



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 11:56 AM UTC

PDB ID : 8W6P / pdb_00008w6p
Title : Crystal structure of dimeric murine SMPDL3A
Authors : Zhang, C.; Liu, P.; Fan, S.; Hou, Y.
Deposited on : 2023-08-29
Resolution : 1.91 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

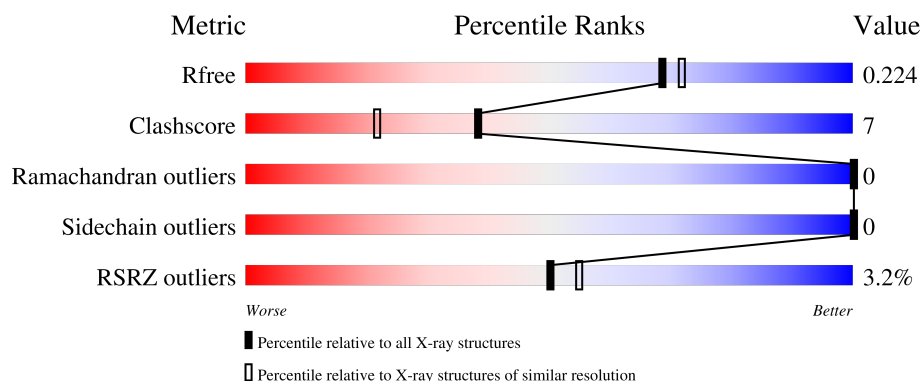
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.91 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	1188 (1.92-1.92)
Clashscore	190562	1209 (1.92-1.92)
Ramachandran outliers	187476	1195 (1.92-1.92)
Sidechain outliers	187428	1195 (1.92-1.92)
RSRZ outliers	180081	1188 (1.92-1.92)

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	413	3% 88% 12%
1	B	413	3% 86% 14%
2	C	2	50% 50%
2	E	2	50% 50%
3	D	2	100%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
4	F	3	67% 33%

2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 7618 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 Acid sphingomyelinase-like phosphodiesterase 3a.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	412	Total	C	N	O	S	0	0	0
			3287	2118	535	620	14			
1	B	413	Total	C	N	O	S	0	0	0
			3292	2121	536	621	14			

- 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	C	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	E	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 3 is an oligosaccharide called alpha-L-fucopyranose-(1-6)-2-acetamido-2-deoxy-beta-D-glucopyranose.



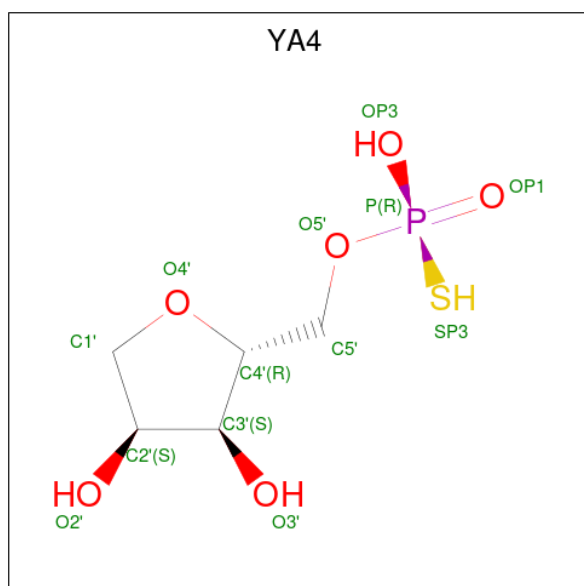
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	D	2	Total	C	N	O	0	0	0
			24	14	1	9			

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	F	3	Total	C	N	O	0	0	0
			39	22	2	15			

- Molecule 5 is [(2 {R},3 {S},4 {S})-3,4-bis(oxidanyl)oxolan-2-yl]methoxy-sulfanyl-phosphinic acid (CCD ID: YA4) (formula: C₅H₁₁O₆PS) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	O	P	S	1	0
			13	5	6	1	1		

- Molecule 6 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆) (labeled as "Ligand of Interest" by depositor).

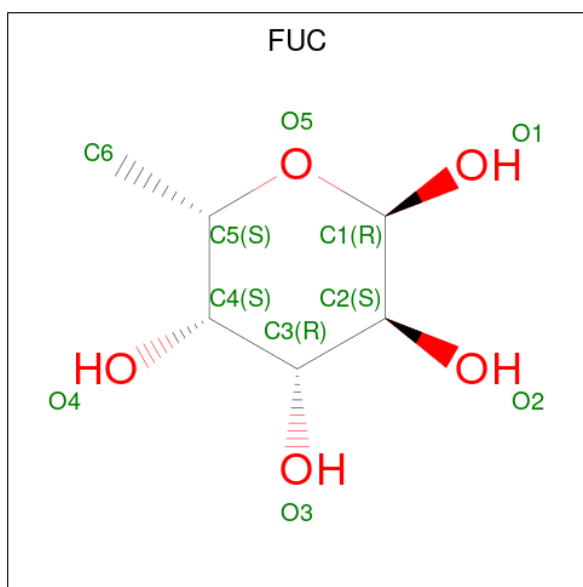


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	1	Total	C	N	O	0	0
			14	8	1	5		
6	A	1	Total	C	N	O	0	0
			14	8	1	5		
6	B	1	Total	C	N	O	0	0
			14	8	1	5		
6	B	1	Total	C	N	O	0	0
			14	8	1	5		
6	B	1	Total	C	N	O	0	0
			14	8	1	5		
6	B	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 7 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

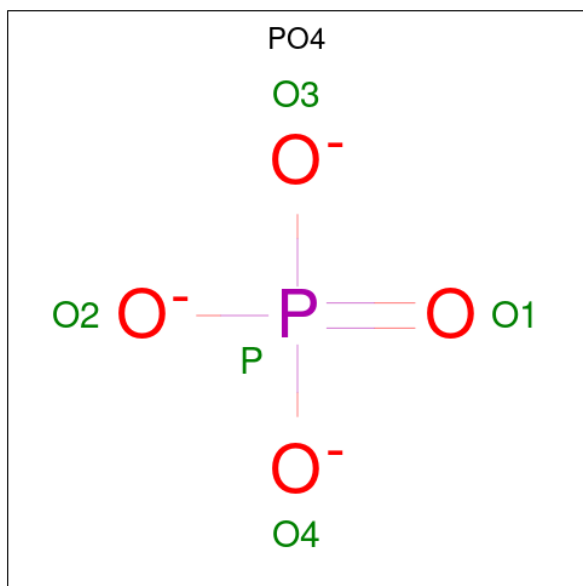
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	2	Total	Zn	0	0
			2	2		
7	B	2	Total	Zn	0	0
			2	2		

- Molecule 8 is alpha-L-fucopyranose (CCD ID: FUC) (formula: C₆H₁₂O₅) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	B	1	Total	C	O	0	0
			10	6	4		

- Molecule 9 is PHOSPHATE ION (CCD ID: PO4) (formula: O_4P) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	B	1	Total	O	P	0	0
			5	4	1		

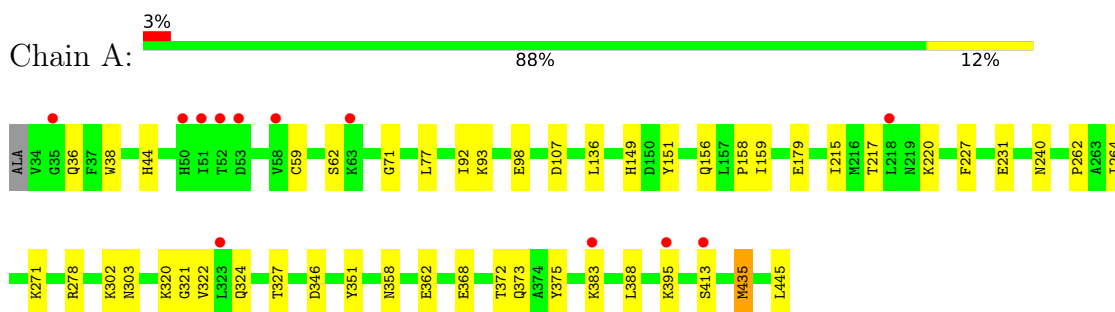
- Molecule 10 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	403	Total 403	O 403	0	0
10	B	401	Total 401	O 401	0	0

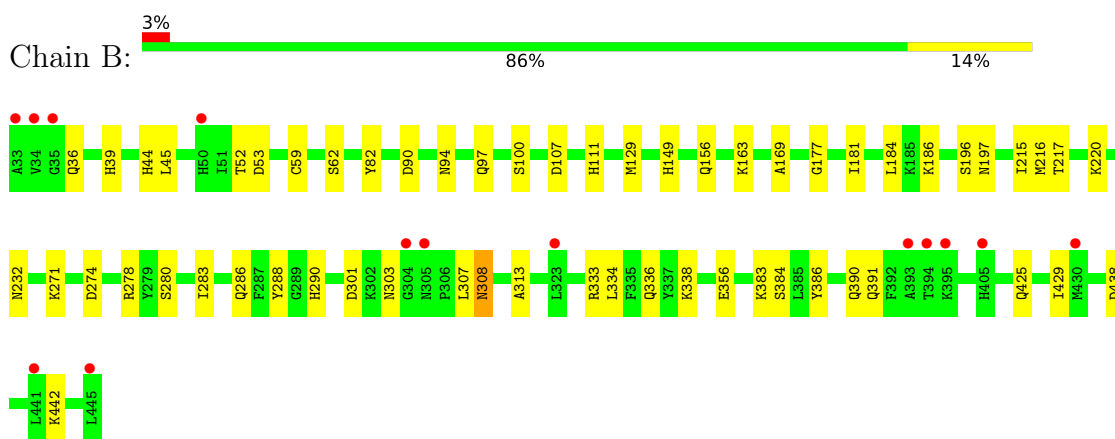
3 Residue-property plots [i](#)

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

- Molecule 1: Acid sphingomyelinase-like phosphodiesterase 3a



- Molecule 1: Acid sphingomyelinase-like phosphodiesterase 3a



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



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





- Molecule 3: α -L-fucopyranose-(1-6)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain D:  100%



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

Chain F:  67% 33%



4 Data and refinement statistics

Property	Value	Source
Space group	P 41	Depositor
Cell constants a, b, c, α , β , γ	122.22Å 122.22Å 79.56Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.27 – 1.91 20.27 – 1.91	Depositor EDS
% Data completeness (in resolution range)	98.0 (20.27-1.91) 98.2 (20.27-1.91)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.28 (at 1.90Å)	Xtriage
Refinement program	PHENIX (1.18.2_3874: ???)	Depositor
R, R_{free}	0.218 , 0.246 (Not available) , 0.224	Depositor DCC
R_{free} test set	2001 reflections (2.19%)	wwPDB-VP
Wilson B-factor (Å ²)	27.0	Xtriage
Anisotropy	0.216	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 52.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	0.058 for h,-k,-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	7618	wwPDB-VP
Average B, all atoms (Å ²)	30.0	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 30.65 % 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 1.2627e-03.*

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: NAG, YA4, BMA, FUC, ZN, PO4

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	0.43	0/3381	0.70	1/4618 (0.0%)
1	B	0.45	0/3386	0.69	4/4625 (0.1%)
All	All	0.44	0/6767	0.70	5/9243 (0.1%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	308	ASN	CB-CA-C	7.53	121.84	109.72
1	B	308	ASN	N-CA-CB	-6.95	99.23	110.77
1	B	186	LYS	CD-CE-NZ	-6.48	91.15	111.90
1	A	435	MET	CB-CG-SD	-5.33	96.69	112.70
1	B	186	LYS	N-CA-C	5.09	117.95	111.69

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3287	0	3189	38	3
1	B	3292	0	3195	50	0
2	C	28	0	25	0	0
2	E	28	0	25	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	D	24	0	22	1	0
4	F	39	0	34	0	0
5	A	13	0	0	1	3
6	A	28	0	26	1	0
6	B	56	0	50	1	0
7	A	2	0	0	0	0
7	B	2	0	0	0	0
8	B	10	0	10	0	0
9	B	5	0	0	1	0
10	A	403	0	0	12	0
10	B	401	0	0	24	0
All	All	7618	0	6576	92	3

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

All (92) 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:A:383:LYS:HG2	10:A:858:HOH:O	1.43	1.16
1:B:82:TYR:OH	10:B:601:HOH:O	1.84	0.94
1:B:39:HIS:O	10:B:602:HOH:O	1.86	0.93
1:B:308:ASN:OD1	10:B:603:HOH:O	1.89	0.88
9:B:506:PO4:O2	10:B:604:HOH:O	1.94	0.84
1:A:413:SER:O	10:A:602:HOH:O	1.96	0.82
1:B:391:GLN:OE1	10:B:605:HOH:O	1.97	0.81
1:A:231:GLU:OE1	10:A:603:HOH:O	2.03	0.77
1:B:336:GLN:OE1	10:B:608:HOH:O	2.03	0.75
1:A:93:LYS:HE2	1:A:136:LEU:HD22	1.68	0.75
1:B:156:GLN:HE22	1:B:215:ILE:N	1.85	0.74
10:A:999:HOH:O	3:D:1:NAG:O4	2.04	0.74
1:B:156:GLN:HE22	1:B:215:ILE:H	1.36	0.74
1:A:240:ASN:ND2	10:A:608:HOH:O	2.19	0.73
1:A:362:GLU:OE1	10:A:604:HOH:O	2.07	0.72
1:A:217:THR:HA	1:A:220:LYS:HD2	1.72	0.70
1:B:44:HIS:CE1	10:B:604:HOH:O	2.44	0.69
1:B:36:GLN:HB3	1:B:334:LEU:HD11	1.75	0.69
1:B:274:ASP:OD2	10:B:606:HOH:O	2.12	0.68
6:A:502:NAG:O3	10:A:606:HOH:O	2.13	0.66
1:B:53:ASP:OD2	10:B:611:HOH:O	2.13	0.66
1:A:322:VAL:O	10:A:607:HOH:O	2.15	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:97:GLN:NE2	10:B:614:HOH:O	2.17	0.64
1:B:216:MET:HE3	10:B:754:HOH:O	1.97	0.63
1:B:271:LYS:NZ	10:B:619:HOH:O	2.30	0.63
1:A:59:CYS:SG	1:A:62:SER:HB3	2.38	0.63
1:B:232:ASN:ND2	10:B:609:HOH:O	2.09	0.62
1:A:156:GLN:HE22	1:A:215:ILE:H	1.48	0.62
6:B:503:NAG:O6	10:B:607:HOH:O	2.02	0.60
1:B:283:ILE:HB	1:B:308:ASN:HD21	1.66	0.59
1:B:356:GLU:OE1	10:B:613:HOH:O	2.17	0.59
1:B:149:HIS:CD2	10:B:604:HOH:O	2.56	0.59
1:B:303:ASN:ND2	10:B:623:HOH:O	2.36	0.59
1:A:321:GLY:H	1:A:324:GLN:NE2	2.01	0.57
1:B:290:HIS:HA	10:B:639:HOH:O	2.04	0.57
1:A:227:PHE:O	1:A:231:GLU:HG3	2.06	0.56
1:B:45:LEU:HD22	1:B:129:MET:HE3	1.89	0.54
1:B:338:LYS:HE2	10:B:878:HOH:O	2.06	0.54
1:A:36:GLN:HG3	1:A:98:GLU:O	2.06	0.54
1:B:36:GLN:OE1	1:B:334:LEU:HD21	2.07	0.54
1:A:445:LEU:C	10:A:619:HOH:O	2.50	0.53
1:B:301:ASP:HB3	1:B:307:LEU:HD11	1.90	0.53
1:A:302:LYS:HG2	10:A:715:HOH:O	2.08	0.53
1:B:278:ARG:NH2	10:B:606:HOH:O	2.02	0.52
1:B:90:ASP:O	1:B:94:ASN:ND2	2.39	0.52
1:A:395:LYS:N	1:A:395:LYS:HD2	2.25	0.52
1:A:44:HIS:CE1	1:A:107:ASP:HB3	2.44	0.52
1:B:220:LYS:CG	10:B:629:HOH:O	2.59	0.51
1:B:338:LYS:HD3	10:B:803:HOH:O	2.11	0.50
1:B:307:LEU:O	1:B:308:ASN:HB2	2.10	0.50
1:B:438:ASP:O	1:B:442:LYS:HG2	2.11	0.49
1:B:163:LYS:N	1:B:163:LYS:HD3	2.28	0.49
1:B:425:GLN:O	1:B:429:ILE:HG13	2.12	0.49
1:B:386:TYR:O	1:B:390:GLN:HG2	2.12	0.49
1:A:156:GLN:CD	10:A:611:HOH:O	2.57	0.48
1:B:52:THR:OG1	10:B:615:HOH:O	2.18	0.48
1:B:286:GLN:NE2	1:B:288:TYR:OH	2.45	0.48
1:A:156:GLN:NE2	1:A:215:ILE:HG12	2.30	0.47
1:A:373:GLN:HG2	10:A:929:HOH:O	2.13	0.47
1:B:44:HIS:CE1	1:B:107:ASP:HB3	2.50	0.47
1:B:169:ALA:HA	1:B:184:LEU:HD23	1.96	0.47
1:B:156:GLN:NE2	1:B:156:GLN:HA	2.29	0.47
1:B:44:HIS:CE1	1:B:111:HIS:CE1	3.03	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:220:LYS:HG3	10:B:629:HOH:O	2.15	0.46
1:A:435:MET:HE3	1:A:435:MET:HB2	1.60	0.46
1:A:156:GLN:HE22	1:A:215:ILE:N	2.11	0.46
1:A:227:PHE:CE2	1:A:271:LYS:HD2	2.51	0.46
1:B:313:ALA:HB2	1:B:333:ARG:HD2	1.99	0.45
1:A:38:TRP:CE2	1:A:92:ILE:HG23	2.52	0.45
1:A:159:ILE:HD13	1:A:220:LYS:CE	2.46	0.45
1:B:59:CYS:SG	1:B:62:SER:HB3	2.57	0.45
1:B:100:SER:HB2	1:B:196:SER:OG	2.18	0.43
1:B:196:SER:OG	1:B:197:ASN:ND2	2.51	0.43
1:A:179:GLU:H	1:A:179:GLU:CD	2.24	0.43
1:A:320:LYS:HB3	1:A:327:THR:HB	2.00	0.43
1:A:62:SER:HA	1:A:77:LEU:O	2.18	0.43
1:B:383:LYS:HG3	1:B:384:SER:N	2.34	0.43
1:A:71:GLY:HA3	1:A:358:ASN:CG	2.45	0.42
1:A:151:TYR:CZ	1:A:158:PRO:HD3	2.55	0.42
1:A:346:ASP:OD2	1:A:372:THR:OG1	2.36	0.42
1:B:177:GLY:O	1:B:181:ILE:HG12	2.19	0.42
1:A:351:TYR:CD1	1:A:368:GLU:HB2	2.55	0.42
1:A:375:TYR:HB3	1:A:388:LEU:CD1	2.50	0.41
1:B:280:SER:HA	1:B:308:ASN:HD22	1.85	0.41
1:A:321:GLY:H	1:A:324:GLN:HE21	1.68	0.41
1:B:217:THR:HA	1:B:220:LYS:HD2	2.03	0.41
1:A:262:PRO:HB2	1:A:264:ILE:O	2.20	0.41
1:A:278:ARG:HH11	1:A:278:ARG:HD3	1.71	0.41
1:B:156:GLN:NE2	1:B:215:ILE:H	2.11	0.41
1:A:375:TYR:HB3	1:A:388:LEU:HD13	2.03	0.41
1:A:149:HIS:NE2	5:A:501:YA4:SP3	2.66	0.40
1:B:280:SER:HA	1:B:308:ASN:ND2	2.36	0.40

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:303:ASN:ND2	5:A:501:YA4:C2'[4_554]	1.79	0.41
1:A:303:ASN:CG	5:A:501:YA4:O2'[4_554]	1.97	0.23
1:A:303:ASN:OD1	5:A:501:YA4:O2'[4_554]	2.19	0.01

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	410/413 (99%)	390 (95%)	20 (5%)	0	100	100
1	B	411/413 (100%)	387 (94%)	24 (6%)	0	100	100
All	All	821/826 (99%)	777 (95%)	44 (5%)	0	100	100

There are no Ramachandran outliers to report.

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	367/367 (100%)	367 (100%)	0	100	100
1	B	367/367 (100%)	367 (100%)	0	100	100
All	All	734/734 (100%)	734 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	154	GLN
1	A	156	GLN
1	A	286	GLN
1	A	308	ASN
1	A	324	GLN
1	A	419	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	156	GLN
1	B	208	ASN
1	B	286	GLN
1	B	308	ASN
1	B	336	GLN
1	B	373	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 ⓘ

9 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	C	1	1,2	14,14,15	0.33	0	17,19,21	0.97	1 (5%)
2	NAG	C	2	2	14,14,15	0.15	0	17,19,21	0.42	0
3	NAG	D	1	1,3	14,14,15	0.42	0	17,19,21	0.67	0
3	FUC	D	2	3	10,10,11	1.67	3 (30%)	14,14,16	1.29	2 (14%)
2	NAG	E	1	1,2	14,14,15	0.33	0	17,19,21	0.57	0
2	NAG	E	2	2	14,14,15	0.28	0	17,19,21	1.73	3 (17%)
4	NAG	F	1	1,4	14,14,15	0.28	0	17,19,21	0.49	0
4	NAG	F	2	4	14,14,15	0.46	0	17,19,21	0.55	0
4	BMA	F	3	4	11,11,12	0.87	0	15,15,17	1.04	1 (6%)

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	C	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	C	2	2	-	0/6/23/26	0/1/1/1
3	NAG	D	1	1,3	-	0/6/23/26	0/1/1/1
3	FUC	D	2	3	-	-	0/1/1/1
2	NAG	E	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	E	2	2	-	1/6/23/26	0/1/1/1
4	NAG	F	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	F	2	4	-	0/6/23/26	0/1/1/1
4	BMA	F	3	4	-	0/2/19/22	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	2	FUC	O5-C5	3.15	1.49	1.43
3	D	2	FUC	C2-C3	2.54	1.56	1.52
3	D	2	FUC	O5-C1	-2.46	1.39	1.43

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	2	NAG	C1-O5-C5	4.20	117.82	112.19
2	E	2	NAG	C2-N2-C7	4.02	128.29	122.90
2	C	1	NAG	C1-O5-C5	3.34	116.67	112.19
2	E	2	NAG	C1-C2-N2	3.02	115.19	110.43
4	F	3	BMA	C1-O5-C5	2.94	116.13	112.19
3	D	2	FUC	O5-C5-C4	2.25	113.60	109.55
3	D	2	FUC	O2-C2-C1	2.10	114.02	109.22

There are no chirality outliers.

All (3) torsion outliers are listed below:

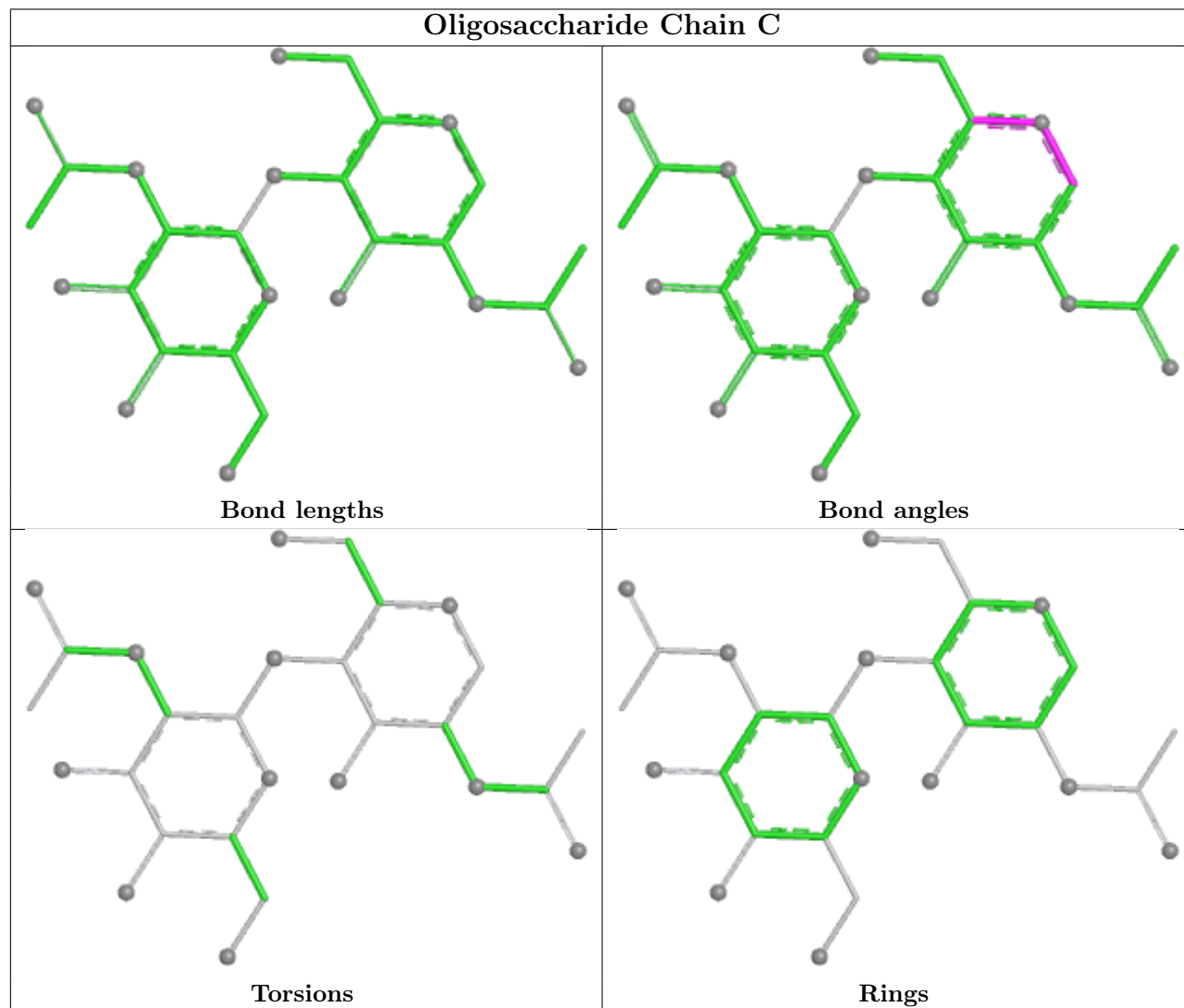
Mol	Chain	Res	Type	Atoms
2	E	2	NAG	C3-C2-N2-C7
2	E	1	NAG	C4-C5-C6-O6
2	E	1	NAG	O5-C5-C6-O6

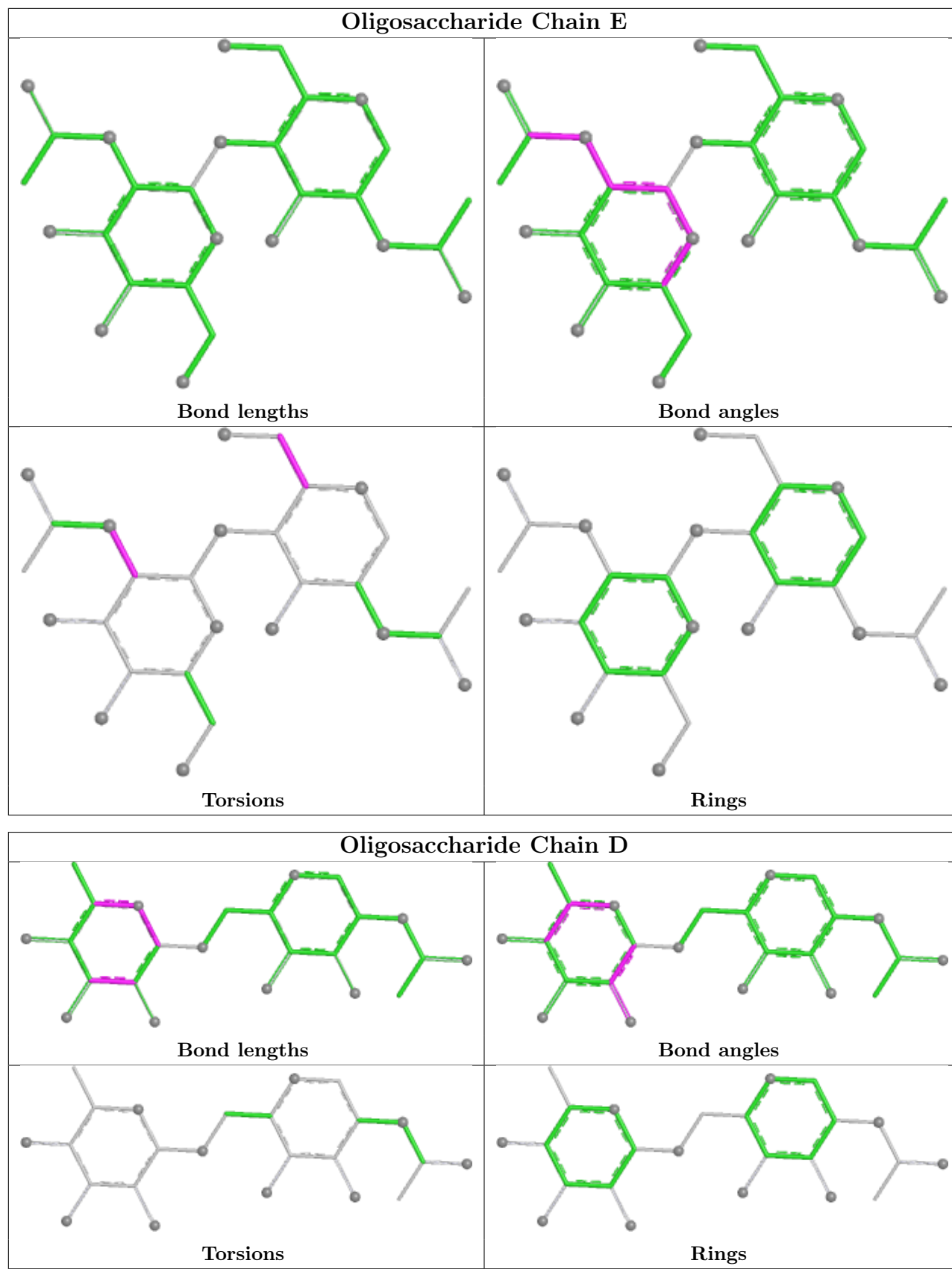
There are no ring outliers.

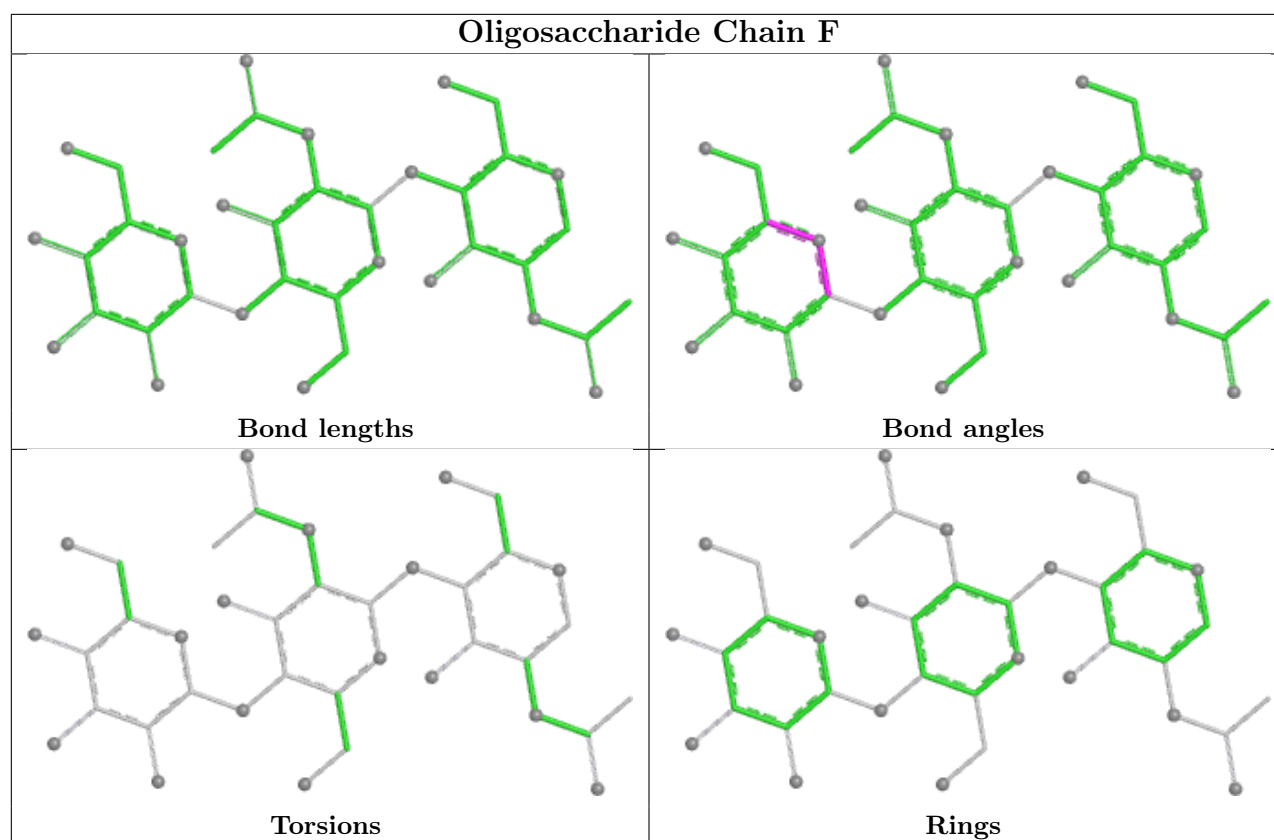
1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	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 13 ligands modelled in this entry, 4 are monoatomic - leaving 9 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	$\# Z > 2$
6	NAG	A	502	1	14,14,15	0.40	0	17,19,21	0.71	1 (5%)
6	NAG	B	501	6	14,14,15	0.49	0	17,19,21	0.69	0
9	PO4	B	506	7	4,4,4	0.92	0	6,6,6	1.11	0
6	NAG	B	503	1	14,14,15	0.81	1 (7%)	17,19,21	0.54	0
6	NAG	B	504	1,8	14,14,15	0.49	0	17,19,21	0.66	0
8	FUC	B	502	6	10,10,11	1.07	1 (10%)	14,14,16	1.34	2 (14%)
6	NAG	A	503	1	14,14,15	0.54	0	17,19,21	0.55	0
6	NAG	B	505	6,1	14,14,15	0.50	0	17,19,21	0.69	0
5	YA4	A	501	1,7	11,13,13	0.99	1 (9%)	12,19,19	1.11	1 (8%)

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
6	NAG	A	502	1	-	2/6/23/26	0/1/1/1
6	NAG	B	501	6	-	4/6/23/26	0/1/1/1
6	NAG	B	503	1	-	0/6/23/26	0/1/1/1
6	NAG	B	504	1,8	-	3/6/23/26	0/1/1/1
8	FUC	B	502	6	-	-	0/1/1/1
6	NAG	A	503	1	-	0/6/23/26	0/1/1/1
6	NAG	B	505	6,1	-	0/6/23/26	0/1/1/1
5	YA4	A	501	1,7	-	2/5/19/19	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	B	502	FUC	C1-C2	2.68	1.58	1.52
6	B	503	NAG	C1-C2	2.54	1.55	1.52
5	A	501	YA4	P-OP3	2.43	1.63	1.56

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	B	502	FUC	C1-O5-C5	2.62	119.15	112.97
8	B	502	FUC	O5-C5-C4	2.53	114.10	109.55
5	A	501	YA4	C1'-C2'-C3'	2.48	105.60	101.63
6	A	502	NAG	C1-O5-C5	2.07	114.96	112.19

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	B	504	NAG	C4-C5-C6-O6
6	A	502	NAG	O5-C5-C6-O6
6	B	501	NAG	O5-C5-C6-O6
6	B	504	NAG	O5-C5-C6-O6
6	B	501	NAG	C4-C5-C6-O6
6	A	502	NAG	C4-C5-C6-O6
5	A	501	YA4	O4'-C4'-C5'-O5'
6	B	501	NAG	C3-C2-N2-C7
6	B	501	NAG	C1-C2-N2-C7

Continued on next page...

Continued from previous page...

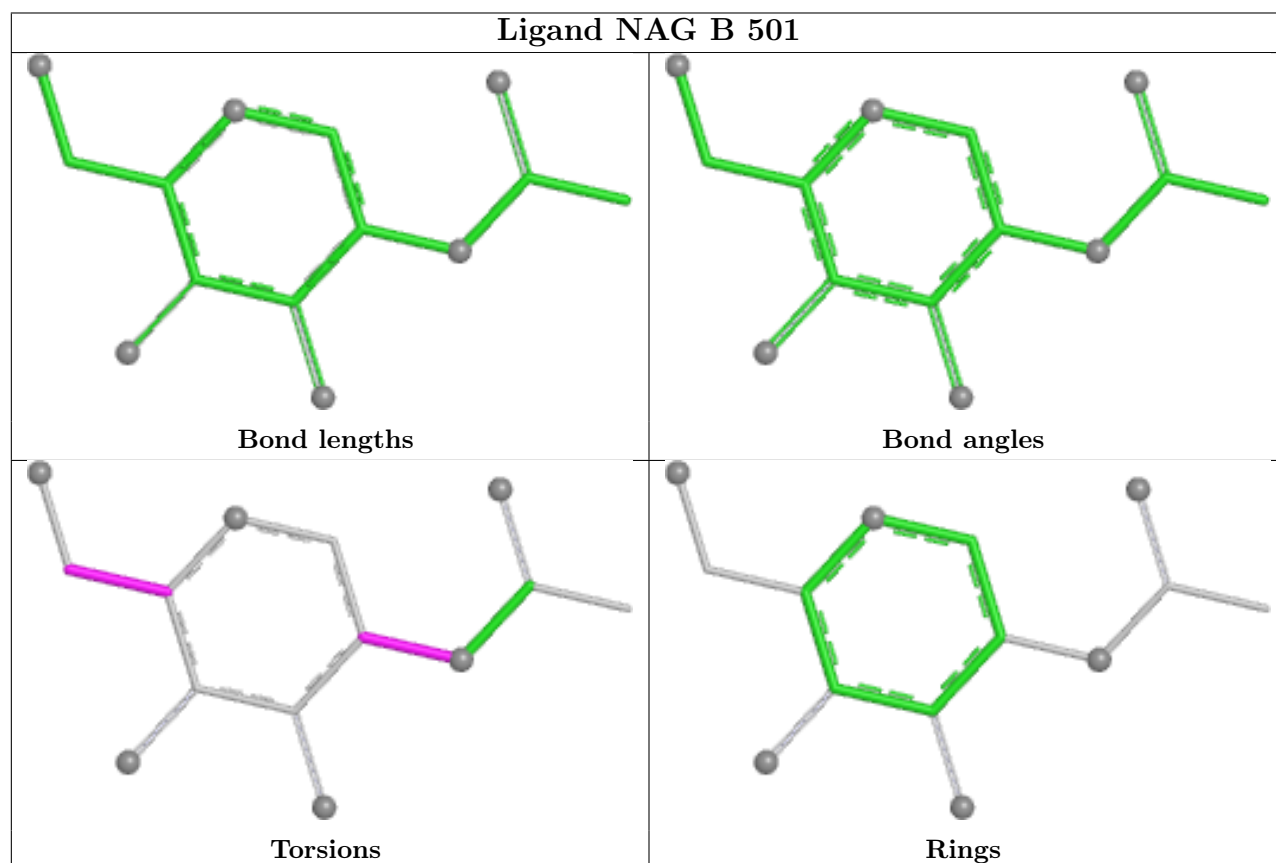
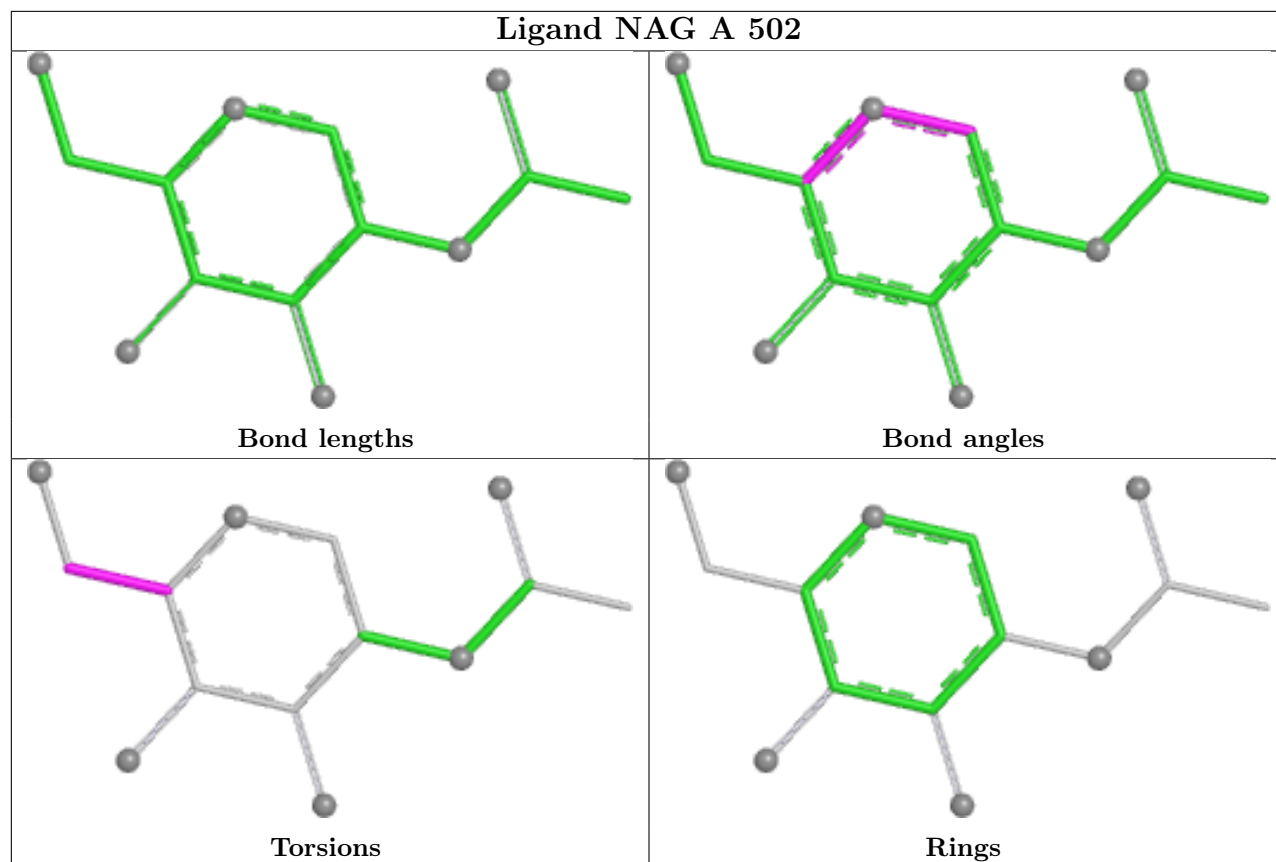
Mol	Chain	Res	Type	Atoms
6	B	504	NAG	C1-C2-N2-C7
5	A	501	YA4	C3'-C4'-C5'-O5'

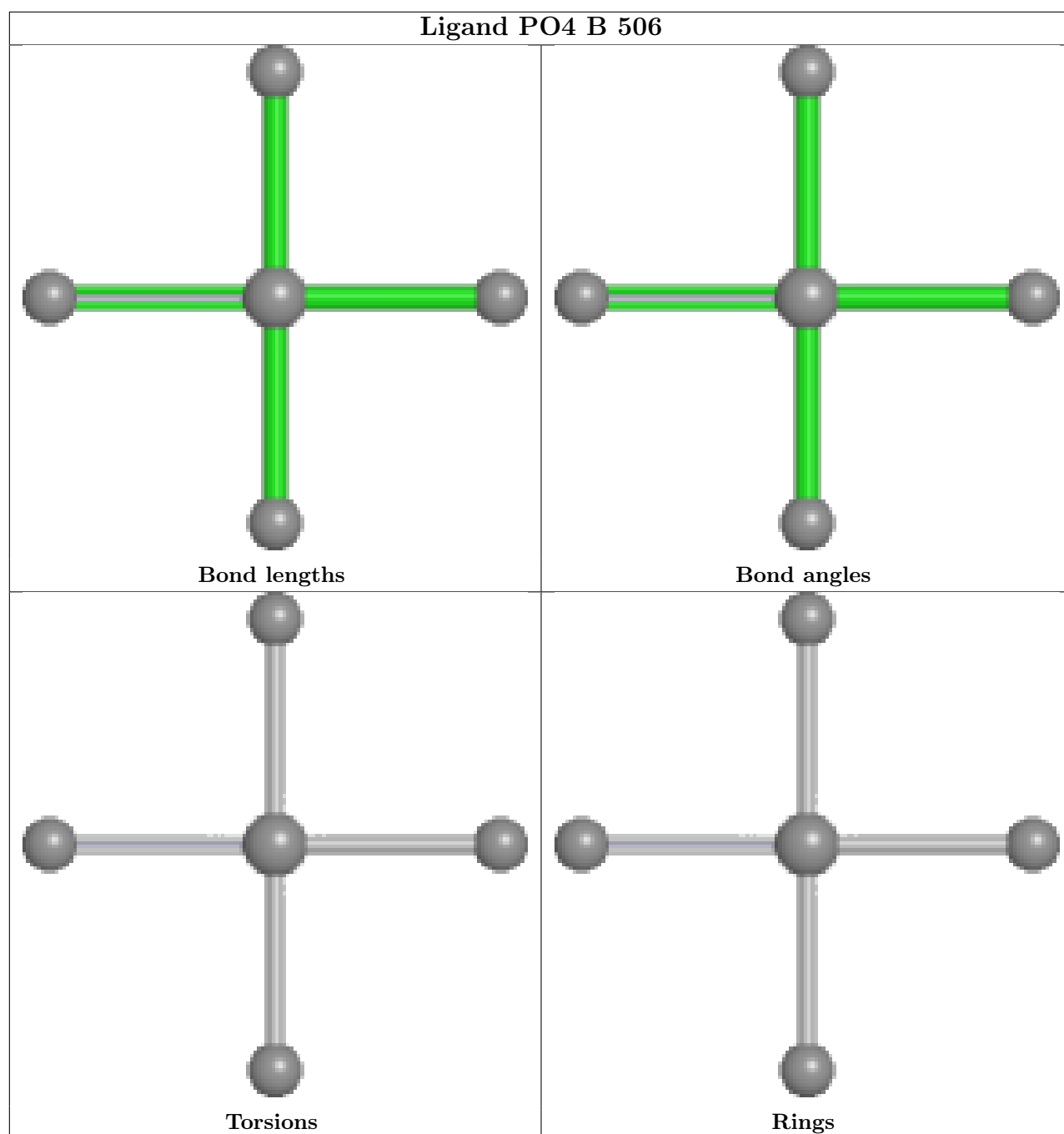
There are no ring outliers.

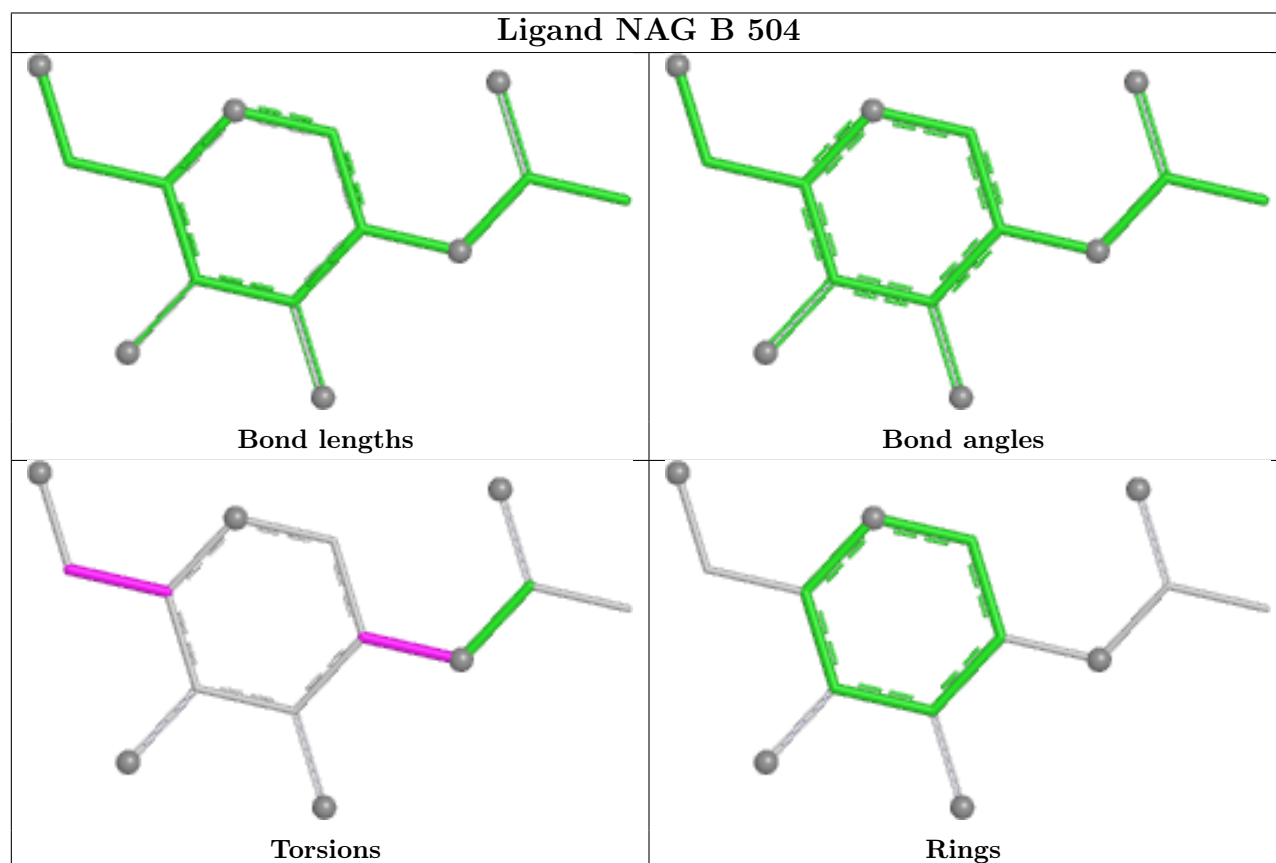
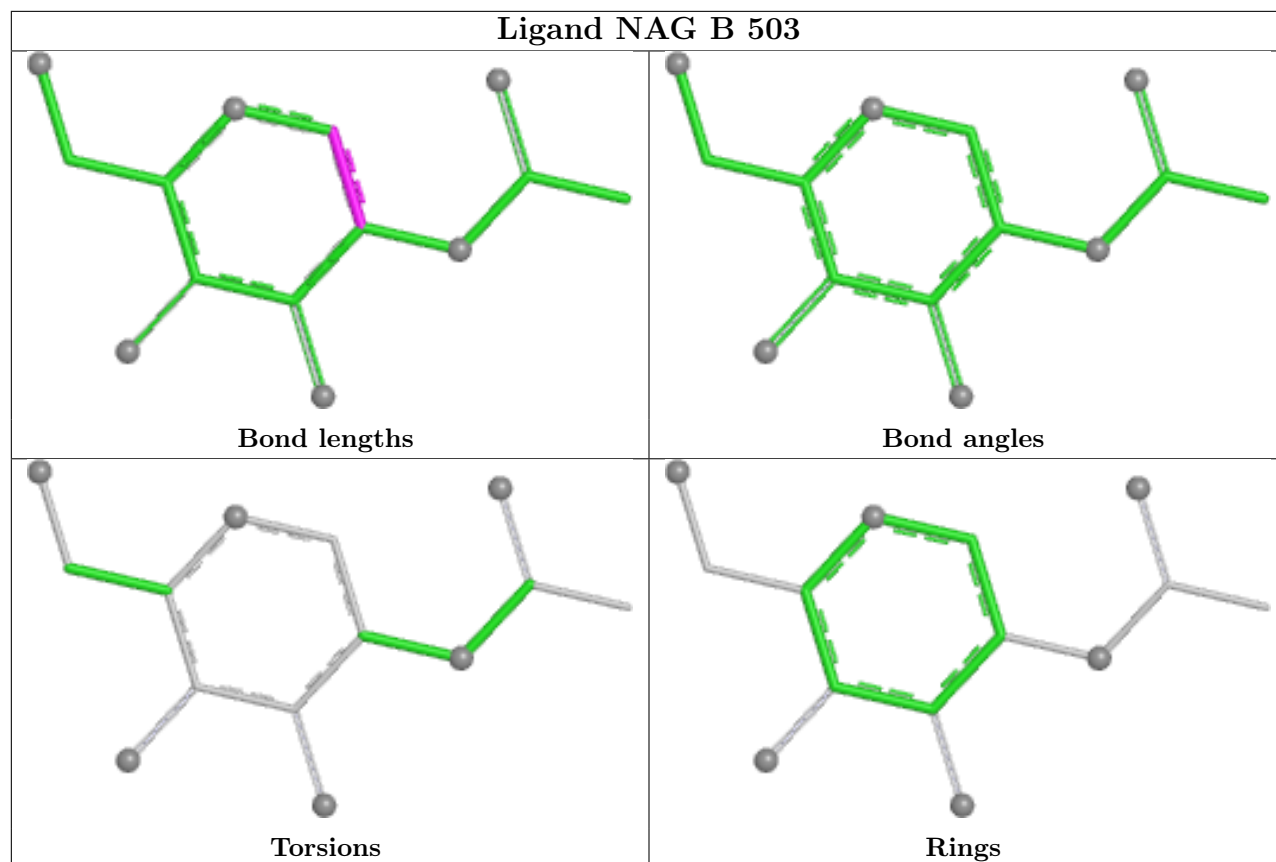
4 monomers are involved in 7 short contacts:

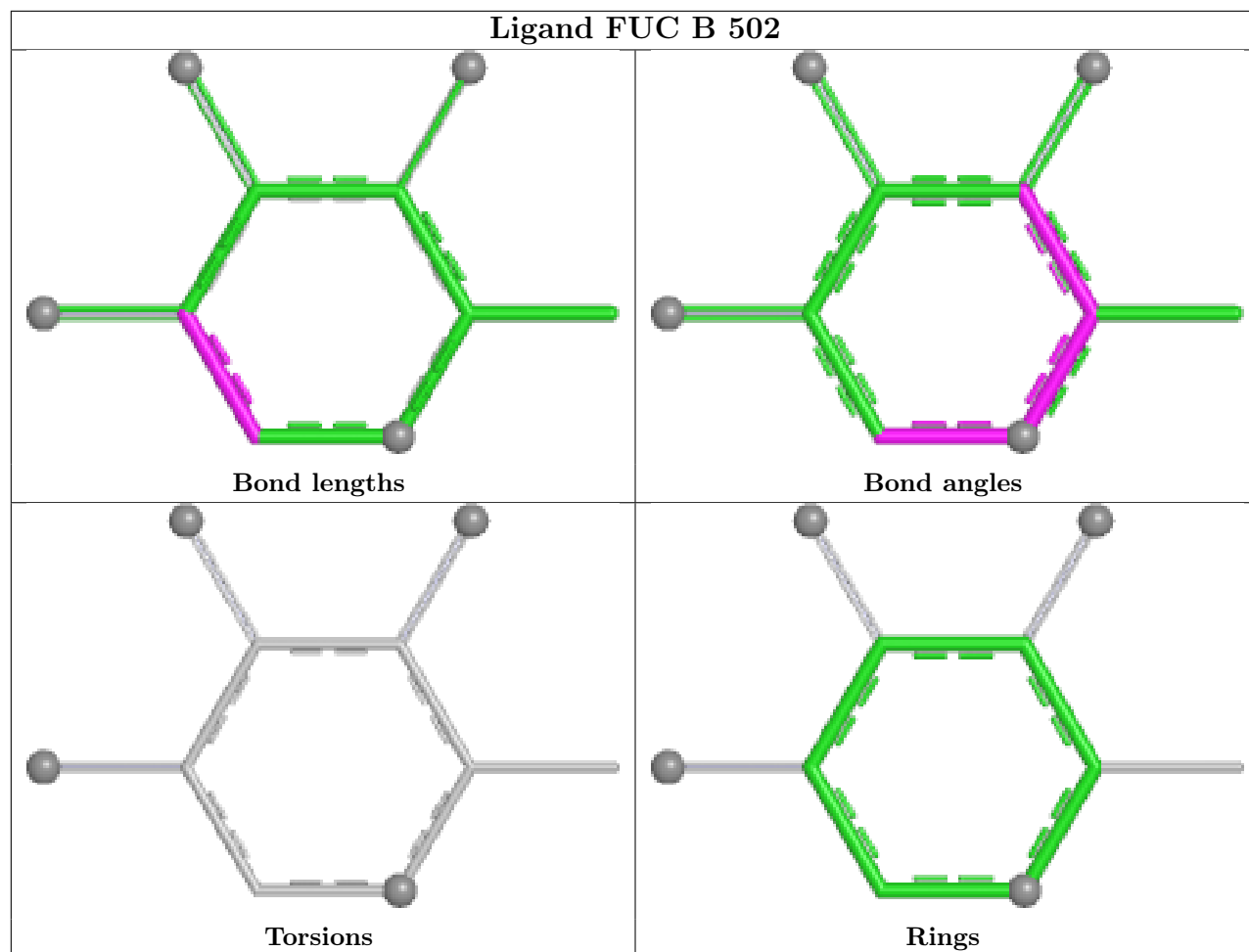
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	502	NAG	1	0
9	B	506	PO4	1	0
6	B	503	NAG	1	0
5	A	501	YA4	1	3

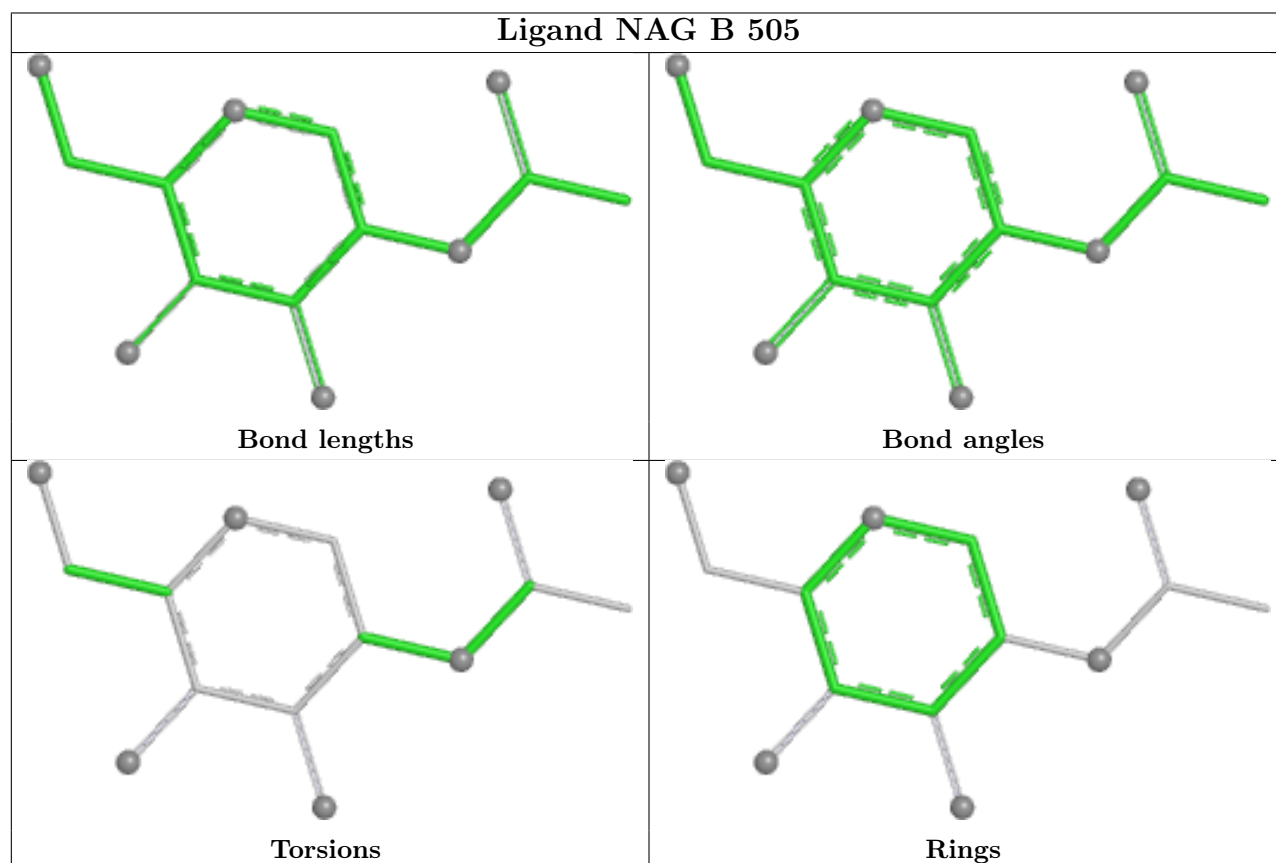
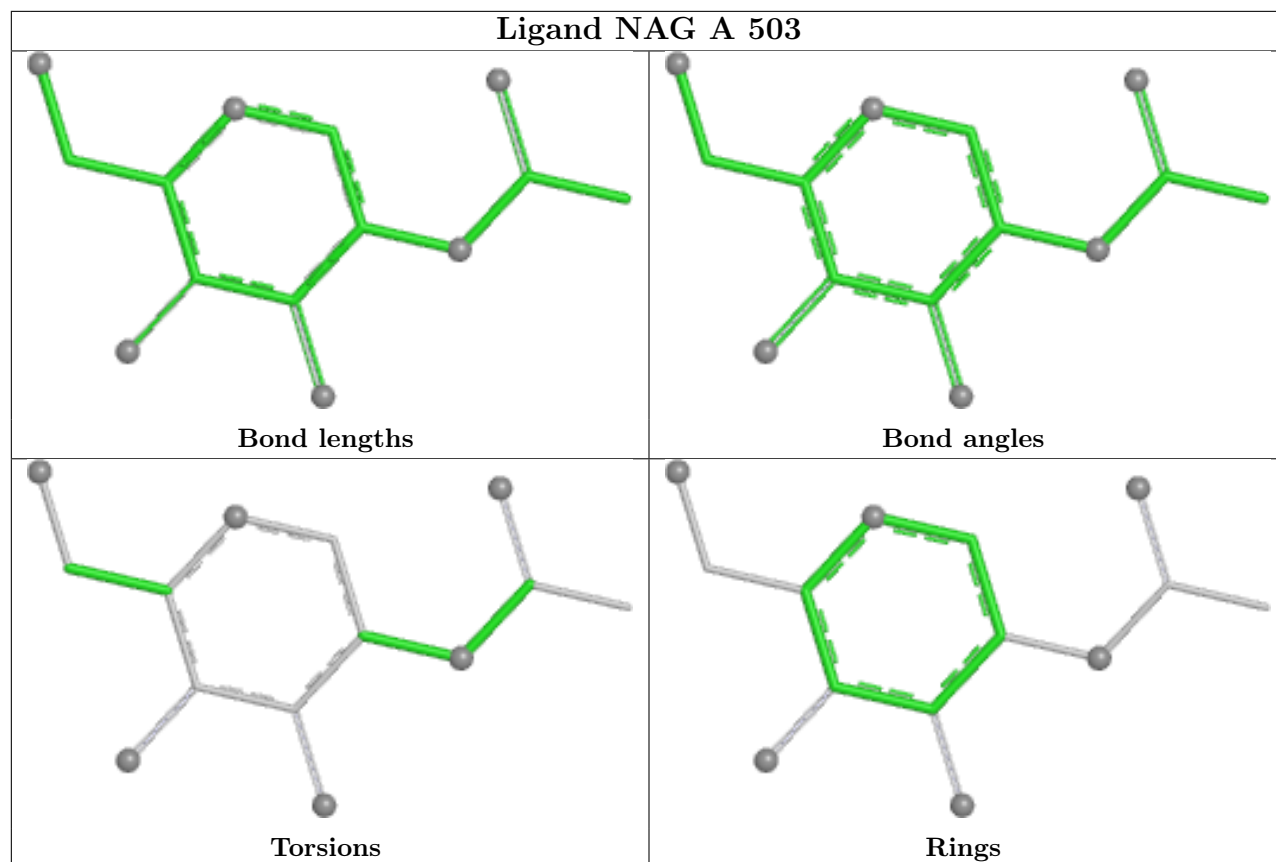
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

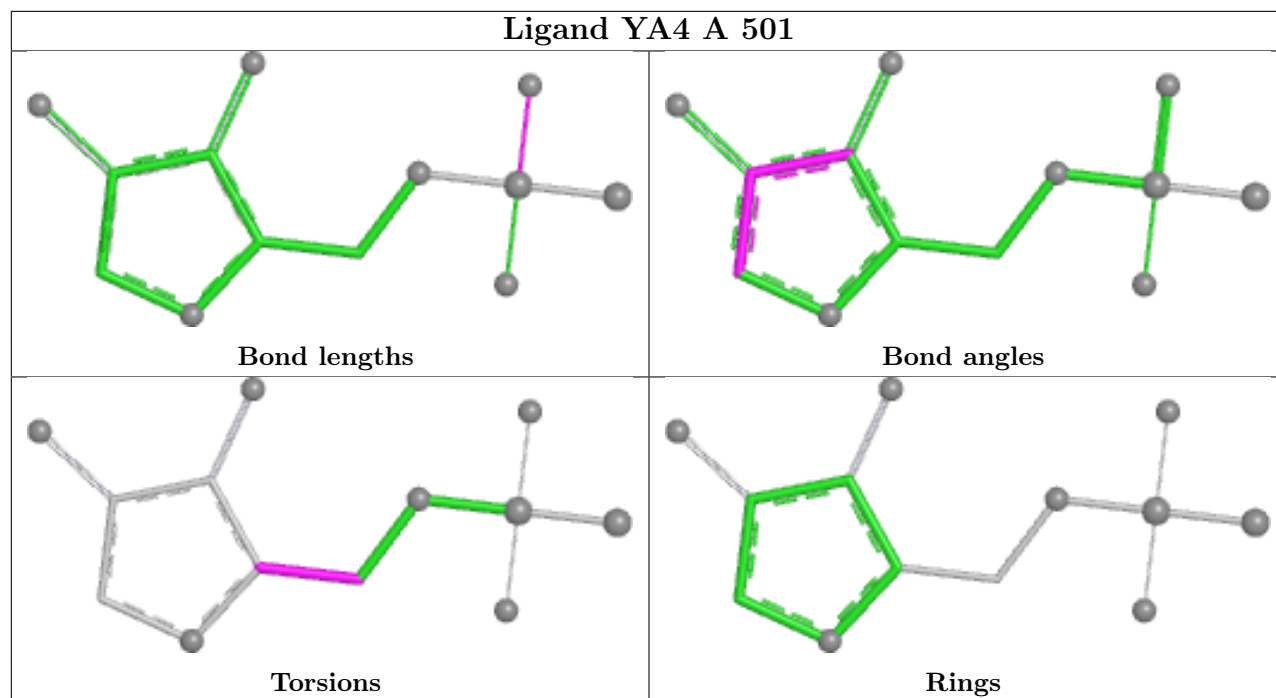












5.7 Other polymers [i](#)

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	412/413 (99%)	0.29	12 (2%) 53 60	16, 27, 43, 52	0
1	B	413/413 (100%)	0.36	14 (3%) 48 53	17, 28, 43, 69	0
All	All	825/826 (99%)	0.33	26 (3%) 50 55	16, 28, 43, 69	0

All (26) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	34	VAL	5.2
1	B	33	ALA	3.6
1	A	35	GLY	3.5
1	B	394	THR	3.5
1	B	323	LEU	3.1
1	A	51	ILE	3.0
1	A	383	LYS	3.0
1	A	58	VAL	2.9
1	A	50	HIS	2.8
1	A	323	LEU	2.7
1	B	445	LEU	2.6
1	B	35	GLY	2.5
1	A	63	LYS	2.5
1	A	52	THR	2.4
1	B	393	ALA	2.4
1	B	50	HIS	2.4
1	B	430	MET	2.3
1	A	53	ASP	2.3
1	B	305	ASN	2.2
1	A	218	LEU	2.2
1	B	441	LEU	2.2
1	B	405	HIS	2.2
1	A	413	SER	2.1
1	B	304	GLY	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	395	LYS	2.1
1	B	395	LYS	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](#)

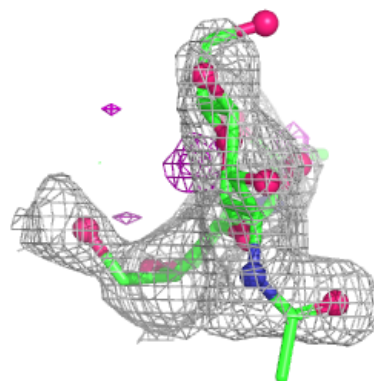
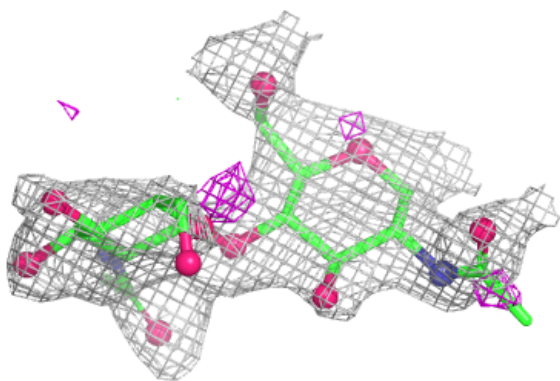
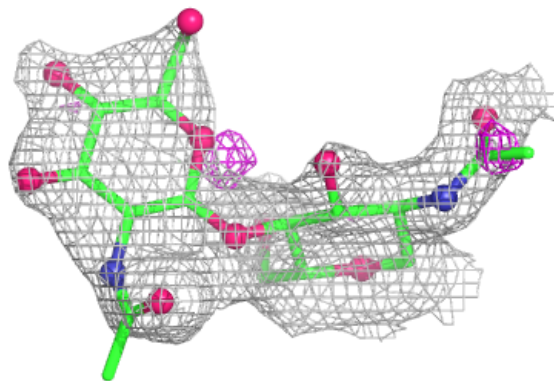
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q < 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	FUC	D	2	10/11	0.58	0.19	46,52,54,58	0
2	NAG	E	2	14/15	0.60	0.18	49,60,67,68	0
2	NAG	C	2	14/15	0.67	0.16	69,71,77,78	0
4	BMA	F	3	11/12	0.68	0.14	56,63,68,69	0
2	NAG	C	1	14/15	0.79	0.15	41,51,58,64	0
4	NAG	F	2	14/15	0.82	0.12	42,49,60,62	0
3	NAG	D	1	14/15	0.85	0.12	32,40,45,50	0
2	NAG	E	1	14/15	0.86	0.12	38,42,48,52	0
4	NAG	F	1	14/15	0.86	0.10	30,33,38,43	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.

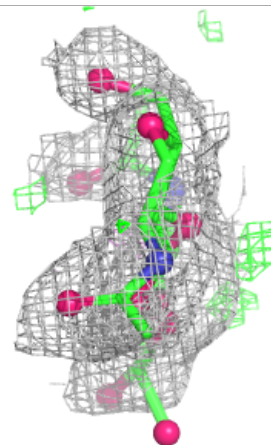
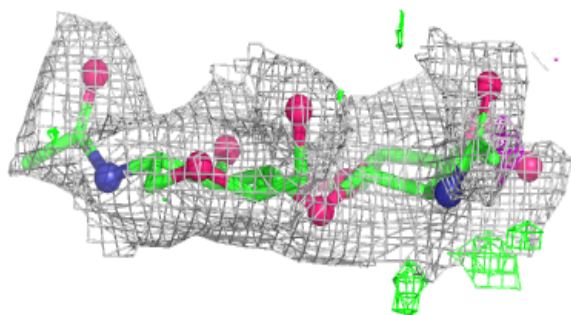
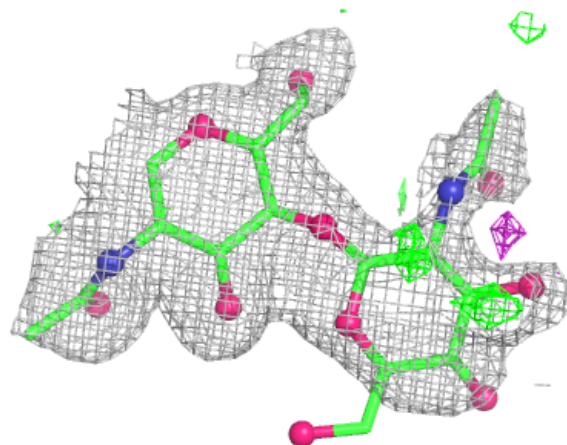
Electron density around Chain C:

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



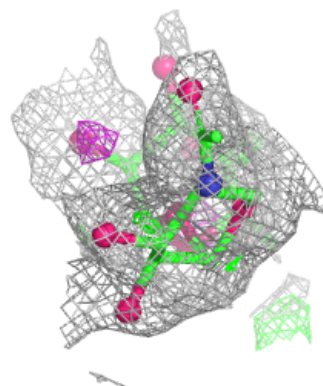
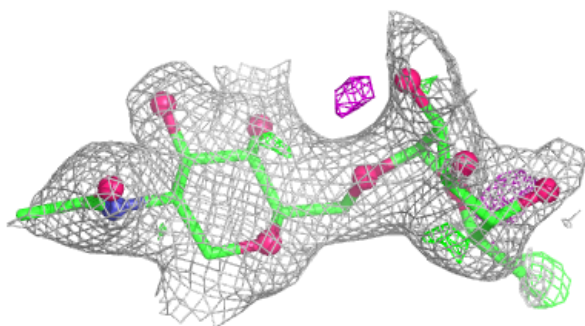
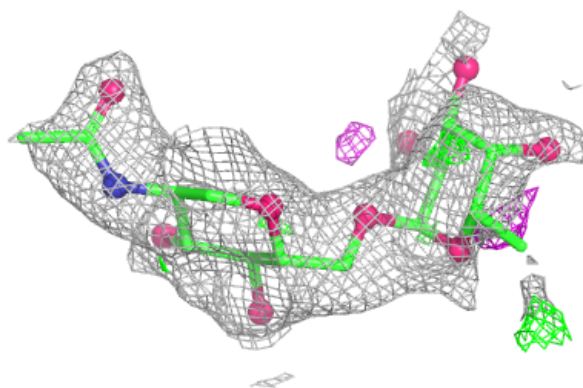
Electron density around Chain E:

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

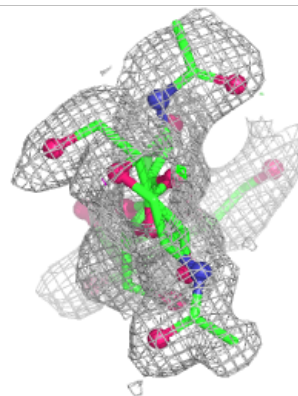
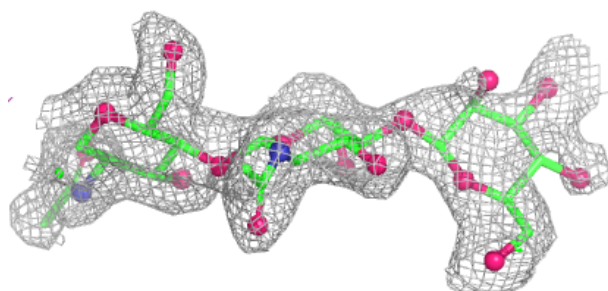
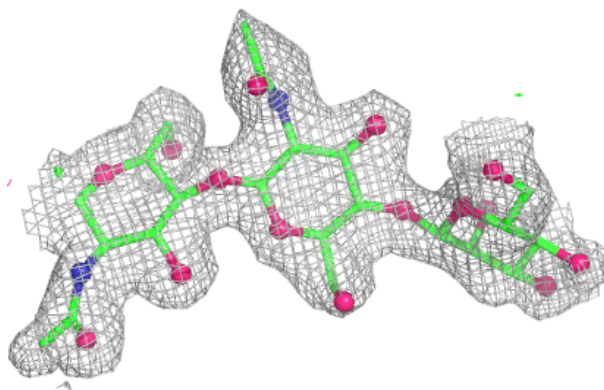


Electron density around Chain D:

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

**Electron density around Chain F:**

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



6.4 Ligands

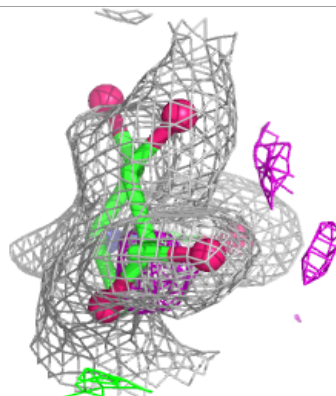
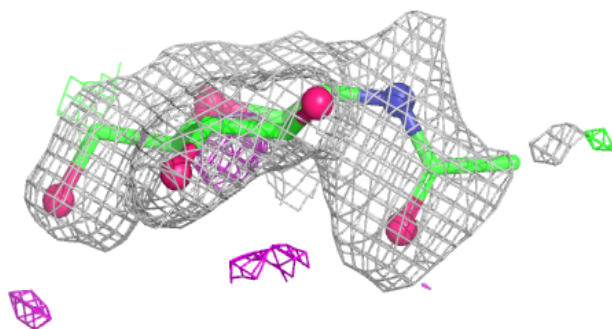
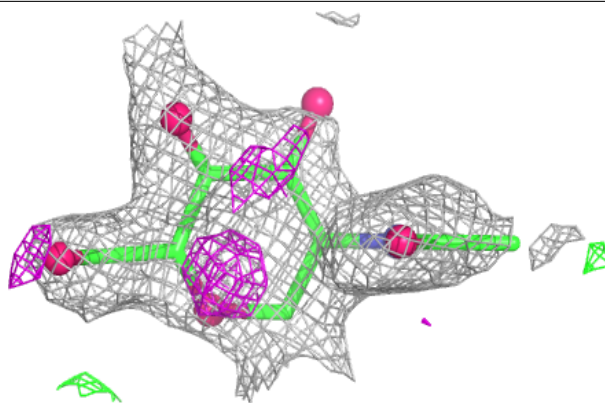
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
6	NAG	B	501	14/15	0.68	0.13	50,55,59,64	0
6	NAG	B	503	14/15	0.71	0.15	34,49,56,62	0
8	FUC	B	502	10/11	0.71	0.15	59,61,63,63	0
6	NAG	A	502	14/15	0.77	0.13	38,47,52,55	0
6	NAG	A	503	14/15	0.82	0.12	33,37,48,52	0
6	NAG	B	504	14/15	0.88	0.09	33,40,52,53	0
6	NAG	B	505	14/15	0.89	0.10	37,39,46,49	0
5	YA4	A	501	13/13	0.93	0.13	25,34,41,41	9
9	PO4	B	506	5/5	0.94	0.09	28,28,34,36	0
7	ZN	B	508	1/1	0.98	0.11	36,36,36,36	0
7	ZN	B	507	1/1	0.99	0.03	29,29,29,29	0
7	ZN	A	504	1/1	0.99	0.07	33,33,33,33	0
7	ZN	A	505	1/1	1.00	0.01	25,25,25,25	0

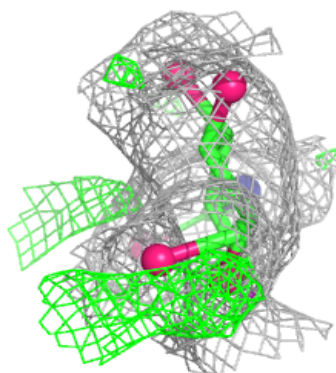
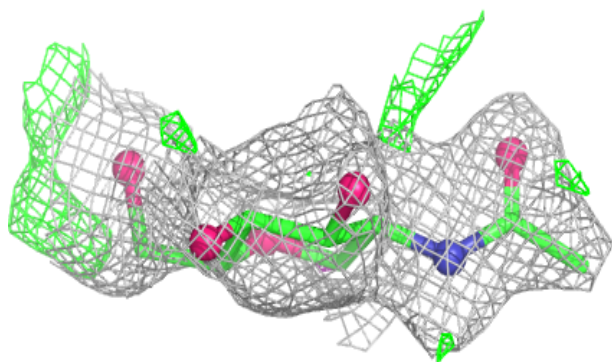
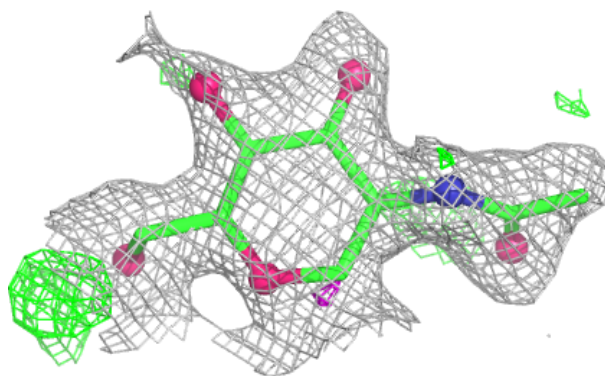
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around NAG B 501:

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

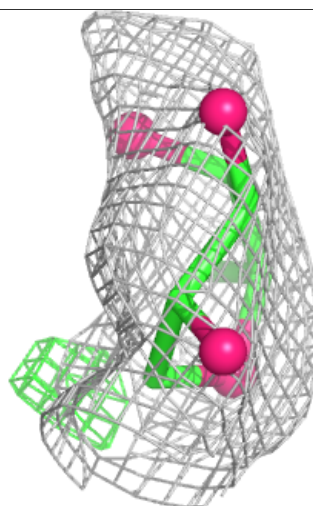
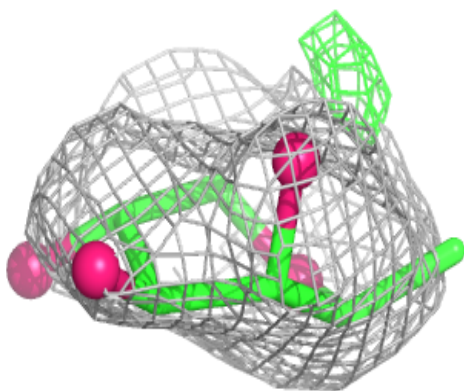
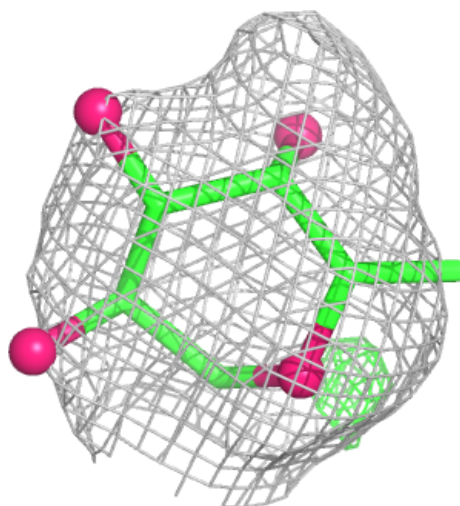
**Electron density around NAG B 503:**

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



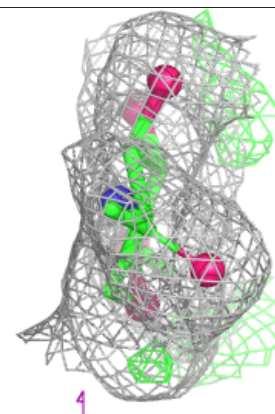
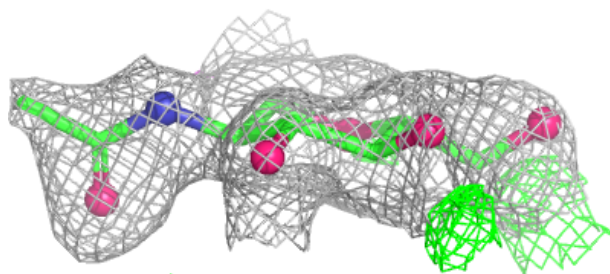
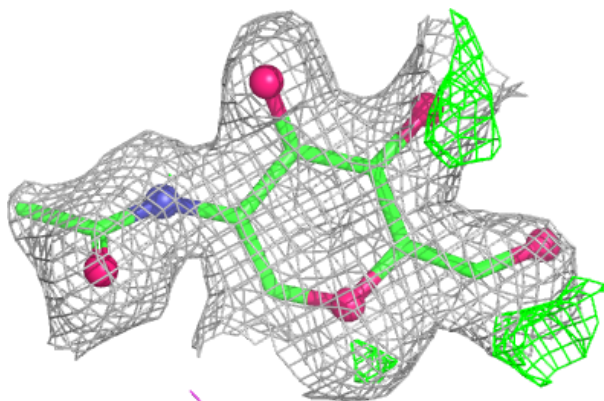
Electron density around FUC B 502:

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

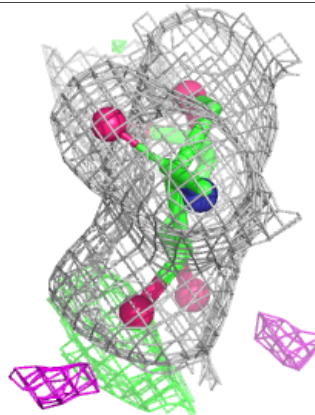
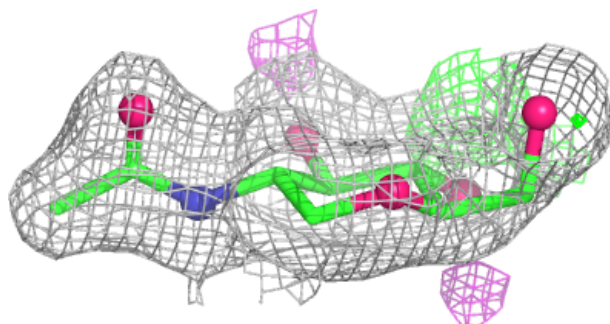
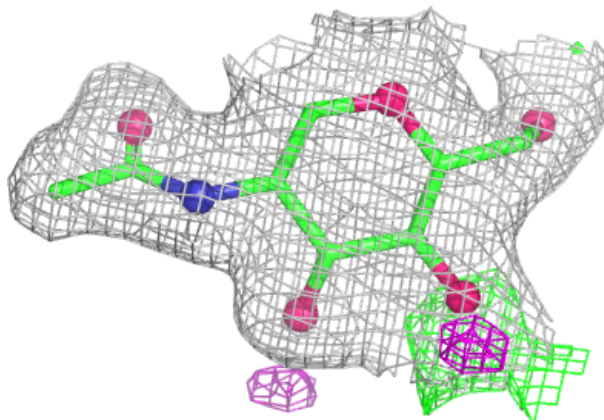


Electron density around NAG A 502:

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

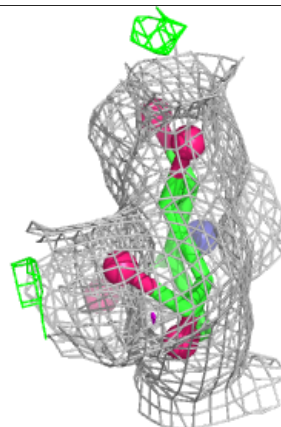
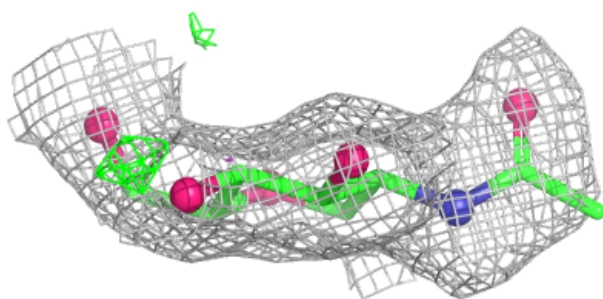
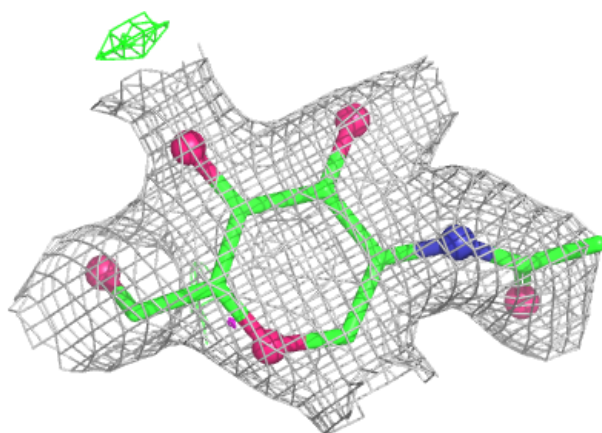
**Electron density around NAG A 503:**

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

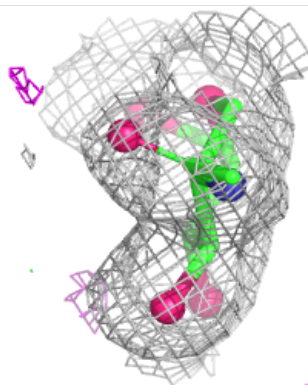
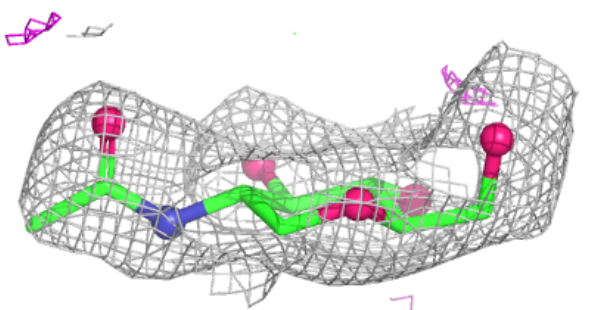
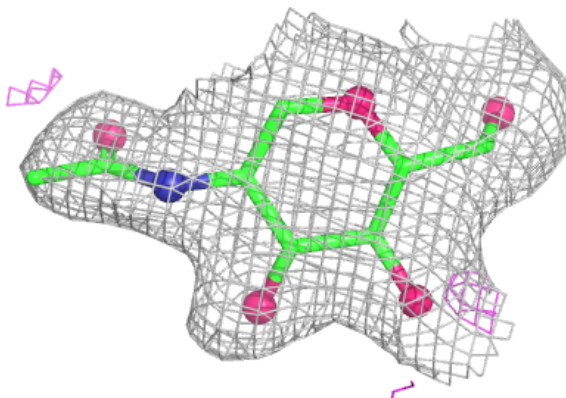


Electron density around NAG B 504:

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

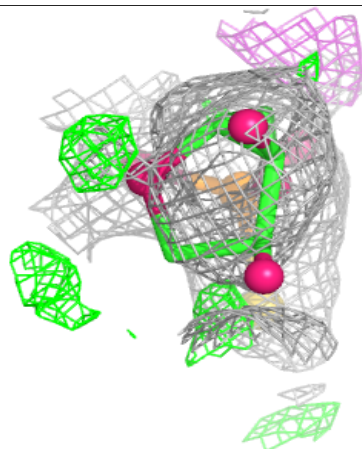
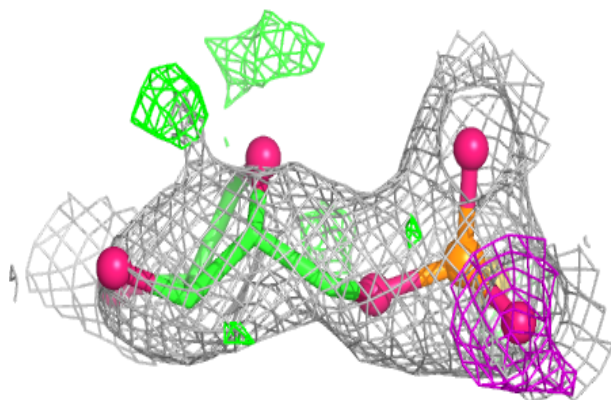
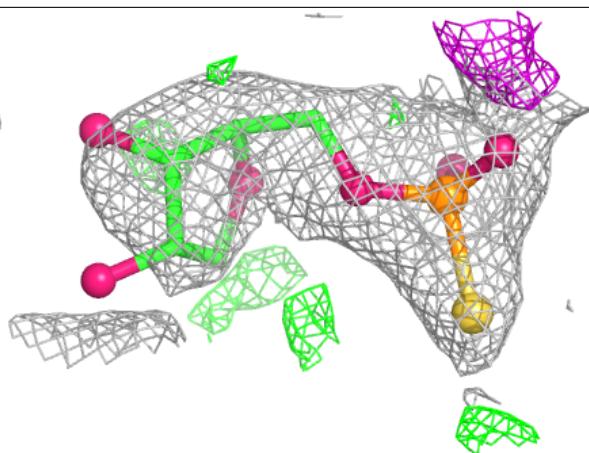
**Electron density around NAG B 505:**

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



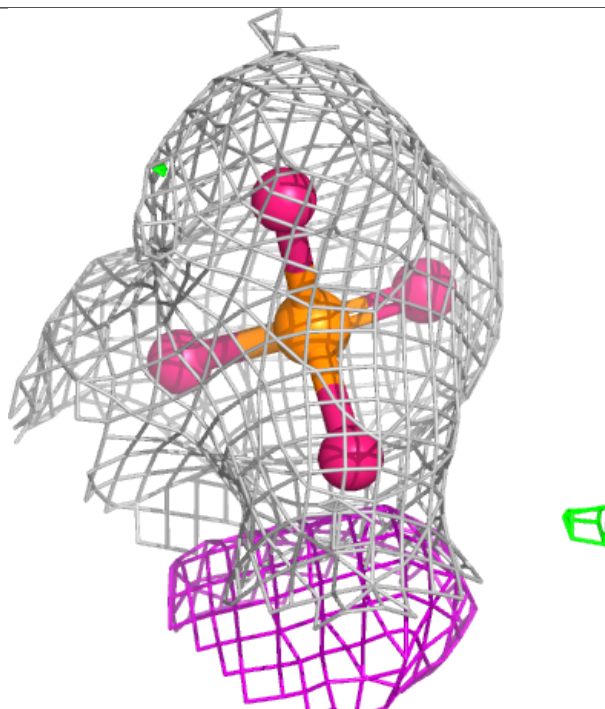
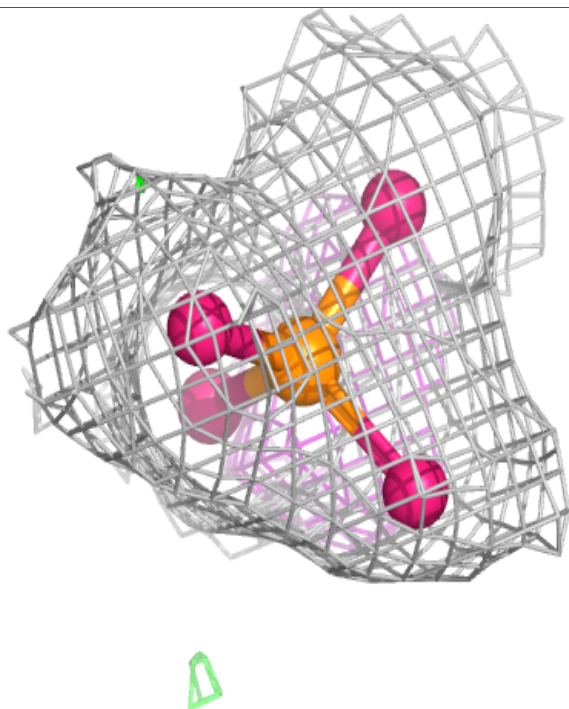
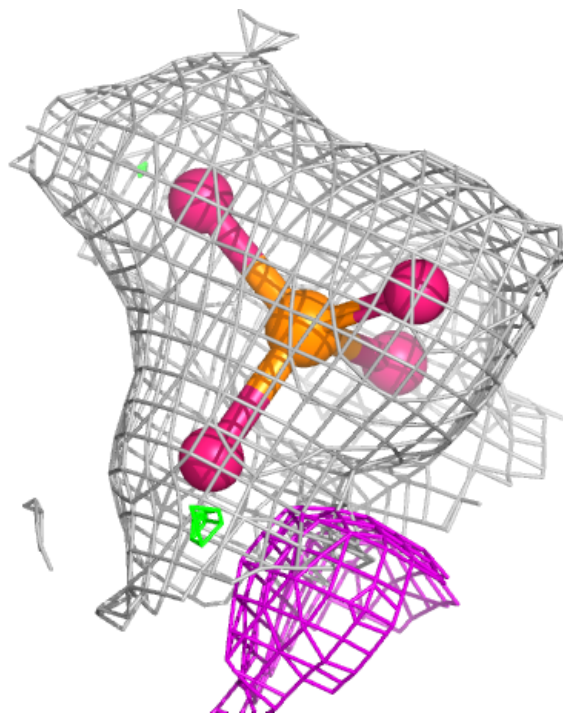
Electron density around YA4 A 501:

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



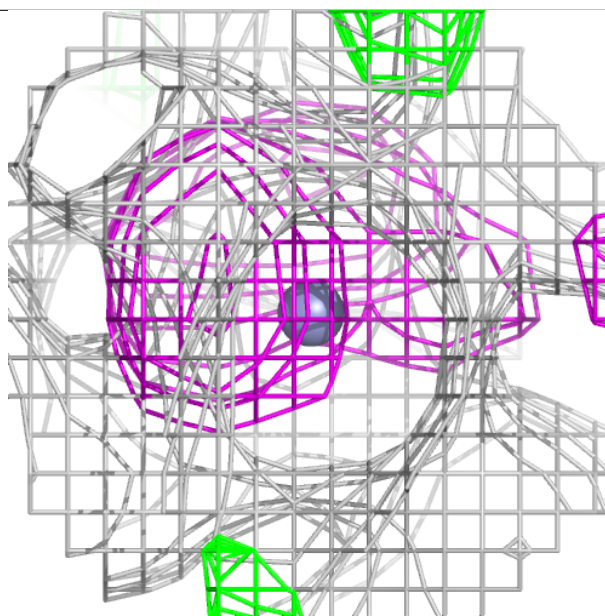
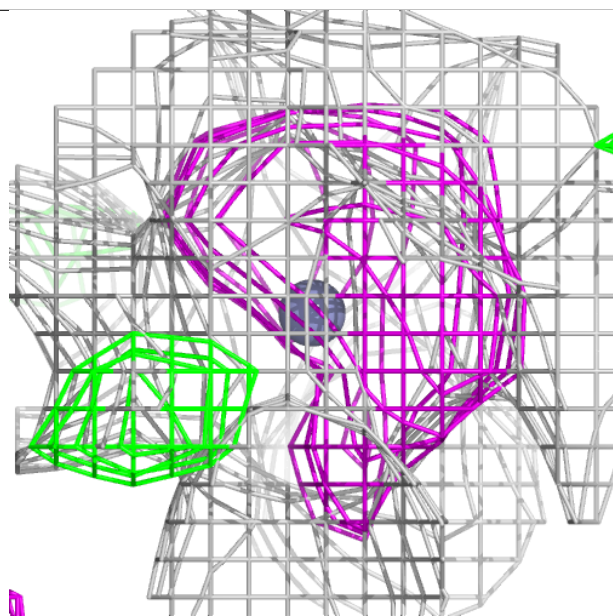
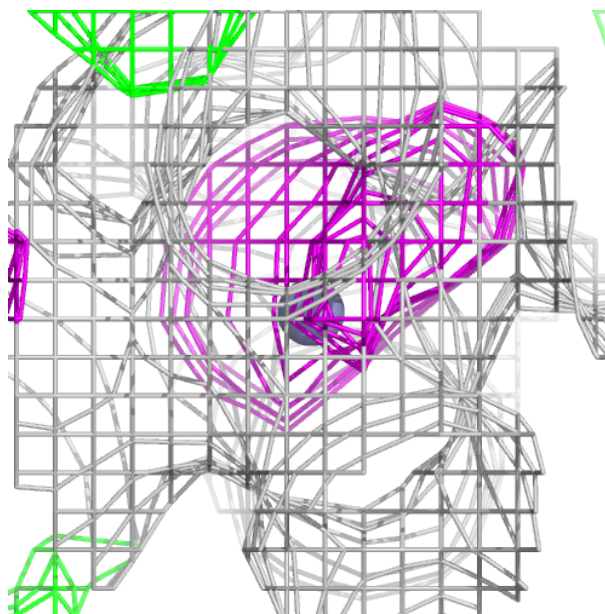
Electron density around PO4 B 506:

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



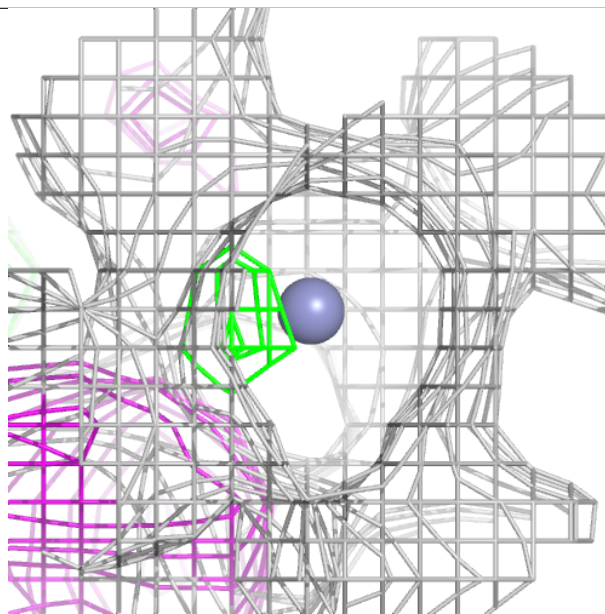
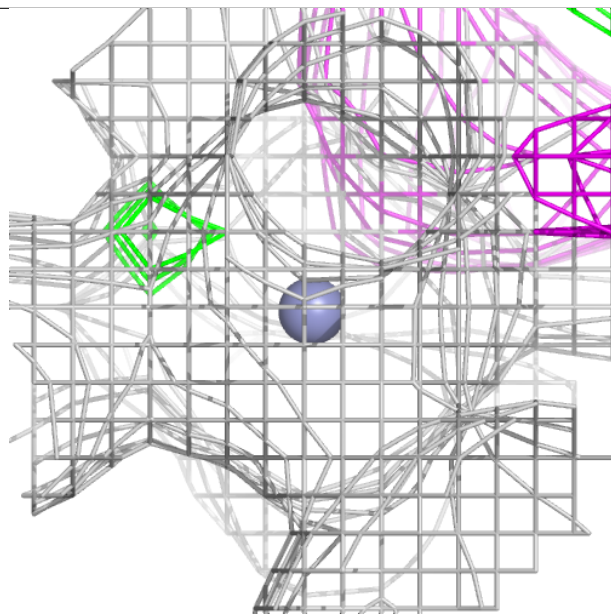
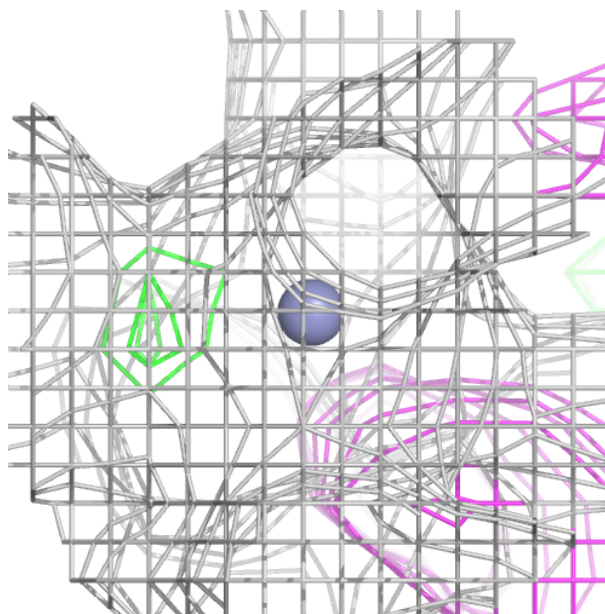
Electron density around ZN B 508:

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



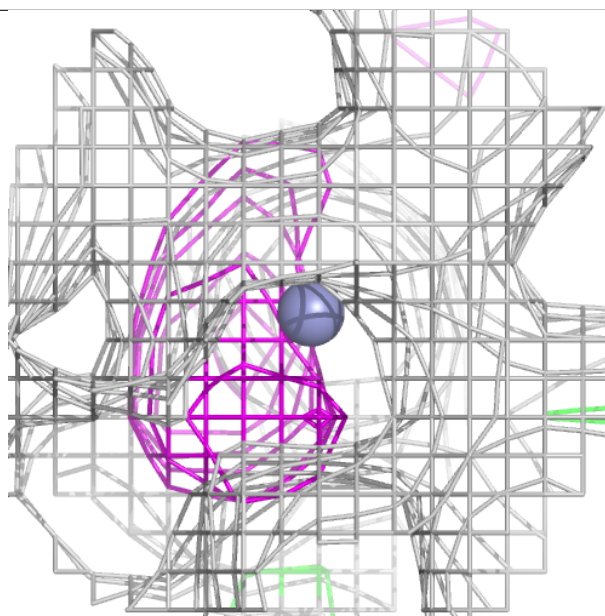
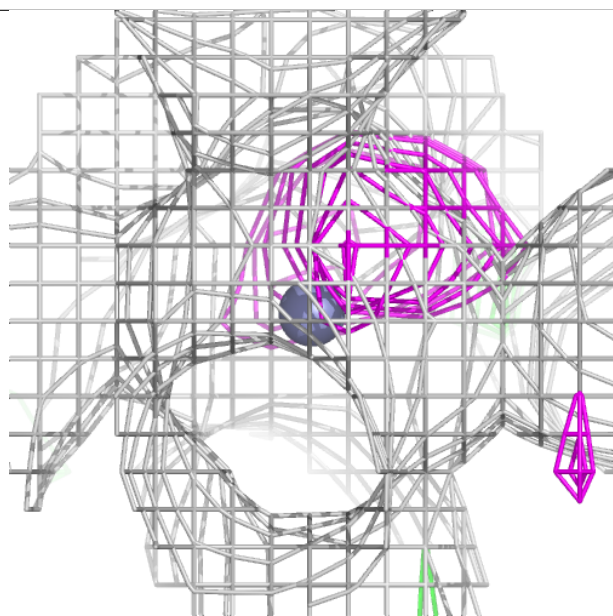
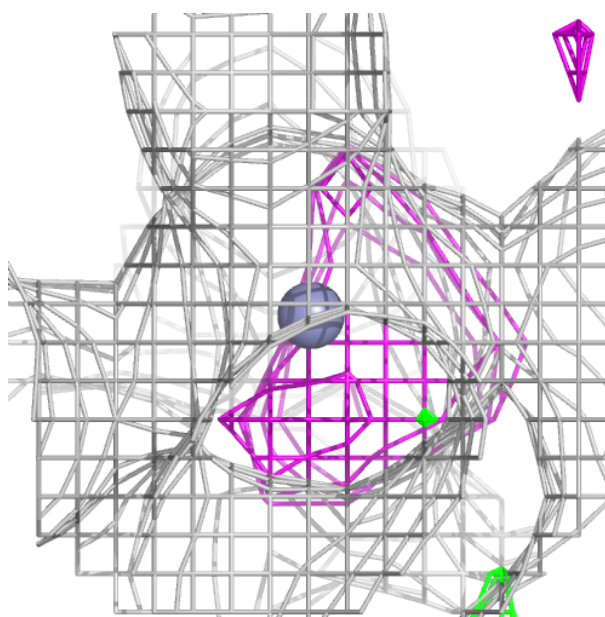
Electron density around ZN B 507:

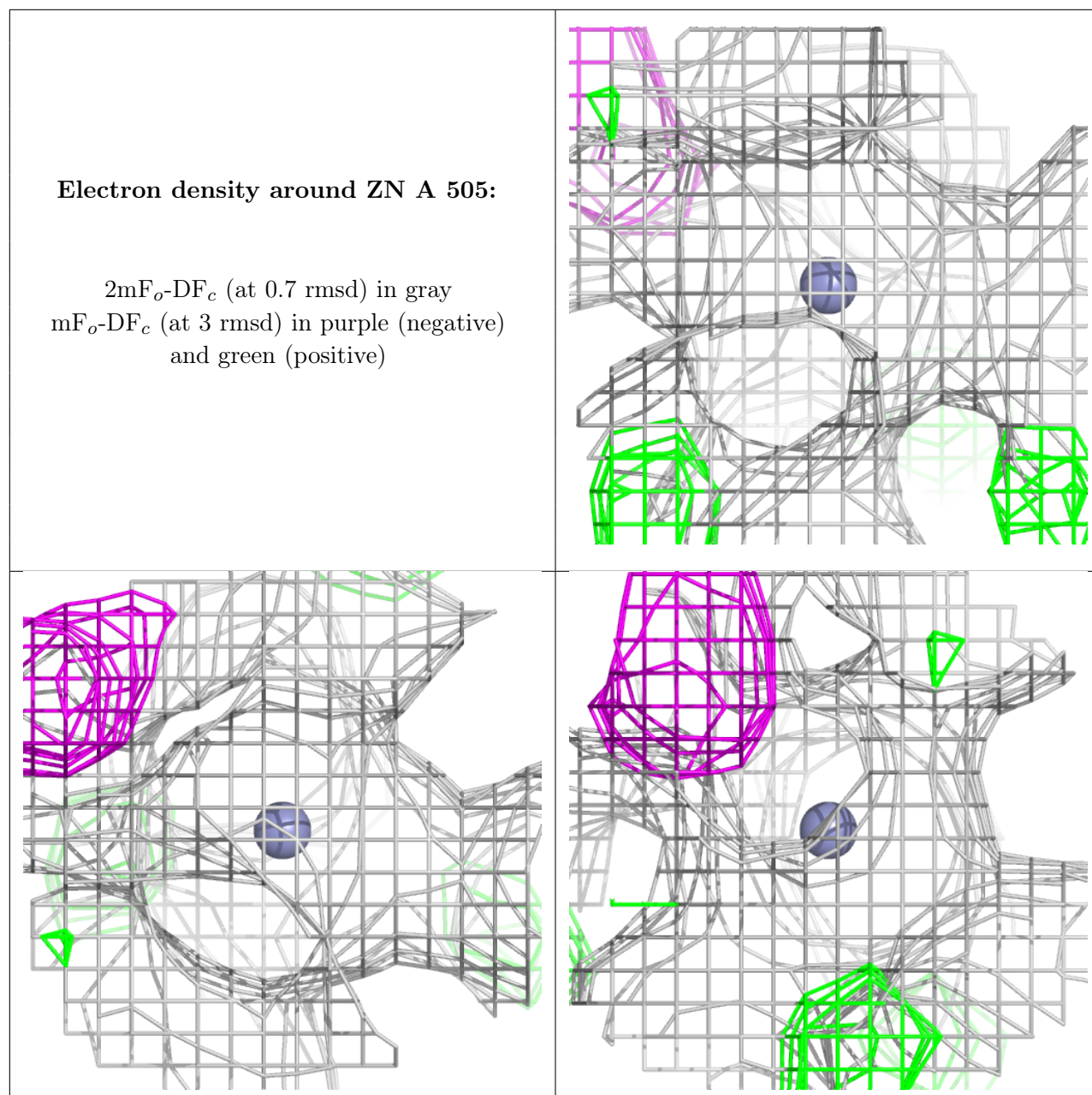
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around ZN A 504:

$2mF_o-DF_c$ (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.