



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 18, 2026 – 12:27 AM UTC

PDB ID : 8Q6R / pdb_00008q6r
Title : Structure of complement FP in complex with the TPP-3077 VHH
Authors : Andersen, G.R.; Pedersen, D.V.
Deposited on : 2023-08-14
Resolution : 1.90 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

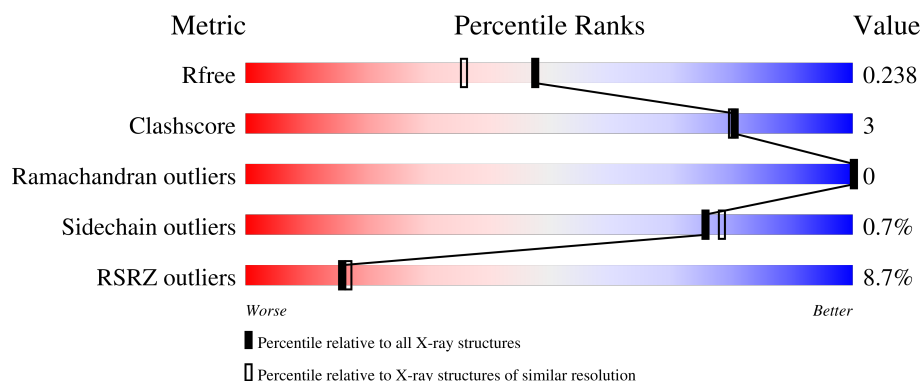
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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.



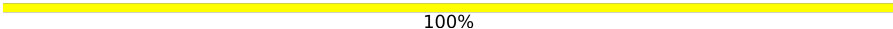
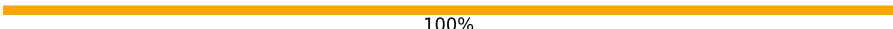
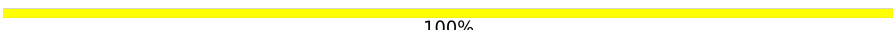
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	7789 (1.90-1.90)
Clashscore	190562	8410 (1.90-1.90)
Ramachandran outliers	187476	8333 (1.90-1.90)
Sidechain outliers	187428	8333 (1.90-1.90)
RSRZ outliers	180081	7790 (1.90-1.90)

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

Mol	Chain	Length	Quality of chain
1	A	125	2% 90% 5%
1	B	125	2% 93% 5%
2	C	108	10% 93% 6%
2	E	108	13% 93% 6%
3	D	221	10% 91% 5%

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Mol	Chain	Length	Quality of chain
3	F	221	 10% 90% 5% 5%
4	G	2	 100%
4	H	2	 100%
4	J	2	 100%
4	K	2	 100%
5	I	2	 50% 50%

2 Entry composition [i](#)

There are 9 unique types of molecules in this entry. The entry contains 13865 atoms, of which 6373 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 The properdin specific VHH TPP-3077.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	119	Total	C	H	N	O	S	0	0	0
			1806	567	896	161	178	4			
1	B	120	Total	C	H	N	O	S	0	0	0
			1823	573	903	164	179	4			

- Molecule 2 is a protein called Properdin.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	C	107	Total	C	H	N	O	S	0	0	0
			1564	500	752	145	155	12			
2	E	107	Total	C	H	N	O	S	0	0	0
			1564	500	752	145	155	12			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	132	ALA	CYS	conflict	UNP P27918
E	132	ALA	CYS	conflict	UNP P27918

- Molecule 3 is a protein called Properdin.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
3	D	211	Total	C	H	N	O	S	0	0	0
			3166	1009	1535	309	291	22			
3	F	211	Total	C	H	N	O	S	0	0	0
			3166	1009	1535	309	291	22			

There are 14 discrepancies between the modelled and reference sequences:

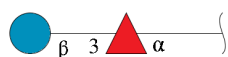
Chain	Residue	Modelled	Actual	Comment	Reference
D	255	GLY	-	expression tag	UNP P27918
D	470	HIS	-	expression tag	UNP P27918

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Chain	Residue	Modelled	Actual	Comment	Reference
D	471	HIS	-	expression tag	UNP P27918
D	472	HIS	-	expression tag	UNP P27918
D	473	HIS	-	expression tag	UNP P27918
D	474	HIS	-	expression tag	UNP P27918
D	475	HIS	-	expression tag	UNP P27918
F	255	GLY	-	expression tag	UNP P27918
F	470	HIS	-	expression tag	UNP P27918
F	471	HIS	-	expression tag	UNP P27918
F	472	HIS	-	expression tag	UNP P27918
F	473	HIS	-	expression tag	UNP P27918
F	474	HIS	-	expression tag	UNP P27918
F	475	HIS	-	expression tag	UNP P27918

- Molecule 4 is an oligosaccharide called beta-D-glucopyranose-(1-3)-alpha-L-fucopyranose.



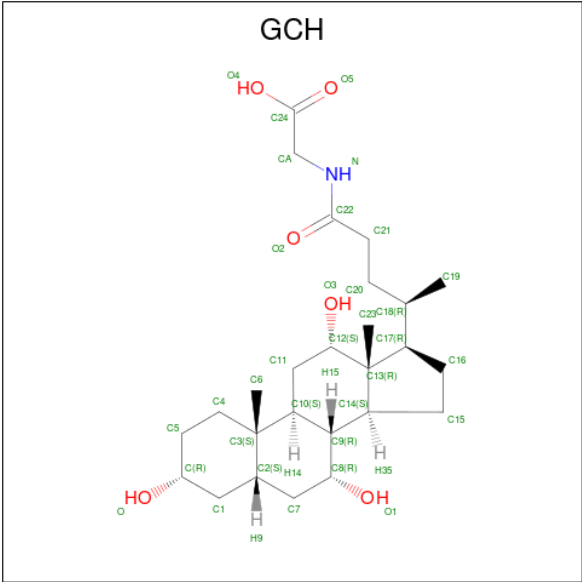
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
4	G	2	Total	C	O	0	0	0
			21	12	9			
4	H	2	Total	C	O	0	0	0
			21	12	9			
4	J	2	Total	C	O	0	0	0
			21	12	9			
4	K	2	Total	C	O	0	0	0
			21	12	9			

- Molecule 5 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



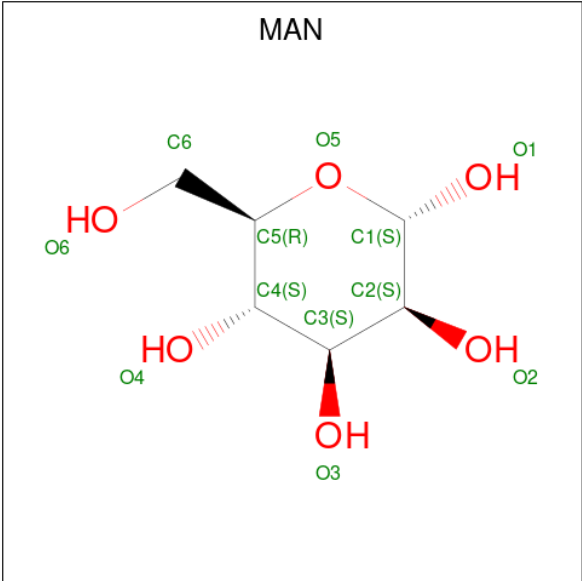
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	I	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 6 is GLYCOCHOLIC ACID (CCD ID: GCH) (formula: C₂₆H₄₃NO₆) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	1	Total	C	N	O	0	0
			33	26	1	6		
6	A	1	Total	C	N	O	0	0
			33	26	1	6		

- Molecule 7 is alpha-D-mannopyranose (CCD ID: MAN) (formula: C₆H₁₂O₆) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	C	1	Total	C	O	0	0
			11	6	5		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	C	1	Total	C	O	0	0
			11	6	5		
7	D	1	Total	C	O	0	0
			11	6	5		
7	D	1	Total	C	O	0	0
			11	6	5		
7	D	1	Total	C	O	0	0
			11	6	5		
7	D	1	Total	C	O	0	0
			11	6	5		
7	D	1	Total	C	O	0	0
			11	6	5		
7	D	1	Total	C	O	0	0
			11	6	5		
7	E	1	Total	C	O	0	0
			11	6	5		
7	E	1	Total	C	O	0	0
			11	6	5		
7	F	1	Total	C	O	0	0
			11	6	5		
7	F	1	Total	C	O	0	0
			11	6	5		
7	F	1	Total	C	O	0	0
			11	6	5		
7	F	1	Total	C	O	0	0
			11	6	5		
7	F	1	Total	C	O	0	0
			11	6	5		
7	F	1	Total	C	O	0	0
			11	6	5		

- Molecule 8 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
8	F	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	82	Total	O	0	0
			82	82		
9	B	79	Total	O	0	0
			79	79		
9	C	20	Total	O	0	0
			20	20		
9	D	74	Total	O	0	0
			74	74		
9	E	22	Total	O	0	0
			22	22		
9	F	87	Total	O	0	0
			87	87		

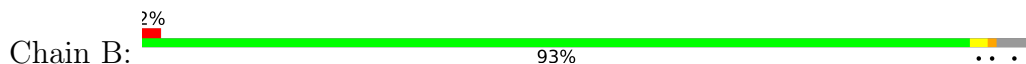
3 Residue-property plots

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: The properdin specific VHH TPP-3077



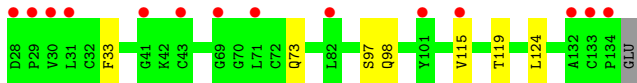
- Molecule 1: The properdin specific VHH TPP-3077



- Molecule 2: Properdin



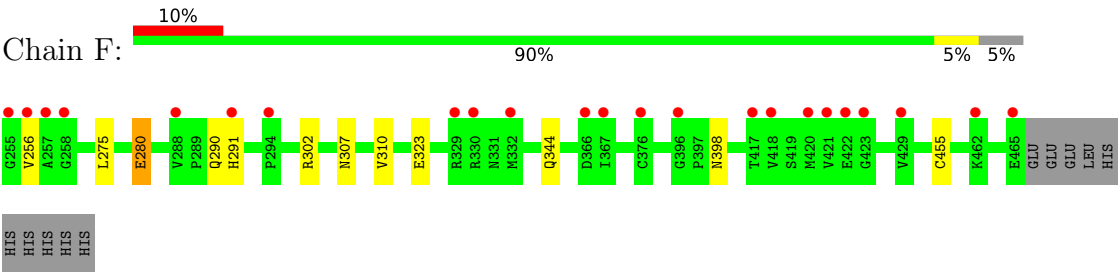
- Molecule 2: Properdin



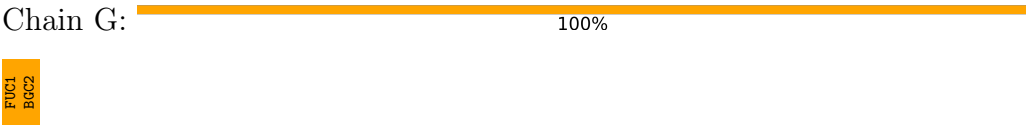
- Molecule 3: Properdin



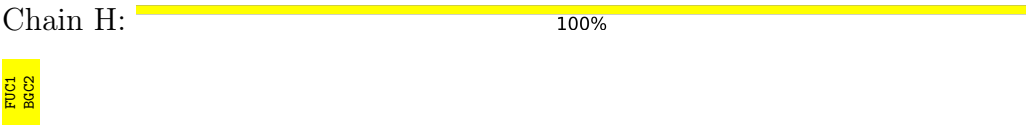
- Molecule 3: Properdin



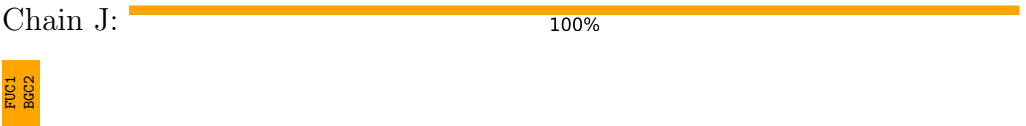
- Molecule 4: beta-D-glucopyranose-(1-3)-alpha-L-fucopyranose



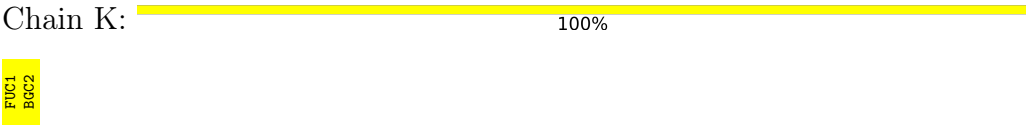
- Molecule 4: beta-D-glucopyranose-(1-3)-alpha-L-fucopyranose



- Molecule 4: beta-D-glucopyranose-(1-3)-alpha-L-fucopyranose



- Molecule 4: beta-D-glucopyranose-(1-3)-alpha-L-fucopyranose



- Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	79.21Å 63.70Å 119.25Å 90.00° 103.75° 90.00°	Depositor
Resolution (Å)	47.86 – 1.90 47.86 – 1.90	Depositor EDS
% Data completeness (in resolution range)	98.1 (47.86-1.90) 98.2 (47.86-1.90)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.05 (at 1.84Å)	Xtriage
Refinement program	PHENIX 1.19.2_4158	Depositor
R, R_{free}	0.202 , 0.238 0.203 , 0.238	Depositor DCC
R_{free} test set	2000 reflections (2.09%)	wwPDB-VP
Wilson B-factor (Å ²)	32.5	Xtriage
Anisotropy	0.408	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 47.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	13865	wwPDB-VP
Average B, all atoms (Å ²)	65.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 32.55 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 9.2355e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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: MAN, GCH, NAG, BGC, FUC

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	0.98	1/926 (0.1%)	1.05	1/1251 (0.1%)
1	B	0.95	0/937	1.03	0/1266
2	C	0.55	0/832	0.75	0/1128
2	E	0.54	0/832	0.74	1/1128 (0.1%)
3	D	0.78	4/1685 (0.2%)	0.94	3/2295 (0.1%)
3	F	0.76	3/1685 (0.2%)	0.87	2/2295 (0.1%)
All	All	0.78	8/6897 (0.1%)	0.91	7/9363 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	2
All	All	0	3

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	398	ASN	C-O	8.85	1.28	1.23
3	D	344	GLN	CB-CG	-8.54	1.26	1.52
3	D	267	SER	CA-C	-7.62	1.45	1.52
1	A	82	MET	SD-CE	-7.05	1.61	1.79
3	F	344	GLN	CB-CG	-7.05	1.31	1.52
3	D	398	ASN	C-O	-6.61	1.20	1.23
3	D	267	SER	C-O	5.63	1.29	1.24
3	F	310	VAL	CA-C	-5.42	1.48	1.53

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	267	SER	O-C-N	-10.32	115.11	121.71
3	F	455	CYS	CA-CB-SG	-5.55	101.64	114.40
2	E	98	GLN	N-CA-CB	-5.43	101.31	111.13
3	F	280	GLU	CB-CA-C	5.34	120.74	109.79
1	A	71	ARG	CB-CA-C	-5.31	98.83	109.35
3	D	344	GLN	N-CA-CB	-5.29	102.13	111.39
3	D	280	GLU	CB-CA-C	5.12	120.29	109.79

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	71	ARG	Sidechain
1	B	6	GLU	Sidechain
1	B	71	ARG	Sidechain

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	910	896	896	4	0
1	B	920	903	903	1	0
2	C	812	752	754	4	0
2	E	812	752	754	3	0
3	D	1631	1535	1544	4	0
3	F	1631	1535	1544	5	0
4	G	21	0	19	2	0
4	H	21	0	19	0	0
4	J	21	0	19	1	0
4	K	21	0	19	0	0
5	I	28	0	25	1	0
6	A	66	0	74	9	0
7	C	22	0	20	0	0
7	D	88	0	80	4	0
7	E	22	0	20	0	0
7	F	88	0	80	2	0
8	F	14	0	13	0	0
9	A	82	0	0	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	B	79	0	0	0	0
9	C	20	0	0	1	0
9	D	74	0	0	1	0
9	E	22	0	0	1	0
9	F	87	0	0	1	0
All	All	7492	6373	6783	36	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 3.

All (36) 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)
6:A:1102:GCH:C7	6:A:1102:GCH:C8	1.76	1.58
6:A:1102:GCH:C17	6:A:1102:GCH:C16	1.75	1.54
6:A:1102:GCH:C16	6:A:1102:GCH:C18	2.49	0.89
2:C:84:SER:O	9:C:301:HOH:O	1.93	0.86
3:D:374:GLN:OE1	9:D:601:HOH:O	1.97	0.81
1:A:44:GLU:OE1	9:A:1201:HOH:O	1.99	0.81
1:A:71:ARG:NH2	9:A:1202:HOH:O	2.15	0.80
2:C:134:PRO:HD2	4:G:1:FUC:H62	1.77	0.67
6:A:1102:GCH:C16	6:A:1102:GCH:C20	2.77	0.62
4:G:1:FUC:O2	4:G:2:BGC:H2	2.00	0.61
2:E:73:GLN:NE2	9:E:301:HOH:O	2.32	0.61
6:A:1102:GCH:C7	6:A:1102:GCH:O1	2.48	0.61
3:D:273:CYS:HA	3:D:310:VAL:HG13	1.84	0.59
4:J:1:FUC:O2	4:J:2:BGC:H2	2.02	0.58
2:E:97:SER:HB3	2:E:124:LEU:HD11	1.89	0.54
2:E:115:VAL:HG21	2:E:119:THR:HG21	1.92	0.50
1:B:82:MET:HE2	1:B:85:LEU:HD21	1.94	0.49
6:A:1102:GCH:C7	6:A:1102:GCH:C9	2.52	0.48
6:A:1102:GCH:C8	6:A:1102:GCH:C2	2.70	0.47
2:C:115:VAL:HG21	2:C:119:THR:HG21	1.97	0.47
3:D:382:TRP:N	7:D:504:MAN:O2	2.42	0.44
6:A:1102:GCH:C16	6:A:1102:GCH:H28	2.45	0.44
5:I:1:NAG:H4	5:I:2:NAG:H2	1.81	0.43
1:A:61:ASP:OD2	7:D:501:MAN:H5	2.18	0.43
7:F:507:MAN:O3	7:F:507:MAN:H61	2.19	0.43
3:F:275:LEU:HD23	3:F:307:ASN:HA	2.01	0.42
3:F:256:VAL:HG12	3:F:291:HIS:HB2	2.01	0.41
2:C:97:SER:HB3	2:C:124:LEU:HD11	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:280:GLU:OE2	3:F:302:ARG:NH2	2.41	0.41
7:D:508:MAN:H61	7:D:508:MAN:O3	2.20	0.41
3:D:344:GLN:HE22	3:D:432:TRP:CG	2.39	0.41
6:A:1101:GCH:H26	6:A:1101:GCH:H19	1.81	0.41
3:F:290:GLN:HA	9:F:635:HOH:O	2.21	0.41
1:A:88:GLU:HG3	9:A:1255:HOH:O	2.21	0.40
3:F:323:GLU:OE1	7:F:503:MAN:O3	2.33	0.40
7:D:505:MAN:H61	7:D:505:MAN:O3	2.20	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	117/125 (94%)	116 (99%)	1 (1%)	0	100	100
1	B	118/125 (94%)	116 (98%)	2 (2%)	0	100	100
2	C	105/108 (97%)	97 (92%)	8 (8%)	0	100	100
2	E	105/108 (97%)	98 (93%)	7 (7%)	0	100	100
3	D	209/221 (95%)	204 (98%)	5 (2%)	0	100	100
3	F	209/221 (95%)	205 (98%)	4 (2%)	0	100	100
All	All	863/908 (95%)	836 (97%)	27 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	98/104 (94%)	97 (99%)	1 (1%)	68	70
1	B	99/104 (95%)	98 (99%)	1 (1%)	68	70
2	C	89/90 (99%)	88 (99%)	1 (1%)	65	67
2	E	89/90 (99%)	88 (99%)	1 (1%)	65	67
3	D	180/190 (95%)	179 (99%)	1 (1%)	78	81
3	F	180/190 (95%)	180 (100%)	0	100	100
All	All	735/768 (96%)	730 (99%)	5 (1%)	76	78

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	GLU
1	B	6	GLU
2	C	33	PHE
3	D	310	VAL
2	E	33	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	73	ASN
1	B	13	GLN
1	B	73	ASN
1	B	120	HIS
2	C	98	GLN
3	D	290	GLN
3	D	363	GLN
3	D	369	HIS
3	F	291	HIS

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 ⓘ

10 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
4	FUC	G	1	2,4	10,10,11	1.48	1 (10%)	14,14,16	1.25	0
4	BGC	G	2	4	11,11,12	1.72	2 (18%)	15,15,17	2.24	1 (6%)
4	FUC	H	1	3,4	10,10,11	1.32	2 (20%)	14,14,16	0.99	0
4	BGC	H	2	4	11,11,12	1.86	2 (18%)	15,15,17	1.55	2 (13%)
5	NAG	I	1	3,5	14,14,15	0.23	0	17,19,21	0.44	0
5	NAG	I	2	5	14,14,15	0.68	1 (7%)	17,19,21	0.94	1 (5%)
4	FUC	J	1	2,4	10,10,11	1.20	1 (10%)	14,14,16	1.11	0
4	BGC	J	2	4	11,11,12	1.69	2 (18%)	15,15,17	2.31	4 (26%)
4	FUC	K	1	3,4	10,10,11	1.91	2 (20%)	14,14,16	1.33	2 (14%)
4	BGC	K	2	4	11,11,12	1.18	2 (18%)	15,15,17	1.38	2 (13%)

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
4	FUC	G	1	2,4	-	-	0/1/1/1
4	BGC	G	2	4	-	2/2/19/22	0/1/1/1
4	FUC	H	1	3,4	-	-	0/1/1/1
4	BGC	H	2	4	-	0/2/19/22	0/1/1/1
5	NAG	I	1	3,5	-	0/6/23/26	0/1/1/1
5	NAG	I	2	5	-	1/6/23/26	0/1/1/1
4	FUC	J	1	2,4	-	-	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	BGC	J	2	4	-	2/2/19/22	0/1/1/1
4	FUC	K	1	3,4	-	-	0/1/1/1
4	BGC	K	2	4	-	0/2/19/22	0/1/1/1

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	K	1	FUC	O5-C1	-4.64	1.35	1.43
4	G	2	BGC	O5-C1	4.60	1.51	1.43
4	J	2	BGC	O5-C1	4.49	1.51	1.43
4	H	2	BGC	O5-C1	4.13	1.50	1.43
4	H	2	BGC	C2-C3	-3.73	1.46	1.52
4	G	1	FUC	C2-C3	2.95	1.57	1.52
4	J	1	FUC	C2-C3	2.59	1.56	1.52
4	K	1	FUC	C2-C3	-2.39	1.48	1.52
4	K	2	BGC	C2-C3	-2.34	1.48	1.52
4	H	1	FUC	C2-C3	2.32	1.56	1.52
4	K	2	BGC	O5-C1	2.31	1.47	1.43
5	I	2	NAG	C1-C2	2.30	1.55	1.52
4	H	1	FUC	O5-C1	-2.15	1.40	1.43
4	G	2	BGC	O5-C5	2.12	1.47	1.43
4	J	2	BGC	O3-C3	2.03	1.48	1.43

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	G	2	BGC	C1-C2-C3	7.46	120.51	109.64
4	J	2	BGC	C1-C2-C3	6.92	119.72	109.64
4	H	2	BGC	C2-C3-C4	-4.11	103.63	110.86
4	J	2	BGC	O5-C1-C2	3.20	118.42	110.79
4	K	2	BGC	O4-C4-C5	-2.96	102.05	109.32
4	K	1	FUC	C3-C4-C5	-2.70	105.71	109.81
5	I	2	NAG	C2-N2-C7	2.61	126.40	122.90
4	J	2	BGC	C2-C3-C4	2.29	114.88	110.86
4	J	2	BGC	C3-C4-C5	2.16	114.16	110.23
4	H	2	BGC	O5-C5-C4	2.08	115.89	110.83
4	K	2	BGC	C1-O5-C5	2.04	114.92	112.19
4	K	1	FUC	O5-C5-C6	-2.01	103.03	107.40

There are no chirality outliers.

All (5) torsion outliers are listed below:

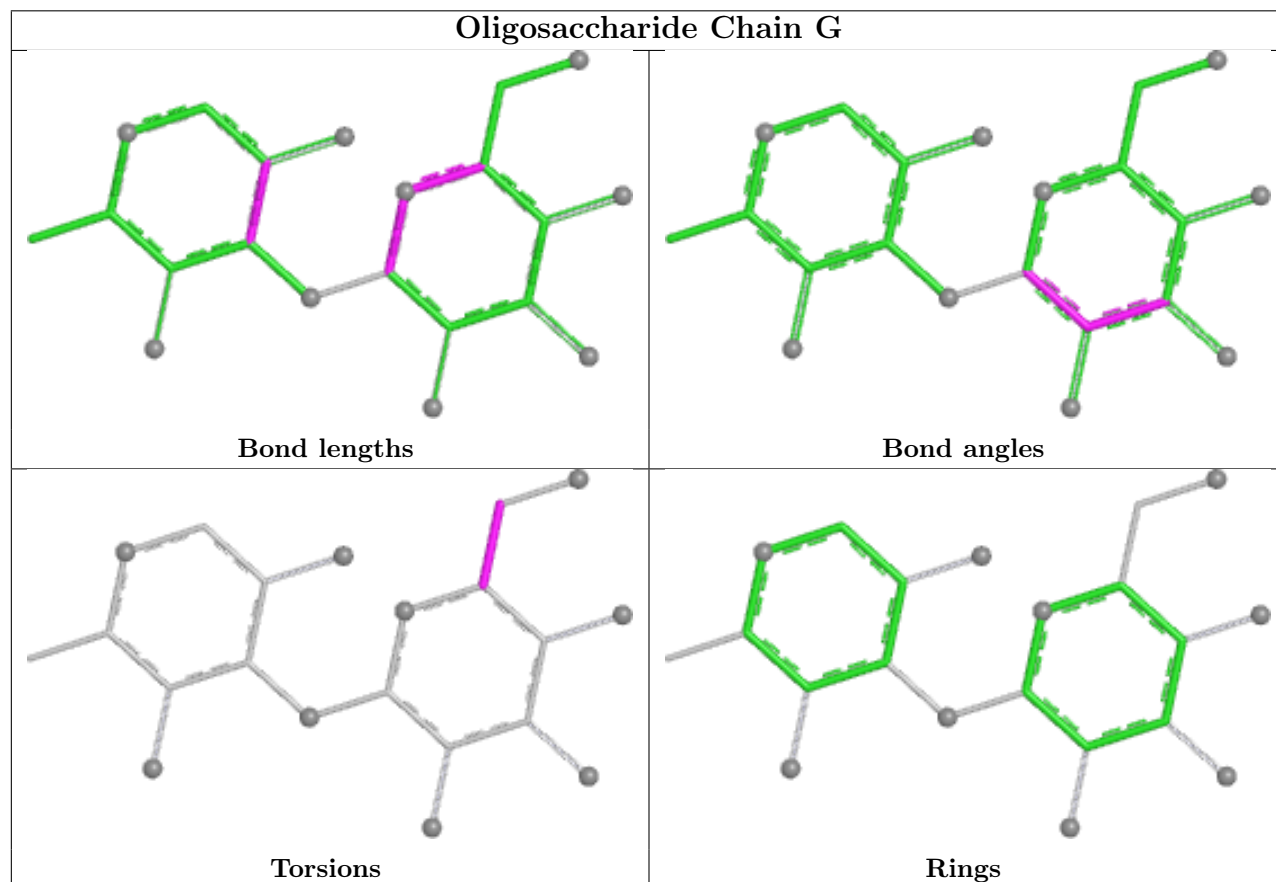
Mol	Chain	Res	Type	Atoms
5	I	2	NAG	C1-C2-N2-C7
4	G	2	BGC	O5-C5-C6-O6
4	J	2	BGC	C4-C5-C6-O6
4	J	2	BGC	O5-C5-C6-O6
4	G	2	BGC	C4-C5-C6-O6

There are no ring outliers.

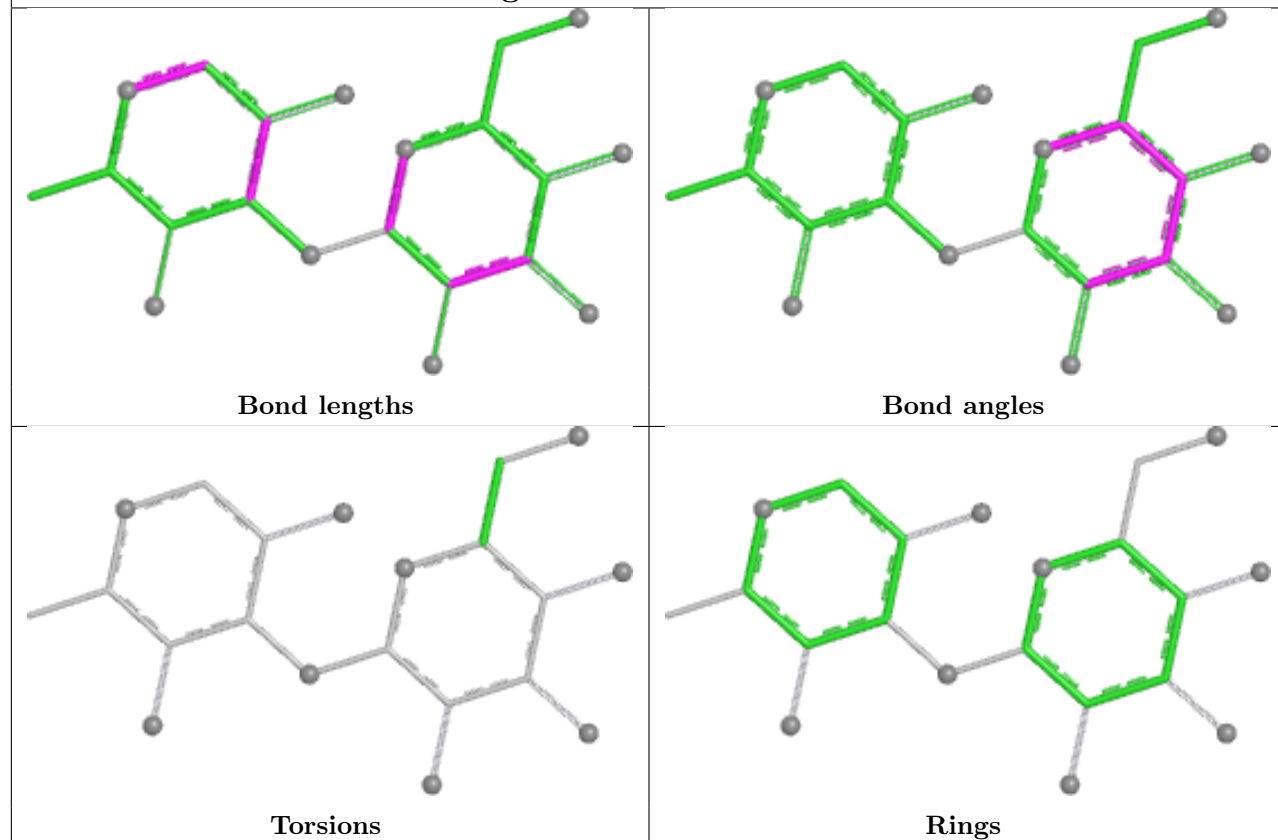
6 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	I	2	NAG	1	0
4	G	1	FUC	2	0
4	J	1	FUC	1	0
5	I	1	NAG	1	0
4	J	2	BGC	1	0
4	G	2	BGC	1	0

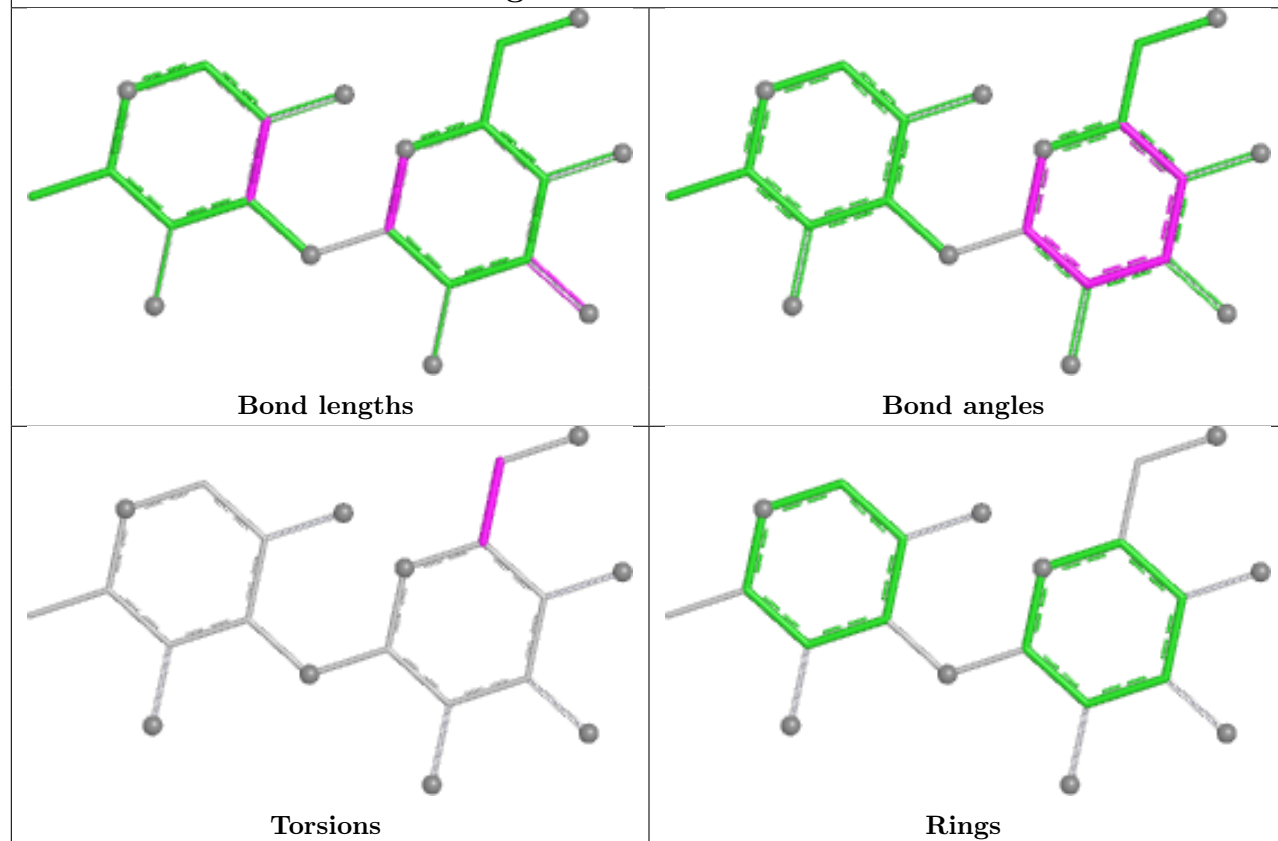
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

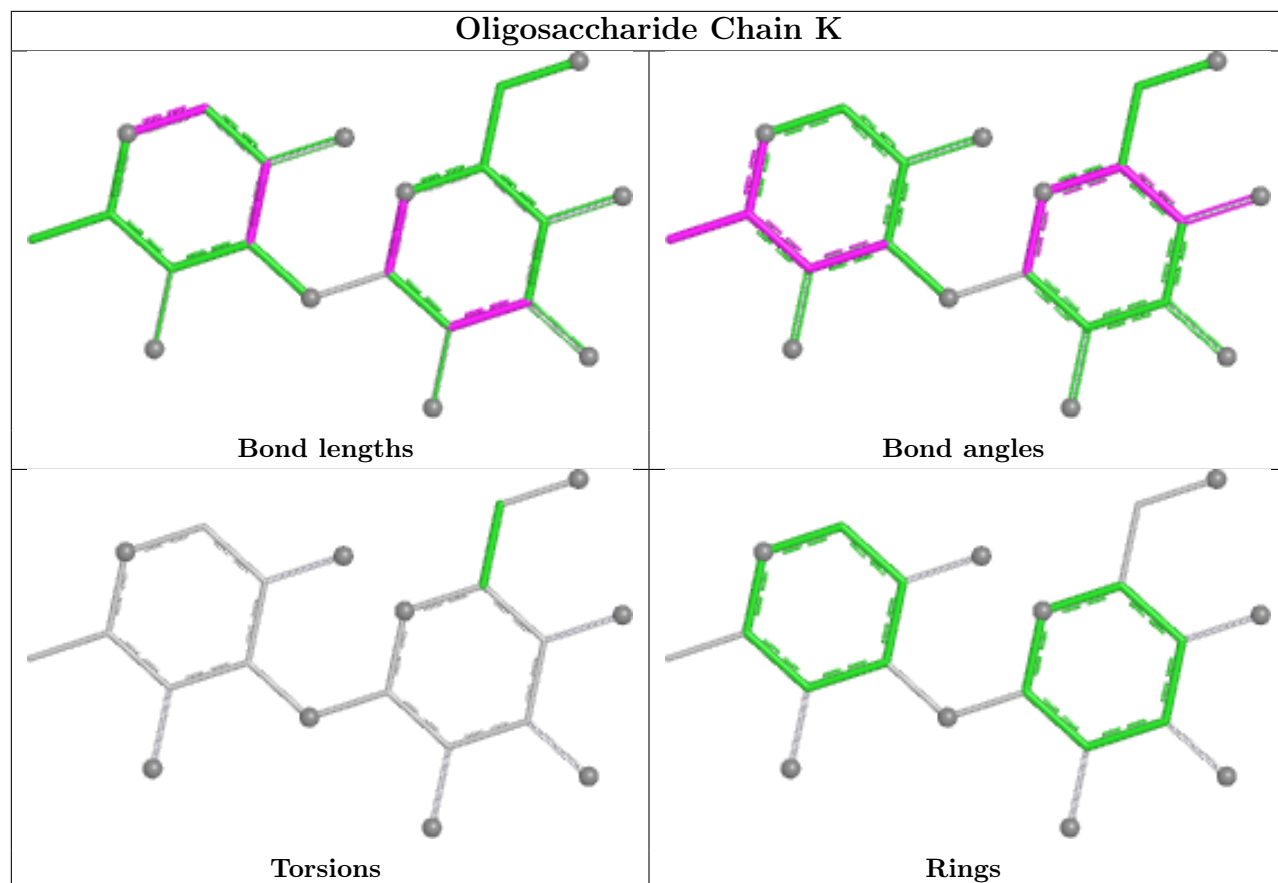


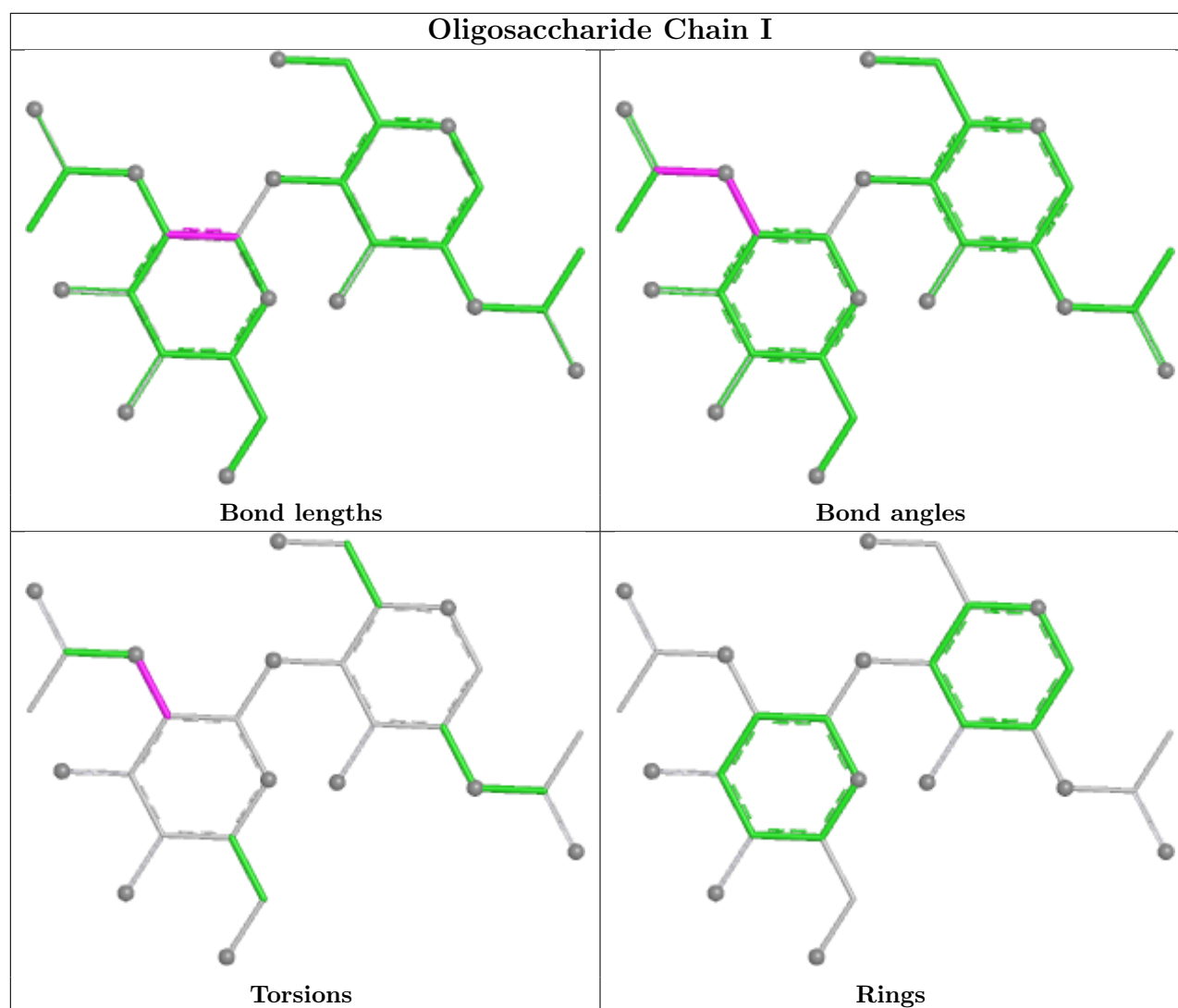
Oligosaccharide Chain H



Oligosaccharide Chain J







5.6 Ligand geometry [i](#)

23 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
7	MAN	E	201	2	11,11,12	0.83	0	15,15,17	0.74	0
7	MAN	F	508	3	11,11,12	1.82	3 (27%)	15,15,17	1.41	2 (13%)
6	GCH	A	1102	-	36,36,36	8.18	27 (75%)	56,56,56	2.57	26 (46%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	MAN	F	507	3	11,11,12	1.15	2 (18%)	15,15,17	1.17	2 (13%)
7	MAN	D	505	3	11,11,12	1.17	1 (9%)	15,15,17	1.20	2 (13%)
7	MAN	F	509	3	11,11,12	1.36	1 (9%)	15,15,17	1.74	2 (13%)
7	MAN	F	504	3	11,11,12	2.51	3 (27%)	15,15,17	1.94	6 (40%)
7	MAN	D	502	3	11,11,12	1.51	3 (27%)	15,15,17	1.33	1 (6%)
7	MAN	F	501	3	11,11,12	1.78	2 (18%)	15,15,17	2.14	4 (26%)
7	MAN	F	506	3	11,11,12	1.20	1 (9%)	15,15,17	1.36	2 (13%)
7	MAN	E	202	2	11,11,12	1.32	0	15,15,17	1.38	3 (20%)
7	MAN	F	502	3	11,11,12	1.16	1 (9%)	15,15,17	1.76	1 (6%)
7	MAN	D	503	3	11,11,12	1.53	2 (18%)	15,15,17	1.55	3 (20%)
6	GCH	A	1101	-	36,36,36	8.06	26 (72%)	56,56,56	3.06	28 (50%)
8	NAG	F	505	3	14,14,15	0.49	0	17,19,21	0.41	0
7	MAN	F	503	3	11,11,12	1.70	2 (18%)	15,15,17	1.31	2 (13%)
7	MAN	C	202	2	11,11,12	1.05	1 (9%)	15,15,17	1.45	3 (20%)
7	MAN	C	201	2	11,11,12	1.06	0	15,15,17	1.19	1 (6%)
7	MAN	D	508	3	11,11,12	1.44	2 (18%)	15,15,17	1.23	1 (6%)
7	MAN	D	504	3	11,11,12	2.16	3 (27%)	15,15,17	2.04	3 (20%)
7	MAN	D	501	3	11,11,12	2.29	5 (45%)	15,15,17	1.54	3 (20%)
7	MAN	D	506	3	11,11,12	1.04	0	15,15,17	1.29	1 (6%)
7	MAN	D	507	3	11,11,12	1.61	2 (18%)	15,15,17	1.78	2 (13%)

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
7	MAN	E	201	2	-	0/2/19/22	0/1/1/1
7	MAN	F	508	3	-	1/2/19/22	0/1/1/1
6	GCH	A	1102	-	-	1/14/79/79	0/4/4/4
7	MAN	F	507	3	-	1/2/19/22	0/1/1/1
7	MAN	D	505	3	-	1/2/19/22	0/1/1/1
7	MAN	F	509	3	-	0/2/19/22	0/1/1/1
7	MAN	F	504	3	-	0/2/19/22	0/1/1/1
7	MAN	D	502	3	-	0/2/19/22	0/1/1/1
7	MAN	F	501	3	-	0/2/19/22	0/1/1/1
7	MAN	F	506	3	-	2/2/19/22	0/1/1/1
7	MAN	E	202	2	-	0/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	MAN	F	502	3	-	0/2/19/22	0/1/1/1
7	MAN	D	503	3	-	0/2/19/22	0/1/1/1
6	GCH	A	1101	-	-	2/14/79/79	0/4/4/4
8	NAG	F	505	3	-	2/6/23/26	0/1/1/1
7	MAN	F	503	3	-	0/2/19/22	0/1/1/1
7	MAN	C	202	2	-	0/2/19/22	0/1/1/1
7	MAN	C	201	2	-	0/2/19/22	0/1/1/1
7	MAN	D	508	3	-	2/2/19/22	0/1/1/1
7	MAN	D	504	3	-	0/2/19/22	0/1/1/1
7	MAN	D	501	3	-	0/2/19/22	0/1/1/1
7	MAN	D	506	3	-	1/2/19/22	0/1/1/1
7	MAN	D	507	3	-	1/2/19/22	0/1/1/1

All (87) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	1102	GCH	C9-C14	-24.03	1.07	1.53
6	A	1101	GCH	C9-C14	-23.07	1.09	1.53
6	A	1102	GCH	C9-C8	-19.83	1.17	1.53
6	A	1101	GCH	C9-C8	-19.42	1.18	1.53
6	A	1101	GCH	C3-C2	-14.62	1.32	1.55
6	A	1101	GCH	C11-C12	-14.35	1.29	1.53
6	A	1102	GCH	C3-C2	-14.23	1.33	1.55
6	A	1102	GCH	C18-C17	-12.90	1.32	1.54
6	A	1102	GCH	C11-C12	-12.90	1.32	1.53
6	A	1102	GCH	C7-C8	12.31	1.76	1.52
6	A	1101	GCH	C18-C17	-12.30	1.33	1.54
6	A	1101	GCH	C7-C8	10.61	1.72	1.52
6	A	1102	GCH	O3-C12	10.51	1.60	1.43
6	A	1102	GCH	C16-C17	10.29	1.75	1.54
6	A	1101	GCH	O3-C12	10.04	1.60	1.43
6	A	1101	GCH	C16-C17	9.25	1.73	1.54
6	A	1102	GCH	C1-C2	8.92	1.68	1.53
6	A	1101	GCH	C1-C2	8.90	1.68	1.53
6	A	1102	GCH	C13-C12	-8.59	1.41	1.54
6	A	1101	GCH	O1-C8	8.09	1.60	1.43
6	A	1101	GCH	C13-C12	-8.02	1.42	1.54
6	A	1101	GCH	C15-C14	7.28	1.69	1.54
6	A	1102	GCH	C13-C17	7.24	1.67	1.55
6	A	1102	GCH	C15-C14	6.72	1.68	1.54
6	A	1102	GCH	C22-N	6.41	1.48	1.33
6	A	1101	GCH	C7-C2	-6.34	1.43	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	1101	GCH	C22-N	6.29	1.48	1.33
6	A	1102	GCH	O1-C8	6.23	1.56	1.43
7	F	504	MAN	O5-C1	-6.18	1.33	1.43
6	A	1101	GCH	C13-C17	6.13	1.65	1.55
6	A	1101	GCH	C13-C14	5.98	1.65	1.55
6	A	1102	GCH	C4-C3	5.93	1.64	1.54
6	A	1101	GCH	C4-C3	5.59	1.63	1.54
6	A	1101	GCH	C5-C	-5.50	1.39	1.51
6	A	1102	GCH	C5-C	-5.43	1.39	1.51
7	D	504	MAN	O5-C1	-5.32	1.34	1.43
6	A	1102	GCH	C20-C18	4.19	1.64	1.54
7	D	507	MAN	C4-C3	4.04	1.62	1.52
7	D	501	MAN	O2-C2	4.04	1.51	1.43
7	D	501	MAN	O5-C5	3.93	1.51	1.43
6	A	1102	GCH	C13-C14	3.89	1.62	1.55
7	F	504	MAN	C1-C2	-3.82	1.43	1.52
6	A	1102	GCH	C7-C2	-3.79	1.47	1.53
7	F	501	MAN	O5-C5	3.69	1.50	1.43
7	F	501	MAN	C1-C2	3.67	1.61	1.52
6	A	1101	GCH	C20-C18	3.64	1.63	1.54
6	A	1102	GCH	C4-C5	3.60	1.60	1.53
7	D	503	MAN	O5-C5	3.53	1.50	1.43
6	A	1102	GCH	C16-C15	3.51	1.63	1.54
6	A	1102	GCH	C1-C	3.51	1.58	1.52
7	F	509	MAN	O5-C5	3.49	1.50	1.43
6	A	1102	GCH	C3-C10	3.46	1.62	1.56
7	F	503	MAN	O5-C1	-3.44	1.37	1.43
6	A	1101	GCH	C19-C18	3.35	1.61	1.53
7	D	502	MAN	C1-C2	3.33	1.60	1.52
6	A	1101	GCH	C1-C	3.29	1.57	1.52
6	A	1102	GCH	C21-C22	3.27	1.57	1.51
6	A	1101	GCH	C16-C15	3.21	1.62	1.54
7	F	504	MAN	O2-C2	-3.09	1.36	1.43
7	F	508	MAN	C2-C3	-3.07	1.47	1.52
6	A	1102	GCH	C19-C18	3.03	1.60	1.53
7	F	508	MAN	O5-C1	-2.98	1.38	1.43
7	D	505	MAN	O5-C5	2.97	1.49	1.43
7	F	508	MAN	O5-C5	2.94	1.49	1.43
7	D	504	MAN	C2-C3	-2.88	1.48	1.52
7	D	504	MAN	O2-C2	-2.83	1.37	1.43
7	D	501	MAN	C1-C2	2.68	1.58	1.52
7	D	508	MAN	O2-C2	-2.56	1.38	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	1101	GCH	C9-C10	2.50	1.58	1.53
7	D	501	MAN	O5-C1	2.50	1.47	1.43
7	D	508	MAN	O5-C5	2.49	1.48	1.43
7	D	502	MAN	O5-C5	2.49	1.48	1.43
6	A	1101	GCH	C21-C22	2.47	1.56	1.51
6	A	1101	GCH	O2-C22	-2.44	1.18	1.23
6	A	1102	GCH	CA-C24	2.40	1.56	1.50
6	A	1102	GCH	O2-C22	-2.37	1.18	1.23
6	A	1101	GCH	C4-C5	2.35	1.58	1.53
7	F	506	MAN	C4-C5	2.34	1.58	1.53
7	F	507	MAN	O5-C5	2.28	1.47	1.43
7	D	503	MAN	O3-C3	-2.25	1.37	1.43
7	F	507	MAN	O5-C1	-2.25	1.39	1.43
7	D	507	MAN	C2-C3	-2.21	1.49	1.52
7	F	503	MAN	O5-C5	2.21	1.47	1.43
7	C	202	MAN	O5-C5	2.15	1.47	1.43
7	D	501	MAN	O4-C4	-2.15	1.37	1.43
7	D	502	MAN	C4-C5	2.13	1.57	1.53
7	F	502	MAN	O5-C5	2.06	1.47	1.43

All (98) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	1101	GCH	C19-C18-C20	-7.20	99.20	110.34
6	A	1101	GCH	O3-C12-C13	-6.23	100.49	111.02
6	A	1102	GCH	O3-C12-C13	-6.23	100.50	111.02
6	A	1101	GCH	O1-C8-C7	-6.06	94.80	109.86
6	A	1101	GCH	C7-C8-C9	6.01	118.06	111.50
6	A	1102	GCH	C7-C8-C9	5.64	117.66	111.50
7	F	501	MAN	C1-O5-C5	5.55	119.62	112.19
7	D	507	MAN	C1-O5-C5	5.54	119.62	112.19
6	A	1101	GCH	C14-C13-C12	5.39	112.34	107.42
7	F	509	MAN	C1-O5-C5	5.36	119.37	112.19
7	D	504	MAN	O2-C2-C3	-5.30	99.18	110.15
6	A	1101	GCH	C11-C12-C13	5.26	116.62	111.26
6	A	1102	GCH	O1-C8-C7	-5.24	96.82	109.86
6	A	1101	GCH	C2-C1-C	-5.20	104.87	112.71
7	F	502	MAN	C1-O5-C5	5.11	119.04	112.19
6	A	1101	GCH	C23-C13-C17	-4.88	103.55	111.20
6	A	1101	GCH	C21-C20-C18	-4.76	105.56	114.46
6	A	1101	GCH	C17-C13-C14	4.65	104.78	100.11
6	A	1102	GCH	C14-C9-C8	4.43	117.73	111.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	1101	GCH	C4-C5-C	4.34	116.23	110.48
6	A	1101	GCH	C15-C14-C9	4.30	124.26	118.36
6	A	1102	GCH	C11-C12-C13	4.21	115.55	111.26
6	A	1102	GCH	C16-C15-C14	4.15	113.27	105.14
6	A	1102	GCH	C17-C13-C12	4.06	121.32	117.67
7	D	502	MAN	C1-O5-C5	3.97	117.50	112.19
6	A	1102	GCH	C23-C13-C12	-3.89	105.17	109.06
6	A	1101	GCH	C14-C9-C8	3.83	116.94	111.85
6	A	1101	GCH	C5-C4-C3	-3.81	106.30	112.74
6	A	1101	GCH	C1-C2-C3	3.68	116.57	112.66
6	A	1102	GCH	C13-C14-C9	3.66	119.36	114.72
6	A	1102	GCH	C23-C13-C17	-3.66	105.47	111.20
7	F	504	MAN	O5-C1-C2	3.61	119.40	110.79
7	D	508	MAN	C1-O5-C5	3.58	116.99	112.19
6	A	1101	GCH	O-C-C5	-3.56	100.86	110.17
7	D	503	MAN	C1-O5-C5	3.54	116.92	112.19
6	A	1102	GCH	C15-C14-C9	3.53	123.20	118.36
7	D	505	MAN	C1-O5-C5	3.52	116.90	112.19
6	A	1102	GCH	C17-C13-C14	3.49	103.61	100.11
7	F	501	MAN	O2-C2-C3	-3.47	102.96	110.15
7	D	504	MAN	O6-C6-C5	-3.45	99.57	111.33
6	A	1101	GCH	C7-C2-C3	-3.38	109.06	112.66
7	F	506	MAN	C1-O5-C5	3.35	116.67	112.19
7	D	501	MAN	C1-O5-C5	3.28	116.58	112.19
6	A	1102	GCH	C15-C16-C17	-3.28	98.72	105.14
7	C	201	MAN	C1-O5-C5	3.27	116.57	112.19
6	A	1102	GCH	O4-C24-CA	3.20	124.97	112.81
7	F	508	MAN	C1-O5-C5	3.20	116.47	112.19
6	A	1101	GCH	C4-C3-C2	3.11	112.22	107.75
6	A	1102	GCH	C16-C17-C18	-3.10	107.49	112.18
7	E	202	MAN	O2-C2-C3	-3.10	103.74	110.15
7	F	504	MAN	C2-C3-C4	-3.08	105.44	110.86
6	A	1102	GCH	C19-C18-C20	-3.04	105.63	110.34
6	A	1102	GCH	C3-C10-C9	3.02	115.20	111.84
7	C	202	MAN	C1-O5-C5	2.95	116.14	112.19
6	A	1101	GCH	C23-C13-C12	-2.94	106.12	109.06
7	F	509	MAN	O2-C2-C1	2.93	115.94	109.22
6	A	1101	GCH	C10-C11-C12	2.90	118.08	114.29
6	A	1101	GCH	C11-C10-C9	2.88	115.16	110.89
7	F	503	MAN	C1-O5-C5	2.88	116.05	112.19
7	E	202	MAN	C1-O5-C5	2.82	115.97	112.19
7	F	506	MAN	O2-C2-C3	-2.77	104.41	110.15

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	D	501	MAN	O2-C2-C3	-2.75	104.46	110.15
7	D	507	MAN	O2-C2-C3	-2.71	104.53	110.15
7	F	501	MAN	O6-C6-C5	-2.67	102.25	111.33
7	D	506	MAN	C1-O5-C5	2.62	115.69	112.19
6	A	1102	GCH	C4-C3-C2	2.57	111.44	107.75
7	F	508	MAN	O2-C2-C3	-2.57	104.83	110.15
6	A	1101	GCH	C21-C22-N	2.55	120.99	116.34
7	F	507	MAN	C1-O5-C5	2.54	115.59	112.19
6	A	1102	GCH	C6-C3-C4	-2.52	104.30	108.31
7	C	202	MAN	O6-C6-C5	-2.49	102.84	111.33
7	C	202	MAN	O2-C2-C3	-2.49	104.99	110.15
6	A	1102	GCH	O2-C22-C21	2.49	126.53	122.02
7	F	504	MAN	O4-C4-C3	-2.47	104.55	110.38
7	F	501	MAN	C2-C3-C4	2.44	115.14	110.86
7	E	202	MAN	O5-C1-C2	2.39	116.49	110.79
6	A	1102	GCH	C4-C5-C	-2.37	107.34	110.48
7	F	504	MAN	O6-C6-C5	-2.28	103.57	111.33
6	A	1101	GCH	C4-C3-C10	-2.18	107.95	111.34
7	F	504	MAN	O2-C2-C3	-2.18	105.64	110.15
6	A	1101	GCH	O4-C24-CA	2.17	121.06	112.81
6	A	1102	GCH	O-C-C1	2.17	114.16	109.84
7	F	504	MAN	O4-C4-C5	-2.16	103.99	109.32
7	F	503	MAN	O6-C6-C5	-2.16	103.97	111.33
7	D	503	MAN	O6-C6-C5	-2.16	103.97	111.33
6	A	1102	GCH	O4-C24-O5	-2.16	117.79	123.33
6	A	1102	GCH	C20-C18-C17	-2.16	105.86	110.33
7	D	503	MAN	O2-C2-C3	-2.13	105.75	110.15
6	A	1101	GCH	C19-C18-C17	2.12	116.07	112.88
7	F	507	MAN	O2-C2-C3	-2.10	105.79	110.15
6	A	1101	GCH	C13-C14-C9	2.08	117.36	114.72
7	D	505	MAN	O2-C2-C3	-2.07	105.87	110.15
6	A	1102	GCH	C10-C11-C12	2.06	116.99	114.29
7	D	504	MAN	O5-C1-C2	2.05	115.68	110.79
6	A	1101	GCH	C13-C17-C18	-2.03	117.02	119.48
6	A	1102	GCH	C16-C17-C13	2.02	105.50	103.54
6	A	1101	GCH	O2-C22-N	-2.02	119.07	123.03
7	D	501	MAN	O2-C2-C1	2.01	113.82	109.22

There are no chirality outliers.

All (14) torsion outliers are listed below:

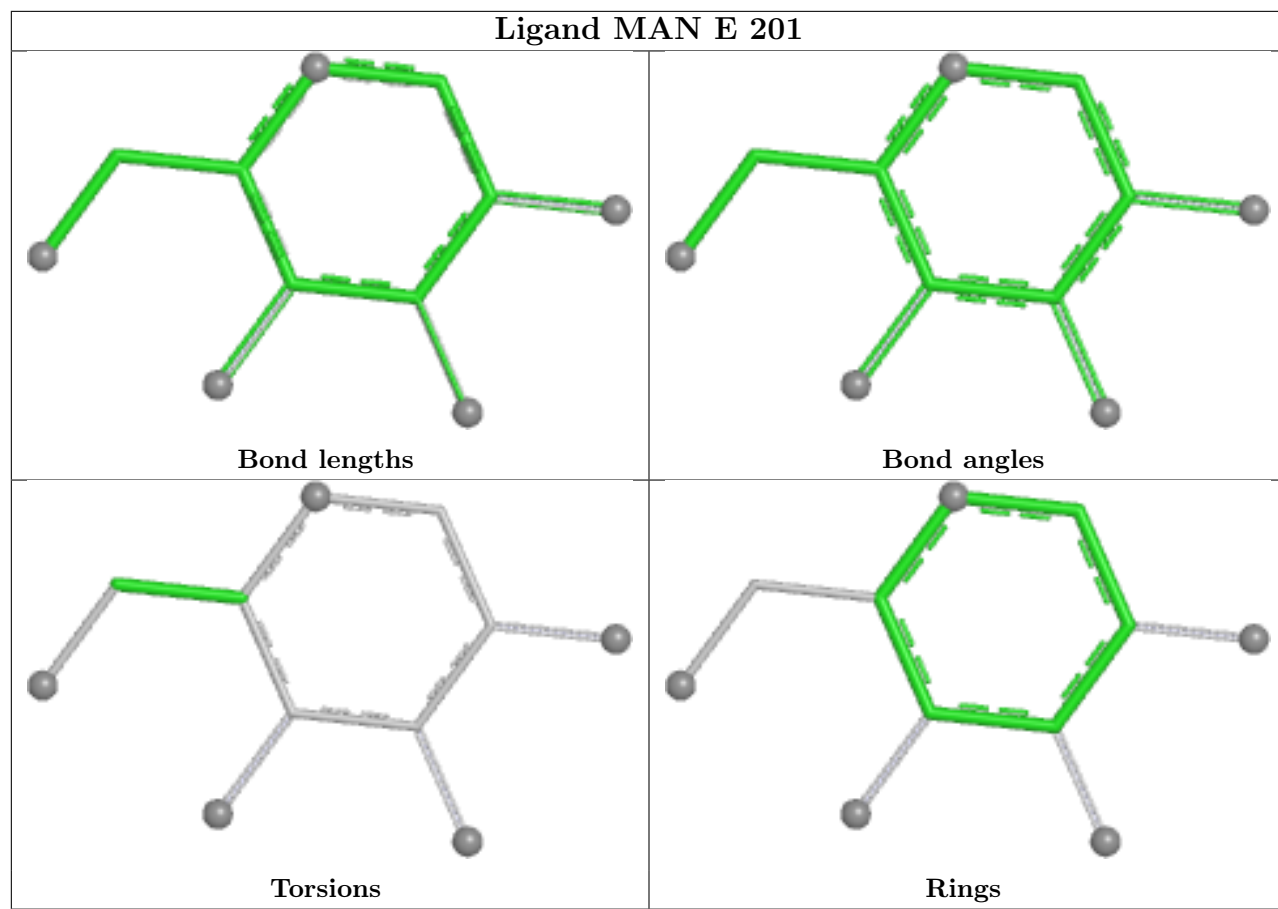
Mol	Chain	Res	Type	Atoms
6	A	1101	GCH	O5-C24-CA-N
8	F	505	NAG	C4-C5-C6-O6
8	F	505	NAG	O5-C5-C6-O6
6	A	1101	GCH	O4-C24-CA-N
7	F	506	MAN	O5-C5-C6-O6
7	D	508	MAN	O5-C5-C6-O6
7	D	505	MAN	O5-C5-C6-O6
7	F	507	MAN	O5-C5-C6-O6
7	F	506	MAN	C4-C5-C6-O6
7	D	507	MAN	O5-C5-C6-O6
7	D	508	MAN	C4-C5-C6-O6
7	F	508	MAN	O5-C5-C6-O6
6	A	1102	GCH	C19-C18-C20-C21
7	D	506	MAN	O5-C5-C6-O6

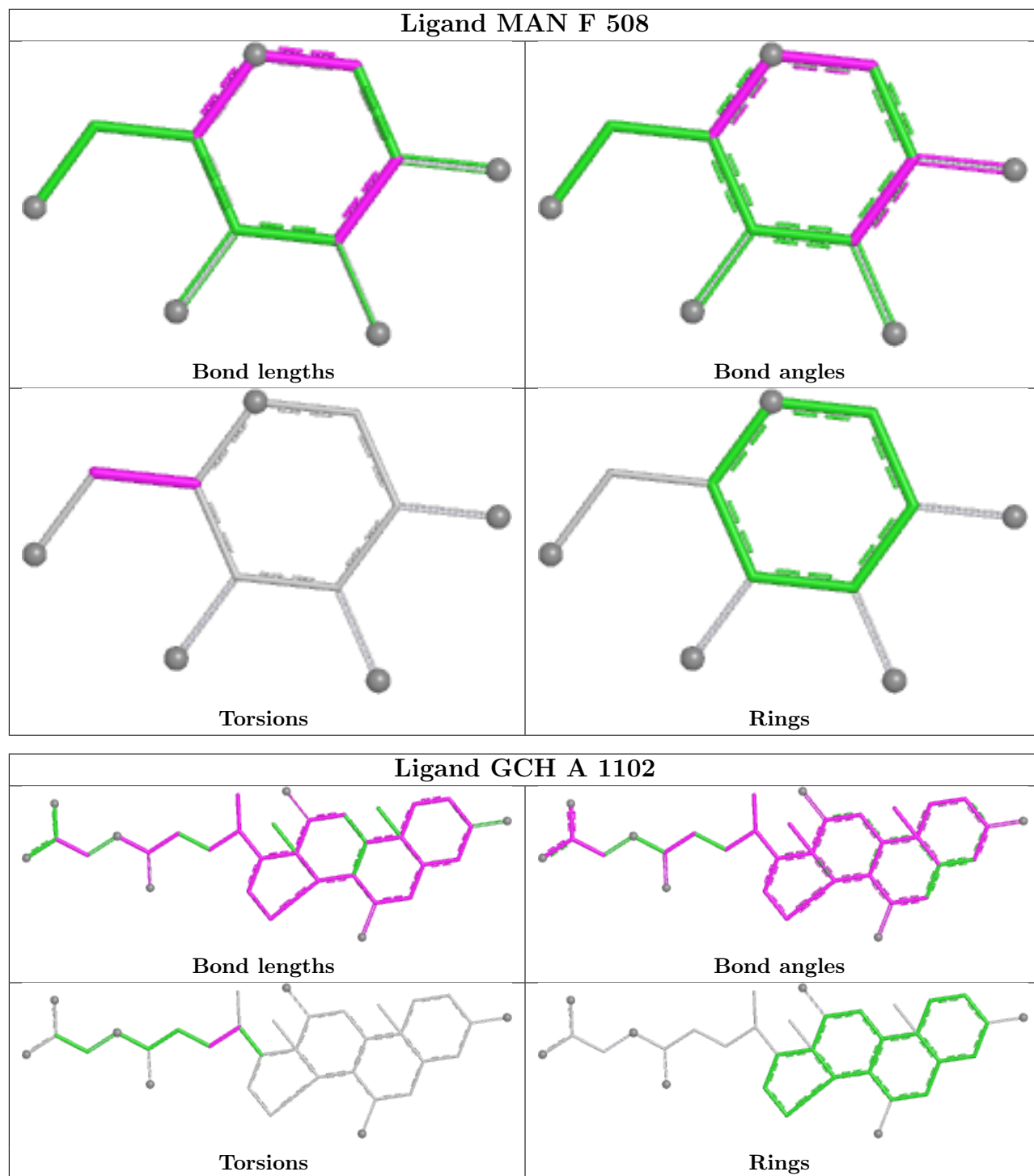
There are no ring outliers.

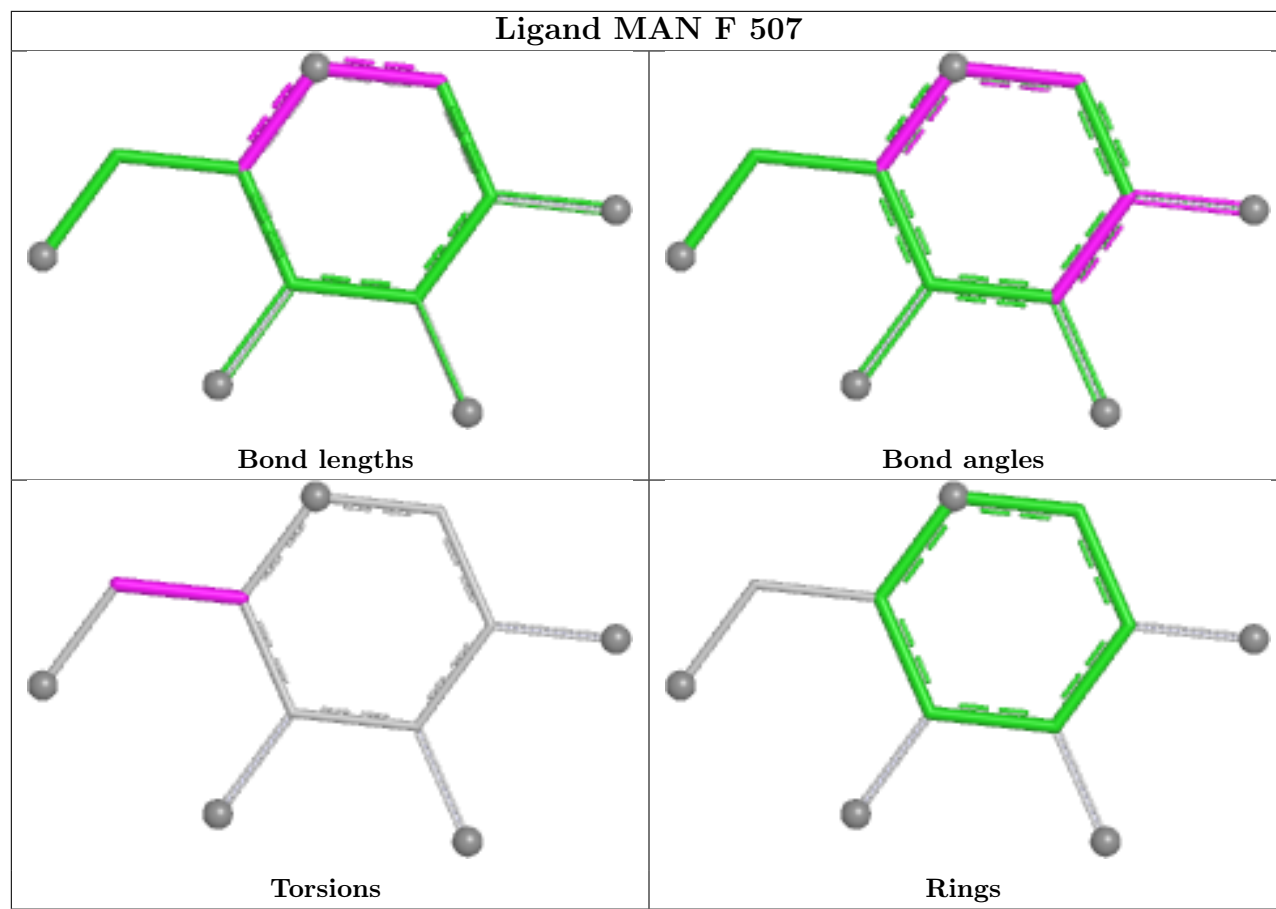
8 monomers are involved in 15 short contacts:

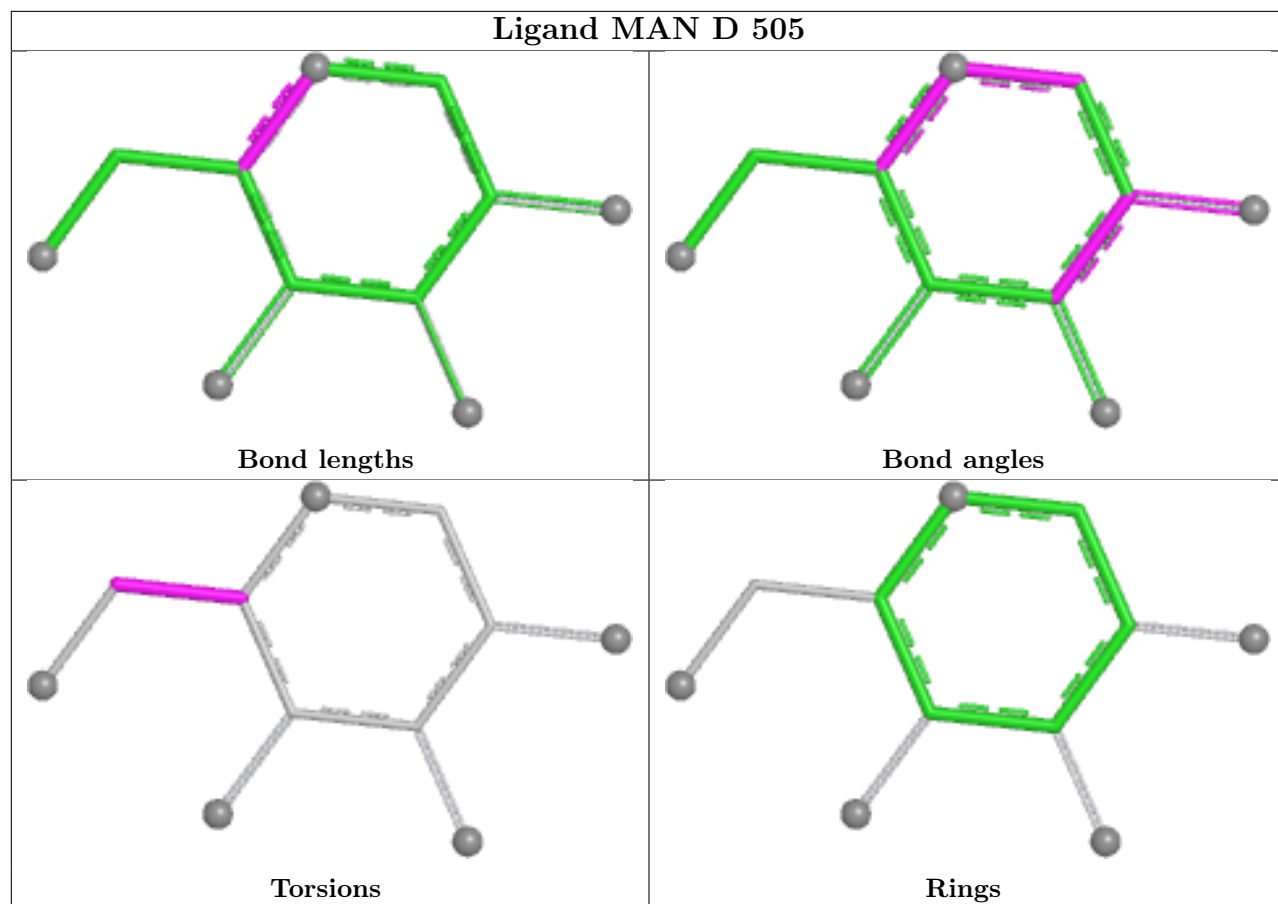
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	1102	GCH	8	0
7	F	507	MAN	1	0
7	D	505	MAN	1	0
6	A	1101	GCH	1	0
7	F	503	MAN	1	0
7	D	508	MAN	1	0
7	D	504	MAN	1	0
7	D	501	MAN	1	0

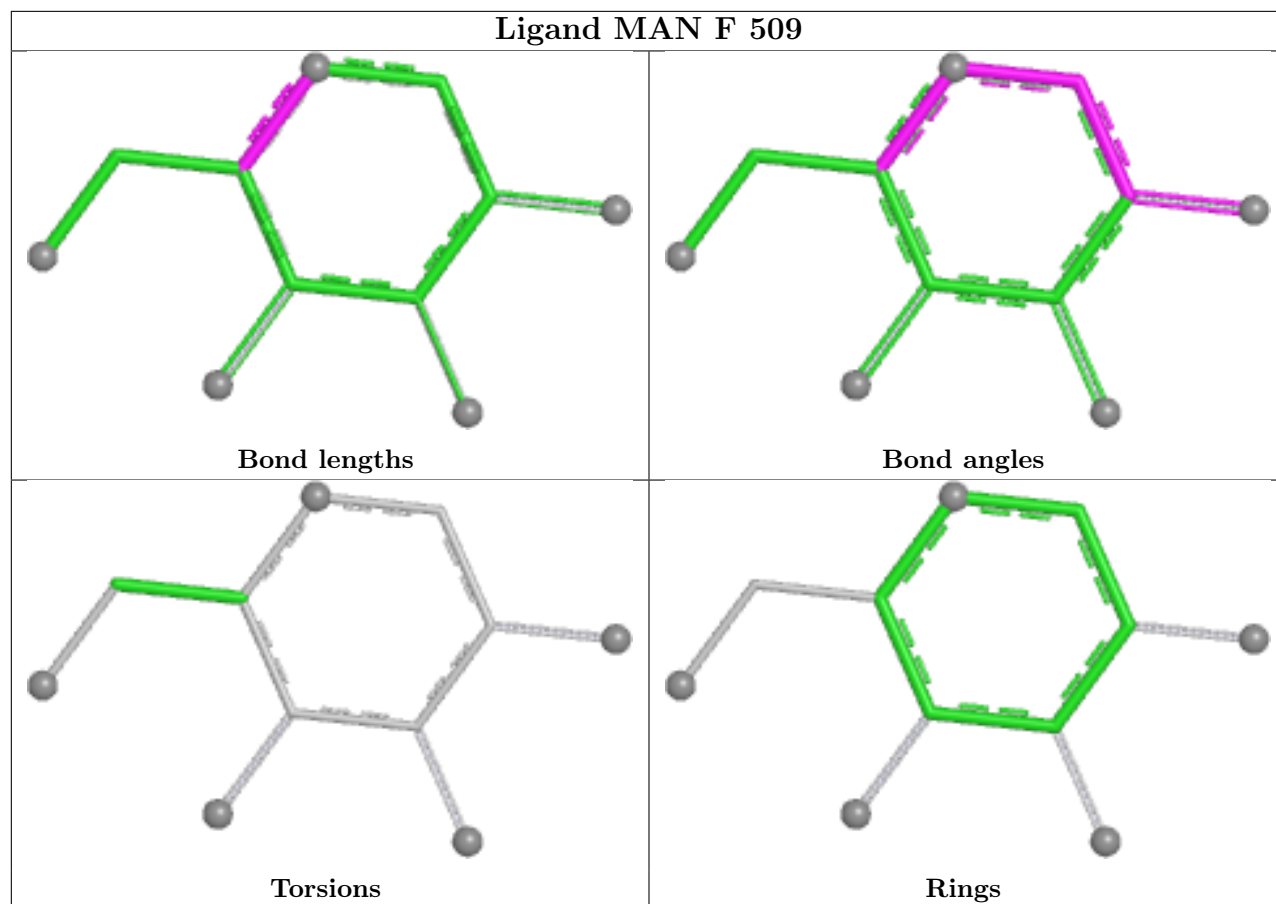
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

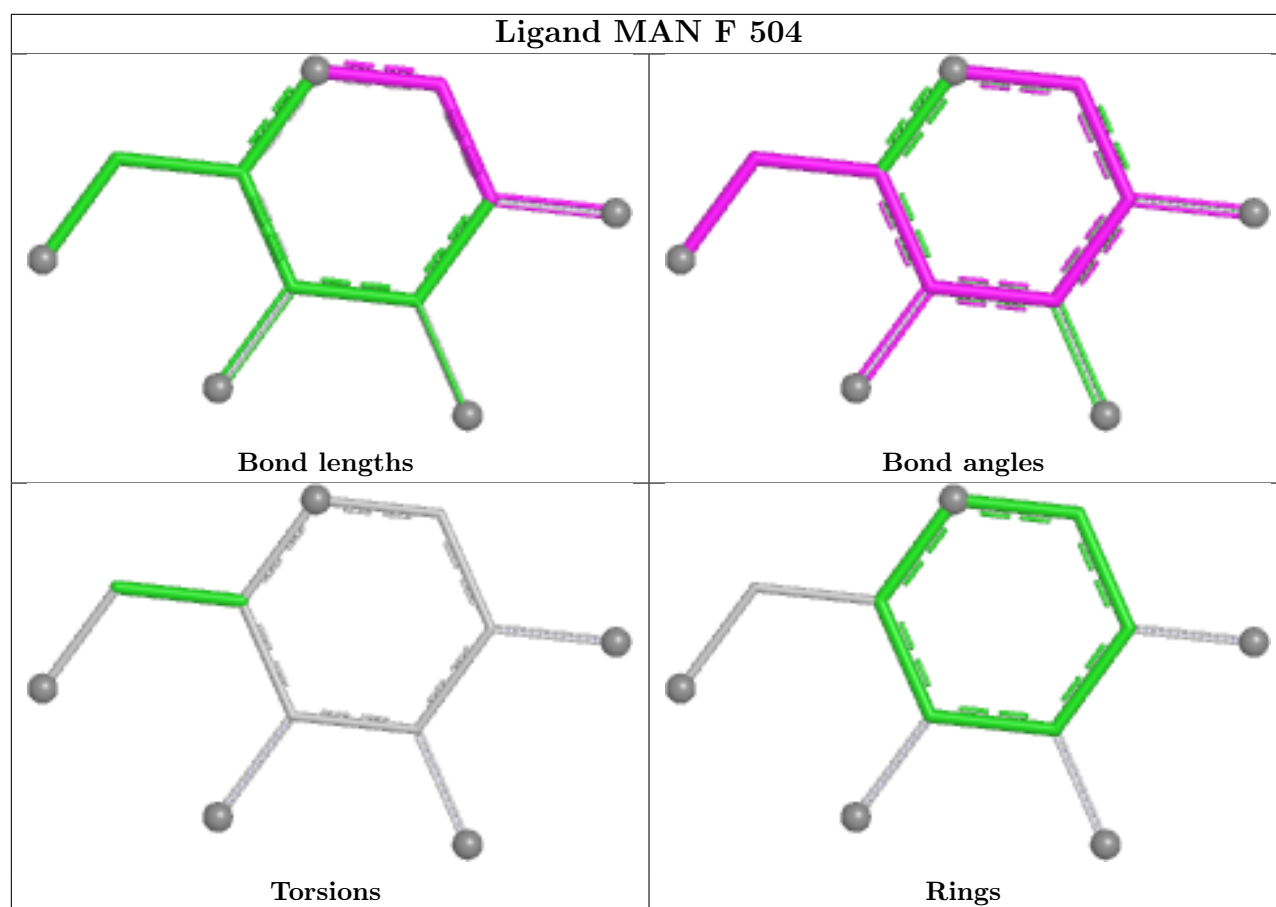


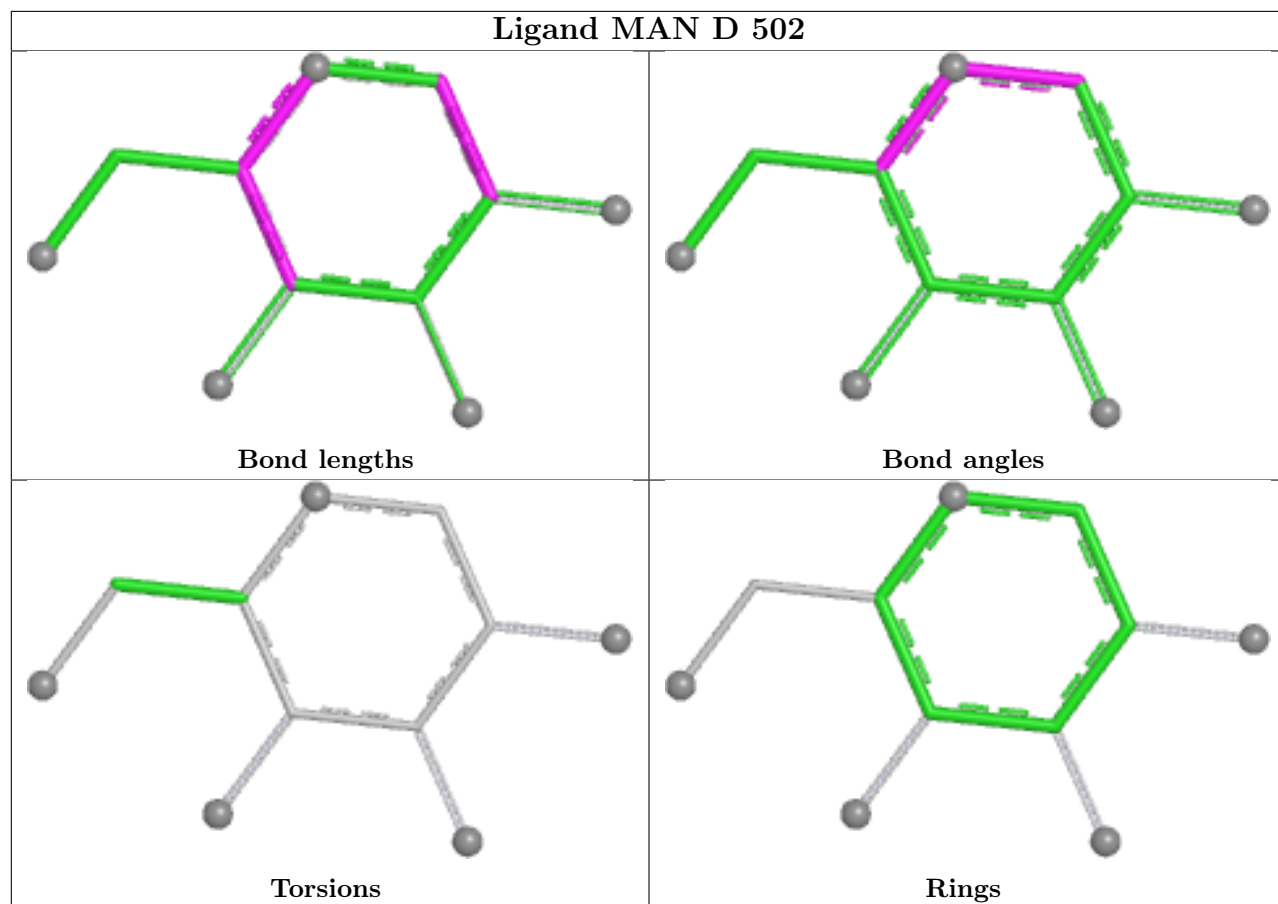


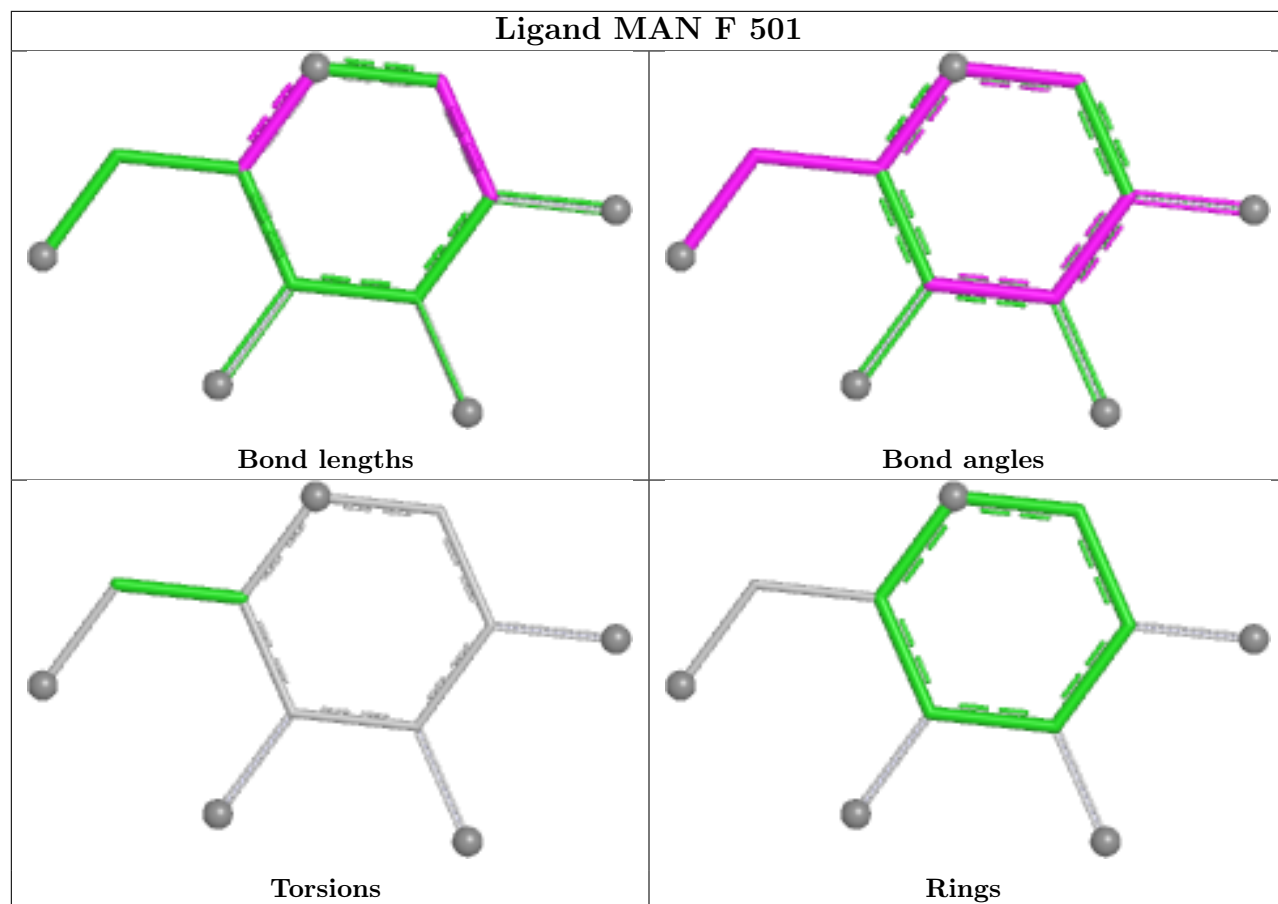


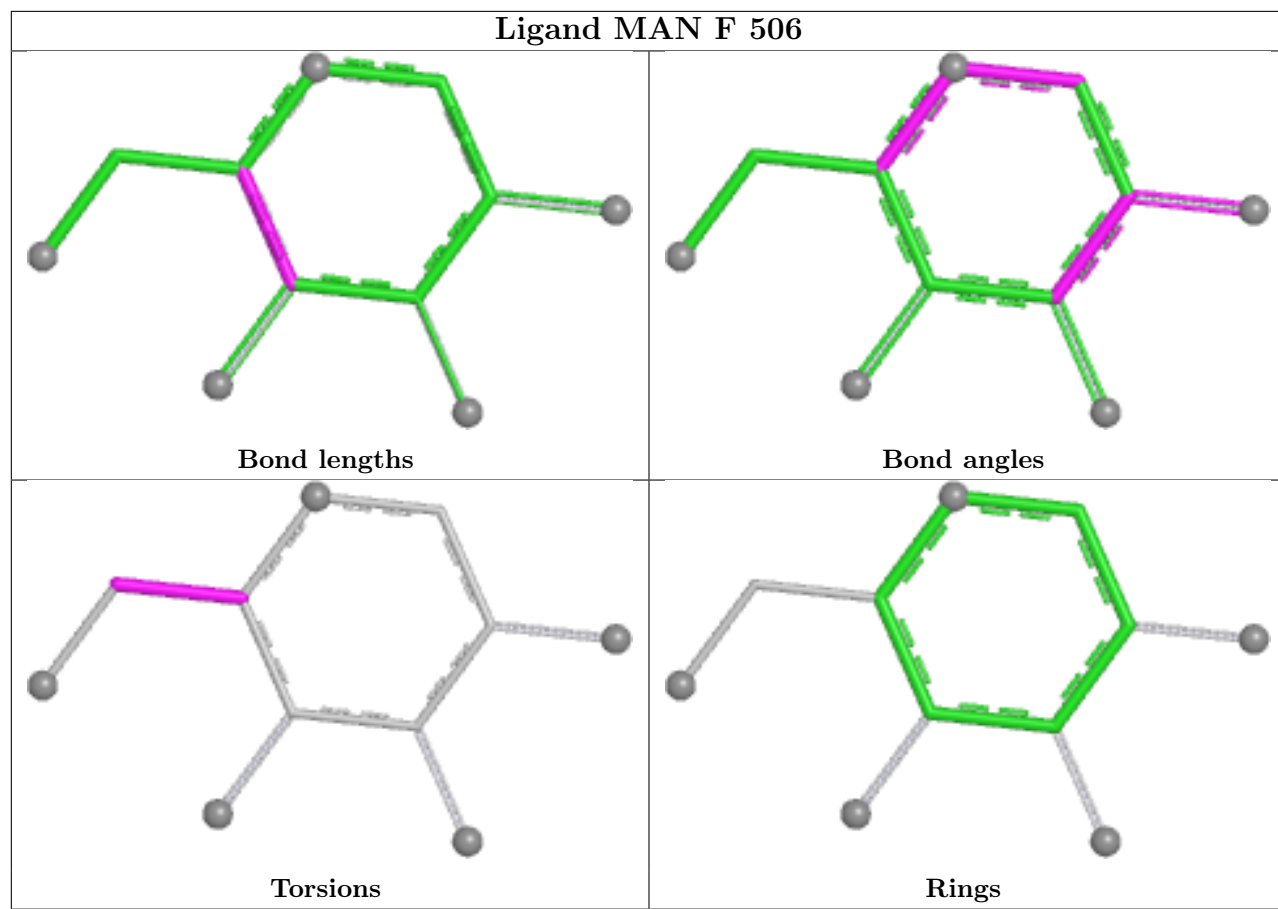


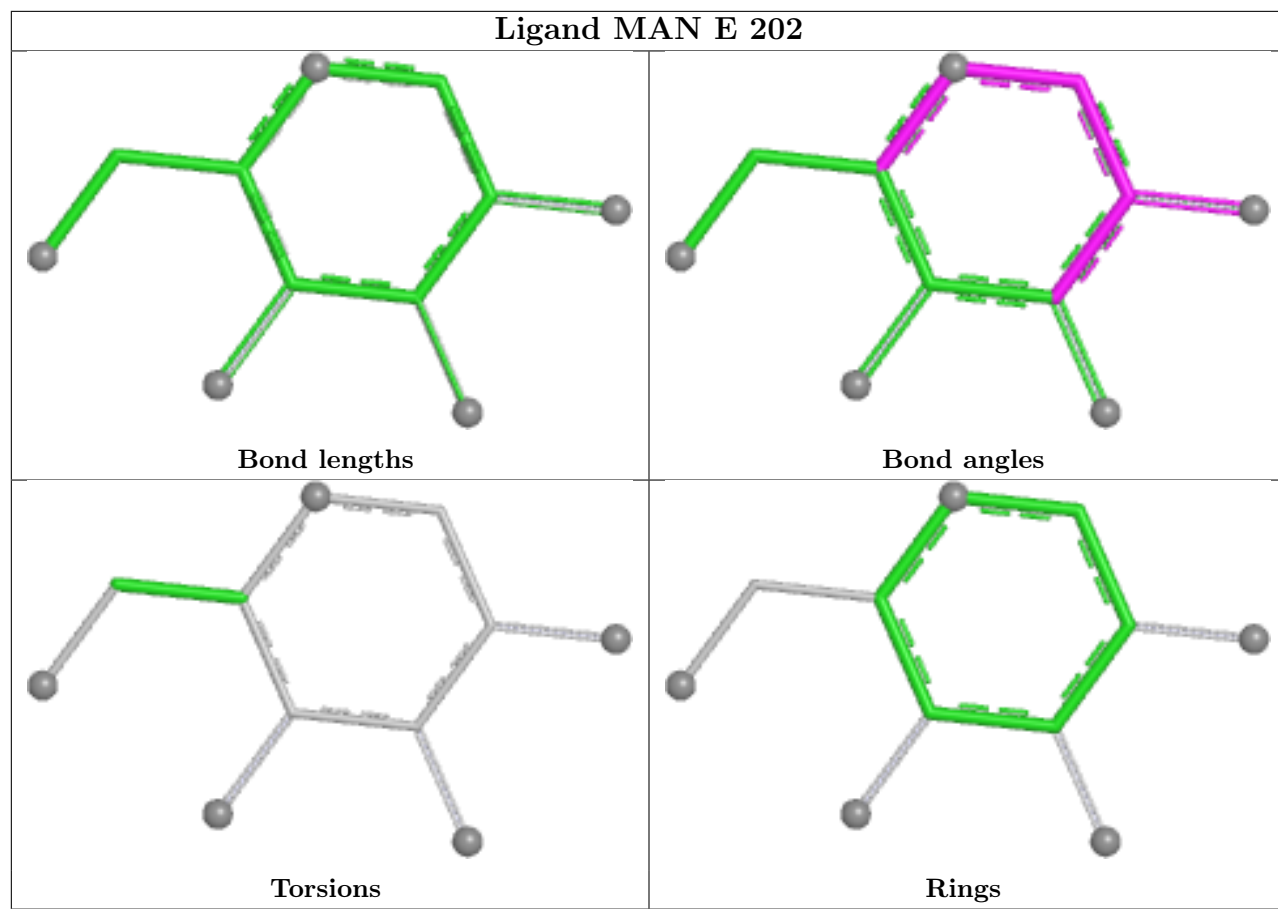


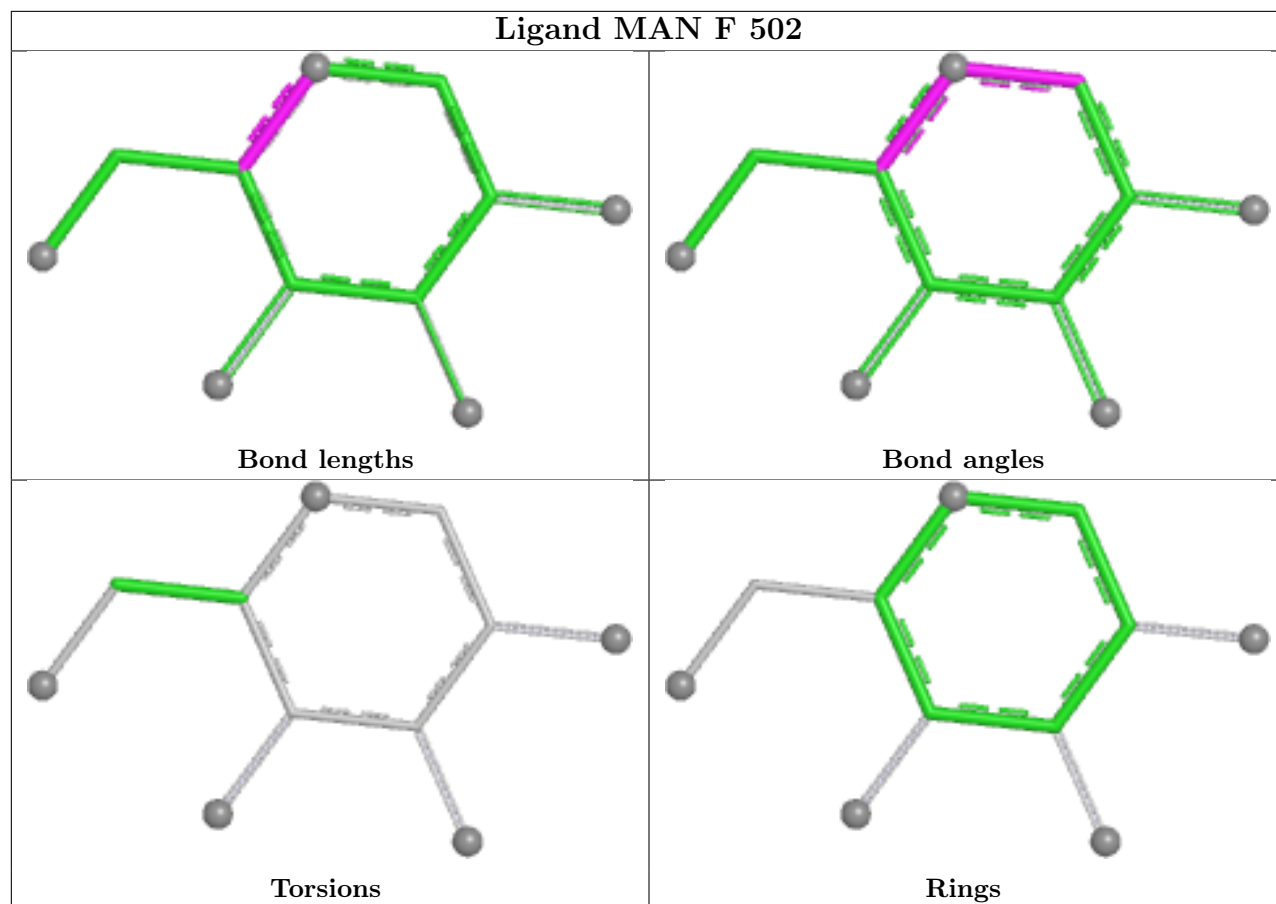


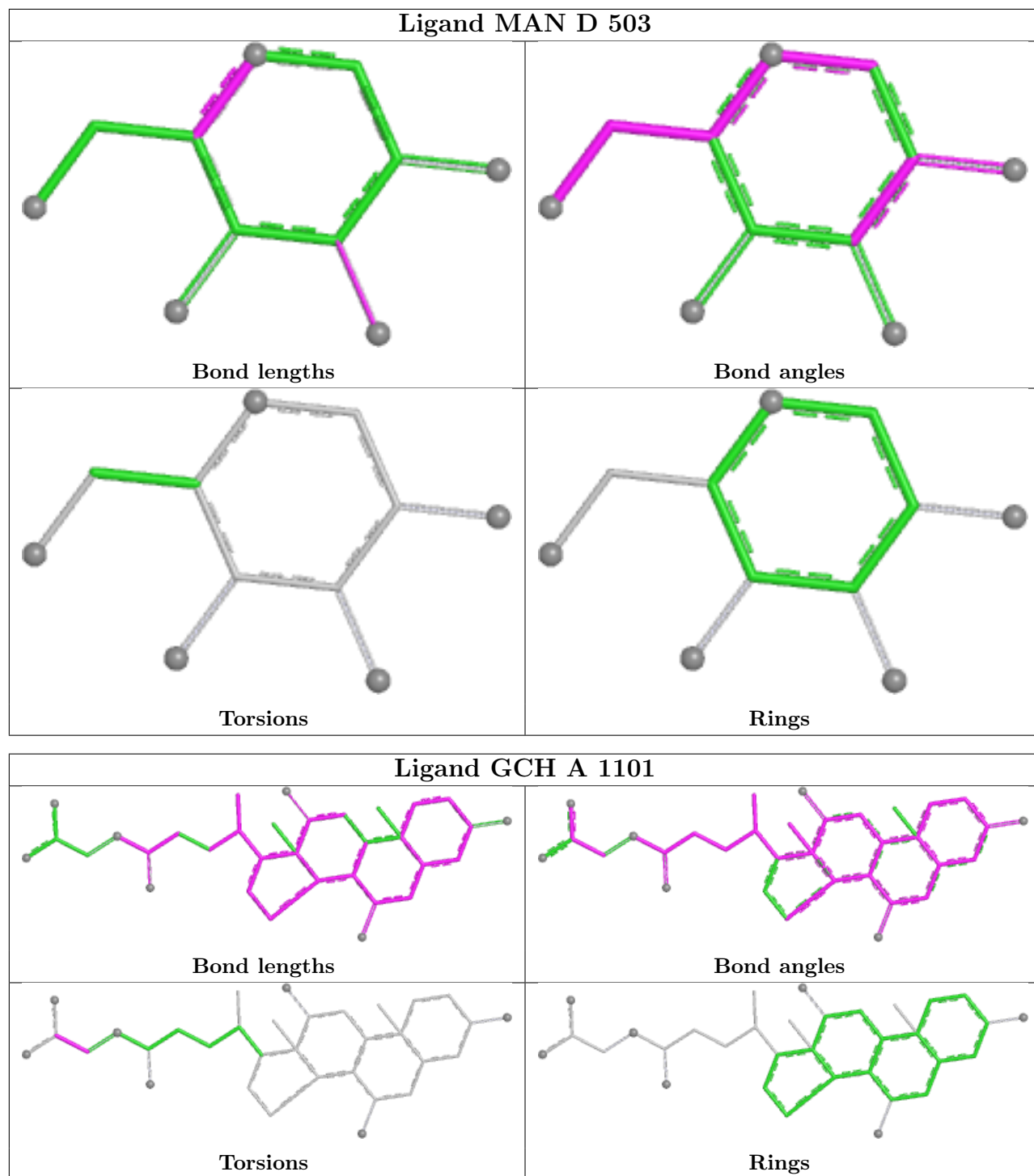


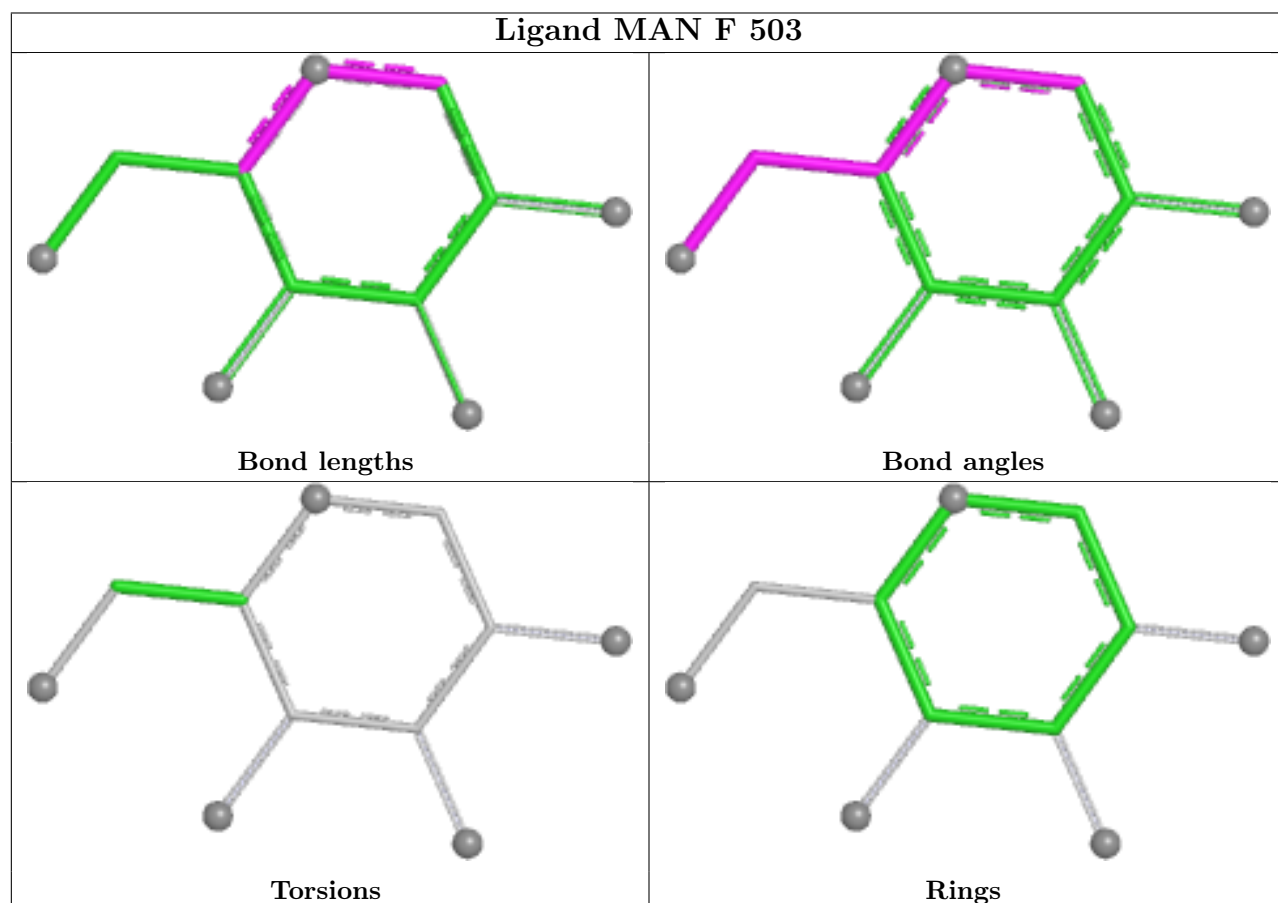
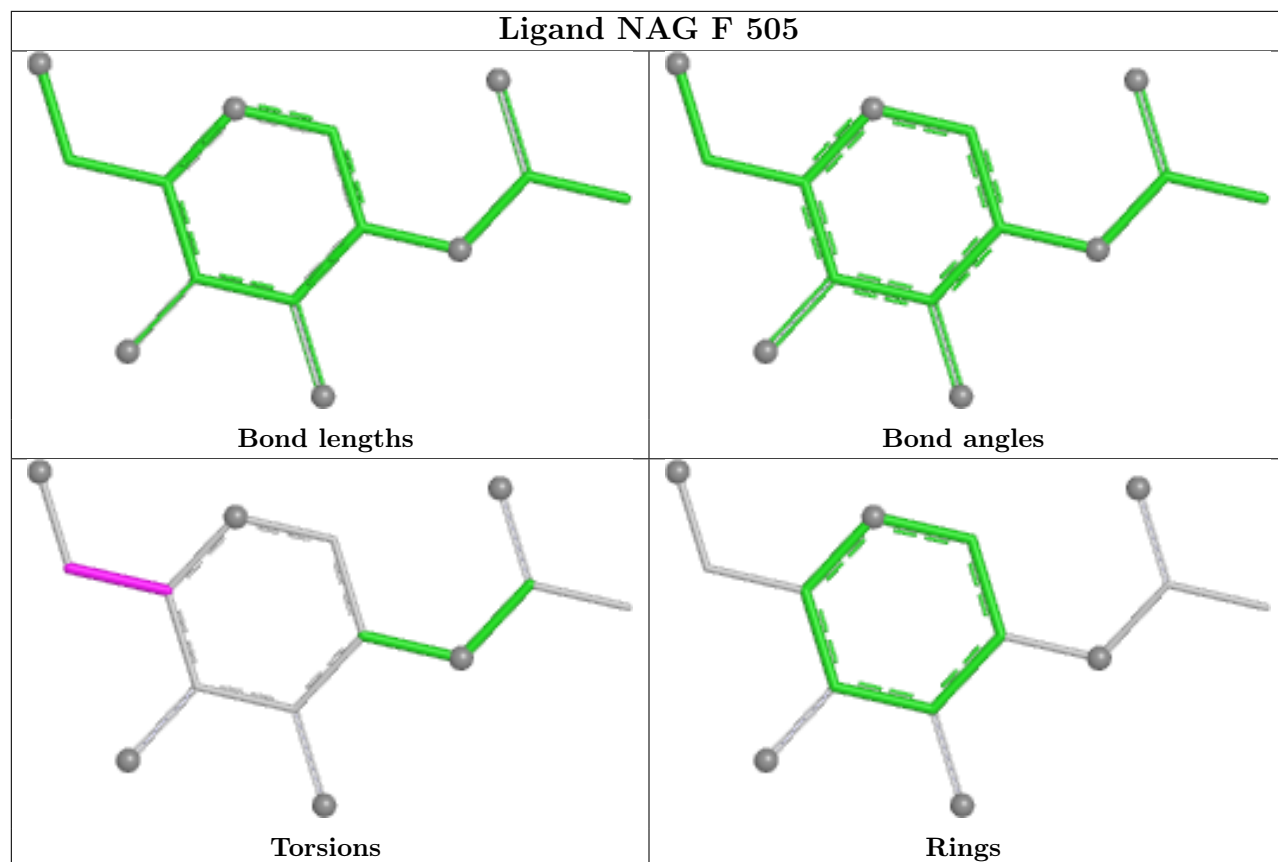


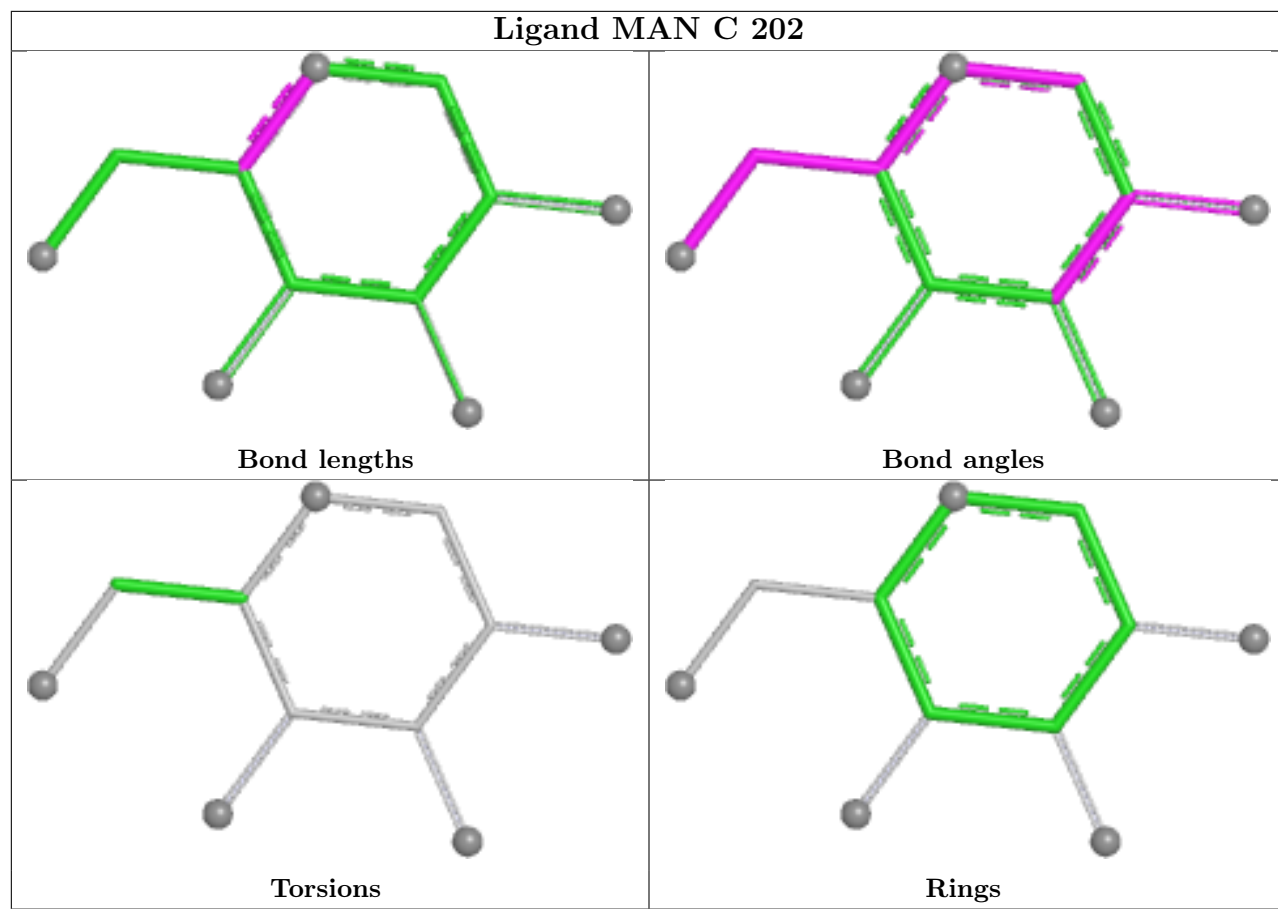


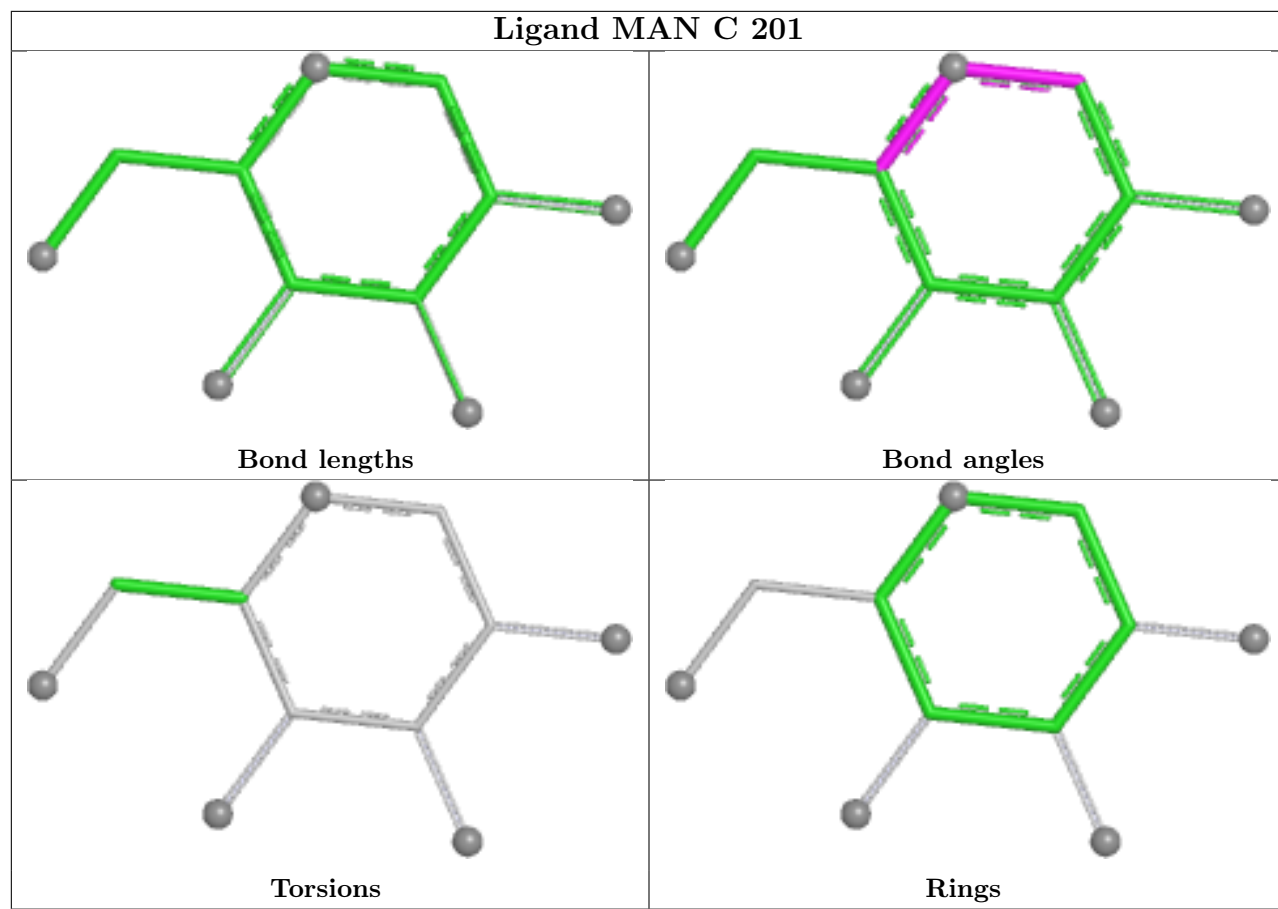


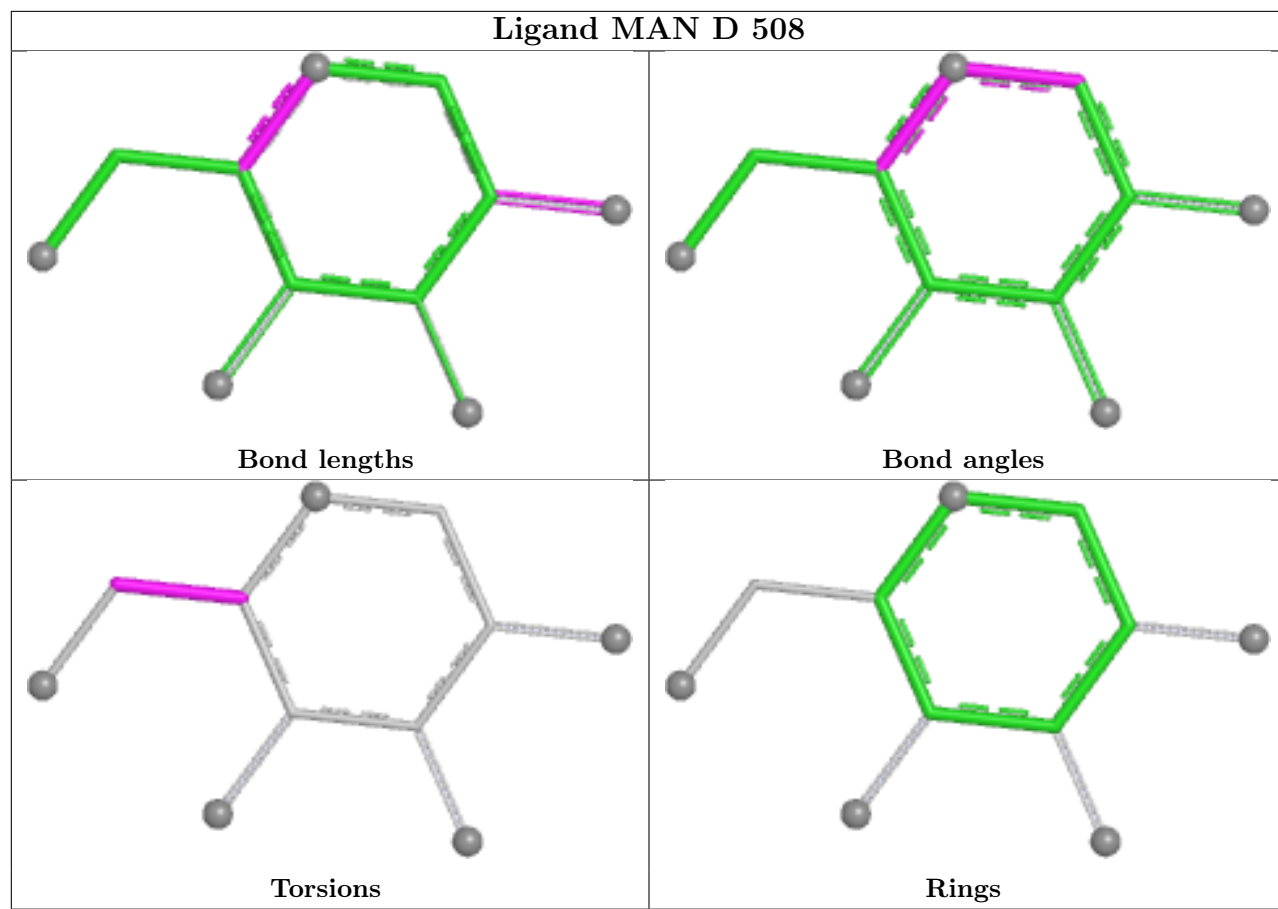


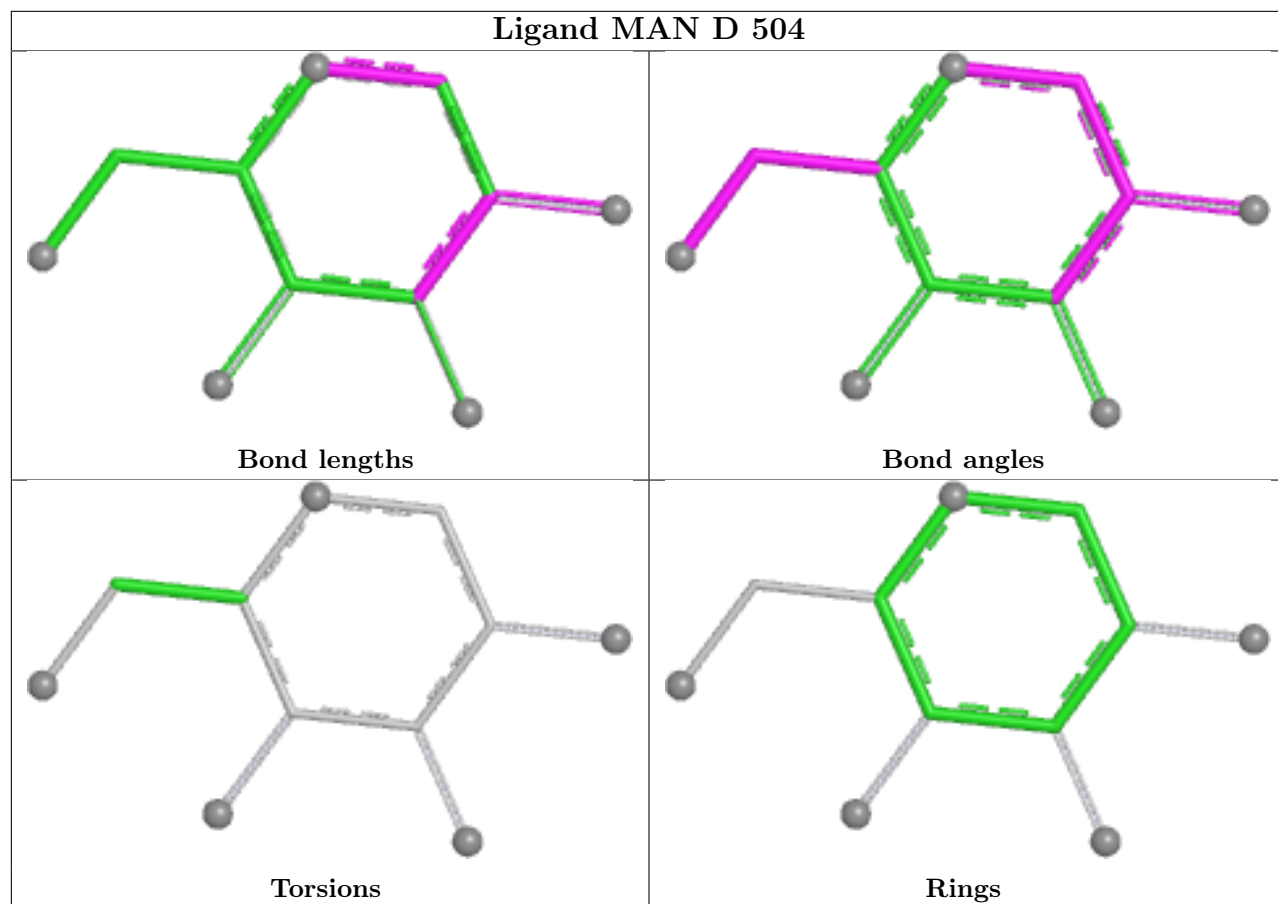


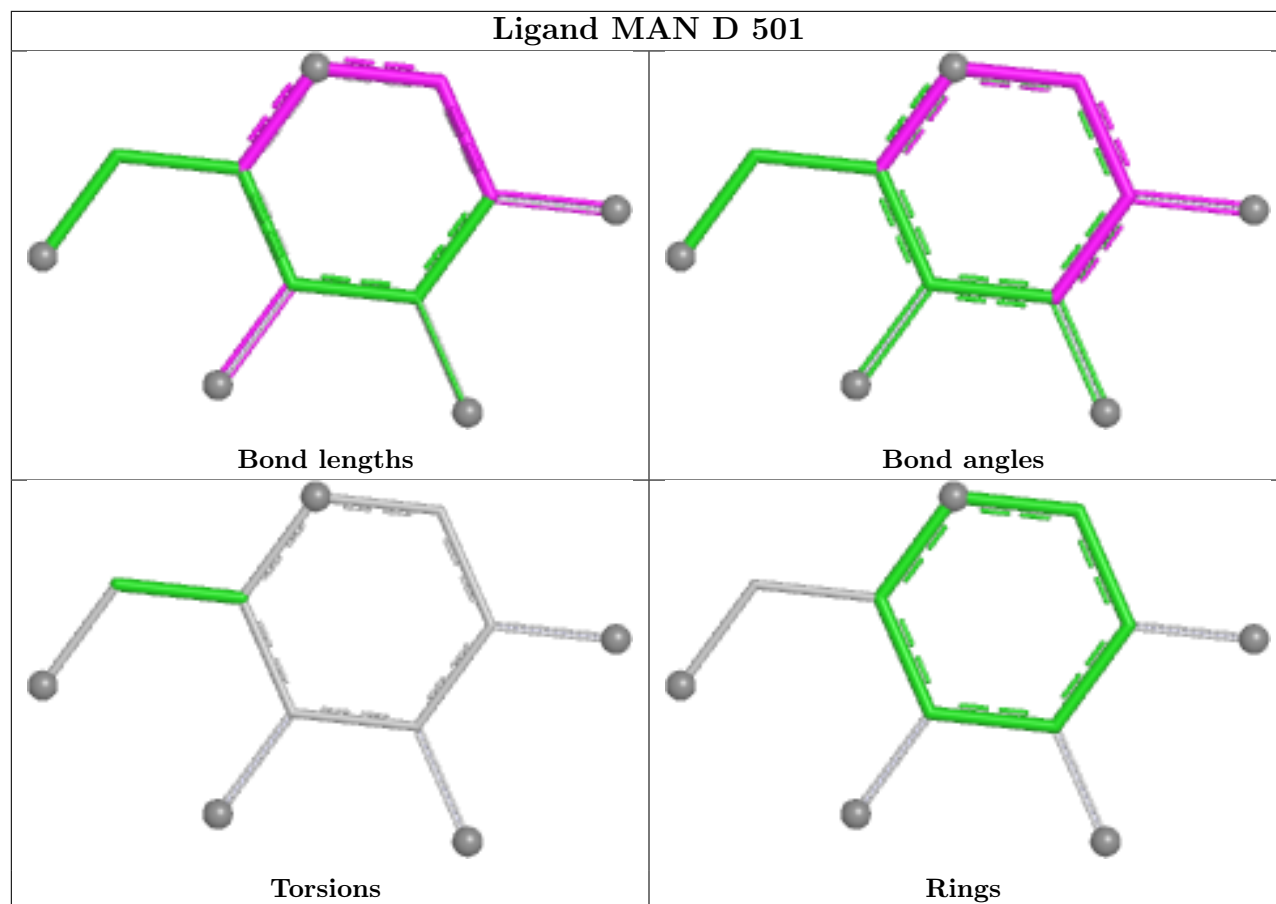


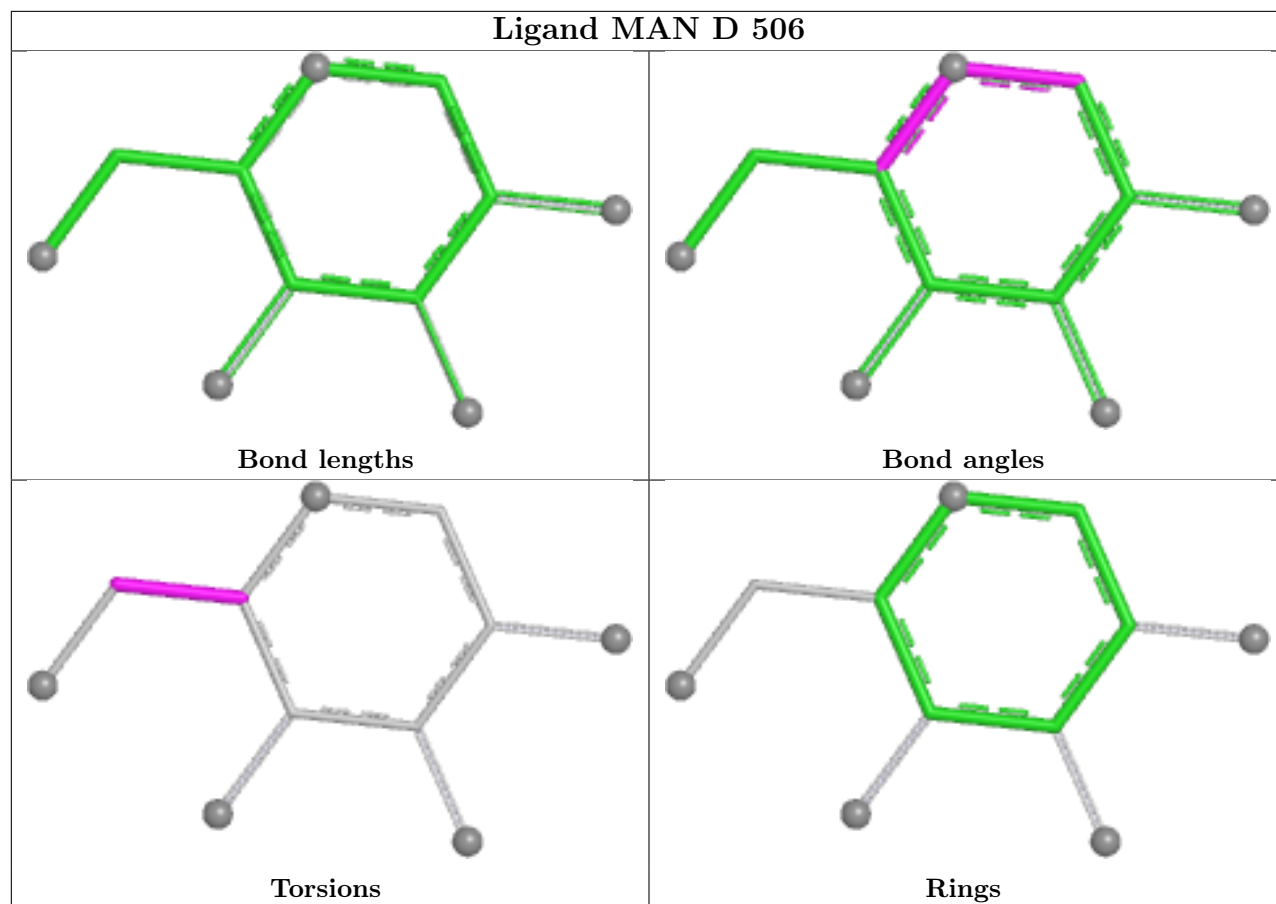


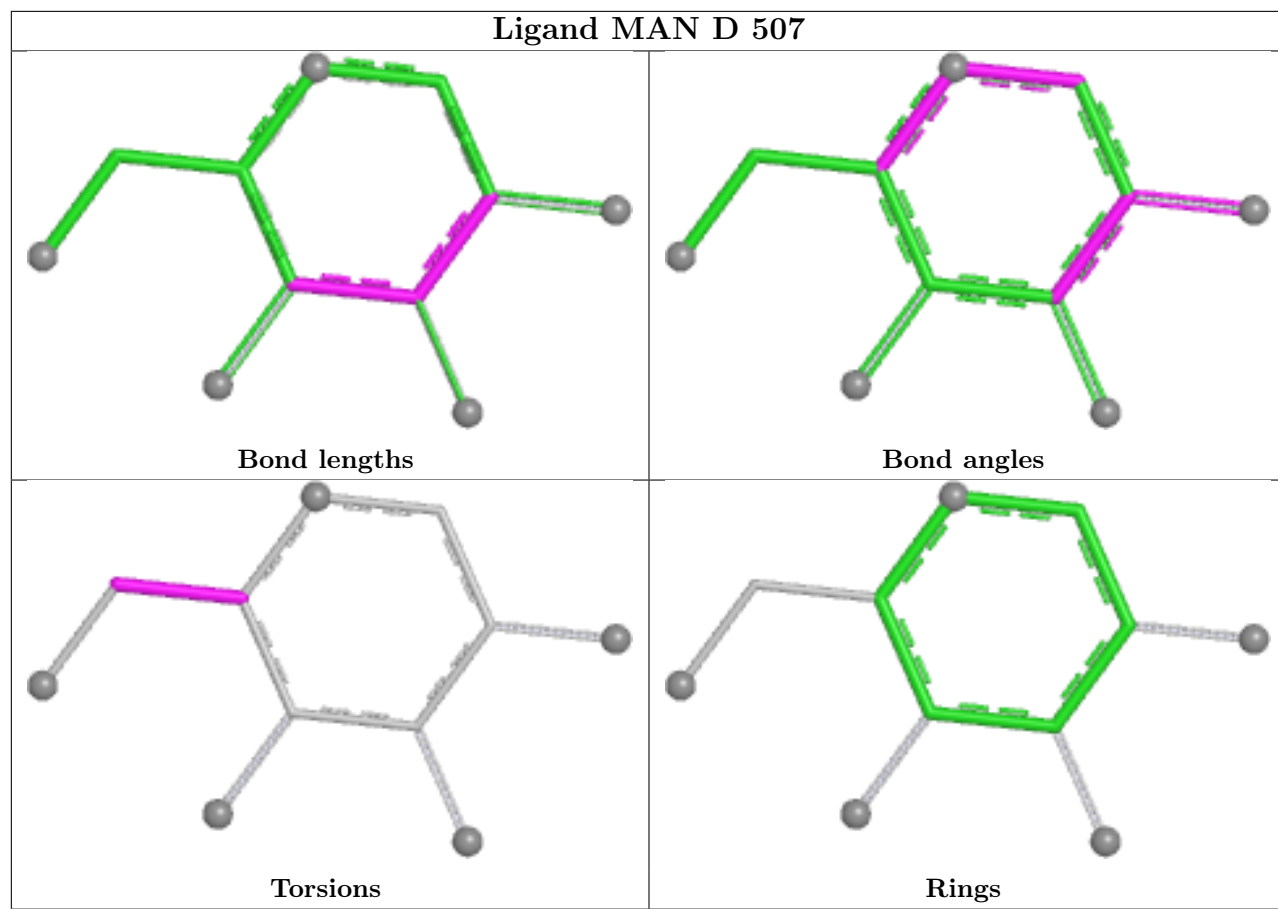












5.7 Other polymers [i](#)

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 ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	119/125 (95%)	-0.06	2 (1%) 69 72	26, 36, 74, 110	0
1	B	120/125 (96%)	0.02	3 (2%) 58 62	29, 38, 78, 122	0
2	C	107/108 (99%)	0.95	11 (10%) 12 12	46, 74, 123, 158	0
2	E	107/108 (99%)	1.12	14 (13%) 7 7	40, 78, 134, 160	0
3	D	211/221 (95%)	0.87	23 (10%) 10 11	33, 64, 121, 144	0
3	F	211/221 (95%)	0.82	23 (10%) 10 11	30, 63, 121, 137	0
All	All	875/908 (96%)	0.66	76 (8%) 16 17	26, 62, 123, 160	0

All (76) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	F	255	GLY	4.8
3	F	256	VAL	4.6
1	A	119	SER	4.4
1	B	120	HIS	4.2
2	C	134	PRO	4.2
2	C	69	GLY	4.2
2	E	69	GLY	4.1
3	D	291	HIS	4.0
3	D	256	VAL	4.0
2	E	134	PRO	3.9
3	D	257	ALA	3.7
3	F	421	VAL	3.7
3	D	421	VAL	3.7
3	D	397	PRO	3.4
3	D	420	MET	3.4
3	F	462	LYS	3.4
2	E	31	LEU	3.4
3	F	258	GLY	3.3
2	C	68	SER	3.3

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Mol	Chain	Res	Type	RSRZ
3	F	422	GLU	3.2
3	D	331	ASN	3.2
3	F	465	GLU	3.2
2	E	82	LEU	3.1
3	D	288	VAL	3.1
3	F	418	VAL	3.1
3	F	330	ARG	3.0
3	D	255	GLY	3.0
2	E	41	GLY	3.0
3	F	332	MET	3.0
3	D	465	GLU	2.9
3	D	396	GLY	2.9
3	D	289	PRO	2.9
3	D	332	MET	2.9
2	C	132	ALA	2.8
2	C	133	CYS	2.8
2	E	133	CYS	2.8
3	D	422	GLU	2.7
3	F	396	GLY	2.7
3	F	367	ILE	2.7
3	D	290	GLN	2.7
3	D	269	CYS	2.6
2	C	29	PRO	2.6
2	C	120	LEU	2.5
2	E	132	ALA	2.5
3	D	292	GLY	2.5
1	A	111	GLN	2.5
3	F	288	VAL	2.5
2	E	71	LEU	2.4
3	D	392	MET	2.4
2	E	101	TYR	2.4
1	B	73	ASN	2.3
2	C	115	VAL	2.3
3	F	429	VAL	2.3
2	E	29	PRO	2.3
3	D	423	GLY	2.2
3	F	423	GLY	2.2
2	C	30	VAL	2.2
3	F	376	CYS	2.2
2	E	28	ASP	2.2
3	D	293	GLY	2.2
3	F	420	MET	2.1

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Mol	Chain	Res	Type	RSRZ
3	F	366	ASP	2.1
2	C	51	VAL	2.1
3	F	417	THR	2.1
1	B	119	SER	2.1
3	D	267	SER	2.1
3	F	291	HIS	2.1
3	F	257	ALA	2.1
3	F	329	ARG	2.1
2	C	31	LEU	2.1
3	D	258	GLY	2.0
2	E	30	VAL	2.0
2	E	115	VAL	2.0
2	E	43	CYS	2.0
3	D	296	CYS	2.0
3	F	294	PRO	2.0

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

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

6.3 Carbohydrates [i](#)

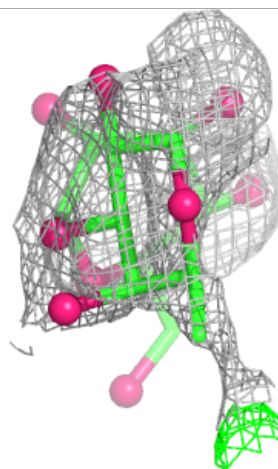
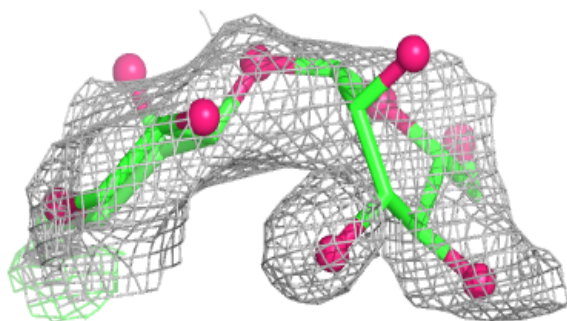
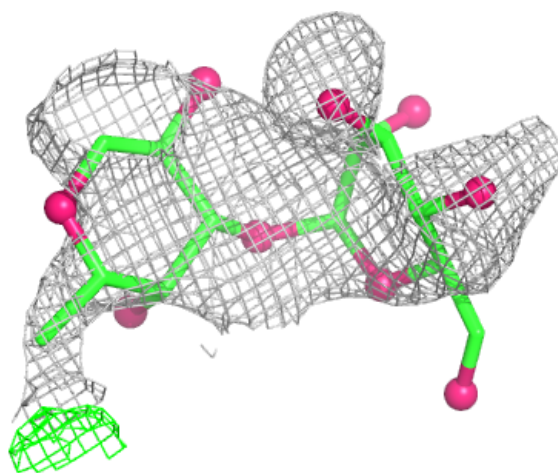
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	FUC	J	1	10/11	0.36	0.17	130,137,150,154	0
5	NAG	I	2	14/15	0.46	0.17	138,148,165,170	0
4	BGC	J	2	11/12	0.50	0.20	106,132,141,146	0
4	FUC	G	1	10/11	0.61	0.13	113,130,141,142	0
5	NAG	I	1	14/15	0.68	0.16	120,136,151,165	0
4	BGC	G	2	11/12	0.71	0.17	100,135,149,151	0
4	BGC	H	2	11/12	0.92	0.10	55,58,64,67	0
4	FUC	H	1	10/11	0.93	0.10	54,61,65,70	0
4	BGC	K	2	11/12	0.93	0.10	44,50,57,60	0
4	FUC	K	1	10/11	0.97	0.06	39,44,49,49	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.

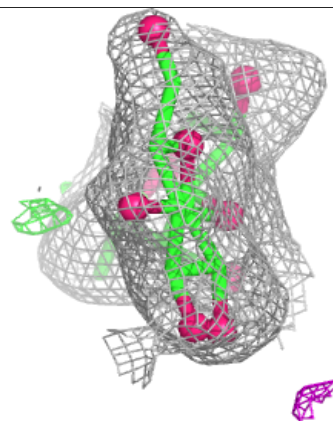
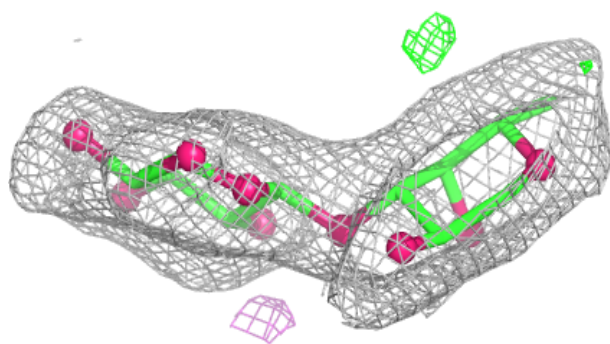
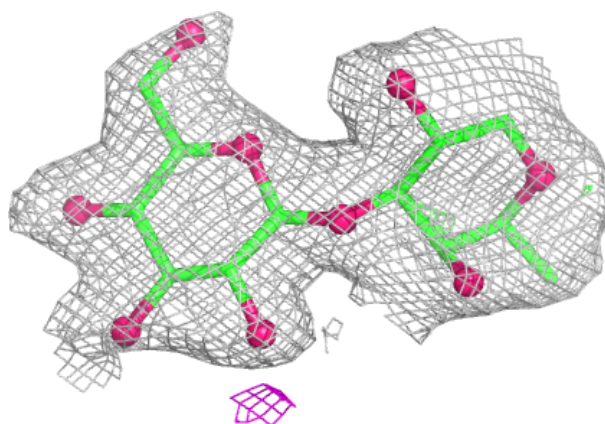
Electron density around Chain G:

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



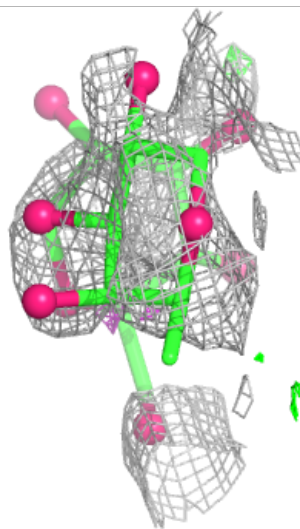
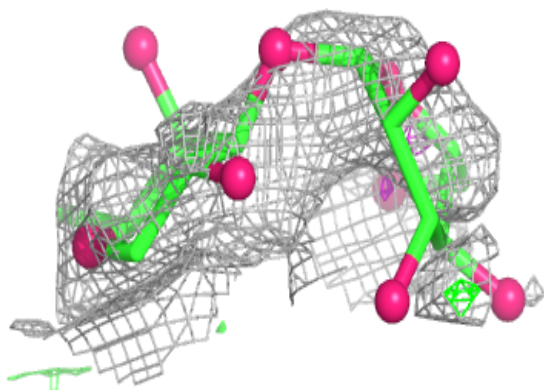
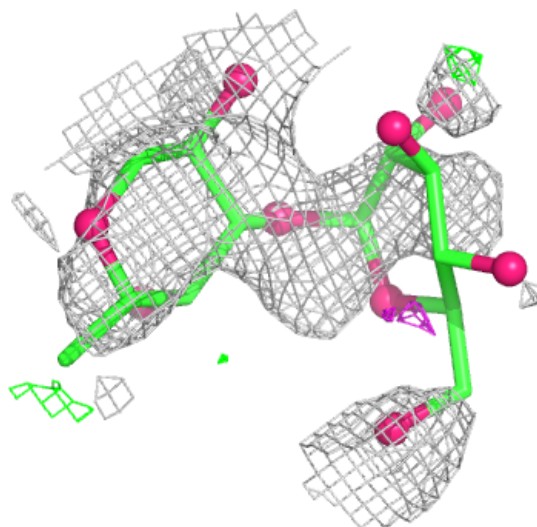
Electron density around Chain H:

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



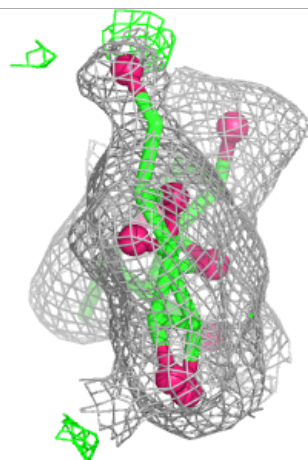
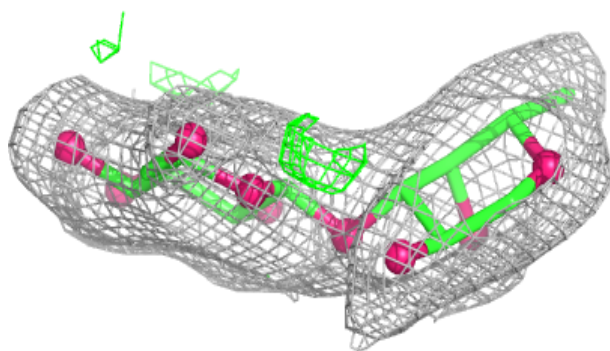
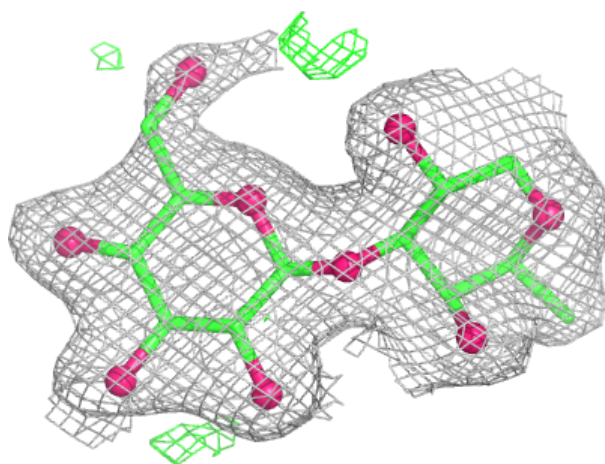
Electron density around Chain J:

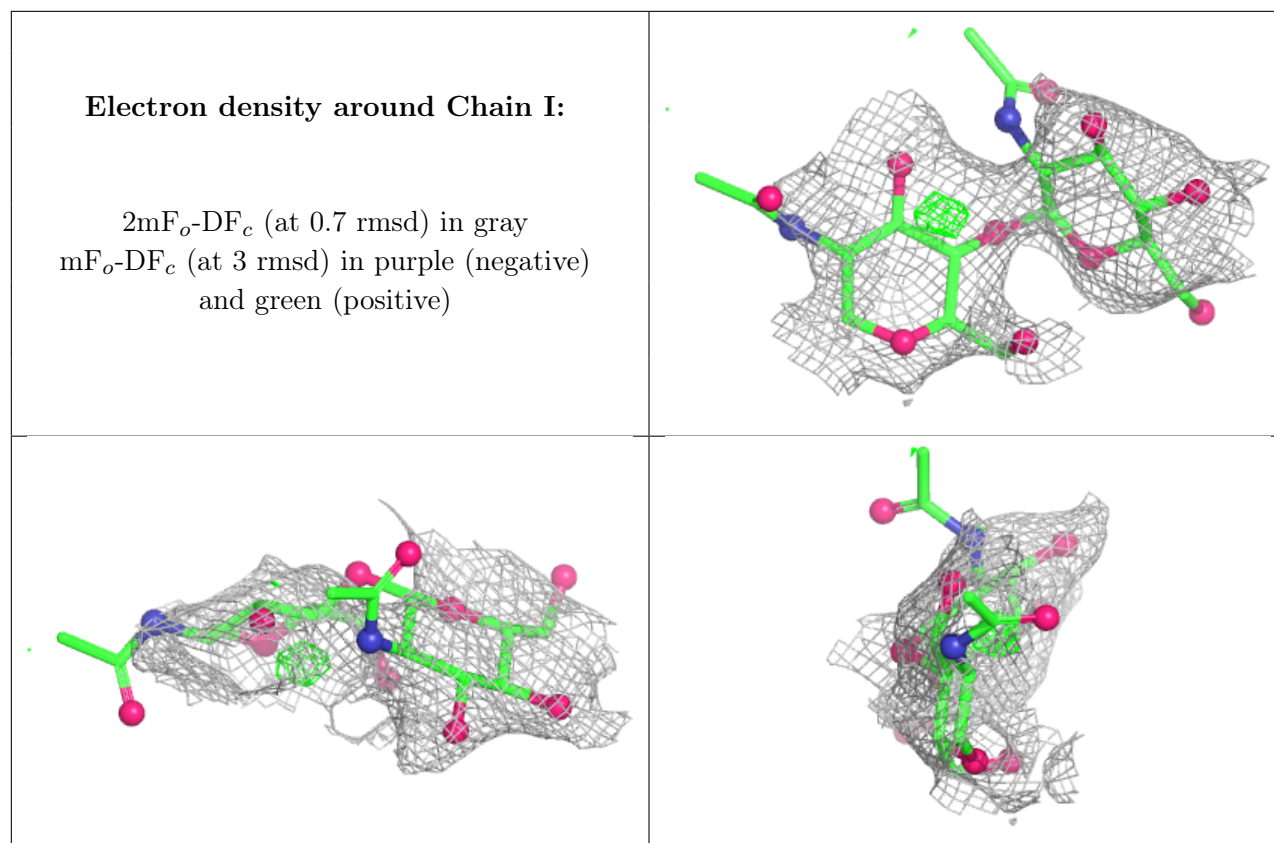
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



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)





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
7	MAN	E	202	11/12	0.42	0.18	80,90,98,102	11
7	MAN	C	202	11/12	0.61	0.21	77,86,101,105	11
7	MAN	D	504	11/12	0.67	0.22	58,79,90,91	0
8	NAG	F	505	14/15	0.67	0.16	107,125,135,136	0
7	MAN	F	504	11/12	0.73	0.22	56,75,90,111	0
7	MAN	F	509	11/12	0.75	0.14	73,85,98,100	0
7	MAN	D	505	11/12	0.76	0.11	69,72,81,82	0
7	MAN	F	507	11/12	0.84	0.11	64,68,71,75	0
7	MAN	F	508	11/12	0.84	0.12	72,79,83,83	0
7	MAN	F	501	11/12	0.84	0.17	40,56,62,67	11
7	MAN	D	506	11/12	0.84	0.11	70,73,79,80	0
7	MAN	D	501	11/12	0.85	0.17	41,49,56,60	11
7	MAN	C	201	11/12	0.87	0.09	61,64,69,73	0
7	MAN	F	506	11/12	0.87	0.09	62,67,74,74	0

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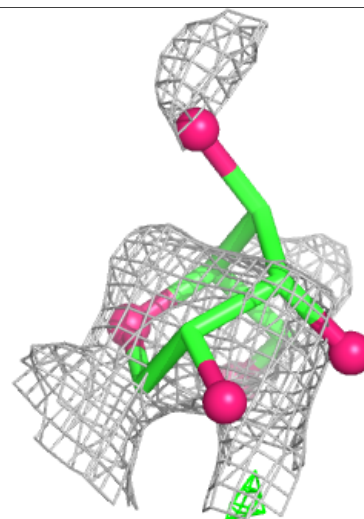
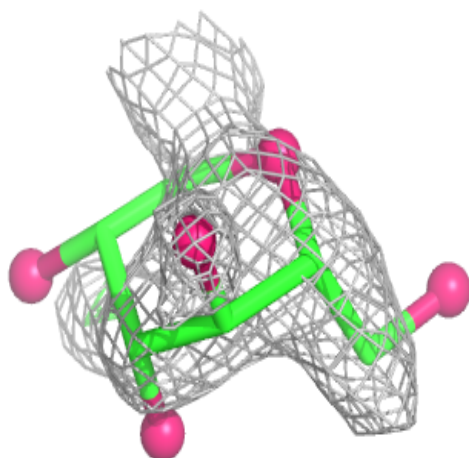
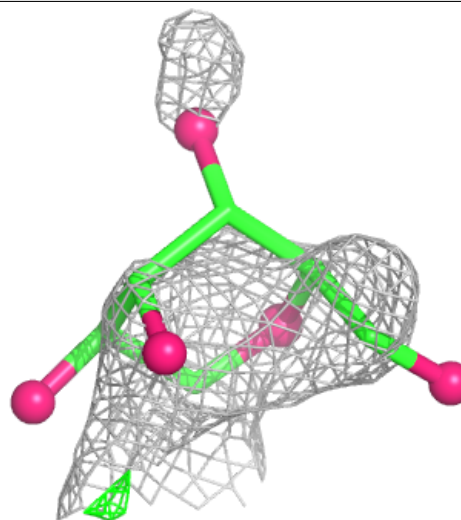
Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
7	MAN	F	502	11/12	0.87	0.12	42,51,56,58	0
7	MAN	D	507	11/12	0.89	0.10	64,67,73,79	0
7	MAN	E	201	11/12	0.90	0.08	67,70,74,75	0
7	MAN	F	503	11/12	0.90	0.11	46,48,51,51	0
6	GCH	A	1101	33/33	0.90	0.15	30,39,95,106	0
7	MAN	D	508	11/12	0.90	0.09	67,70,77,79	0
6	GCH	A	1102	33/33	0.91	0.13	31,39,72,84	0
7	MAN	D	503	11/12	0.91	0.09	43,47,51,52	0
7	MAN	D	502	11/12	0.93	0.08	43,50,56,57	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.

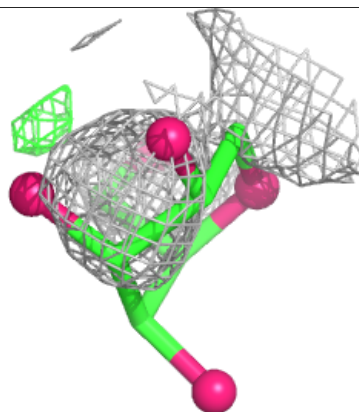
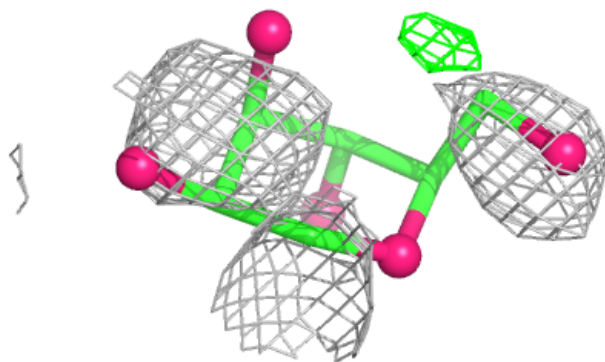
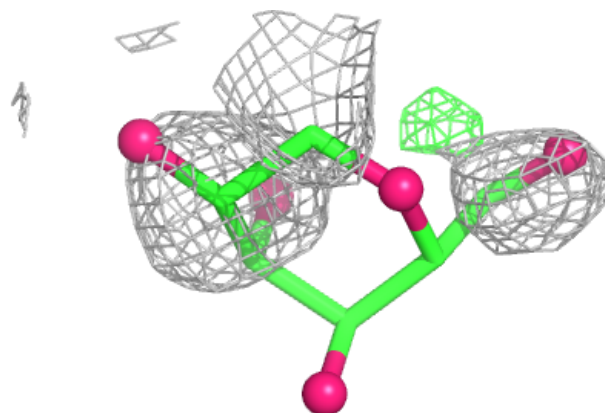
Electron density around MAN E 202:

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



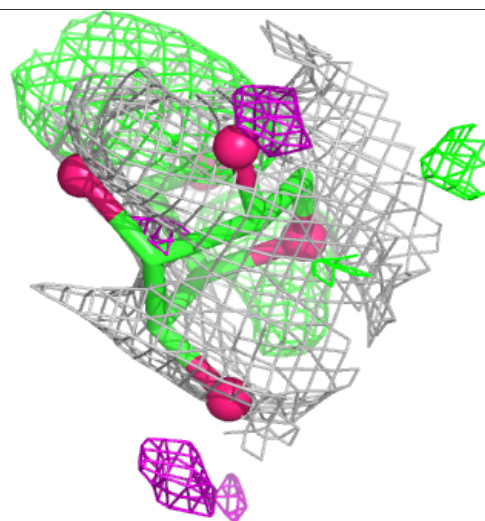
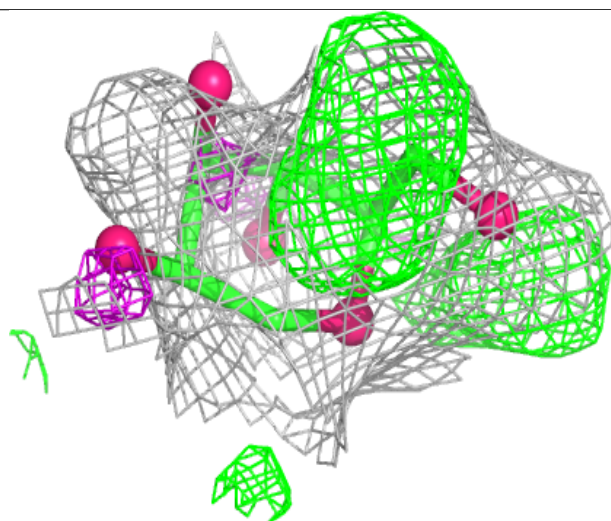
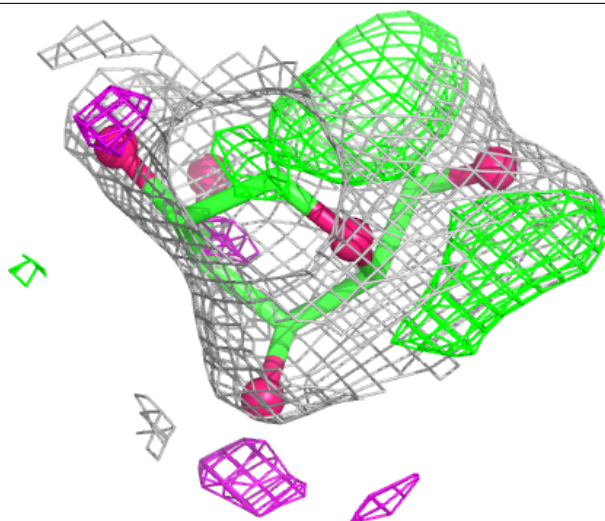
Electron density around MAN C 202:

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



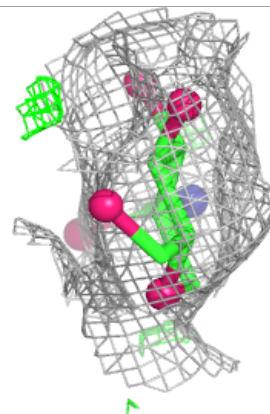
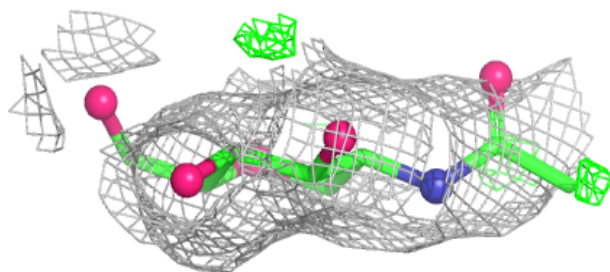
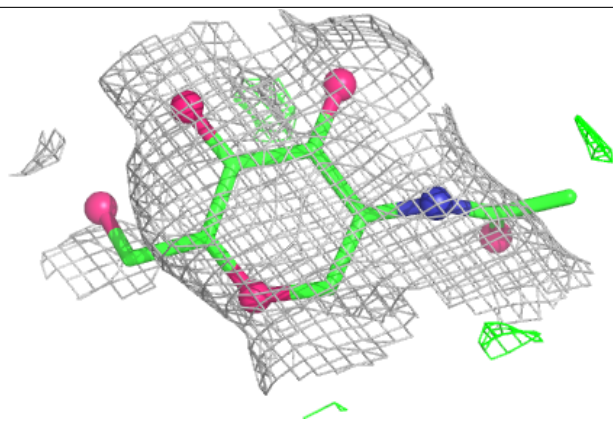
Electron density around MAN D 504:

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



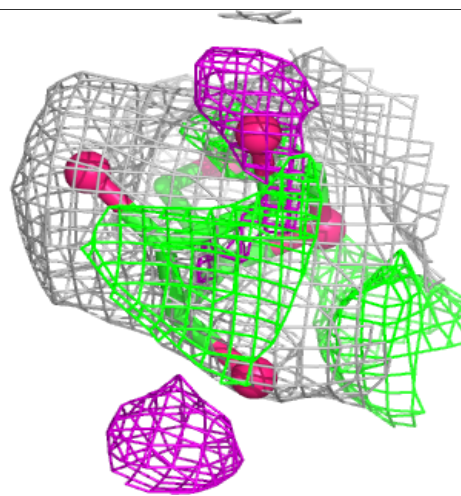
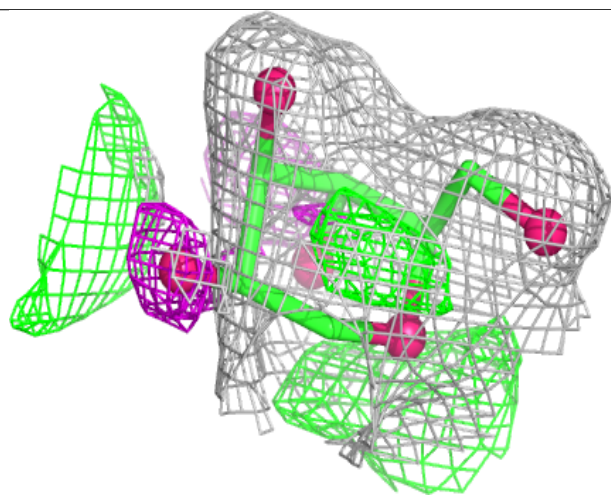
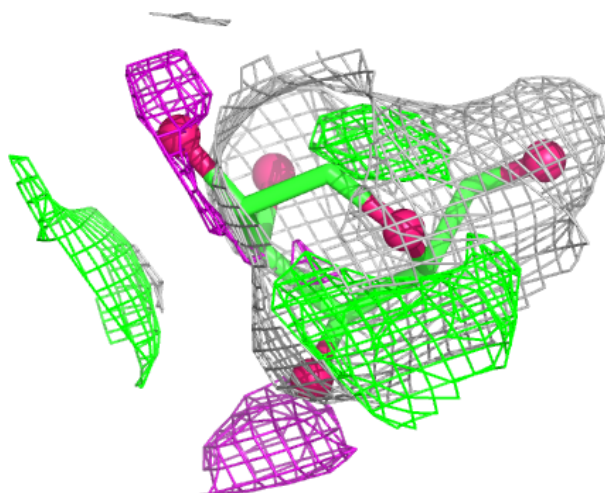
Electron density around NAG F 505:

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and green (positive)



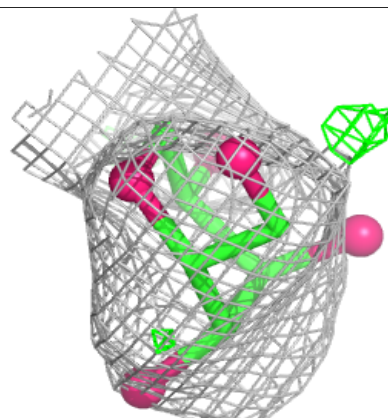
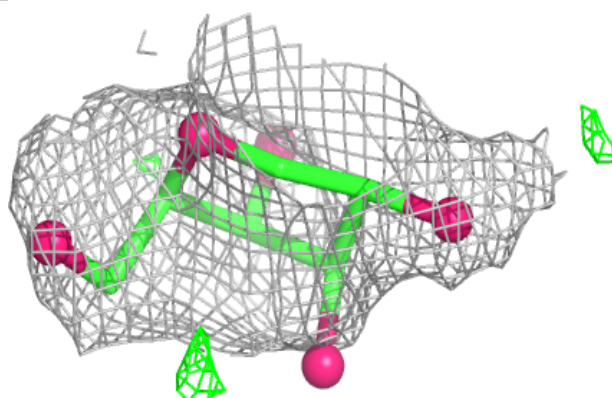
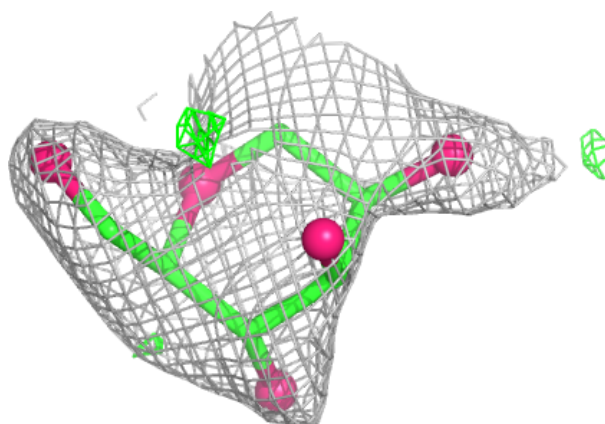
Electron density around MAN F 504:

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



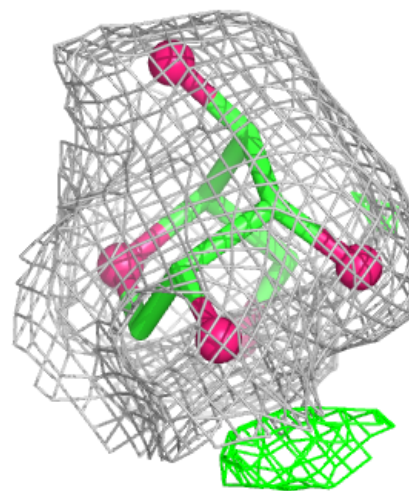
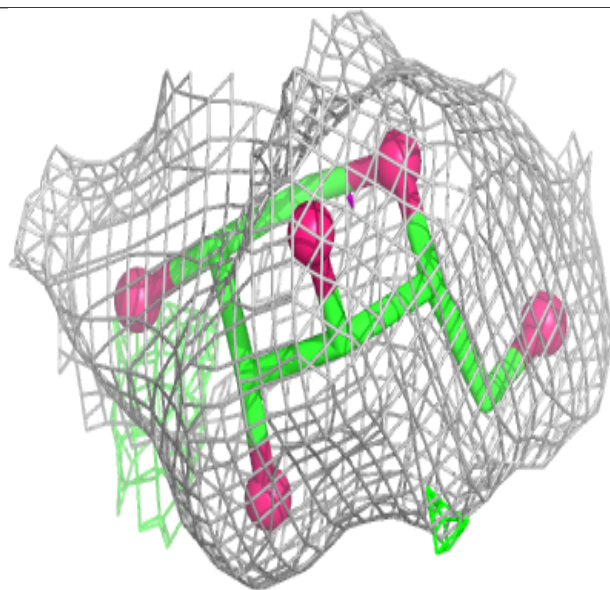
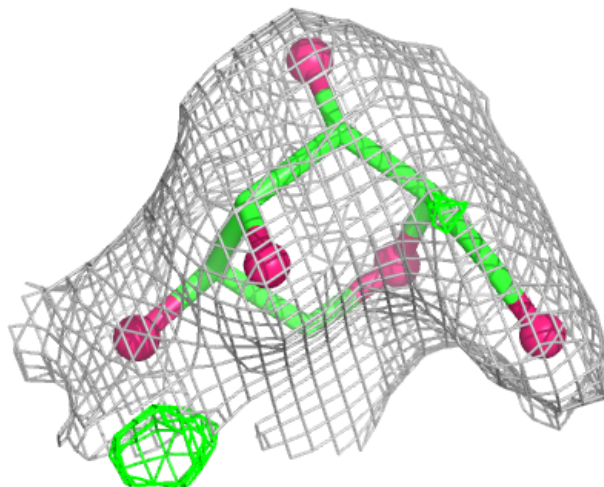
Electron density around MAN F 509:

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and green (positive)



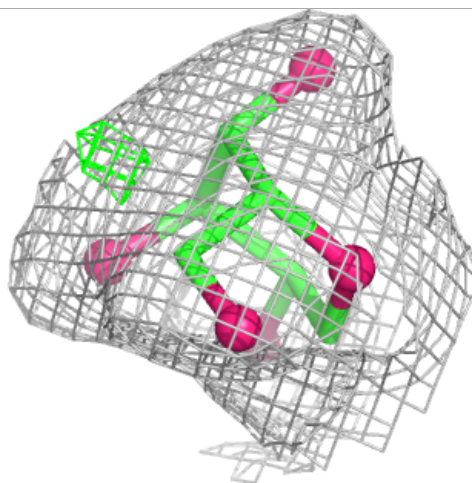
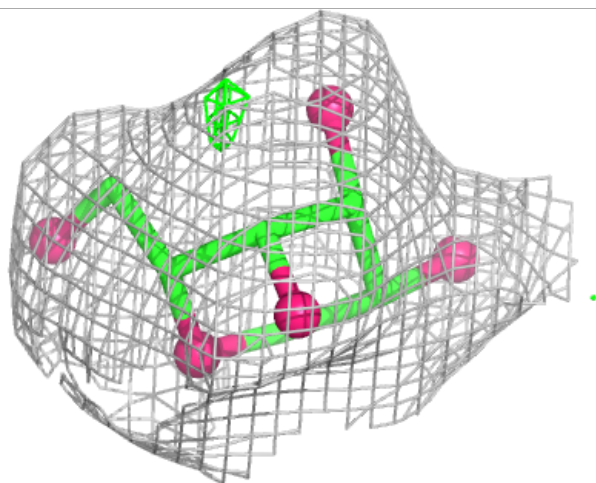
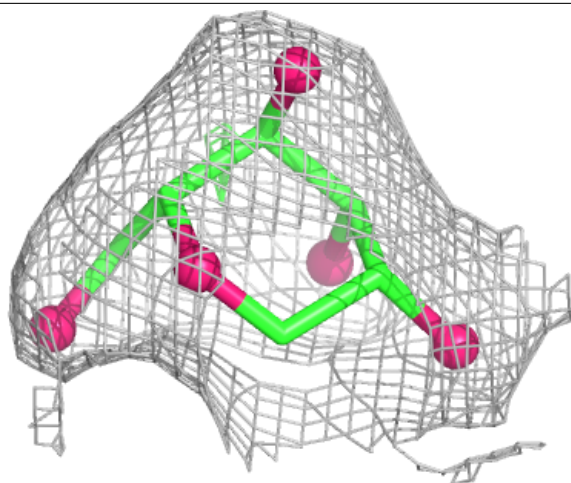
Electron density around MAN D 505:

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



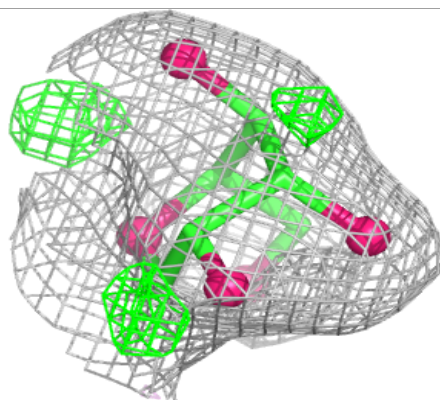
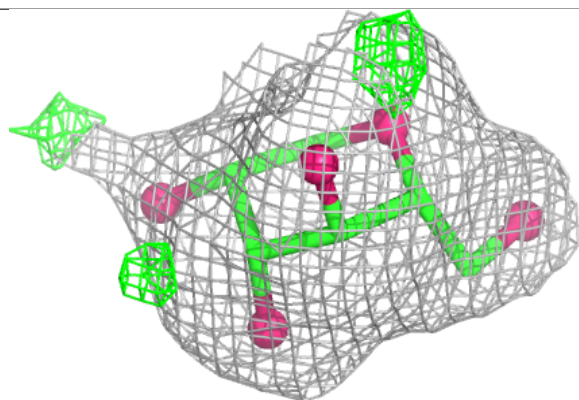
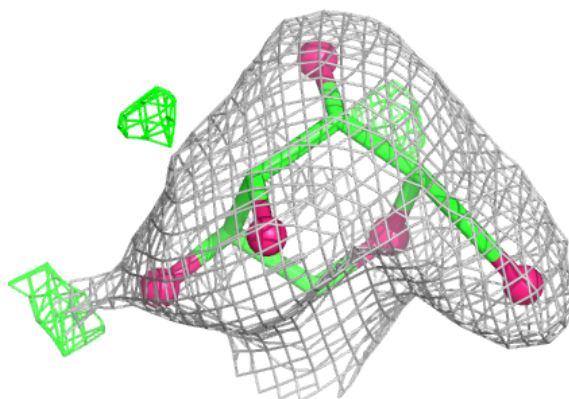
Electron density around MAN F 507:

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and green (positive)

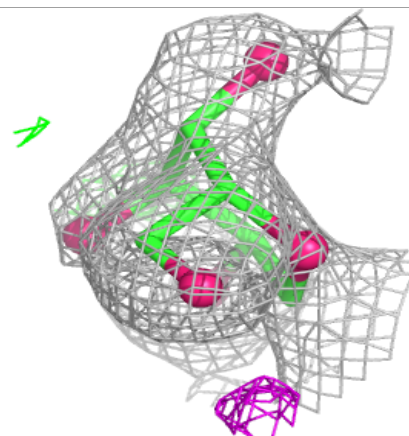
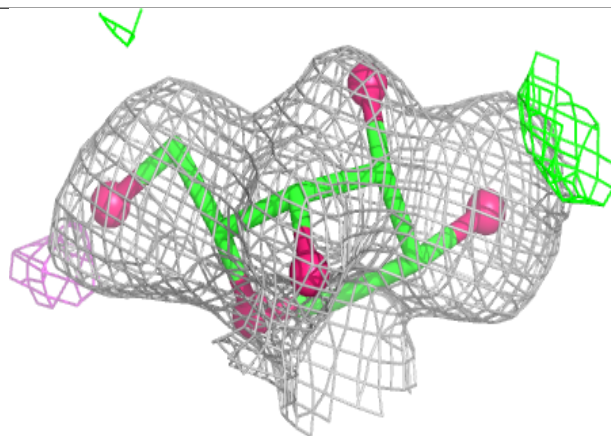
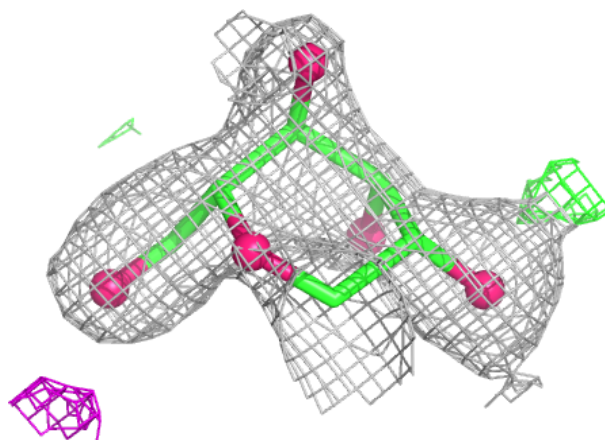


Electron density around MAN F 508:

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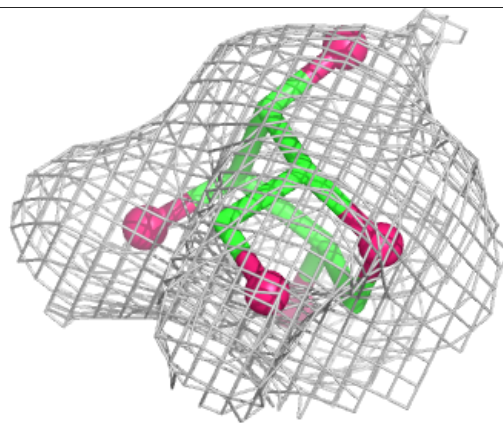
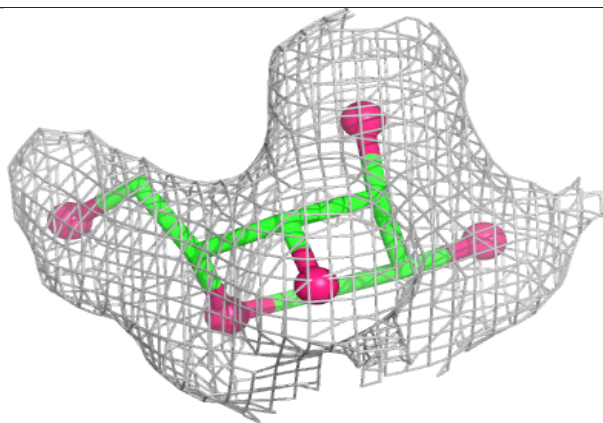
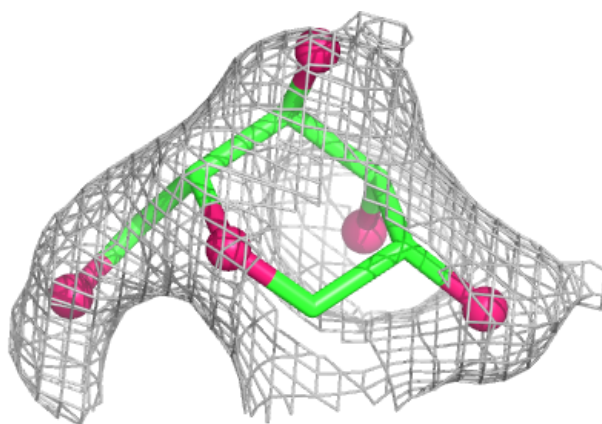
**Electron density around MAN F 501:**

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and green (positive)



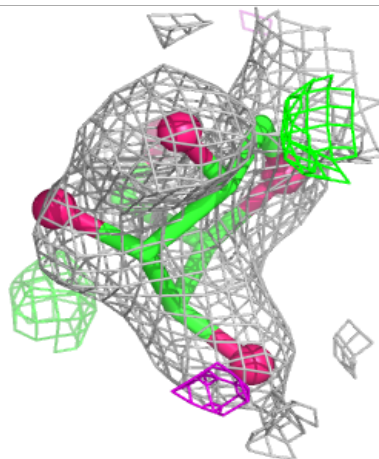
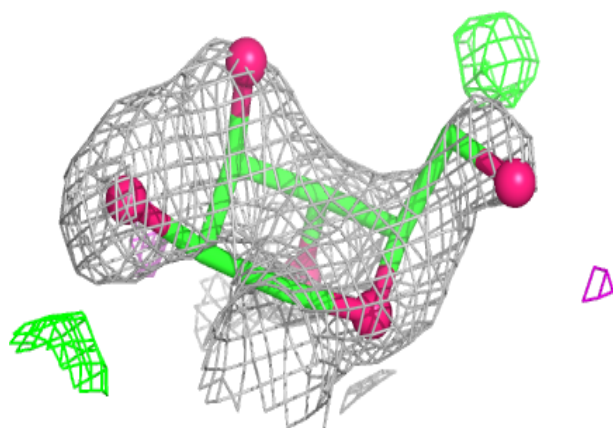
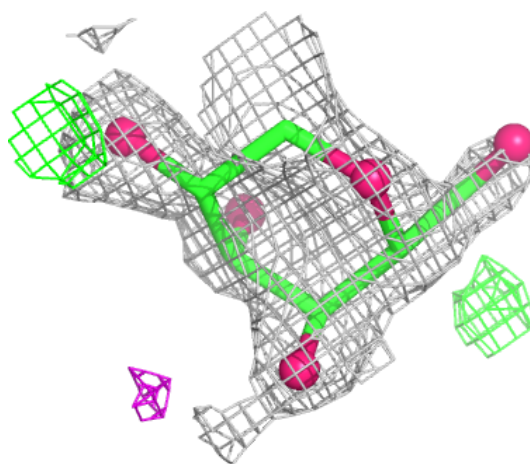
Electron density around MAN D 506:

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and green (positive)



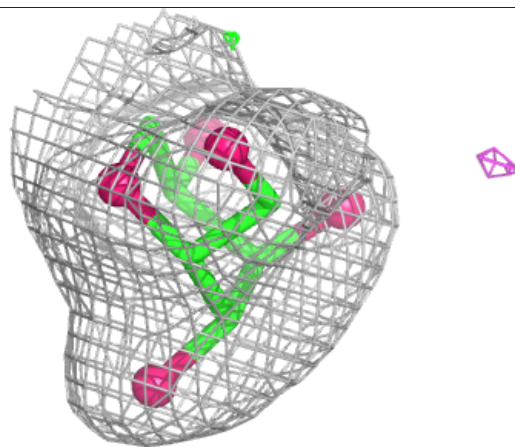
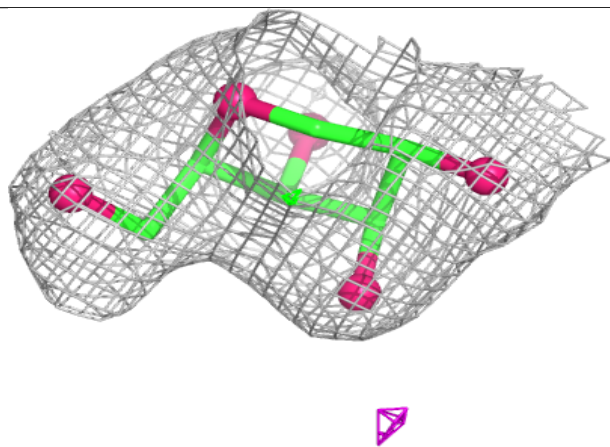
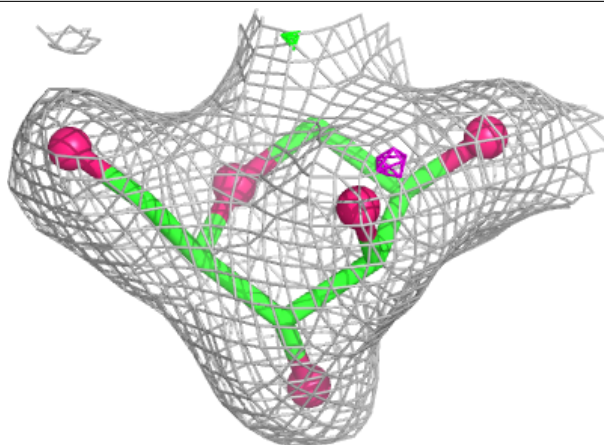
Electron density around MAN D 501:

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and green (positive)



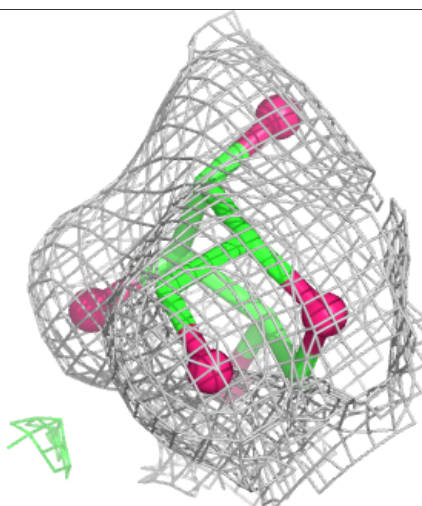
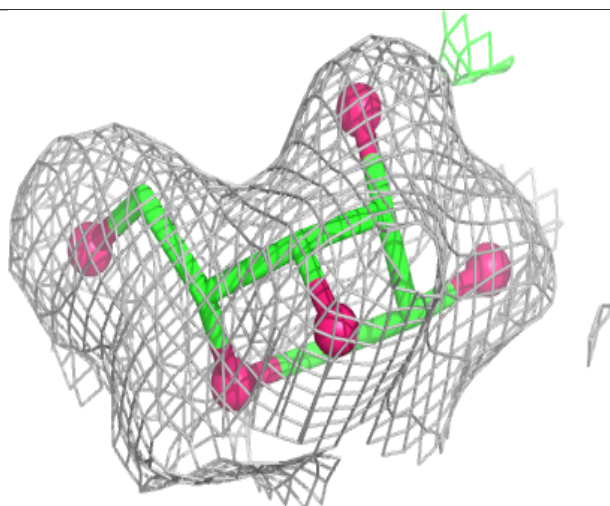
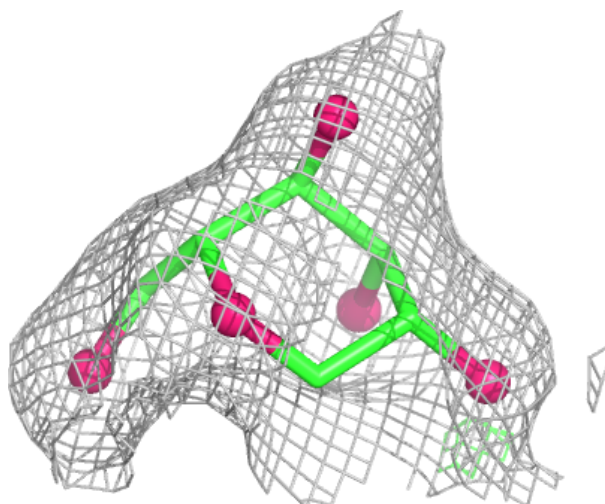
Electron density around MAN C 201:

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and green (positive)



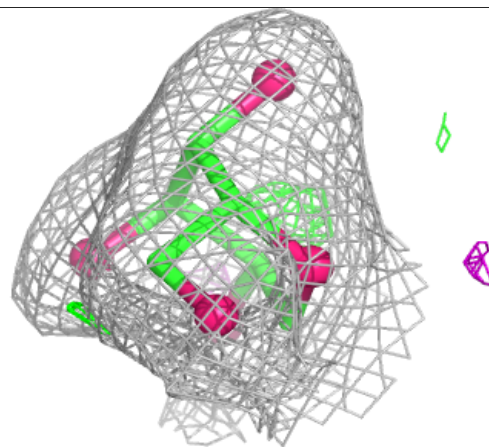
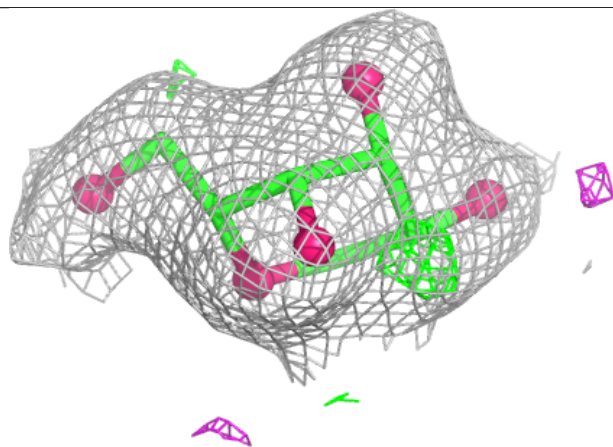
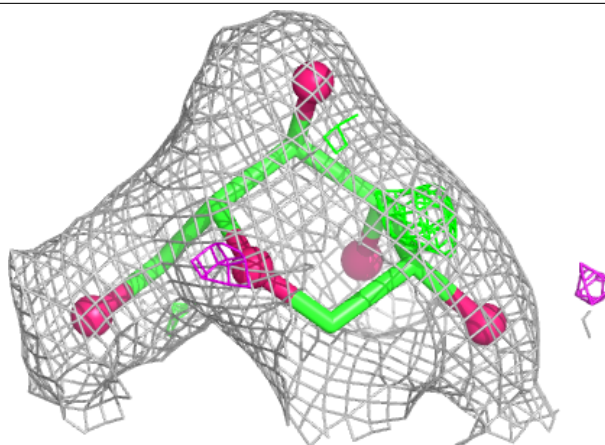
Electron density around MAN F 506:

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and green (positive)



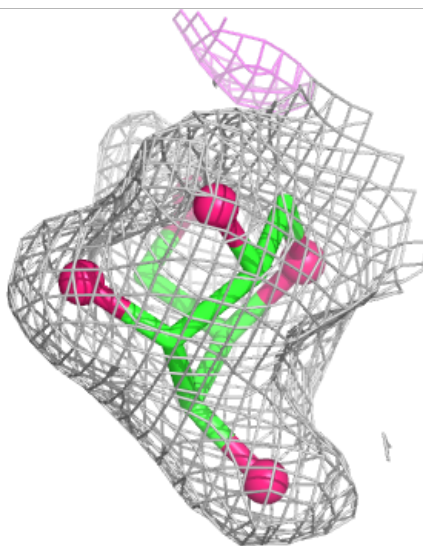
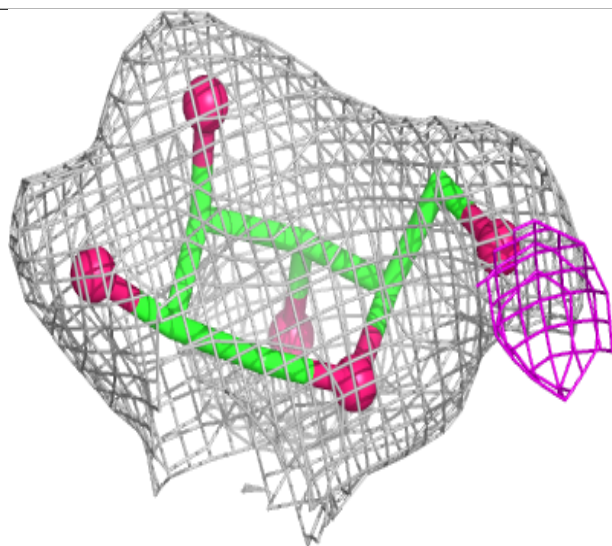
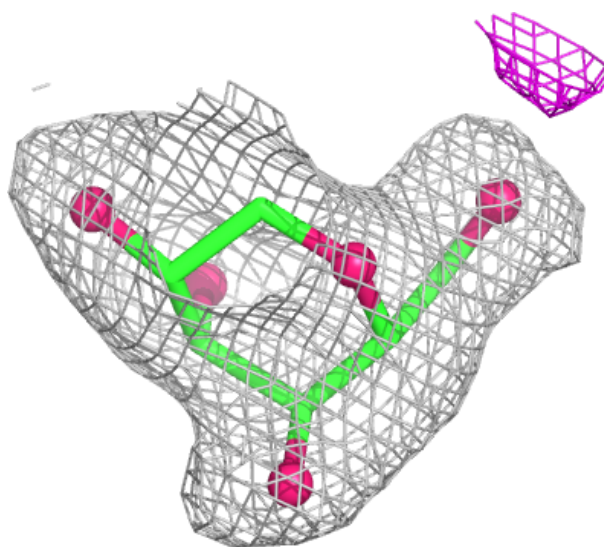
Electron density around MAN F 502:

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and green (positive)



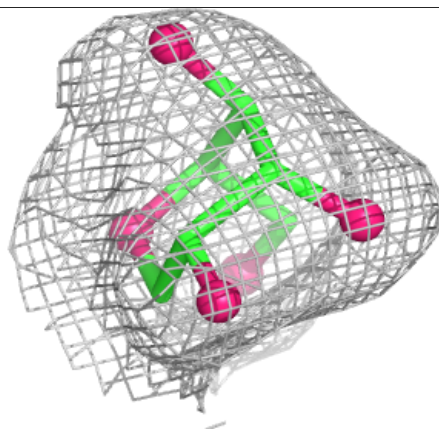
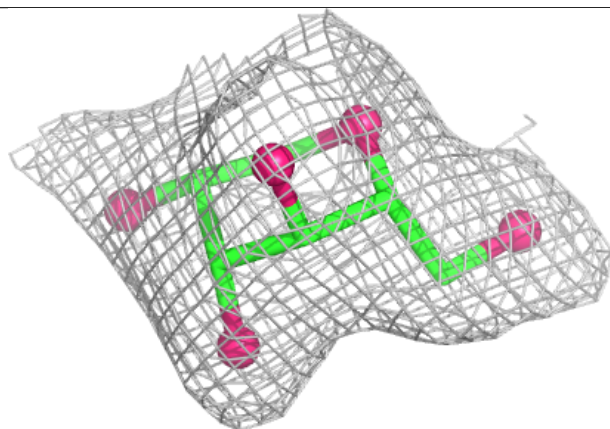
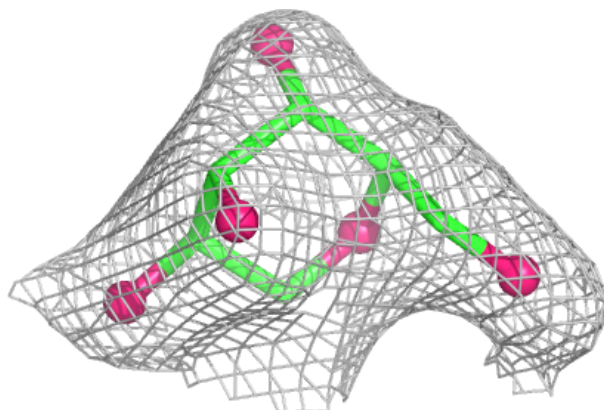
Electron density around MAN D 507:

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and green (positive)



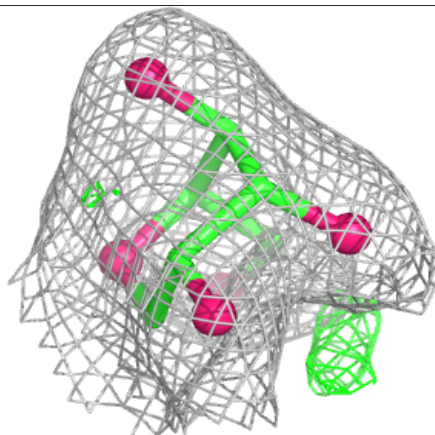
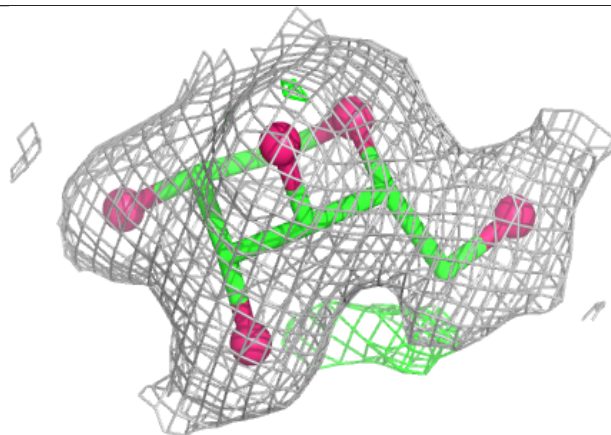
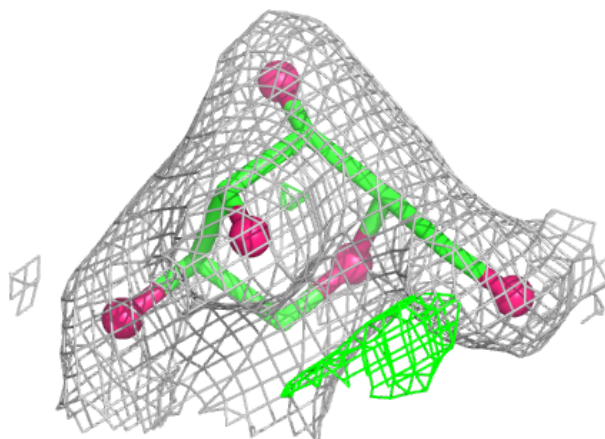
Electron density around MAN E 201:

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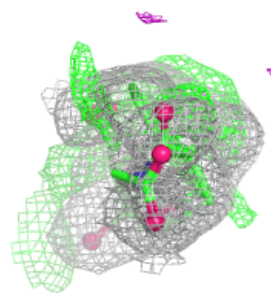
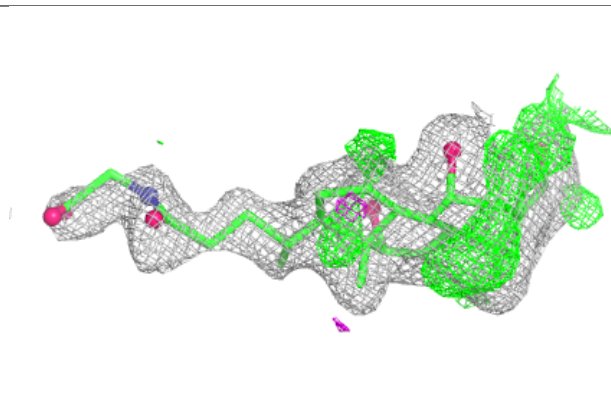
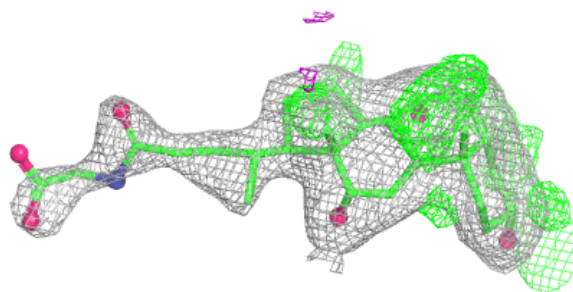


Electron density around MAN F 503:

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and green (positive)

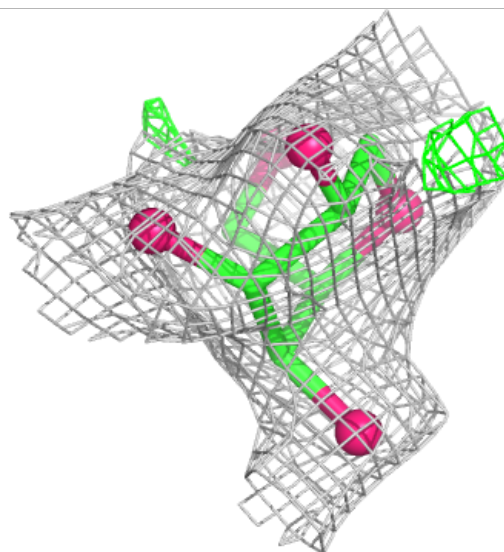
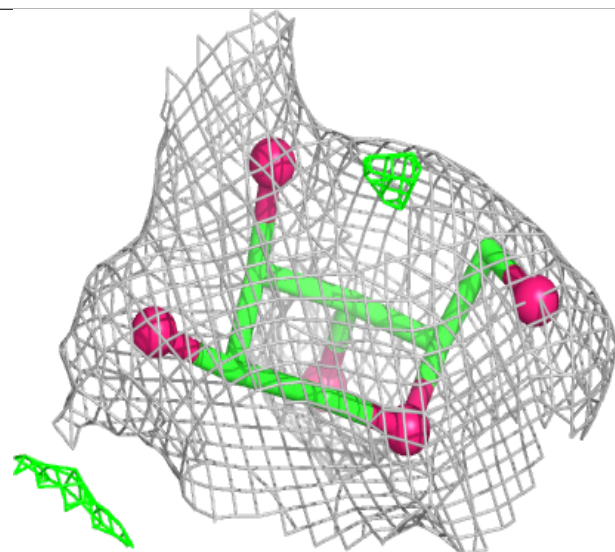
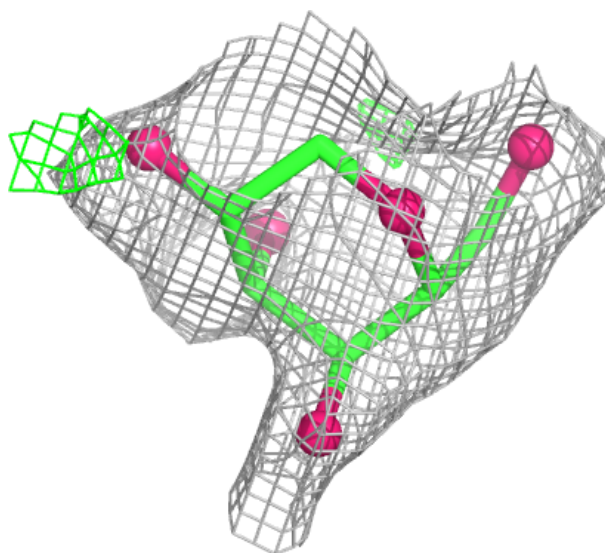
**Electron density around GCH A 1101:**

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



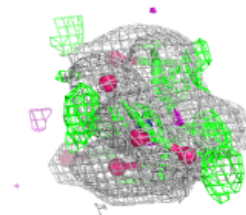
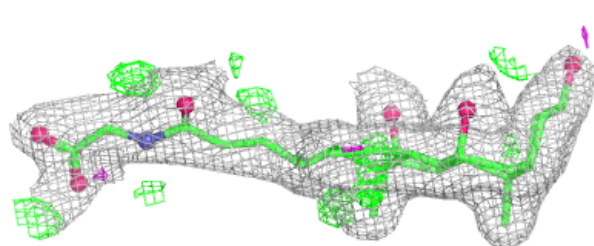
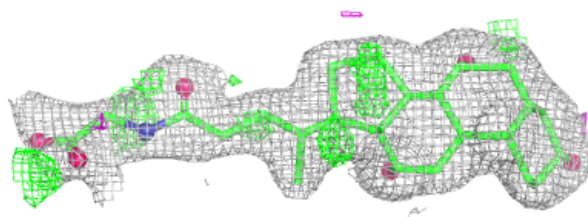
Electron density around MAN D 508:

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



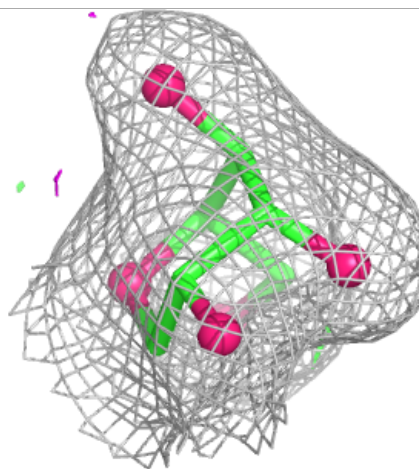
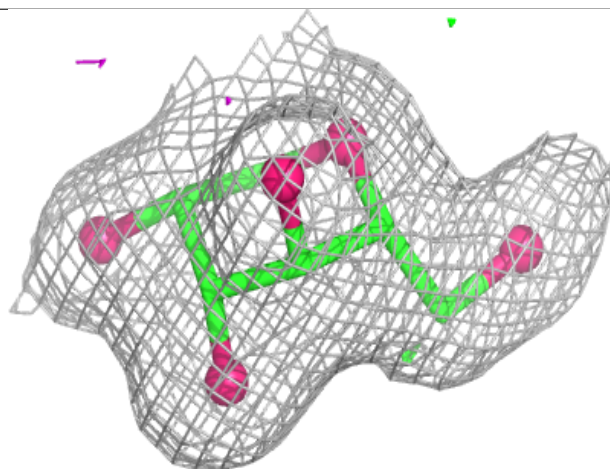
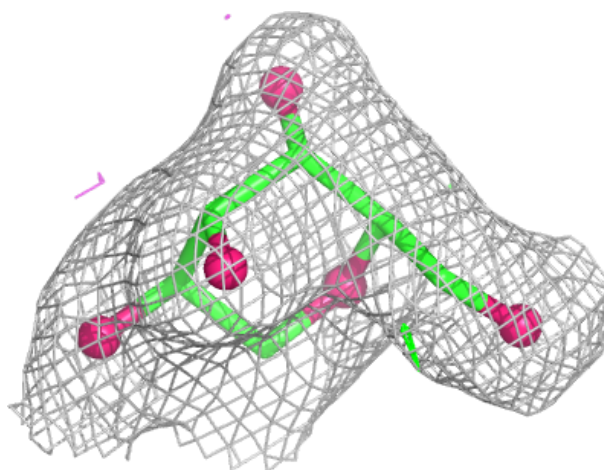
Electron density around GCH A 1102:

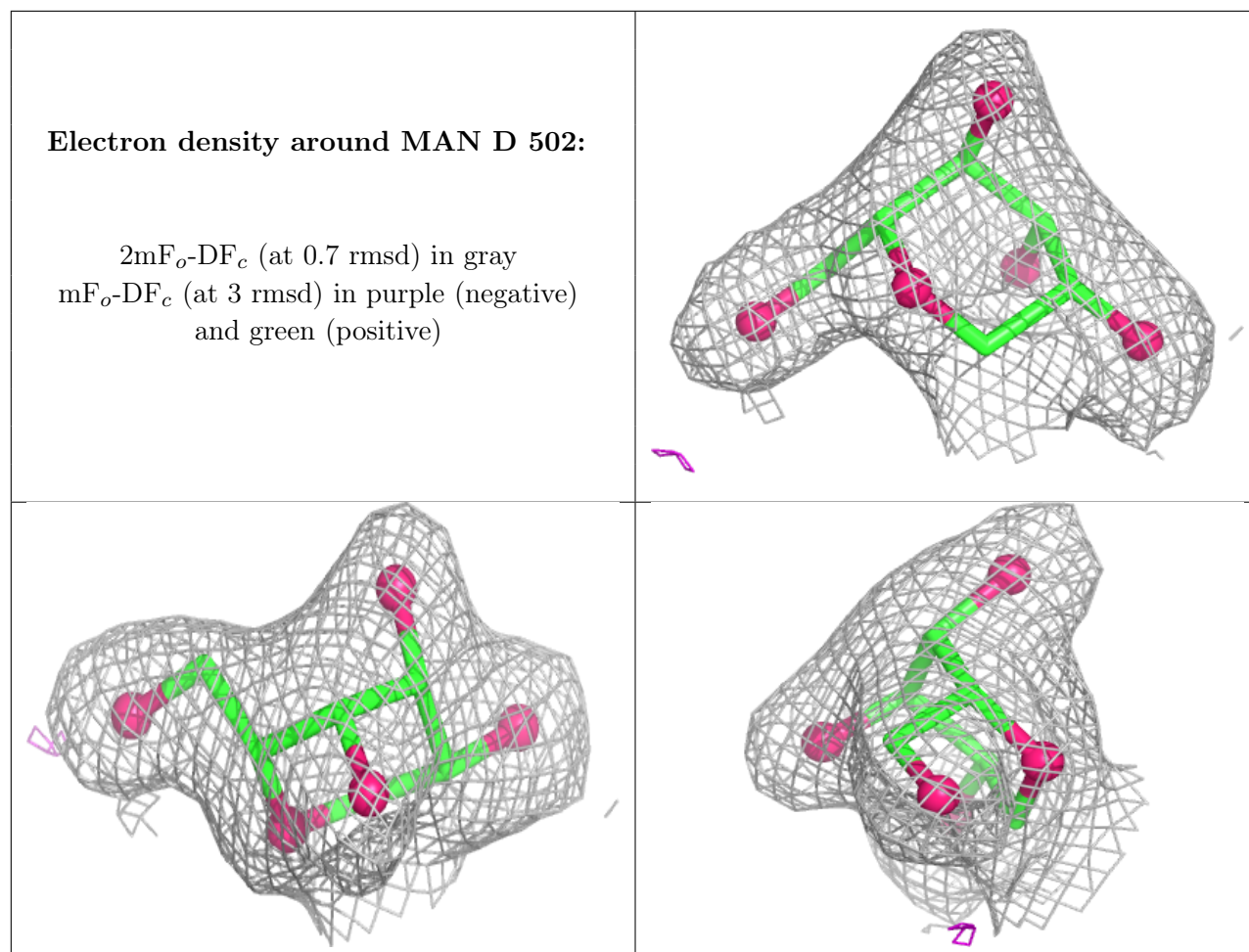
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around MAN D 503:

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





6.5 Other polymers [i](#)

There are no such residues in this entry.