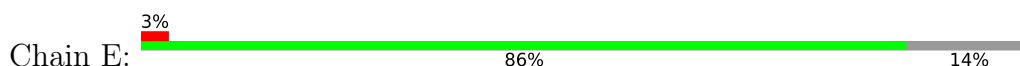
- Molecule 1: ATP-dependent Clp protease proteolytic subunit



- Molecule 1: ATP-dependent Clp protease proteolytic subunit

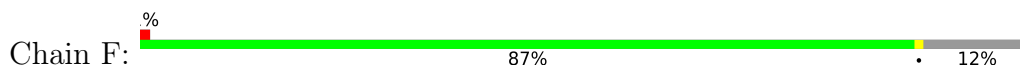


- Molecule 1: ATP-dependent Clp protease proteolytic subunit

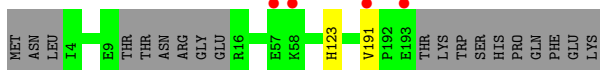
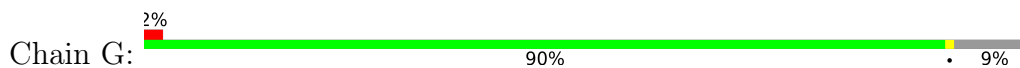


- Molecule 1: ATP-dependent Clp protease proteolytic subunit

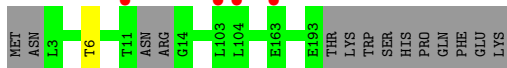
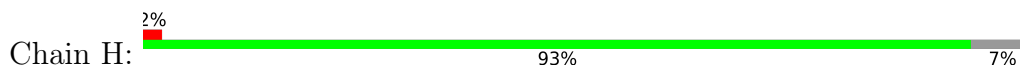




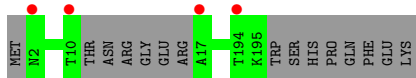
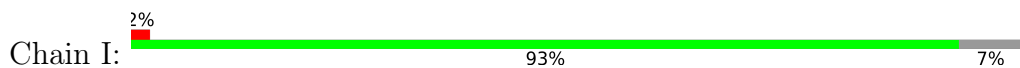
- Molecule 1: ATP-dependent Clp protease proteolytic subunit



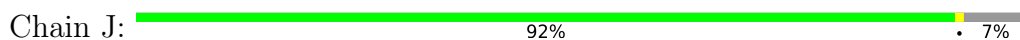
- Molecule 1: ATP-dependent Clp protease proteolytic subunit



- Molecule 1: ATP-dependent Clp protease proteolytic subunit



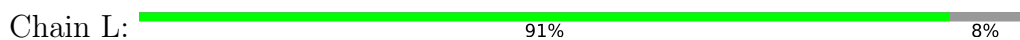
- Molecule 1: ATP-dependent Clp protease proteolytic subunit



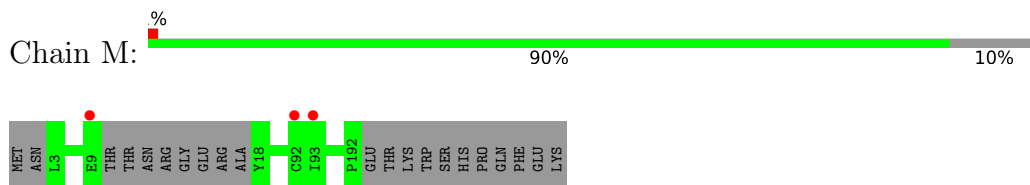
- Molecule 1: ATP-dependent Clp protease proteolytic subunit



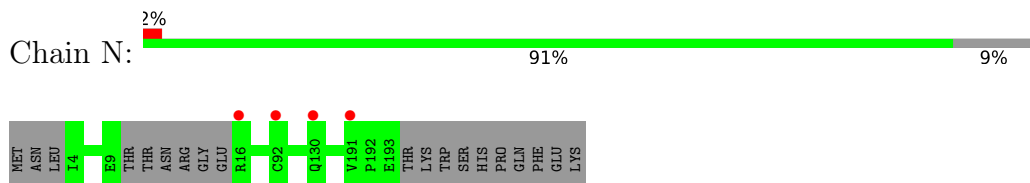
- Molecule 1: ATP-dependent Clp protease proteolytic subunit



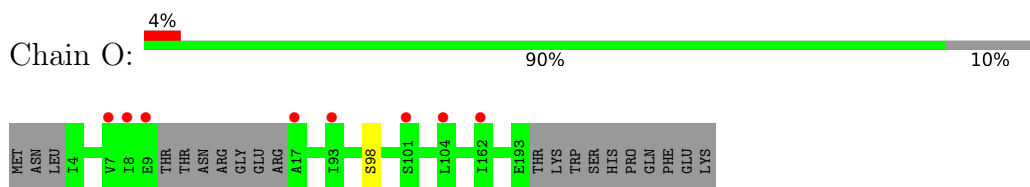
- Molecule 1: ATP-dependent Clp protease proteolytic subunit



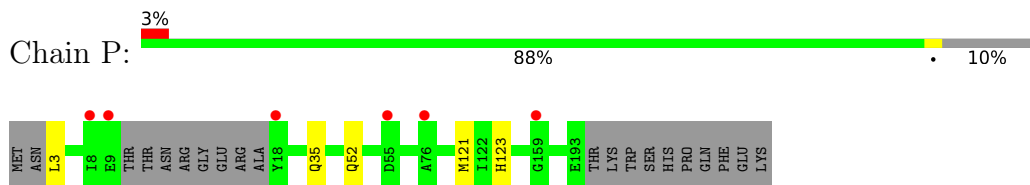
- Molecule 1: ATP-dependent Clp protease proteolytic subunit



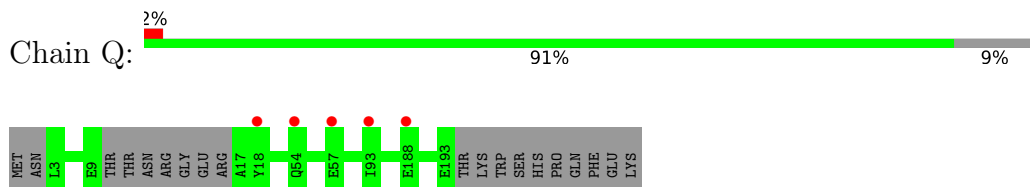
- Molecule 1: ATP-dependent Clp protease proteolytic subunit



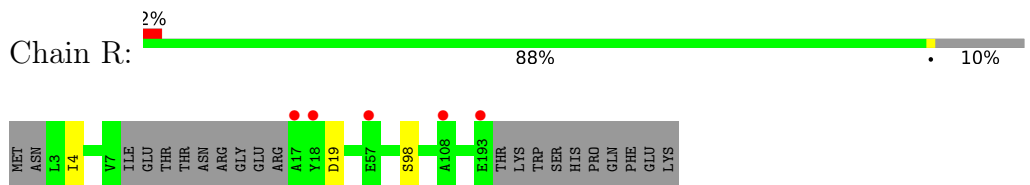
- Molecule 1: ATP-dependent Clp protease proteolytic subunit



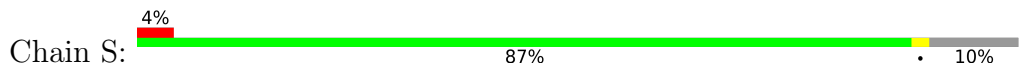
- Molecule 1: ATP-dependent Clp protease proteolytic subunit

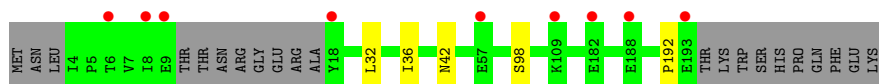


- Molecule 1: ATP-dependent Clp protease proteolytic subunit

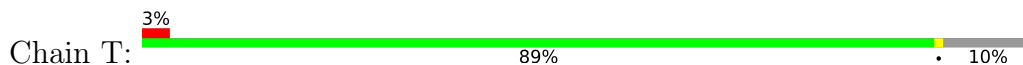


- Molecule 1: ATP-dependent Clp protease proteolytic subunit

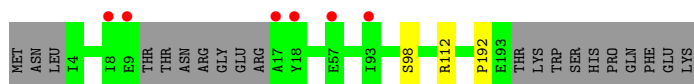
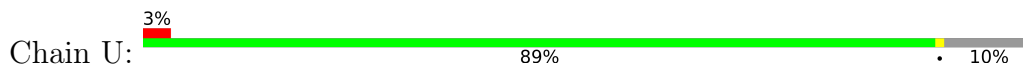




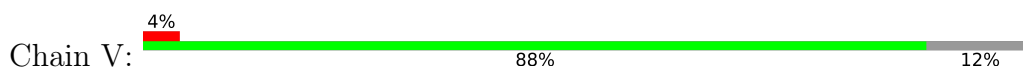
- Molecule 1: ATP-dependent Clp protease proteolytic subunit



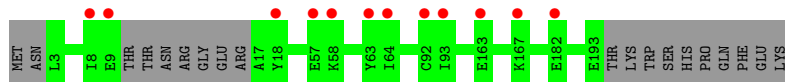
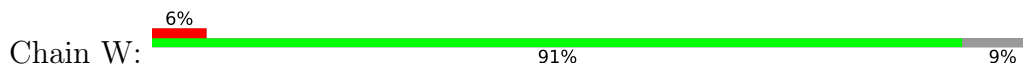
- Molecule 1: ATP-dependent Clp protease proteolytic subunit



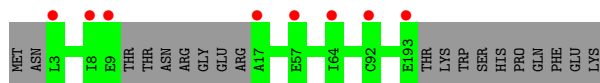
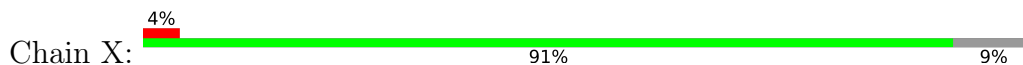
- Molecule 1: ATP-dependent Clp protease proteolytic subunit



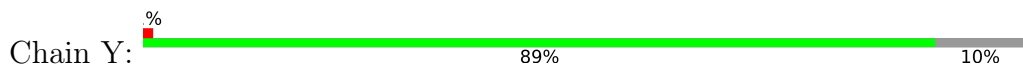
- Molecule 1: ATP-dependent Clp protease proteolytic subunit



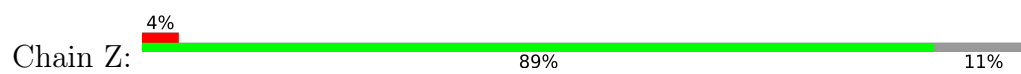
- Molecule 1: ATP-dependent Clp protease proteolytic subunit



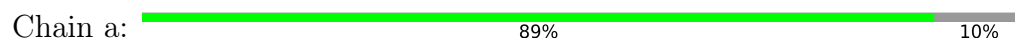
- Molecule 1: ATP-dependent Clp protease proteolytic subunit



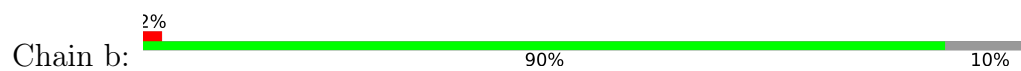
- Molecule 1: ATP-dependent Clp protease proteolytic subunit



- Molecule 1: ATP-dependent Clp protease proteolytic subunit



- Molecule 1: ATP-dependent Clp protease proteolytic subunit



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	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
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.50 (at 2.68Å)	Xtrriage
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 <sup>2</sup> )	72.2	Xtrriage
Anisotropy	0.378	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 40.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.52$ , $\langle L^2 \rangle = 0.35$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	40791	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	84.0	wwPDB-VP

Xtrriage'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.*

<sup>1</sup>Intensities estimated from amplitudes.

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

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

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(°)	Ideal(°)
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

All (30) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	123	HIS
1	B	191	VAL
1	C	35	GLN
1	C	42	ASN
1	E	20	ILE
1	F	6	THR
1	F	75	PHE
1	G	123	HIS
1	G	191	VAL
1	H	6	THR
1	J	52	GLN
1	J	191	VAL
1	L	82	GLN
1	P	3	LEU
1	P	35	GLN
1	P	52	GLN
1	P	121	MET
1	P	123	HIS
1	R	4	ILE
1	R	19	ASP
1	S	32	LEU
1	S	36	ILE
1	S	42	ASN
1	T	27	ASP
1	T	112	ARG
1	U	112	ARG
1	V	112	ARG
1	Y	123	HIS
1	Z	18	TYR
1	b	112	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	123	HIS
1	D	42	ASN
1	D	151	ASN
1	E	123	HIS
1	G	89	GLN
1	K	123	HIS
1	L	82	GLN
1	O	42	ASN
1	O	47	GLN

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Mol	Chain	Res	Type
1	O	89	GLN
1	P	35	GLN
1	S	123	HIS
1	X	42	ASN
1	Y	173	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%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
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	-
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	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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	-

All (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
2	a	301	VSZ	C4-C9	-5.27	1.49	1.54
2	N	301	VSZ	C4-C9	-5.24	1.49	1.54
2	S	301	VSZ	C4-C9	-4.89	1.49	1.54
2	Y	301	VSZ	C4-C9	-4.83	1.49	1.54
2	X	301	VSZ	C4-C1	4.80	1.58	1.50
2	C	301	VSZ	C4-C9	-4.74	1.50	1.54
2	M	301	VSZ	C4-C9	-4.60	1.50	1.54
2	H	301	VSZ	C4-C9	-4.52	1.50	1.54
2	I	301	VSZ	C4-C9	-4.40	1.50	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	G	301	VSZ	C4-C9	-4.37	1.50	1.54
2	T	301	VSZ	C4-C9	-4.16	1.50	1.54
2	L	301	VSZ	C4-C9	-4.14	1.50	1.54
2	K	301	VSZ	C4-C9	-3.98	1.50	1.54
2	F	301	VSZ	C4-C9	-3.77	1.50	1.54
2	A	301	VSZ	C4-C9	-3.60	1.51	1.54
2	W	301	VSZ	C4-C9	-3.44	1.51	1.54
2	R	301	VSZ	C4-C1	3.41	1.55	1.50
2	O	301	VSZ	C4-C9	-3.40	1.51	1.54
2	P	301	VSZ	C4-C9	-3.27	1.51	1.54
2	D	301	VSZ	C4-C9	-3.20	1.51	1.54
2	A	301	VSZ	C4-C5	-3.02	1.50	1.55
2	b	301	VSZ	C4-C9	-2.86	1.51	1.54
2	V	301	VSZ	C4-C9	-2.70	1.51	1.54
2	M	301	VSZ	C22-C21	-2.59	1.47	1.54
2	K	301	VSZ	C22-C21	-2.55	1.47	1.54
2	U	301	VSZ	C22-C21	-2.54	1.47	1.54
2	Z	301	VSZ	C22-C21	-2.39	1.48	1.54
2	U	301	VSZ	C9-C11	-2.36	1.47	1.52
2	R	301	VSZ	C4-C9	-2.35	1.52	1.54
2	I	301	VSZ	C22-C21	-2.28	1.48	1.54
2	G	301	VSZ	C4-C5	-2.27	1.51	1.55
2	A	301	VSZ	C21-C25	-2.26	1.48	1.52
2	N	301	VSZ	C22-C21	-2.26	1.48	1.54
2	D	301	VSZ	C22-C21	-2.24	1.48	1.54
2	a	301	VSZ	C22-C21	-2.23	1.48	1.54
2	U	301	VSZ	O10-C9	-2.22	1.37	1.42
2	C	301	VSZ	C22-C21	-2.22	1.48	1.54
2	G	301	VSZ	C22-C21	-2.17	1.48	1.54
2	Y	301	VSZ	C22-C21	-2.17	1.48	1.54
2	Q	301	VSZ	C22-C21	-2.14	1.48	1.54
2	O	301	VSZ	C4-C5	-2.13	1.52	1.55
2	F	301	VSZ	C22-C21	-2.12	1.48	1.54
2	E	301	VSZ	C21-C25	-2.10	1.49	1.52
2	J	301	VSZ	C4-C9	-2.04	1.52	1.54
2	E	301	VSZ	O10-C9	-2.04	1.38	1.42
2	N	301	VSZ	O10-C9	-2.03	1.38	1.42
2	Q	301	VSZ	C4-C5	-2.03	1.52	1.55
2	B	301	VSZ	C22-C21	-2.03	1.49	1.54
2	E	301	VSZ	C4-C5	-2.03	1.52	1.55
2	H	301	VSZ	C21-C25	-2.02	1.49	1.52

All (82) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
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
2	B	301	VSZ	O10-C9-C4	-3.67	102.31	109.28
2	X	301	VSZ	C9-C4-C1	3.65	118.22	110.65
2	X	301	VSZ	C18-C14-N13	3.57	120.08	110.36
2	E	301	VSZ	O10-C9-C4	-3.54	102.56	109.28
2	X	301	VSZ	C15-C14-C18	-3.53	102.56	111.38
2	M	301	VSZ	O10-C9-C4	-3.29	103.02	109.28
2	R	301	VSZ	C15-C14-N13	-3.27	103.34	111.43
2	E	301	VSZ	C15-C14-C18	-3.06	103.72	111.38
2	K	301	VSZ	O10-C9-C4	-3.00	103.57	109.28
2	N	301	VSZ	C22-C21-N20	-2.94	105.19	111.34
2	K	301	VSZ	C22-C21-N20	-2.85	105.38	111.34
2	X	301	VSZ	C6-C5-C4	-2.78	106.58	111.74
2	X	301	VSZ	C15-C14-N13	-2.77	104.59	111.43
2	D	301	VSZ	C15-C14-C18	-2.69	104.65	111.38
2	W	301	VSZ	C22-C21-N20	-2.69	105.72	111.34
2	L	301	VSZ	O10-C9-C4	-2.68	104.18	109.28
2	R	301	VSZ	C15-C14-C18	-2.67	104.70	111.38
2	I	301	VSZ	C22-C21-N20	-2.64	105.82	111.34
2	J	301	VSZ	C15-C14-C18	-2.64	104.78	111.38
2	R	301	VSZ	C6-C5-C4	-2.61	106.89	111.74
2	Q	301	VSZ	O10-C9-C4	-2.60	104.34	109.28
2	b	301	VSZ	O3-C1-C4	-2.60	118.66	125.23
2	G	301	VSZ	C22-C21-N20	-2.59	105.94	111.34
2	E	301	VSZ	C25-C21-N20	-2.58	104.65	110.28
2	Y	301	VSZ	C15-C14-C18	-2.55	104.99	111.38
2	G	301	VSZ	C6-C5-C4	-2.54	107.02	111.74
2	C	301	VSZ	C22-C21-N20	-2.54	106.04	111.34
2	Z	301	VSZ	O10-C9-C4	-2.49	104.54	109.28
2	N	301	VSZ	C15-C14-C18	-2.49	105.16	111.38
2	B	301	VSZ	C15-C14-C18	-2.48	105.17	111.38
2	I	301	VSZ	O10-C9-C4	-2.48	104.57	109.28
2	F	301	VSZ	C22-C21-N20	-2.42	106.28	111.34
2	C	301	VSZ	O10-C9-C4	-2.41	104.69	109.28
2	C	301	VSZ	O3-C1-C4	-2.38	119.20	125.23
2	W	301	VSZ	O10-C9-C11	-2.38	105.51	110.63
2	Y	301	VSZ	C6-C5-C4	-2.37	107.33	111.74
2	D	301	VSZ	C22-C21-N20	-2.37	106.39	111.34
2	G	301	VSZ	C15-C14-C18	-2.37	105.46	111.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	W	301	VSZ	C6-C5-C4	-2.37	107.35	111.74
2	Q	301	VSZ	C22-C21-N20	-2.36	106.42	111.34
2	a	301	VSZ	O10-C9-C11	-2.34	105.58	110.63
2	P	301	VSZ	O10-C9-C4	-2.33	104.86	109.28
2	V	301	VSZ	C15-C14-N13	-2.33	105.68	111.43
2	B	301	VSZ	C9-C4-C1	-2.31	105.87	110.65
2	F	301	VSZ	C6-C5-C4	-2.29	107.48	111.74
2	R	301	VSZ	O3-C1-C4	-2.28	119.47	125.23
2	L	301	VSZ	C7-C5-C6	-2.26	104.28	110.59
2	C	301	VSZ	C7-C5-C6	-2.24	104.32	110.59
2	N	301	VSZ	O10-C9-C4	-2.23	105.05	109.28
2	b	301	VSZ	C15-C14-C18	-2.22	105.82	111.38
2	R	301	VSZ	C9-C4-C1	2.21	115.22	110.65
2	O	301	VSZ	C22-C21-N20	-2.19	106.77	111.34
2	M	301	VSZ	C15-C14-N13	-2.18	106.04	111.43
2	K	301	VSZ	C6-C5-C4	-2.18	107.70	111.74
2	L	301	VSZ	C15-C14-N13	-2.17	106.07	111.43
2	R	301	VSZ	C18-C14-N13	2.16	116.24	110.36
2	Q	301	VSZ	C6-C5-C4	-2.15	107.74	111.74
2	A	301	VSZ	C42-C23-C22	-2.15	105.27	113.84
2	H	301	VSZ	O10-C9-C4	-2.14	105.21	109.28
2	G	301	VSZ	O10-C9-C4	-2.14	105.21	109.28
2	K	301	VSZ	C23-C22-C21	-2.14	105.87	111.17
2	U	301	VSZ	C22-C21-N20	-2.12	106.91	111.34
2	A	301	VSZ	C9-C4-C1	-2.12	106.25	110.65
2	a	301	VSZ	C18-C14-N13	-2.12	104.61	110.36
2	J	301	VSZ	O3-C1-C4	-2.11	119.90	125.23
2	J	301	VSZ	O10-C9-C11	-2.10	106.10	110.63
2	F	301	VSZ	O26-C25-C21	-2.09	114.50	121.70
2	L	301	VSZ	C22-C21-N20	-2.09	106.98	111.34
2	U	301	VSZ	C9-C4-C1	-2.08	106.33	110.65
2	J	301	VSZ	C7-C5-C6	-2.06	104.82	110.59
2	D	301	VSZ	C23-C22-C21	-2.05	106.07	111.17
2	B	301	VSZ	C25-C21-N20	-2.05	105.80	110.28
2	Z	301	VSZ	C6-C5-C4	-2.04	107.96	111.74
2	F	301	VSZ	O3-C1-C4	-2.03	120.10	125.23
2	H	301	VSZ	C15-C14-N13	-2.03	106.42	111.43
2	b	301	VSZ	O10-C9-C11	-2.02	106.27	110.63
2	Y	301	VSZ	C9-C4-C1	-2.00	106.50	110.65

There are no chirality outliers.

All (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
2	E	301	VSZ	N13-C11-C9-O10
2	F	301	VSZ	C9-C4-C5-C7
2	F	301	VSZ	C1-C4-C5-C6
2	F	301	VSZ	C1-C4-C5-C7
2	F	301	VSZ	O3-C1-C4-C9
2	G	301	VSZ	N13-C11-C9-O10
2	H	301	VSZ	C9-C4-C5-C6
2	H	301	VSZ	C9-C4-C5-C7
2	H	301	VSZ	C1-C4-C5-C6
2	H	301	VSZ	C1-C4-C5-C7
2	I	301	VSZ	N13-C11-C9-O10
2	I	301	VSZ	C9-C4-C5-C6
2	I	301	VSZ	C9-C4-C5-C7
2	I	301	VSZ	C1-C4-C5-C6
2	I	301	VSZ	C1-C4-C5-C7
2	I	301	VSZ	O3-C1-C4-C5
2	M	301	VSZ	N13-C11-C9-O10
2	M	301	VSZ	O3-C1-C4-C5
2	N	301	VSZ	N13-C11-C9-O10
2	N	301	VSZ	O3-C1-C4-C5
2	O	301	VSZ	O12-C11-C9-O10
2	O	301	VSZ	N13-C11-C9-O10
2	O	301	VSZ	O3-C1-C4-C5
2	P	301	VSZ	N13-C11-C9-O10
2	Q	301	VSZ	O12-C11-C9-O10
2	Q	301	VSZ	N13-C11-C9-O10
2	Q	301	VSZ	O3-C1-C4-C5
2	R	301	VSZ	C22-C21-C25-O26
2	R	301	VSZ	C22-C21-C25-O27
2	S	301	VSZ	N13-C11-C9-O10
2	T	301	VSZ	N13-C11-C9-O10
2	T	301	VSZ	O3-C1-C4-C5
2	T	301	VSZ	N20-C21-C25-O26
2	U	301	VSZ	N13-C11-C9-O10
2	U	301	VSZ	O3-C1-C4-C5
2	V	301	VSZ	C9-C4-C5-C6
2	V	301	VSZ	C9-C4-C5-C7
2	V	301	VSZ	C1-C4-C5-C6

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Mol	Chain	Res	Type	Atoms
2	V	301	VSZ	C1-C4-C5-C7
2	W	301	VSZ	N13-C11-C9-O10
2	X	301	VSZ	N13-C11-C9-O10
2	Y	301	VSZ	C9-C4-C5-C7
2	Y	301	VSZ	C1-C4-C5-C6
2	Y	301	VSZ	C1-C4-C5-C7
2	Z	301	VSZ	N13-C11-C9-O10
2	Z	301	VSZ	C9-C4-C5-C7
2	Z	301	VSZ	C1-C4-C5-C7
2	Z	301	VSZ	O3-C1-C4-C5
2	a	301	VSZ	N13-C11-C9-O10
2	a	301	VSZ	C9-C4-C5-C7
2	a	301	VSZ	C1-C4-C5-C7
2	b	301	VSZ	N13-C11-C9-O10
2	b	301	VSZ	C22-C21-C25-O26
2	E	301	VSZ	O12-C11-C9-O10
2	M	301	VSZ	O12-C11-C9-O10
2	N	301	VSZ	O12-C11-C9-O10
2	P	301	VSZ	O12-C11-C9-O10
2	S	301	VSZ	O12-C11-C9-O10
2	T	301	VSZ	O12-C11-C9-O10
2	U	301	VSZ	O12-C11-C9-O10
2	W	301	VSZ	O12-C11-C9-O10
2	X	301	VSZ	O12-C11-C9-O10
2	Z	301	VSZ	O12-C11-C9-O10
2	a	301	VSZ	O12-C11-C9-O10
2	C	301	VSZ	N13-C11-C9-O10
2	F	301	VSZ	N13-C11-C9-O10
2	K	301	VSZ	N13-C11-C9-O10
2	Y	301	VSZ	N13-C11-C9-O10
2	B	301	VSZ	N20-C21-C25-O27
2	E	301	VSZ	N20-C21-C25-O26
2	G	301	VSZ	N20-C21-C25-O27
2	K	301	VSZ	N20-C21-C25-O27
2	L	301	VSZ	N20-C21-C25-O26
2	N	301	VSZ	N20-C21-C25-O27
2	O	301	VSZ	N20-C21-C25-O27
2	P	301	VSZ	N20-C21-C25-O27
2	R	301	VSZ	N20-C21-C25-O26
2	X	301	VSZ	N20-C21-C25-O27
2	b	301	VSZ	N20-C21-C25-O26
2	E	301	VSZ	C22-C21-C25-O26

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Mol	Chain	Res	Type	Atoms
2	L	301	VSZ	C22-C21-C25-O27
2	C	301	VSZ	O12-C11-C9-O10
2	F	301	VSZ	O12-C11-C9-O10
2	I	301	VSZ	O12-C11-C9-O10
2	K	301	VSZ	O12-C11-C9-O10
2	V	301	VSZ	O12-C11-C9-O10
2	Y	301	VSZ	O12-C11-C9-O10
2	A	301	VSZ	N13-C11-C9-O10
2	D	301	VSZ	N13-C11-C9-O10
2	H	301	VSZ	N13-C11-C9-O10
2	J	301	VSZ	N13-C11-C9-O10
2	L	301	VSZ	N13-C11-C9-O10
2	R	301	VSZ	N13-C11-C9-O10
2	V	301	VSZ	N13-C11-C9-O10
2	B	301	VSZ	N20-C21-C25-O26
2	E	301	VSZ	N20-C21-C25-O27
2	F	301	VSZ	N20-C21-C25-O26
2	G	301	VSZ	N20-C21-C25-O26
2	H	301	VSZ	N20-C21-C25-O27
2	K	301	VSZ	N20-C21-C25-O26
2	L	301	VSZ	N20-C21-C25-O27
2	N	301	VSZ	N20-C21-C25-O26
2	O	301	VSZ	N20-C21-C25-O26
2	P	301	VSZ	N20-C21-C25-O26
2	R	301	VSZ	N20-C21-C25-O27
2	T	301	VSZ	N20-C21-C25-O27
2	X	301	VSZ	N20-C21-C25-O26
2	b	301	VSZ	N20-C21-C25-O27
2	E	301	VSZ	C22-C21-C25-O27
2	G	301	VSZ	C22-C21-C25-O27
2	L	301	VSZ	C22-C21-C25-O26
2	N	301	VSZ	C22-C21-C25-O26
2	N	301	VSZ	C22-C21-C25-O27
2	O	301	VSZ	C22-C21-C25-O27
2	T	301	VSZ	C22-C21-C25-O26
2	T	301	VSZ	C22-C21-C25-O27
2	b	301	VSZ	C22-C21-C25-O27
2	B	301	VSZ	O12-C11-C9-O10
2	D	301	VSZ	O12-C11-C9-O10
2	G	301	VSZ	O12-C11-C9-O10
2	H	301	VSZ	O12-C11-C9-O10
2	J	301	VSZ	O12-C11-C9-O10

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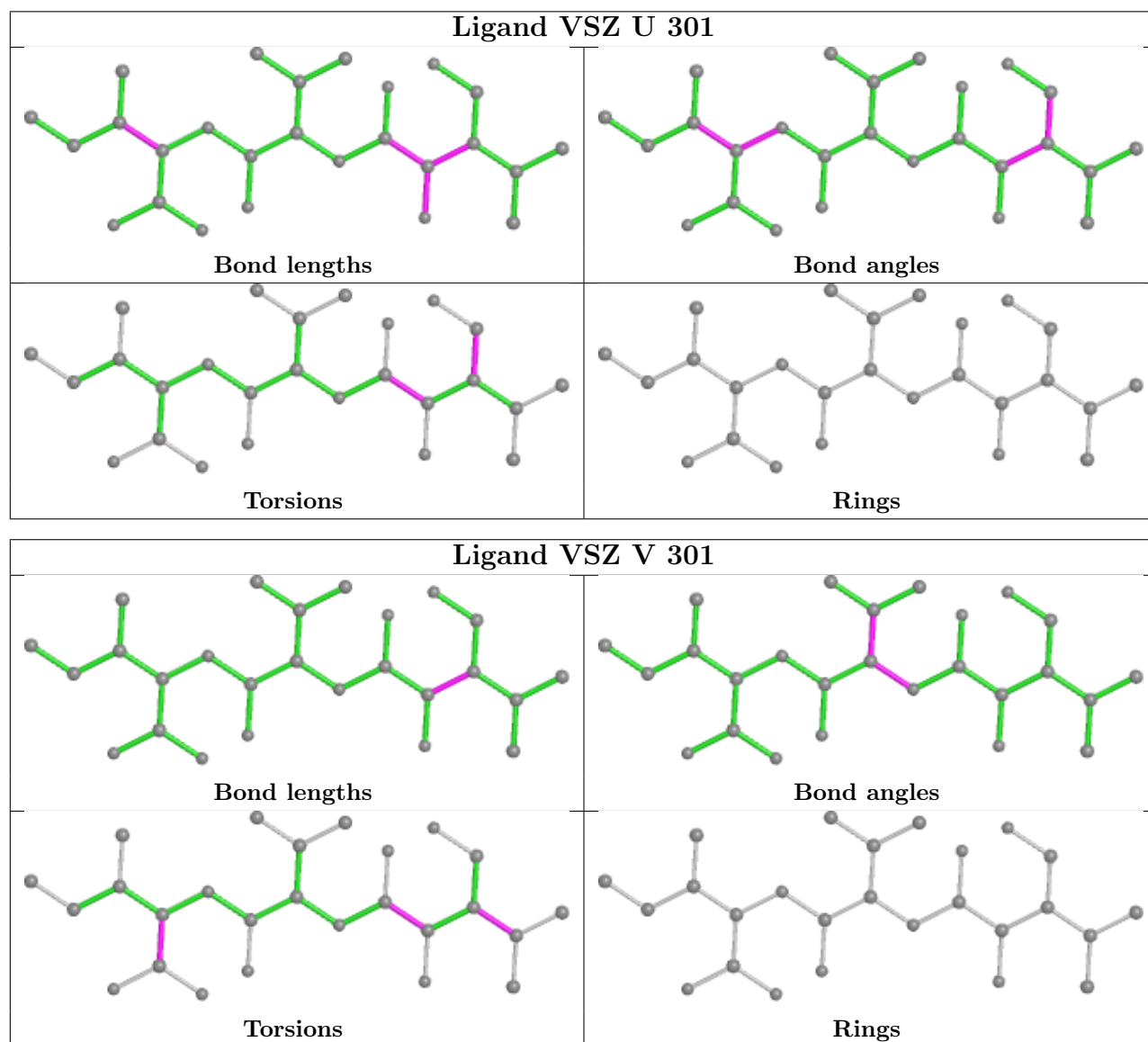
Mol	Chain	Res	Type	Atoms
2	L	301	VSZ	O12-C11-C9-O10
2	R	301	VSZ	O12-C11-C9-O10
2	b	301	VSZ	O12-C11-C9-O10
2	Q	301	VSZ	O12-C11-C9-C4
2	W	301	VSZ	C1-C4-C5-C7
2	R	301	VSZ	C5-C4-C9-O10
2	T	301	VSZ	C5-C4-C9-O10
2	H	301	VSZ	O3-C1-C4-C5
2	A	301	VSZ	O3-C1-C4-C9
2	B	301	VSZ	O3-C1-C4-C9
2	E	301	VSZ	O3-C1-C4-C9
2	K	301	VSZ	O3-C1-C4-C9
2	F	301	VSZ	N20-C21-C25-O27
2	H	301	VSZ	N20-C21-C25-O26
2	V	301	VSZ	N20-C21-C25-O27
2	a	301	VSZ	N20-C21-C25-O26
2	a	301	VSZ	N20-C21-C25-O27
2	R	301	VSZ	C1-C4-C9-O10
2	G	301	VSZ	C22-C21-C25-O26
2	K	301	VSZ	C22-C21-C25-O27
2	A	301	VSZ	O12-C11-C9-O10
2	A	301	VSZ	C9-C4-C5-C7
2	F	301	VSZ	C9-C4-C5-C6
2	W	301	VSZ	C9-C4-C5-C7
2	Y	301	VSZ	C9-C4-C5-C6
2	Z	301	VSZ	C9-C4-C5-C6
2	Z	301	VSZ	C1-C4-C5-C6
2	a	301	VSZ	C9-C4-C5-C6
2	a	301	VSZ	C1-C4-C5-C6

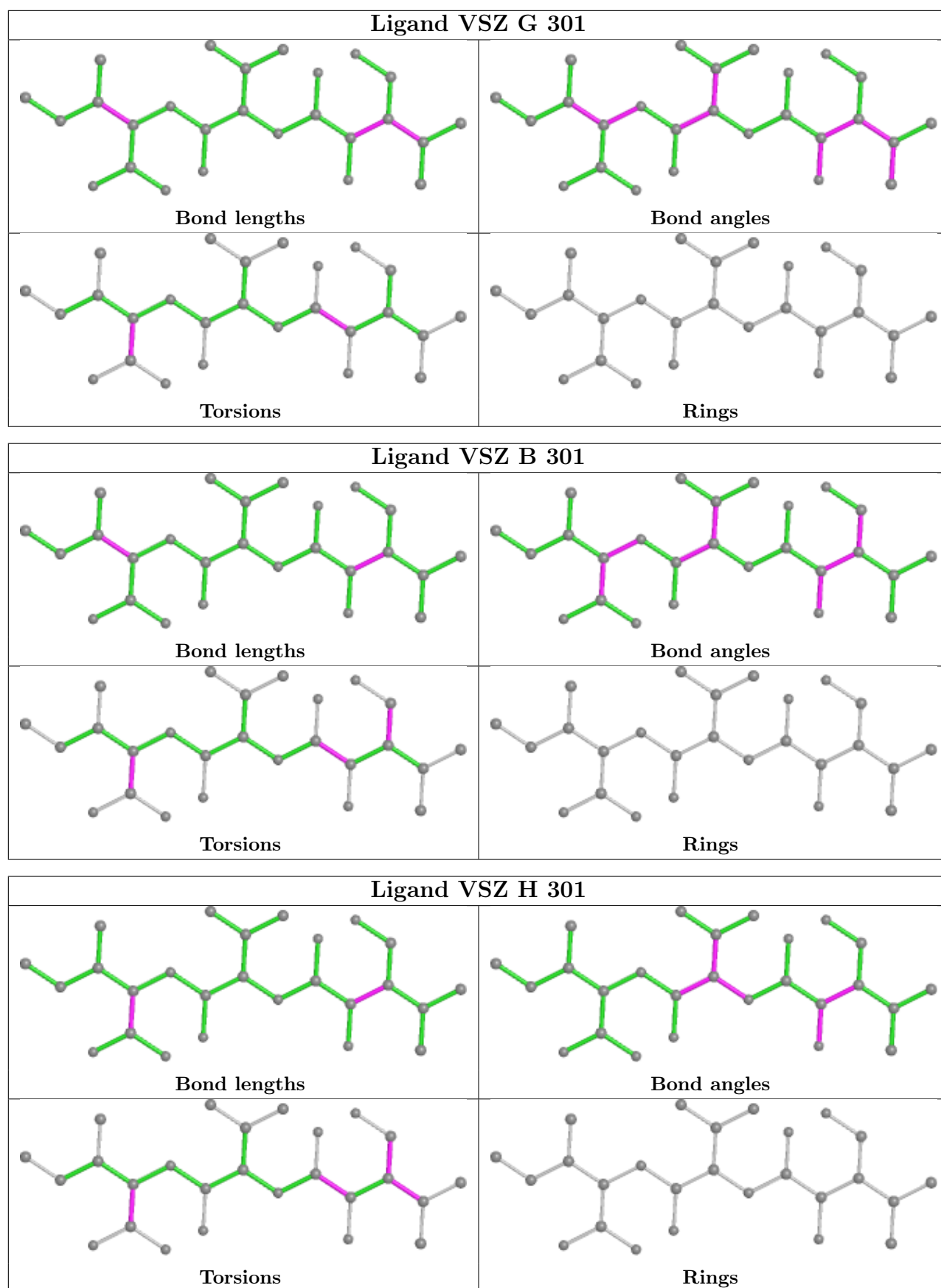
There are no ring outliers.

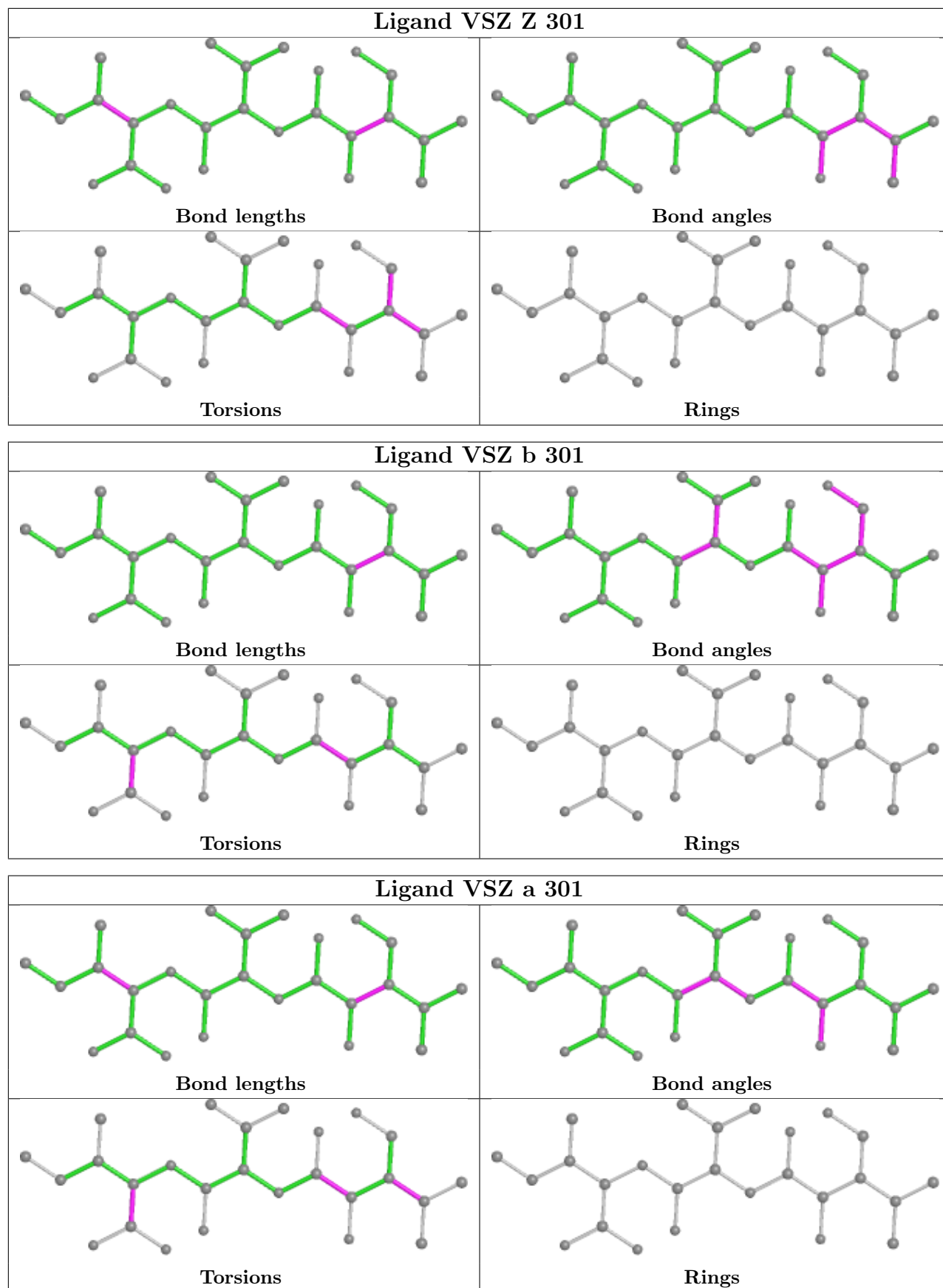
No monomer is involved in short contacts.

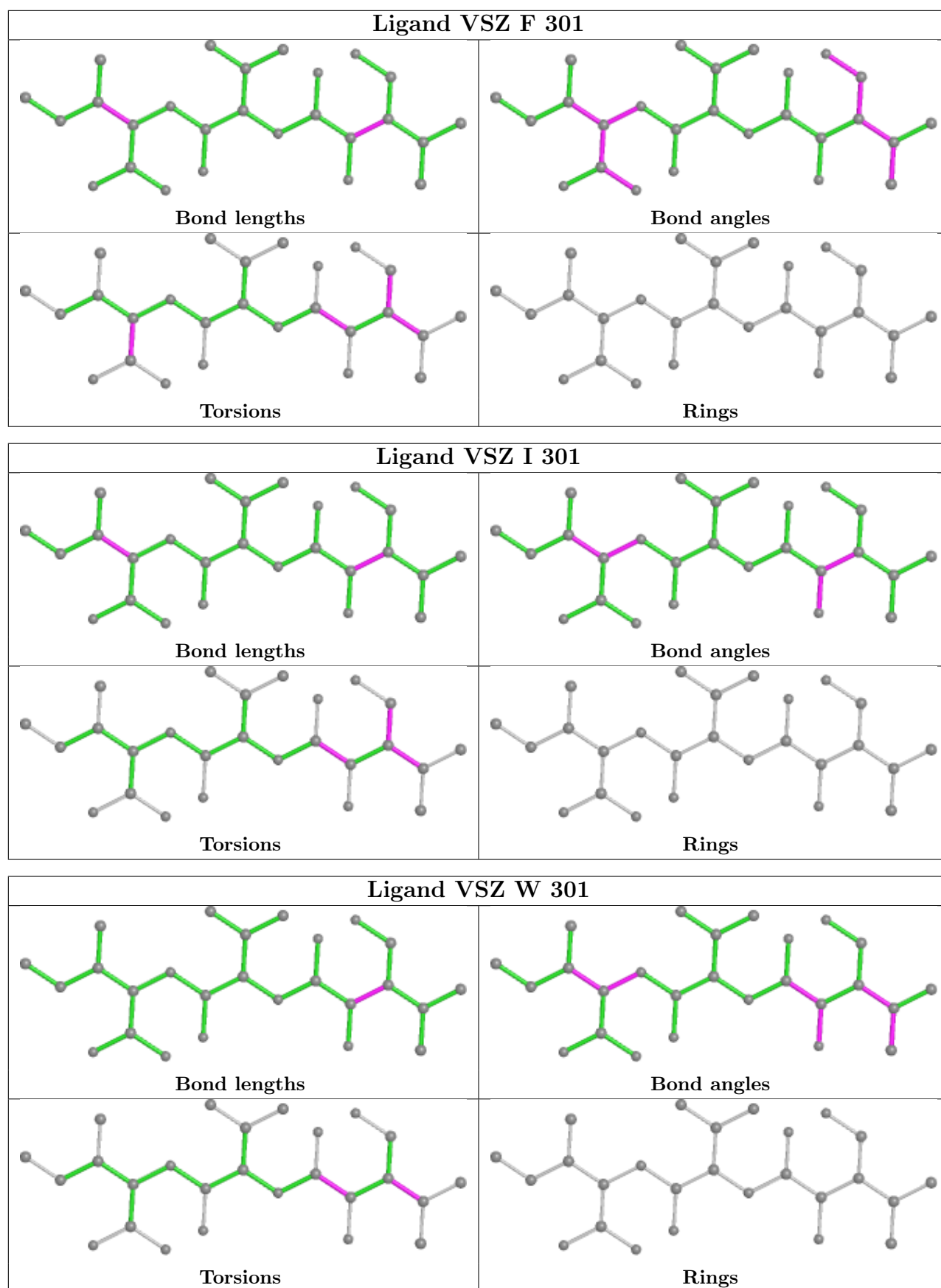
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier.

The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

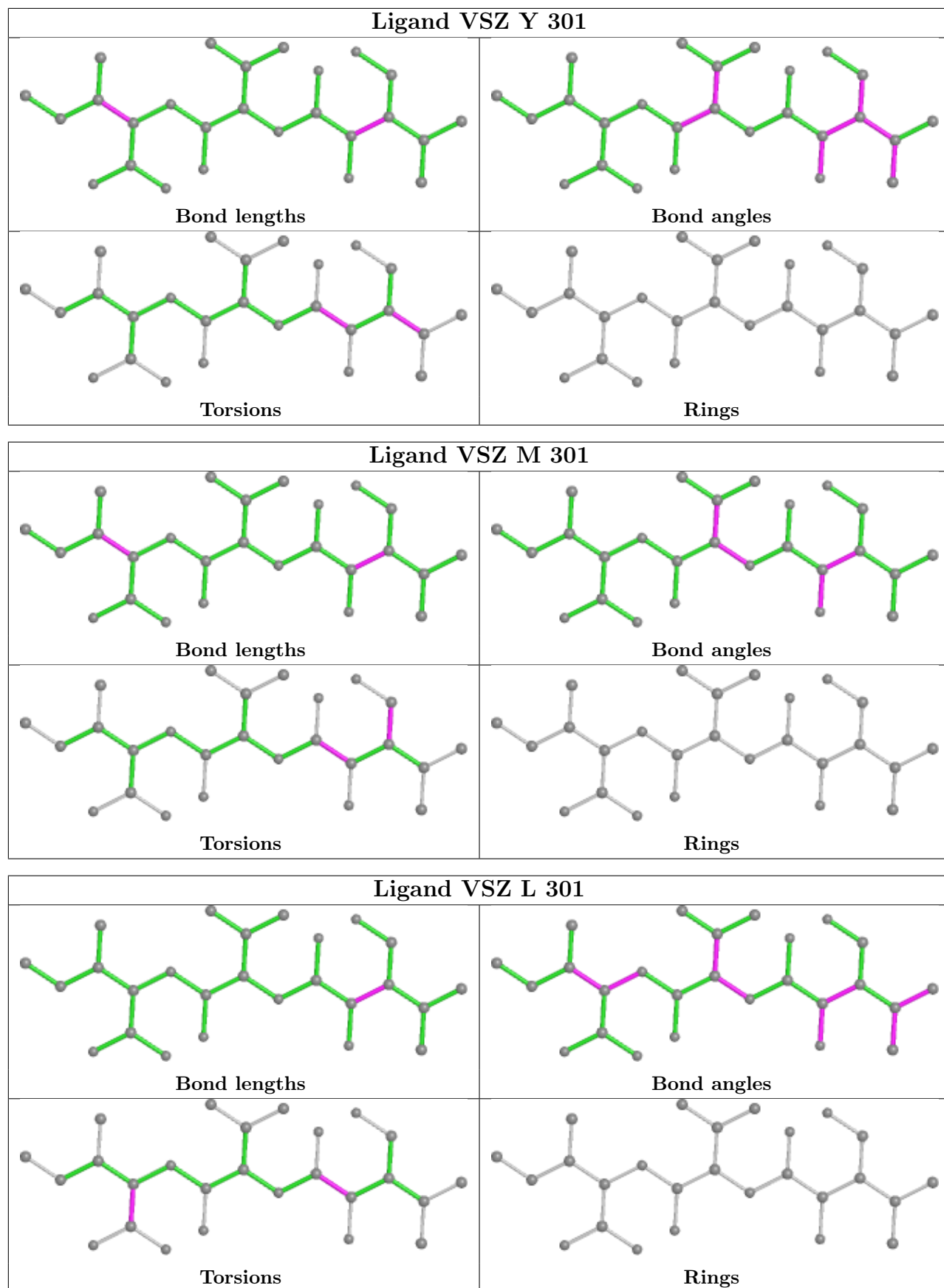


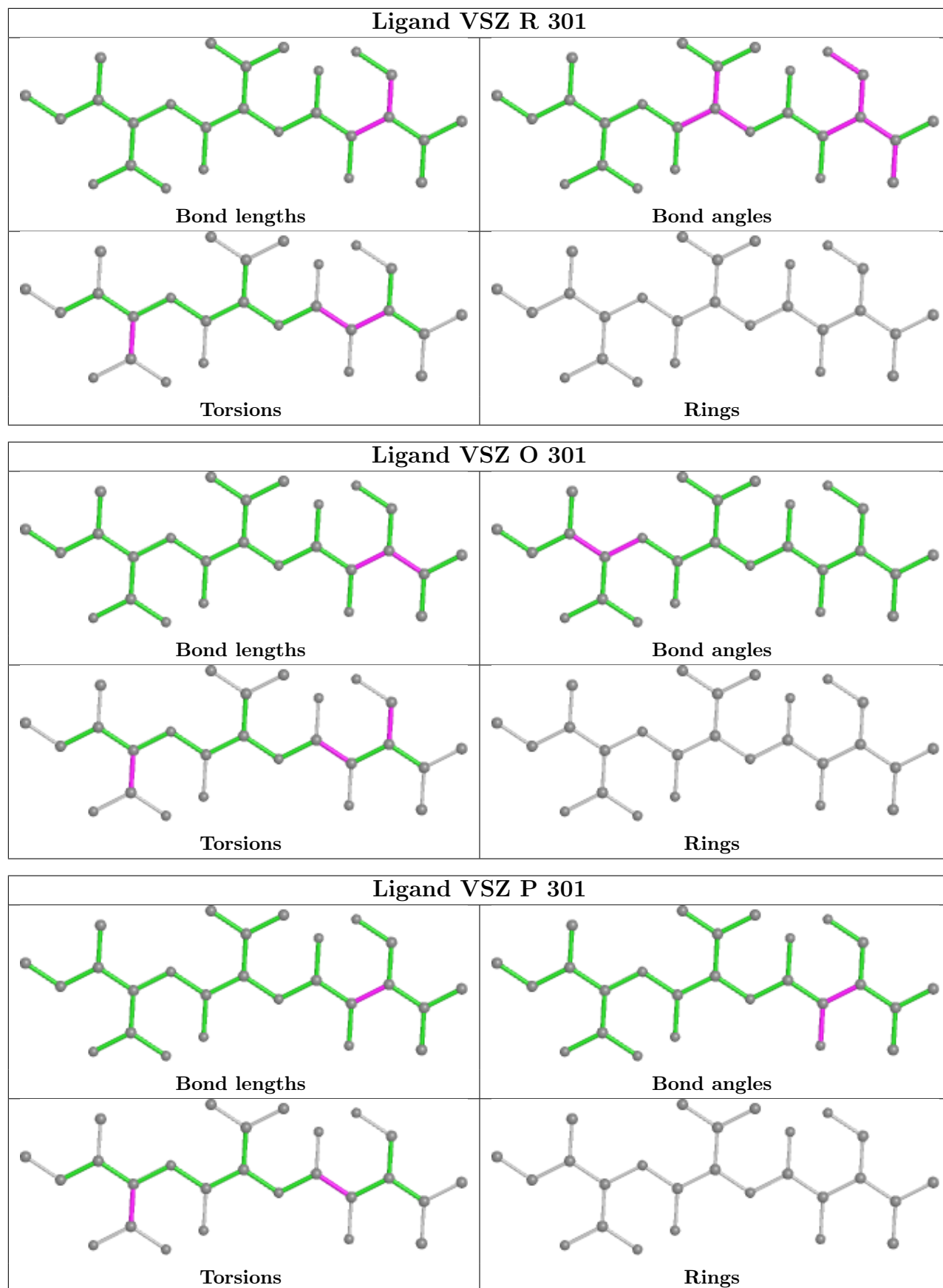


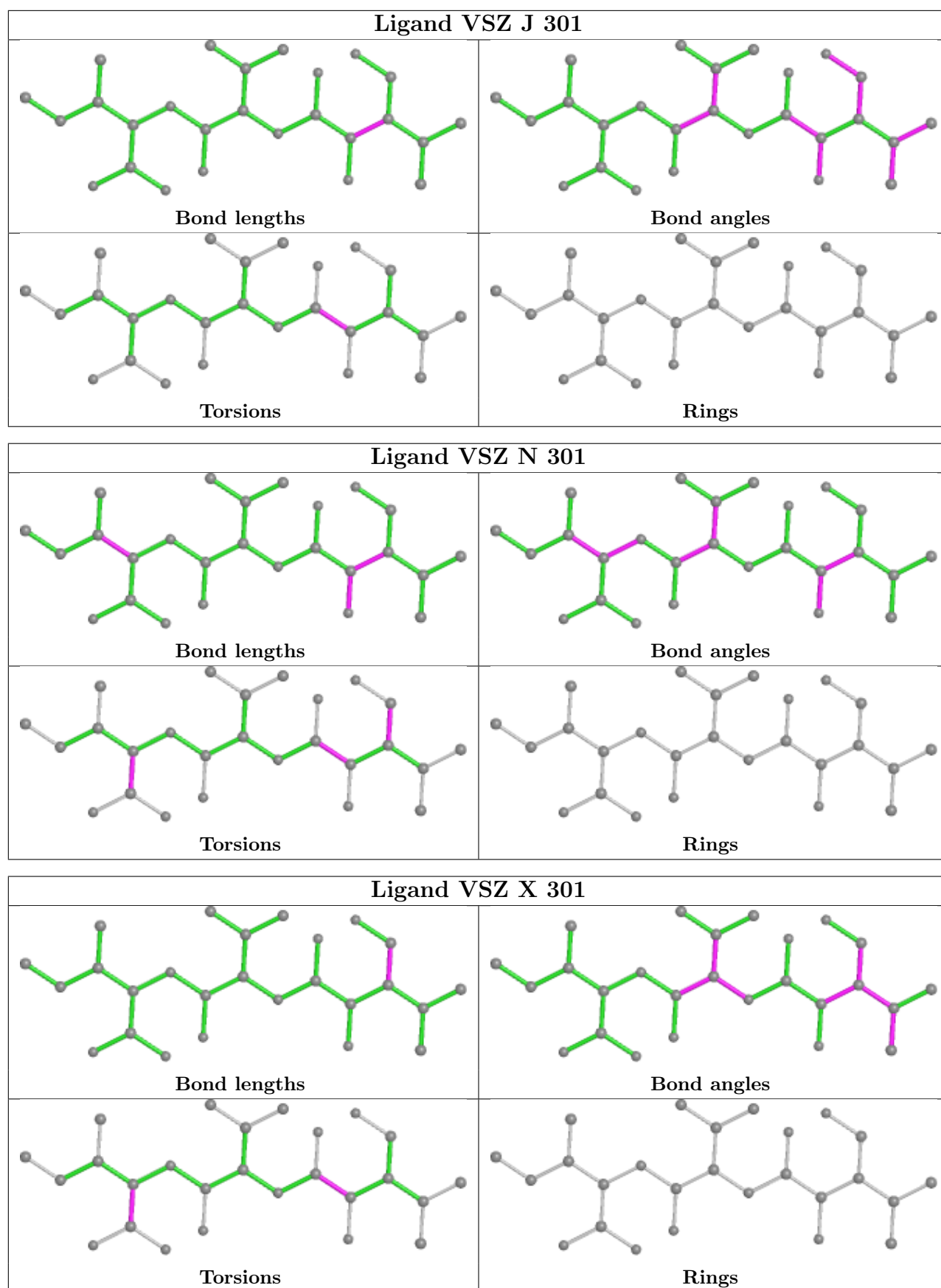


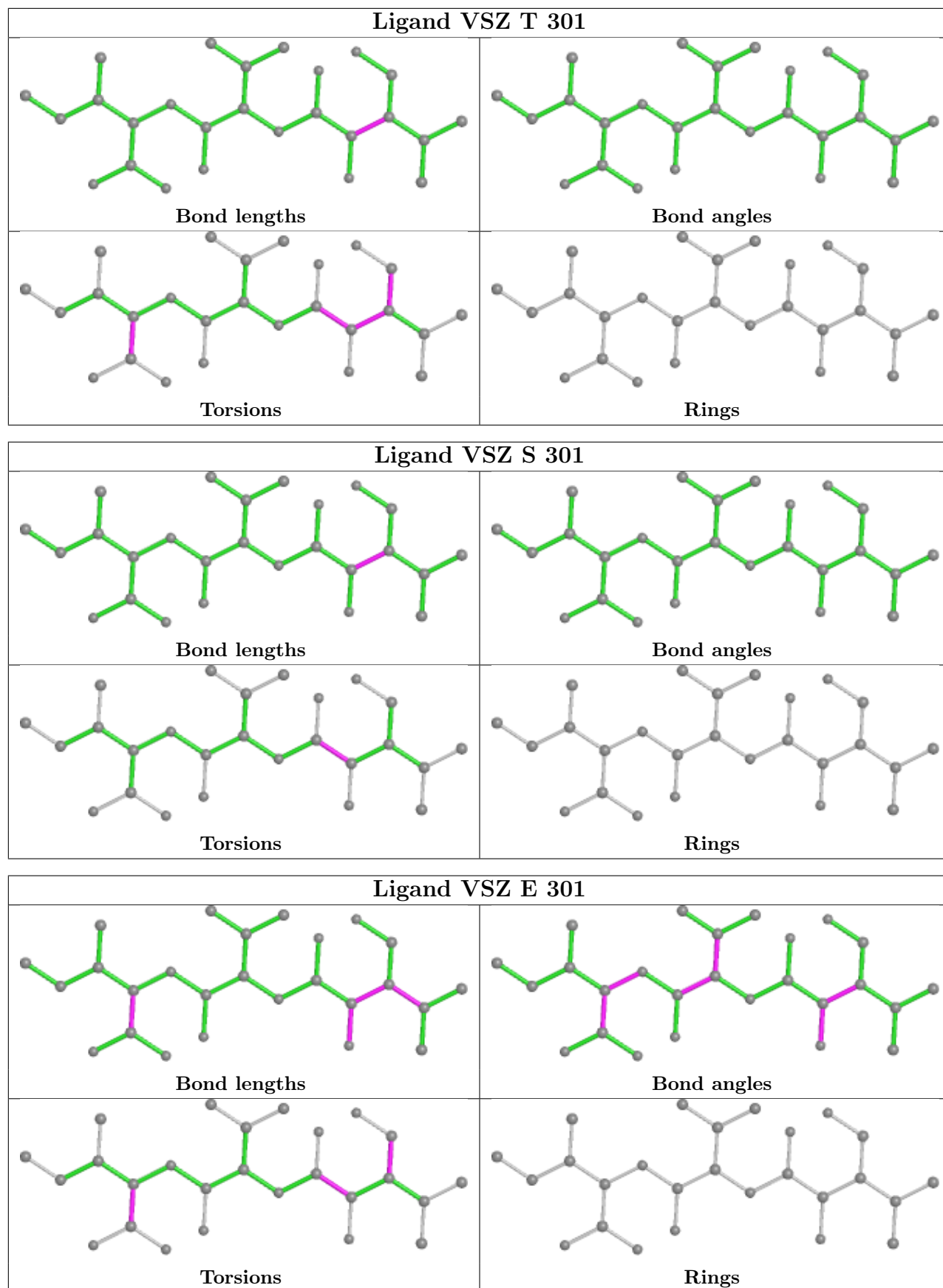


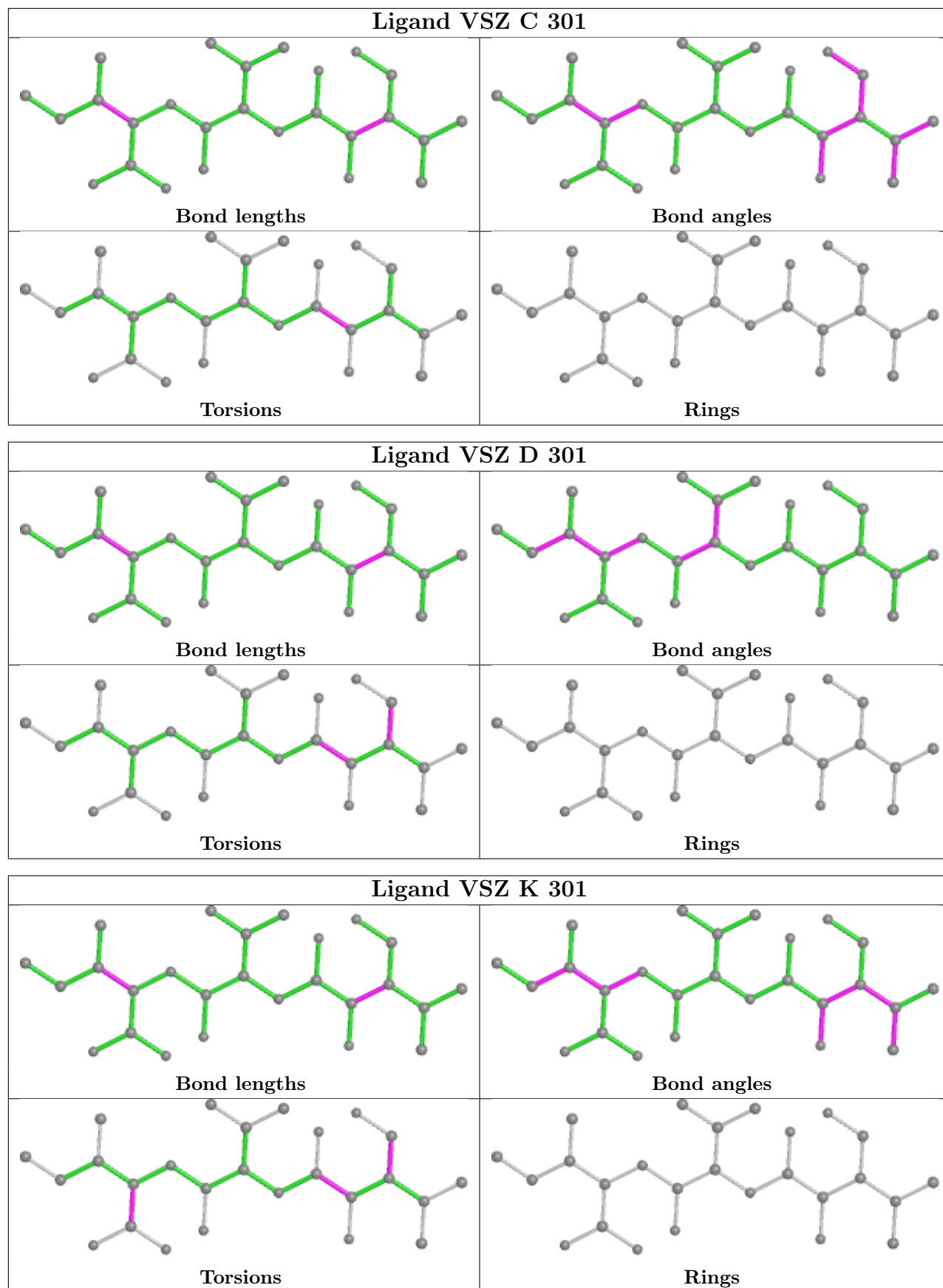


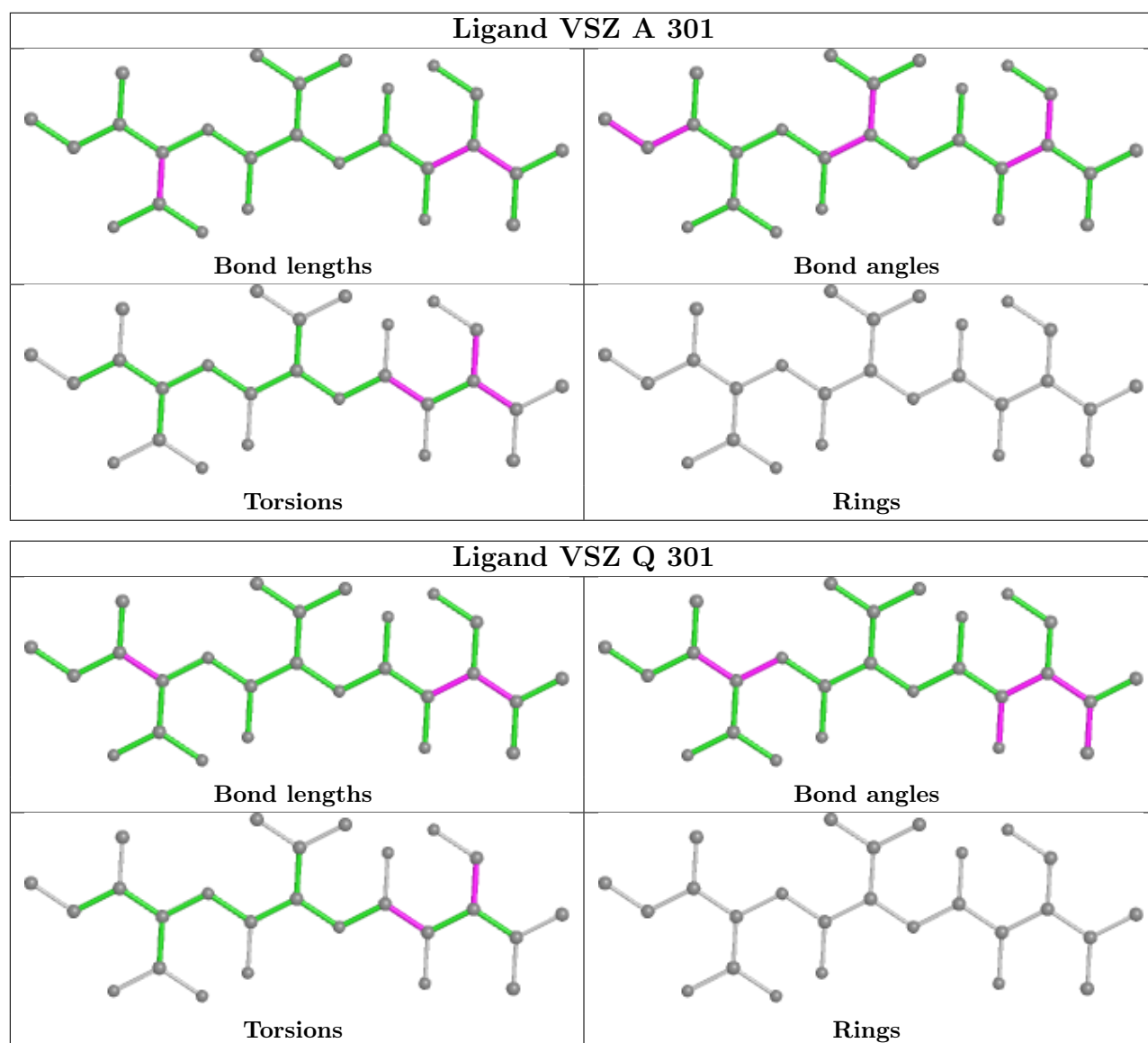












## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

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<sup>th</sup> 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 <sup>2</sup> )	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 <sup>2</sup> )	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

All (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
1	W	8	ILE	4.7
1	O	8	ILE	4.7
1	S	9	GLU	4.5
1	Q	57	GLU	4.4
1	W	9	GLU	4.3
1	J	14	GLY	3.9
1	F	193	GLU	3.7
1	R	17	ALA	3.5
1	Z	191	VAL	3.5
1	F	18	TYR	3.4
1	U	18	TYR	3.4
1	Z	85	LYS	3.4
1	X	8	ILE	3.3
1	G	57	GLU	3.2
1	S	188	GLU	3.2
1	W	18	TYR	3.2
1	P	9	GLU	3.2
1	A	2	ASN	3.2
1	W	58	LYS	3.2
1	B	15	GLU	3.2
1	V	192	PRO	3.1
1	S	193	GLU	3.1
1	B	2	ASN	3.1
1	I	2	ASN	3.0
1	W	92	CYS	3.0
1	P	18	TYR	3.0
1	T	17	ALA	3.0

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	G	58	LYS	2.9
1	M	92	CYS	2.9
1	R	193	GLU	2.9
1	b	3	LEU	2.9
1	A	14	GLY	2.9
1	I	10	THR	2.8
1	Y	9	GLU	2.8
1	A	193	GLU	2.8
1	E	104	LEU	2.8
1	V	48	LEU	2.8
1	W	63	TYR	2.8
1	M	9	GLU	2.8
1	Q	18	TYR	2.8
1	Y	8	ILE	2.8
1	O	9	GLU	2.7
1	E	103	LEU	2.7
1	W	167	LYS	2.7
1	U	9	GLU	2.7
1	O	162	ILE	2.7
1	C	92	CYS	2.7
1	U	17	ALA	2.7
1	D	193	GLU	2.7
1	T	57	GLU	2.6
1	S	18	TYR	2.6
1	C	15	GLU	2.6
1	I	17	ALA	2.6
1	G	191	VAL	2.6
1	E	97	ALA	2.6
1	X	9	GLU	2.6
1	S	8	ILE	2.6
1	b	17	ALA	2.6
1	W	182	GLU	2.6
1	O	101	SER	2.6
1	Z	8	ILE	2.6
1	P	76	ALA	2.5
1	E	96	ALA	2.5
1	W	64	ILE	2.5
1	X	17	ALA	2.5
1	T	18	TYR	2.5
1	P	55	ASP	2.5
1	M	93	ILE	2.5
1	C	193	GLU	2.4

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	D	15	GLU	2.4
1	Q	93	ILE	2.4
1	K	14	GLY	2.4
1	H	11	THR	2.4
1	V	44	ILE	2.4
1	W	57	GLU	2.4
1	W	163	GLU	2.4
1	N	92	CYS	2.4
1	A	12	ASN	2.4
1	D	92	CYS	2.4
1	X	193	GLU	2.4
1	H	103	LEU	2.3
1	R	57	GLU	2.3
1	S	182	GLU	2.3
1	W	93	ILE	2.3
1	H	163	GLU	2.3
1	U	57	GLU	2.3
1	U	93	ILE	2.3
1	N	191	VAL	2.3
1	Z	182	GLU	2.3
1	D	104	LEU	2.3
1	G	193	GLU	2.3
1	S	57	GLU	2.3
1	S	6	THR	2.3
1	D	8	ILE	2.3
1	Z	193	GLU	2.3
1	O	104	LEU	2.2
1	V	23	ARG	2.2
1	Q	188	GLU	2.2
1	b	57	GLU	2.2
1	D	57	GLU	2.2
1	L	11	THR	2.2
1	Z	57	GLU	2.2
1	X	3	LEU	2.2
1	D	129	ALA	2.2
1	X	64	ILE	2.1
1	Q	54	GLN	2.1
1	I	194	THR	2.1
1	X	57	GLU	2.1
1	Z	188	GLU	2.1
1	T	191	VAL	2.1
1	C	57	GLU	2.1

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Mol	Chain	Res	Type	RSRZ
1	b	130	GLN	2.1
1	R	18	TYR	2.1
1	N	130	GLN	2.1
1	V	76	ALA	2.1
1	V	75	PHE	2.1
1	P	159	GLY	2.1
1	O	93	ILE	2.1
1	E	167	LYS	2.1
1	B	193	GLU	2.0
1	F	23	ARG	2.0
1	N	16	ARG	2.0
1	T	8	ILE	2.0
1	R	108	ALA	2.0
1	X	92	CYS	2.0
1	H	104	LEU	2.0
1	P	8	ILE	2.0
1	S	109	LYS	2.0
1	T	76	ALA	2.0
1	b	18	TYR	2.0
1	E	121	MET	2.0
1	Z	7	VAL	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	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

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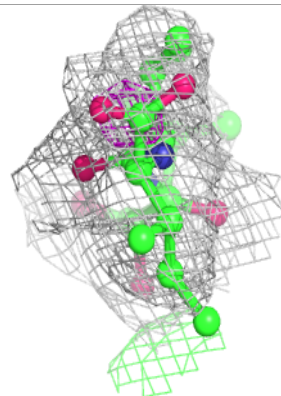
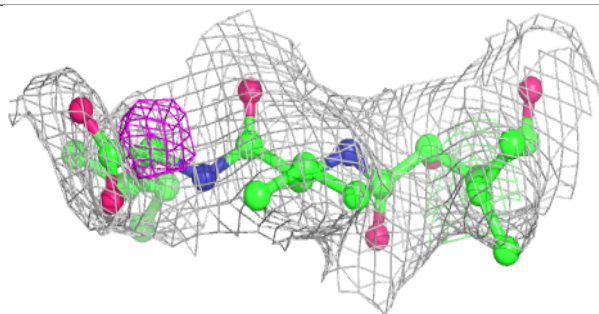
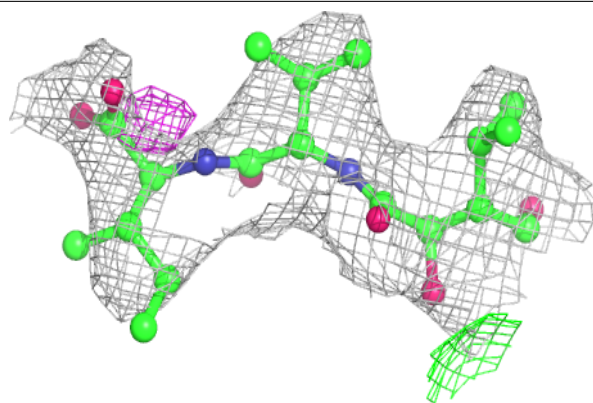
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
2	VSZ	O	301	26/26	0.88	0.17	78,81,90,92	0
2	VSZ	R	301	26/26	0.88	0.25	96,99,104,105	0
2	VSZ	b	301	26/26	0.88	0.23	83,85,94,95	0
2	VSZ	Z	301	26/26	0.90	0.20	81,85,90,92	0
2	VSZ	S	301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

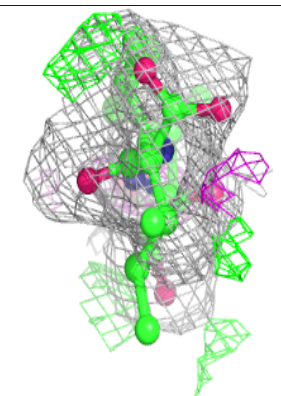
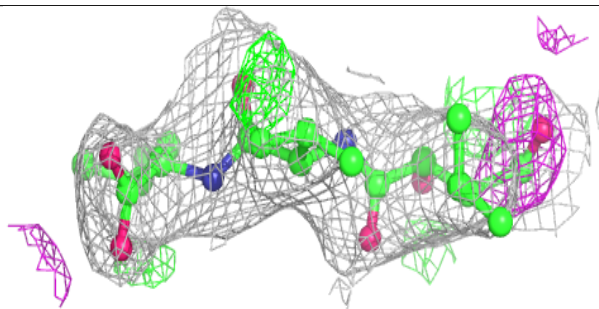
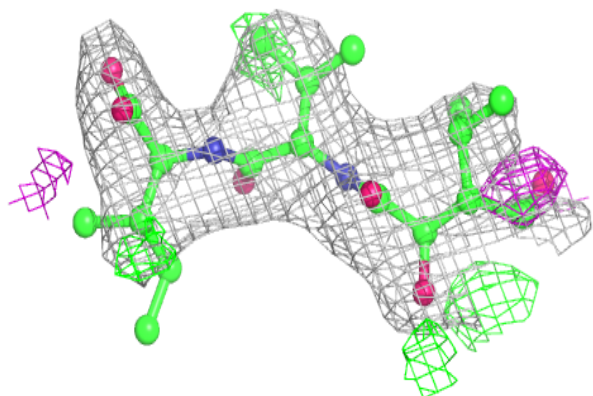
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

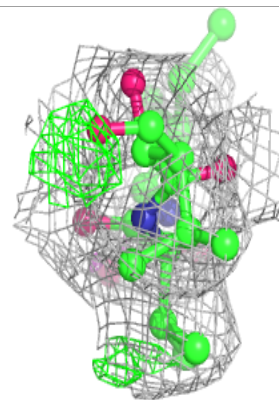
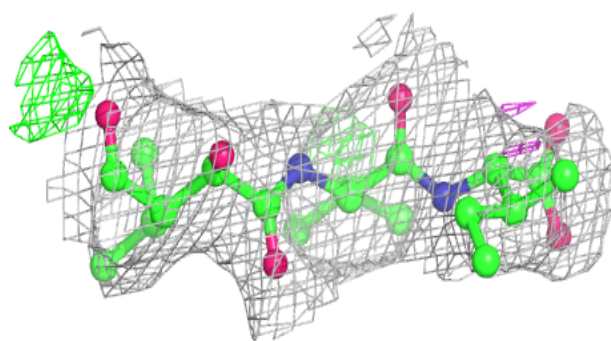
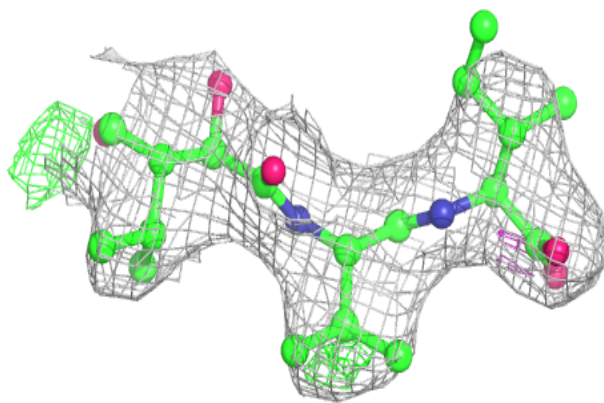
**Electron density around VSZ X 301:**

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

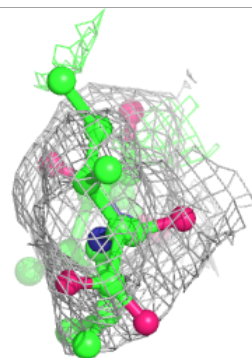
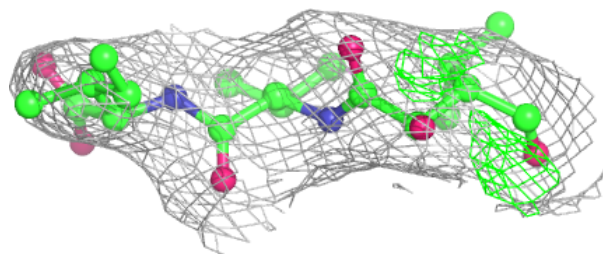
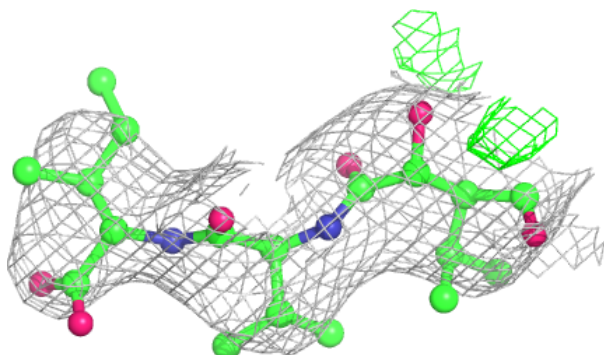


**Electron density around VSZ O 301:**

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

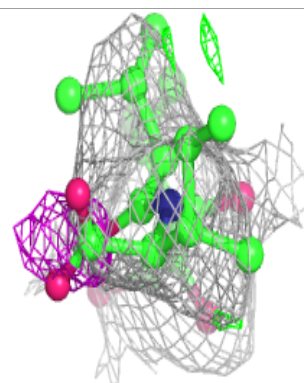
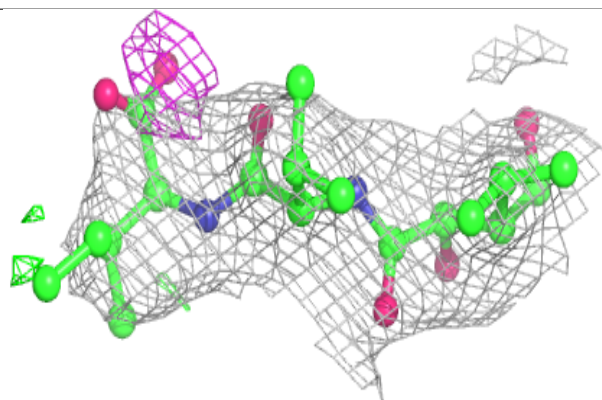
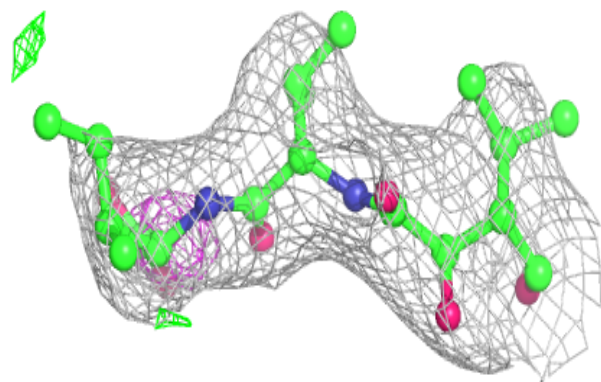
**Electron density around VSZ R 301:**

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

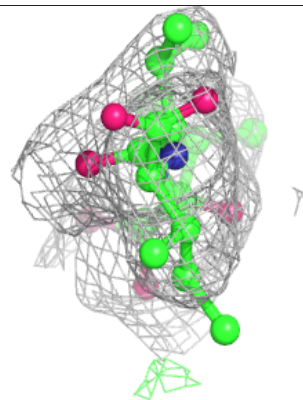
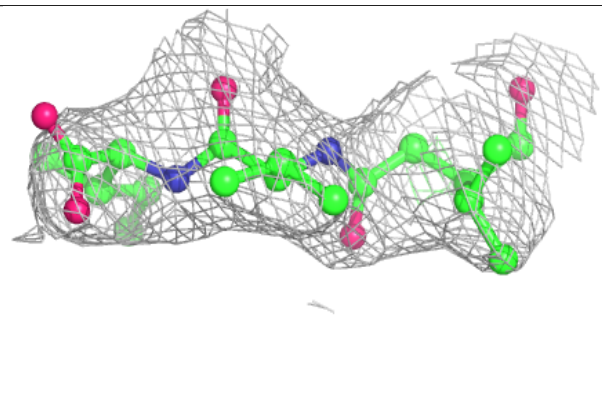
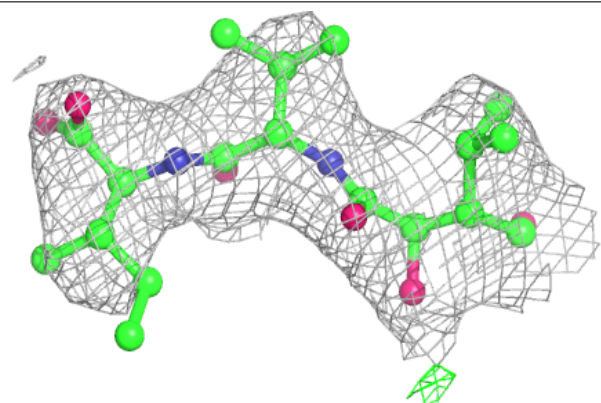


**Electron density around VSZ b 301:**

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

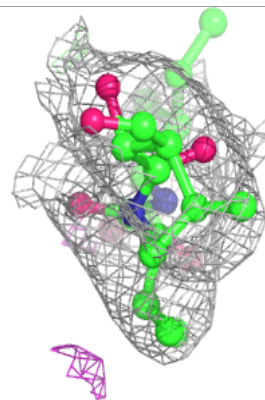
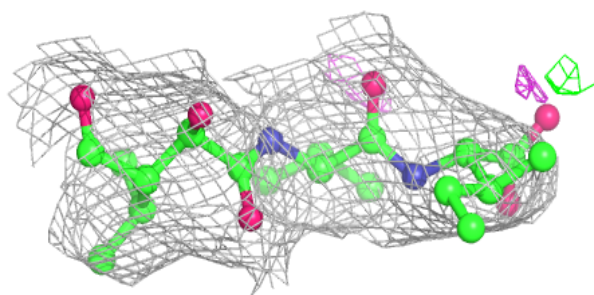
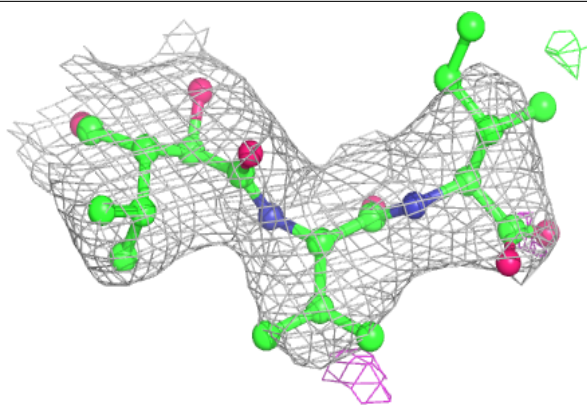
**Electron density around VSZ Z 301:**

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

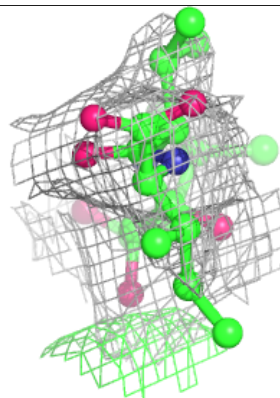
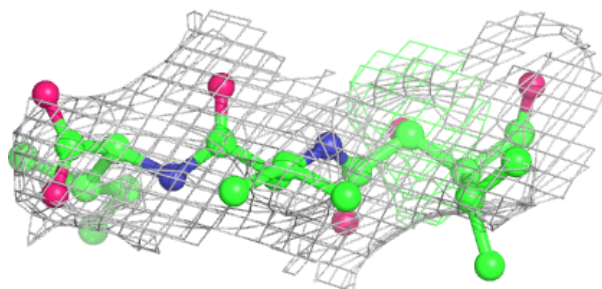
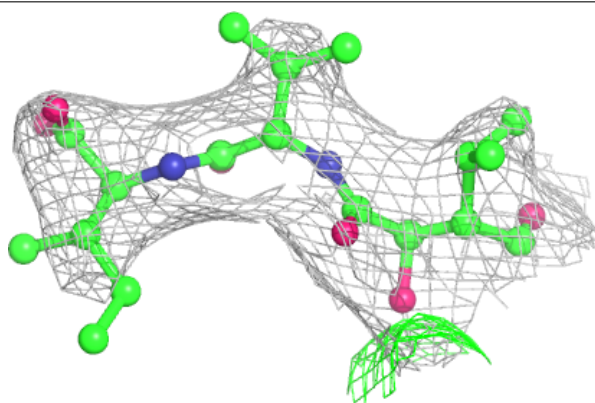


**Electron density around VSZ S 301:**

$2mF_o-DF_c$  (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:**

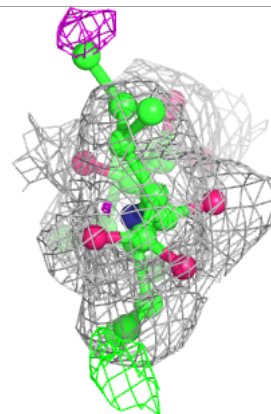
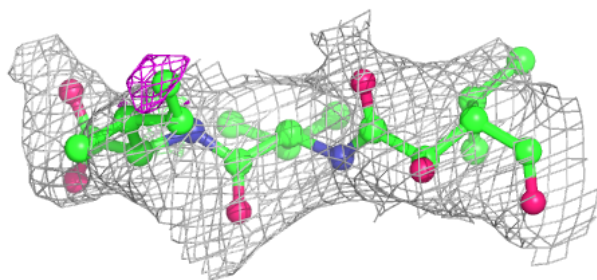
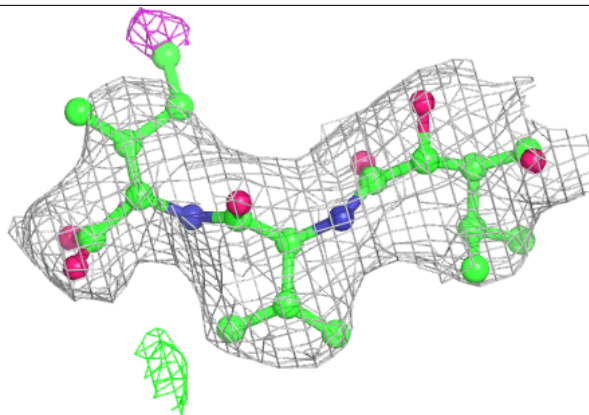
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



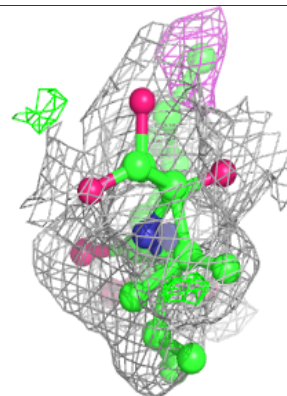
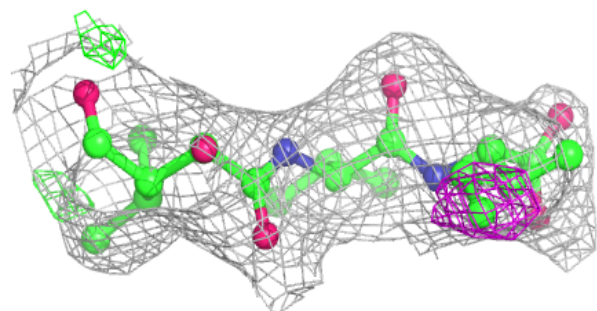
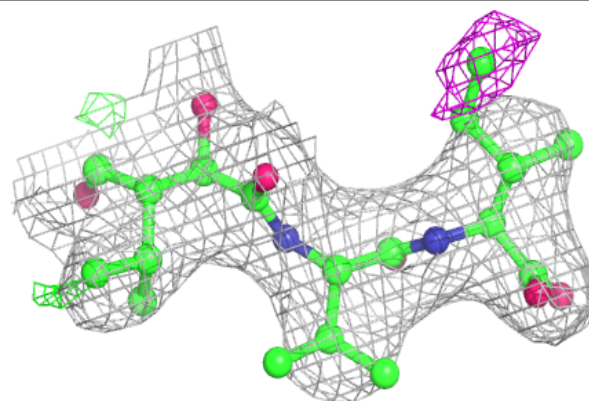


**Electron density around VSZ N 301:**

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

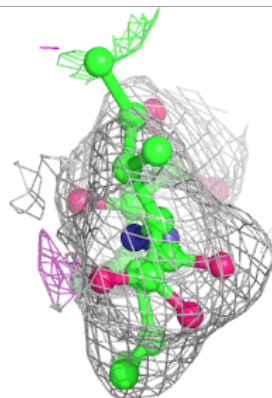
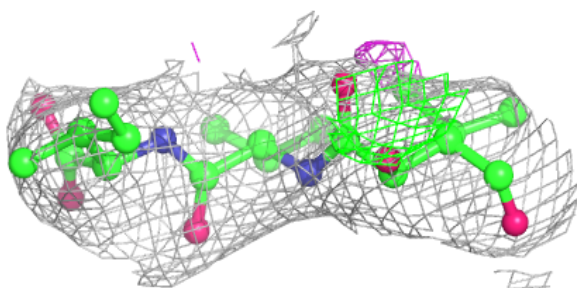
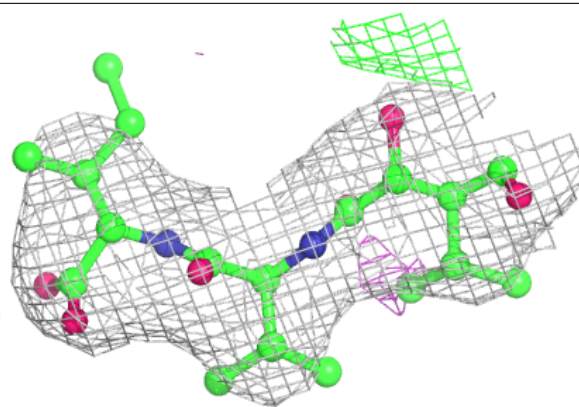
**Electron density around VSZ D 301:**

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

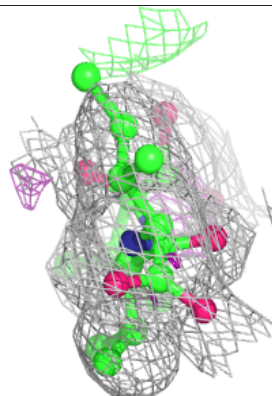
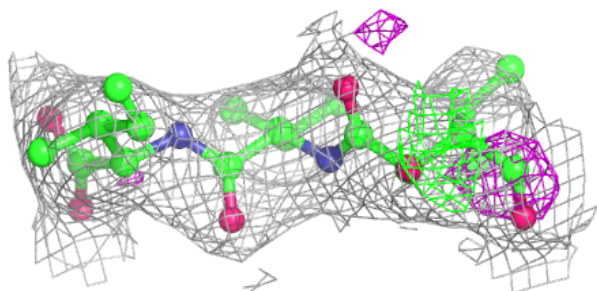
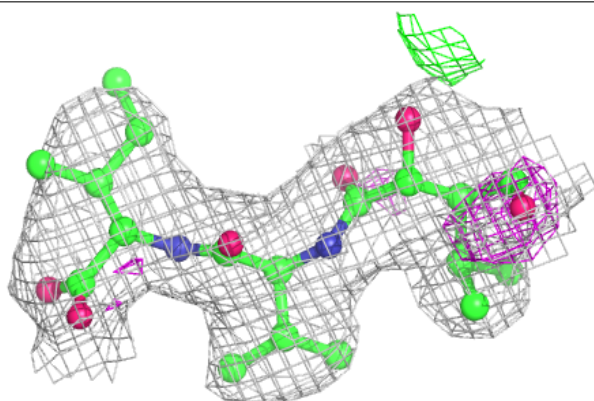


**Electron density around VSZ E 301:**

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

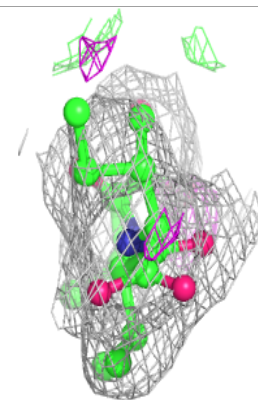
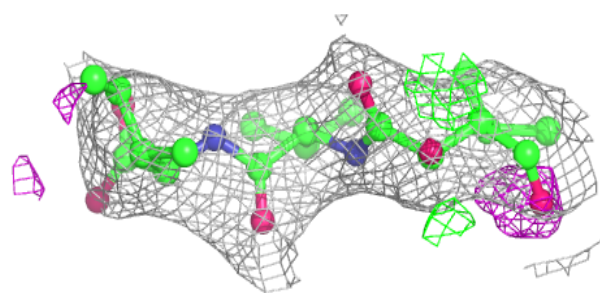
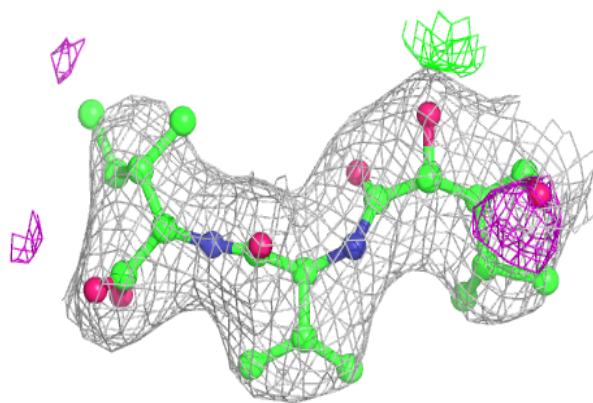
**Electron density around VSZ L 301:**

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

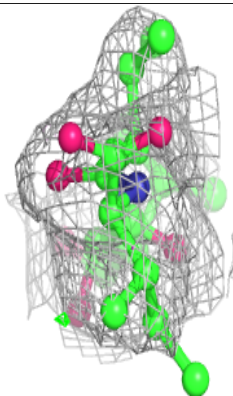
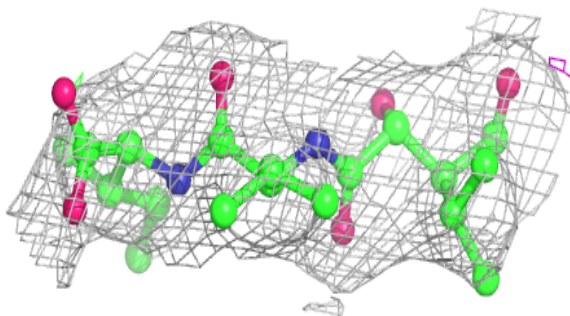
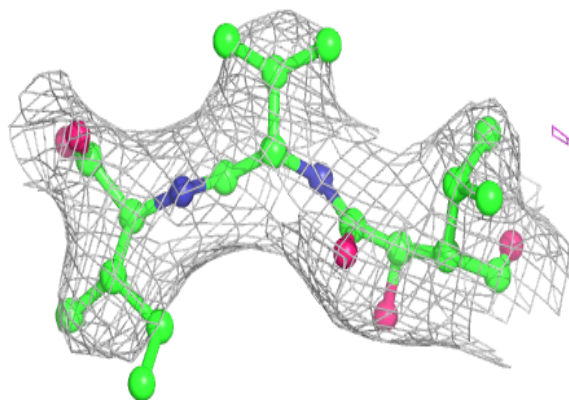


**Electron density around VSZ A 301:**

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

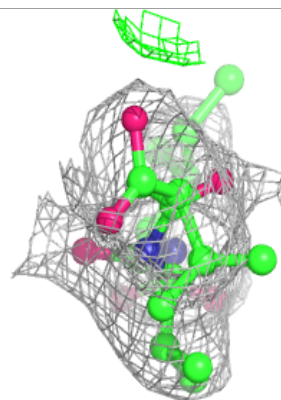
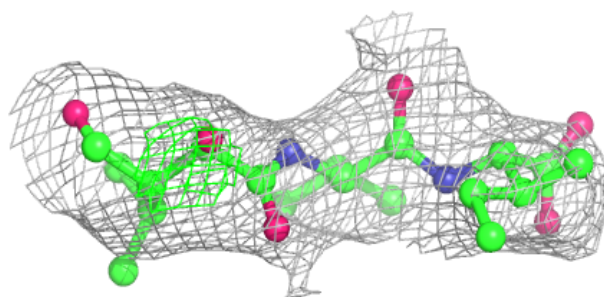
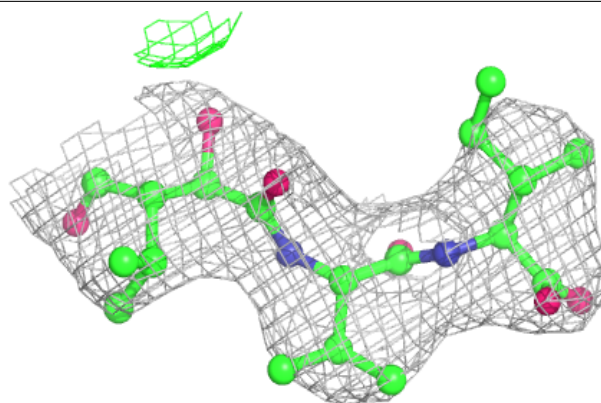
**Electron density around VSZ W 301:**

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

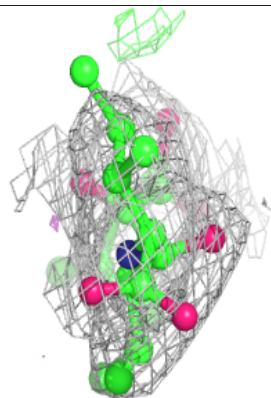
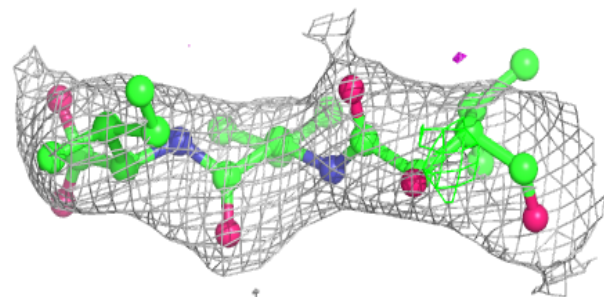
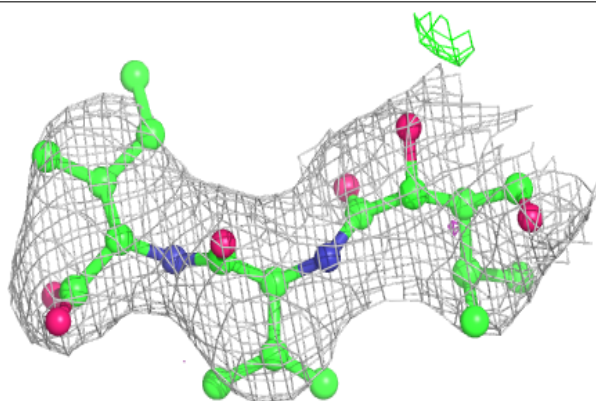


**Electron density around VSZ F 301:**

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

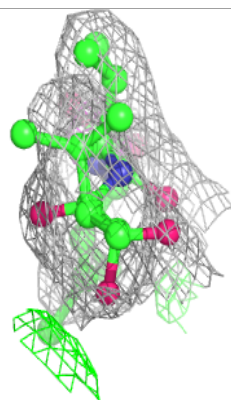
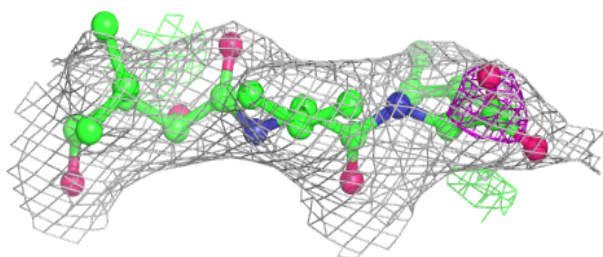
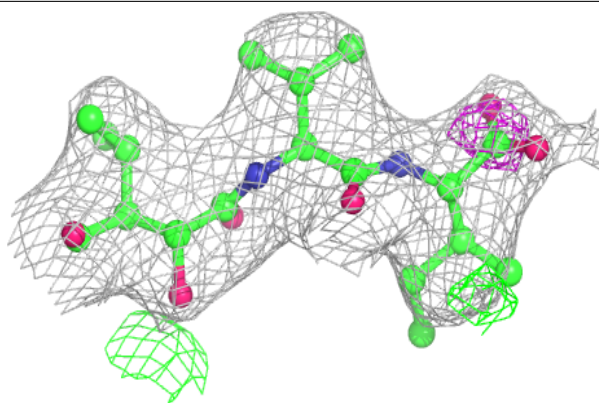
**Electron density around VSZ G 301:**

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

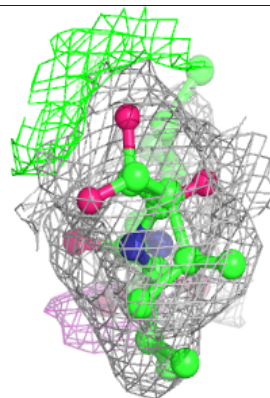
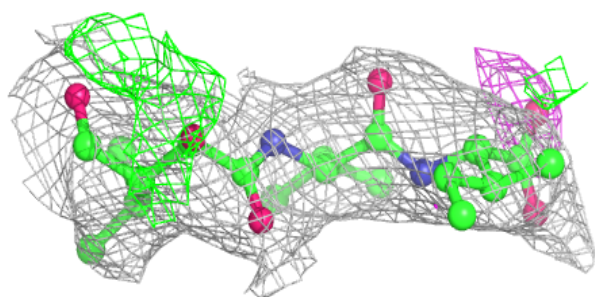
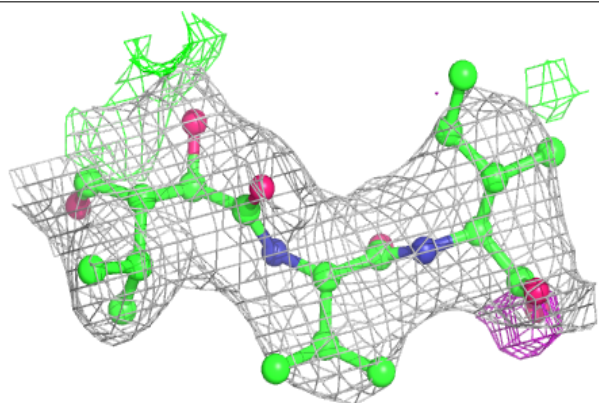


**Electron density around VSZ I 301:**

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

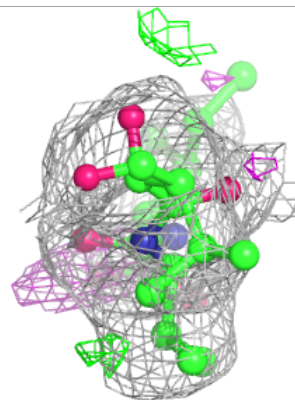
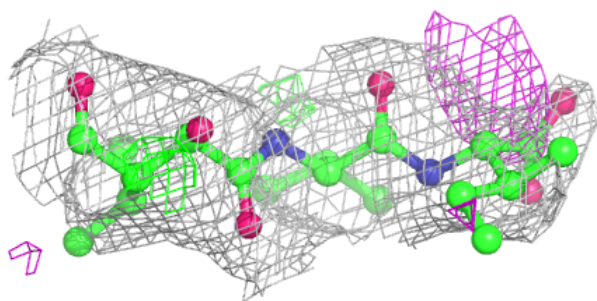
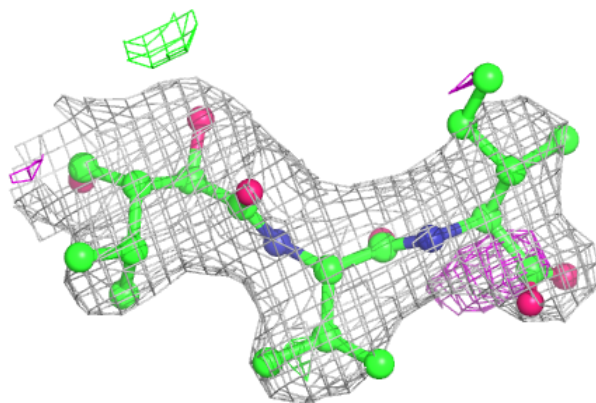
**Electron density around VSZ K 301:**

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

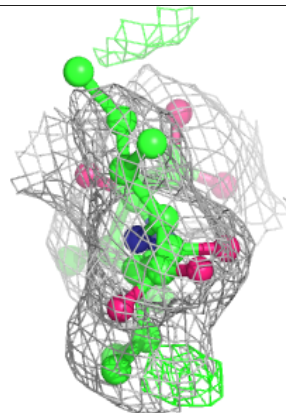
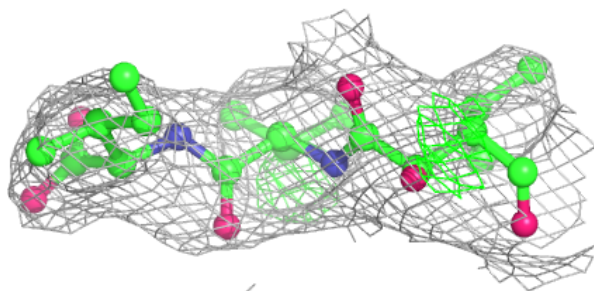
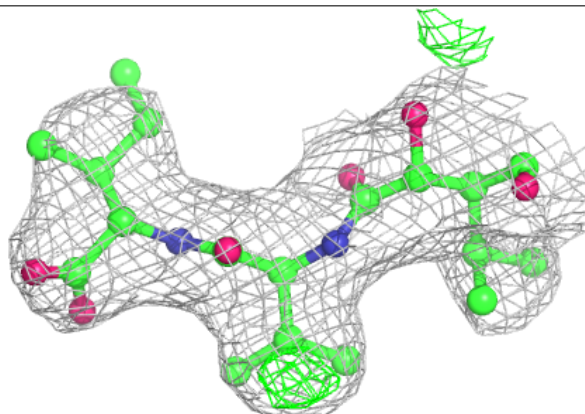


**Electron density around VSZ U 301:**

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

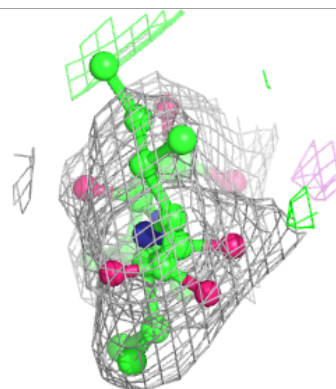
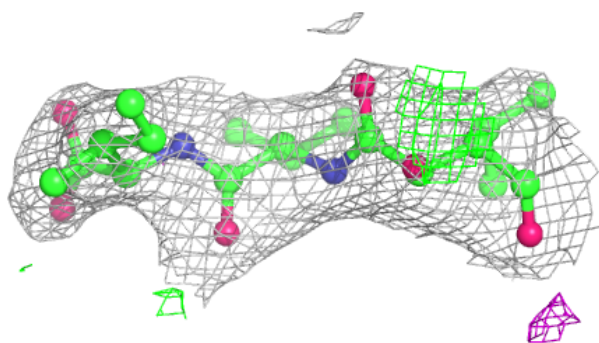
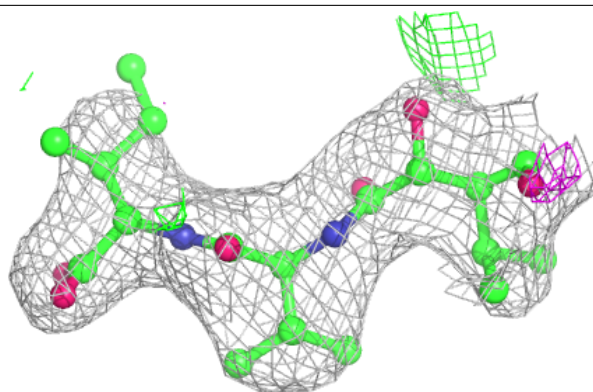
**Electron density around VSZ C 301:**

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

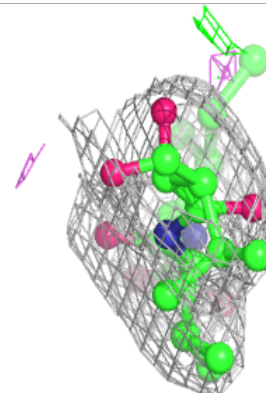
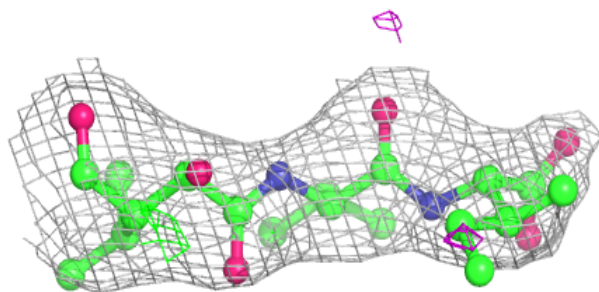
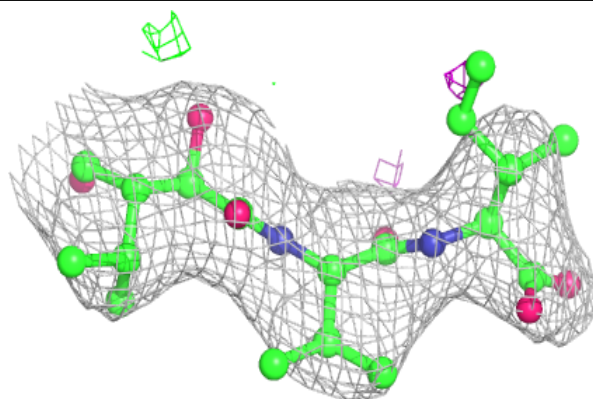


**Electron density around VSZ P 301:**

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

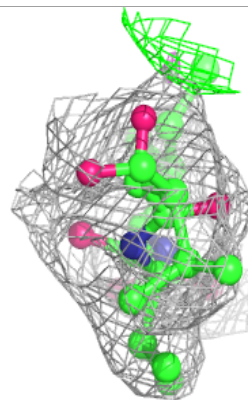
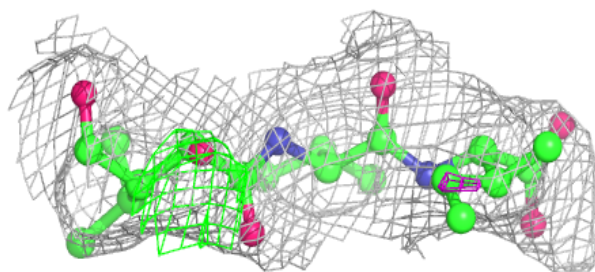
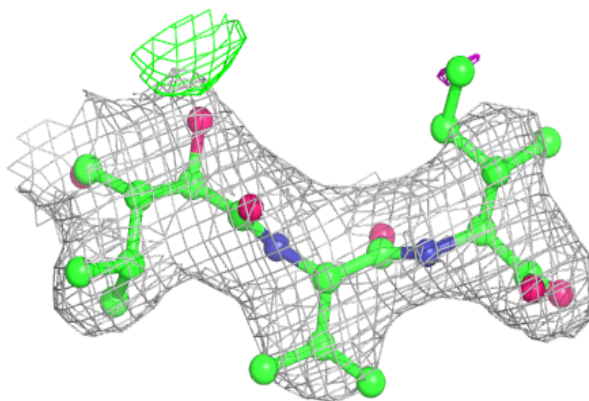
**Electron density around VSZ Q 301:**

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

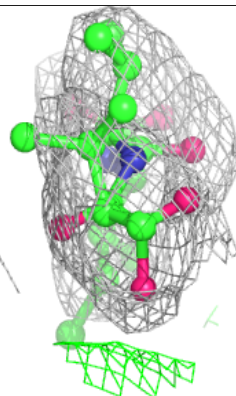
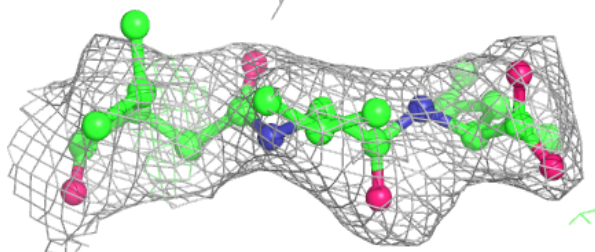
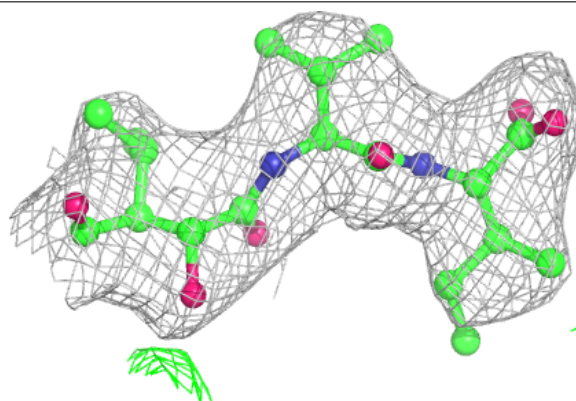


**Electron density around VSZ M 301:**

$2mF_o-DF_c$  (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:**

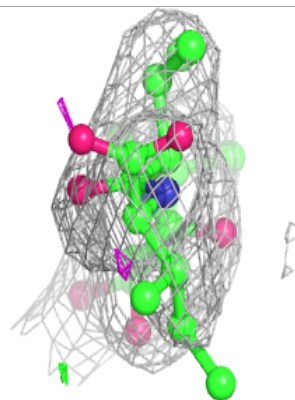
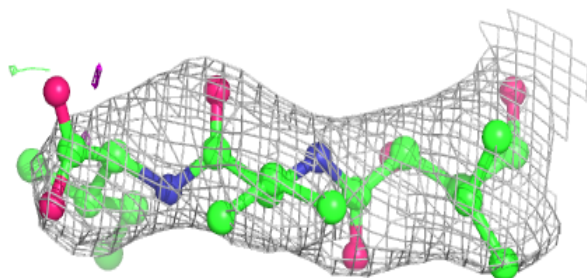
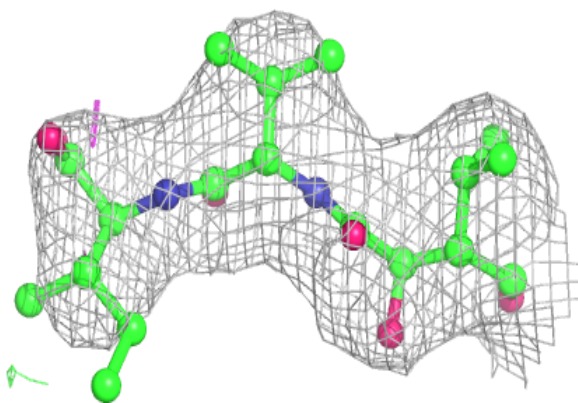
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



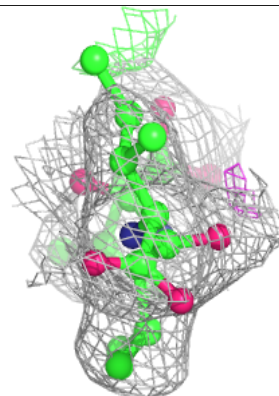
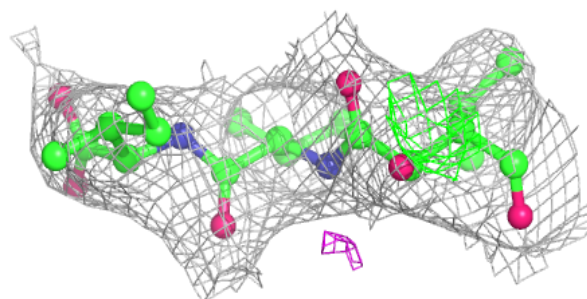
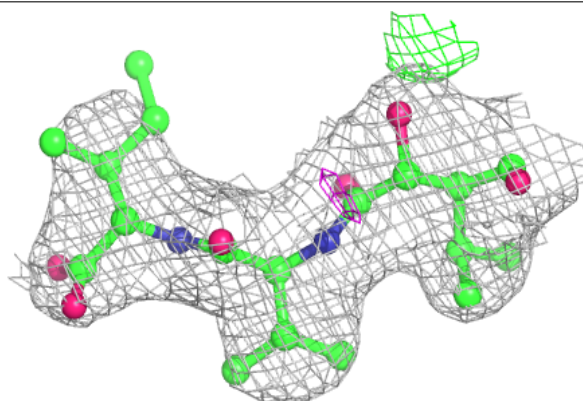


**Electron density around VSZ a 301:**

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

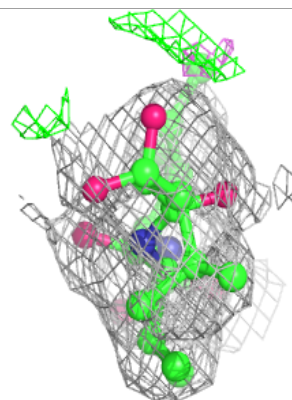
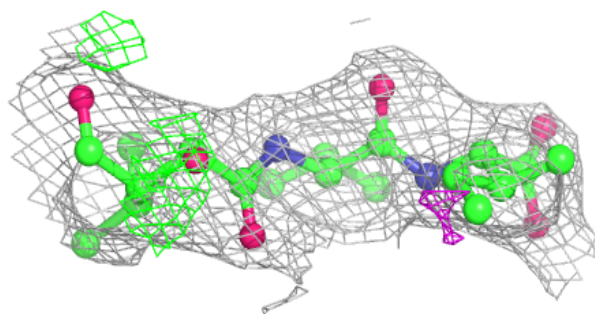
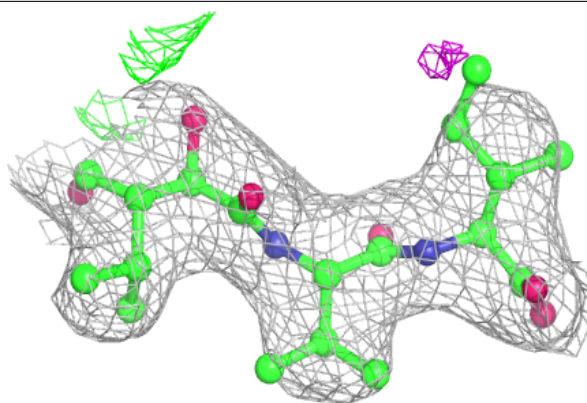
**Electron density around VSZ T 301:**

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

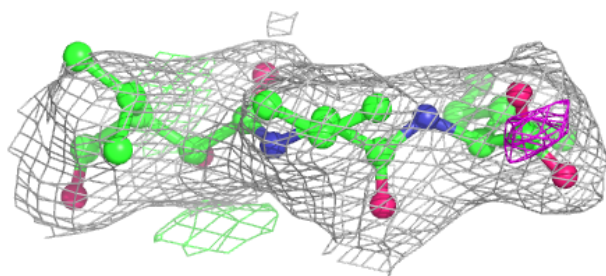
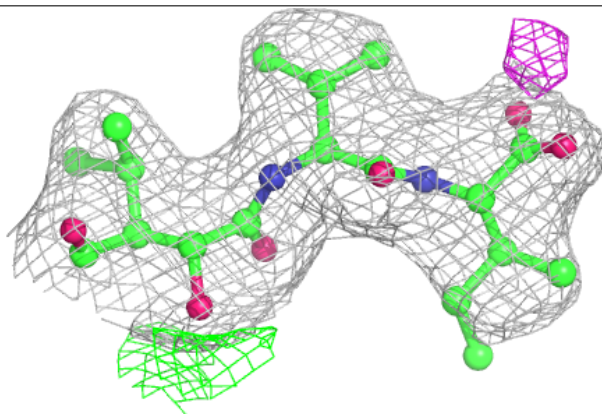


**Electron density around VSZ B 301:**

$2mF_o-DF_c$  (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.