



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 05:17 AM UTC

PDB ID : 7YIV / pdb_00007yiv
Title : The Crystal Structure of Human Tissue Nonspecific Alkaline Phosphatase (ALPL) at Basic pH
Authors : Cao, Y.; Qin, A.; Yu, Y.T.; Yao, D.Q.; Zhang, Q.; Rao, B.; Xia, Y.; Lu, Y.
Deposited on : 2022-07-18
Resolution : 3.18 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

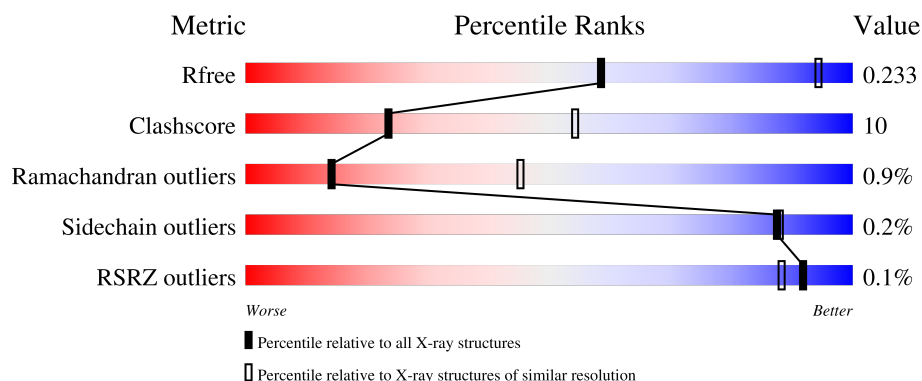
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.18 Å.

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



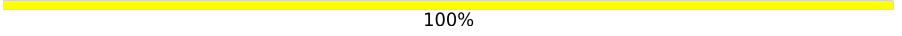
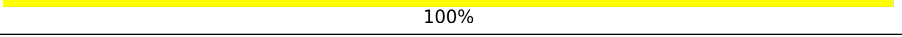
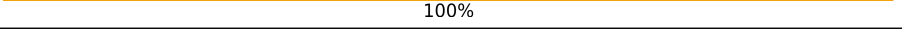
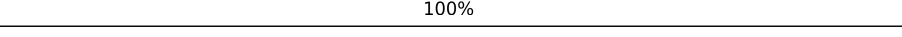
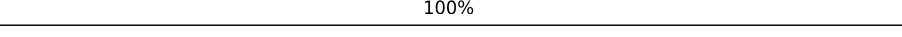
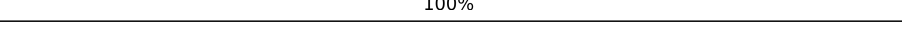
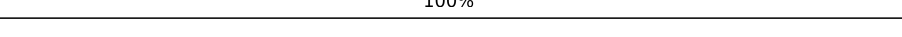
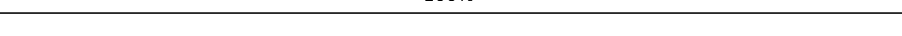
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	2001 (3.20-3.16)
Clashscore	190562	2119 (3.20-3.16)
Ramachandran outliers	187476	2070 (3.20-3.16)
Sidechain outliers	187428	2069 (3.20-3.16)
RSRZ outliers	180081	2001 (3.20-3.16)

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

Mol	Chain	Length	Quality of chain
1	A	518	 69% 24% 7%
1	B	518	 72% 21% 7%
1	C	518	 69% 23% 7%
1	D	518	 73% 19% 7%
1	E	518	 68% 25% 7%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	518	 66% 27% 7%
1	G	518	 74% 19% 7%
1	H	518	 73% 20% 7%
2	I	2	 100%
2	J	2	 50% 50%
2	K	2	 100%
2	L	2	 50% 50%
2	M	2	 50% 50%
2	N	2	 50% 50%
2	O	2	 100%
2	P	2	 100%
2	Q	2	 100%
2	R	2	 50% 50%
2	S	2	 100%
2	T	2	 50% 50%
2	U	2	 100%
2	V	2	 50% 50%
2	W	2	 50% 50%
2	X	2	 100%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 30673 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 Alkaline phosphatase, tissue-nonspecific isozyme.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	484	Total	C	N	O	S	0	0	0
			3748	2345	665	719	19			
1	D	482	Total	C	N	O	S	0	0	0
			3738	2339	663	717	19			
1	C	484	Total	C	N	O	S	0	0	0
			3748	2345	665	719	19			
1	B	484	Total	C	N	O	S	0	0	0
			3748	2345	665	719	19			
1	G	484	Total	C	N	O	S	0	0	0
			3748	2345	665	719	19			
1	H	484	Total	C	N	O	S	0	0	0
			3748	2345	665	719	19			
1	F	483	Total	C	N	O	S	0	0	0
			3743	2342	664	718	19			
1	E	484	Total	C	N	O	S	0	0	0
			3748	2345	665	719	19			

There are 280 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	MET	-	initiating methionine	UNP P05186
A	0	LYS	-	expression tag	UNP P05186
A	1	THR	-	expression tag	UNP P05186
A	2	ILE	-	expression tag	UNP P05186
A	3	ILE	-	expression tag	UNP P05186
A	4	ALA	-	expression tag	UNP P05186
A	5	LEU	-	expression tag	UNP P05186
A	6	SER	-	expression tag	UNP P05186
A	7	TYR	-	expression tag	UNP P05186
A	8	ILE	-	expression tag	UNP P05186
A	9	PHE	-	expression tag	UNP P05186
A	10	CYS	-	expression tag	UNP P05186
A	11	LEU	-	expression tag	UNP P05186

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
A	12	VAL	-	expression tag	UNP P05186
A	13	PHE	-	expression tag	UNP P05186
A	14	ALA	-	expression tag	UNP P05186
A	15	GLY	-	expression tag	UNP P05186
A	16	ARG	-	expression tag	UNP P05186
A	17	ALA	-	expression tag	UNP P05186
A	501	ALA	-	expression tag	UNP P05186
A	502	ALA	-	expression tag	UNP P05186
A	503	ALA	-	expression tag	UNP P05186
A	504	GLU	-	expression tag	UNP P05186
A	505	ASN	-	expression tag	UNP P05186
A	506	LEU	-	expression tag	UNP P05186
A	507	TYR	-	expression tag	UNP P05186
A	508	PHE	-	expression tag	UNP P05186
A	509	GLN	-	expression tag	UNP P05186
A	510	GLY	-	expression tag	UNP P05186
A	511	CYS	-	expression tag	UNP P05186
A	512	CYS	-	expression tag	UNP P05186
A	513	PRO	-	expression tag	UNP P05186
A	514	GLY	-	expression tag	UNP P05186
A	515	CYS	-	expression tag	UNP P05186
A	516	CYS	-	expression tag	UNP P05186
D	-1	MET	-	initiating methionine	UNP P05186
D	0	LYS	-	expression tag	UNP P05186
D	1	THR	-	expression tag	UNP P05186
D	2	ILE	-	expression tag	UNP P05186
D	3	ILE	-	expression tag	UNP P05186
D	4	ALA	-	expression tag	UNP P05186
D	5	LEU	-	expression tag	UNP P05186
D	6	SER	-	expression tag	UNP P05186
D	7	TYR	-	expression tag	UNP P05186
D	8	ILE	-	expression tag	UNP P05186
D	9	PHE	-	expression tag	UNP P05186
D	10	CYS	-	expression tag	UNP P05186
D	11	LEU	-	expression tag	UNP P05186
D	12	VAL	-	expression tag	UNP P05186
D	13	PHE	-	expression tag	UNP P05186
D	14	ALA	-	expression tag	UNP P05186
D	15	GLY	-	expression tag	UNP P05186
D	16	ARG	-	expression tag	UNP P05186
D	17	ALA	-	expression tag	UNP P05186
D	501	ALA	-	expression tag	UNP P05186

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
D	502	ALA	-	expression tag	UNP P05186
D	503	ALA	-	expression tag	UNP P05186
D	504	GLU	-	expression tag	UNP P05186
D	505	ASN	-	expression tag	UNP P05186
D	506	LEU	-	expression tag	UNP P05186
D	507	TYR	-	expression tag	UNP P05186
D	508	PHE	-	expression tag	UNP P05186
D	509	GLN	-	expression tag	UNP P05186
D	510	GLY	-	expression tag	UNP P05186
D	511	CYS	-	expression tag	UNP P05186
D	512	CYS	-	expression tag	UNP P05186
D	513	PRO	-	expression tag	UNP P05186
D	514	GLY	-	expression tag	UNP P05186
D	515	CYS	-	expression tag	UNP P05186
D	516	CYS	-	expression tag	UNP P05186
C	-1	MET	-	initiating methionine	UNP P05186
C	0	LYS	-	expression tag	UNP P05186
C	1	THR	-	expression tag	UNP P05186
C	2	ILE	-	expression tag	UNP P05186
C	3	ILE	-	expression tag	UNP P05186
C	4	ALA	-	expression tag	UNP P05186
C	5	LEU	-	expression tag	UNP P05186
C	6	SER	-	expression tag	UNP P05186
C	7	TYR	-	expression tag	UNP P05186
C	8	ILE	-	expression tag	UNP P05186
C	9	PHE	-	expression tag	UNP P05186
C	10	CYS	-	expression tag	UNP P05186
C	11	LEU	-	expression tag	UNP P05186
C	12	VAL	-	expression tag	UNP P05186
C	13	PHE	-	expression tag	UNP P05186
C	14	ALA	-	expression tag	UNP P05186
C	15	GLY	-	expression tag	UNP P05186
C	16	ARG	-	expression tag	UNP P05186
C	17	ALA	-	expression tag	UNP P05186
C	501	ALA	-	expression tag	UNP P05186
C	502	ALA	-	expression tag	UNP P05186
C	503	ALA	-	expression tag	UNP P05186
C	504	GLU	-	expression tag	UNP P05186
C	505	ASN	-	expression tag	UNP P05186
C	506	LEU	-	expression tag	UNP P05186
C	507	TYR	-	expression tag	UNP P05186
C	508	PHE	-	expression tag	UNP P05186

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
C	509	GLN	-	expression tag	UNP P05186
C	510	GLY	-	expression tag	UNP P05186
C	511	CYS	-	expression tag	UNP P05186
C	512	CYS	-	expression tag	UNP P05186
C	513	PRO	-	expression tag	UNP P05186
C	514	GLY	-	expression tag	UNP P05186
C	515	CYS	-	expression tag	UNP P05186
C	516	CYS	-	expression tag	UNP P05186
B	-1	MET	-	initiating methionine	UNP P05186
B	0	LYS	-	expression tag	UNP P05186
B	1	THR	-	expression tag	UNP P05186
B	2	ILE	-	expression tag	UNP P05186
B	3	ILE	-	expression tag	UNP P05186
B	4	ALA	-	expression tag	UNP P05186
B	5	LEU	-	expression tag	UNP P05186
B	6	SER	-	expression tag	UNP P05186
B	7	TYR	-	expression tag	UNP P05186
B	8	ILE	-	expression tag	UNP P05186
B	9	PHE	-	expression tag	UNP P05186
B	10	CYS	-	expression tag	UNP P05186
B	11	LEU	-	expression tag	UNP P05186
B	12	VAL	-	expression tag	UNP P05186
B	13	PHE	-	expression tag	UNP P05186
B	14	ALA	-	expression tag	UNP P05186
B	15	GLY	-	expression tag	UNP P05186
B	16	ARG	-	expression tag	UNP P05186
B	17	ALA	-	expression tag	UNP P05186
B	501	ALA	-	expression tag	UNP P05186
B	502	ALA	-	expression tag	UNP P05186
B	503	ALA	-	expression tag	UNP P05186
B	504	GLU	-	expression tag	UNP P05186
B	505	ASN	-	expression tag	UNP P05186
B	506	LEU	-	expression tag	UNP P05186
B	507	TYR	-	expression tag	UNP P05186
B	508	PHE	-	expression tag	UNP P05186
B	509	GLN	-	expression tag	UNP P05186
B	510	GLY	-	expression tag	UNP P05186
B	511	CYS	-	expression tag	UNP P05186
B	512	CYS	-	expression tag	UNP P05186
B	513	PRO	-	expression tag	UNP P05186
B	514	GLY	-	expression tag	UNP P05186
B	515	CYS	-	expression tag	UNP P05186

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	516	CYS	-	expression tag	UNP P05186
G	-1	MET	-	initiating methionine	UNP P05186
G	0	LYS	-	expression tag	UNP P05186
G	1	THR	-	expression tag	UNP P05186
G	2	ILE	-	expression tag	UNP P05186
G	3	ILE	-	expression tag	UNP P05186
G	4	ALA	-	expression tag	UNP P05186
G	5	LEU	-	expression tag	UNP P05186
G	6	SER	-	expression tag	UNP P05186
G	7	TYR	-	expression tag	UNP P05186
G	8	ILE	-	expression tag	UNP P05186
G	9	PHE	-	expression tag	UNP P05186
G	10	CYS	-	expression tag	UNP P05186
G	11	LEU	-	expression tag	UNP P05186
G	12	VAL	-	expression tag	UNP P05186
G	13	PHE	-	expression tag	UNP P05186
G	14	ALA	-	expression tag	UNP P05186
G	15	GLY	-	expression tag	UNP P05186
G	16	ARG	-	expression tag	UNP P05186
G	17	ALA	-	expression tag	UNP P05186
G	501	ALA	-	expression tag	UNP P05186
G	502	ALA	-	expression tag	UNP P05186
G	503	ALA	-	expression tag	UNP P05186
G	504	GLU	-	expression tag	UNP P05186
G	505	ASN	-	expression tag	UNP P05186
G	506	LEU	-	expression tag	UNP P05186
G	507	TYR	-	expression tag	UNP P05186
G	508	PHE	-	expression tag	UNP P05186
G	509	GLN	-	expression tag	UNP P05186
G	510	GLY	-	expression tag	UNP P05186
G	511	CYS	-	expression tag	UNP P05186
G	512	CYS	-	expression tag	UNP P05186
G	513	PRO	-	expression tag	UNP P05186
G	514	GLY	-	expression tag	UNP P05186
G	515	CYS	-	expression tag	UNP P05186
G	516	CYS	-	expression tag	UNP P05186
H	-1	MET	-	initiating methionine	UNP P05186
H	0	LYS	-	expression tag	UNP P05186
H	1	THR	-	expression tag	UNP P05186
H	2	ILE	-	expression tag	UNP P05186
H	3	ILE	-	expression tag	UNP P05186
H	4	ALA	-	expression tag	UNP P05186

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
H	5	LEU	-	expression tag	UNP P05186
H	6	SER	-	expression tag	UNP P05186
H	7	TYR	-	expression tag	UNP P05186
H	8	ILE	-	expression tag	UNP P05186
H	9	PHE	-	expression tag	UNP P05186
H	10	CYS	-	expression tag	UNP P05186
H	11	LEU	-	expression tag	UNP P05186
H	12	VAL	-	expression tag	UNP P05186
H	13	PHE	-	expression tag	UNP P05186
H	14	ALA	-	expression tag	UNP P05186
H	15	GLY	-	expression tag	UNP P05186
H	16	ARG	-	expression tag	UNP P05186
H	17	ALA	-	expression tag	UNP P05186
H	501	ALA	-	expression tag	UNP P05186
H	502	ALA	-	expression tag	UNP P05186
H	503	ALA	-	expression tag	UNP P05186
H	504	GLU	-	expression tag	UNP P05186
H	505	ASN	-	expression tag	UNP P05186
H	506	LEU	-	expression tag	UNP P05186
H	507	TYR	-	expression tag	UNP P05186
H	508	PHE	-	expression tag	UNP P05186
H	509	GLN	-	expression tag	UNP P05186
H	510	GLY	-	expression tag	UNP P05186
H	511	CYS	-	expression tag	UNP P05186
H	512	CYS	-	expression tag	UNP P05186
H	513	PRO	-	expression tag	UNP P05186
H	514	GLY	-	expression tag	UNP P05186
H	515	CYS	-	expression tag	UNP P05186
H	516	CYS	-	expression tag	UNP P05186
F	-1	MET	-	initiating methionine	UNP P05186
F	0	LYS	-	expression tag	UNP P05186
F	1	THR	-	expression tag	UNP P05186
F	2	ILE	-	expression tag	UNP P05186
F	3	ILE	-	expression tag	UNP P05186
F	4	ALA	-	expression tag	UNP P05186
F	5	LEU	-	expression tag	UNP P05186
F	6	SER	-	expression tag	UNP P05186
F	7	TYR	-	expression tag	UNP P05186
F	8	ILE	-	expression tag	UNP P05186
F	9	PHE	-	expression tag	UNP P05186
F	10	CYS	-	expression tag	UNP P05186
F	11	LEU	-	expression tag	UNP P05186

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
F	12	VAL	-	expression tag	UNP P05186
F	13	PHE	-	expression tag	UNP P05186
F	14	ALA	-	expression tag	UNP P05186
F	15	GLY	-	expression tag	UNP P05186
F	16	ARG	-	expression tag	UNP P05186
F	17	ALA	-	expression tag	UNP P05186
F	501	ALA	-	expression tag	UNP P05186
F	502	ALA	-	expression tag	UNP P05186
F	503	ALA	-	expression tag	UNP P05186
F	504	GLU	-	expression tag	UNP P05186
F	505	ASN	-	expression tag	UNP P05186
F	506	LEU	-	expression tag	UNP P05186
F	507	TYR	-	expression tag	UNP P05186
F	508	PHE	-	expression tag	UNP P05186
F	509	GLN	-	expression tag	UNP P05186
F	510	GLY	-	expression tag	UNP P05186
F	511	CYS	-	expression tag	UNP P05186
F	512	CYS	-	expression tag	UNP P05186
F	513	PRO	-	expression tag	UNP P05186
F	514	GLY	-	expression tag	UNP P05186
F	515	CYS	-	expression tag	UNP P05186
F	516	CYS	-	expression tag	UNP P05186
E	-1	MET	-	initiating methionine	UNP P05186
E	0	LYS	-	expression tag	UNP P05186
E	1	THR	-	expression tag	UNP P05186
E	2	ILE	-	expression tag	UNP P05186
E	3	ILE	-	expression tag	UNP P05186
E	4	ALA	-	expression tag	UNP P05186
E	5	LEU	-	expression tag	UNP P05186
E	6	SER	-	expression tag	UNP P05186
E	7	TYR	-	expression tag	UNP P05186
E	8	ILE	-	expression tag	UNP P05186
E	9	PHE	-	expression tag	UNP P05186
E	10	CYS	-	expression tag	UNP P05186
E	11	LEU	-	expression tag	UNP P05186
E	12	VAL	-	expression tag	UNP P05186
E	13	PHE	-	expression tag	UNP P05186
E	14	ALA	-	expression tag	UNP P05186
E	15	GLY	-	expression tag	UNP P05186
E	16	ARG	-	expression tag	UNP P05186
E	17	ALA	-	expression tag	UNP P05186
E	501	ALA	-	expression tag	UNP P05186

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
E	502	ALA	-	expression tag	UNP P05186
E	503	ALA	-	expression tag	UNP P05186
E	504	GLU	-	expression tag	UNP P05186
E	505	ASN	-	expression tag	UNP P05186
E	506	LEU	-	expression tag	UNP P05186
E	507	TYR	-	expression tag	UNP P05186
E	508	PHE	-	expression tag	UNP P05186
E	509	GLN	-	expression tag	UNP P05186
E	510	GLY	-	expression tag	UNP P05186
E	511	CYS	-	expression tag	UNP P05186
E	512	CYS	-	expression tag	UNP P05186
E	513	PRO	-	expression tag	UNP P05186
E	514	GLY	-	expression tag	UNP P05186
E	515	CYS	-	expression tag	UNP P05186
E	516	CYS	-	expression tag	UNP P05186

- Molecule 2 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



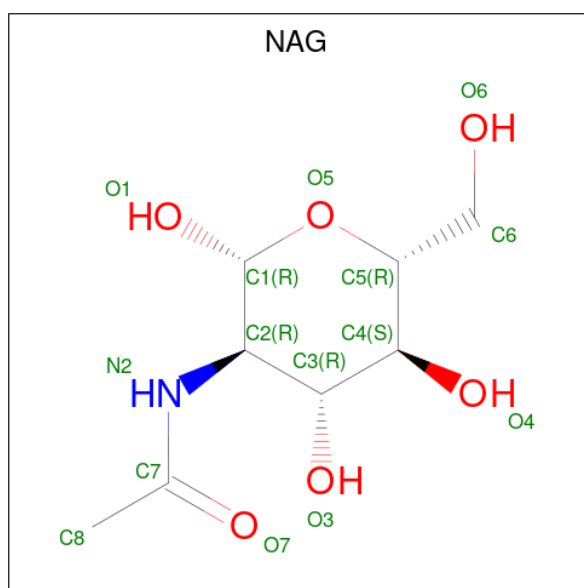
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	I	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	J	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	K	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	L	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	M	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	N	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	O	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	P	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	Q	2	Total	C	N	O	0	0	0
			28	16	2	10			

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	R	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	S	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	T	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	U	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	V	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	W	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	X	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 3 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	D	1	Total	C	N	O	0	0
			14	8	1	5		
3	D	1	Total	C	N	O	0	0
			14	8	1	5		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	C	1	Total	C	N	O	0	0
			14	8	1	5		
3	C	1	Total	C	N	O	0	0
			14	8	1	5		
3	B	1	Total	C	N	O	0	0
			14	8	1	5		
3	B	1	Total	C	N	O	0	0
			14	8	1	5		
3	G	1	Total	C	N	O	0	0
			14	8	1	5		
3	G	1	Total	C	N	O	0	0
			14	8	1	5		
3	H	1	Total	C	N	O	0	0
			14	8	1	5		
3	H	1	Total	C	N	O	0	0
			14	8	1	5		
3	F	1	Total	C	N	O	0	0
			14	8	1	5		
3	F	1	Total	C	N	O	0	0
			14	8	1	5		
3	E	1	Total	C	N	O	0	0
			14	8	1	5		
3	E	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 4 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Mg	0	0
			1	1		
4	D	1	Total	Mg	0	0
			1	1		
4	C	1	Total	Mg	0	0
			1	1		
4	B	1	Total	Mg	0	0
			1	1		
4	G	1	Total	Mg	0	0
			1	1		
4	H	1	Total	Mg	0	0
			1	1		
4	F	1	Total	Mg	0	0
			1	1		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	E	1	Total	Mg	0	0
			1	1		

- Molecule 5 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	2	Total	Zn	0	0
			2	2		
5	D	2	Total	Zn	0	0
			2	2		
5	C	2	Total	Zn	0	0
			2	2		
5	B	2	Total	Zn	0	0
			2	2		
5	G	2	Total	Zn	0	0
			2	2		
5	H	2	Total	Zn	0	0
			2	2		
5	F	2	Total	Zn	0	0
			2	2		
5	E	2	Total	Zn	0	0
			2	2		

- Molecule 6 is CALCIUM ION (CCD ID: CA) (formula: Ca) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	1	Total	Ca	0	0
			1	1		
6	D	1	Total	Ca	0	0
			1	1		
6	C	1	Total	Ca	0	0
			1	1		
6	B	1	Total	Ca	0	0
			1	1		
6	G	1	Total	Ca	0	0
			1	1		
6	H	1	Total	Ca	0	0
			1	1		
6	F	1	Total	Ca	0	0
			1	1		

Continued on next page...

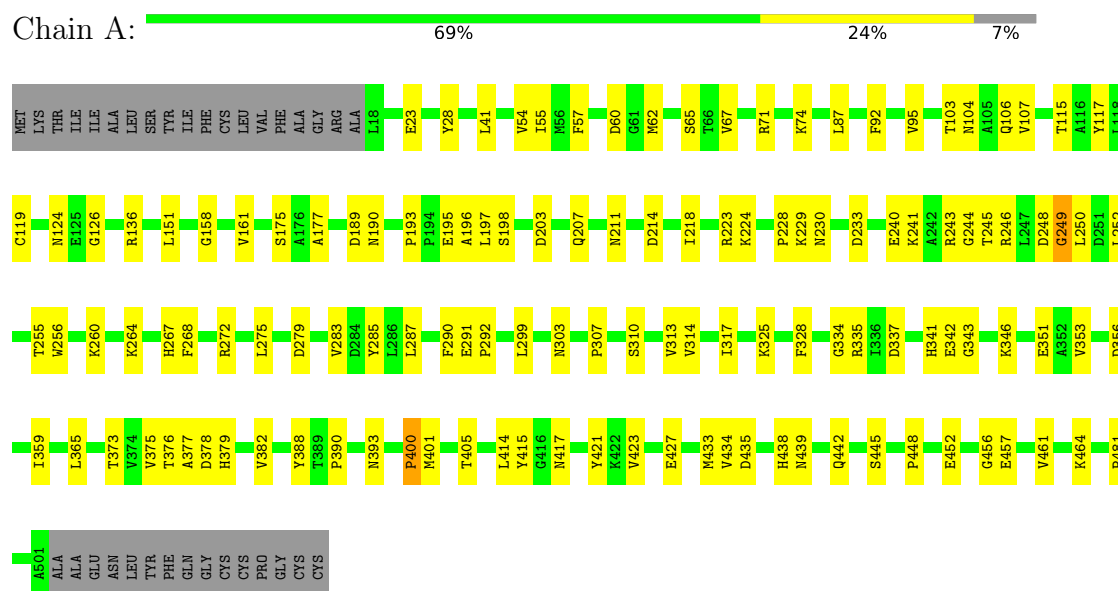
Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	E	1	Total	Ca	0	0
			1	1		

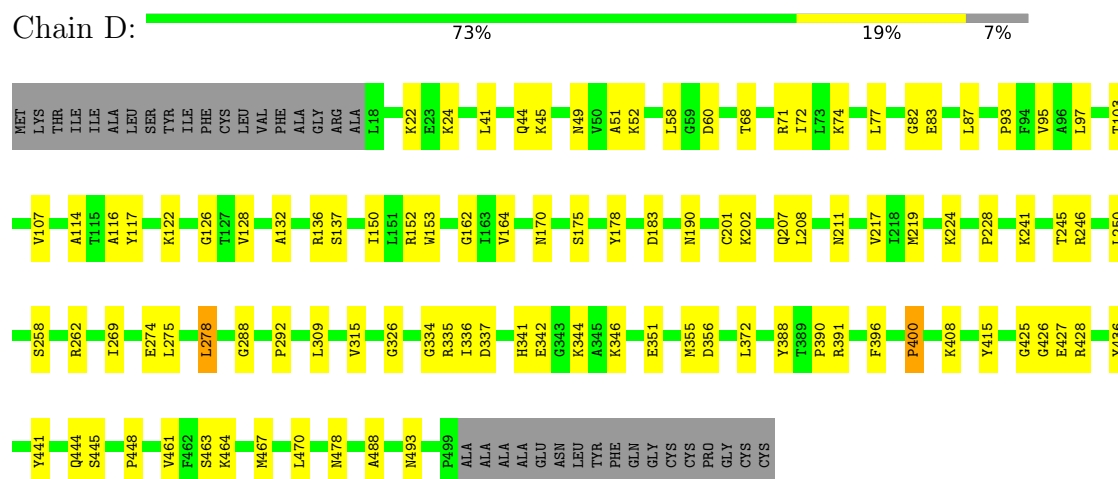
3 Residue-property plots

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

- Molecule 1: Alkaline phosphatase, tissue-nonspecific isozyme

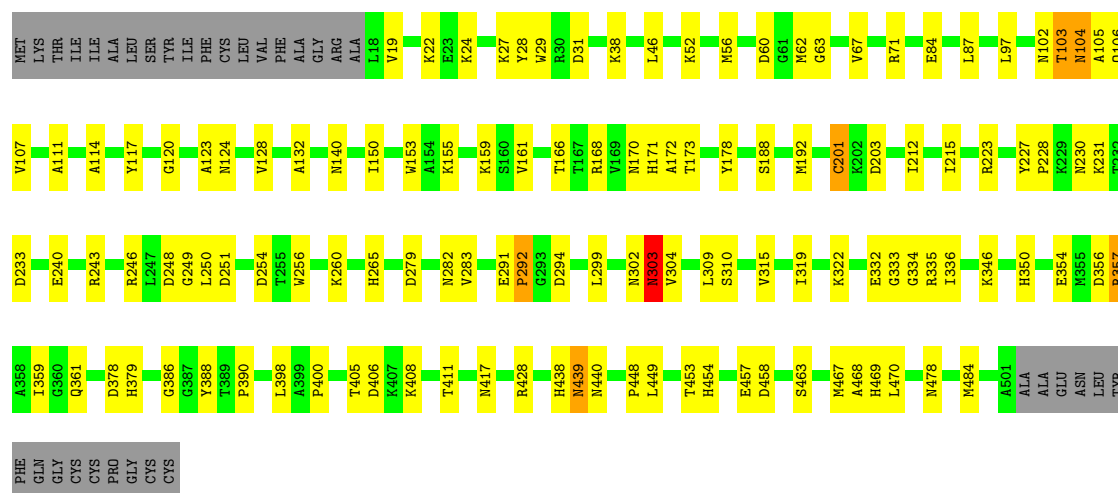


- Molecule 1: Alkaline phosphatase, tissue-nonspecific isozyme



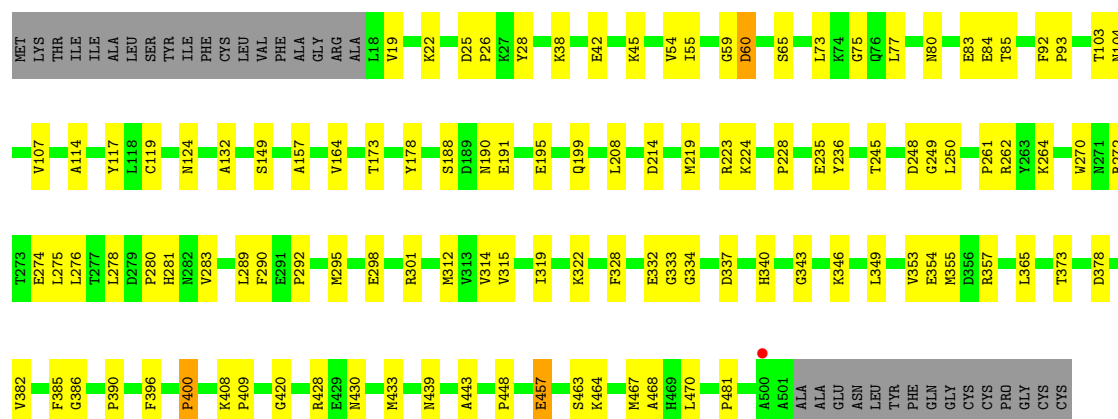
- Molecule 1: Alkaline phosphatase, tissue-nonspecific isozyme

Chain C:



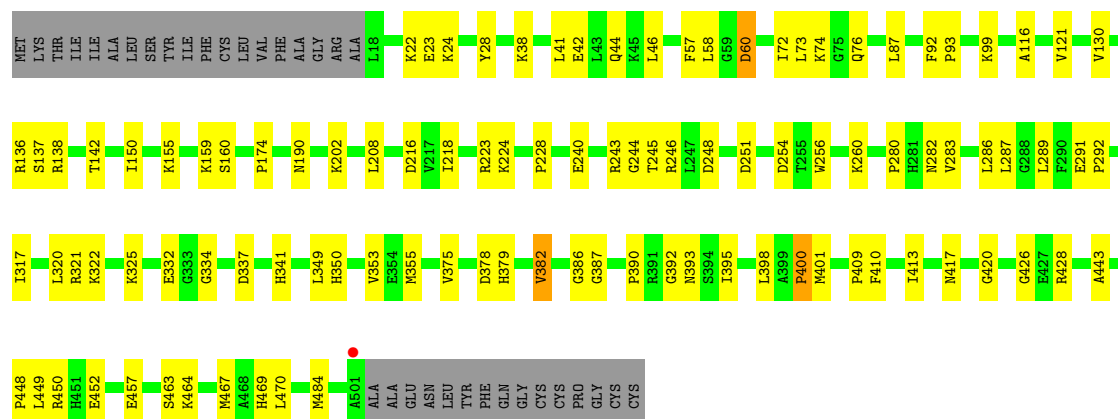
- Molecule 1: Alkaline phosphatase, tissue-nonspecific isozyme

Chain B:



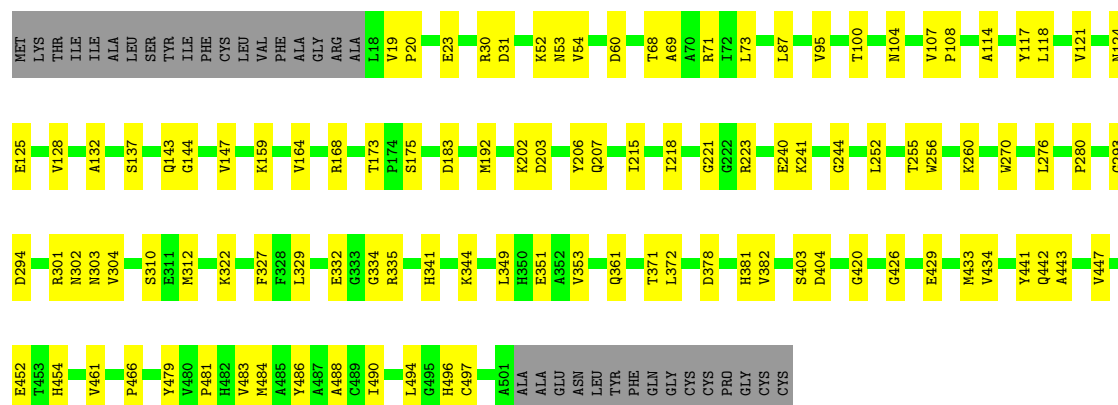
- Molecule 1: Alkaline phosphatase, tissue-nonspecific isozyme

Chain G:



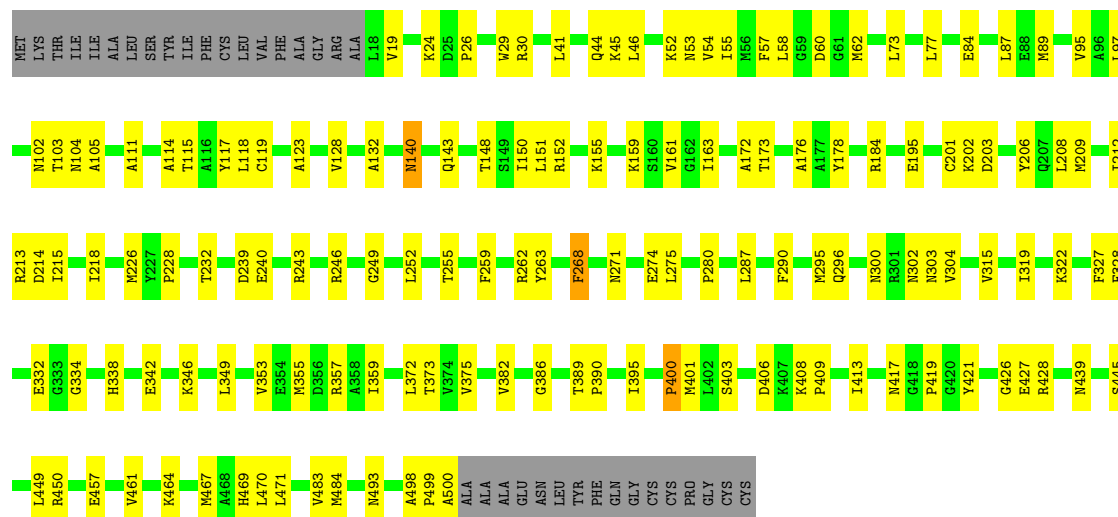
- Molecule 1: Alkaline phosphatase, tissue-nonspecific isozyme

Chain H:  73% 20% 7%



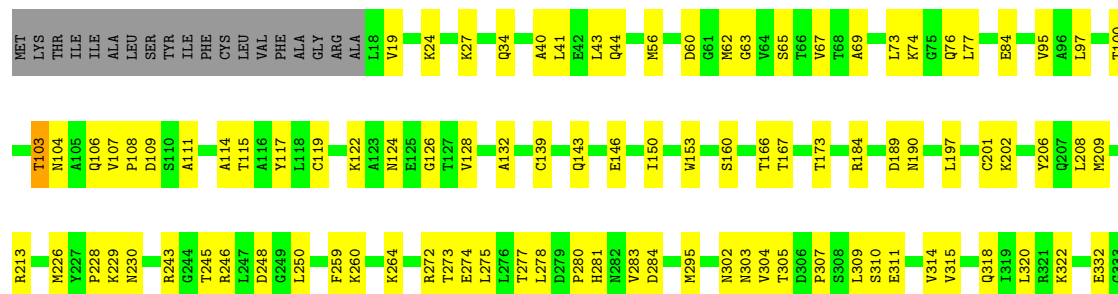
- Molecule 1: Alkaline phosphatase, tissue-nonspecific isozyme

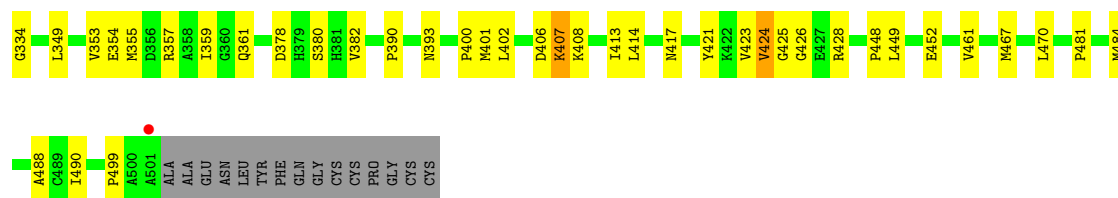
Chain F:  66% 27% 7%



- Molecule 1: Alkaline phosphatase, tissue-nonspecific isozyme

Chain E:  68% 25% 7%





- Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain I: 100%

MAG1
MAG2

- Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain J: 50% 50%

MAG1
MAG2

- Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain K: 100%

MAG1
MAG2

- Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain L: 50% 50%

MAG1
MAG2

- Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain M: 50% 50%

MAG1
MAG2

- Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain N: 50% 50%



- Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain O:  100%



- Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain P:  100%



- Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain Q:  100%



- Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain R:  50% 50%



- Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain S:  100%



- Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain T:  50% 50%



- Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain U:  100%

MAG1
MAG2

- Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain V:  50% 50%

MAG1
MAG2

- Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain W:  50% 50%

MAG1
MAG2

- Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain X:  100%

MAG1
MAG2

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	158.62Å 167.35Å 188.78Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	25.05 – 3.18 25.05 – 3.18	Depositor EDS
% Data completeness (in resolution range)	98.6 (25.05-3.18) 98.7 (25.05-3.18)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.28 (at 3.17Å)	Xtriage
Refinement program	PHENIX 1.19.2_4158	Depositor
R, R_{free}	0.172 , 0.234 0.174 , 0.233	Depositor DCC
R_{free} test set	1996 reflections (2.34%)	wwPDB-VP
Wilson B-factor (Å ²)	70.3	Xtriage
Anisotropy	0.464	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 27.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	30673	wwPDB-VP
Average B, all atoms (Å ²)	68.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.25% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: CA, NAG, ZN, MG

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	0.52	0/3834	0.80	3/5201 (0.1%)
1	B	0.54	0/3834	0.80	0/5201
1	C	0.54	0/3834	0.78	3/5201 (0.1%)
1	D	0.50	0/3824	0.77	0/5187
1	E	0.47	0/3834	0.75	4/5201 (0.1%)
1	F	0.46	1/3829 (0.0%)	0.72	0/5194
1	G	0.49	0/3834	0.76	2/5201 (0.0%)
1	H	0.44	0/3834	0.73	1/5201 (0.0%)
All	All	0.50	1/30657 (0.0%)	0.76	13/41587 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	C	0	1
1	D	0	1
1	E	0	1
1	H	0	1
All	All	0	4

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	140	ASN	CA-C	5.20	1.59	1.52

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	103	THR	CA-C-N	6.47	133.67	122.09
1	C	103	THR	C-N-CA	6.47	133.67	122.09
1	E	401	MET	CA-CB-CG	6.21	126.53	114.10
1	E	139	CYS	CA-C-N	-5.48	111.06	121.54
1	E	139	CYS	C-N-CA	-5.48	111.06	121.54
1	A	400	PRO	CA-C-N	-5.48	113.61	122.82
1	A	400	PRO	C-N-CA	-5.48	113.61	122.82
1	E	401	MET	CB-CG-SD	5.32	128.67	112.70
1	G	401	MET	CA-CB-CG	5.29	124.68	114.10
1	H	304	VAL	N-CA-C	-5.16	106.63	111.48
1	G	401	MET	CB-CG-SD	5.15	128.14	112.70
1	C	357	ARG	CG-CD-NE	-5.15	100.68	112.00
1	A	401	MET	CA-CB-CG	5.12	124.33	114.10

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	104	ASN	Peptide
1	D	152	ARG	Sidechain
1	E	103	THR	Peptide
1	H	433	MET	Peptide

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3748	0	3628	86	0
1	B	3748	0	3629	83	0
1	C	3748	0	3629	83	0
1	D	3738	0	3619	75	0
1	E	3748	0	3628	93	0
1	F	3743	0	3624	101	0
1	G	3748	0	3628	67	0
1	H	3748	0	3629	73	0
2	I	28	0	25	0	0
2	J	28	0	25	0	0
2	K	28	0	25	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	L	28	0	25	2	0
2	M	28	0	25	0	0
2	N	28	0	25	1	0
2	O	28	0	25	2	0
2	P	28	0	25	1	0
2	Q	28	0	25	1	0
2	R	28	0	25	0	0
2	S	28	0	25	0	0
2	T	28	0	25	0	0
2	U	28	0	25	1	0
2	V	28	0	25	1	0
2	W	28	0	25	2	0
2	X	28	0	25	1	0
3	A	28	0	26	0	0
3	B	28	0	26	2	0
3	C	28	0	26	1	0
3	D	28	0	26	0	0
3	E	28	0	26	1	0
3	F	28	0	26	1	0
3	G	28	0	26	0	0
3	H	28	0	26	1	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
4	E	1	0	0	0	0
4	F	1	0	0	0	0
4	G	1	0	0	0	0
4	H	1	0	0	0	0
5	A	2	0	0	0	0
5	B	2	0	0	0	0
5	C	2	0	0	0	0
5	D	2	0	0	1	0
5	E	2	0	0	0	0
5	F	2	0	0	0	0
5	G	2	0	0	0	0
5	H	2	0	0	0	0
6	A	1	0	0	0	0
6	B	1	0	0	0	0
6	C	1	0	0	0	0
6	D	1	0	0	0	0
6	E	1	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	F	1	0	0	0	0
6	G	1	0	0	0	0
6	H	1	0	0	0	0
All	All	30673	0	29622	615	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 10.

All (615) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:246:ARG:HH11	1:F:252:LEU:HD11	1.23	1.02
1:D:275:LEU:HD11	1:D:315:VAL:HG21	1.43	0.99
1:B:59:GLY:HA2	1:B:355:MET:HE1	1.55	0.86
1:G:60:ASP:HB2	1:G:334:GLY:HA2	1.57	0.86
1:B:54:VAL:HG23	1:B:328:PHE:HD1	1.41	0.86
1:B:275:LEU:HD11	1:B:315:VAL:HG21	1.57	0.84
1:C:56:MET:HE2	1:C:484:MET:HE1	1.59	0.84
1:B:333:GLY:HA3	1:B:355:MET:HE2	1.60	0.82
1:A:107:VAL:HG21	1:B:386:GLY:HA2	1.62	0.81
1:A:314:VAL:HG13	1:A:365:LEU:HD11	1.64	0.79
1:H:173:THR:HG21	1:H:332:GLU:HG3	1.64	0.78
1:G:246:ARG:NH2	1:G:248:ASP:OD2	2.16	0.78
1:E:246:ARG:NH2	1:E:248:ASP:OD2	2.15	0.77
1:D:41:LEU:O	1:D:44:GLN:HG3	1.85	0.76
1:A:310:SER:O	1:A:314:VAL:HG23	1.86	0.76
1:F:87:LEU:HD13	1:F:89:MET:HE3	1.68	0.76
1:D:132:ALA:HB3	1:C:24:LYS:HA	1.69	0.75
1:A:195:GLU:HA	1:A:198:SER:HB3	1.69	0.74
1:B:346:LYS:HD3	1:B:439:ASN:HA	1.67	0.74
1:F:390:PRO:HD3	1:F:400:PRO:HG3	1.71	0.73
1:E:248:ASP:HB3	1:E:250:LEU:HG	1.70	0.73
1:G:450:ARG:H	1:H:404:ASP:HB2	1.52	0.72
1:D:45:LYS:HE2	1:B:276:LEU:O	1.90	0.72
1:F:246:ARG:NH1	1:F:252:LEU:HD11	2.03	0.71
1:B:467:MET:HE3	1:B:470:LEU:HD11	1.71	0.71
1:H:104:ASN:HB2	1:H:124:ASN:HA	1.72	0.71
1:F:409:PRO:O	1:F:428:ARG:NH2	2.23	0.71
1:F:386:GLY:HA2	1:E:107:VAL:HG21	1.72	0.70
1:E:423:VAL:HA	1:E:428:ARG:HA	1.74	0.70
1:G:24:LYS:HA	1:H:132:ALA:HB3	1.72	0.70

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:268:PHE:HD1	1:F:287:LEU:HD12	1.58	0.69
1:E:390:PRO:HD3	1:E:400:PRO:HG3	1.75	0.69
1:C:60:ASP:OD2	1:C:332:GLU:OE2	2.10	0.69
1:F:406:ASP:OD2	1:F:428:ARG:NH1	2.25	0.69
1:A:230:ASN:OD1	1:A:243:ARG:NH1	2.26	0.68
1:G:448:PRO:O	1:H:403:SER:OG	2.11	0.68
1:B:59:GLY:CA	1:B:355:MET:HE1	2.24	0.68
1:E:208:LEU:HD23	1:E:226:MET:HE1	1.75	0.68
1:G:22:LYS:HD2	1:G:28:TYR:CE1	2.29	0.67
1:E:209:MET:HE2	1:E:226:MET:HE3	1.76	0.67
1:B:430:ASN:ND2	1:B:433:MET:HE2	2.09	0.67
1:B:173:THR:HG21	1:B:332:GLU:HG3	1.76	0.67
1:G:150:ILE:HD13	1:G:484:MET:HE3	1.76	0.66
1:C:390:PRO:HD3	1:C:400:PRO:HG3	1.76	0.66
1:H:486:TYR:CE2	1:H:496:HIS:HB2	2.30	0.66
1:B:60:ASP:OD2	1:B:332:GLU:OE2	2.14	0.66
1:A:252:LEU:HA	1:A:255:THR:HB	1.78	0.66
1:G:160:SER:HB3	1:G:320:LEU:HD22	1.78	0.66
1:F:240:GLU:HG2	1:F:243:ARG:NH2	2.11	0.66
1:C:346:LYS:HD3	1:C:439:ASN:HA	1.78	0.65
1:C:463:SER:HB3	1:C:468:ALA:HB1	1.79	0.65
1:G:155:LYS:NZ	1:G:216:ASP:OD1	2.29	0.65
1:C:240:GLU:O	1:C:243:ARG:HG3	1.97	0.64
1:B:390:PRO:HD3	1:B:400:PRO:HG3	1.80	0.64
1:A:248:ASP:HB3	1:A:250:LEU:HD23	1.79	0.64
1:B:38:LYS:O	1:B:42:GLU:HG3	1.97	0.64
1:E:417:ASN:HB2	1:E:449:LEU:HD12	1.79	0.64
1:D:337:ASP:OD2	5:D:604:ZN:ZN	1.46	0.64
1:G:337:ASP:OD2	1:G:341:HIS:CD2	2.50	0.64
1:B:409:PRO:O	1:B:428:ARG:NH2	2.30	0.64
1:H:20:PRO:HB2	1:H:23:GLU:HG3	1.79	0.64
1:E:60:ASP:HB2	1:E:334:GLY:HA2	1.80	0.63
1:A:126:GLY:HA3	1:A:136:ARG:HD2	1.79	0.63
1:H:344:LYS:HG2	1:H:442:GLN:HG2	1.79	0.63
1:E:228:PRO:HA	1:E:246:ARG:HB2	1.80	0.63
1:E:74:LYS:HD2	1:E:353:VAL:HG13	1.79	0.63
1:H:137:SER:OG	1:H:183:ASP:OD2	2.12	0.63
1:F:403:SER:OG	1:E:448:PRO:O	2.16	0.63
1:A:356:ASP:HA	1:A:359:ILE:HD12	1.81	0.62
1:A:256:TRP:CD1	1:A:260:LYS:HZ1	2.18	0.62
1:E:114:ALA:HA	1:E:117:TYR:CZ	2.34	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:54:VAL:HG23	1:B:328:PHE:CD1	2.31	0.62
1:G:57:PHE:HB3	1:G:355:MET:HE3	1.80	0.62
1:C:155:LYS:HG2	1:C:212:ILE:HD11	1.82	0.62
1:A:60:ASP:HB2	1:A:334:GLY:HA2	1.80	0.62
1:F:102:ASN:HB2	1:F:105:ALA:HB3	1.80	0.62
1:F:408:LYS:NZ	1:F:427:GLU:HG3	2.15	0.61
1:E:281:HIS:HA	1:E:322:LYS:HE2	1.81	0.61
1:G:57:PHE:HB2	1:G:375:VAL:HG22	1.81	0.61
1:A:390:PRO:HD3	1:A:400:PRO:HG3	1.82	0.61
1:G:60:ASP:HB3	1:G:337:ASP:HB2	1.82	0.61
1:F:52:LYS:O	1:F:159:LYS:NZ	2.32	0.61
2:Q:1:NAG:H61	2:Q:2:NAG:N2	2.16	0.61
1:B:420:GLY:HA3	1:B:443:ALA:O	2.01	0.60
1:E:202:LYS:HB3	1:E:206:TYR:CD1	2.36	0.60
1:D:137:SER:OG	1:D:183:ASP:OD2	2.19	0.60
1:H:280:PRO:O	1:H:322:LYS:HE2	2.01	0.60
1:D:390:PRO:HD3	1:D:400:PRO:HG3	1.82	0.60
1:D:224:LYS:HG2	1:D:292:PRO:O	2.02	0.60
1:C:166:THR:HG23	1:C:309:LEU:HD13	1.84	0.60
1:G:409:PRO:O	1:G:428:ARG:NH2	2.35	0.60
1:C:103:THR:HG21	1:C:132:ALA:HB2	1.84	0.60
1:G:390:PRO:HD3	1:G:400:PRO:HG3	1.83	0.59
1:E:488:ALA:HB3	1:E:490:ILE:HG12	1.84	0.59
1:H:52:LYS:O	1:H:159:LYS:HE3	2.03	0.59
1:E:408:LYS:HG2	2:X:1:NAG:H82	1.85	0.59
1:A:104:ASN:HB2	1:A:124:ASN:HA	1.85	0.59
1:F:115:THR:O	1:F:119:CYS:HB2	2.03	0.59
1:H:192:MET:CE	1:H:203:ASP:HB3	2.33	0.59
1:H:341:HIS:CE1	1:H:454:HIS:HE2	2.19	0.59
1:C:228:PRO:HB3	1:C:249:GLY:HA2	1.85	0.58
1:B:104:ASN:HB2	1:B:124:ASN:HA	1.85	0.58
1:F:152:ARG:HB2	1:F:212:ILE:HD11	1.85	0.58
1:E:274:GLU:OE2	2:W:1:NAG:H62	2.04	0.58
1:A:60:ASP:HB3	1:A:337:ASP:HB2	1.84	0.58
1:A:342:GLU:O	1:A:442:GLN:NE2	2.36	0.58
1:E:355:MET:O	1:E:359:ILE:HG13	2.03	0.58
1:C:102:ASN:HB2	1:C:105:ALA:HB3	1.85	0.58
1:F:226:MET:HA	1:F:252:LEU:HD12	1.85	0.58
3:H:602:NAG:O7	3:H:602:NAG:O3	2.18	0.58
1:F:57:PHE:HB3	1:F:355:MET:HE3	1.86	0.58
1:A:106:GLN:HB2	1:B:83:GLU:OE2	2.03	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:337:ASP:OD2	1:D:341:HIS:NE2	2.36	0.57
1:D:103:THR:HG22	1:C:19:VAL:HG22	1.86	0.57
1:F:262:ARG:NH1	1:F:263:TYR:OH	2.37	0.57
1:E:229:LYS:HD2	1:E:245:THR:HA	1.85	0.57
1:A:299:LEU:HD13	1:A:439:ASN:ND2	2.20	0.57
1:F:97:LEU:HG	1:E:95:VAL:HG11	1.86	0.57
1:G:228:PRO:HA	1:G:246:ARG:HB2	1.85	0.57
1:H:335:ARG:HB2	1:H:351:GLU:OE1	2.05	0.57
1:C:104:ASN:ND2	1:C:124:ASN:HB3	2.19	0.56
1:F:240:GLU:HG2	1:F:243:ARG:CZ	2.35	0.56
1:A:246:ARG:NH2	1:A:248:ASP:OD2	2.37	0.56
1:C:256:TRP:CD1	1:C:260:LYS:HZ3	2.24	0.56
1:H:53:ASN:HB2	1:H:371:THR:HG23	1.88	0.56
1:H:164:VAL:HG23	1:H:329:LEU:HD11	1.87	0.56
1:E:143:GLN:HA	1:E:146:GLU:OE2	2.06	0.56
1:G:256:TRP:CD1	1:G:260:LYS:HZ3	2.24	0.55
1:D:448:PRO:HB2	1:C:405:THR:HG21	1.89	0.55
1:G:130:VAL:HG11	1:G:142:THR:HG23	1.88	0.55
1:C:291:GLU:HG3	1:C:292:PRO:HD2	1.88	0.55
1:H:276:LEU:O	1:F:45:LYS:HE2	2.07	0.55
1:A:343:GLY:O	1:A:442:GLN:HA	2.06	0.55
1:H:486:TYR:CZ	1:H:496:HIS:HB2	2.42	0.55
1:A:190:ASN:HB2	1:A:245:THR:O	2.06	0.55
1:E:104:ASN:HB2	1:E:124:ASN:HA	1.89	0.55
1:C:265:HIS:ND1	1:C:282:ASN:OD1	2.40	0.55
1:C:467:MET:HA	1:C:469:HIS:CE1	2.41	0.55
1:B:22:LYS:HE3	1:B:28:TYR:CZ	2.42	0.55
1:G:38:LYS:O	1:G:42:GLU:HG3	2.06	0.54
1:F:268:PHE:HA	1:F:287:LEU:O	2.07	0.54
1:C:223:ARG:NH1	1:C:233:ASP:OD2	2.41	0.54
1:B:54:VAL:CG2	1:B:328:PHE:HD1	2.18	0.54
1:B:223:ARG:HD3	1:B:289:LEU:O	2.07	0.54
1:D:228:PRO:HA	1:D:246:ARG:HB2	1.90	0.54
2:N:1:NAG:H61	2:N:2:NAG:HN2	1.73	0.54
1:E:481:PRO:HA	1:E:484:MET:HE2	1.89	0.54
1:A:207:GLN:HB3	1:A:211:ASN:ND2	2.23	0.54
1:A:275:LEU:HD12	1:A:290:PHE:CZ	2.43	0.54
1:H:429:GLU:OE2	1:H:434:VAL:HG11	2.07	0.54
1:C:170:ASN:HA	1:C:178:TYR:OH	2.07	0.54
1:A:433:MET:HB2	1:A:434:VAL:HG13	1.90	0.53
1:H:341:HIS:CE1	1:H:454:HIS:NE2	2.75	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:346:LYS:HD3	1:F:439:ASN:HA	1.89	0.53
1:G:76:GLN:NE2	1:G:393:ASN:O	2.40	0.53
1:F:232:THR:HA	1:F:243:ARG:HG2	1.90	0.53
1:F:493:ASN:ND2	1:E:34:GLN:OE1	2.32	0.53
1:E:150:ILE:HA	1:E:153:TRP:CE3	2.43	0.53
1:A:55:ILE:HB	1:A:373:THR:HG23	1.89	0.53
1:C:188:SER:HA	1:C:203:ASP:OD2	2.09	0.53
1:G:190:ASN:HB2	1:G:245:THR:O	2.09	0.53
1:D:24:LYS:HA	1:C:132:ALA:HB3	1.91	0.53
1:D:493:ASN:HD21	1:C:38:LYS:NZ	2.07	0.53
1:B:275:LEU:HD11	1:B:315:VAL:CG2	2.34	0.53
1:B:114:ALA:HA	1:B:117:TYR:CZ	2.43	0.53
1:F:60:ASP:HB2	1:F:334:GLY:HA2	1.91	0.53
1:H:488:ALA:O	1:H:490:ILE:HG23	2.08	0.53
1:E:173:THR:HG21	1:E:332:GLU:HG3	1.91	0.53
1:E:273:THR:O	1:E:277:THR:N	2.41	0.53
1:E:424:VAL:HG23	1:E:425:GLY:H	1.74	0.53
1:E:230:ASN:HA	1:E:243:ARG:HB3	1.91	0.53
1:H:240:GLU:HG3	1:H:241:LYS:N	2.23	0.53
1:A:335:ARG:HB2	1:A:351:GLU:OE1	2.09	0.52
1:B:340:HIS:O	1:B:343:GLY:N	2.41	0.52
1:H:121:VAL:HG21	1:H:147:VAL:HG11	1.92	0.52
1:F:173:THR:HB	1:F:332:GLU:OE2	2.08	0.52
1:A:228:PRO:HB3	1:A:249:GLY:HA2	1.91	0.52
1:D:228:PRO:HD3	1:D:250:LEU:O	2.09	0.52
1:F:148:THR:HB	1:F:152:ARG:HG2	1.90	0.52
1:G:72:ILE:O	1:G:76:GLN:HG3	2.10	0.52
1:C:406:ASP:O	1:C:408:LYS:HG3	2.09	0.52
1:C:467:MET:HB3	1:C:470:LEU:HD22	1.92	0.52
1:F:215:ILE:HB	1:F:218:ILE:HD11	1.92	0.52
1:F:419:PRO:HG3	1:F:450:ARG:O	2.10	0.52
1:A:223:ARG:HD2	1:A:233:ASP:OD1	2.09	0.52
1:E:275:LEU:HG	1:E:315:VAL:HG21	1.92	0.52
1:C:319:ILE:O	1:C:322:LYS:HD3	2.10	0.52
1:G:417:ASN:HB2	1:G:449:LEU:HD12	1.92	0.52
1:D:467:MET:HE3	1:D:470:LEU:HD11	1.92	0.52
1:G:92:PHE:CZ	1:G:464:LYS:HE2	2.44	0.52
1:B:103:THR:HG21	1:B:132:ALA:HB1	1.92	0.51
1:H:143:GLN:HG2	1:H:144:GLY:N	2.26	0.51
1:E:166:THR:HG23	1:E:309:LEU:HD13	1.93	0.51
1:E:274:GLU:O	1:E:278:LEU:HG	2.10	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:60:ASP:HB2	1:D:334:GLY:HA2	1.92	0.51
1:C:71:ARG:HA	1:C:87:LEU:HD21	1.91	0.51
1:B:274:GLU:OE2	2:O:1:NAG:H62	2.09	0.51
1:H:69:ALA:HB1	1:H:349:LEU:HD21	1.93	0.51
1:D:107:VAL:HB	1:C:388:TYR:HA	1.93	0.51
1:C:192:MET:HE1	1:C:201:CYS:O	2.11	0.51
1:F:498:ALA:O	1:F:500:ALA:N	2.43	0.51
1:B:349:LEU:O	1:B:353:VAL:HG23	2.11	0.51
1:F:54:VAL:CG1	1:F:484:MET:HE3	2.41	0.51
1:E:150:ILE:HD13	1:E:484:MET:HE3	1.93	0.51
1:D:408:LYS:HG3	2:L:1:NAG:H82	1.92	0.51
1:G:349:LEU:O	1:G:353:VAL:HG23	2.10	0.51
1:A:267:HIS:O	1:A:268:PHE:HB3	2.10	0.51
1:D:116:ALA:O	1:D:478:ASN:HA	2.11	0.51
1:A:229:LYS:HD2	1:A:245:THR:HA	1.93	0.51
1:A:390:PRO:O	1:A:393:ASN:HB2	2.10	0.51
1:G:46:LEU:HB3	1:G:469:HIS:CE1	2.45	0.51
1:F:58:LEU:HD22	1:F:117:TYR:CE1	2.46	0.51
1:F:203:ASP:OD1	1:F:203:ASP:N	2.42	0.51
1:A:60:ASP:HB3	1:A:337:ASP:CB	2.41	0.50
1:C:140:ASN:N	1:C:140:ASN:OD1	2.44	0.50
1:C:168:ARG:HB2	1:C:171:HIS:HB2	1.93	0.50
1:C:408:LYS:O	1:C:428:ARG:NH2	2.44	0.50
1:G:223:ARG:HA	1:G:289:LEU:HD23	1.92	0.50
1:D:49:ASN:OD1	1:B:281:HIS:NE2	2.45	0.50
1:C:356:ASP:HA	1:C:359:ILE:HD12	1.93	0.50
1:D:425:GLY:C	1:D:427:GLU:H	2.19	0.50
1:C:103:THR:HG22	1:C:123:ALA:C	2.35	0.50
1:B:157:ALA:HA	1:F:213:ARG:NH1	2.26	0.50
1:B:261:PRO:HG2	1:B:264:LYS:HG2	1.92	0.50
1:B:195:GLU:O	1:B:199:GLN:HG3	2.11	0.50
1:H:223:ARG:HH11	1:H:270:TRP:HB2	1.75	0.50
1:F:228:PRO:HA	1:F:246:ARG:HB2	1.93	0.50
1:F:395:ILE:HG13	1:F:413:ILE:HD11	1.92	0.50
1:E:69:ALA:HB1	1:E:349:LEU:HD21	1.94	0.50
1:E:84:GLU:CD	1:E:84:GLU:H	2.19	0.50
1:E:314:VAL:O	1:E:318:GLN:HG3	2.12	0.50
1:D:107:VAL:HG21	1:C:386:GLY:HA2	1.93	0.50
1:D:275:LEU:HD11	1:D:315:VAL:CG2	2.29	0.50
1:B:235:GLU:HB3	1:B:236:TYR:CD1	2.46	0.50
3:B:601:NAG:O7	3:B:601:NAG:O3	2.26	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:202:LYS:HD3	1:H:206:TYR:CE1	2.46	0.50
2:U:1:NAG:H61	2:U:2:NAG:N2	2.27	0.50
1:A:62:MET:HE3	1:A:67:VAL:CG1	2.42	0.50
1:A:193:PRO:HD2	1:A:196:ALA:HB3	1.93	0.50
1:F:41:LEU:HD23	1:E:470:LEU:HD21	1.94	0.50
1:F:319:ILE:O	1:F:322:LYS:HG3	2.12	0.50
1:B:119:CYS:HA	1:B:149:SER:HA	1.93	0.50
1:B:408:LYS:HG3	2:P:1:NAG:H82	1.94	0.50
1:H:420:GLY:HA3	1:H:443:ALA:O	2.12	0.49
1:F:114:ALA:HA	1:F:117:TYR:CZ	2.47	0.49
1:B:228:PRO:HB3	1:B:249:GLY:HA2	1.93	0.49
1:G:410:PHE:HB2	1:H:447:VAL:HG21	1.94	0.49
1:E:305:THR:HG22	2:W:1:NAG:H81	1.93	0.49
1:D:68:THR:HG21	1:C:457:GLU:HA	1.94	0.49
1:H:95:VAL:HA	1:H:461:VAL:O	2.12	0.49
1:C:63:GLY:O	1:C:67:VAL:HG13	2.13	0.49
1:H:54:VAL:CG1	1:H:484:MET:HE3	2.43	0.49
1:H:168:ARG:HG3	1:H:168:ARG:HH11	1.77	0.49
1:F:155:LYS:HE2	1:F:159:LYS:O	2.13	0.49
1:E:264:LYS:HD2	1:E:284:ASP:OD2	2.12	0.49
1:D:275:LEU:CD1	1:D:315:VAL:HG21	2.30	0.49
1:B:319:ILE:O	1:B:322:LYS:HD3	2.13	0.49
1:A:115:THR:O	1:A:119:CYS:HB2	2.12	0.49
1:F:29:TRP:CZ3	1:E:122:LYS:HD2	2.48	0.49
1:F:151:LEU:HD13	1:F:163:ILE:HD11	1.94	0.49
1:A:218:ILE:HB	1:A:287:LEU:HD12	1.94	0.49
1:F:290:PHE:HB2	1:F:295:MET:HE3	1.94	0.49
1:C:161:VAL:HG23	1:C:215:ILE:HG23	1.95	0.49
1:B:290:PHE:HB2	1:B:295:MET:HE3	1.95	0.49
1:G:280:PRO:C	1:G:282:ASN:H	2.21	0.49
1:H:117:TYR:HE2	1:H:378:ASP:HB3	1.78	0.49
1:F:29:TRP:CH2	1:E:122:LYS:HD2	2.48	0.49
1:F:46:LEU:HD13	1:E:44:GLN:HG2	1.95	0.49
1:D:335:ARG:HB2	1:D:351:GLU:OE1	2.12	0.48
1:C:60:ASP:O	1:C:336:ILE:HB	2.13	0.48
1:F:19:VAL:HG13	1:E:103:THR:CG2	2.43	0.48
1:A:279:ASP:O	1:A:283:VAL:HG23	2.14	0.48
1:H:256:TRP:CD1	1:H:260:LYS:HZ3	2.31	0.48
1:E:63:GLY:HA3	1:E:380:SER:OG	2.13	0.48
1:E:402:LEU:HD13	1:E:407:LYS:O	2.13	0.48
1:C:315:VAL:O	1:C:319:ILE:HG13	2.13	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:99:LYS:HG2	1:H:71:ARG:NH1	2.28	0.48
1:H:203:ASP:O	1:H:207:GLN:HG3	2.13	0.48
1:F:172:ALA:HB2	1:F:184:ARG:CZ	2.43	0.48
1:F:209:MET:HG3	1:F:252:LEU:HB3	1.95	0.48
1:A:421:TYR:HB3	1:A:448:PRO:HB3	1.96	0.48
1:B:333:GLY:CA	1:B:355:MET:HE2	2.37	0.48
1:F:467:MET:HE3	1:F:470:LEU:HD11	1.95	0.48
1:A:117:TYR:CE2	1:A:378:ASP:HB3	2.49	0.48
1:B:73:LEU:O	1:B:77:LEU:HG	2.14	0.48
1:A:158:GLY:HA3	1:A:325:LYS:HD2	1.96	0.48
1:F:132:ALA:HB3	1:E:24:LYS:HA	1.95	0.48
1:G:240:GLU:O	1:G:243:ARG:HG3	2.13	0.48
1:H:71:ARG:HA	1:H:87:LEU:HD21	1.95	0.48
1:B:262:ARG:NH1	1:E:27:LYS:HD3	2.28	0.48
1:H:73:LEU:HD22	1:H:349:LEU:HB3	1.96	0.48
1:F:55:ILE:O	1:F:373:THR:HA	2.14	0.48
1:F:150:ILE:HD13	1:F:484:MET:HE2	1.96	0.48
1:E:190:ASN:HB2	1:E:245:THR:O	2.13	0.48
1:D:262:ARG:HG3	1:H:497:CYS:HA	1.96	0.47
1:C:52:LYS:O	1:C:159:LYS:HE3	2.13	0.47
1:C:332:GLU:HG2	1:C:334:GLY:N	2.29	0.47
1:B:214:ASP:OD1	1:B:214:ASP:N	2.44	0.47
1:A:203:ASP:O	1:A:207:GLN:HG3	2.14	0.47
1:D:22:LYS:NZ	1:B:80:ASN:OD1	2.47	0.47
1:C:248:ASP:HB3	1:C:250:LEU:H	1.79	0.47
1:H:104:ASN:ND2	1:H:124:ASN:HB3	2.29	0.47
1:H:301:ARG:HG2	1:H:302:ASN:N	2.28	0.47
1:D:150:ILE:HA	1:D:153:TRP:CE3	2.50	0.47
1:G:159:LYS:HE3	1:G:325:LYS:O	2.15	0.47
1:H:117:TYR:HA	1:H:481:PRO:HD3	1.96	0.47
1:H:117:TYR:CE2	1:H:378:ASP:HB3	2.49	0.47
1:F:353:VAL:O	1:F:357:ARG:HG2	2.14	0.47
1:E:167:THR:HG23	1:E:334:GLY:HA3	1.96	0.47
1:C:104:ASN:HB2	1:C:124:ASN:HA	1.97	0.47
1:C:228:PRO:HA	1:C:246:ARG:HB2	1.97	0.47
1:B:164:VAL:CG1	1:B:312:MET:HE3	2.44	0.47
1:H:60:ASP:HB2	1:H:334:GLY:HA2	1.97	0.47
1:H:479:TYR:O	1:H:483:VAL:HG23	2.15	0.47
1:F:173:THR:HG21	1:F:332:GLU:HG3	1.95	0.47
1:F:214:ASP:OD1	1:F:214:ASP:N	2.48	0.47
1:H:100:THR:O	1:H:108:PRO:HG3	2.15	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:255:THR:HG22	1:F:259:PHE:CE2	2.50	0.47
1:E:189:ASP:HB2	1:E:197:LEU:HD21	1.97	0.47
1:A:189:ASP:HB2	1:A:197:LEU:HD21	1.97	0.47
1:D:126:GLY:HA3	1:D:136:ARG:HD2	1.96	0.47
1:C:97:LEU:HD23	1:C:97:LEU:HA	1.74	0.47
1:C:303:ASN:HD22	3:C:602:NAG:C7	2.27	0.47
1:F:103:THR:HG21	1:F:132:ALA:HB2	1.96	0.47
1:A:103:THR:CG2	1:B:19:VAL:HG13	2.45	0.47
1:A:117:TYR:HE2	1:A:378:ASP:HB3	1.80	0.47
1:C:22:LYS:HD2	1:C:28:TYR:CE1	2.50	0.47
1:B:224:LYS:HG2	1:B:292:PRO:O	2.15	0.47
1:G:426:GLY:CA	1:H:426:GLY:HA2	2.45	0.47
1:H:168:ARG:HG3	1:H:294:ASP:OD1	2.14	0.47
1:E:413:ILE:O	1:E:414:LEU:HD23	2.15	0.47
1:A:341:HIS:ND1	1:A:452:GLU:O	2.46	0.46
1:A:456:GLY:HA3	1:B:385:PHE:CZ	2.50	0.46
1:C:279:ASP:O	1:C:283:VAL:HG23	2.15	0.46
1:B:275:LEU:CD1	1:B:315:VAL:HG21	2.37	0.46
1:B:346:LYS:HG3	1:B:396:PHE:CZ	2.50	0.46
1:G:286:LEU:HD12	1:G:287:LEU:H	1.80	0.46
1:A:92:PHE:CE1	1:A:464:LYS:HE2	2.50	0.46
1:B:84:GLU:CD	1:B:84:GLU:H	2.23	0.46
1:G:150:ILE:HD13	1:G:484:MET:CE	2.42	0.46
1:H:128:VAL:HG11	1:H:175:SER:OG	2.15	0.46
1:E:160:SER:HB3	1:E:320:LEU:CD2	2.45	0.46
1:A:23:GLU:HG2	1:A:28:TYR:CE2	2.51	0.46
1:A:151:LEU:HD13	1:A:177:ALA:HB1	1.96	0.46
1:G:420:GLY:HA3	1:G:443:ALA:O	2.15	0.46
1:D:122:LYS:HB2	1:C:29:TRP:CE2	2.50	0.46
1:A:214:ASP:OD1	1:A:214:ASP:N	2.44	0.46
1:G:41:LEU:O	1:G:44:GLN:HB2	2.15	0.46
1:E:354:GLU:OE1	1:E:357:ARG:HD2	2.16	0.46
1:B:235:GLU:HG3	1:B:270:TRP:HZ3	1.81	0.46
1:G:283:VAL:O	1:G:322:LYS:NZ	2.48	0.46
1:F:228:PRO:HB3	1:F:249:GLY:HA2	1.98	0.46
1:A:240:GLU:O	1:A:243:ARG:HG3	2.16	0.46
1:D:51:ALA:HB3	1:D:488:ALA:HA	1.97	0.46
1:C:150:ILE:HA	1:C:153:TRP:CE3	2.50	0.46
1:E:378:ASP:N	1:E:378:ASP:OD1	2.42	0.46
1:C:27:LYS:HD3	1:C:31:ASP:OD2	2.15	0.46
1:F:53:ASN:HD22	1:F:327:PHE:H	1.64	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:77:LEU:HD23	1:D:77:LEU:HA	1.73	0.46
1:C:379:HIS:CE1	1:C:454:HIS:CD2	3.04	0.46
1:B:60:ASP:CB	1:B:334:GLY:HA2	2.45	0.46
1:F:58:LEU:HD23	1:F:173:THR:HG21	1.98	0.46
1:E:160:SER:HB3	1:E:320:LEU:HD23	1.98	0.46
1:B:430:ASN:HD22	1:B:433:MET:HE2	1.75	0.46
1:H:114:ALA:O	1:H:118:LEU:HB2	2.15	0.46
1:E:421:TYR:HE1	1:E:423:VAL:HG22	1.80	0.46
1:D:408:LYS:CG	2:L:1:NAG:H82	2.47	0.45
1:F:54:VAL:O	1:F:328:PHE:HA	2.17	0.45
1:F:155:LYS:HE3	1:F:161:VAL:HG22	1.98	0.45
1:F:202:LYS:HD2	1:F:206:TYR:CE1	2.51	0.45
1:B:195:GLU:CD	1:B:195:GLU:H	2.24	0.45
1:G:93:PRO:HD2	1:G:463:SER:O	2.16	0.45
1:F:118:LEU:HD12	1:F:176:ALA:HB3	1.98	0.45
1:C:155:LYS:HA	1:C:155:LYS:HD3	1.83	0.45
1:G:317:ILE:O	1:G:321:ARG:HG2	2.16	0.45
1:G:386:GLY:HA2	1:H:107:VAL:HG21	1.98	0.45
1:H:381:HIS:HB3	1:H:452:GLU:OE2	2.16	0.45
1:F:271:ASN:OD1	1:F:274:GLU:HG3	2.16	0.45
1:D:72:ILE:HG23	1:D:82:GLY:HA3	1.99	0.45
1:G:23:GLU:HG2	1:G:28:TYR:CE2	2.51	0.45
1:G:426:GLY:HA2	1:H:426:GLY:HA2	1.97	0.45
1:F:280:PRO:O	1:F:322:LYS:HE2	2.16	0.45
1:F:457:GLU:HB2	1:E:65:SER:HA	1.99	0.45
2:O:1:NAG:H61	2:O:2:NAG:C7	2.46	0.45
1:H:164:VAL:HG12	1:H:312:MET:HE3	1.98	0.45
1:F:103:THR:HG22	1:F:123:ALA:C	2.41	0.45
1:A:71:ARG:HA	1:A:87:LEU:HD21	1.98	0.45
1:A:195:GLU:CA	1:A:198:SER:HB3	2.44	0.45
1:B:283:VAL:O	1:B:322:LYS:HE2	2.16	0.45
1:G:92:PHE:CE1	1:G:464:LYS:HE2	2.51	0.45
1:G:208:LEU:HD11	1:G:218:ILE:HD13	1.98	0.45
1:F:53:ASN:ND2	1:F:327:PHE:CD2	2.85	0.45
1:F:239:ASP:OD1	1:F:240:GLU:N	2.50	0.45
1:E:117:TYR:HA	1:E:481:PRO:HD3	1.99	0.45
1:E:357:ARG:HG2	1:E:357:ARG:HH11	1.81	0.45
1:A:376:THR:OG1	1:A:377:ALA:N	2.48	0.45
1:C:103:THR:HG21	1:C:132:ALA:CB	2.47	0.45
1:B:346:LYS:HA	1:B:396:PHE:CE1	2.51	0.45
1:F:111:ALA:HB1	1:F:128:VAL:HG12	1.99	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:170:ASN:HA	1:D:178:TYR:OH	2.17	0.45
1:A:229:LYS:HG3	1:A:230:ASN:N	2.32	0.45
1:D:388:TYR:HA	1:C:107:VAL:HB	1.99	0.45
1:B:93:PRO:HD2	1:B:463:SER:O	2.16	0.45
1:F:57:PHE:HB2	1:F:375:VAL:HG22	1.98	0.45
1:D:95:VAL:HA	1:D:461:VAL:O	2.18	0.44
1:D:342:GLU:OE2	1:D:344:LYS:HE3	2.17	0.44
1:B:60:ASP:HB3	1:B:334:GLY:HA2	1.99	0.44
1:B:248:ASP:HB3	1:B:250:LEU:H	1.82	0.44
1:G:457:GLU:HA	1:H:68:THR:HG21	1.98	0.44
1:C:398:LEU:HD23	1:C:411:THR:HG22	1.99	0.44
1:B:92:PHE:CE1	1:B:464:LYS:HE2	2.52	0.44
1:H:104:ASN:HB2	1:H:125:GLU:H	1.82	0.44
1:D:207:GLN:HB3	1:D:211:ASN:ND2	2.33	0.44
1:F:26:PRO:O	1:F:30:ARG:HG3	2.18	0.44
1:F:417:ASN:HB2	1:F:449:LEU:HD12	1.99	0.44
1:D:372:LEU:HD12	1:D:464:LYS:O	2.17	0.44
1:B:278:LEU:O	1:B:280:PRO:HD3	2.18	0.44
1:G:73:LEU:HD21	1:G:350:HIS:CE1	2.52	0.44
1:F:46:LEU:HB3	1:F:469:HIS:NE2	2.31	0.44
1:F:372:LEU:HD12	1:F:464:LYS:O	2.17	0.44
1:E:109:ASP:HB2	1:E:184:ARG:HH12	1.82	0.44
1:D:51:ALA:HB3	1:D:488:ALA:CA	2.48	0.44
1:A:291:GLU:HG3	1:A:292:PRO:HD2	1.99	0.44
1:D:74:LYS:NZ	1:D:356:ASP:OD1	2.48	0.44
1:B:55:ILE:O	1:B:373:THR:HA	2.18	0.44
1:F:73:LEU:O	1:F:77:LEU:HG	2.17	0.44
1:E:56:MET:HE1	1:E:117:TYR:O	2.18	0.44
1:E:310:SER:HB3	1:E:361:GLN:HG3	1.99	0.44
1:D:83:GLU:OE2	1:C:106:GLN:HB2	2.18	0.44
1:D:278:LEU:HA	1:D:278:LEU:HD12	1.78	0.44
1:C:299:LEU:HD11	1:C:350:HIS:CG	2.53	0.44
1:C:299:LEU:HD11	1:C:350:HIS:ND1	2.33	0.44
1:C:168:ARG:HG3	1:C:294:ASP:OD1	2.18	0.44
1:E:111:ALA:HB1	1:E:128:VAL:HG12	1.98	0.44
1:D:114:ALA:HA	1:D:117:TYR:CE2	2.53	0.44
1:C:150:ILE:HD13	1:C:484:MET:HE3	2.00	0.44
1:B:45:LYS:H	1:B:45:LYS:HG2	1.60	0.44
1:E:41:LEU:O	1:E:44:GLN:HB2	2.18	0.44
1:A:435:ASP:OD2	1:A:438:HIS:HB2	2.18	0.43
1:D:60:ASP:O	1:D:336:ILE:HB	2.18	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:97:LEU:HA	1:D:97:LEU:HD23	1.77	0.43
1:D:428:ARG:NH1	1:D:444:GLN:OE1	2.51	0.43
1:E:40:ALA:O	1:E:43:LEU:HB2	2.17	0.43
1:E:213:ARG:O	1:E:260:LYS:NZ	2.51	0.43
1:C:46:LEU:HD13	1:C:469:HIS:CD2	2.53	0.43
1:F:302:ASN:O	1:F:304:VAL:N	2.51	0.43
1:D:60:ASP:CB	1:D:334:GLY:HA2	2.48	0.43
1:G:58:LEU:HD22	1:G:58:LEU:HA	1.87	0.43
1:H:104:ASN:HD22	1:H:125:GLU:HG3	1.83	0.43
1:H:332:GLU:CD	1:H:334:GLY:HA3	2.43	0.43
1:F:195:GLU:H	1:F:195:GLU:HG3	1.38	0.43
1:D:448:PRO:HB2	1:C:405:THR:CG2	2.48	0.43
1:C:251:ASP:OD2	1:C:254:ASP:HB2	2.18	0.43
1:B:117:TYR:HA	1:B:481:PRO:HD3	2.01	0.43
1:B:248:ASP:OD2	1:B:250:LEU:HD12	2.18	0.43
1:G:378:ASP:N	1:G:378:ASP:OD1	2.50	0.43
1:H:341:HIS:CE1	1:H:454:HIS:CD2	3.05	0.43
1:F:62:MET:HE2	1:F:62:MET:HB3	1.88	0.43
1:F:338:HIS:O	1:F:342:GLU:HG3	2.17	0.43
1:E:109:ASP:OD2	1:E:126:GLY:N	2.45	0.43
1:A:54:VAL:HB	1:A:328:PHE:HD1	1.83	0.43
1:A:240:GLU:OE1	1:A:243:ARG:NH2	2.52	0.43
1:A:313:VAL:O	1:A:317:ILE:HG13	2.18	0.43
3:F:601:NAG:O7	3:F:601:NAG:O3	2.31	0.43
1:A:224:LYS:HG2	1:A:292:PRO:O	2.19	0.43
1:D:162:GLY:HA2	1:D:217:VAL:O	2.18	0.43
1:C:302:ASN:O	1:C:304:VAL:N	2.51	0.43
1:G:395:ILE:HG13	1:G:413:ILE:HD11	2.01	0.43
1:G:410:PHE:CB	1:H:447:VAL:HG21	2.47	0.43
1:F:172:ALA:HB2	1:F:184:ARG:NH2	2.33	0.43
1:D:309:LEU:HD23	1:D:355:MET:HA	2.00	0.43
1:D:342:GLU:CD	1:D:344:LYS:HE3	2.44	0.43
1:C:448:PRO:O	1:C:449:LEU:HD23	2.19	0.43
1:H:221:GLY:HA3	1:H:293:GLY:O	2.19	0.43
1:H:252:LEU:HA	1:H:255:THR:HB	2.01	0.43
1:E:417:ASN:OD1	1:E:452:GLU:HG2	2.19	0.43
1:F:84:GLU:H	1:F:84:GLU:CD	2.27	0.43
1:E:275:LEU:CD1	1:E:315:VAL:HG11	2.48	0.43
1:B:463:SER:HB3	1:B:468:ALA:HB1	2.00	0.43
1:F:359:ILE:HD13	1:F:375:VAL:HG21	2.00	0.43
1:F:408:LYS:HZ1	1:F:427:GLU:HG3	1.84	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:92:PHE:CZ	1:A:464:LYS:HE2	2.54	0.42
1:A:405:THR:HG21	1:B:448:PRO:HB2	2.00	0.42
1:C:173:THR:HB	1:C:332:GLU:OE2	2.18	0.42
1:G:174:PRO:HD3	1:G:332:GLU:OE1	2.18	0.42
1:H:30:ARG:O	1:H:31:ASP:C	2.62	0.42
1:F:296:GLN:HG3	1:F:300:ASN:HB2	1.99	0.42
1:D:269:ILE:O	1:D:288:GLY:HA2	2.19	0.42
1:E:97:LEU:HD23	1:E:97:LEU:HA	1.82	0.42
1:A:417:ASN:OD1	1:A:452:GLU:HG2	2.20	0.42
1:D:436:TYR:HA	1:D:441:TYR:CG	2.54	0.42
1:G:291:GLU:HG3	1:G:292:PRO:HD2	2.01	0.42
1:A:57:PHE:HB2	1:A:375:VAL:HG22	2.02	0.42
1:A:264:LYS:HD3	1:A:285:TYR:HE2	1.84	0.42
1:D:93:PRO:HD2	1:D:463:SER:O	2.20	0.42
1:D:128:VAL:HG11	1:D:175:SER:OG	2.19	0.42
1:C:230:ASN:O	1:C:243:ARG:HD3	2.19	0.42
1:G:398:LEU:HD23	1:G:398:LEU:HA	1.87	0.42
1:A:95:VAL:HA	1:A:461:VAL:O	2.20	0.42
1:B:314:VAL:HG22	1:B:365:LEU:HD11	2.00	0.42
1:G:337:ASP:OD1	1:G:379:HIS:HE1	2.03	0.42
1:H:104:ASN:CB	1:H:125:GLU:H	2.31	0.42
1:D:71:ARG:HA	1:D:87:LEU:HD21	2.00	0.42
1:H:54:VAL:HG12	1:H:484:MET:HE3	2.01	0.42
1:H:215:ILE:HB	1:H:218:ILE:HD11	2.01	0.42
1:F:104:ASN:HB3	1:E:19:VAL:HG22	2.02	0.42
1:E:272:ARG:NH2	1:E:311:GLU:OE2	2.52	0.42
1:E:423:VAL:HG23	1:E:423:VAL:O	2.20	0.42
1:E:467:MET:HE3	1:E:467:MET:HB3	1.93	0.42
1:D:241:LYS:HB3	1:D:241:LYS:HE3	1.79	0.42
1:C:333:GLY:O	1:C:335:ARG:N	2.46	0.42
1:B:178:TYR:CE2	1:B:208:LEU:HD13	2.54	0.42
1:B:188:SER:HB3	1:B:191:GLU:OE1	2.19	0.42
1:B:298:GLU:OE2	1:B:301:ARG:NH1	2.52	0.42
1:G:38:LYS:HA	1:G:38:LYS:HD3	1.74	0.42
1:H:310:SER:HB3	1:H:361:GLN:HE21	1.85	0.42
1:H:441:TYR:CE2	1:H:443:ALA:HA	2.54	0.42
1:D:269:ILE:CG2	1:D:274:GLU:HB3	2.50	0.42
1:D:425:GLY:O	1:D:427:GLU:N	2.52	0.42
1:C:114:ALA:HA	1:C:117:TYR:CE2	2.55	0.42
1:G:467:MET:HE3	1:G:470:LEU:HD11	2.01	0.42
1:F:401:MET:HB2	1:F:401:MET:HE3	1.79	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:213:ARG:HB3	1:E:259:PHE:CD2	2.55	0.42
1:A:414:LEU:HD23	1:A:414:LEU:HA	1.70	0.42
1:C:438:HIS:O	1:C:440:ASN:N	2.53	0.42
1:B:354:GLU:HA	1:B:357:ARG:HG3	2.02	0.42
1:F:471:LEU:HG	1:F:483:VAL:HG11	2.02	0.42
1:C:84:GLU:CD	1:C:84:GLU:H	2.28	0.41
1:C:111:ALA:HB1	1:C:128:VAL:HG13	2.02	0.41
2:V:1:NAG:H62	2:V:2:NAG:O7	2.21	0.41
1:A:275:LEU:HD12	1:A:290:PHE:HZ	1.83	0.41
1:C:310:SER:OG	1:C:354:GLU:OE2	2.30	0.41
1:G:136:ARG:C	1:G:138:ARG:H	2.28	0.41
1:F:95:VAL:HA	1:F:461:VAL:O	2.19	0.41
1:E:302:ASN:C	1:E:304:VAL:H	2.29	0.41
1:D:164:VAL:HG22	1:D:219:MET:HB2	2.02	0.41
1:C:227:TYR:HB3	1:C:231:LYS:HD3	2.02	0.41
1:C:357:ARG:O	1:C:361:GLN:HG2	2.20	0.41
1:G:224:LYS:O	1:G:244:GLY:HA2	2.20	0.41
1:F:426:GLY:HA2	1:E:426:GLY:O	2.20	0.41
1:A:74:LYS:HG3	1:A:353:VAL:HG13	2.02	0.41
1:D:103:THR:HG21	1:D:132:ALA:HB1	2.02	0.41
1:D:178:TYR:CE2	1:D:208:LEU:HD13	2.55	0.41
1:D:202:LYS:HD2	1:D:202:LYS:HA	1.65	0.41
1:F:178:TYR:CD1	1:F:208:LEU:HA	2.55	0.41
1:F:421:TYR:HB2	1:F:445:SER:OG	2.21	0.41
1:E:95:VAL:HA	1:E:461:VAL:O	2.20	0.41
1:E:295:MET:HE1	1:E:307:PRO:HD2	2.02	0.41
1:A:65:SER:HA	1:B:457:GLU:HB3	2.01	0.41
1:A:457:GLU:HB3	1:B:65:SER:HA	2.02	0.41
1:B:190:ASN:HB2	1:B:245:THR:O	2.21	0.41
1:H:60:ASP:OD2	1:H:332:GLU:OE2	2.39	0.41
1:A:41:LEU:HD23	1:B:470:LEU:HD21	2.03	0.41
1:A:161:VAL:HA	1:A:328:PHE:O	2.21	0.41
1:G:202:LYS:HE3	1:G:202:LYS:HB3	1.79	0.41
1:F:41:LEU:O	1:F:44:GLN:HB2	2.21	0.41
1:F:349:LEU:HD23	1:F:349:LEU:HA	1.92	0.41
1:A:117:TYR:HA	1:A:481:PRO:HD3	2.03	0.41
1:A:346:LYS:HE2	1:A:439:ASN:OD1	2.20	0.41
1:D:58:LEU:HD22	1:D:58:LEU:HA	1.80	0.41
1:B:60:ASP:HA	1:B:378:ASP:OD1	2.21	0.41
1:H:159:LYS:HB3	1:H:327:PHE:HA	2.02	0.41
1:A:415:TYR:O	1:A:445:SER:HA	2.21	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:190:ASN:HB2	1:D:245:THR:O	2.21	0.41
1:D:258:SER:O	1:H:494:LEU:HD23	2.20	0.41
1:B:25:ASP:O	1:B:26:PRO:C	2.63	0.41
1:B:272:ARG:HG2	1:B:276:LEU:HD23	2.02	0.41
3:B:602:NAG:H83	3:B:602:NAG:H3	2.02	0.41
1:E:302:ASN:CG	1:E:305:THR:OG1	2.63	0.41
1:A:62:MET:HE3	1:A:67:VAL:HG12	2.02	0.41
1:A:423:VAL:HG13	1:A:427:GLU:O	2.20	0.41
1:A:435:ASP:CG	1:A:438:HIS:HB2	2.46	0.41
1:D:52:LYS:O	1:D:326:GLY:HA3	2.21	0.41
1:D:346:LYS:HG3	1:D:396:PHE:CZ	2.56	0.41
1:D:415:TYR:O	1:D:445:SER:HA	2.20	0.41
1:C:417:ASN:OD1	1:C:453:THR:HG23	2.21	0.41
1:B:219:MET:HG2	1:B:290:PHE:HE2	1.85	0.41
1:G:116:ALA:HA	1:G:121:VAL:O	2.21	0.41
1:G:251:ASP:OD2	1:G:254:ASP:HB2	2.21	0.41
1:H:372:LEU:HD13	1:H:466:PRO:O	2.21	0.41
1:F:275:LEU:CD1	1:F:315:VAL:HG21	2.51	0.41
1:E:62:MET:O	1:E:62:MET:HG2	2.21	0.41
1:E:73:LEU:O	1:E:77:LEU:HG	2.21	0.41
1:E:76:GLN:NE2	1:E:393:ASN:O	2.47	0.41
1:G:337:ASP:CG	1:G:341:HIS:CD2	2.98	0.41
1:A:175:SER:O	1:A:177:ALA:N	2.54	0.40
1:A:272:ARG:HG3	1:A:307:PRO:HB3	2.04	0.40
1:B:60:ASP:O	1:B:337:ASP:HB2	2.21	0.40
1:G:160:SER:HB3	1:G:320:LEU:CD2	2.49	0.40
1:H:349:LEU:O	1:H:353:VAL:HG23	2.21	0.40
1:E:62:MET:HG2	1:E:67:VAL:HG12	2.03	0.40
1:D:83:GLU:CD	1:D:391:ARG:HD2	2.46	0.40
1:C:283:VAL:O	1:C:322:LYS:NZ	2.55	0.40
1:C:378:ASP:CG	1:C:379:HIS:CD2	2.99	0.40
1:B:75:GLY:HA3	1:B:85:THR:OG1	2.20	0.40
1:F:19:VAL:HG13	1:E:103:THR:HG21	2.04	0.40
1:F:24:LYS:HA	1:E:132:ALA:HB3	2.02	0.40
1:E:100:THR:O	1:E:108:PRO:HG3	2.21	0.40
1:E:115:THR:O	1:E:119:CYS:HB2	2.21	0.40
1:E:283:VAL:O	1:E:322:LYS:NZ	2.49	0.40
1:A:189:ASP:OD1	1:A:189:ASP:N	2.54	0.40
1:A:378:ASP:CG	1:A:379:HIS:CD2	2.99	0.40
1:D:71:ARG:NH2	1:C:458:ASP:OD2	2.48	0.40
1:G:74:LYS:HD2	1:G:87:LEU:HD23	2.03	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:389:THR:OG1	1:E:106:GLN:HB3	2.21	0.40
1:G:382:VAL:HG22	1:G:452:GLU:OE2	2.22	0.40
1:G:392:GLY:O	1:G:393:ASN:C	2.64	0.40
1:F:114:ALA:HA	1:F:117:TYR:CE2	2.55	0.40
1:E:278:LEU:O	1:E:280:PRO:HD3	2.22	0.40
1:E:406:ASP:O	1:E:408:LYS:HG3	2.21	0.40
3:E:602:NAG:O7	3:E:602:NAG:H3	2.21	0.40
1:A:175:SER:C	1:A:177:ALA:H	2.30	0.40
1:A:228:PRO:HD3	1:A:250:LEU:O	2.22	0.40
1:A:388:TYR:HA	1:B:107:VAL:HB	2.02	0.40
1:C:120:GLY:C	1:C:478:ASN:HB2	2.46	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	482/518 (93%)	441 (92%)	37 (8%)	4 (1%)	16	47
1	B	482/518 (93%)	446 (92%)	32 (7%)	4 (1%)	16	47
1	C	482/518 (93%)	448 (93%)	29 (6%)	5 (1%)	12	43
1	D	480/518 (93%)	448 (93%)	29 (6%)	3 (1%)	21	53
1	E	482/518 (93%)	450 (93%)	27 (6%)	5 (1%)	12	43
1	F	481/518 (93%)	446 (93%)	28 (6%)	7 (2%)	8	35
1	G	482/518 (93%)	439 (91%)	38 (8%)	5 (1%)	12	43
1	H	482/518 (93%)	448 (93%)	31 (6%)	3 (1%)	21	53
All	All	3853/4144 (93%)	3566 (93%)	251 (6%)	36 (1%)	14	45

All (36) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	F	303	ASN
1	E	424	VAL
1	D	278	LEU
1	C	172	ALA
1	B	60	ASP
1	F	499	PRO
1	A	244	GLY
1	D	426	GLY
1	C	62	MET
1	B	457	GLU
1	F	140	ASN
1	F	268	PHE
1	E	499	PRO
1	C	439	ASN
1	G	60	ASP
1	E	303	ASN
1	A	241	LYS
1	C	303	ASN
1	B	400	PRO
1	G	400	PRO
1	E	407	LYS
1	A	249	GLY
1	C	292	PRO
1	G	137	SER
1	F	143	GLN
1	H	244	GLY
1	B	382	VAL
1	F	400	PRO
1	A	382	VAL
1	G	382	VAL
1	F	382	VAL
1	G	387	GLY
1	H	19	VAL
1	D	400	PRO
1	H	382	VAL
1	E	382	VAL

5.3.2 Protein sidechains ⓘ

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

The Analysed column shows the number of residues for which the sidechain conformation was

analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	398/424 (94%)	397 (100%)	1 (0%)	86	86
1	B	398/424 (94%)	398 (100%)	0	100	100
1	C	398/424 (94%)	396 (100%)	2 (0%)	81	83
1	D	398/424 (94%)	397 (100%)	1 (0%)	86	86
1	E	398/424 (94%)	397 (100%)	1 (0%)	86	86
1	F	398/424 (94%)	397 (100%)	1 (0%)	86	86
1	G	398/424 (94%)	398 (100%)	0	100	100
1	H	398/424 (94%)	397 (100%)	1 (0%)	86	86
All	All	3184/3392 (94%)	3177 (100%)	7 (0%)	87	88

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	303	ASN
1	D	201	CYS
1	C	201	CYS
1	C	303	ASN
1	H	303	ASN
1	F	201	CYS
1	E	201	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (36) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	124	ASN
1	A	296	GLN
1	A	451	HIS
1	A	477	GLN
1	D	124	ASN
1	D	199	GLN
1	D	379	HIS
1	D	478	ASN
1	D	493	ASN
1	C	34	GLN
1	C	104	ASN
1	B	32	GLN
1	B	475	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	477	GLN
1	G	53	ASN
1	G	199	GLN
1	H	104	ASN
1	H	124	ASN
1	H	190	ASN
1	H	267	HIS
1	H	350	HIS
1	H	361	GLN
1	H	442	GLN
1	H	477	GLN
1	F	53	ASN
1	F	78	HIS
1	F	143	GLN
1	F	230	ASN
1	F	296	GLN
1	F	300	ASN
1	F	350	HIS
1	E	32	GLN
1	E	190	ASN
1	E	296	GLN
1	E	318	GLN
1	E	477	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

32 monosaccharides 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	NAG	I	1	1,2	14,14,15	0.69	1 (7%)	17,19,21	0.96	1 (5%)
2	NAG	I	2	2	14,14,15	0.89	1 (7%)	17,19,21	0.81	1 (5%)
2	NAG	J	1	1,2	14,14,15	0.30	0	17,19,21	1.07	1 (5%)
2	NAG	J	2	2	14,14,15	0.66	0	17,19,21	0.38	0
2	NAG	K	1	1,2	14,14,15	0.66	1 (7%)	17,19,21	0.62	0
2	NAG	K	2	2	14,14,15	1.22	3 (21%)	17,19,21	1.10	1 (5%)
2	NAG	L	1	1,2	14,14,15	0.56	0	17,19,21	1.10	1 (5%)
2	NAG	L	2	2	14,14,15	0.65	1 (7%)	17,19,21	0.83	0
2	NAG	M	1	1,2	14,14,15	0.83	1 (7%)	17,19,21	0.47	0
2	NAG	M	2	2	14,14,15	0.41	0	17,19,21	0.44	0
2	NAG	N	1	1,2	14,14,15	0.49	0	17,19,21	0.71	0
2	NAG	N	2	2	14,14,15	0.77	1 (7%)	17,19,21	0.69	1 (5%)
2	NAG	O	1	1,2	14,14,15	0.90	1 (7%)	17,19,21	0.60	0
2	NAG	O	2	2	14,14,15	0.91	1 (7%)	17,19,21	1.34	1 (5%)
2	NAG	P	1	1,2	14,14,15	0.35	0	17,19,21	0.58	0
2	NAG	P	2	2	14,14,15	0.67	1 (7%)	17,19,21	0.81	0
2	NAG	Q	1	1,2	14,14,15	0.55	0	17,19,21	0.84	1 (5%)
2	NAG	Q	2	2	14,14,15	1.16	1 (7%)	17,19,21	1.15	1 (5%)
2	NAG	R	1	1,2	14,14,15	0.48	0	17,19,21	0.78	0
2	NAG	R	2	2	14,14,15	0.64	0	17,19,21	0.88	1 (5%)
2	NAG	S	1	1,2	14,14,15	0.73	0	17,19,21	0.57	0
2	NAG	S	2	2	14,14,15	0.60	0	17,19,21	0.65	0
2	NAG	T	1	1,2	14,14,15	0.43	0	17,19,21	0.96	1 (5%)
2	NAG	T	2	2	14,14,15	0.50	0	17,19,21	0.77	0
2	NAG	U	1	1,2	14,14,15	0.77	1 (7%)	17,19,21	0.48	0
2	NAG	U	2	2	14,14,15	1.00	1 (7%)	17,19,21	0.67	0
2	NAG	V	1	1,2	14,14,15	0.61	0	17,19,21	0.92	1 (5%)
2	NAG	V	2	2	14,14,15	0.40	0	17,19,21	0.73	0
2	NAG	W	1	1,2	14,14,15	0.39	0	17,19,21	0.80	0
2	NAG	W	2	2	14,14,15	0.51	0	17,19,21	0.59	0
2	NAG	X	1	1,2	14,14,15	0.34	0	17,19,21	0.55	0
2	NAG	X	2	2	14,14,15	0.93	1 (7%)	17,19,21	1.00	1 (5%)

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	NAG	I	1	1,2	-	3/6/23/26	0/1/1/1
2	NAG	I	2	2	-	2/6/23/26	0/1/1/1
2	NAG	J	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	J	2	2	-	1/6/23/26	0/1/1/1
2	NAG	K	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	K	2	2	-	0/6/23/26	0/1/1/1
2	NAG	L	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	L	2	2	-	4/6/23/26	0/1/1/1
2	NAG	M	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	M	2	2	-	0/6/23/26	0/1/1/1
2	NAG	N	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	N	2	2	-	2/6/23/26	0/1/1/1
2	NAG	O	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	O	2	2	-	2/6/23/26	0/1/1/1
2	NAG	P	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	P	2	2	-	4/6/23/26	0/1/1/1
2	NAG	Q	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	Q	2	2	-	2/6/23/26	0/1/1/1
2	NAG	R	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	R	2	2	-	2/6/23/26	0/1/1/1
2	NAG	S	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	S	2	2	-	3/6/23/26	0/1/1/1
2	NAG	T	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	T	2	2	-	4/6/23/26	0/1/1/1
2	NAG	U	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	U	2	2	-	0/6/23/26	0/1/1/1
2	NAG	V	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	V	2	2	-	3/6/23/26	0/1/1/1
2	NAG	W	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	W	2	2	-	2/6/23/26	0/1/1/1
2	NAG	X	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	X	2	2	-	2/6/23/26	0/1/1/1

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	Q	2	NAG	O5-C1	4.00	1.50	1.43
2	U	2	NAG	C1-C2	3.47	1.57	1.52
2	K	2	NAG	O5-C1	-3.35	1.38	1.43
2	X	2	NAG	C1-C2	3.19	1.56	1.52
2	O	2	NAG	O5-C1	3.10	1.48	1.43
2	I	2	NAG	C1-C2	3.03	1.56	1.52
2	M	1	NAG	O5-C1	-3.01	1.38	1.43
2	O	1	NAG	O5-C1	-2.76	1.39	1.43
2	U	1	NAG	C1-C2	2.48	1.55	1.52
2	K	1	NAG	O5-C1	-2.25	1.39	1.43
2	K	2	NAG	C1-C2	2.24	1.55	1.52
2	I	1	NAG	O5-C1	-2.12	1.40	1.43
2	N	2	NAG	O5-C1	2.07	1.47	1.43
2	L	2	NAG	O5-C1	2.05	1.47	1.43
2	K	2	NAG	C3-C2	2.03	1.56	1.52
2	P	2	NAG	C1-C2	2.00	1.55	1.52

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	O	2	NAG	C1-O5-C5	4.22	117.84	112.19
2	L	1	NAG	C1-O5-C5	3.60	117.02	112.19
2	Q	2	NAG	C1-O5-C5	3.50	116.88	112.19
2	J	1	NAG	C1-O5-C5	3.21	116.49	112.19
2	V	1	NAG	C1-O5-C5	3.09	116.33	112.19
2	X	2	NAG	C1-O5-C5	2.93	116.11	112.19
2	K	2	NAG	C4-C3-C2	2.90	115.26	111.02
2	Q	1	NAG	C1-O5-C5	2.67	115.77	112.19
2	T	1	NAG	C1-O5-C5	2.63	115.72	112.19
2	I	2	NAG	C2-N2-C7	2.44	126.17	122.90
2	I	1	NAG	C3-C4-C5	2.42	114.62	110.23
2	N	2	NAG	C1-O5-C5	2.41	115.42	112.19
2	R	2	NAG	C2-N2-C7	2.08	125.69	122.90

There are no chirality outliers.

All (54) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	R	2	NAG	C1-C2-N2-C7
2	V	2	NAG	C1-C2-N2-C7
2	P	2	NAG	O5-C5-C6-O6
2	L	1	NAG	O5-C5-C6-O6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
2	S	1	NAG	O5-C5-C6-O6
2	J	1	NAG	O5-C5-C6-O6
2	L	2	NAG	O5-C5-C6-O6
2	N	2	NAG	O5-C5-C6-O6
2	W	2	NAG	O5-C5-C6-O6
2	X	1	NAG	O5-C5-C6-O6
2	O	2	NAG	C4-C5-C6-O6
2	Q	2	NAG	O5-C5-C6-O6
2	P	2	NAG	C4-C5-C6-O6
2	V	2	NAG	O5-C5-C6-O6
2	L	1	NAG	C4-C5-C6-O6
2	Q	2	NAG	C4-C5-C6-O6
2	T	1	NAG	O5-C5-C6-O6
2	O	2	NAG	O5-C5-C6-O6
2	S	1	NAG	C4-C5-C6-O6
2	N	1	NAG	O5-C5-C6-O6
2	X	1	NAG	C4-C5-C6-O6
2	R	1	NAG	O5-C5-C6-O6
2	J	1	NAG	C4-C5-C6-O6
2	N	2	NAG	C4-C5-C6-O6
2	T	1	NAG	C4-C5-C6-O6
2	U	1	NAG	O5-C5-C6-O6
2	R	1	NAG	C4-C5-C6-O6
2	N	1	NAG	C4-C5-C6-O6
2	U	1	NAG	C4-C5-C6-O6
2	T	2	NAG	O5-C5-C6-O6
2	I	1	NAG	O5-C5-C6-O6
2	W	2	NAG	C4-C5-C6-O6
2	V	2	NAG	C4-C5-C6-O6
2	L	2	NAG	C4-C5-C6-O6
2	X	2	NAG	O5-C5-C6-O6
2	P	1	NAG	C4-C5-C6-O6
2	S	2	NAG	C4-C5-C6-O6
2	J	2	NAG	O5-C5-C6-O6
2	R	2	NAG	O5-C5-C6-O6
2	T	2	NAG	C4-C5-C6-O6
2	S	2	NAG	O5-C5-C6-O6
2	P	2	NAG	C1-C2-N2-C7
2	X	2	NAG	C4-C5-C6-O6
2	I	1	NAG	C4-C5-C6-O6
2	P	1	NAG	O5-C5-C6-O6
2	I	2	NAG	C3-C2-N2-C7

Continued on next page...

Continued from previous page...

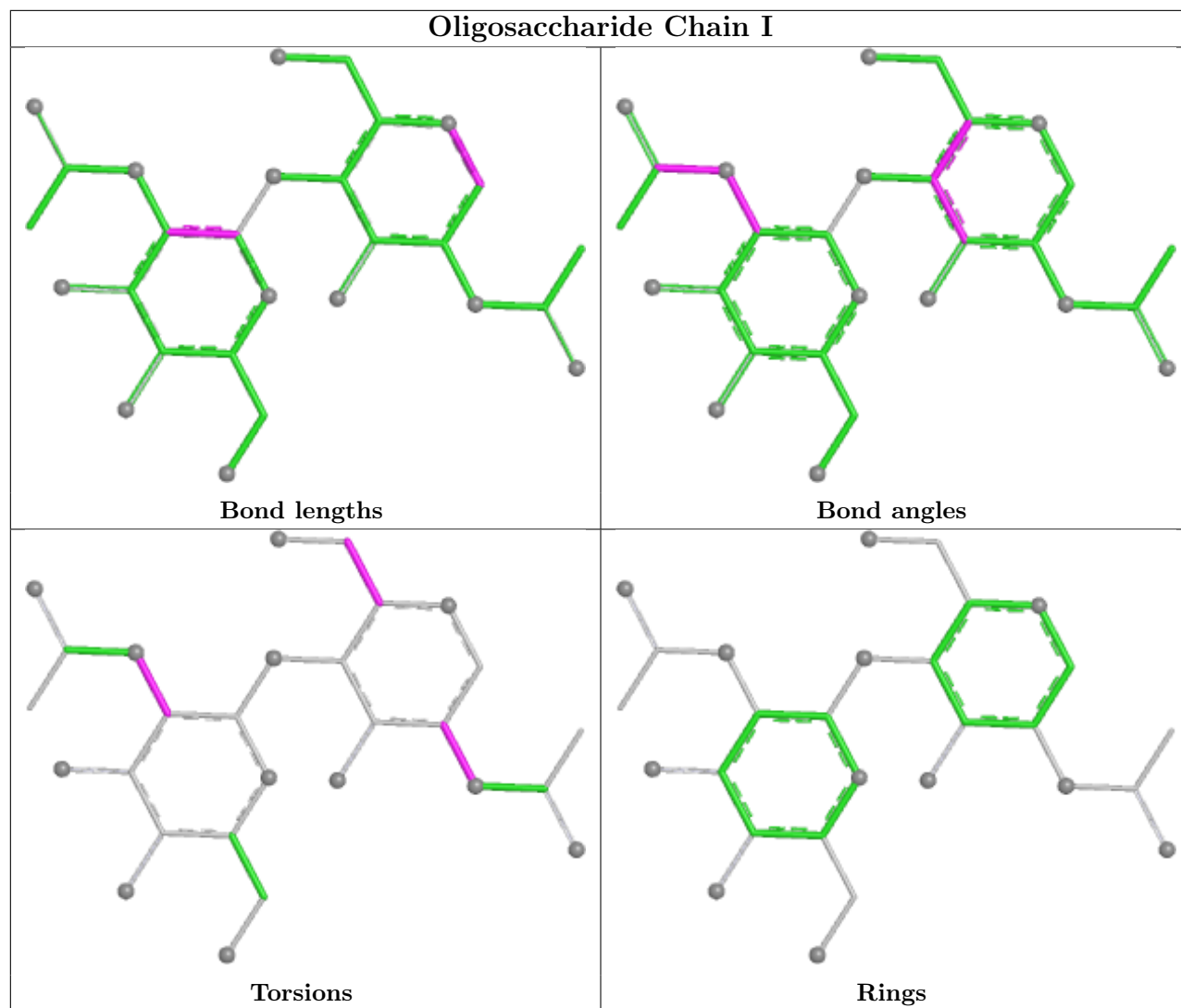
Mol	Chain	Res	Type	Atoms
2	L	2	NAG	C3-C2-N2-C7
2	T	2	NAG	C3-C2-N2-C7
2	I	1	NAG	C1-C2-N2-C7
2	I	2	NAG	C1-C2-N2-C7
2	L	2	NAG	C1-C2-N2-C7
2	S	2	NAG	C1-C2-N2-C7
2	T	2	NAG	C1-C2-N2-C7
2	P	2	NAG	C3-C2-N2-C7

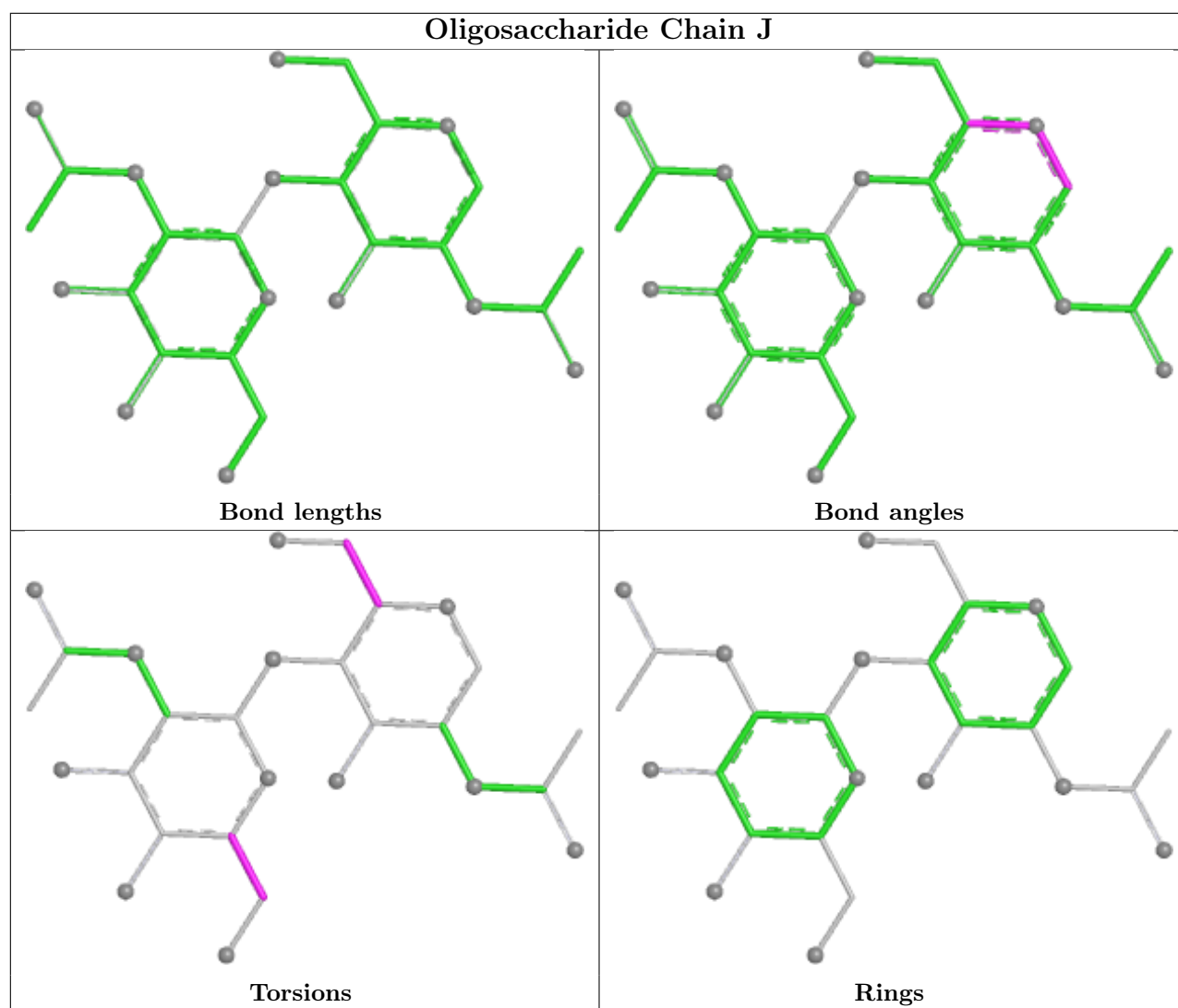
There are no ring outliers.

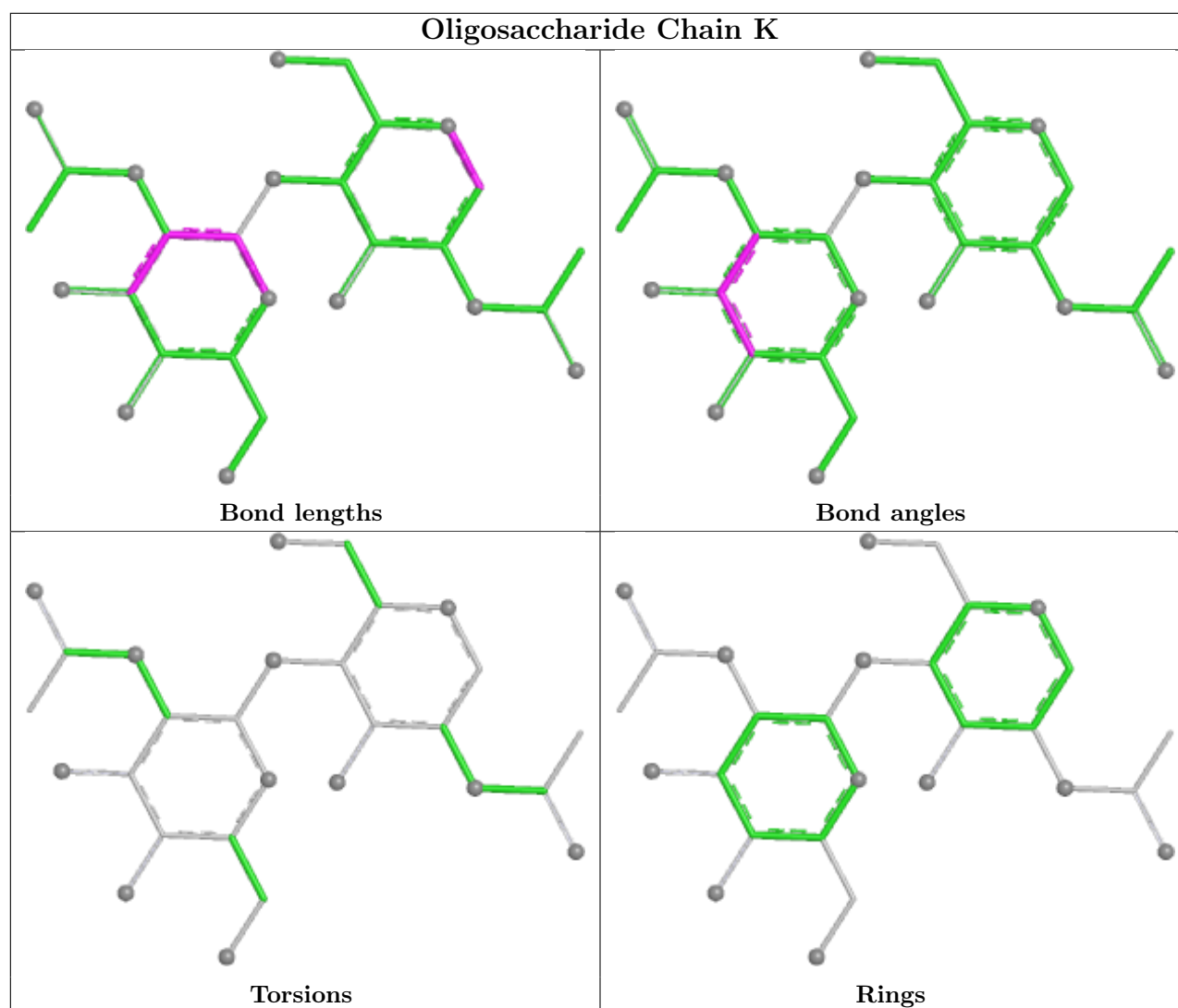
14 monomers are involved in 12 short contacts:

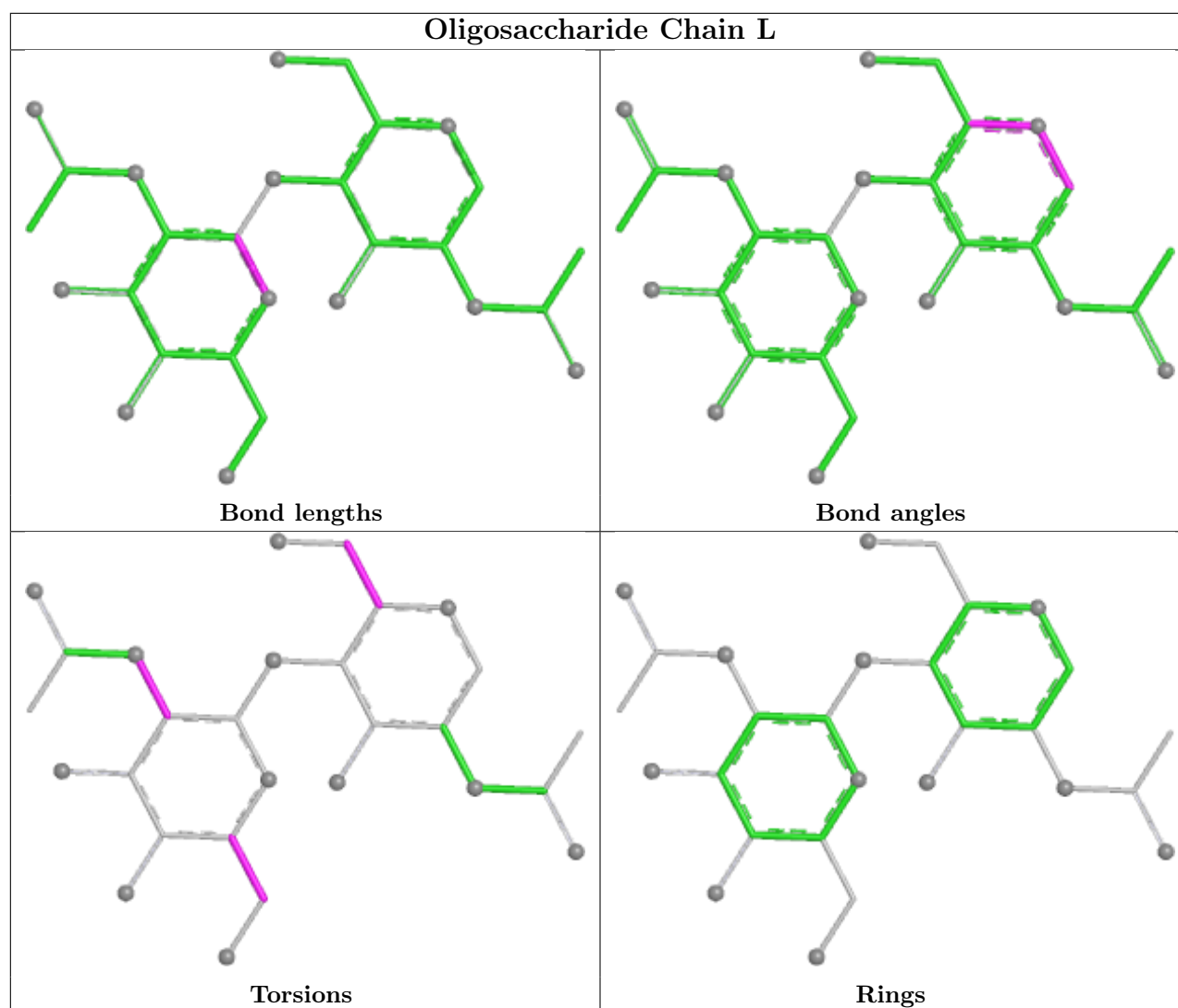
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	V	2	NAG	1	0
2	W	1	NAG	2	0
2	X	1	NAG	1	0
2	N	2	NAG	1	0
2	N	1	NAG	1	0
2	O	1	NAG	2	0
2	P	1	NAG	1	0
2	O	2	NAG	1	0
2	Q	1	NAG	1	0
2	U	2	NAG	1	0
2	L	1	NAG	2	0
2	Q	2	NAG	1	0
2	V	1	NAG	1	0
2	U	1	NAG	1	0

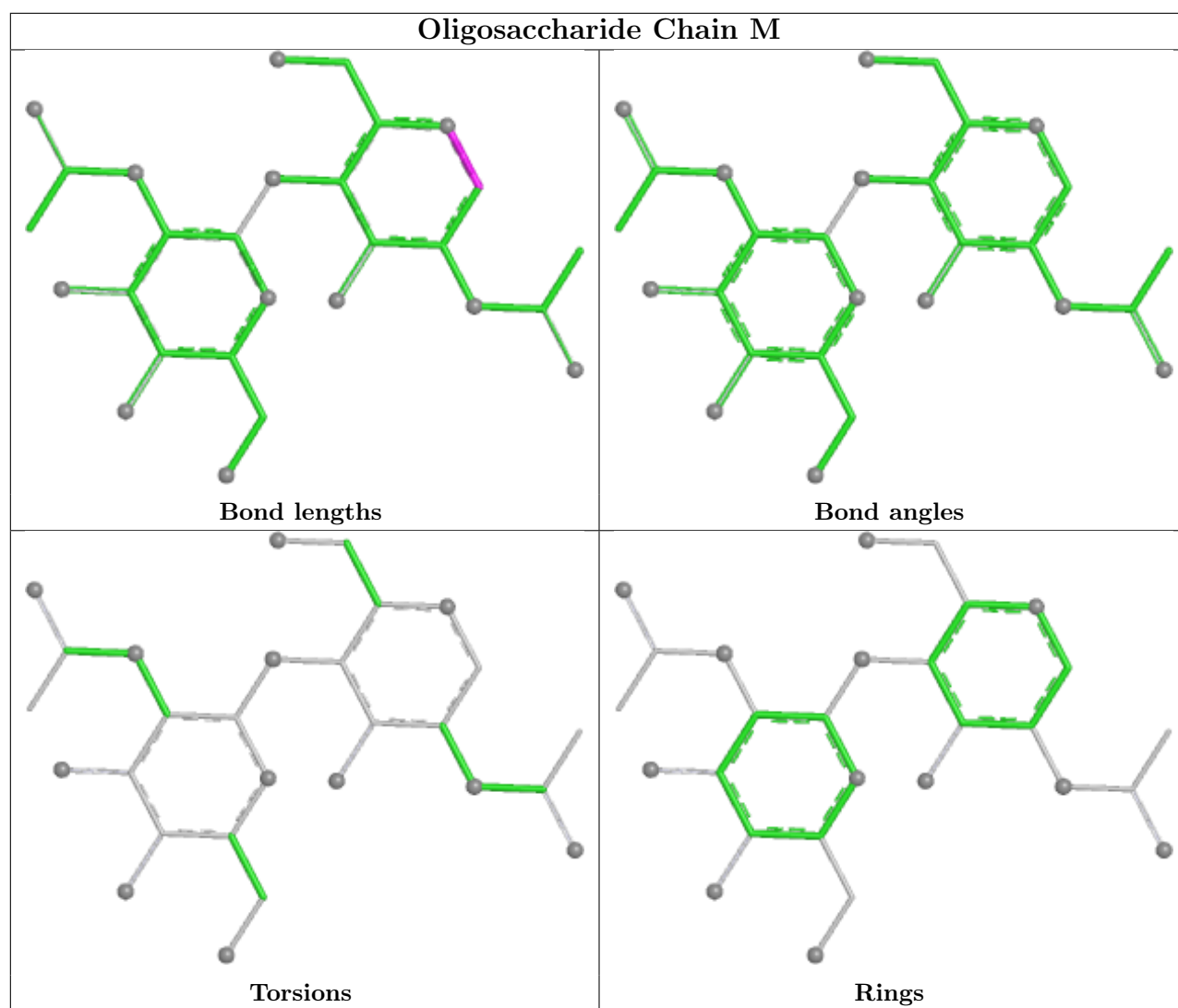
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

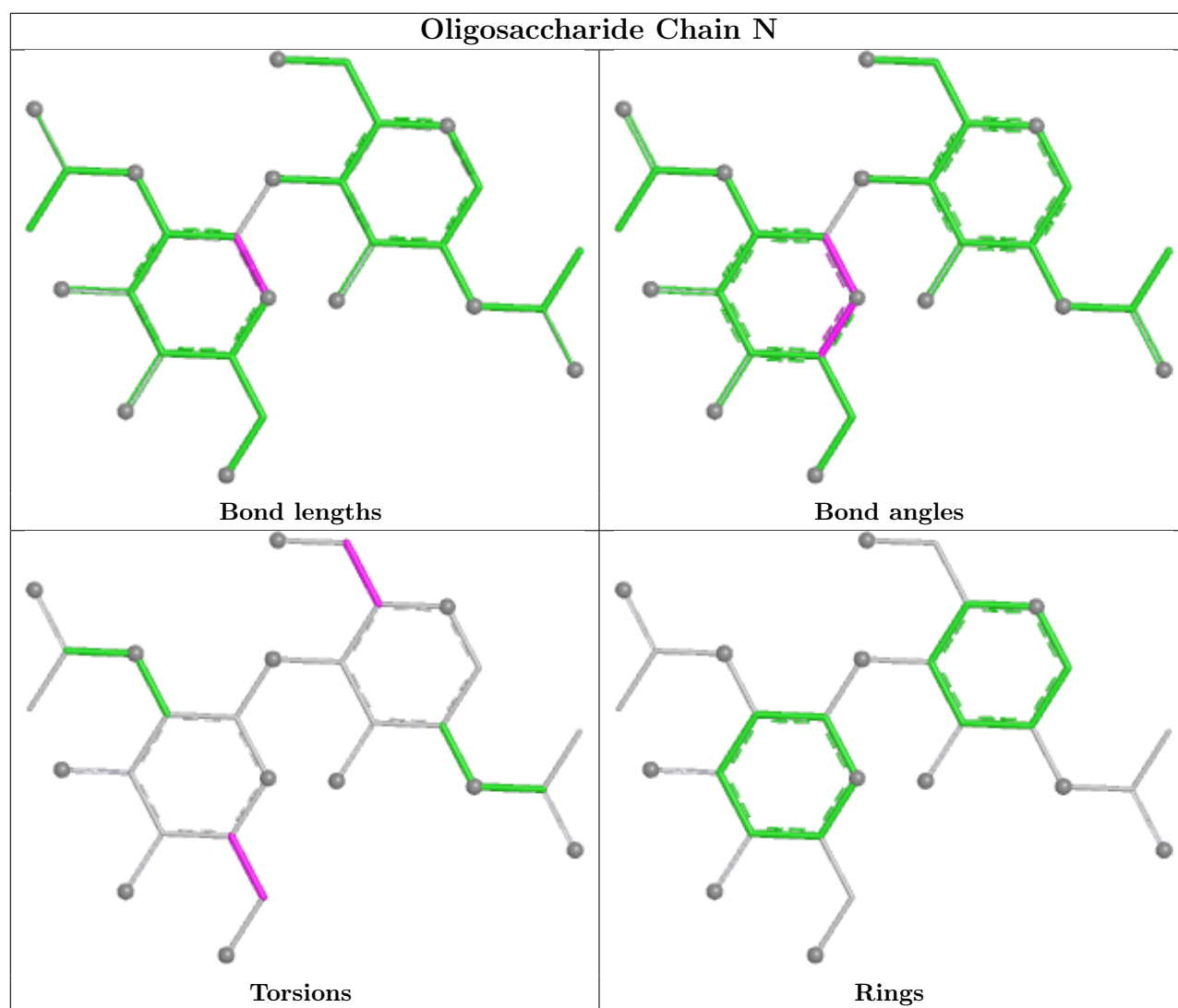


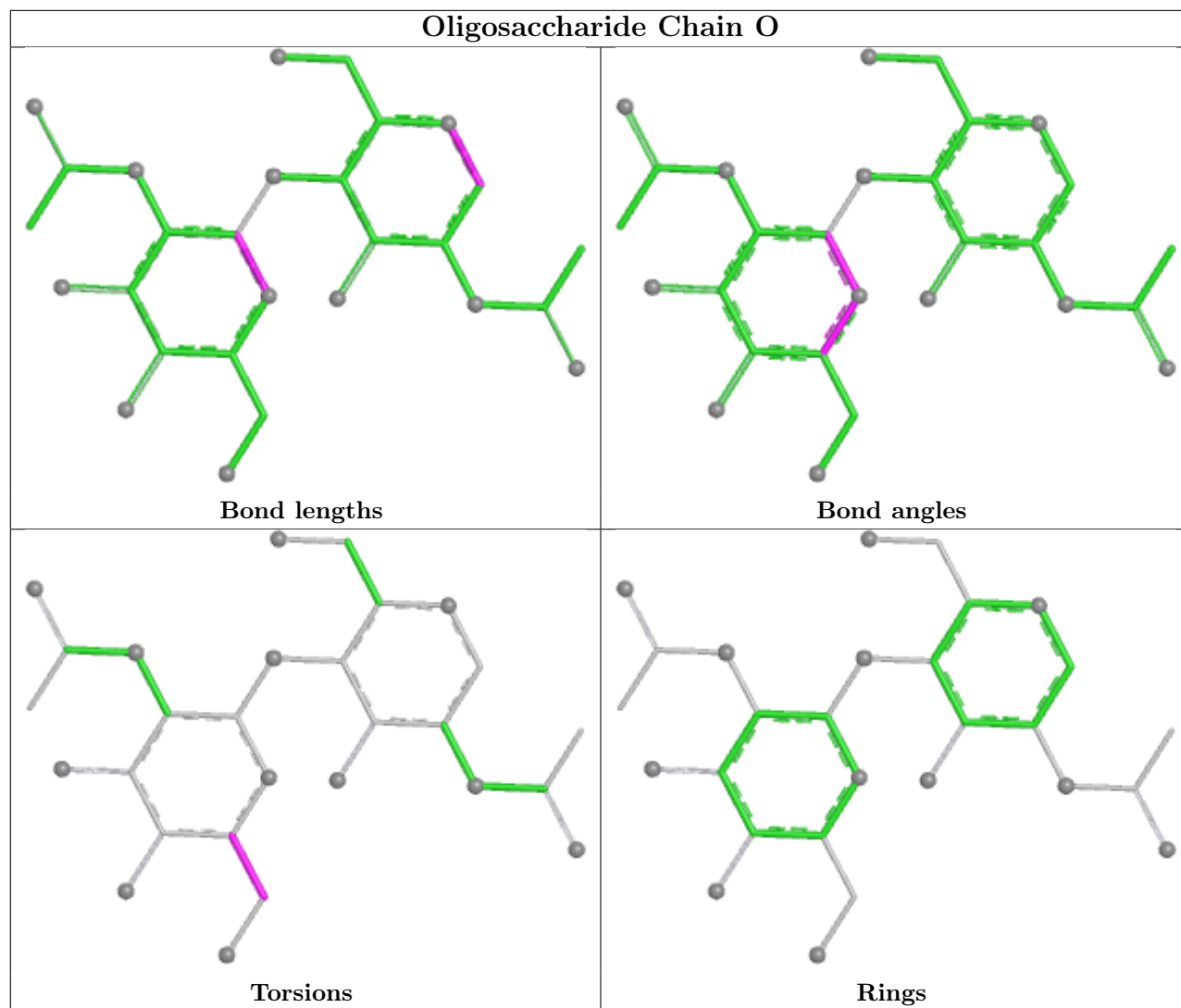


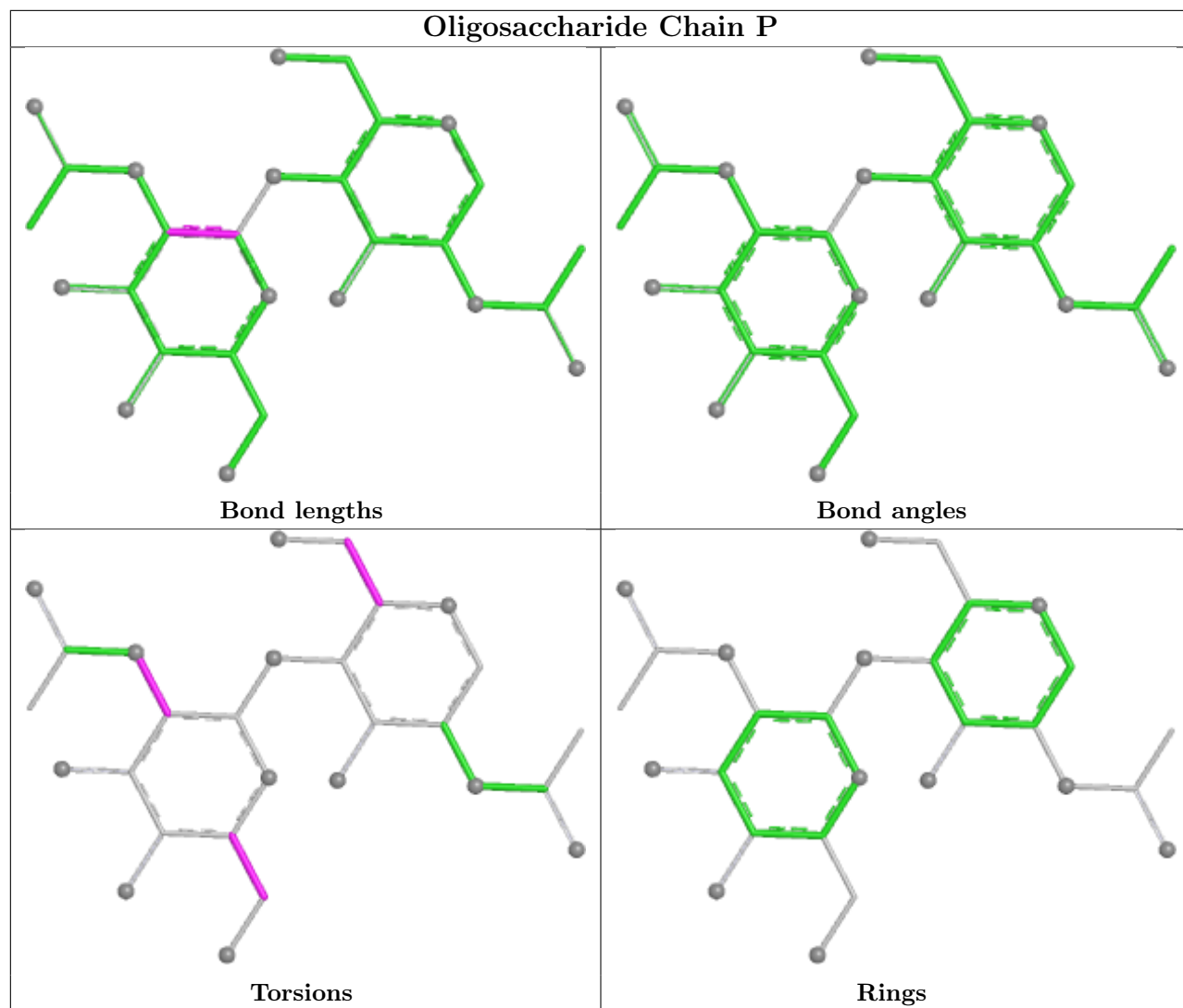


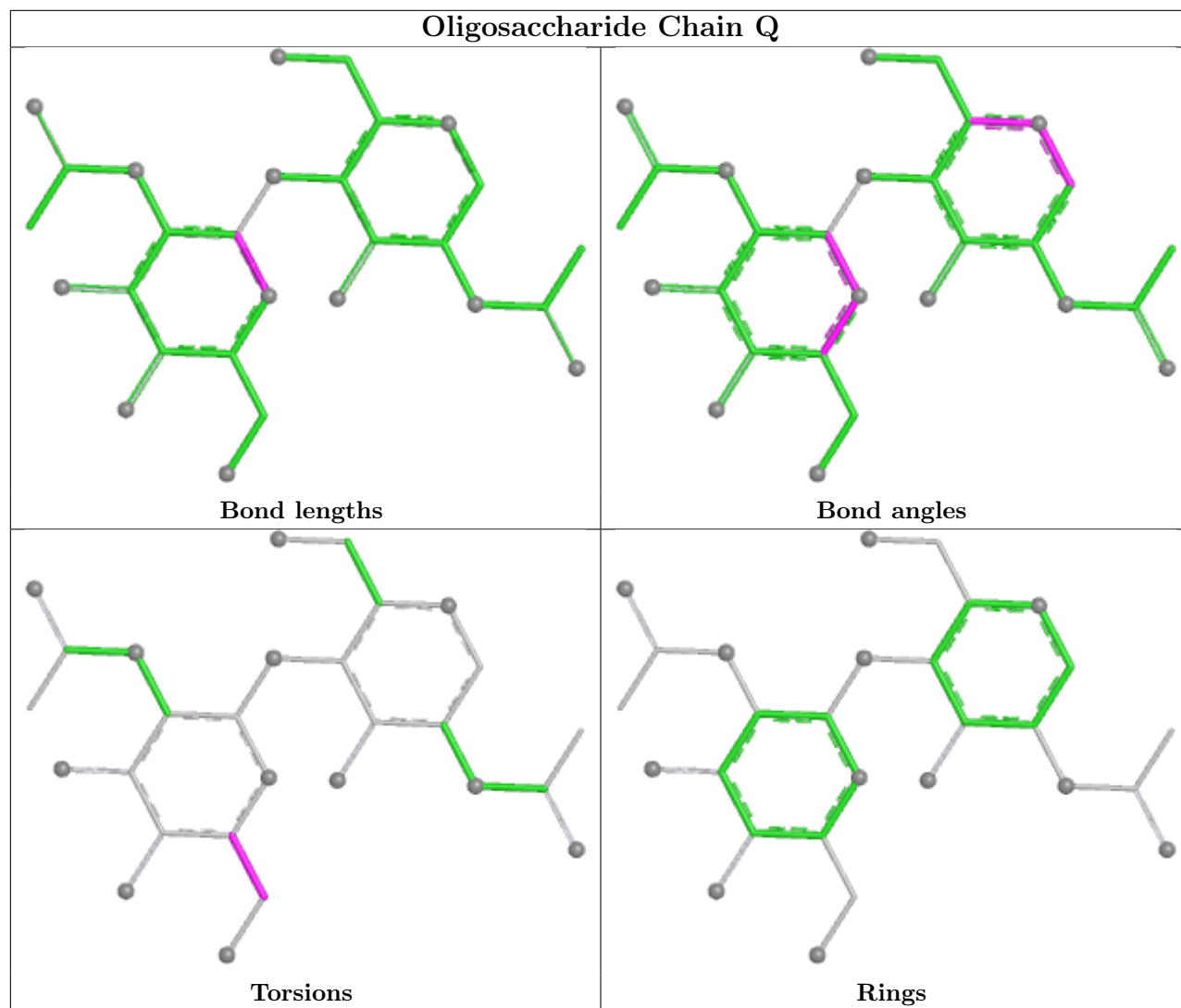


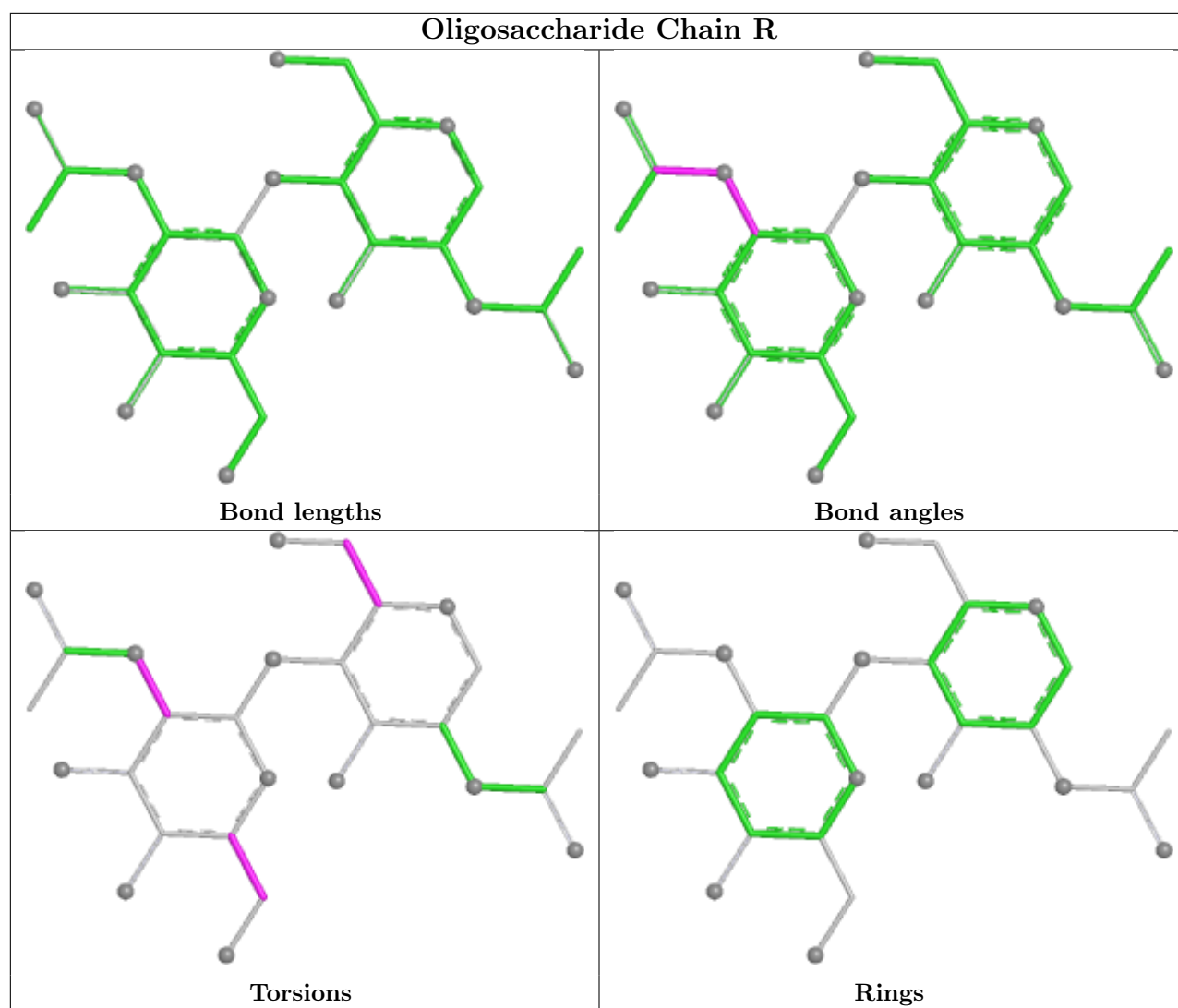


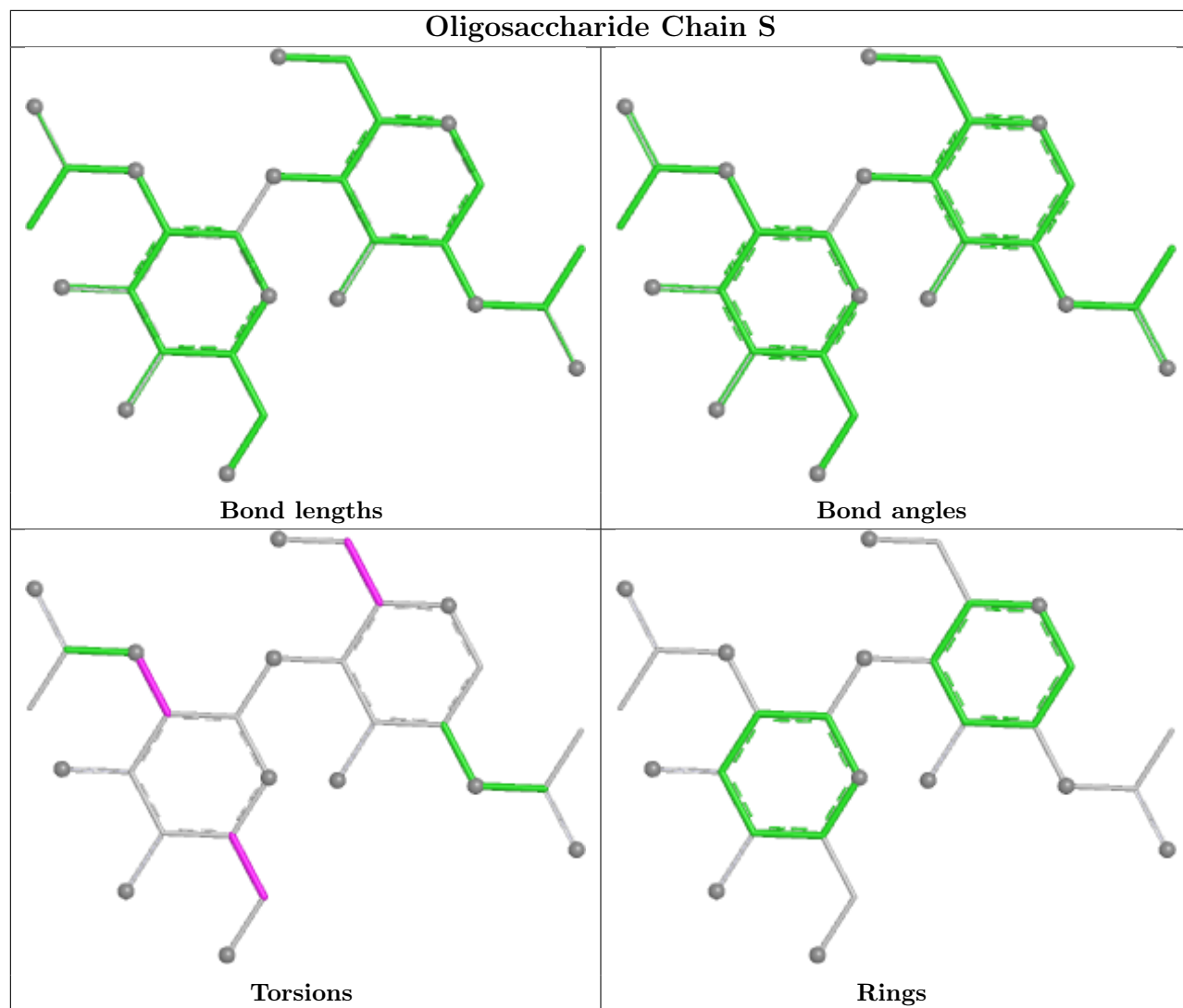


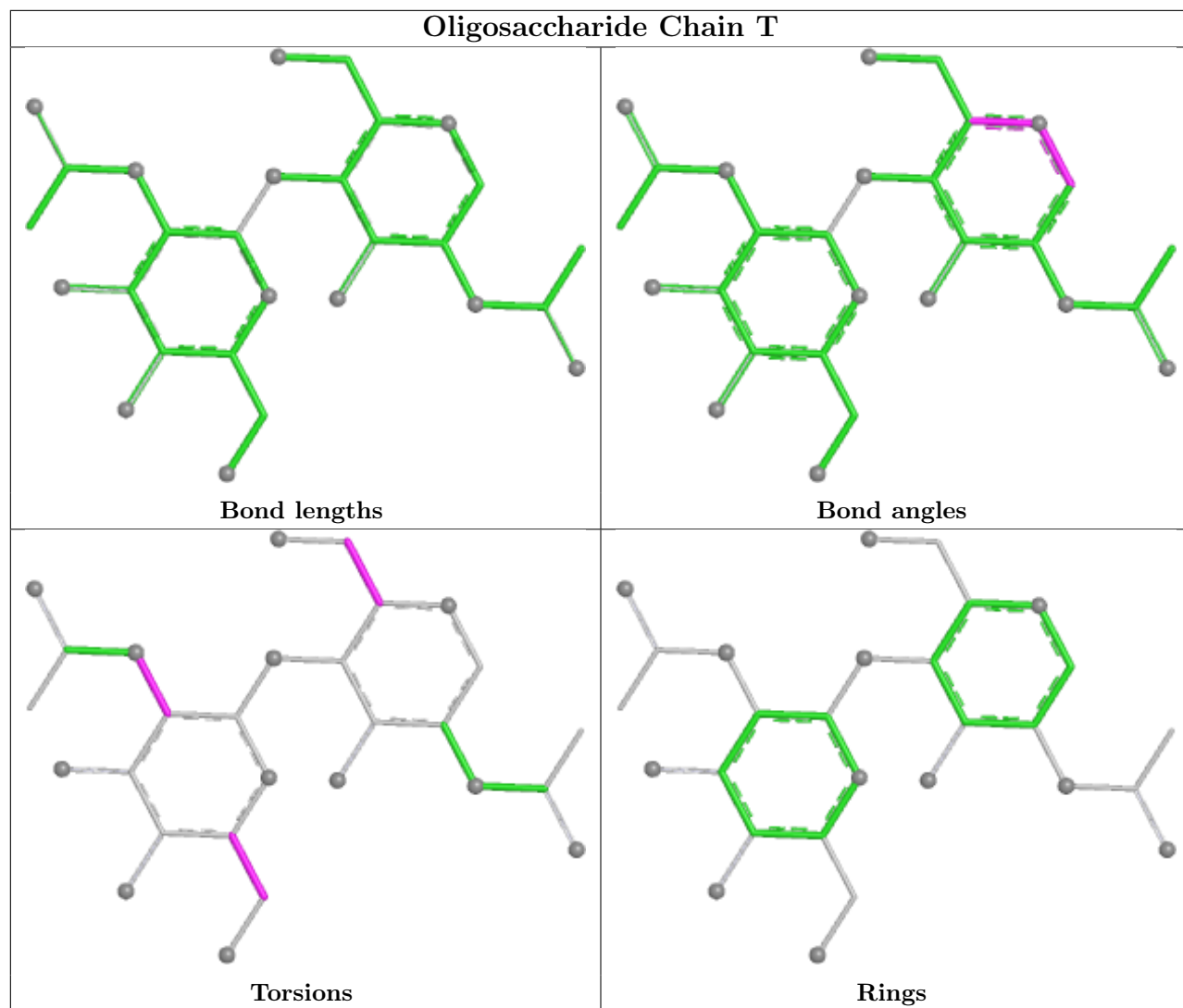


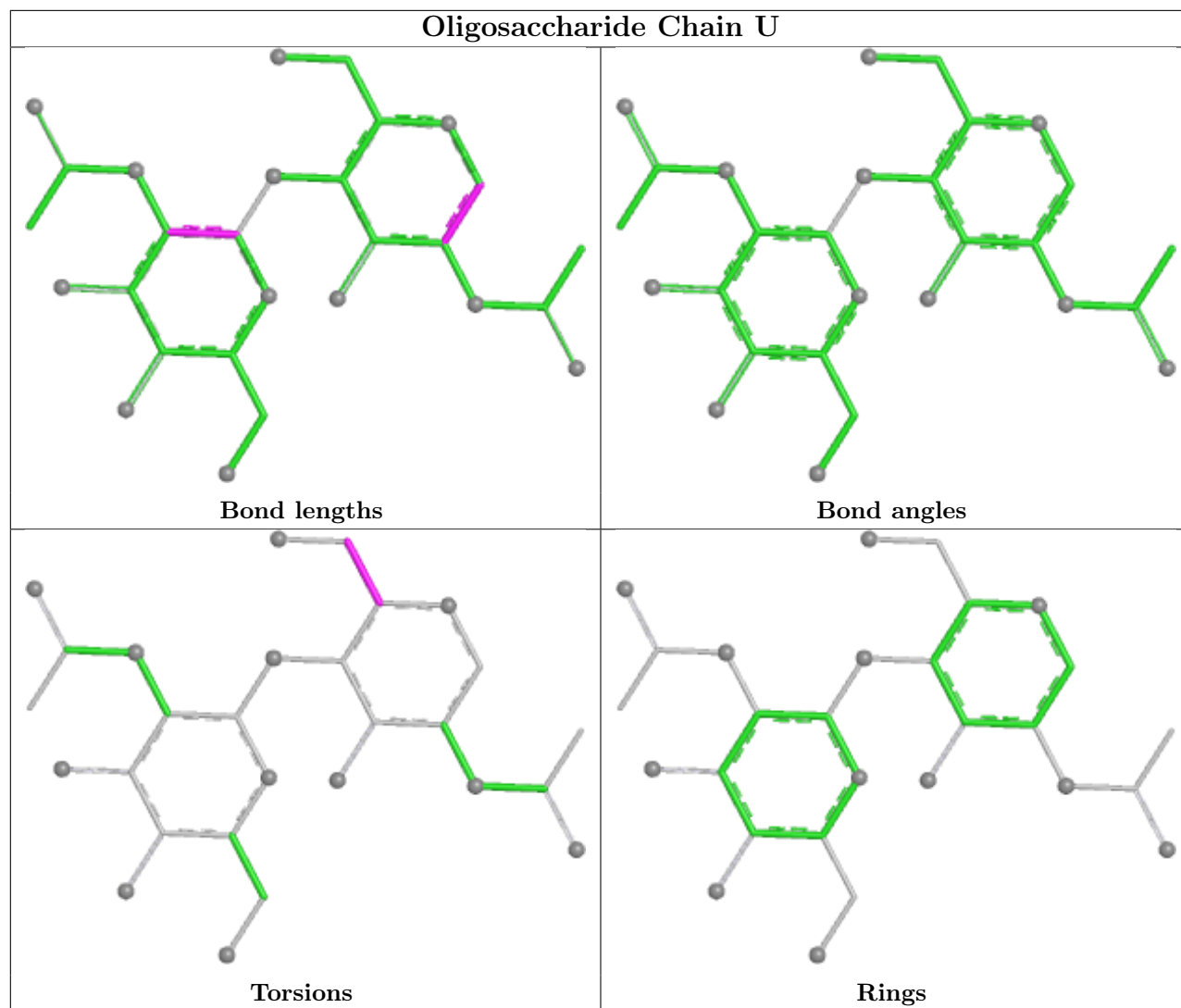


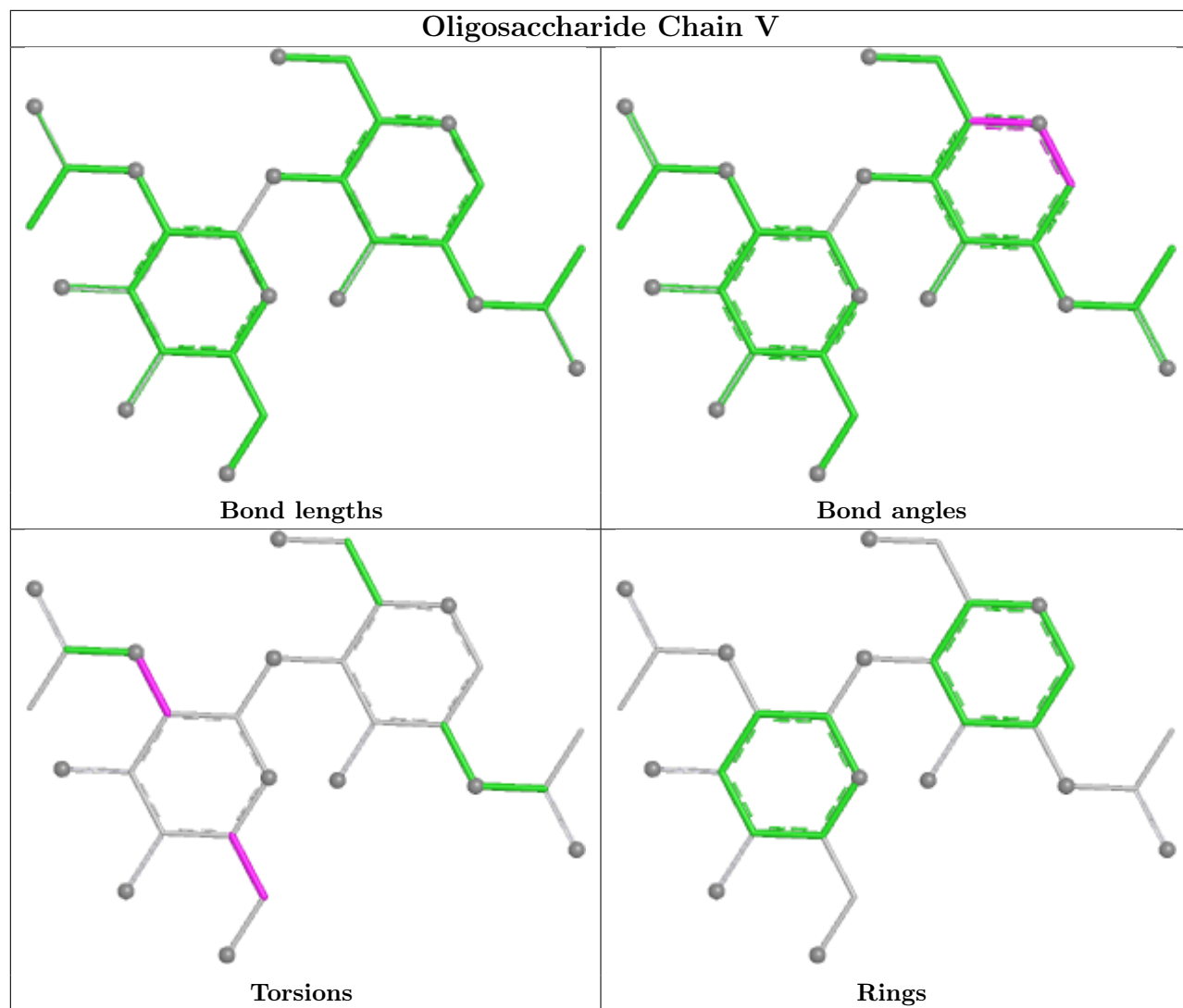


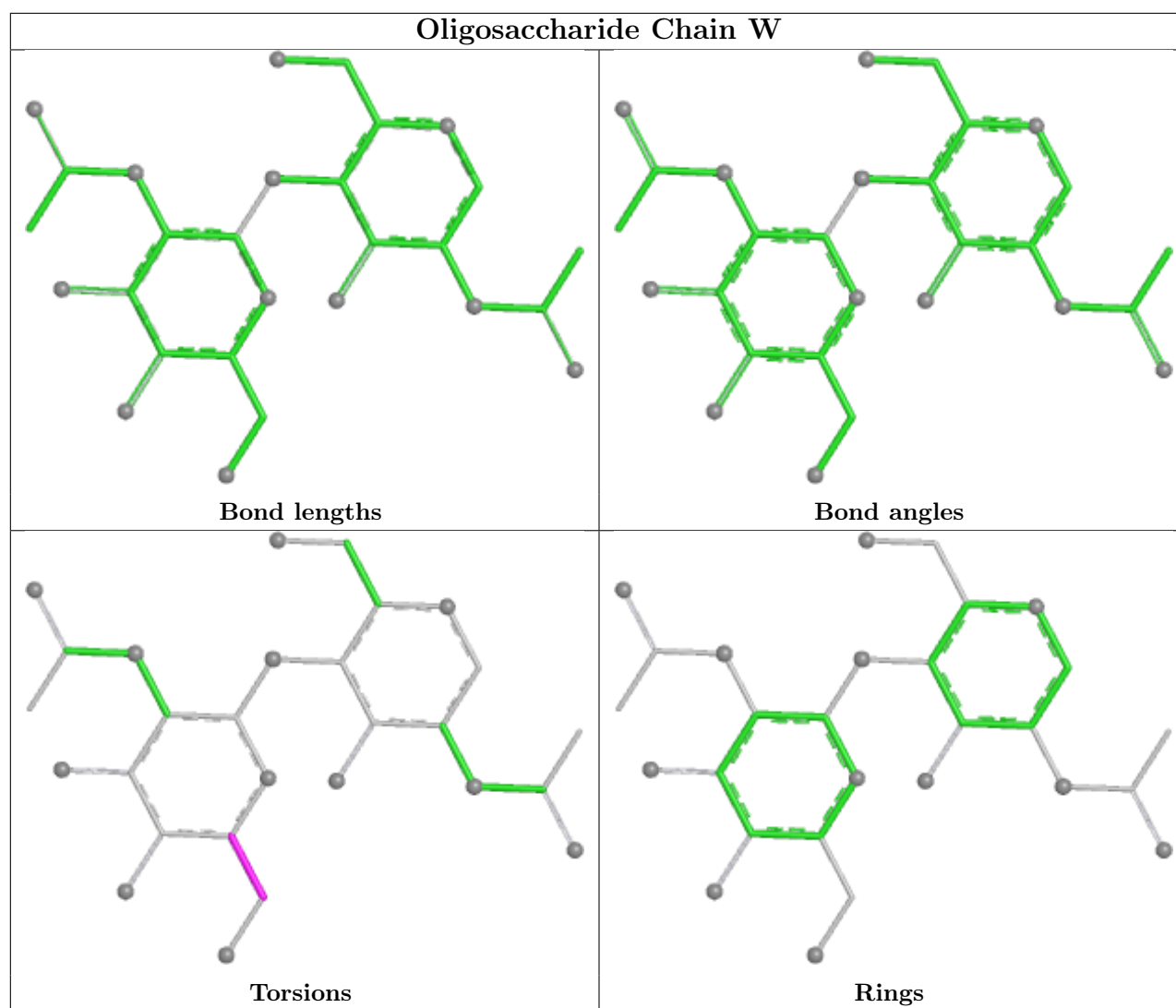


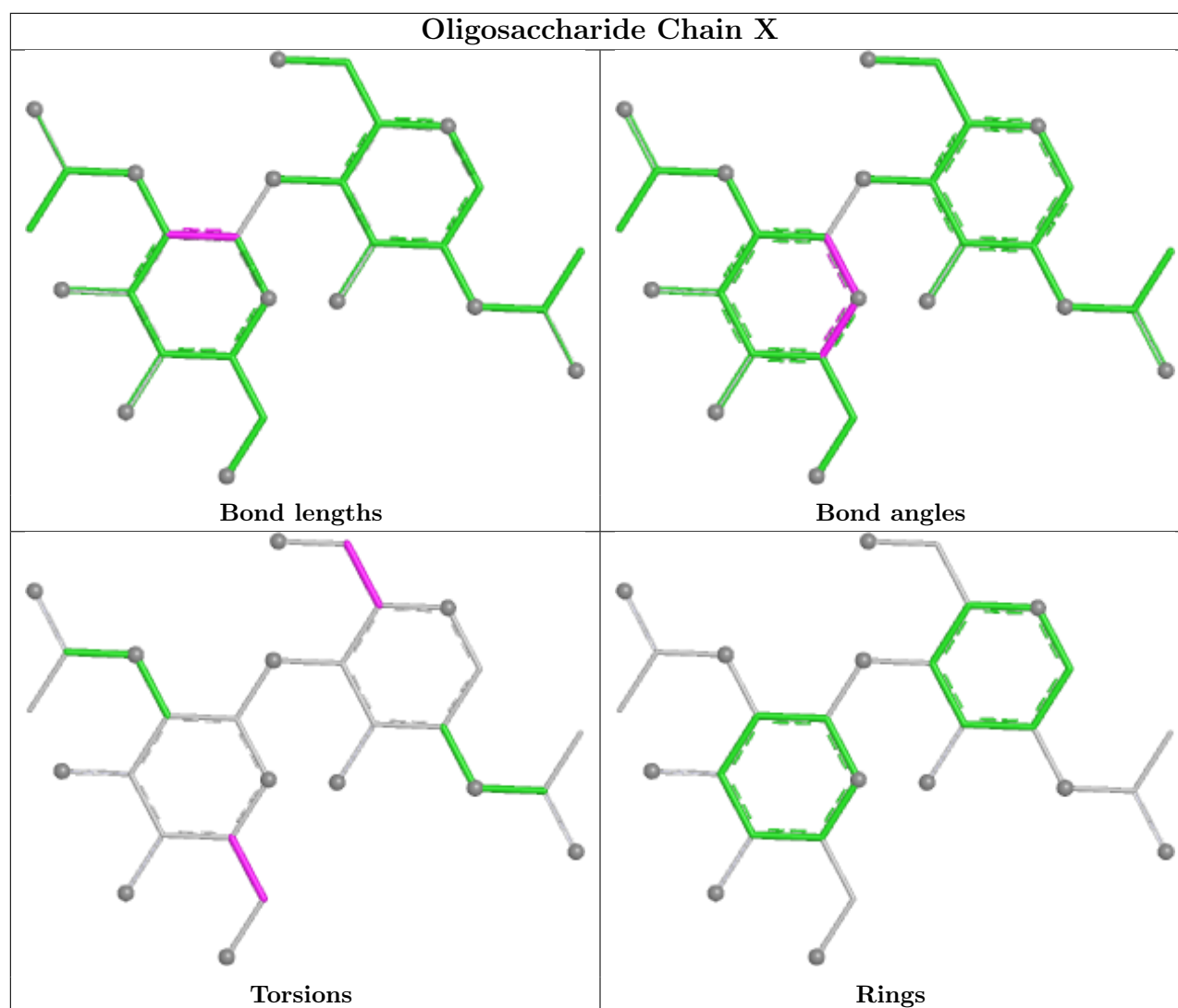












5.6 Ligand geometry [i](#)

Of 48 ligands modelled in this entry, 32 are monoatomic - leaving 16 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	NAG	F	602	1	14,14,15	0.92	2 (14%)	17,19,21	1.29	1 (5%)
3	NAG	H	602	1	14,14,15	1.23	2 (14%)	17,19,21	1.00	1 (5%)
3	NAG	A	602	1	14,14,15	1.27	1 (7%)	17,19,21	1.26	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	NAG	G	601	1	14,14,15	1.14	2 (14%)	17,19,21	0.93	1 (5%)
3	NAG	F	601	1	14,14,15	1.26	2 (14%)	17,19,21	0.54	0
3	NAG	C	602	1	14,14,15	0.95	1 (7%)	17,19,21	0.68	0
3	NAG	D	602	1	14,14,15	1.96	2 (14%)	17,19,21	1.28	2 (11%)
3	NAG	B	602	1	14,14,15	0.74	0	17,19,21	1.76	4 (23%)
3	NAG	H	601	1	14,14,15	0.69	0	17,19,21	0.44	0
3	NAG	C	601	1	14,14,15	1.12	2 (14%)	17,19,21	0.75	1 (5%)
3	NAG	E	601	1	14,14,15	0.92	1 (7%)	17,19,21	0.75	0
3	NAG	E	602	1	14,14,15	0.98	1 (7%)	17,19,21	1.28	2 (11%)
3	NAG	D	601	1	14,14,15	0.61	0	17,19,21	0.59	0
3	NAG	B	601	1	14,14,15	1.23	2 (14%)	17,19,21	1.03	2 (11%)
3	NAG	A	601	1	14,14,15	0.89	2 (14%)	17,19,21	0.98	1 (5%)
3	NAG	G	602	1	14,14,15	1.13	1 (7%)	17,19,21	1.10	1 (5%)

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
3	NAG	F	602	1	-	2/6/23/26	0/1/1/1
3	NAG	H	602	1	-	3/6/23/26	0/1/1/1
3	NAG	A	602	1	-	2/6/23/26	0/1/1/1
3	NAG	G	601	1	-	2/6/23/26	0/1/1/1
3	NAG	F	601	1	-	3/6/23/26	0/1/1/1
3	NAG	C	602	1	-	3/6/23/26	0/1/1/1
3	NAG	D	602	1	-	3/6/23/26	0/1/1/1
3	NAG	B	602	1	-	6/6/23/26	0/1/1/1
3	NAG	H	601	1	-	2/6/23/26	0/1/1/1
3	NAG	C	601	1	-	0/6/23/26	0/1/1/1
3	NAG	E	601	1	-	1/6/23/26	0/1/1/1
3	NAG	E	602	1	-	3/6/23/26	0/1/1/1
3	NAG	D	601	1	-	2/6/23/26	0/1/1/1
3	NAG	B	601	1	-	3/6/23/26	0/1/1/1
3	NAG	A	601	1	-	2/6/23/26	0/1/1/1
3	NAG	G	602	1	-	3/6/23/26	0/1/1/1

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	602	NAG	C1-C2	6.16	1.60	1.52
3	A	602	NAG	O5-C1	4.25	1.50	1.43
3	G	602	NAG	C1-C2	3.94	1.57	1.52
3	B	601	NAG	C1-C2	3.91	1.57	1.52
3	D	602	NAG	O5-C1	3.63	1.49	1.43
3	F	601	NAG	C1-C2	3.40	1.57	1.52
3	G	601	NAG	C1-C2	3.28	1.56	1.52
3	C	602	NAG	O5-C1	3.25	1.49	1.43
3	H	602	NAG	C1-C2	3.24	1.56	1.52
3	E	602	NAG	O5-C1	3.11	1.48	1.43
3	F	601	NAG	O5-C1	3.06	1.48	1.43
3	C	601	NAG	O5-C1	3.01	1.48	1.43
3	E	601	NAG	C1-C2	2.95	1.56	1.52
3	H	602	NAG	O5-C1	2.82	1.48	1.43
3	C	601	NAG	C1-C2	2.72	1.56	1.52
3	G	601	NAG	O5-C1	2.40	1.47	1.43
3	F	602	NAG	O5-C1	2.33	1.47	1.43
3	F	602	NAG	C1-C2	2.32	1.55	1.52
3	A	601	NAG	C1-C2	2.15	1.55	1.52
3	A	601	NAG	O5-C1	2.08	1.47	1.43
3	B	601	NAG	O5-C1	2.01	1.47	1.43

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	602	NAG	C2-N2-C7	4.91	129.48	122.90
3	A	602	NAG	C1-O5-C5	4.42	118.11	112.19
3	E	602	NAG	C1-O5-C5	4.24	117.87	112.19
3	F	602	NAG	C1-O5-C5	4.21	117.83	112.19
3	G	602	NAG	C1-O5-C5	3.61	117.02	112.19
3	D	602	NAG	C1-O5-C5	3.44	116.79	112.19
3	A	601	NAG	C1-O5-C5	3.19	116.46	112.19
3	G	601	NAG	C1-O5-C5	3.19	116.45	112.19
3	H	602	NAG	C2-N2-C7	2.99	126.91	122.90
3	D	602	NAG	C2-N2-C7	2.96	126.87	122.90
3	B	601	NAG	C1-O5-C5	2.63	115.72	112.19
3	B	601	NAG	C2-N2-C7	2.57	126.34	122.90
3	C	601	NAG	C1-O5-C5	2.50	115.54	112.19
3	B	602	NAG	C3-C4-C5	2.27	114.34	110.23
3	B	602	NAG	C1-O5-C5	2.22	115.16	112.19
3	E	602	NAG	C2-N2-C7	2.19	125.83	122.90
3	B	602	NAG	C1-C2-N2	2.01	113.60	110.43

There are no chirality outliers.

All (40) torsion outliers are listed below:

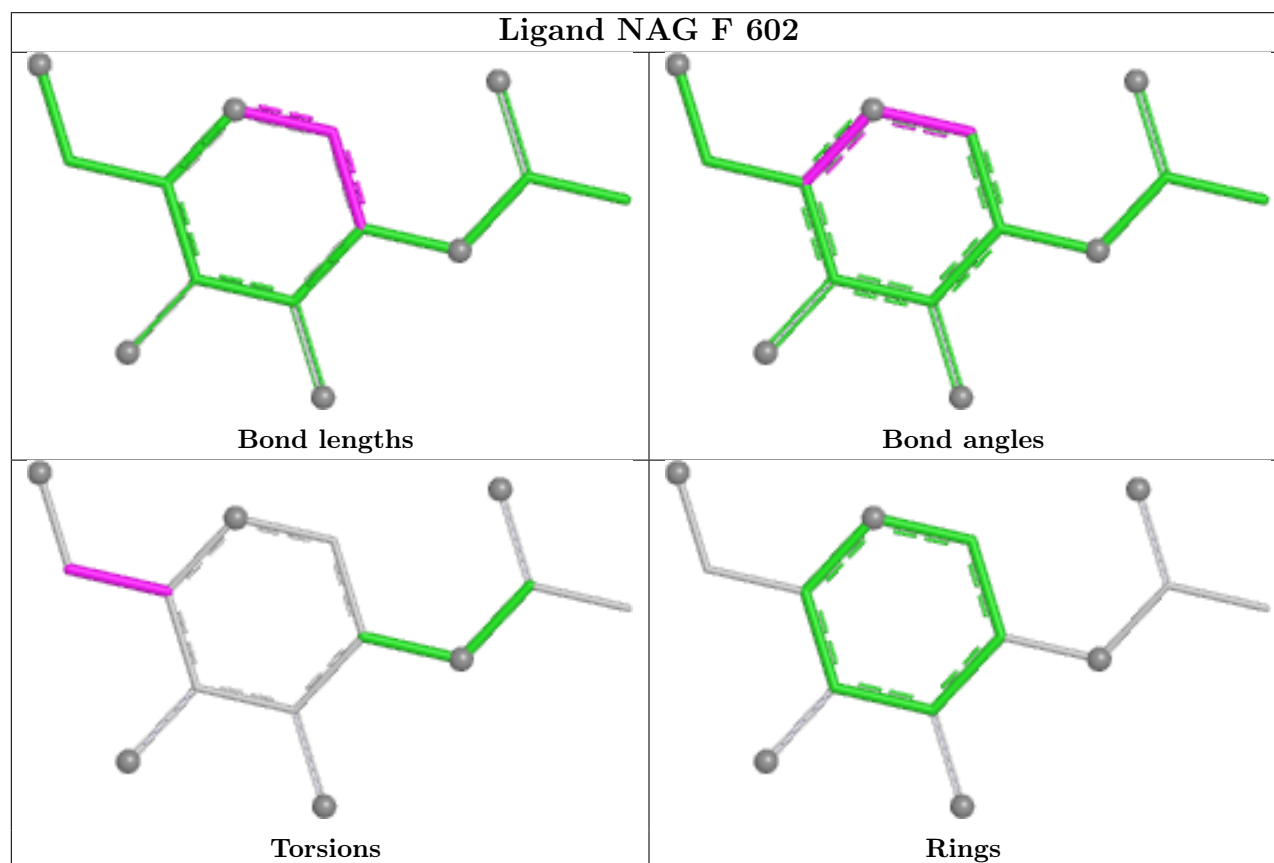
Mol	Chain	Res	Type	Atoms
3	D	602	NAG	C1-C2-N2-C7
3	H	602	NAG	C3-C2-N2-C7
3	B	602	NAG	O5-C5-C6-O6
3	G	601	NAG	C4-C5-C6-O6
3	B	601	NAG	O5-C5-C6-O6
3	A	602	NAG	O5-C5-C6-O6
3	B	602	NAG	C4-C5-C6-O6
3	G	601	NAG	O5-C5-C6-O6
3	F	601	NAG	O5-C5-C6-O6
3	G	602	NAG	O5-C5-C6-O6
3	D	602	NAG	O5-C5-C6-O6
3	H	601	NAG	O5-C5-C6-O6
3	A	602	NAG	C4-C5-C6-O6
3	H	602	NAG	O5-C5-C6-O6
3	F	602	NAG	O5-C5-C6-O6
3	A	601	NAG	C4-C5-C6-O6
3	F	602	NAG	C4-C5-C6-O6
3	G	602	NAG	C4-C5-C6-O6
3	E	602	NAG	C4-C5-C6-O6
3	B	601	NAG	C4-C5-C6-O6
3	H	601	NAG	C4-C5-C6-O6
3	A	601	NAG	O5-C5-C6-O6
3	C	602	NAG	C8-C7-N2-C2
3	C	602	NAG	O7-C7-N2-C2
3	B	602	NAG	C8-C7-N2-C2
3	B	602	NAG	O7-C7-N2-C2
3	D	601	NAG	O5-C5-C6-O6
3	E	602	NAG	O5-C5-C6-O6
3	F	601	NAG	C4-C5-C6-O6
3	C	602	NAG	O5-C5-C6-O6
3	H	602	NAG	C4-C5-C6-O6
3	D	601	NAG	C4-C5-C6-O6
3	E	601	NAG	O5-C5-C6-O6
3	B	601	NAG	C3-C2-N2-C7
3	E	602	NAG	C3-C2-N2-C7
3	D	602	NAG	C4-C5-C6-O6
3	B	602	NAG	C1-C2-N2-C7
3	F	601	NAG	C3-C2-N2-C7
3	G	602	NAG	C1-C2-N2-C7
3	B	602	NAG	C3-C2-N2-C7

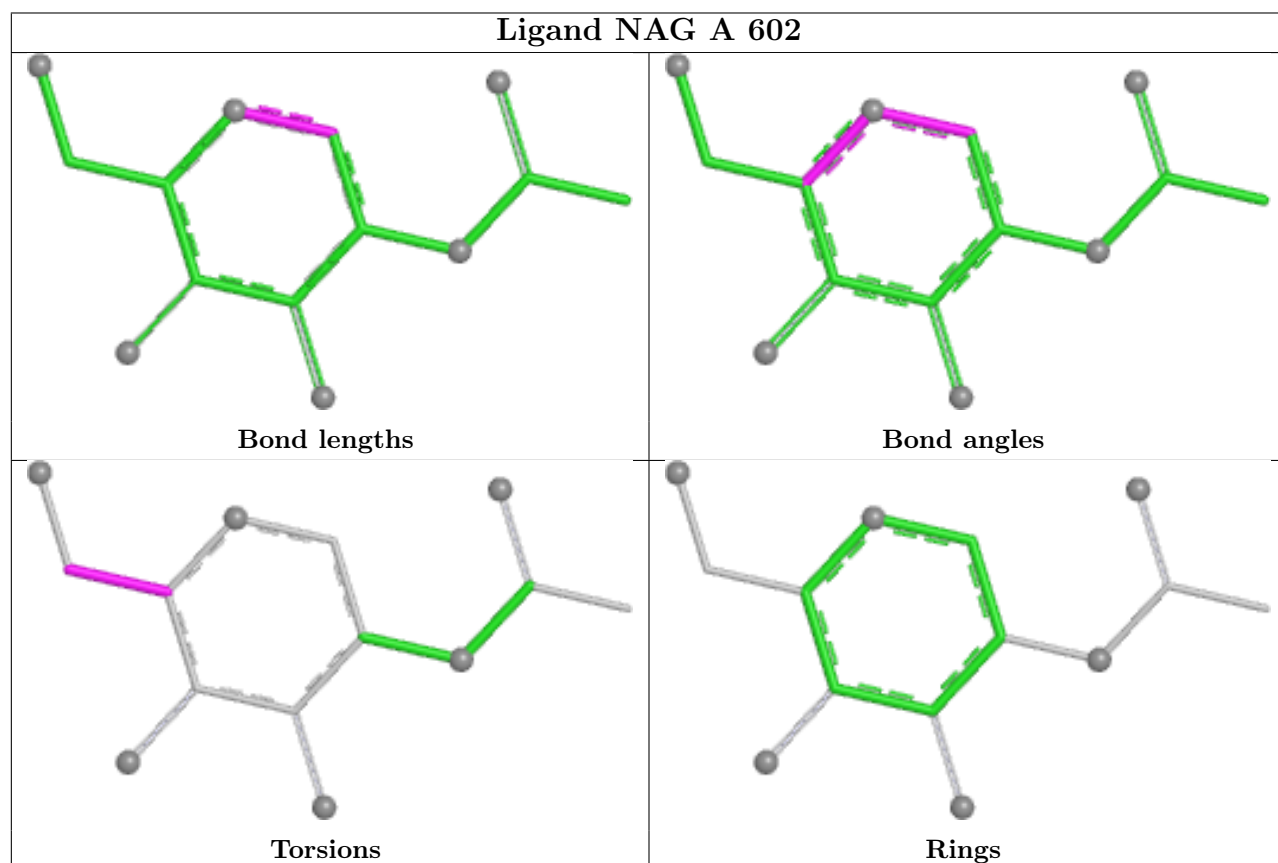
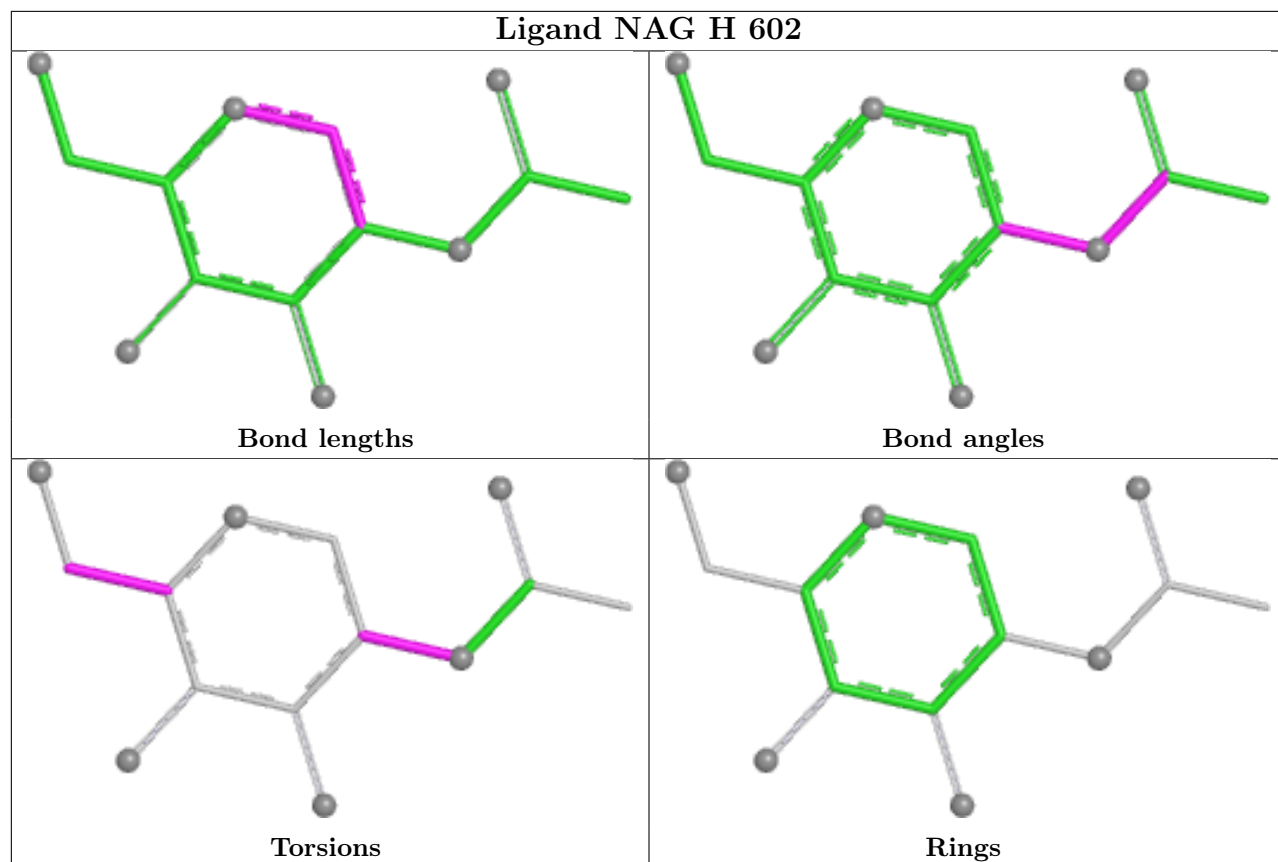
There are no ring outliers.

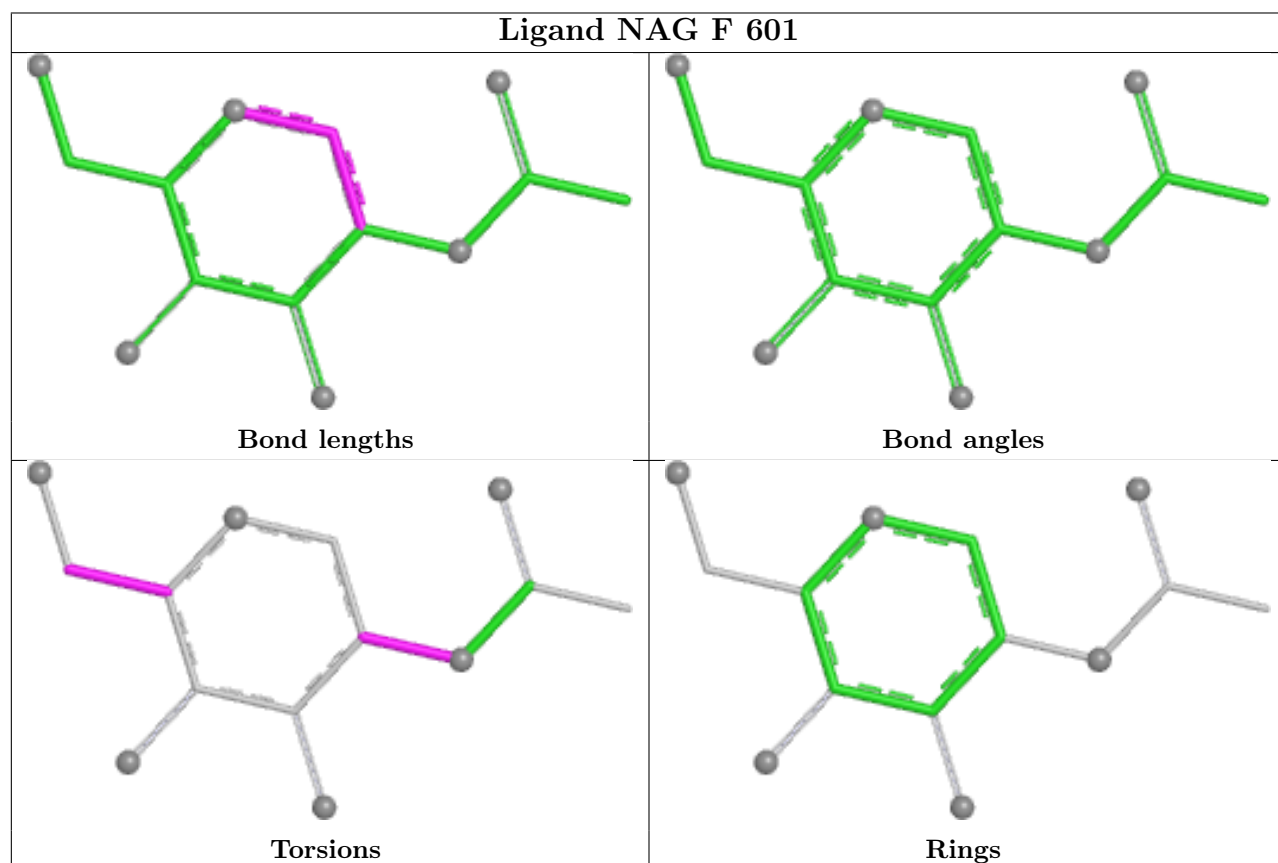
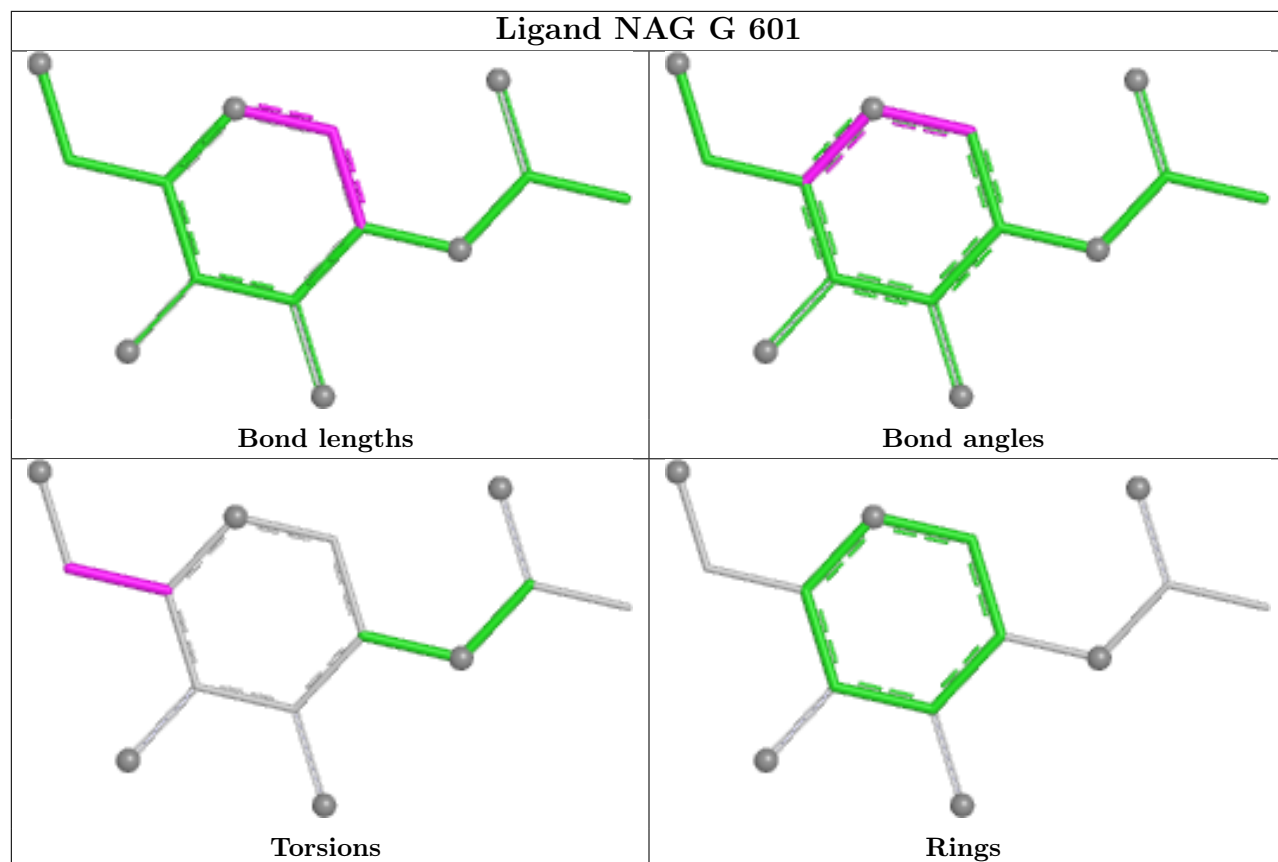
6 monomers are involved in 6 short contacts:

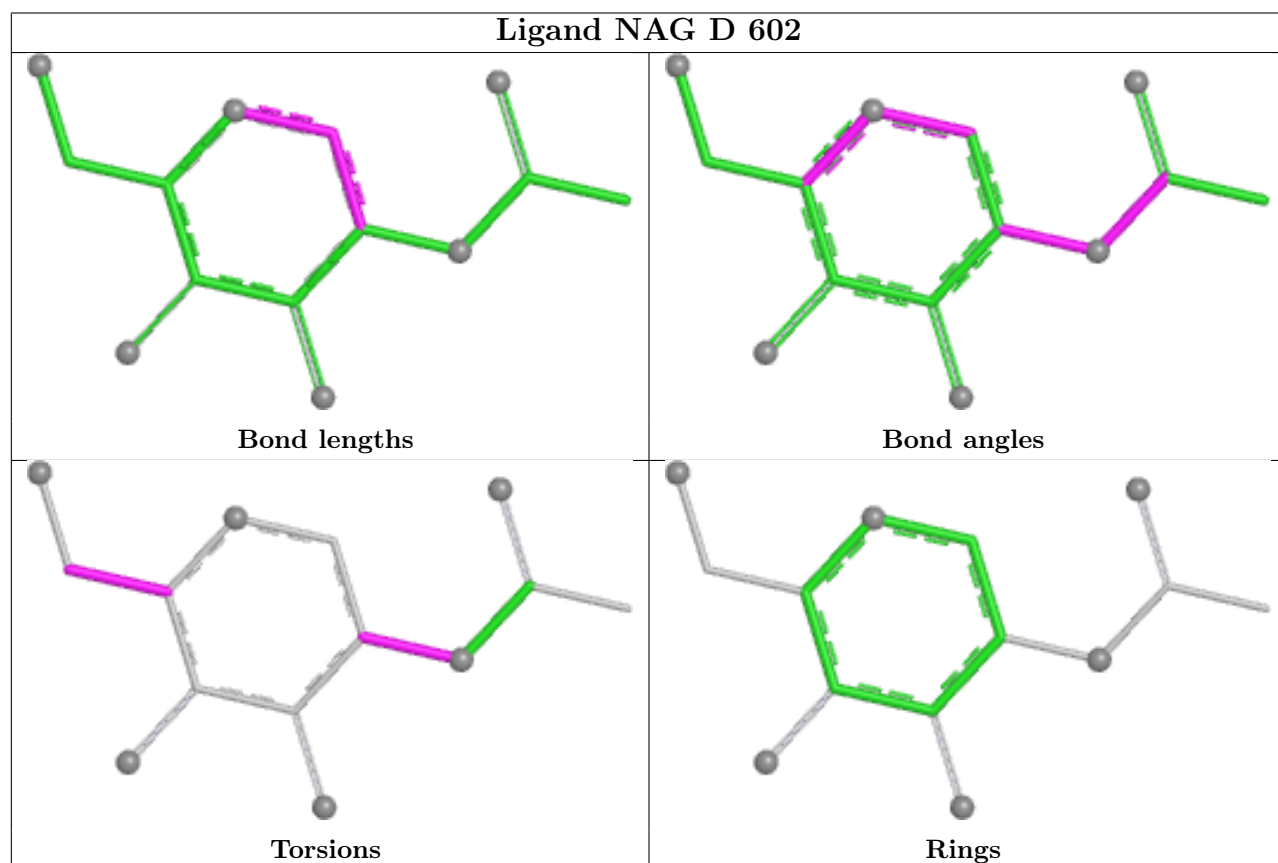
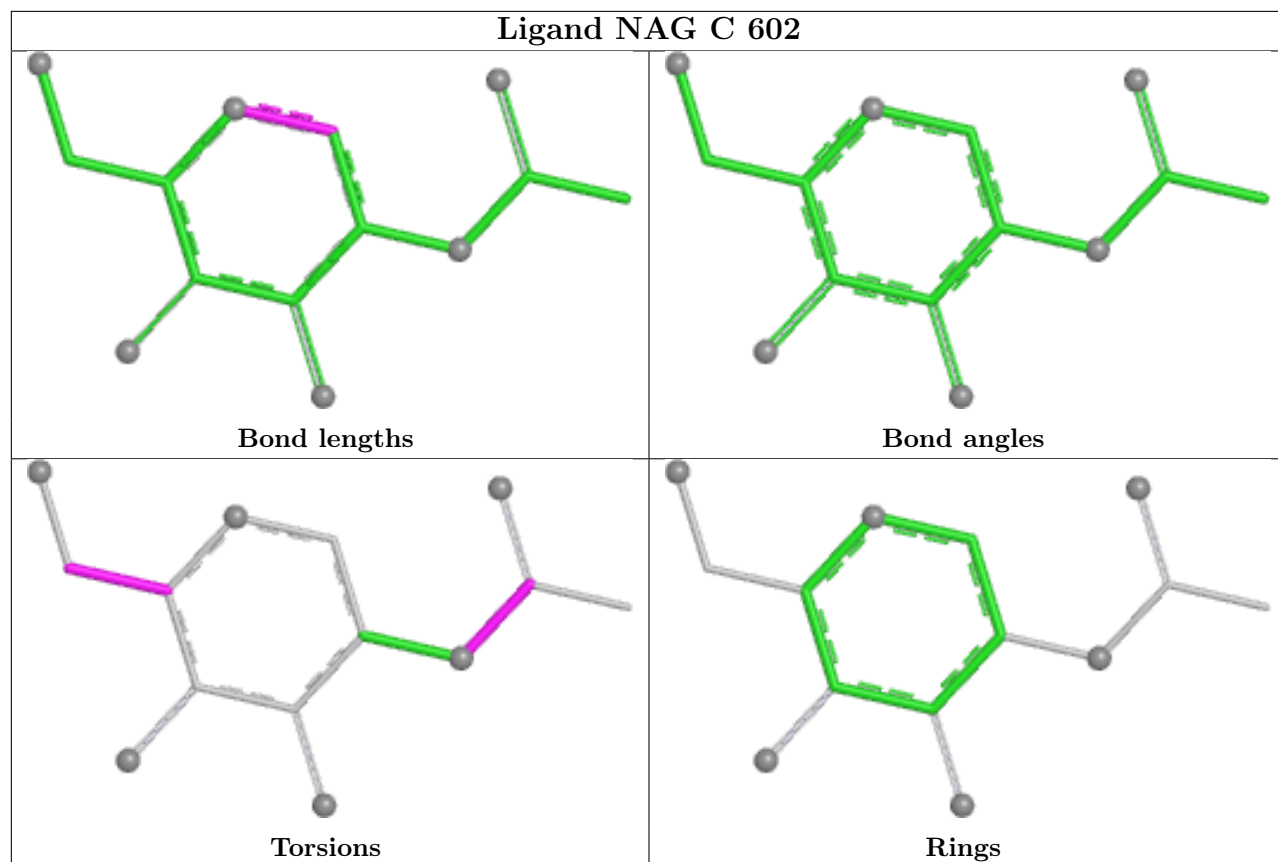
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	H	602	NAG	1	0
3	F	601	NAG	1	0
3	C	602	NAG	1	0
3	B	602	NAG	1	0
3	E	602	NAG	1	0
3	B	601	NAG	1	0

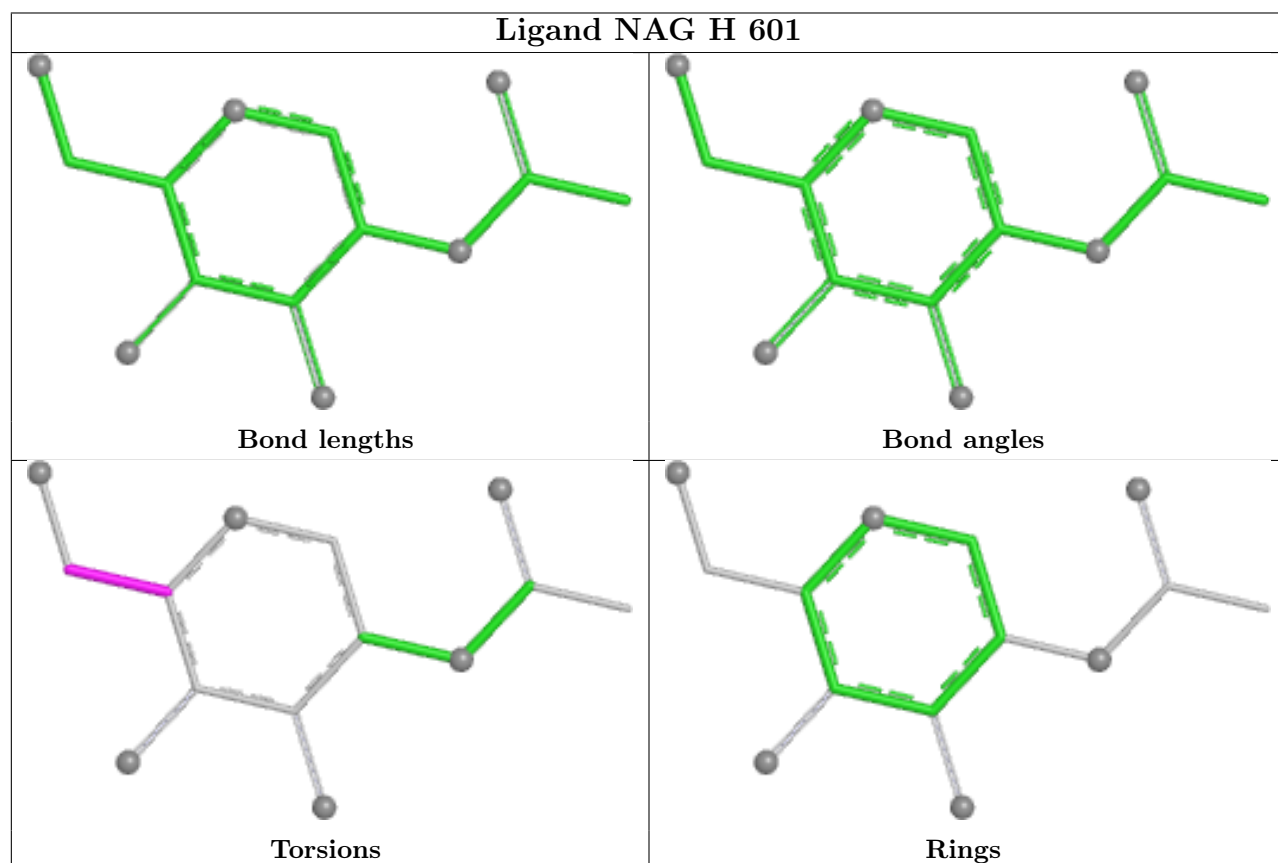
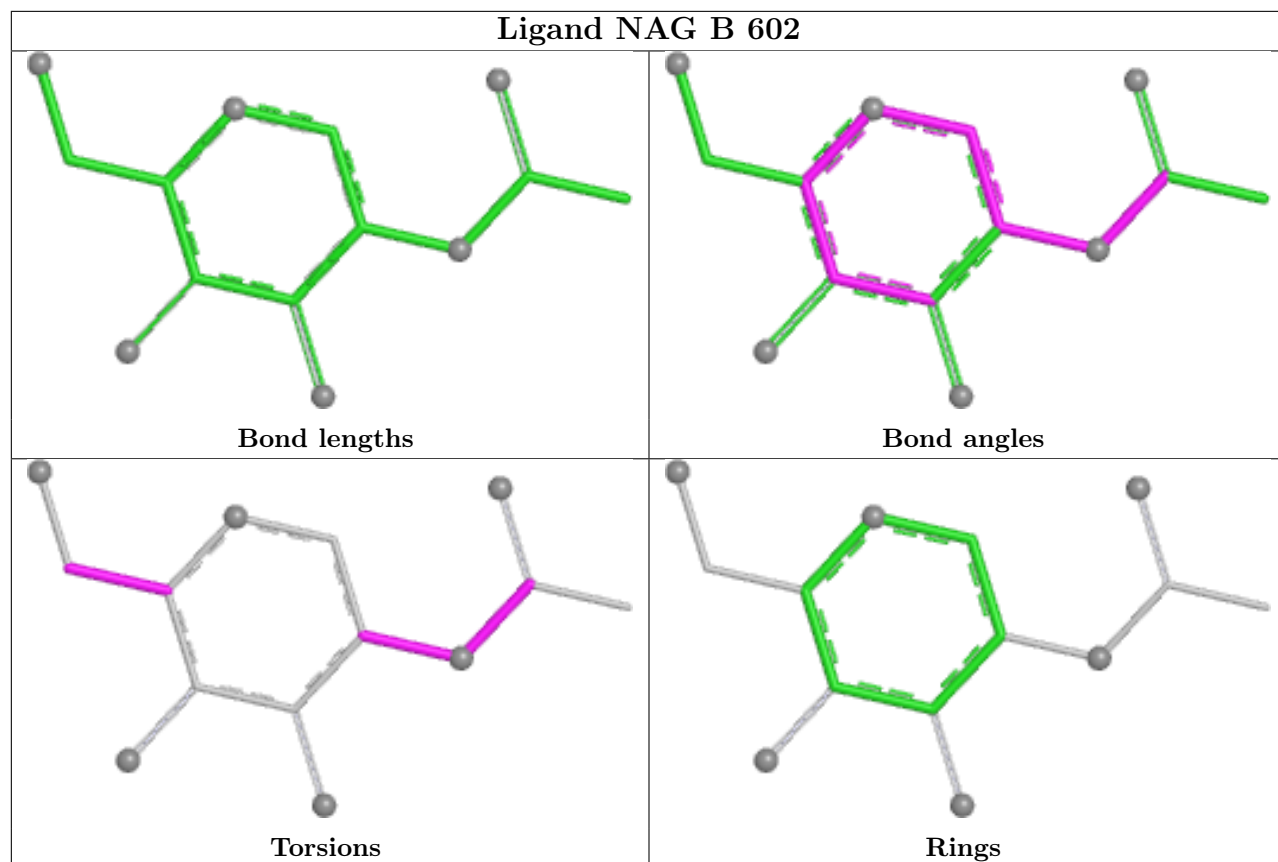
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

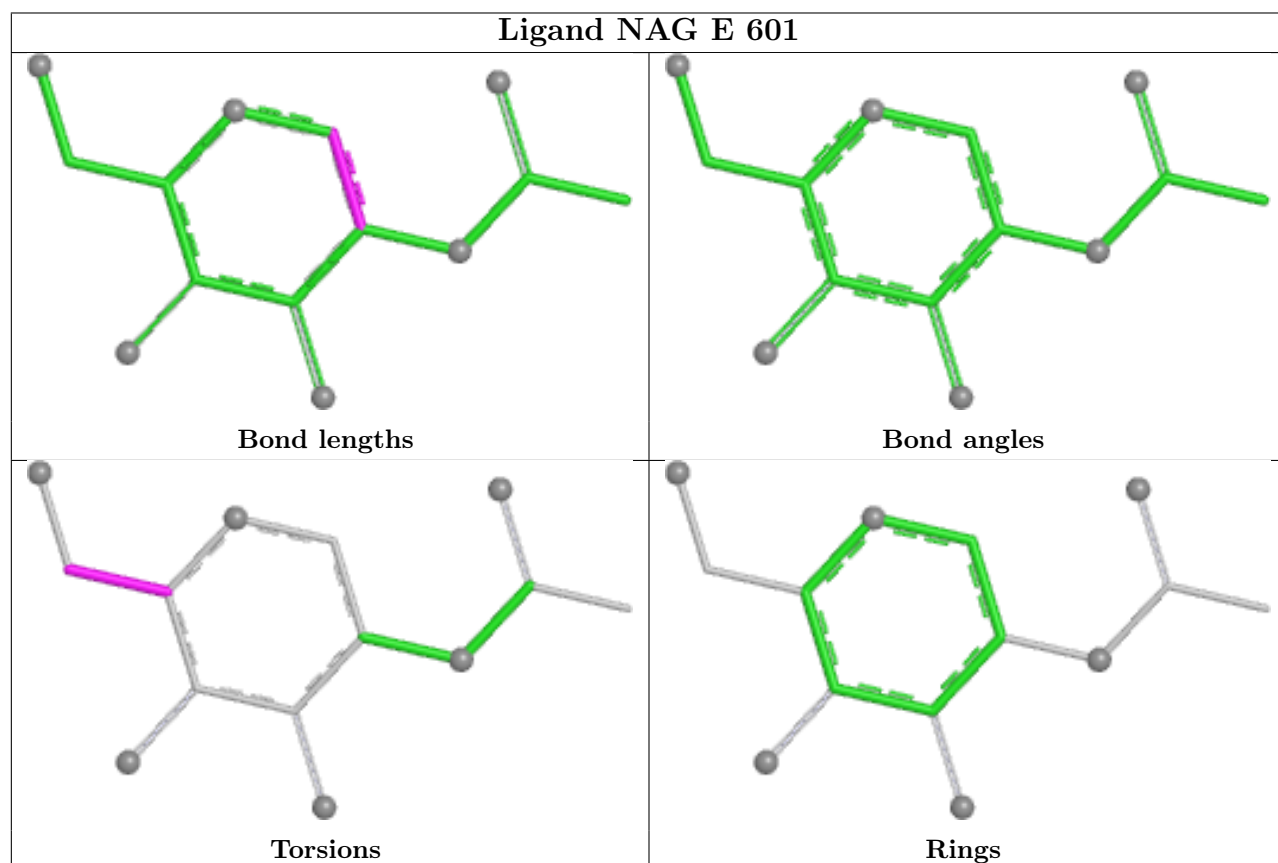
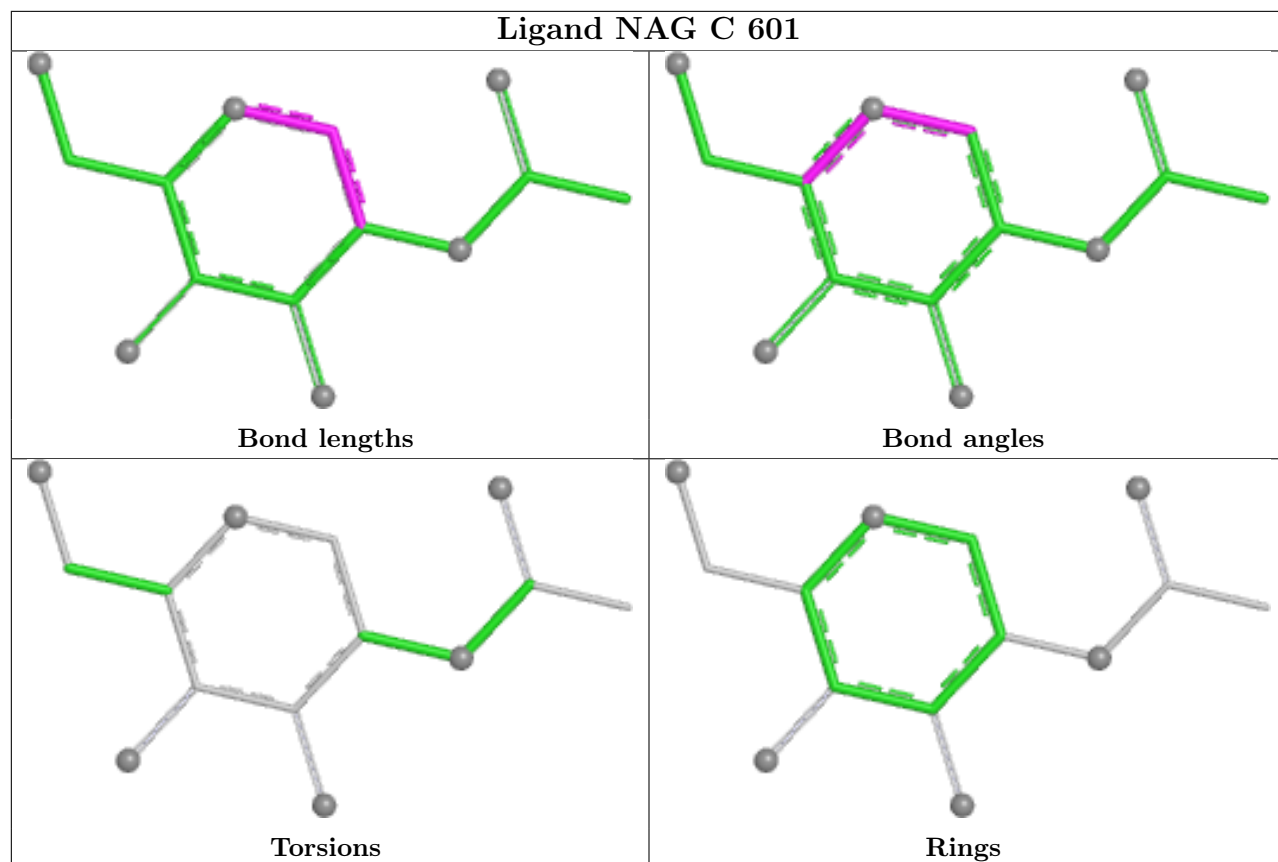


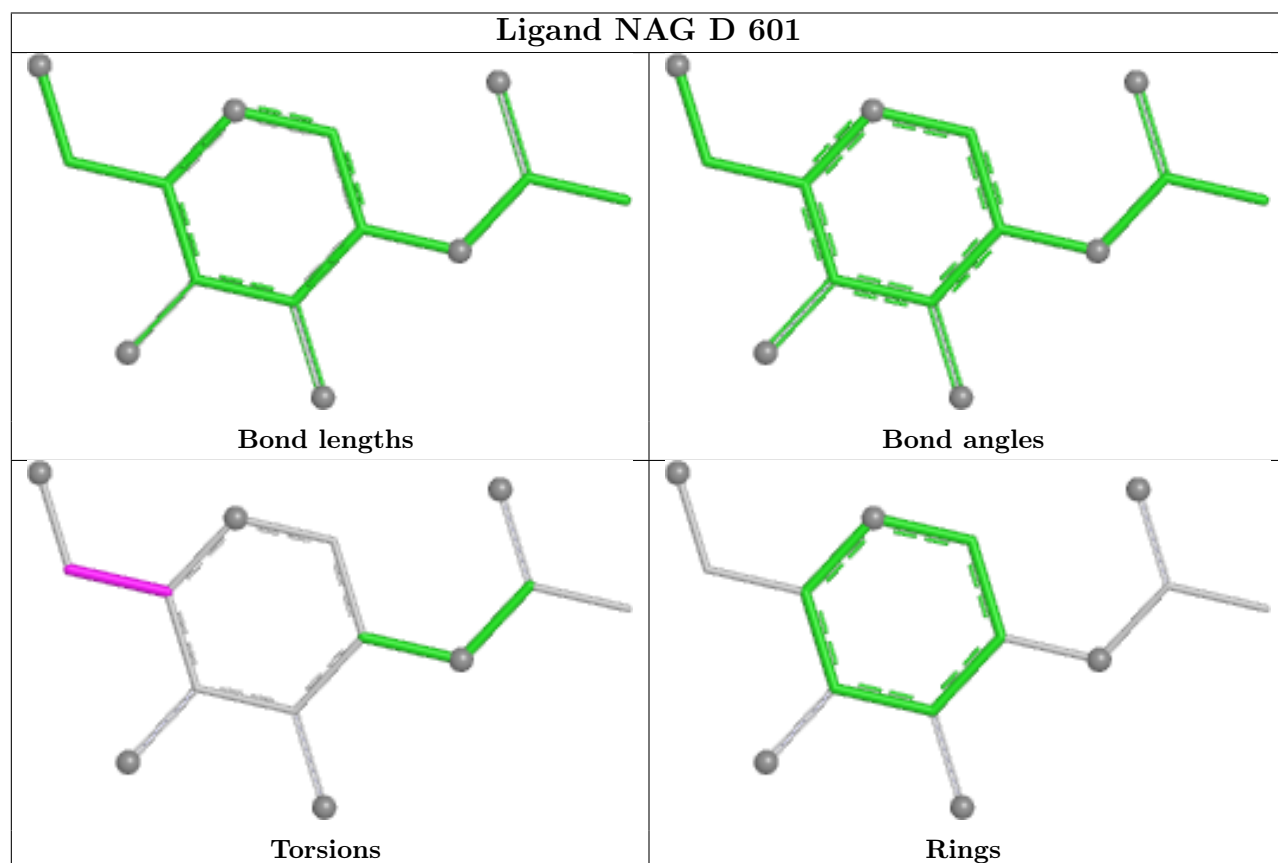
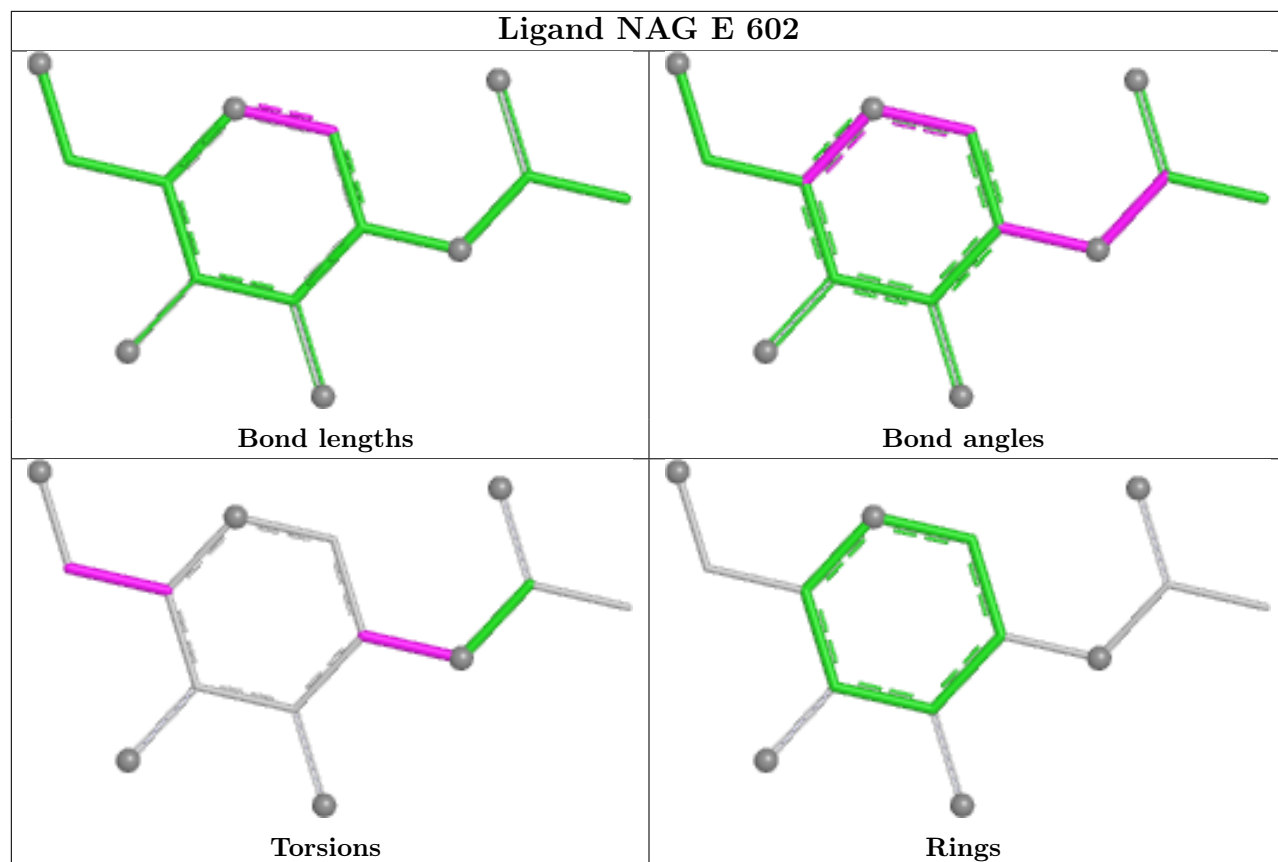


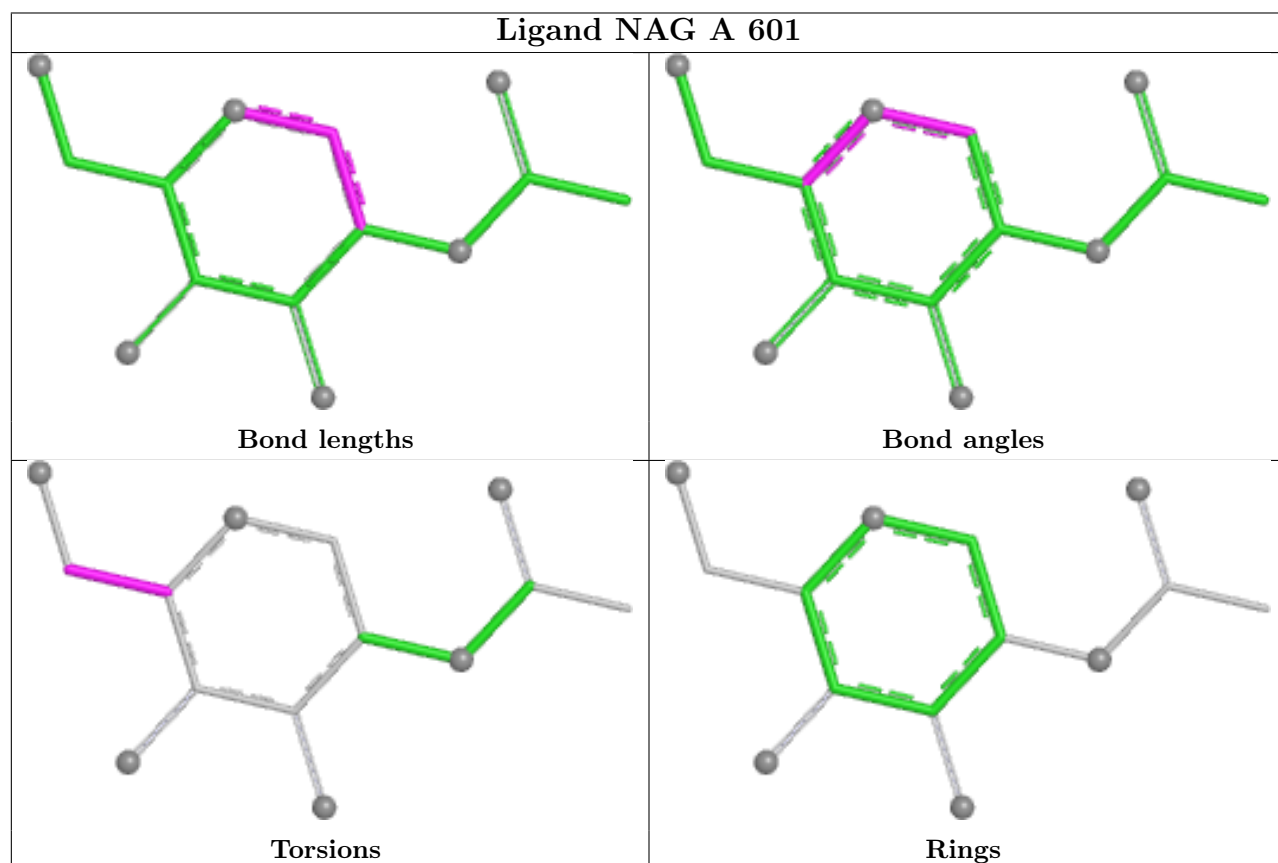
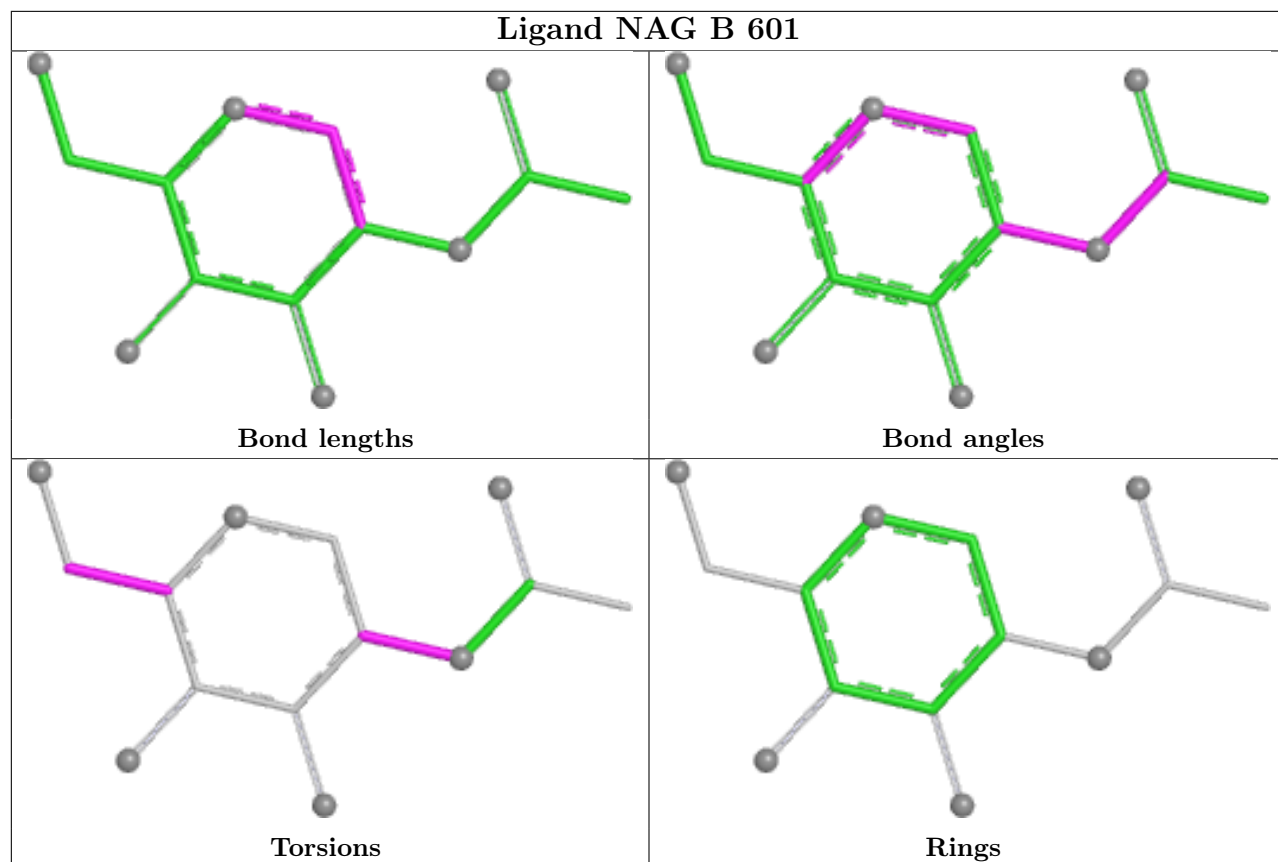


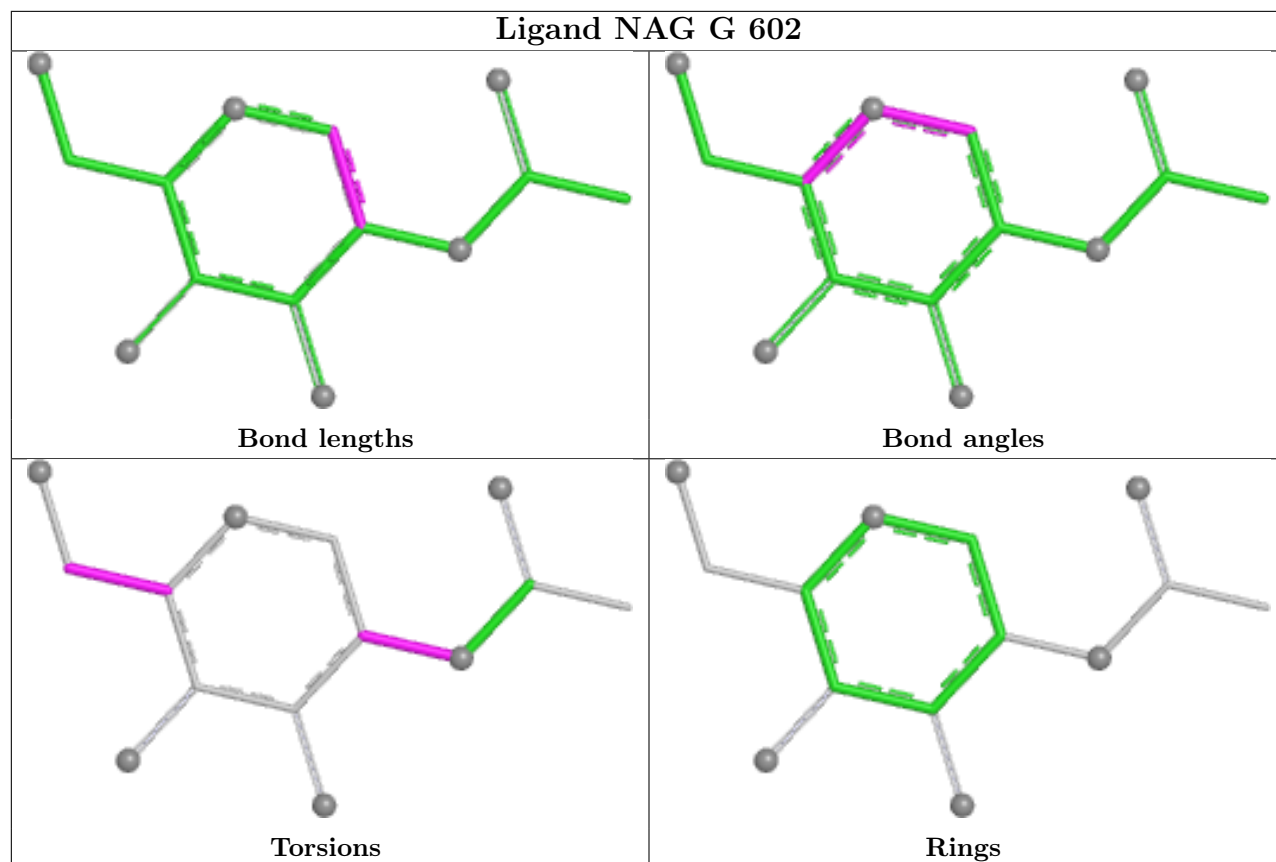












5.7 Other polymers [i](#)

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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	484/518 (93%)	-0.56	0 100 100	44, 64, 93, 110	0
1	B	484/518 (93%)	-0.72	1 (0%) 91 85	40, 55, 80, 121	0
1	C	484/518 (93%)	-0.61	0 100 100	39, 59, 86, 111	0
1	D	482/518 (93%)	-0.63	0 100 100	42, 62, 91, 110	0
1	E	484/518 (93%)	-0.50	1 (0%) 91 85	54, 73, 98, 114	0
1	F	483/518 (93%)	-0.56	0 100 100	54, 69, 95, 117	0
1	G	484/518 (93%)	-0.53	1 (0%) 91 85	45, 69, 95, 118	0
1	H	484/518 (93%)	-0.51	0 100 100	48, 73, 100, 121	0
All	All	3869/4144 (93%)	-0.58	3 (0%) 92 88	39, 66, 94, 121	0

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	501	ALA	3.0
1	G	501	ALA	2.4
1	B	500	ALA	2.2

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](#)

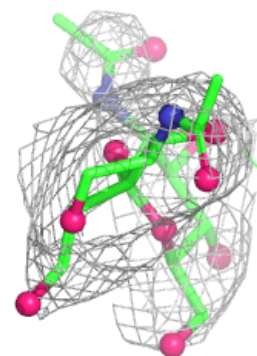
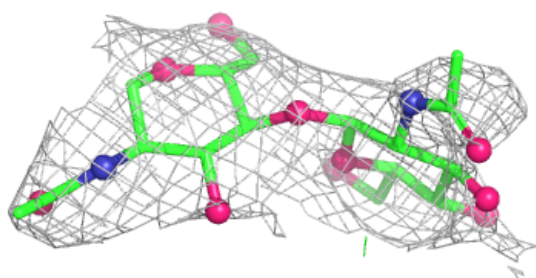
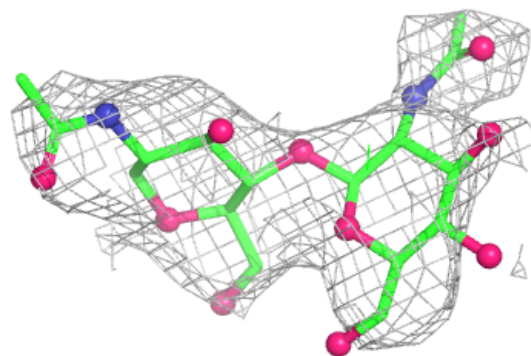
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	NAG	U	2	14/15	0.40	0.13	106,125,128,132	0
2	NAG	I	2	14/15	0.47	0.12	105,118,124,127	0
2	NAG	R	2	14/15	0.52	0.10	99,123,131,133	0
2	NAG	L	2	14/15	0.64	0.10	103,116,125,125	0
2	NAG	K	2	14/15	0.65	0.10	81,105,121,122	0
2	NAG	V	2	14/15	0.67	0.09	89,110,114,116	0
2	NAG	S	2	14/15	0.71	0.09	101,112,118,119	0
2	NAG	X	2	14/15	0.74	0.10	100,117,122,123	0
2	NAG	T	2	14/15	0.75	0.08	87,107,125,126	0
2	NAG	X	1	14/15	0.75	0.10	79,94,101,102	0
2	NAG	P	2	14/15	0.75	0.09	98,107,115,118	0
2	NAG	R	1	14/15	0.76	0.10	97,109,121,123	0
2	NAG	W	2	14/15	0.77	0.09	101,113,124,125	0
2	NAG	O	2	14/15	0.77	0.08	82,102,110,111	0
2	NAG	Q	2	14/15	0.77	0.10	93,113,121,124	0
2	NAG	N	2	14/15	0.79	0.09	97,108,111,114	0
2	NAG	N	1	14/15	0.81	0.08	88,97,101,102	0
2	NAG	M	2	14/15	0.81	0.09	101,119,128,132	0
2	NAG	J	2	14/15	0.83	0.09	112,125,131,131	0
2	NAG	Q	1	14/15	0.86	0.10	81,96,98,101	0
2	NAG	V	1	14/15	0.86	0.09	77,90,100,102	0
2	NAG	W	1	14/15	0.87	0.09	81,104,113,117	0
2	NAG	P	1	14/15	0.87	0.07	75,88,98,100	0
2	NAG	S	1	14/15	0.88	0.08	74,98,105,108	0
2	NAG	U	1	14/15	0.88	0.09	79,95,108,111	0
2	NAG	I	1	14/15	0.88	0.08	82,99,108,114	0
2	NAG	L	1	14/15	0.90	0.08	75,90,106,108	0
2	NAG	J	1	14/15	0.91	0.07	80,95,111,112	0
2	NAG	T	1	14/15	0.92	0.07	73,84,98,101	0
2	NAG	K	1	14/15	0.92	0.08	73,79,93,102	0
2	NAG	M	1	14/15	0.94	0.08	77,97,116,122	0
2	NAG	O	1	14/15	0.95	0.06	57,69,78,86	0

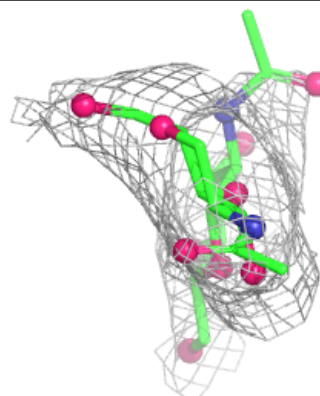
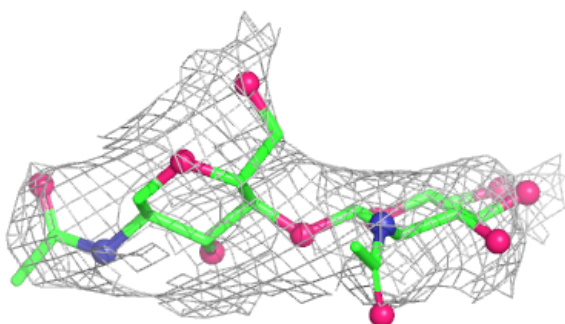
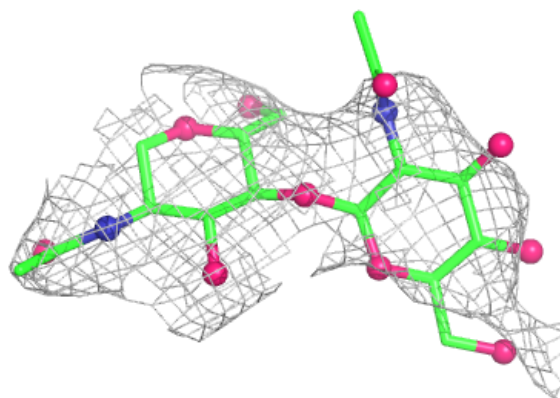
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around Chain I:

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

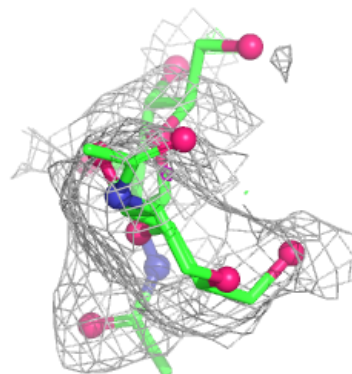
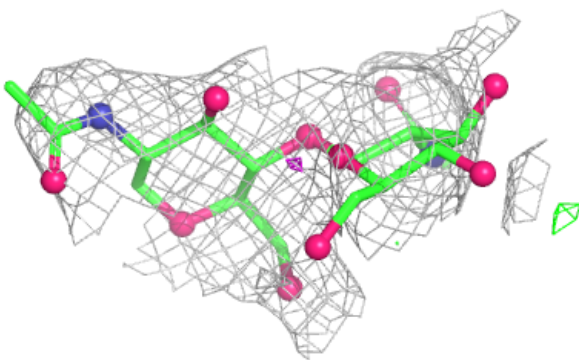
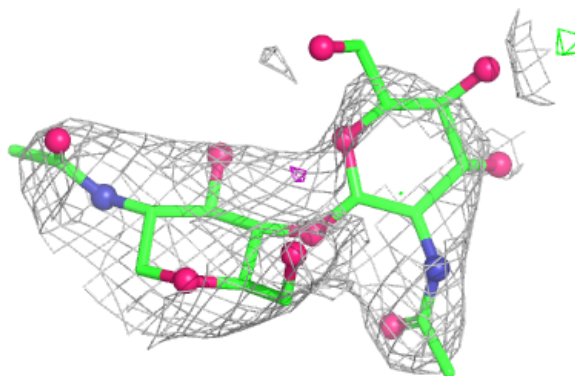
**Electron density around Chain J:**

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

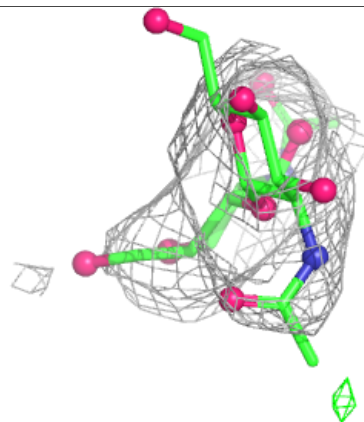
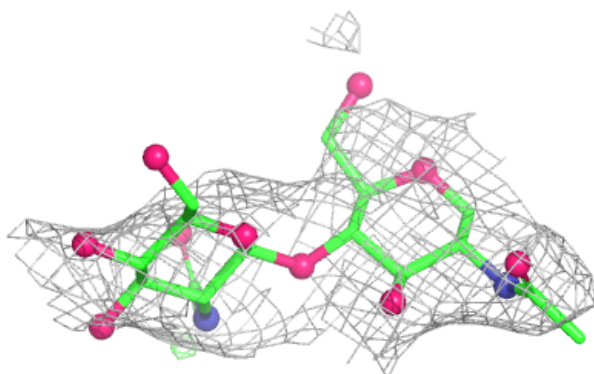
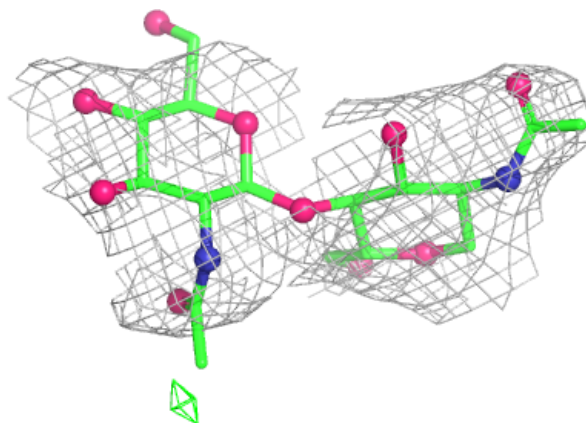


Electron density around Chain K:

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

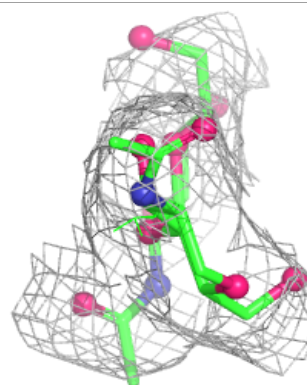
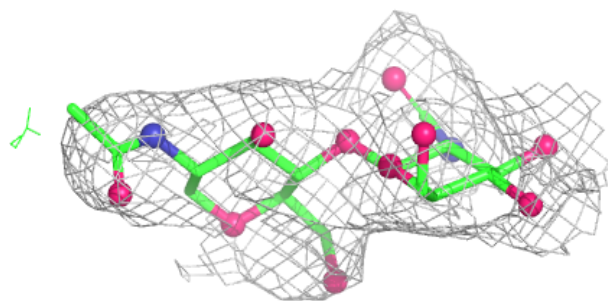
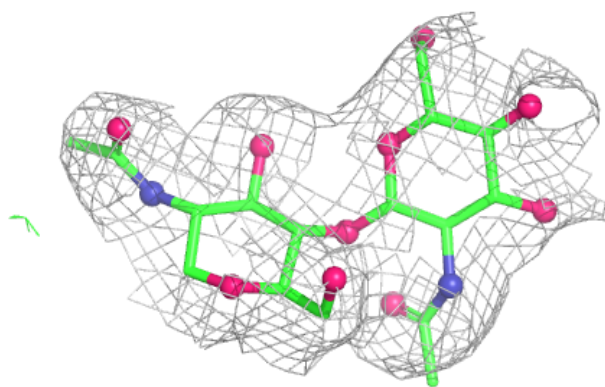
**Electron density around Chain L:**

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

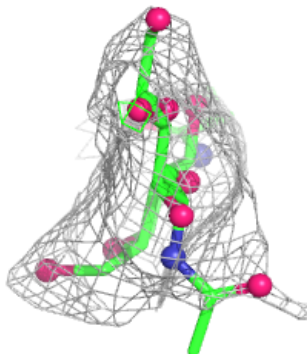
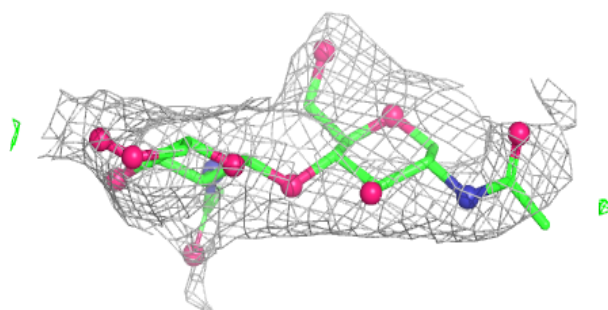
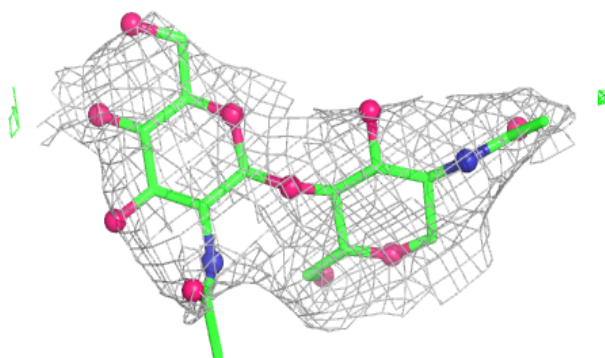


Electron density around Chain M:

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

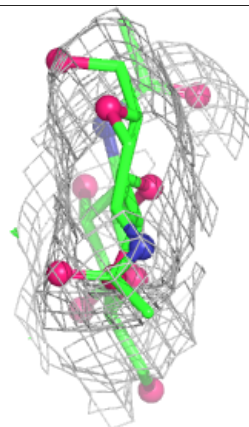
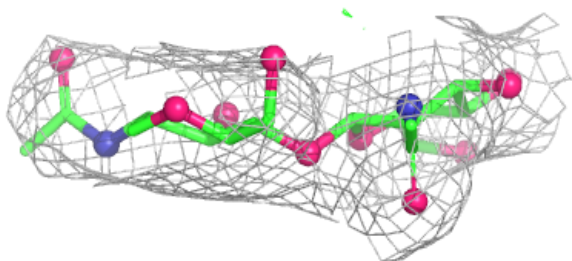
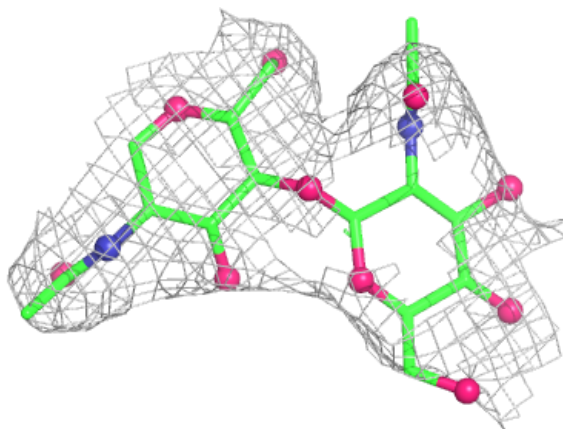
**Electron density around Chain N:**

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

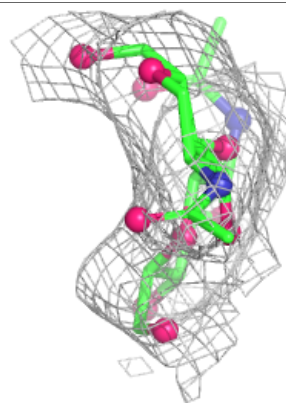
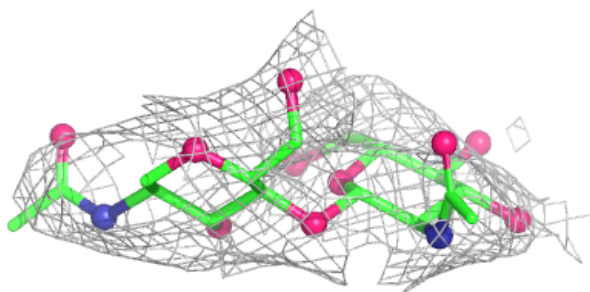
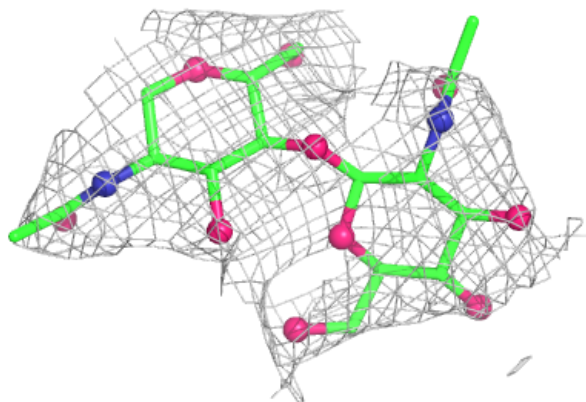


Electron density around Chain O:

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

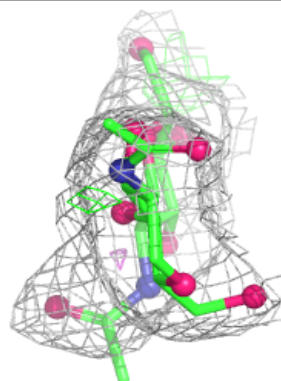
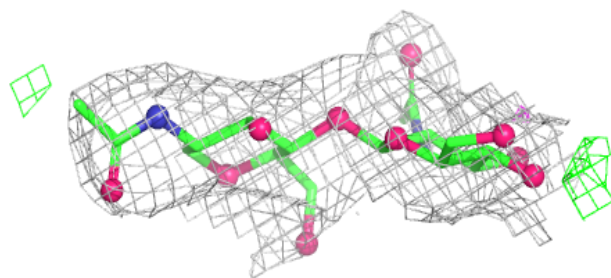
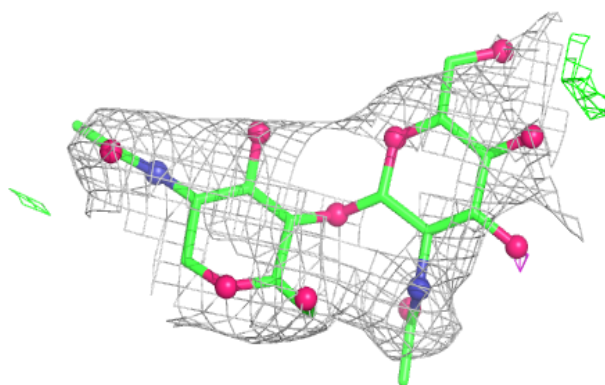
**Electron density around Chain P:**

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



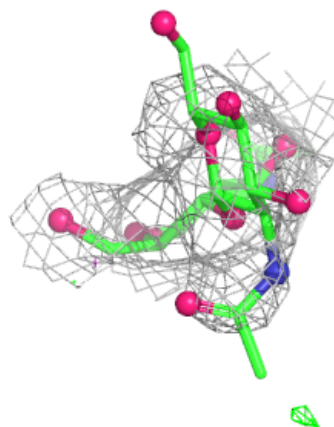
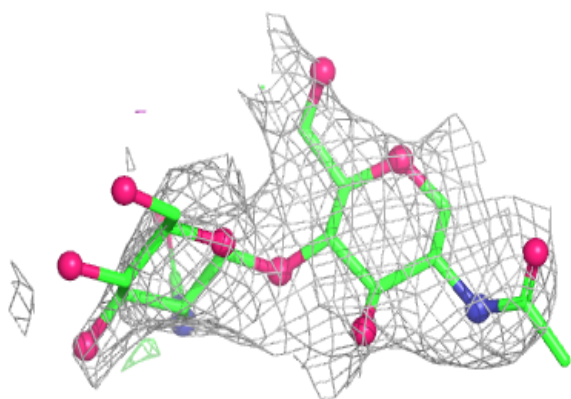
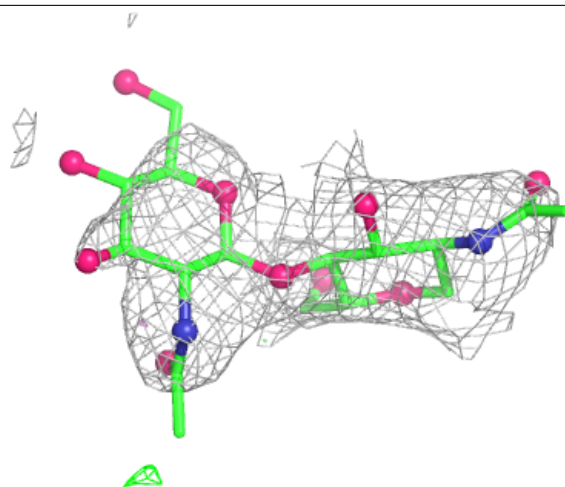
Electron density around Chain Q:

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



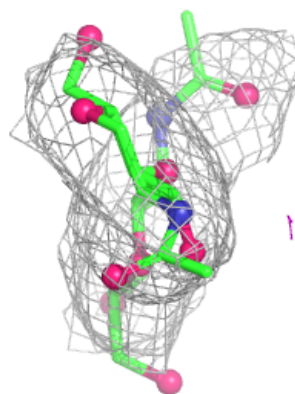
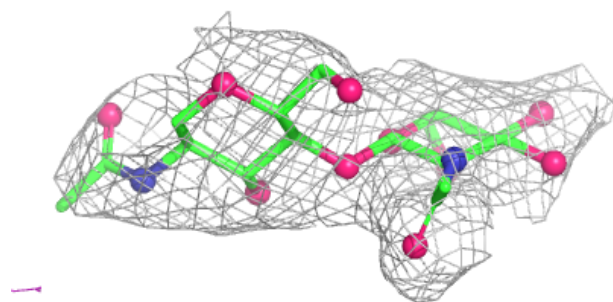
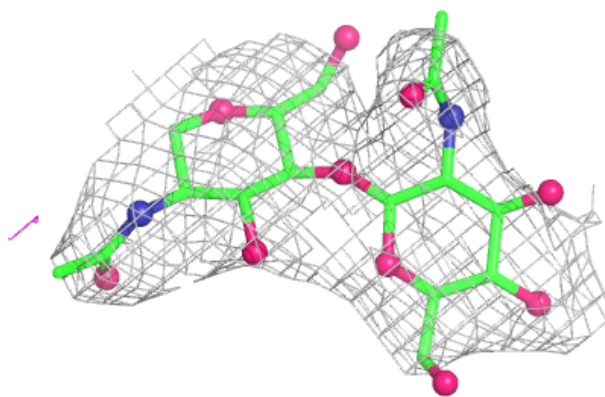
Electron density around Chain R:

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

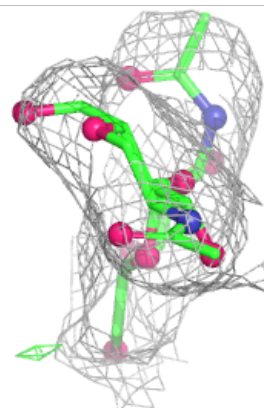
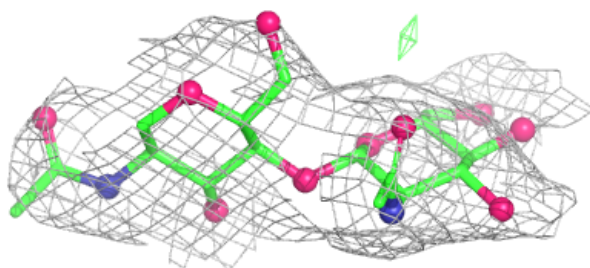
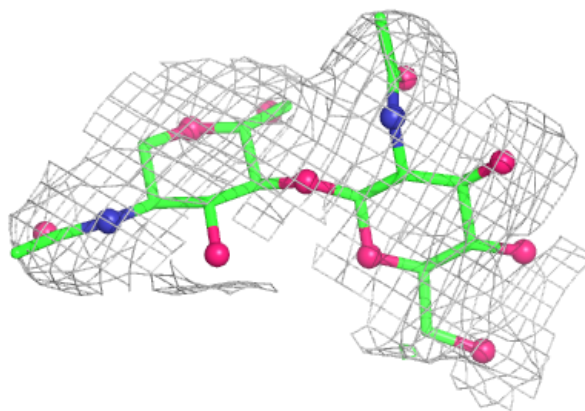


Electron density around Chain S:

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

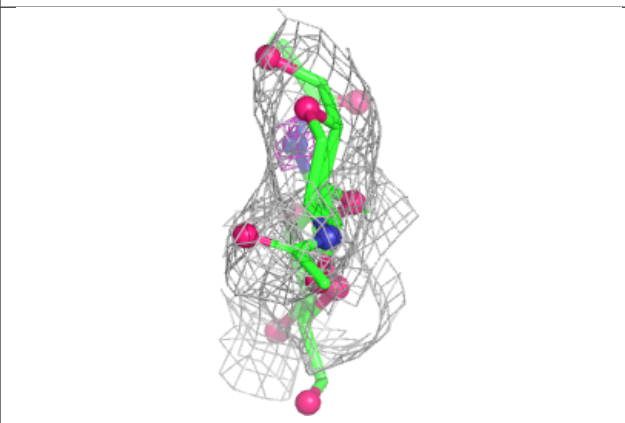
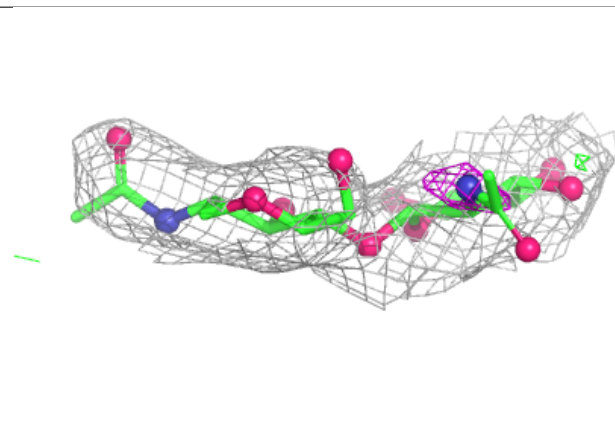
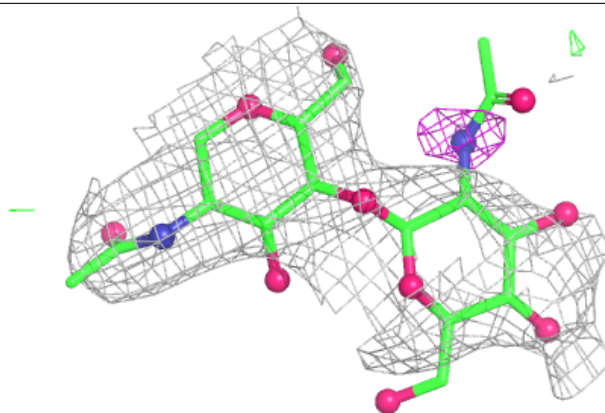
**Electron density around Chain T:**

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

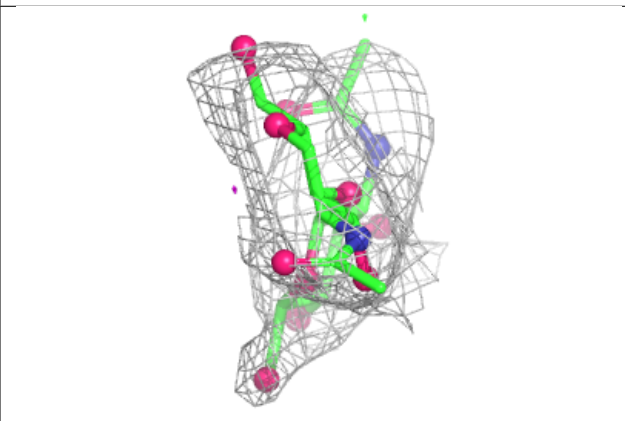
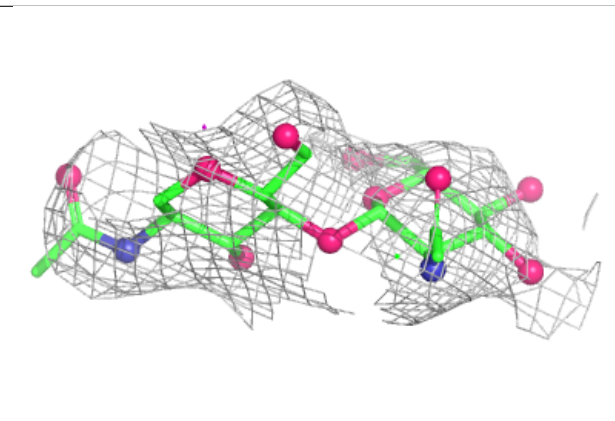
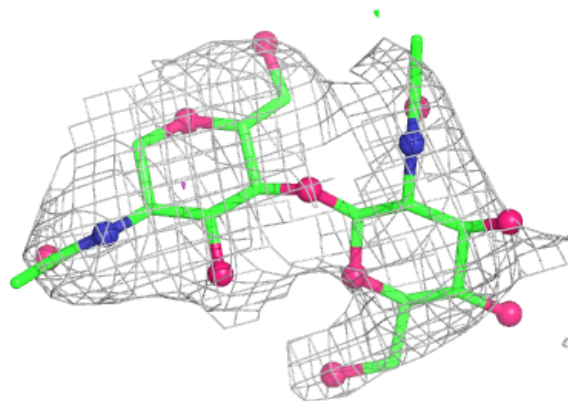


Electron density around Chain U:

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

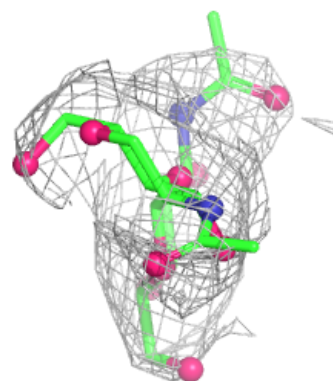
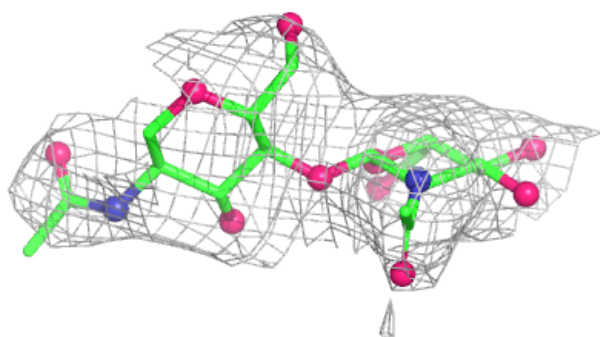
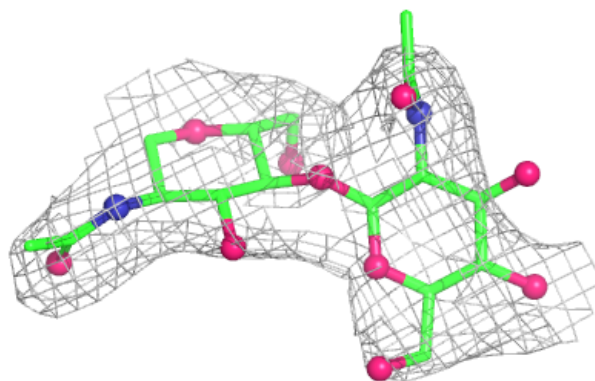
**Electron density around Chain V:**

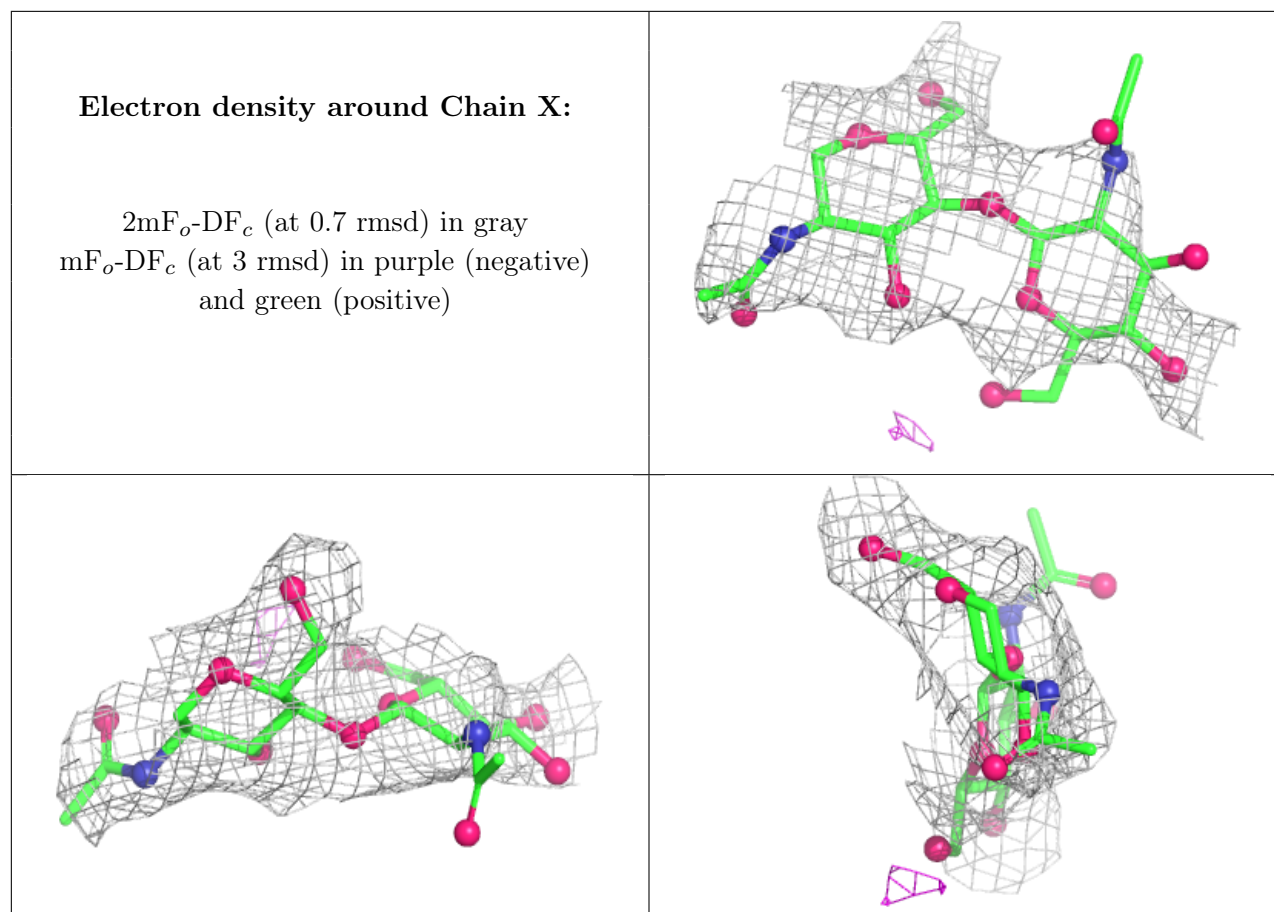
$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around Chain W:

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





6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	NAG	F	602	14/15	0.48	0.13	90,104,118,121	0
3	NAG	H	602	14/15	0.55	0.13	92,99,111,112	0
3	NAG	E	602	14/15	0.57	0.12	104,112,117,121	0
3	NAG	G	602	14/15	0.59	0.10	101,116,123,123	0
3	NAG	D	602	14/15	0.59	0.13	85,111,120,121	0
3	NAG	G	601	14/15	0.64	0.11	103,110,113,114	0
3	NAG	B	601	14/15	0.65	0.12	87,108,114,116	0
3	NAG	C	601	14/15	0.65	0.14	92,105,113,113	0
3	NAG	F	601	14/15	0.67	0.10	105,126,129,129	0
3	NAG	A	601	14/15	0.68	0.10	78,99,116,121	0
3	NAG	H	601	14/15	0.68	0.09	93,109,113,117	0
3	NAG	D	601	14/15	0.72	0.12	91,110,116,120	0

Continued on next page...

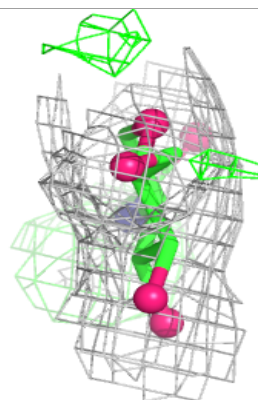
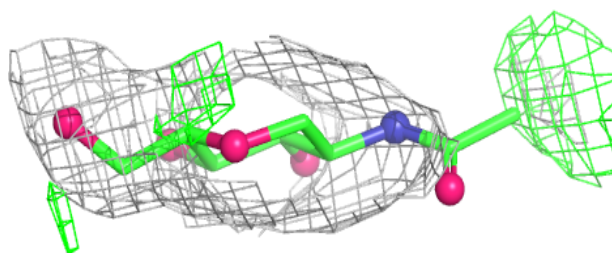
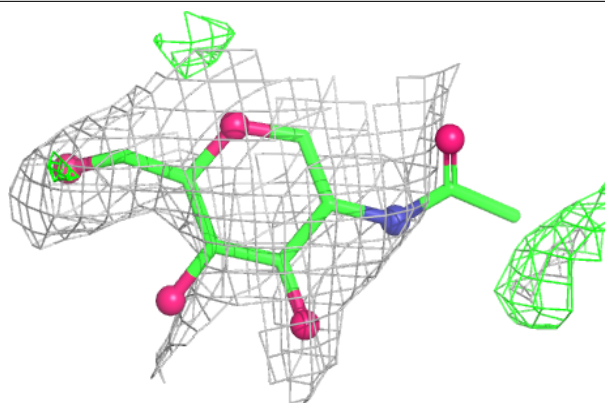
Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	NAG	A	602	14/15	0.73	0.10	80,96,104,105	0
3	NAG	C	602	14/15	0.73	0.10	87,100,106,107	0
3	NAG	B	602	14/15	0.76	0.12	76,92,103,106	0
3	NAG	E	601	14/15	0.77	0.09	94,107,111,116	0
4	MG	C	603	1/1	0.82	0.21	55,55,55,55	0
4	MG	A	603	1/1	0.85	0.14	64,64,64,64	0
4	MG	H	603	1/1	0.86	0.21	73,73,73,73	0
4	MG	D	603	1/1	0.89	0.17	62,62,62,62	0
4	MG	B	603	1/1	0.90	0.20	50,50,50,50	0
4	MG	E	603	1/1	0.92	0.23	58,58,58,58	0
4	MG	G	603	1/1	0.94	0.09	61,61,61,61	0
5	ZN	G	604	1/1	0.94	0.17	102,102,102,102	0
5	ZN	D	604	1/1	0.95	0.16	132,132,132,132	0
4	MG	F	603	1/1	0.95	0.15	54,54,54,54	0
6	CA	C	605	1/1	0.95	0.04	82,82,82,82	0
6	CA	D	605	1/1	0.96	0.06	70,70,70,70	0
6	CA	A	605	1/1	0.96	0.06	88,88,88,88	0
5	ZN	A	606	1/1	0.97	0.08	91,91,91,91	0
5	ZN	A	604	1/1	0.97	0.07	67,67,67,67	0
6	CA	G	605	1/1	0.97	0.05	77,77,77,77	0
5	ZN	F	606	1/1	0.98	0.06	90,90,90,90	0
5	ZN	E	604	1/1	0.98	0.07	74,74,74,74	0
5	ZN	E	606	1/1	0.98	0.03	68,68,68,68	0
5	ZN	C	606	1/1	0.98	0.06	76,76,76,76	0
5	ZN	C	604	1/1	0.98	0.13	76,76,76,76	0
5	ZN	G	606	1/1	0.98	0.07	83,83,83,83	0
5	ZN	H	604	1/1	0.98	0.07	113,113,113,113	0
6	CA	F	605	1/1	0.98	0.03	73,73,73,73	0
6	CA	E	605	1/1	0.98	0.03	90,90,90,90	0
5	ZN	F	604	1/1	0.99	0.06	80,80,80,80	0
5	ZN	D	606	1/1	0.99	0.02	80,80,80,80	0
6	CA	B	605	1/1	0.99	0.04	62,62,62,62	0
5	ZN	B	604	1/1	0.99	0.08	53,53,53,53	0
6	CA	H	605	1/1	0.99	0.03	74,74,74,74	0
5	ZN	B	606	1/1	0.99	0.08	90,90,90,90	0
5	ZN	H	606	1/1	0.99	0.07	82,82,82,82	0

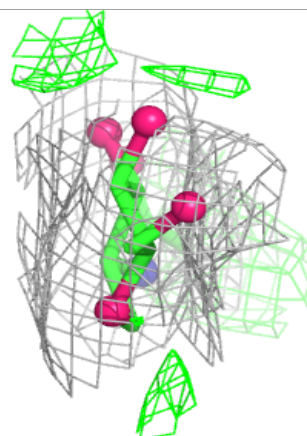
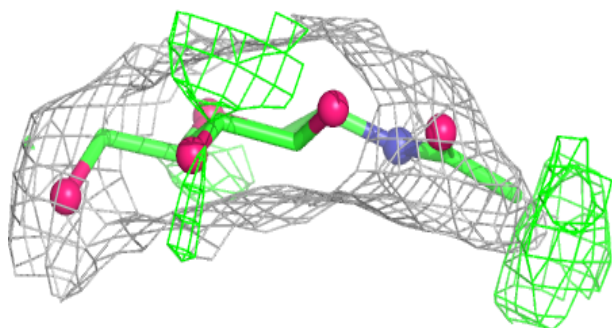
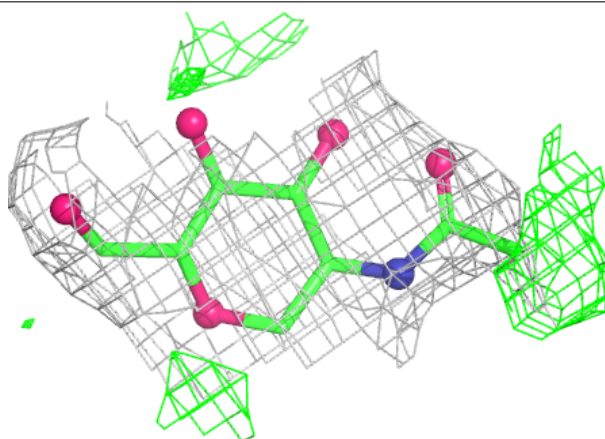
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around NAG F 602:

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

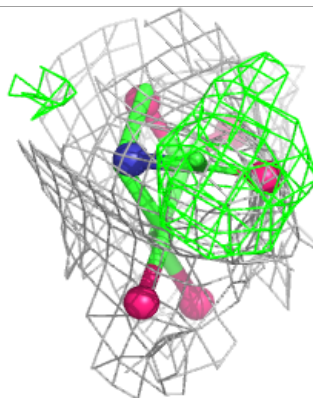
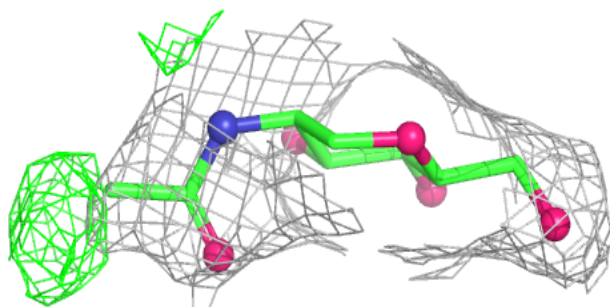
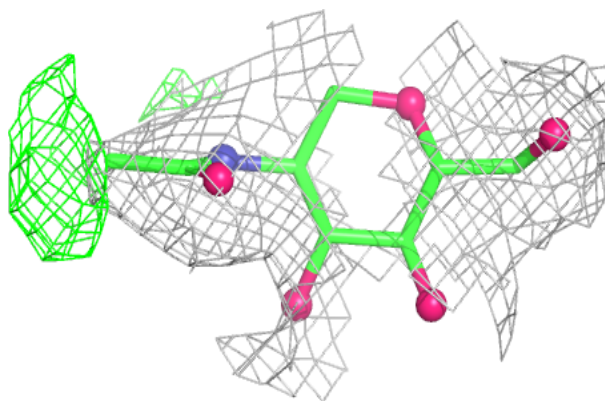
**Electron density around NAG H 602:**

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

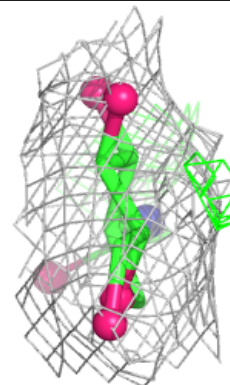
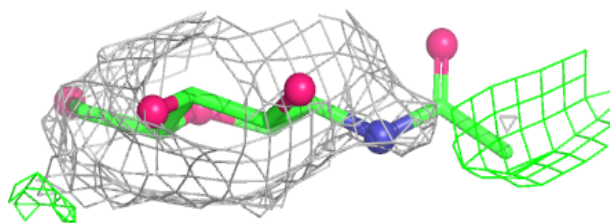
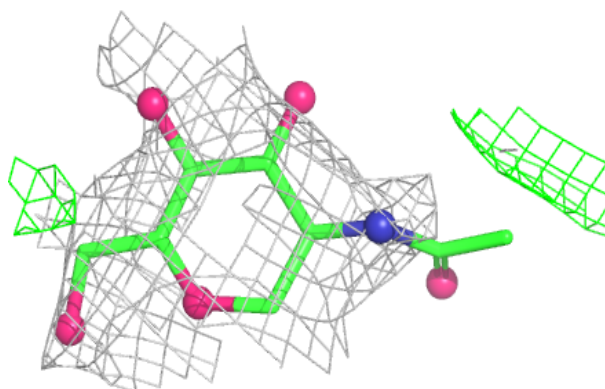


Electron density around NAG E 602:

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

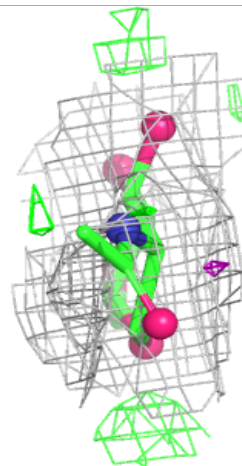
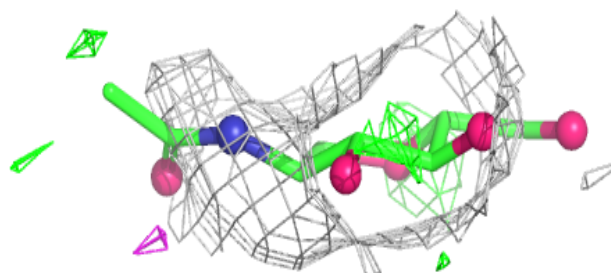
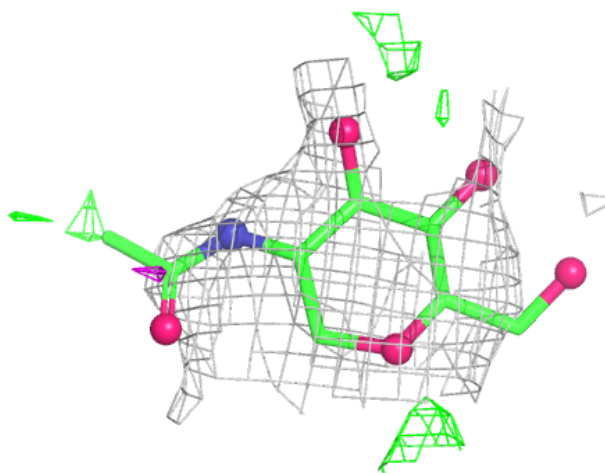
**Electron density around NAG G 602:**

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



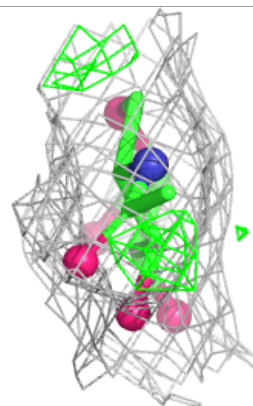
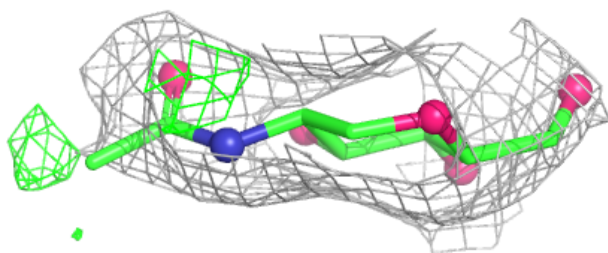
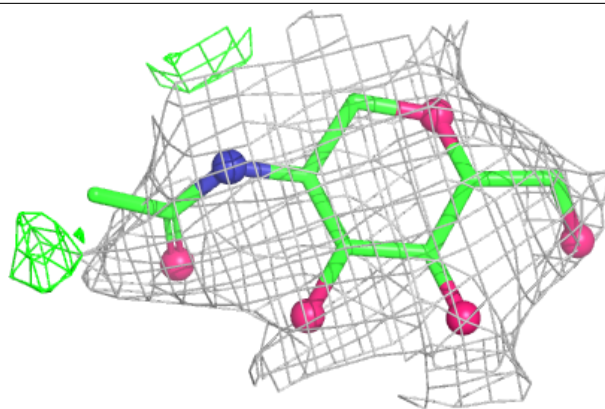
Electron density around NAG D 602:

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



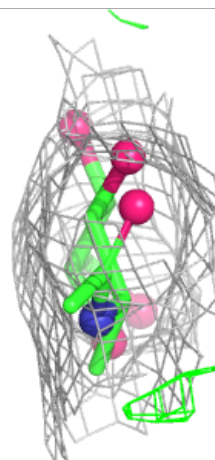
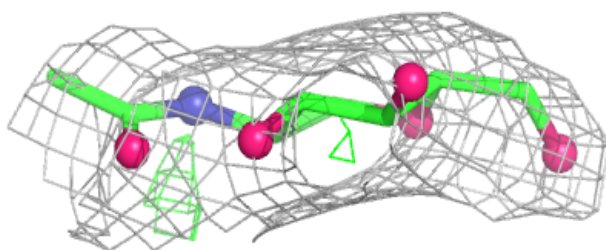
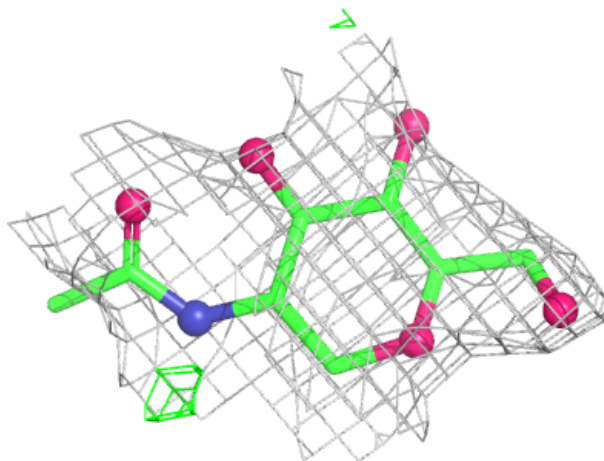
Electron density around NAG G 601:

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



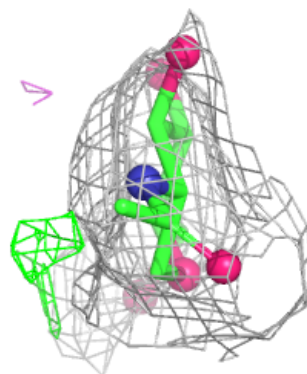
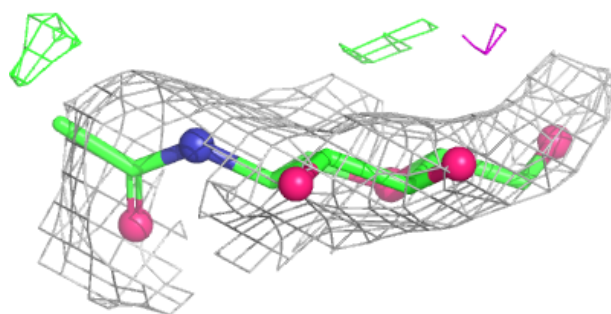
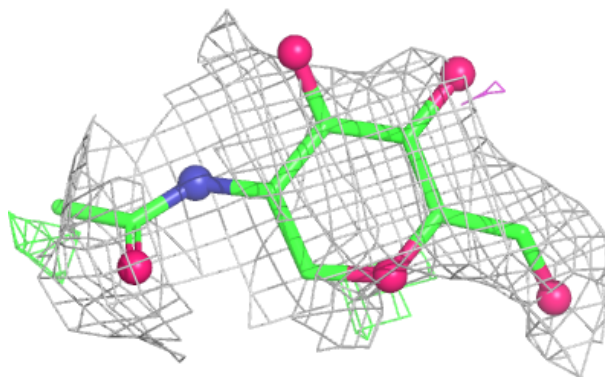
Electron density around NAG B 601:

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

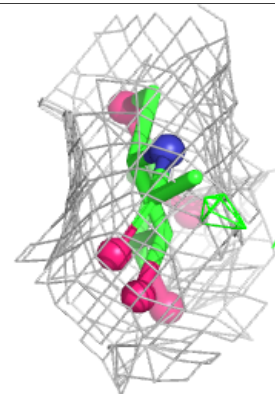
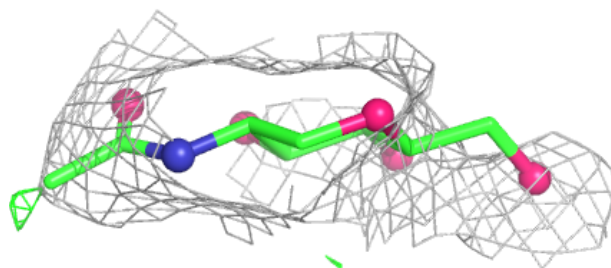
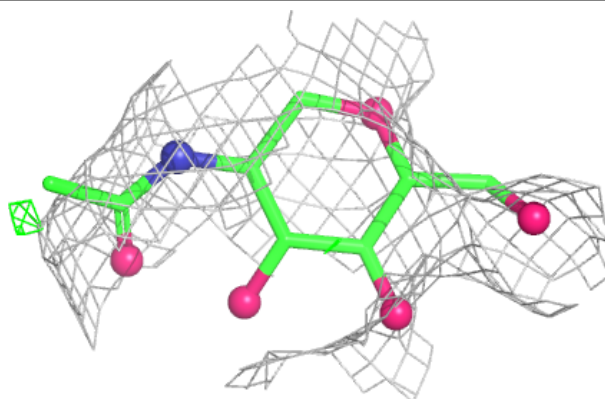


Electron density around NAG C 601:

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

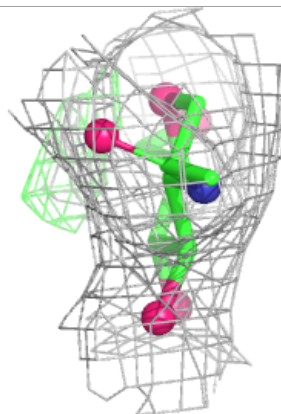
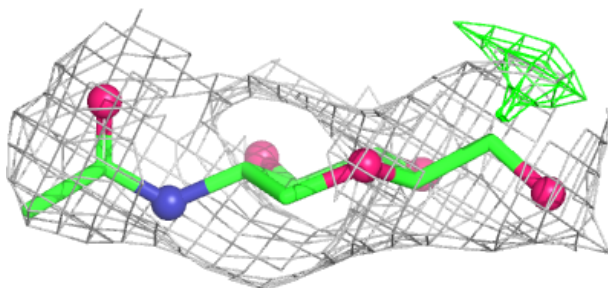
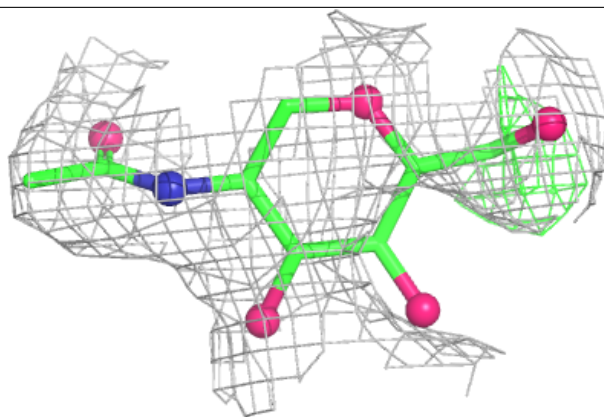
**Electron density around NAG F 601:**

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

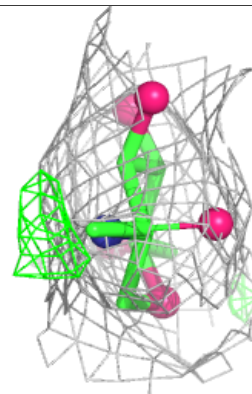
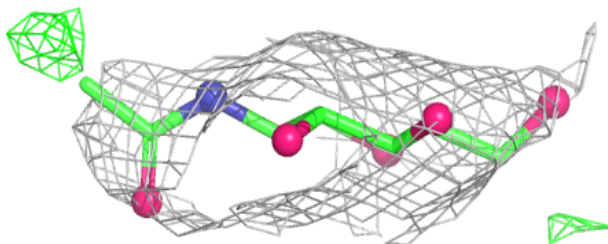
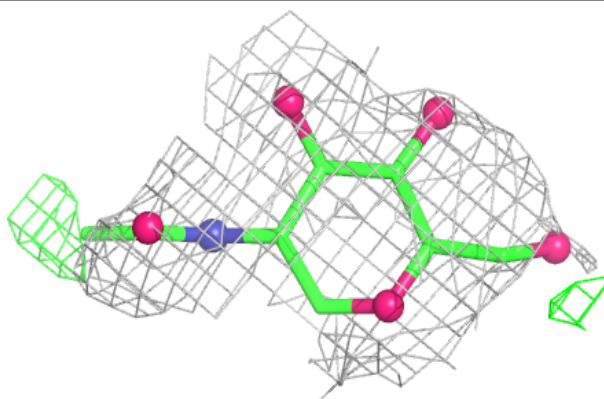


Electron density around NAG A 601:

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

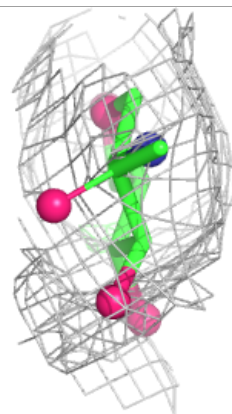
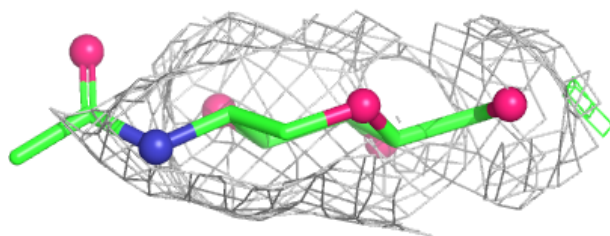
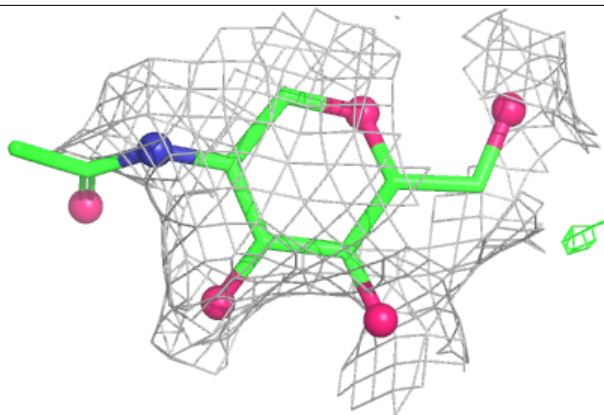
**Electron density around NAG H 601:**

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



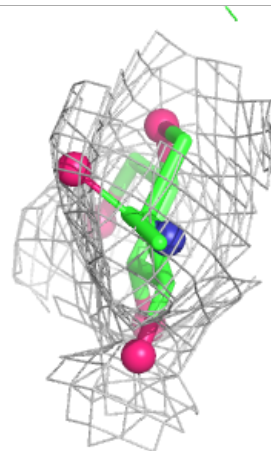
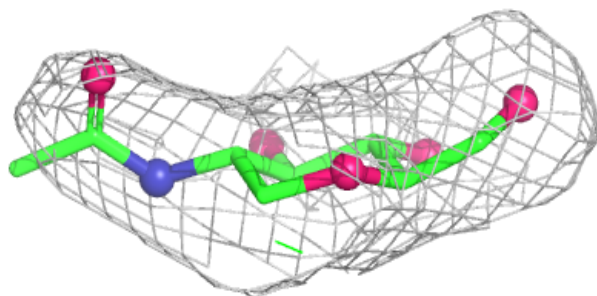
Electron density around NAG D 601:

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



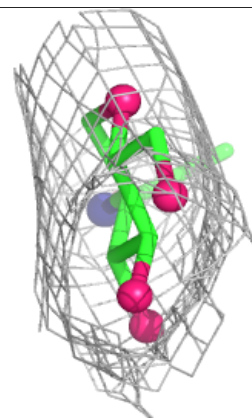
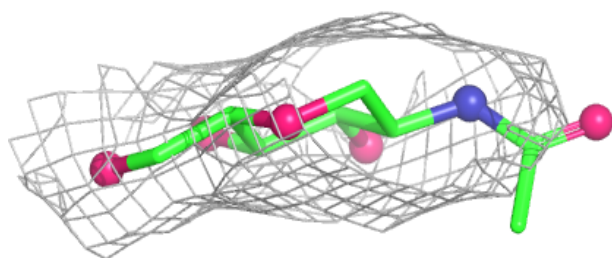
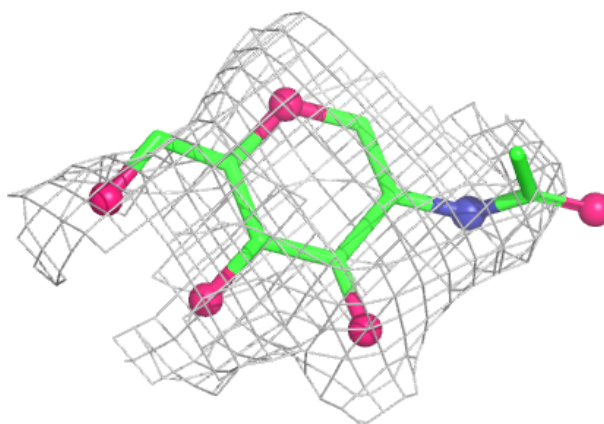
Electron density around NAG A 602:

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



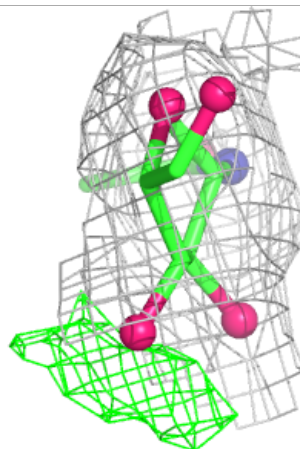
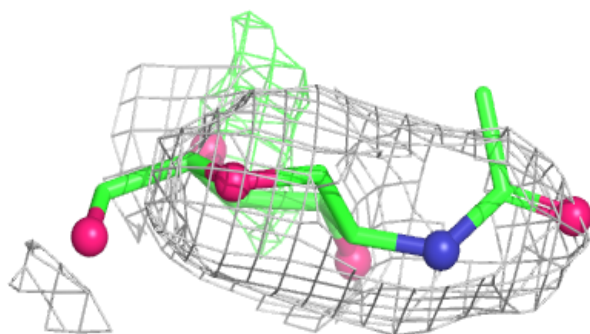
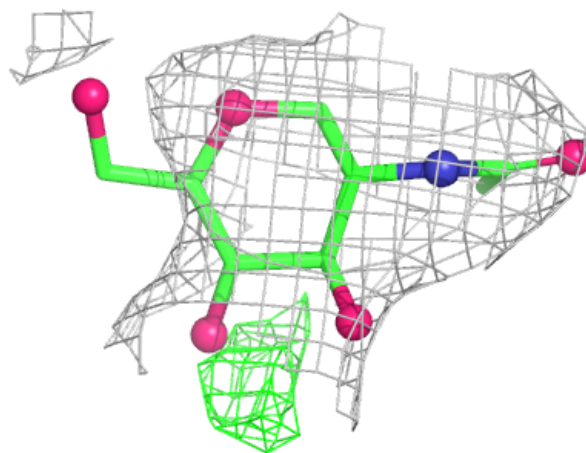
Electron density around NAG C 602:

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



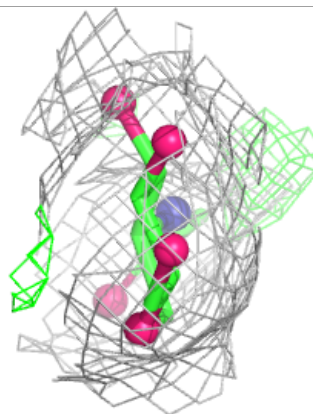
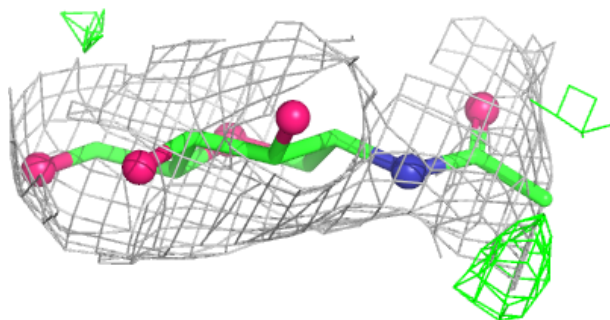
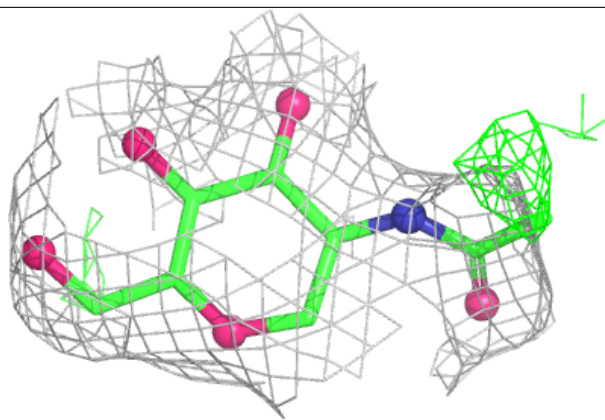
Electron density around NAG B 602:

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



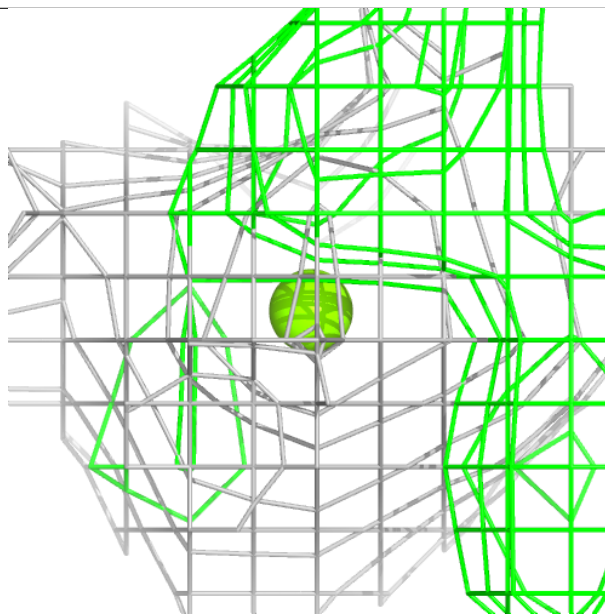
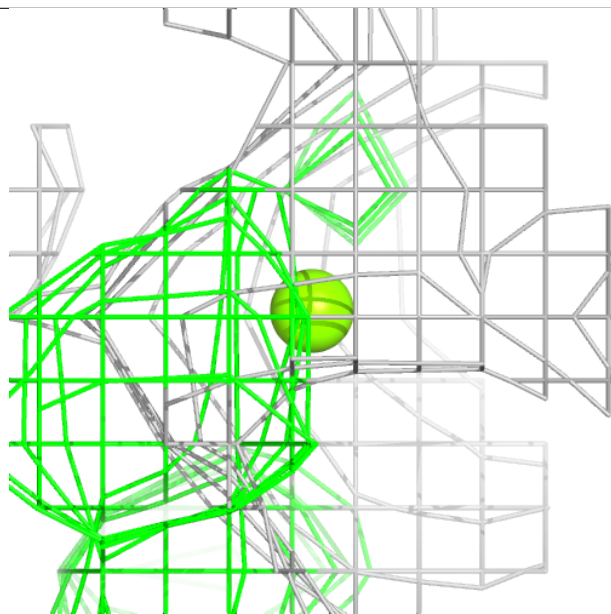
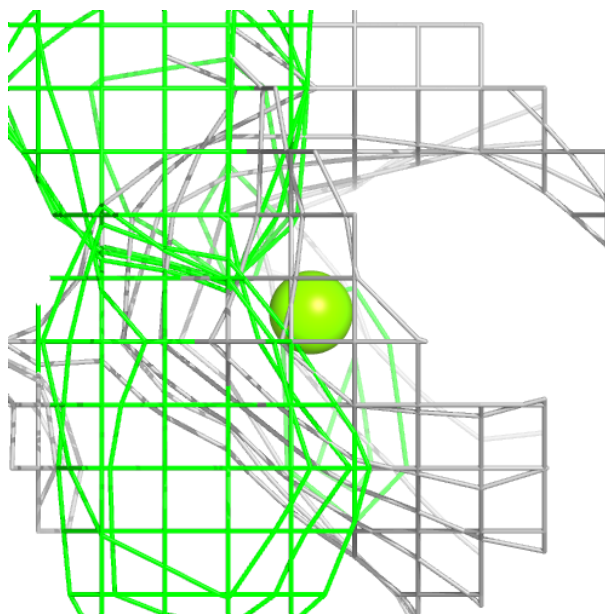
Electron density around NAG E 601:

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



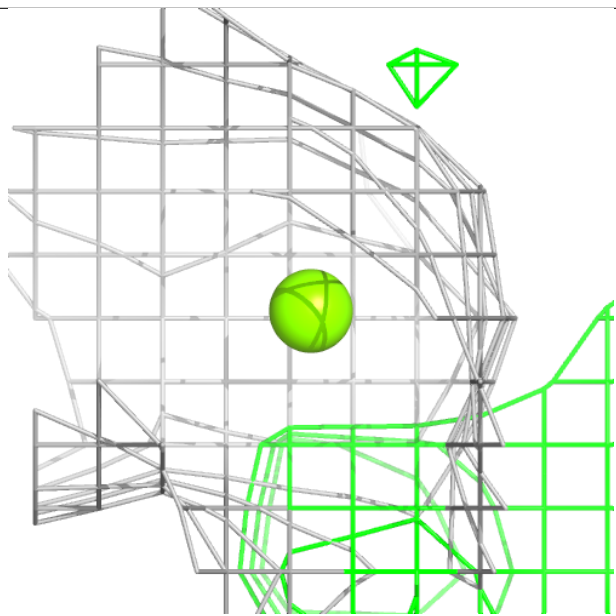
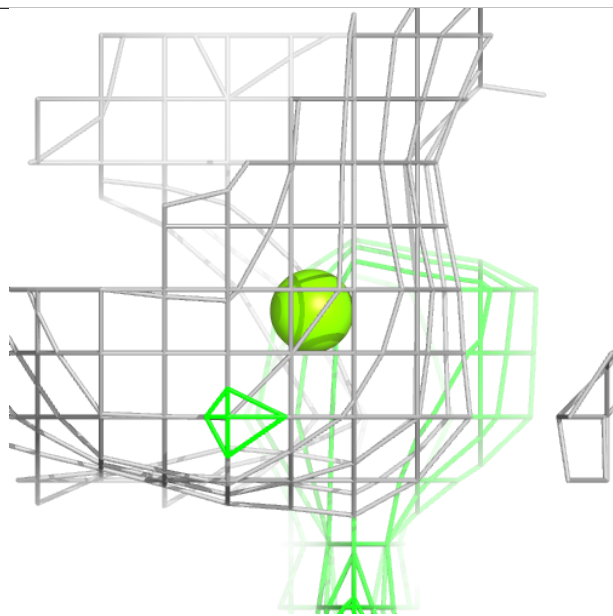
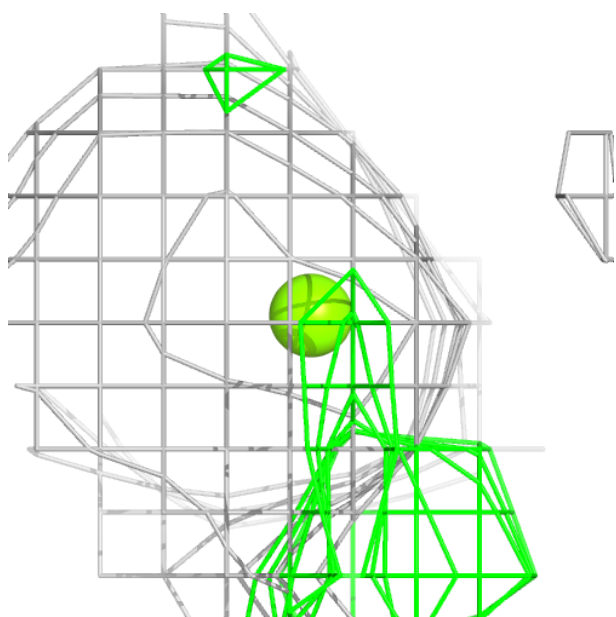
Electron density around MG C 603:

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



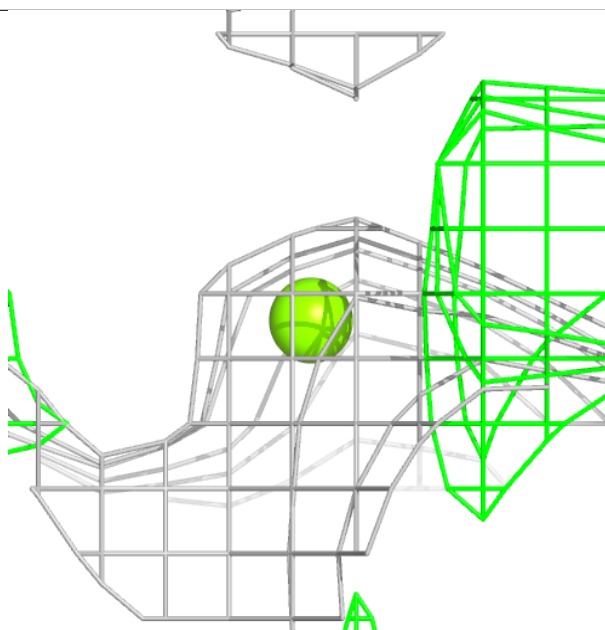
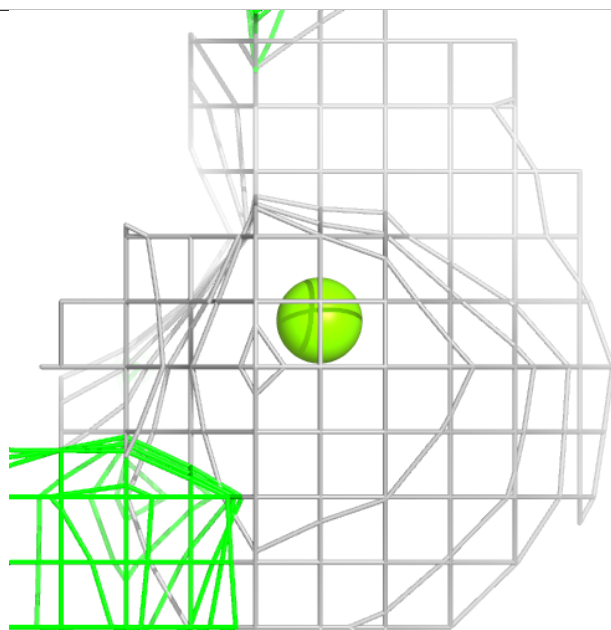
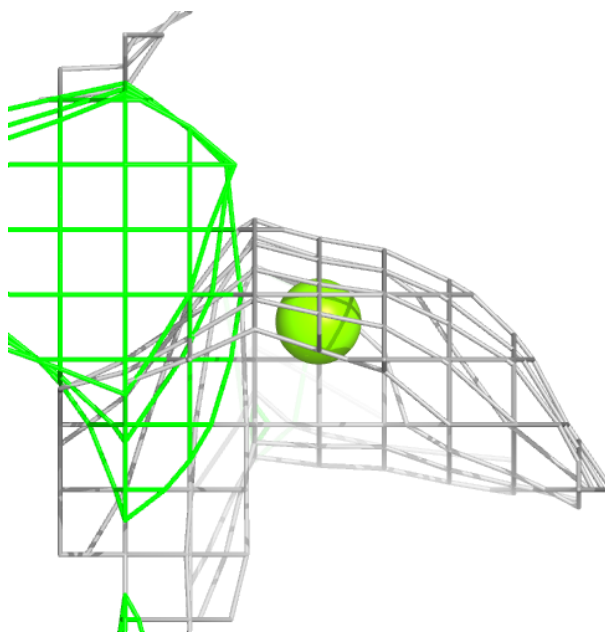
Electron density around MG A 603:

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



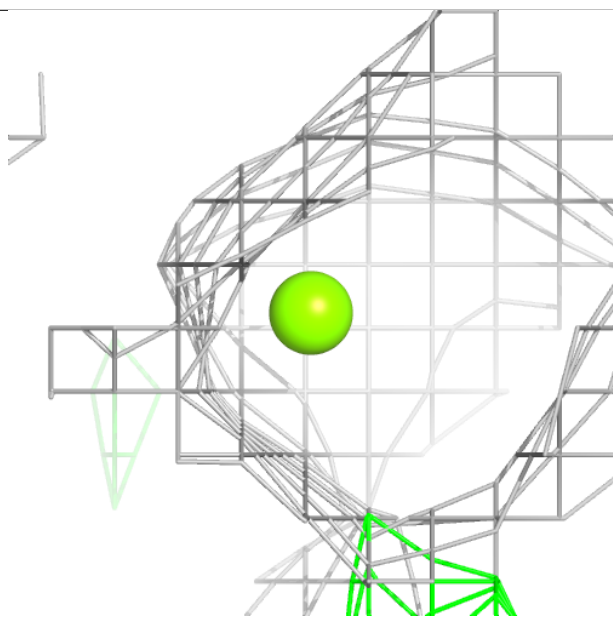
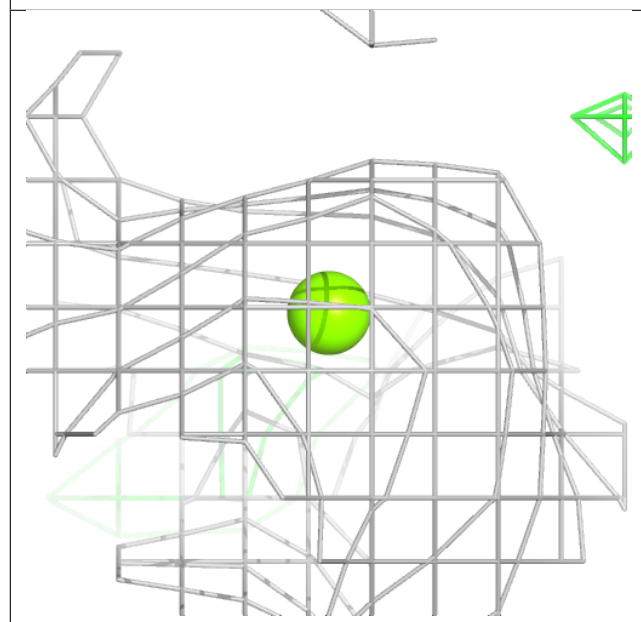
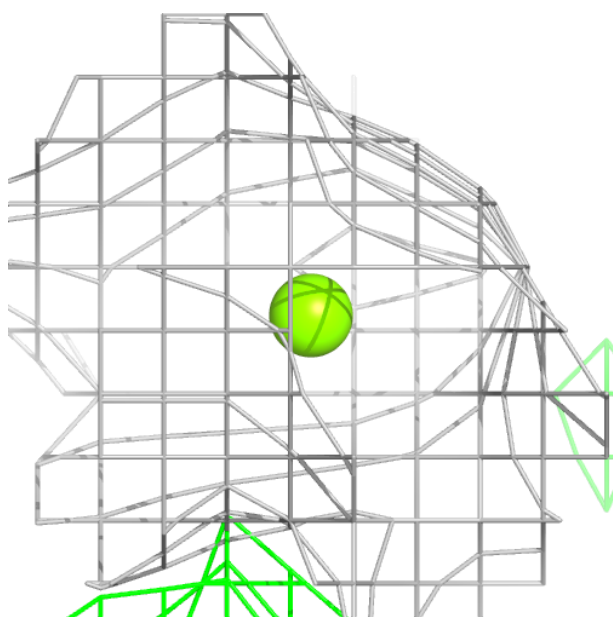
Electron density around MG H 603:

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



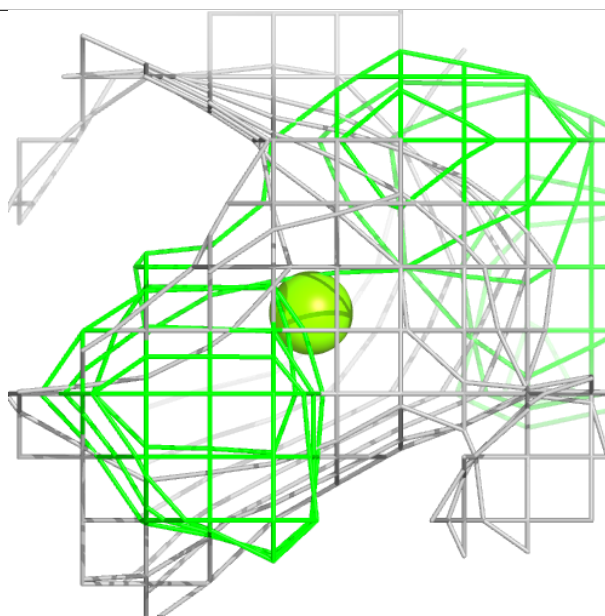
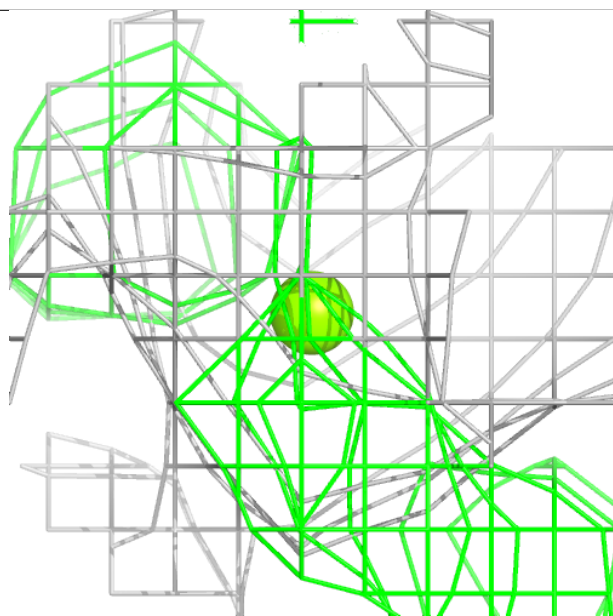
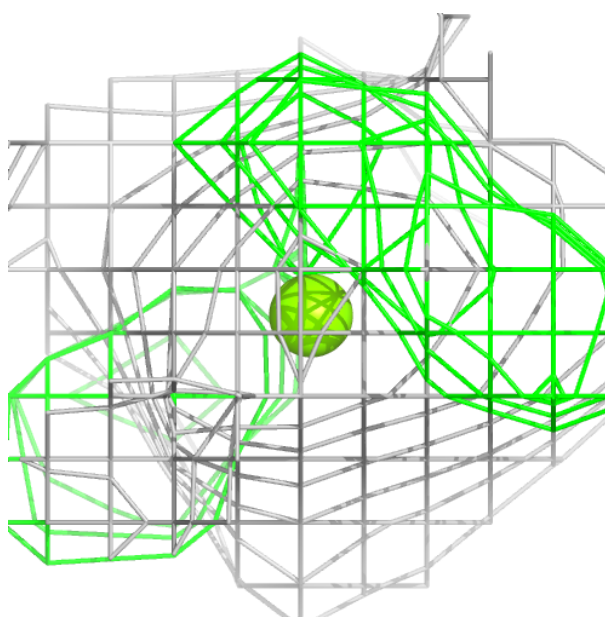
Electron density around MG D 603:

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



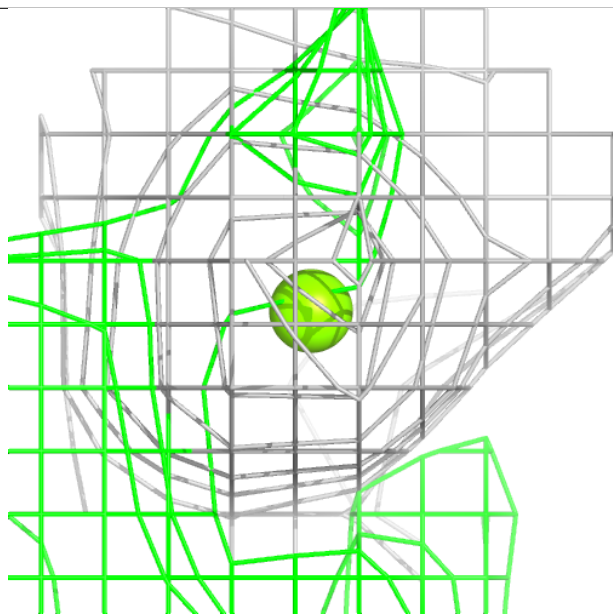
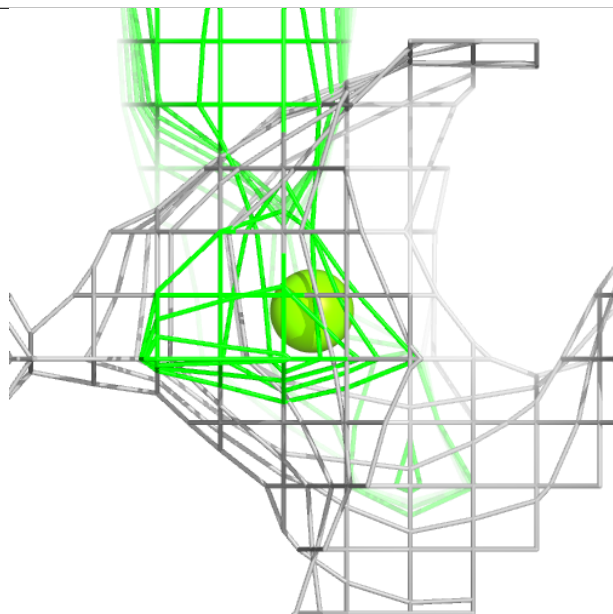
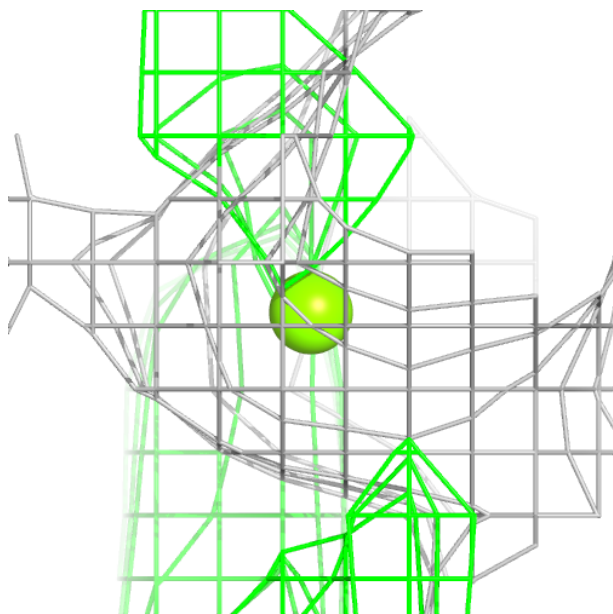
Electron density around MG B 603:

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



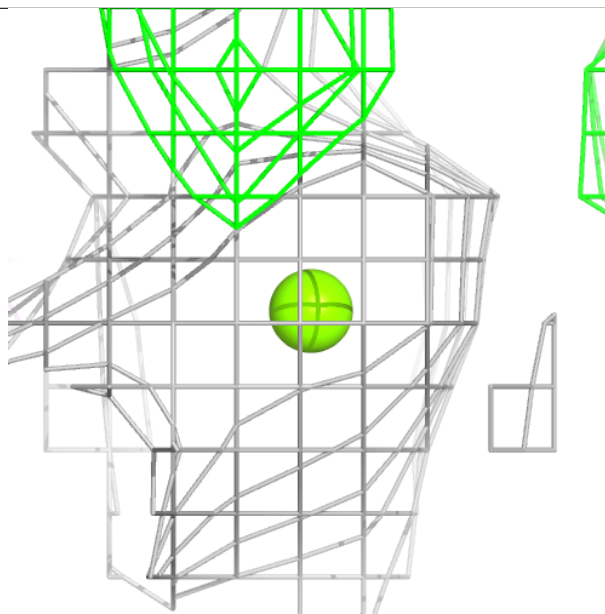
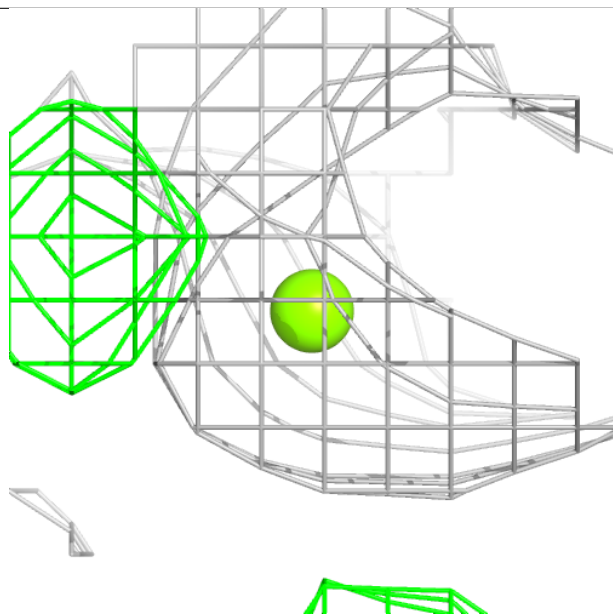
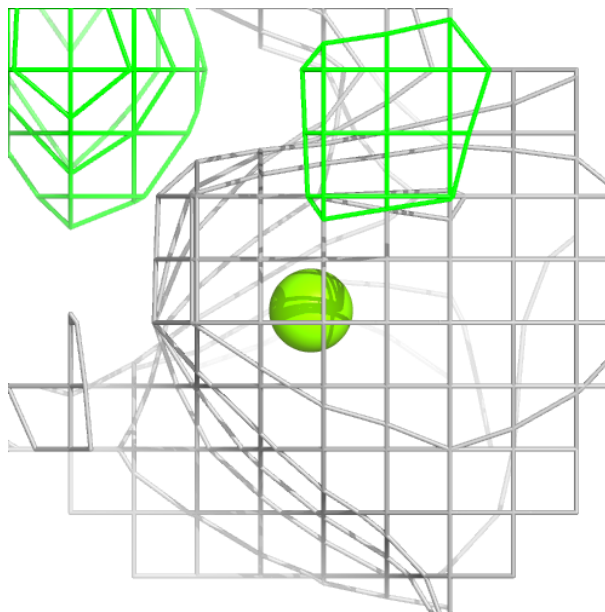
Electron density around MG E 603:

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



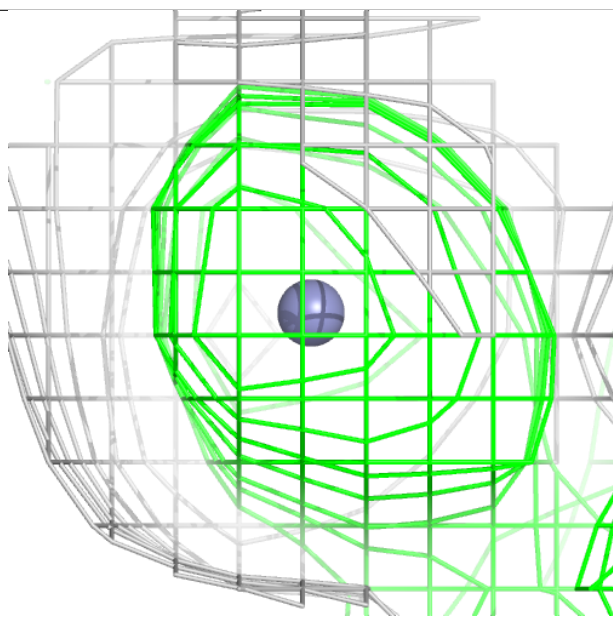
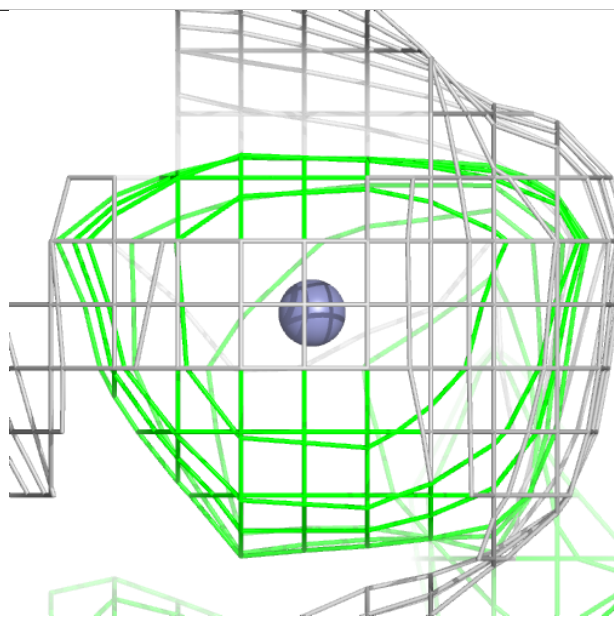
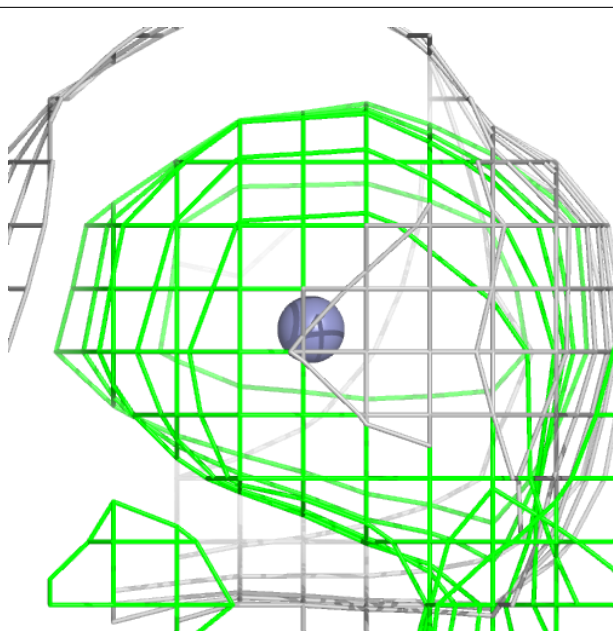
Electron density around MG G 603:

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



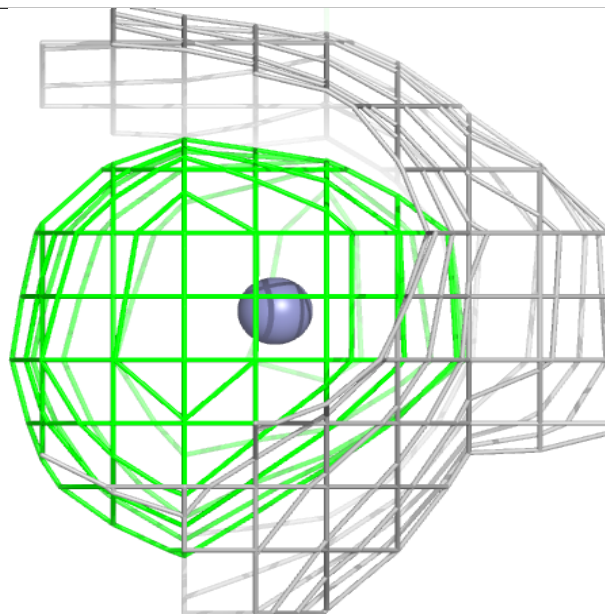
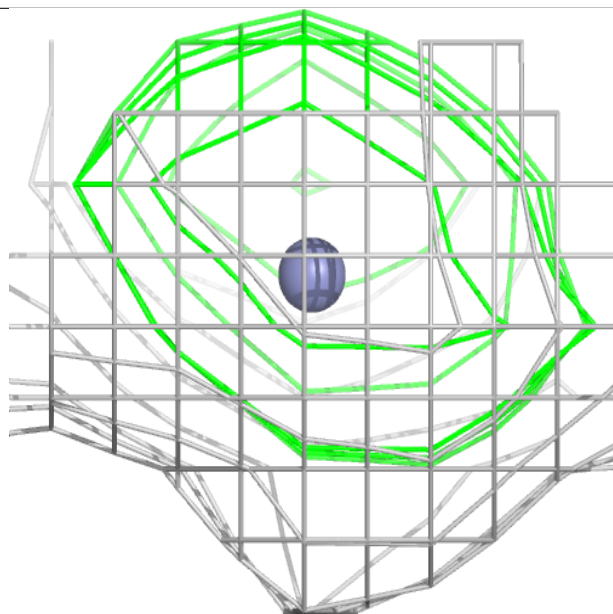
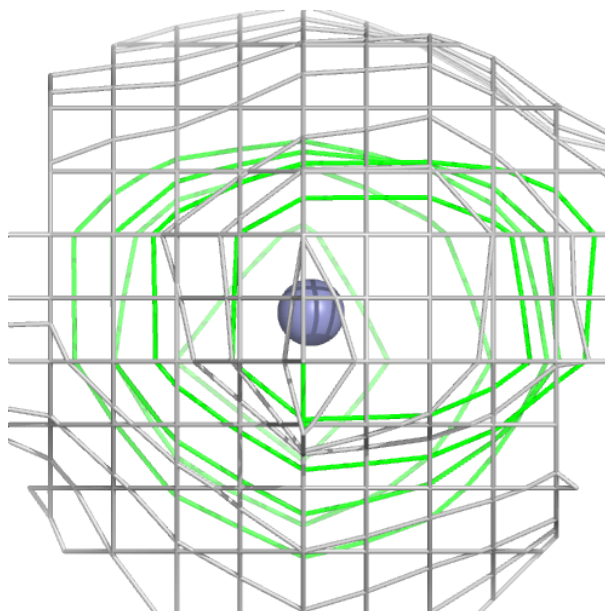
Electron density around ZN G 604:

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



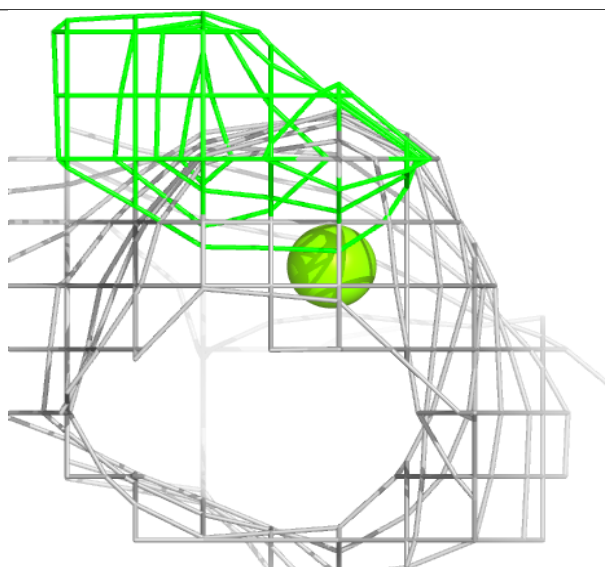
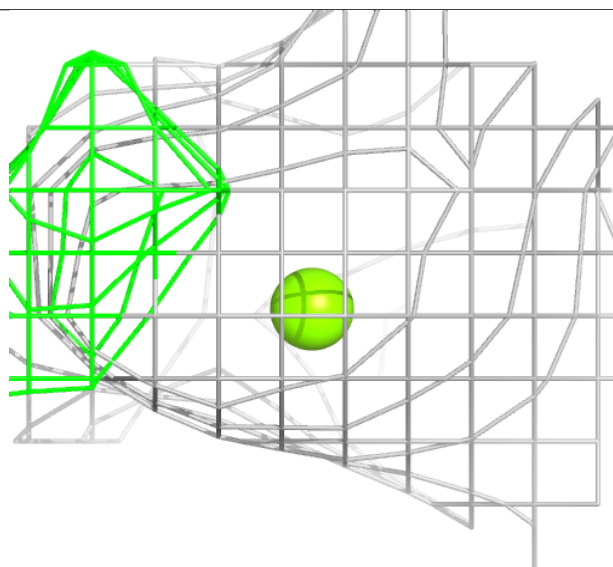
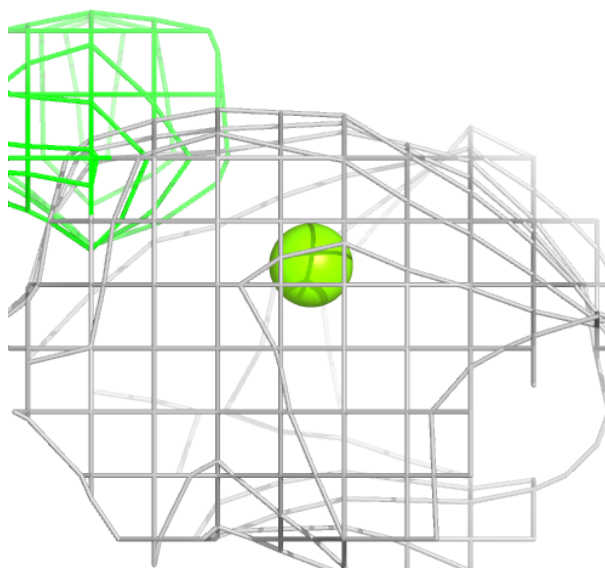
Electron density around ZN D 604:

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



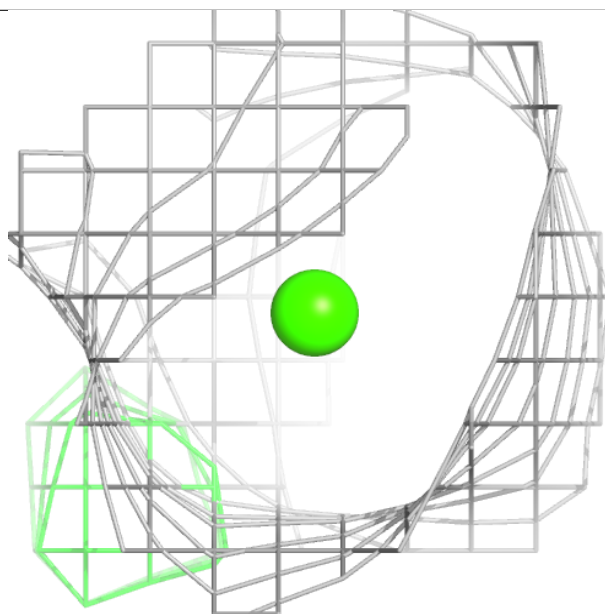
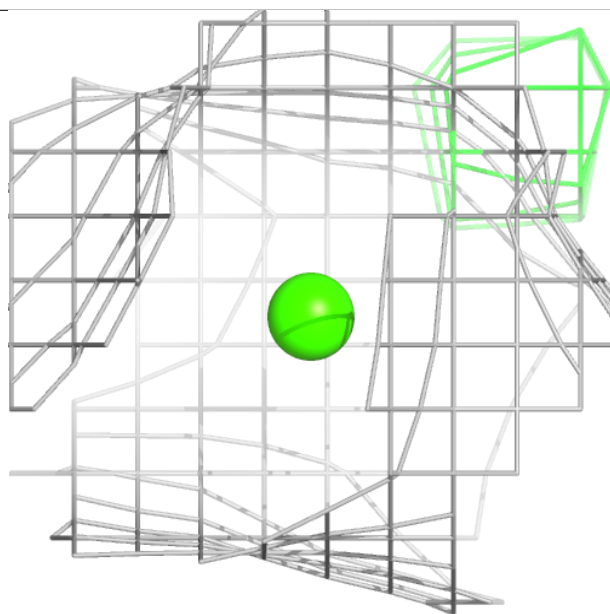
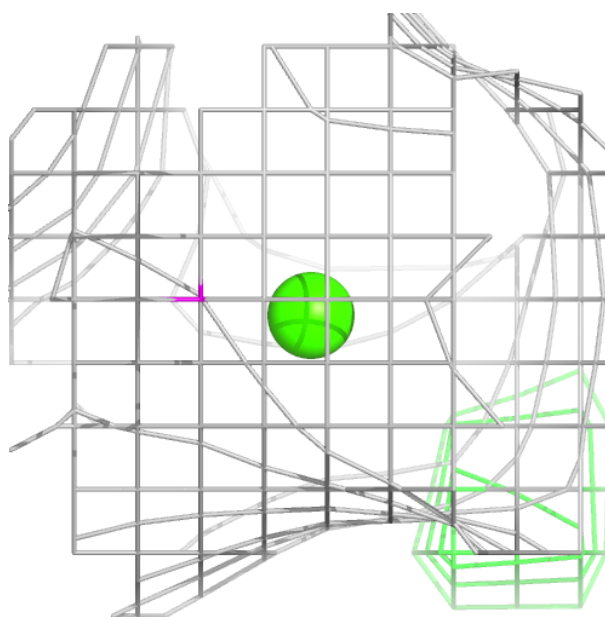
Electron density around MG F 603:

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



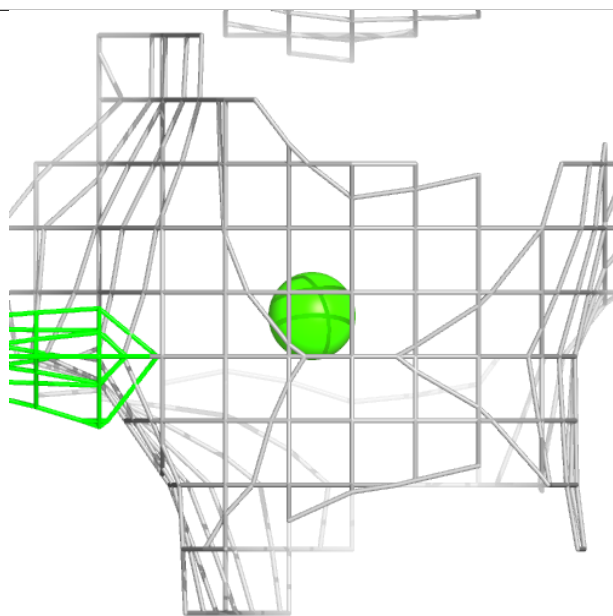
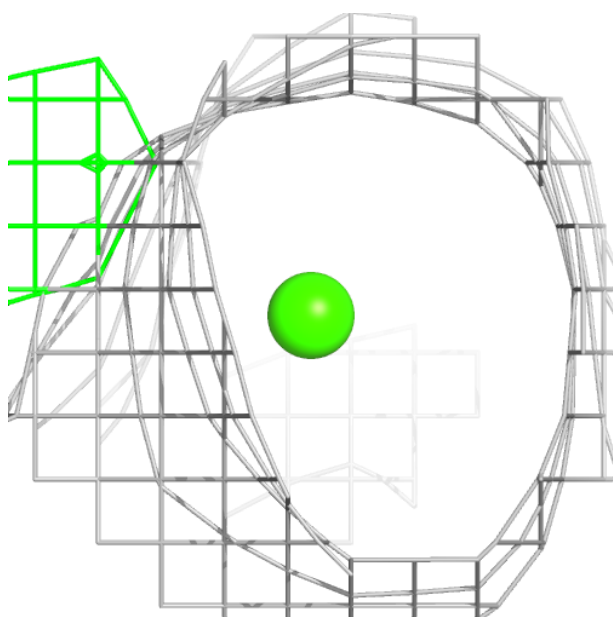
Electron density around CA C 605:

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



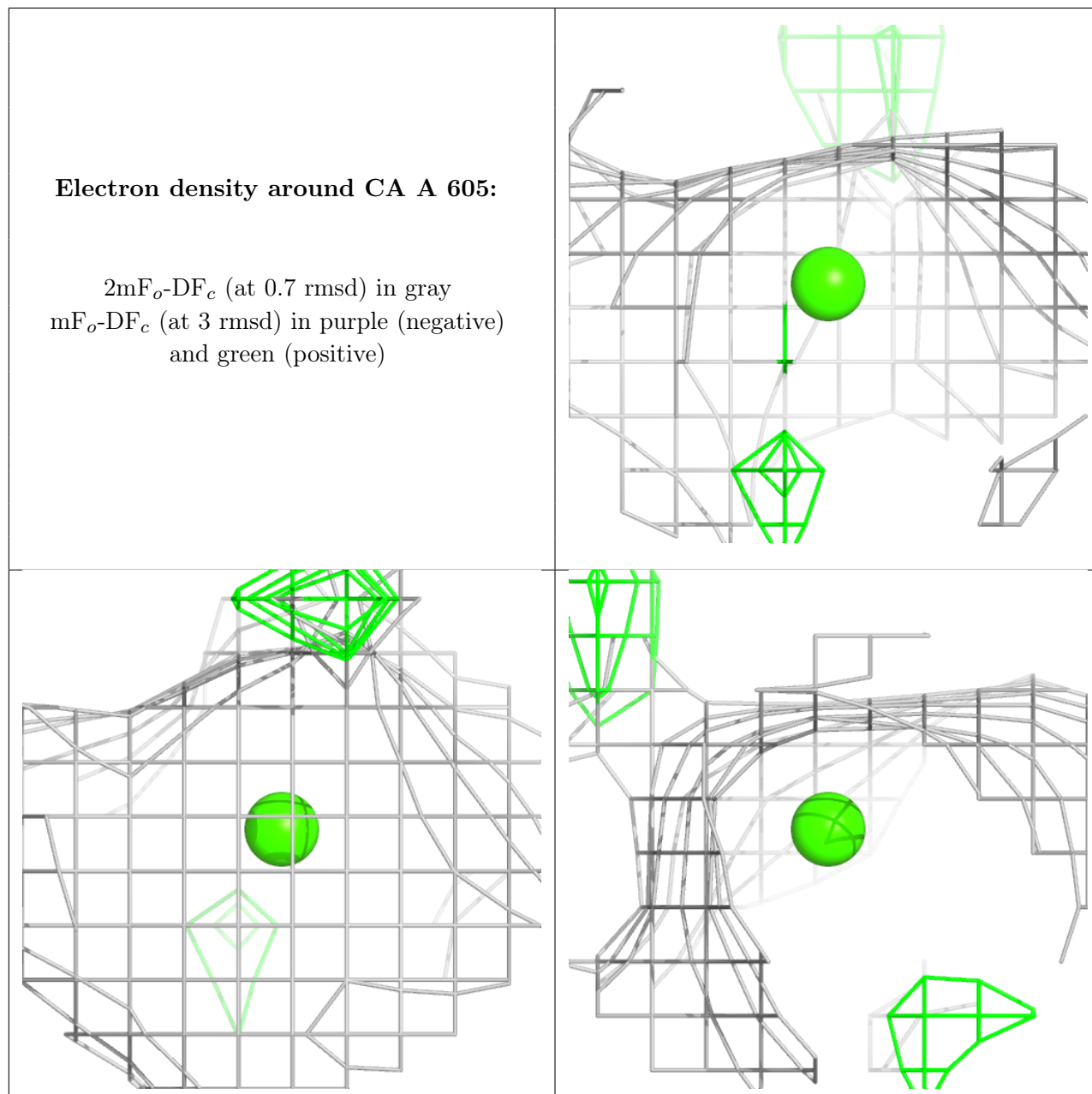
Electron density around CA D 605:

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



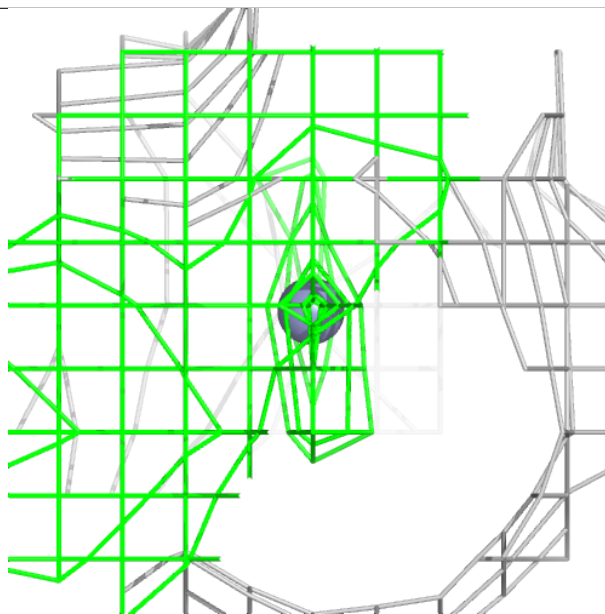
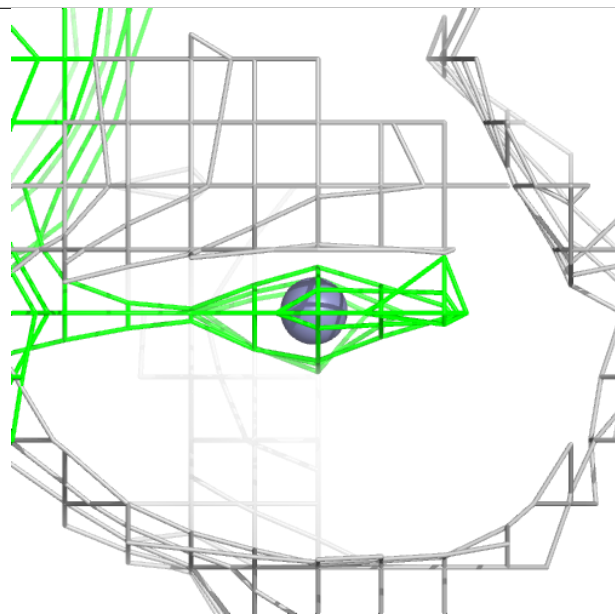
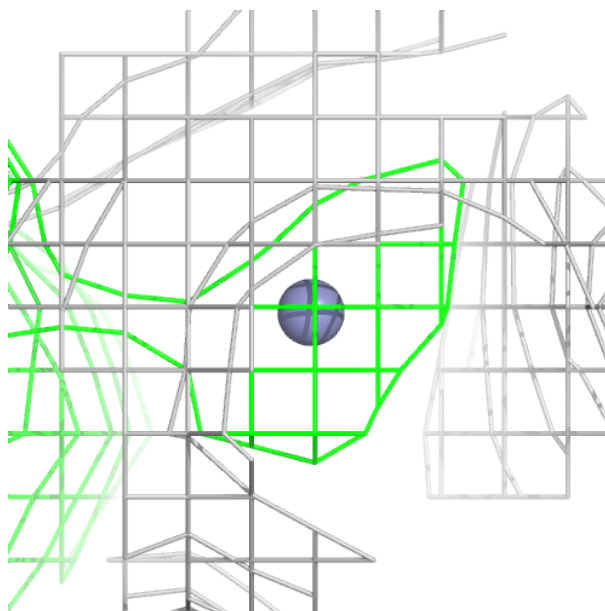
Electron density around CA A 605:

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



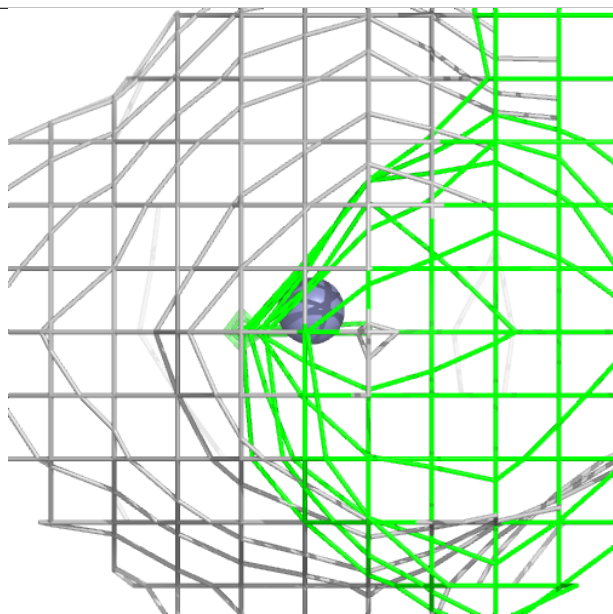
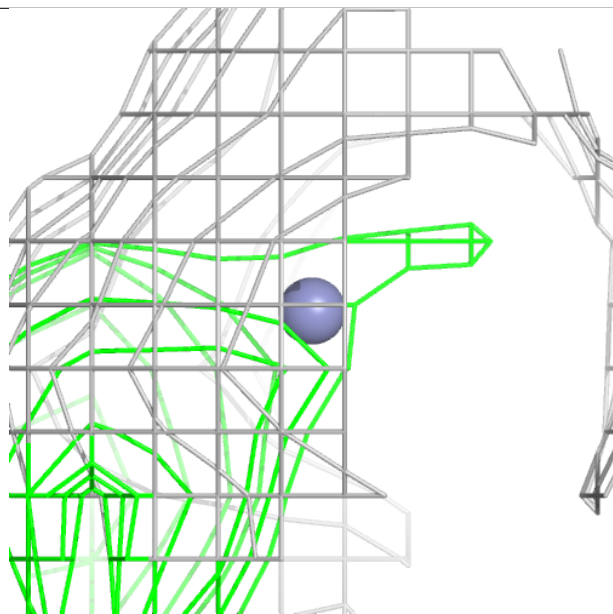
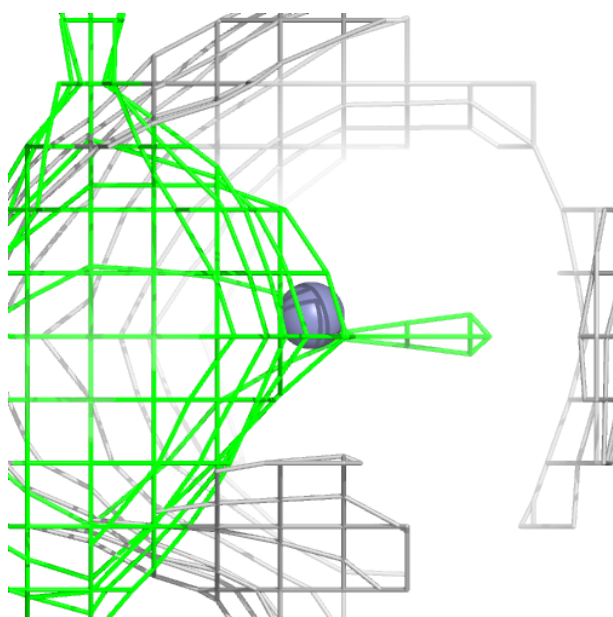
Electron density around ZN A 606:

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



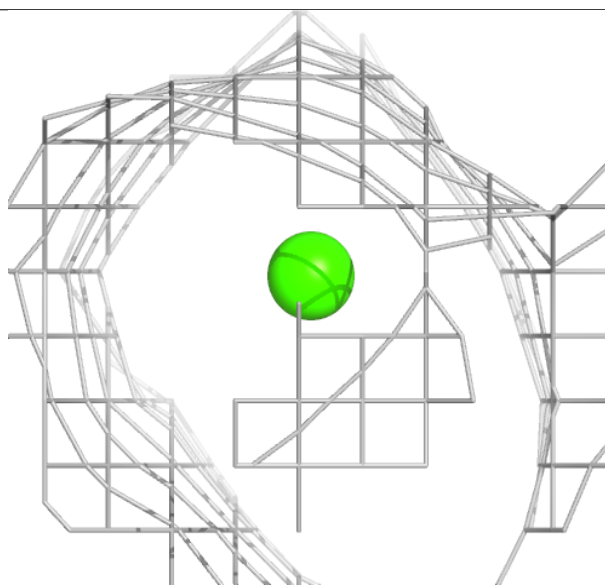
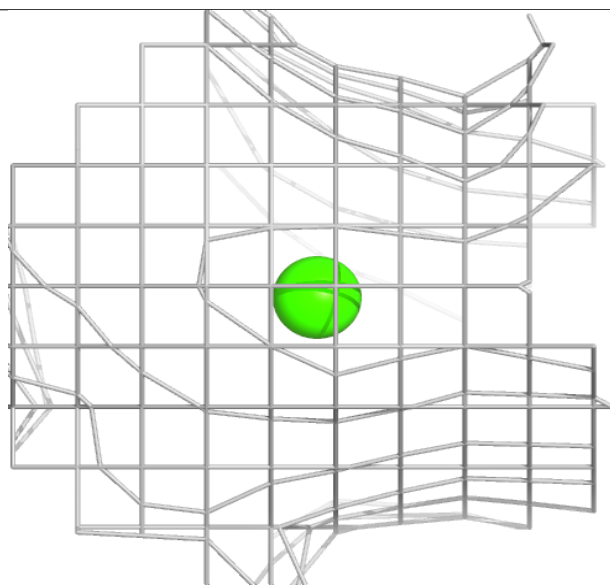
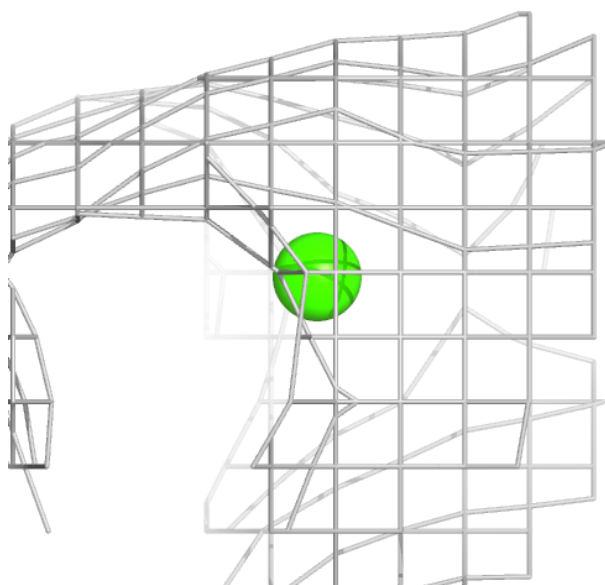
Electron density around ZN A 604:

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



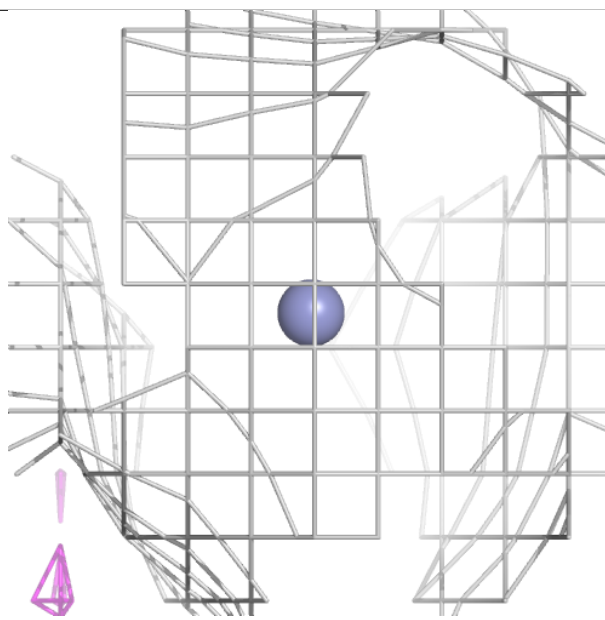
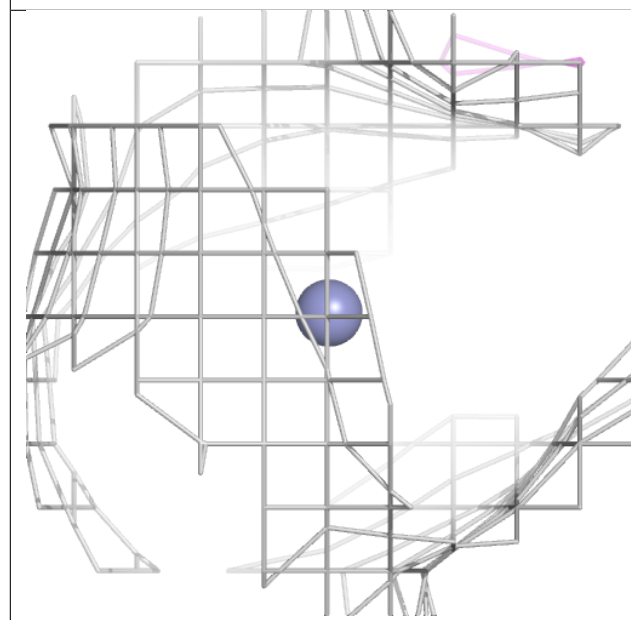
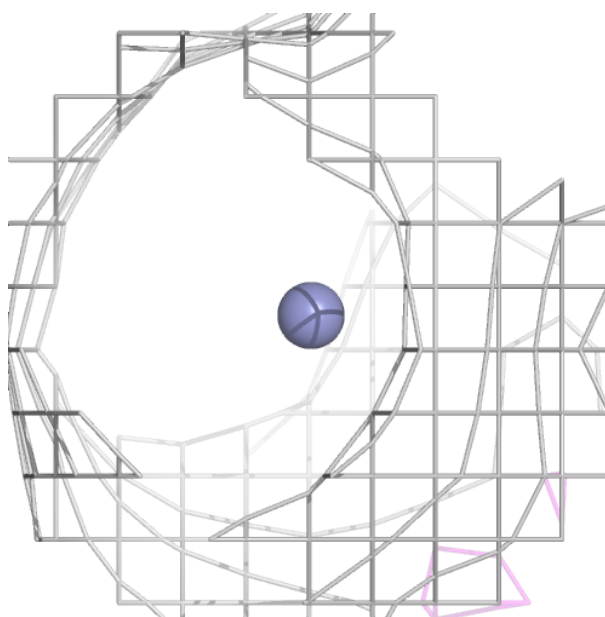
Electron density around CA G 605:

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



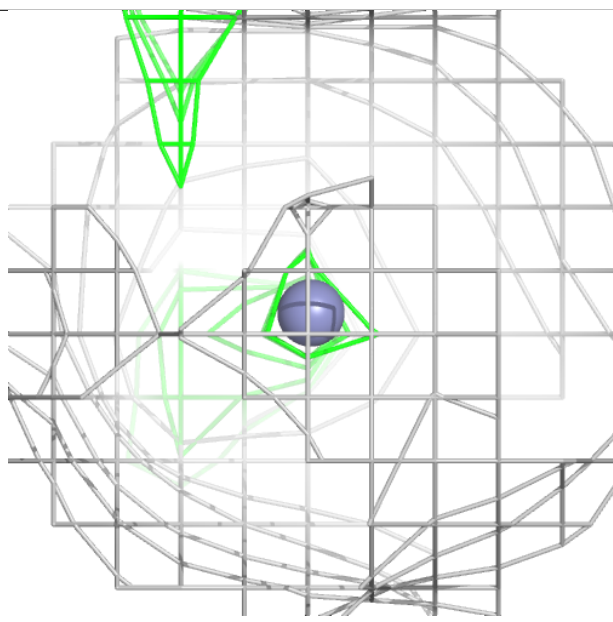
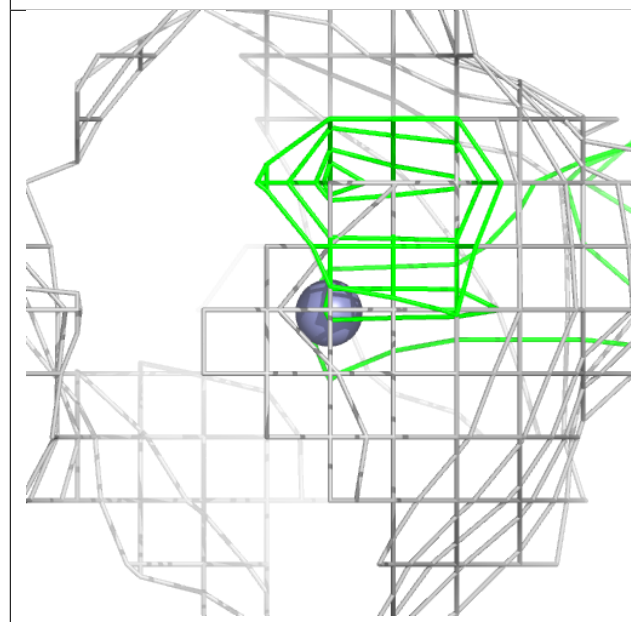
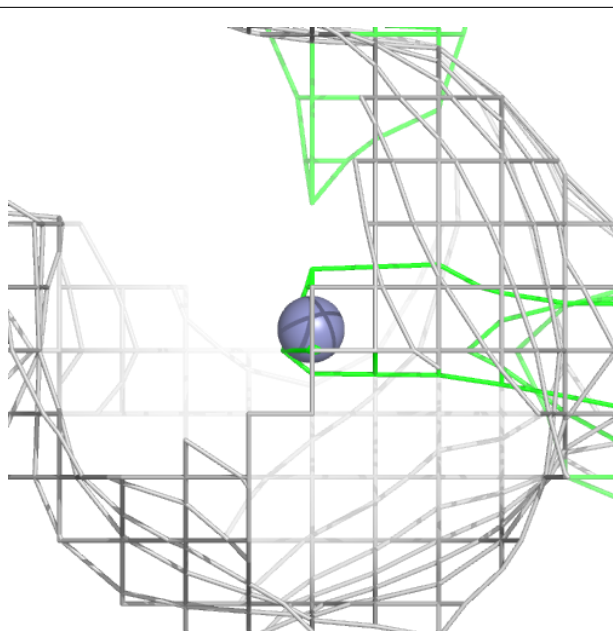
Electron density around ZN F 606:

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



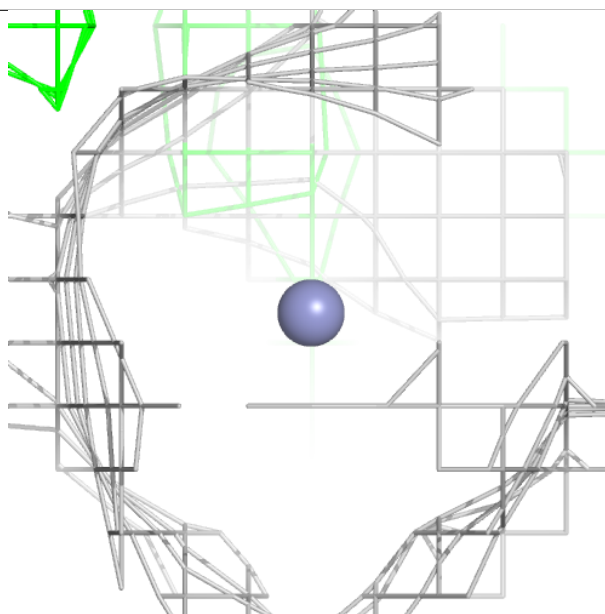
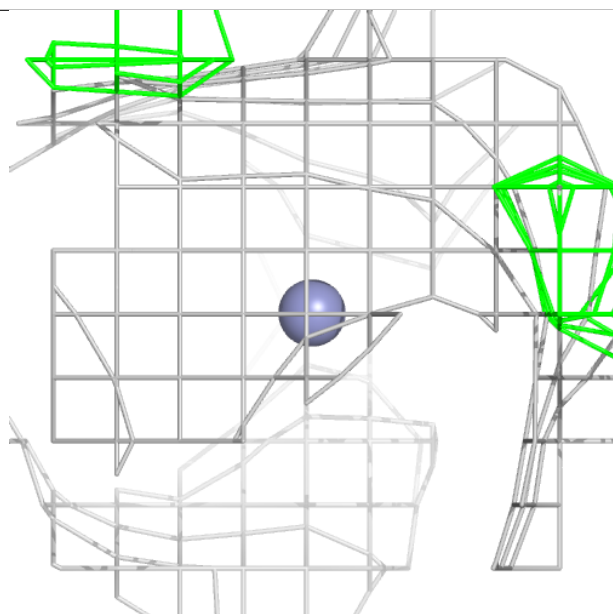
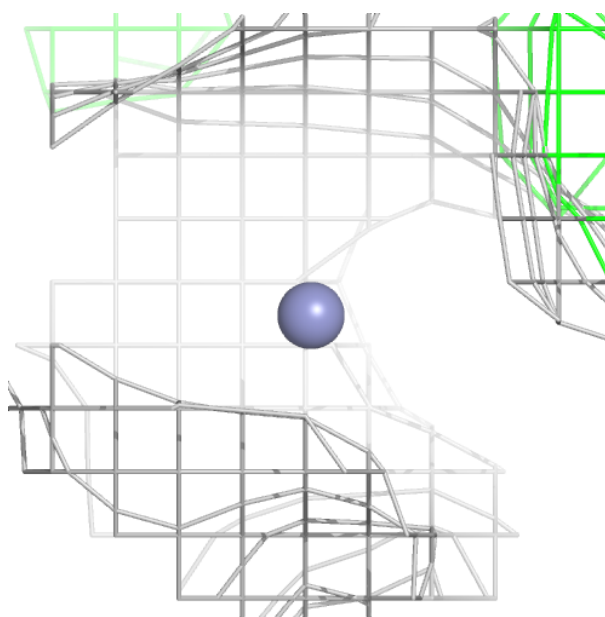
Electron density around ZN E 604:

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



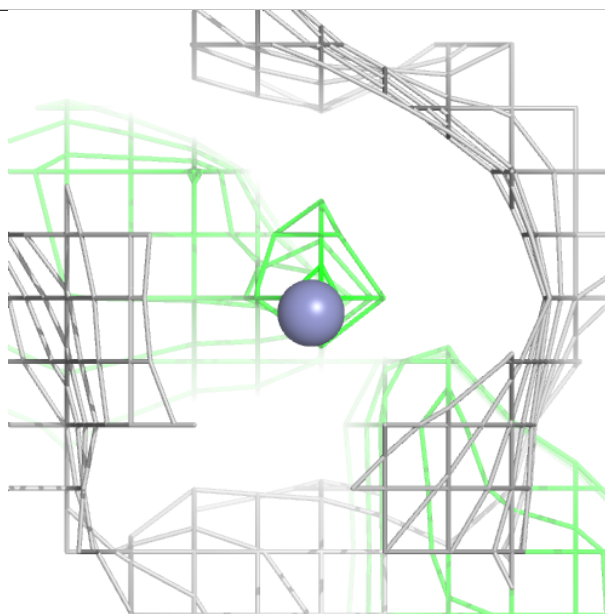
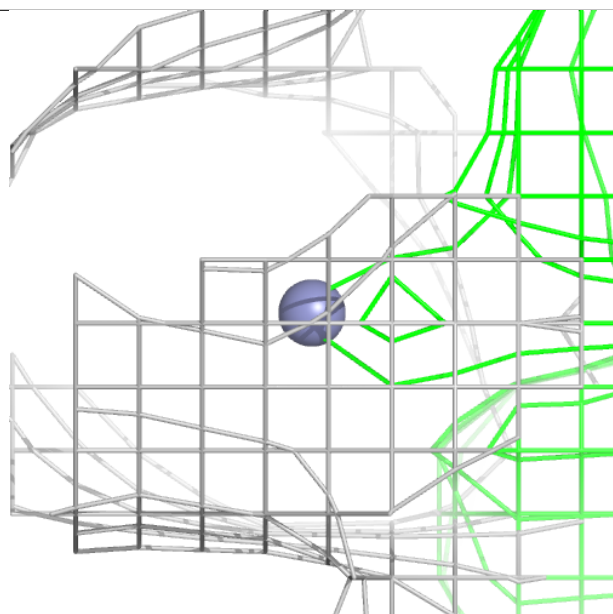
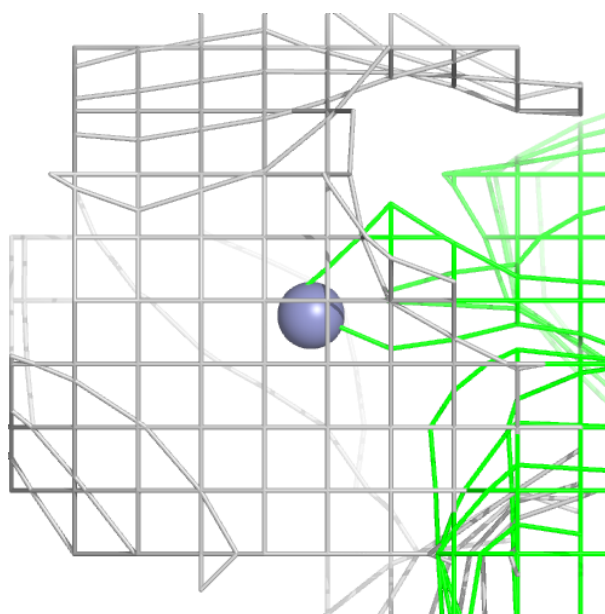
Electron density around ZN E 606:

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



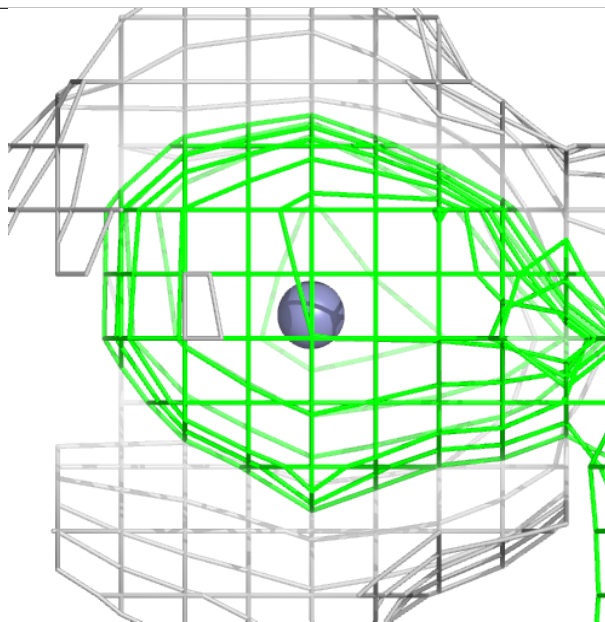
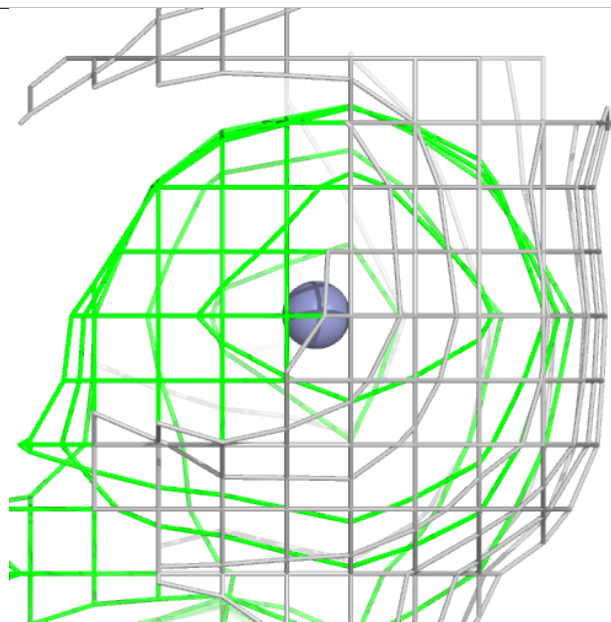
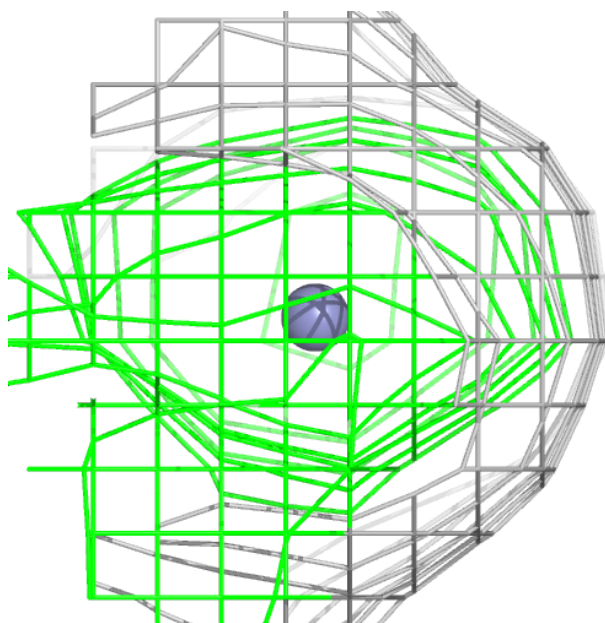
Electron density around ZN C 606:

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



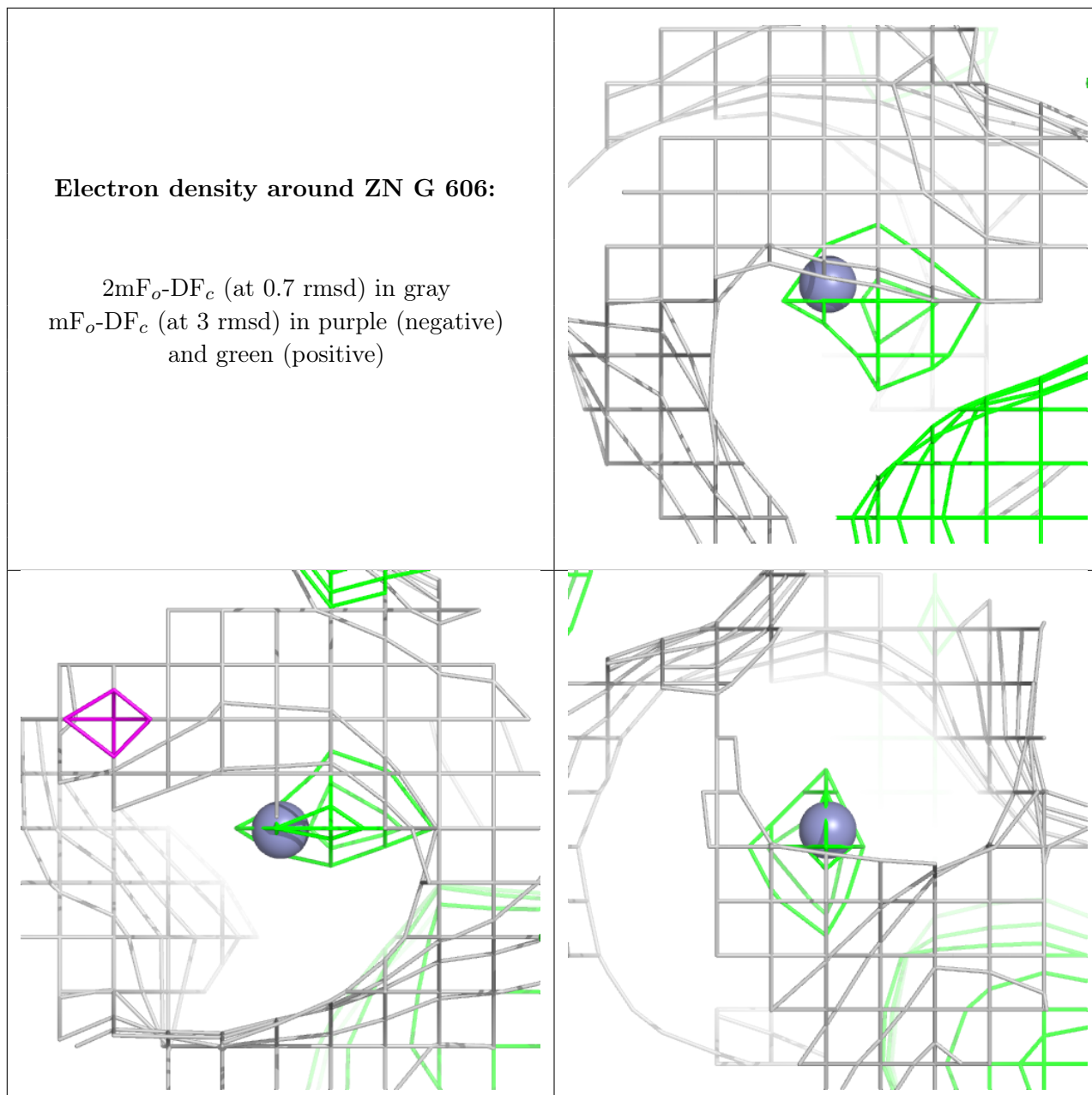
Electron density around ZN C 604:

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



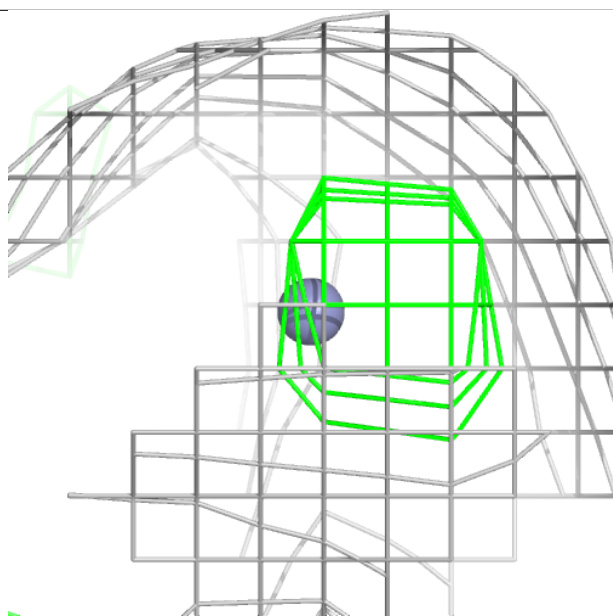
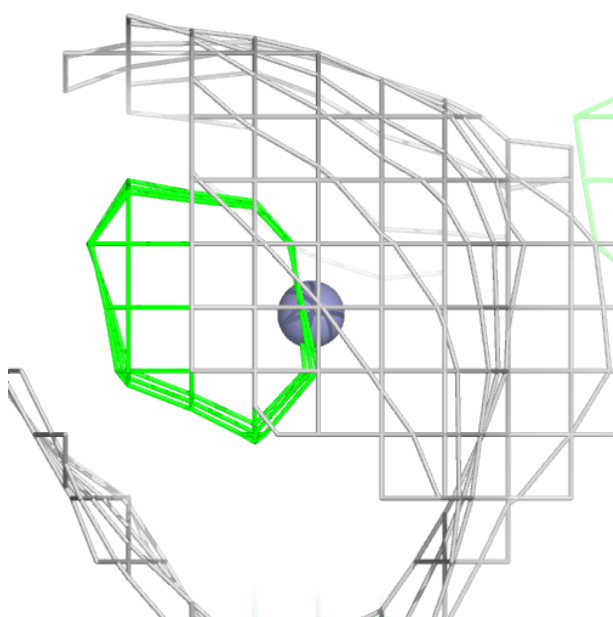
Electron density around ZN G 606:

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



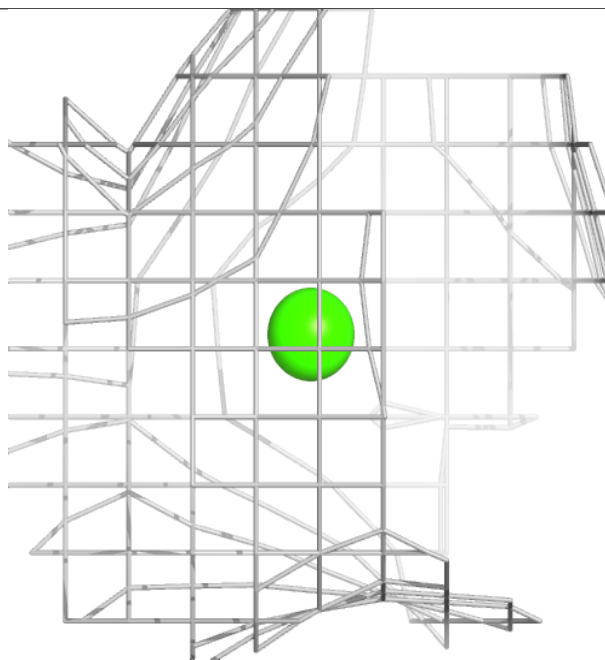
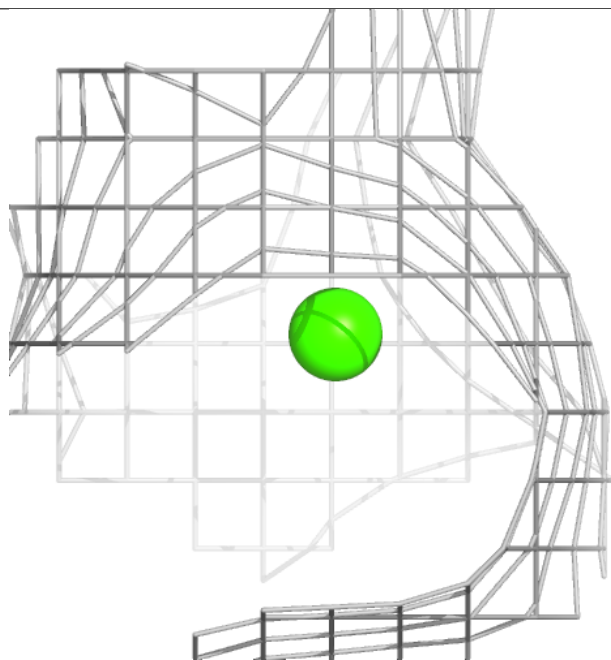
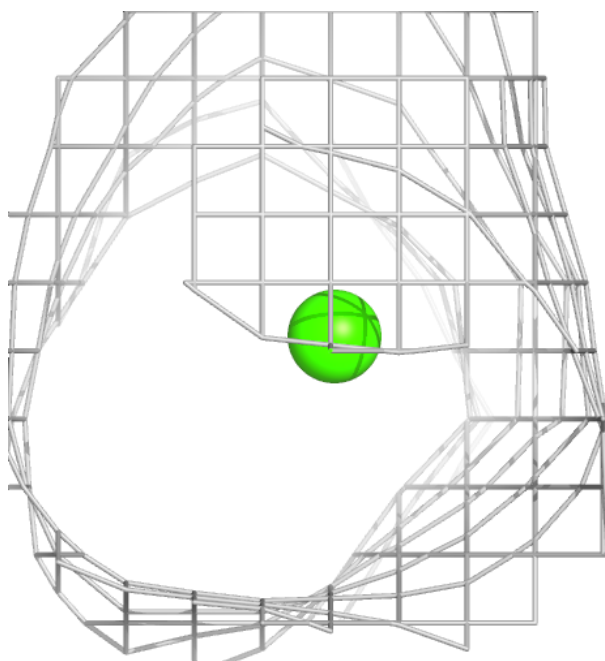
Electron density around ZN H 604:

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



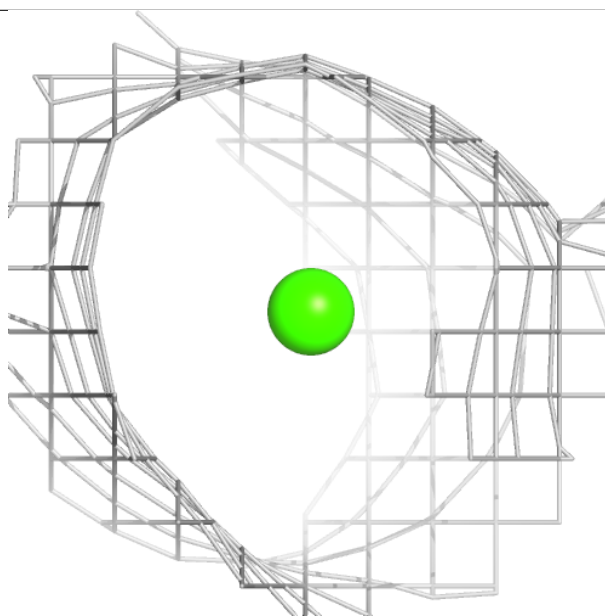
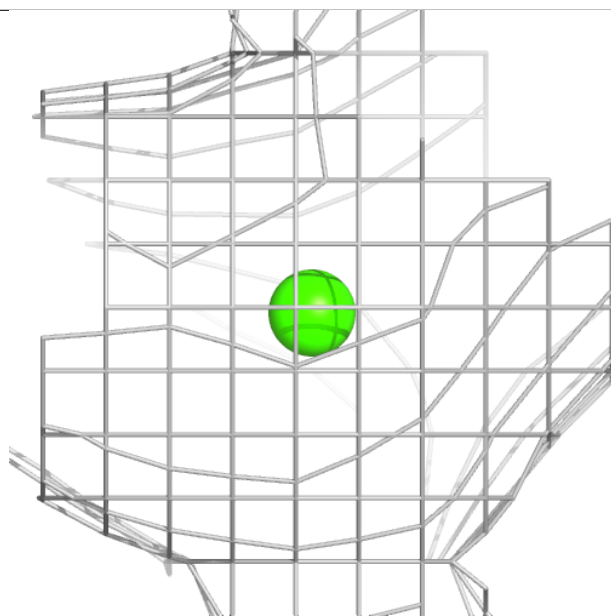
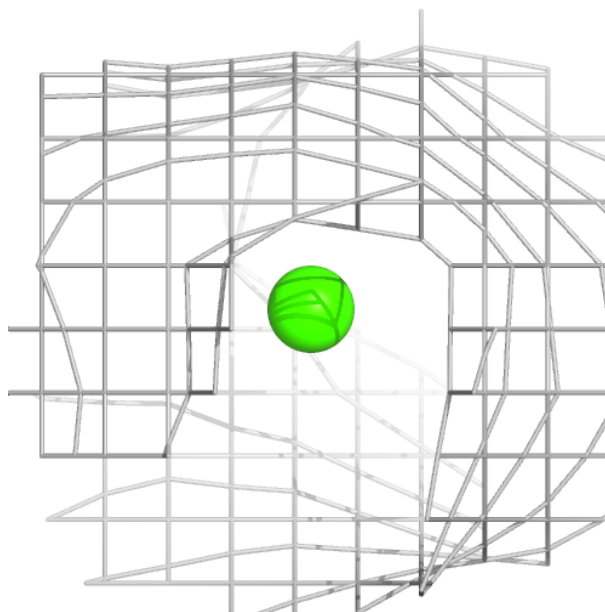
Electron density around CA F 605:

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



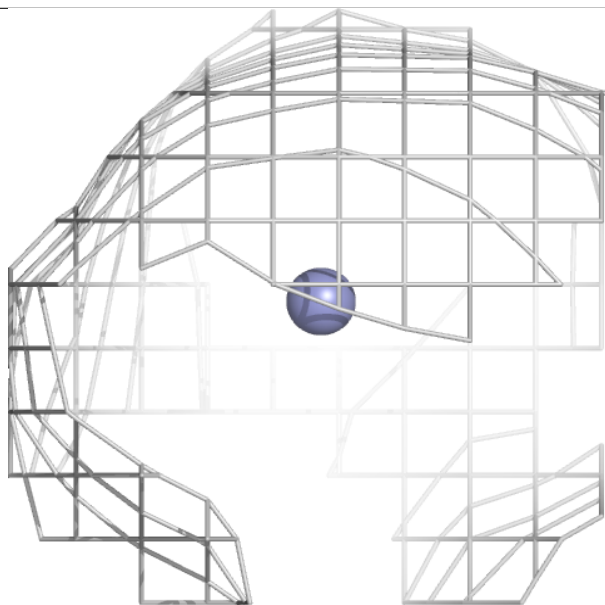
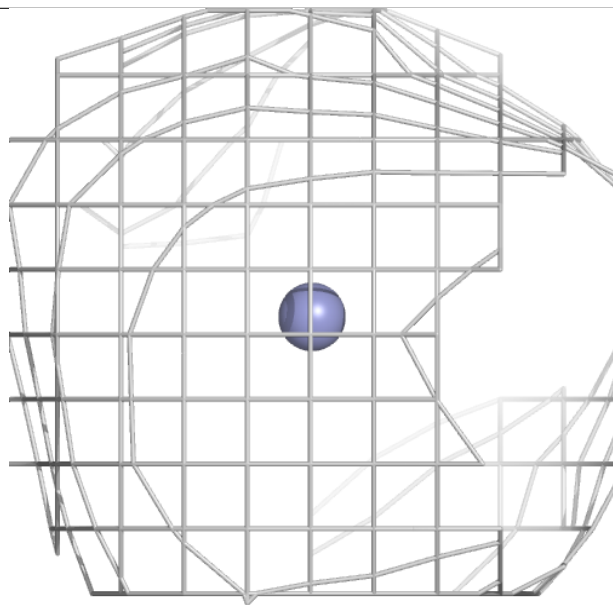
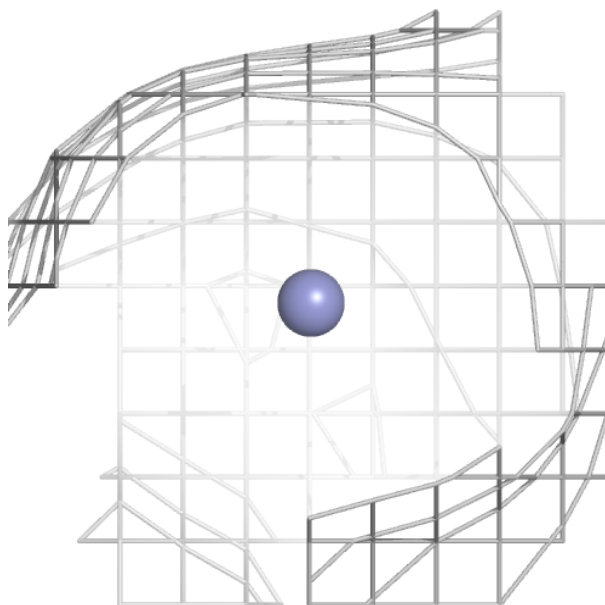
Electron density around CA E 605:

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



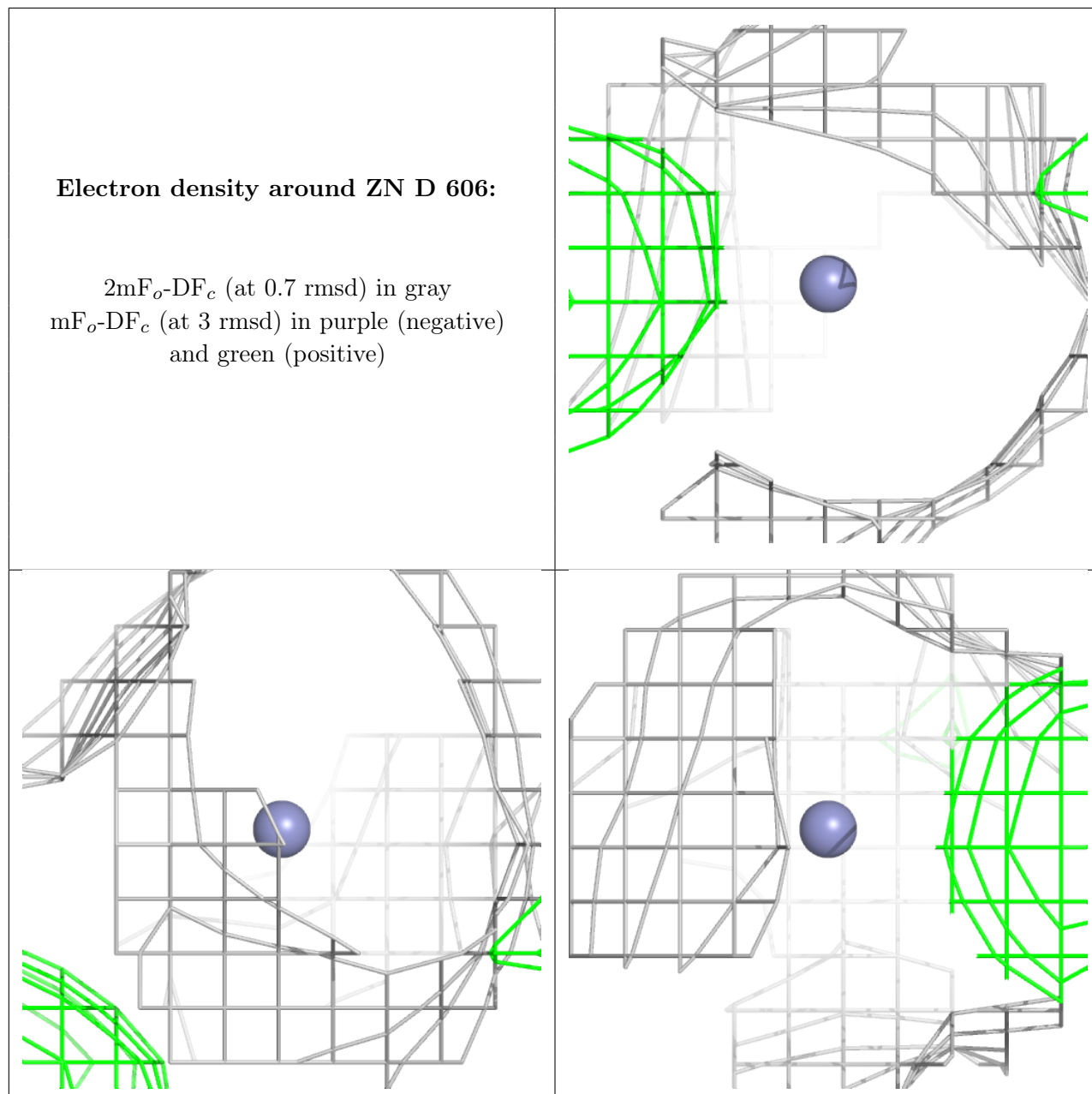
Electron density around ZN F 604:

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



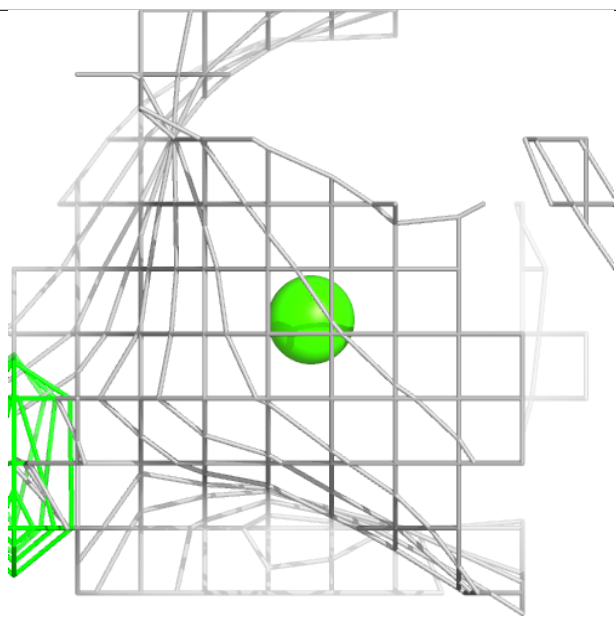
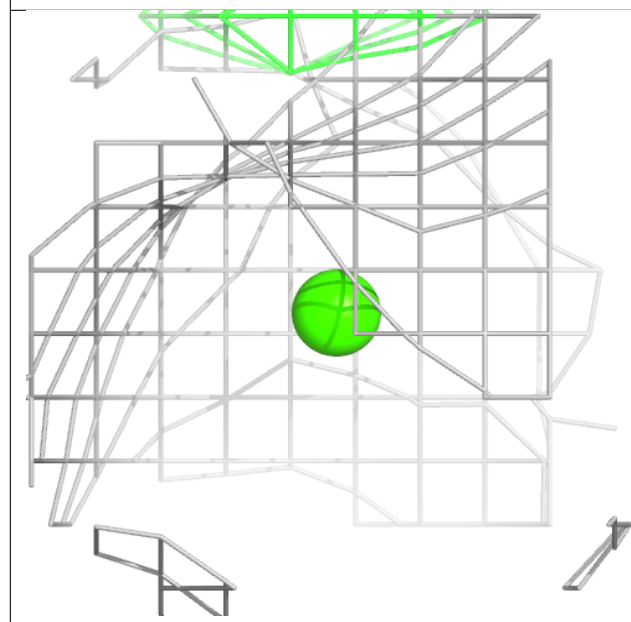
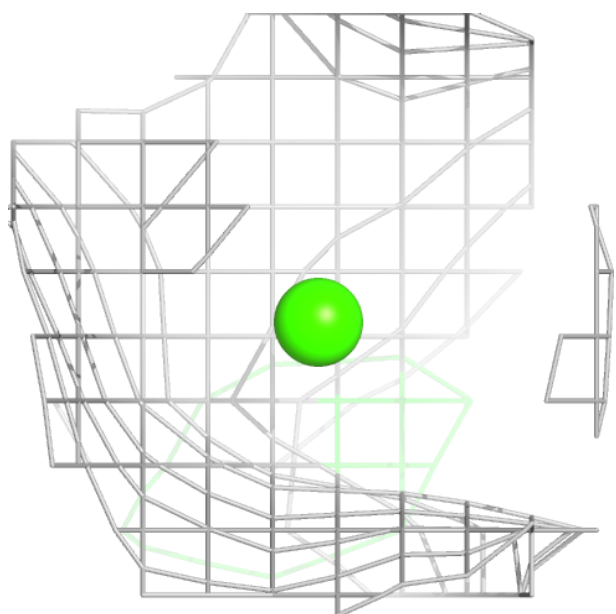
Electron density around ZN D 606:

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



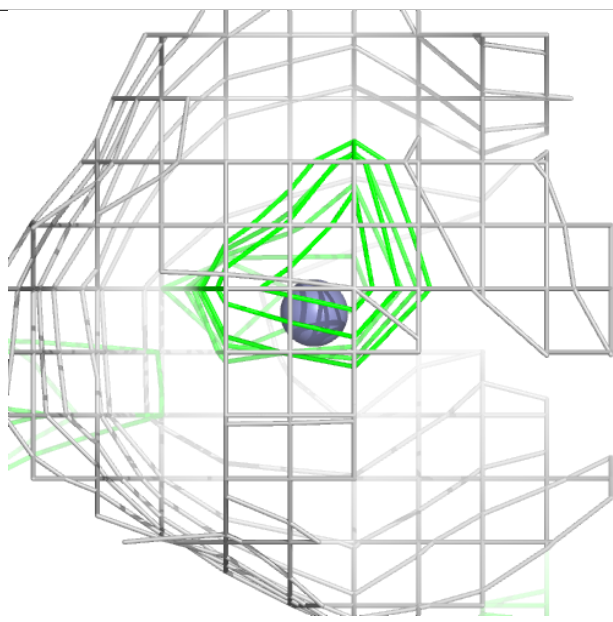
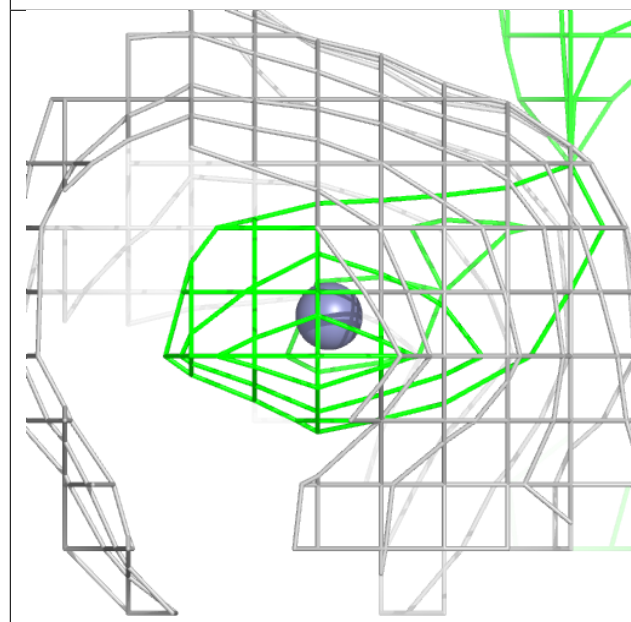
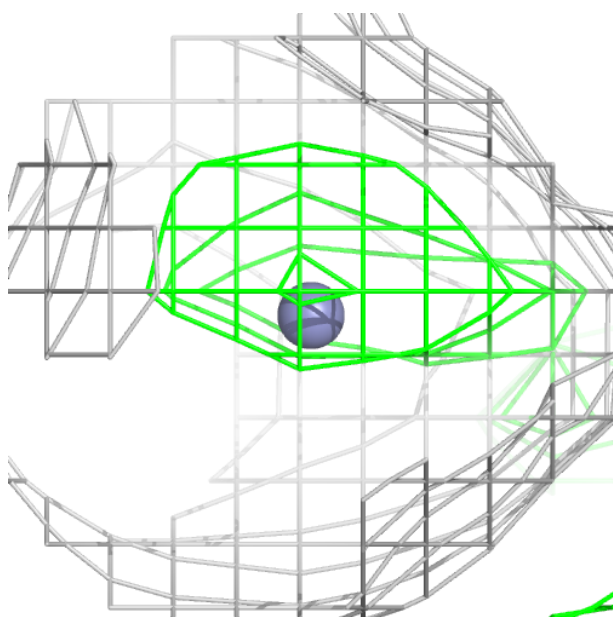
Electron density around CA B 605:

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



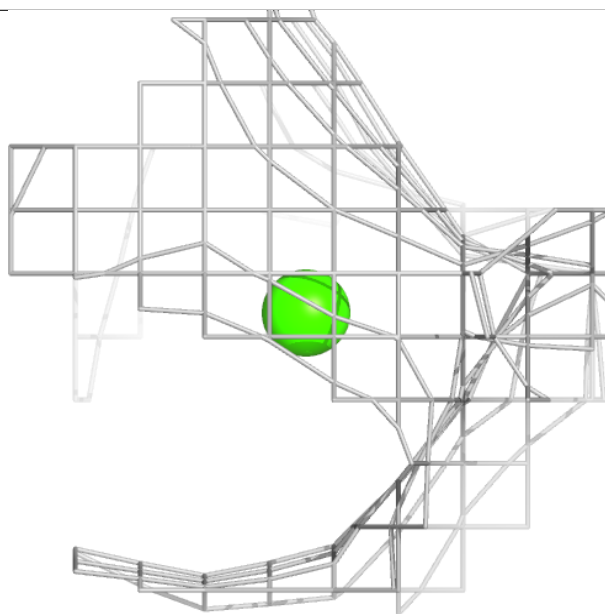
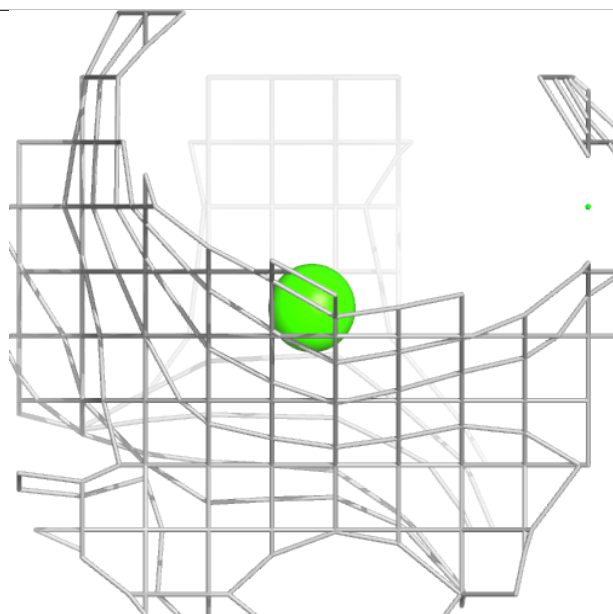
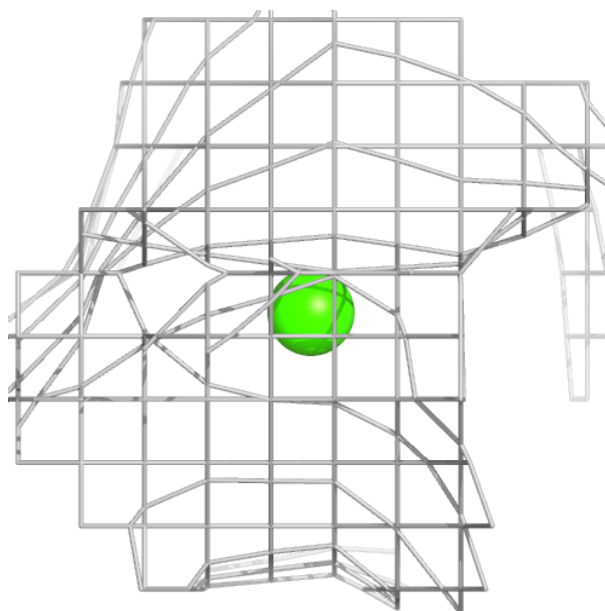
Electron density around ZN B 604:

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



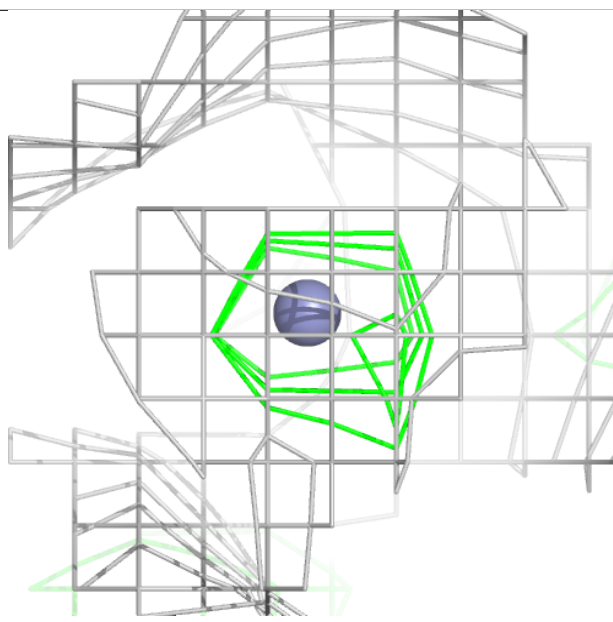
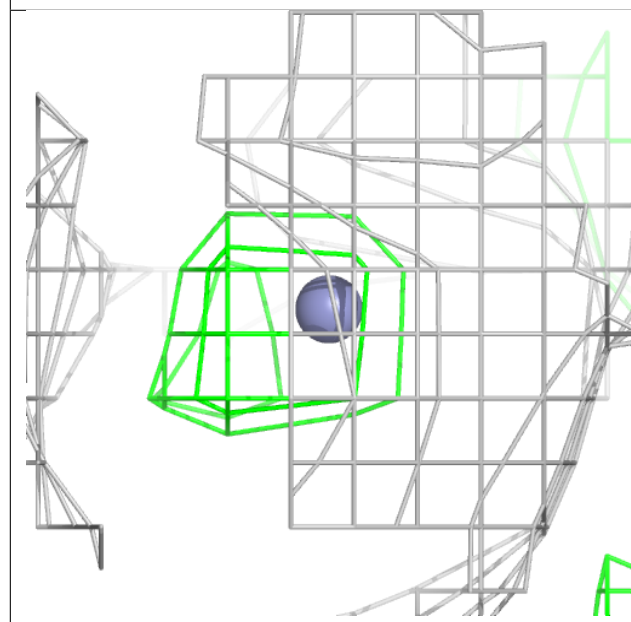
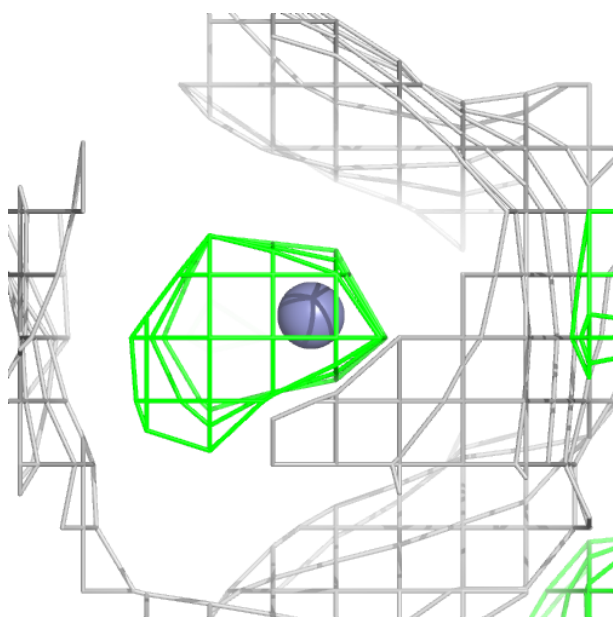
Electron density around CA H 605:

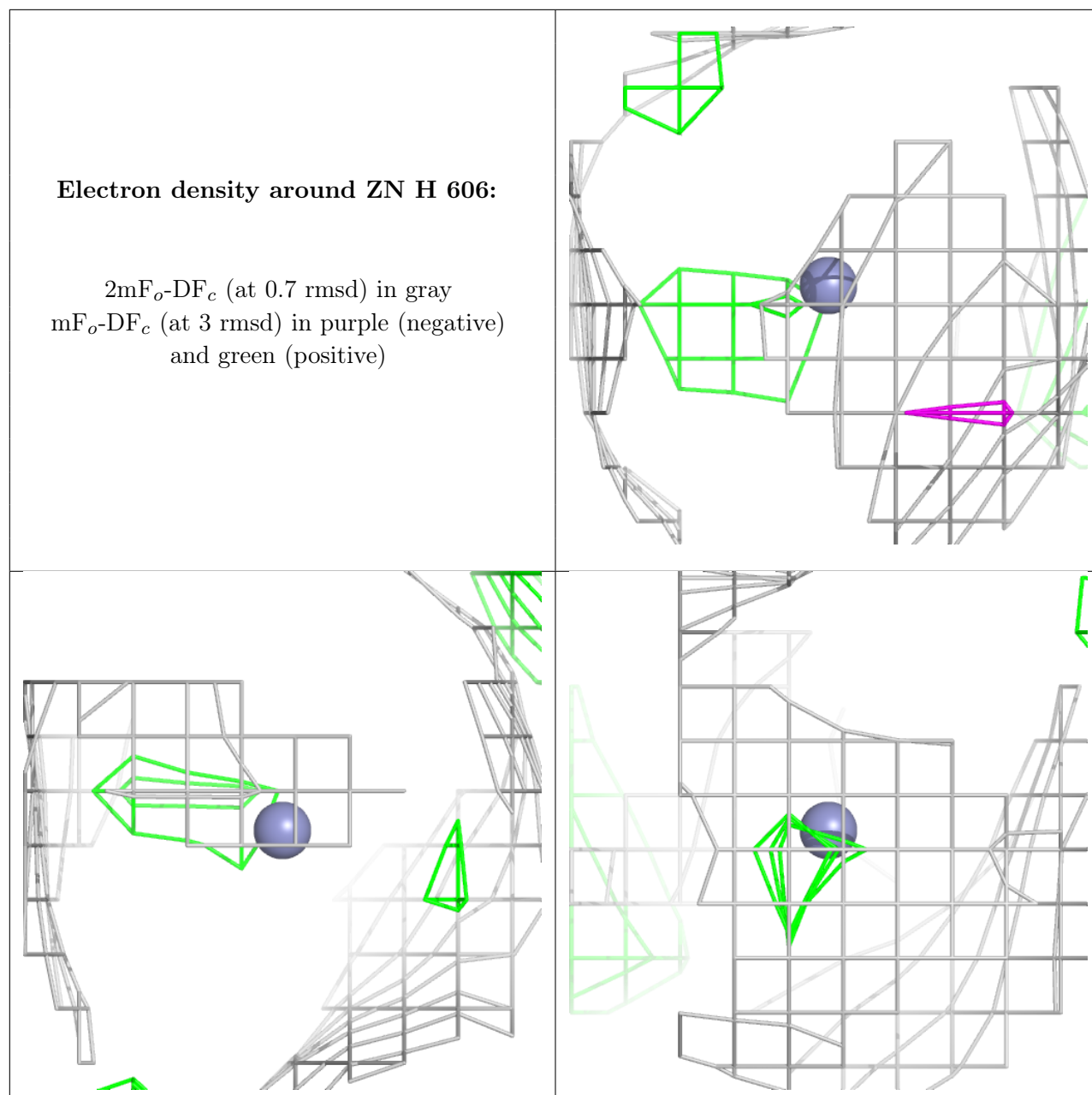
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around ZN B 606:

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





6.5 Other polymers ⓘ

There are no such residues in this entry.