



wwPDB X-ray Structure Validation Summary Report ⓘ

Jul 14, 2026 – 02:13 PM EDT

PDB ID : 9Q3Y / pdb_00009q3y
Title : GluN1b-GluN2B ATD in complex with radiprodil
Authors : Regan, M.C.; Furukawa, H.
Deposited on : 2025-08-19
Resolution : 2.74 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ 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 : 9.0.015 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.50

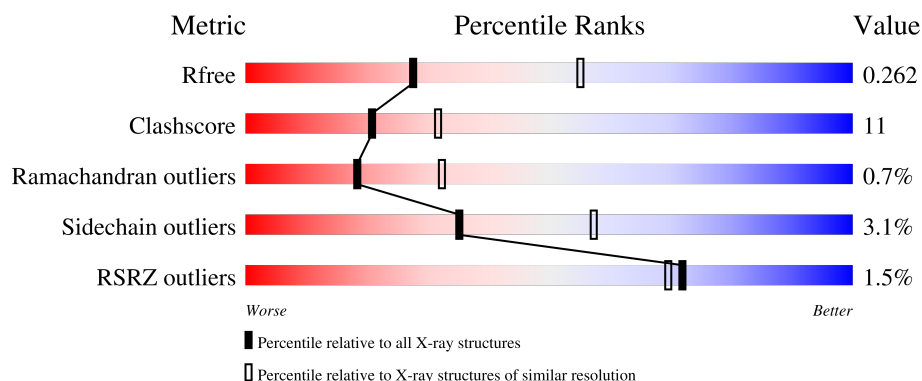
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.74 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	1819 (2.76-2.72)
Clashscore	190562	1866 (2.76-2.72)
Ramachandran outliers	187476	1830 (2.76-2.72)
Sidechain outliers	187428	1831 (2.76-2.72)
RSRZ outliers	180081	1819 (2.76-2.72)

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	359	2% 80% 19% .
2	B	363	% 77% 18% ..
2	D	363	% 78% 20% .
3	C	358	2% 80% 18% .
4	E	5	100%

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 11408 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 Glutamate receptor ionotropic, NMDA 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	359	Total	C	N	O	S	0	0	0
			2765	1763	482	509	11			

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	61	GLN	ASN	conflict	UNP A0A1L8F5J9
A	?	-	PRO	deletion	UNP A0A1L8F5J9
A	?	-	THR	deletion	UNP A0A1L8F5J9
A	?	-	ASP	deletion	UNP A0A1L8F5J9
A	?	-	HIS	deletion	UNP A0A1L8F5J9
A	186	GLY	GLU	conflict	UNP A0A1L8F5J9
A	209	GLY	LYS	conflict	UNP A0A1L8F5J9
A	?	-	GLU	deletion	UNP A0A1L8F5J9
A	210	PRO	SER	conflict	UNP A0A1L8F5J9
A	371	GLN	ASN	conflict	UNP A0A1L8F5J9

- Molecule 2 is a protein called Glutamate receptor ionotropic, NMDA 2B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	359	Total	C	N	O	S	0	1	0
			2805	1801	451	537	16			
2	D	363	Total	C	N	O	S	0	0	0
			2754	1771	442	525	16			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	348	ASP	ASN	conflict	UNP Q00960
D	348	ASP	ASN	conflict	UNP Q00960

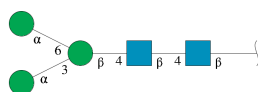
- Molecule 3 is a protein called Glutamate receptor ionotropic, NMDA 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	358	Total	C	N	O	S	0	0	0
			2739	1743	476	509	11			

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	61	GLN	ASN	conflict	UNP A0A1L8F5J9
C	?	-	PRO	deletion	UNP A0A1L8F5J9
C	?	-	THR	deletion	UNP A0A1L8F5J9
C	?	-	ASP	deletion	UNP A0A1L8F5J9
C	209	GLY	GLU	conflict	UNP A0A1L8F5J9
C	?	-	LYS	deletion	UNP A0A1L8F5J9
C	?	-	GLU	deletion	UNP A0A1L8F5J9
C	210	PRO	SER	conflict	UNP A0A1L8F5J9
C	371	GLN	ASN	conflict	UNP A0A1L8F5J9

- Molecule 4 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



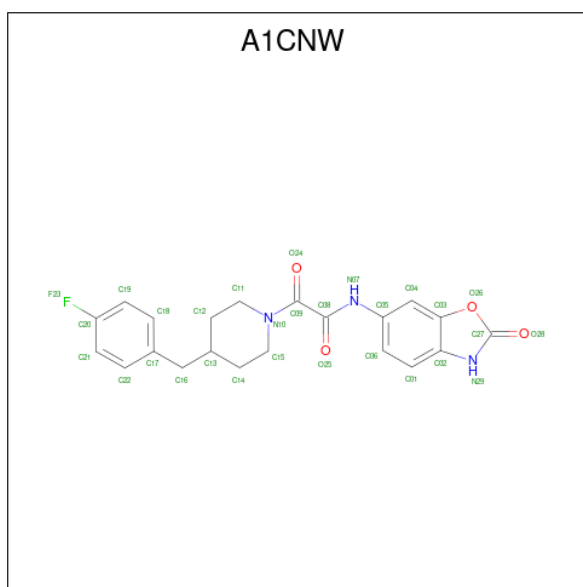
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	E	5	Total	C	N	O	0	0	0
			61	34	2	25			

- Molecule 5 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
5	A	1	Total	C	N	O	0	0
			14	8	1	5		
5	B	1	Total	C	N	O	0	0
			14	8	1	5		
5	B	1	Total	C	N	O	0	0
			14	8	1	5		
5	C	1	Total	C	N	O	0	0
			14	8	1	5		
5	C	1	Total	C	N	O	0	0
			14	8	1	5		
5	D	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 6 is radiprodil (CCD ID: A1CNW) (formula: $C_{21}H_{20}FN_3O_4$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	A	1	Total 29	C 21	F 1	N 3	O 4	0	0
6	D	1	Total 29	C 21	F 1	N 3	O 4	0	0

- Molecule 7 is SODIUM ION (CCD ID: NA) (formula: Na) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total Na 1 1	0	0
7	C	1	Total Na 1 1	0	0

- Molecule 8 is CHLORIDE ION (CCD ID: CL) (formula: Cl) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	2	Total Cl 2 2	0	0
8	B	3	Total Cl 3 3	0	0
8	C	3	Total Cl 3 3	0	0
8	D	1	Total Cl 1 1	0	0

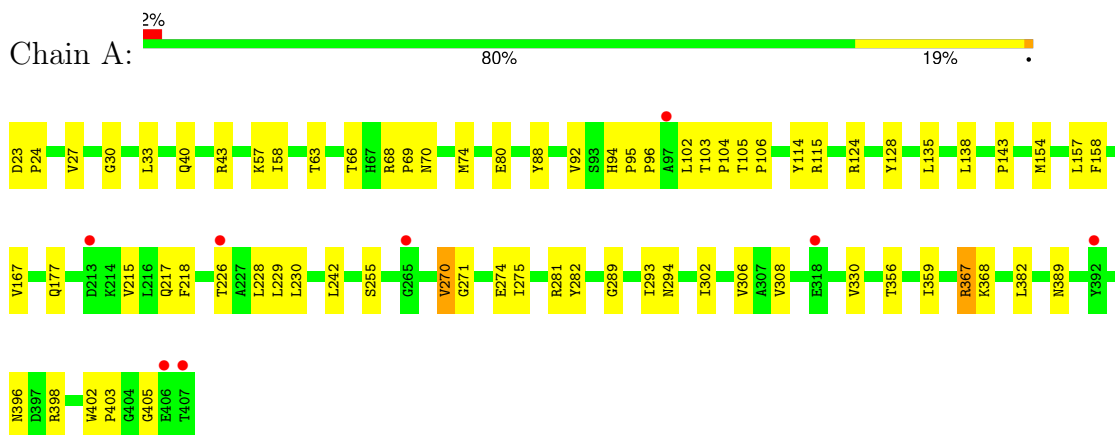
- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	52	Total 52	O 52	0	0
9	B	32	Total 32	O 32	0	0
9	C	26	Total 26	O 26	0	0
9	D	21	Total 21	O 21	0	0

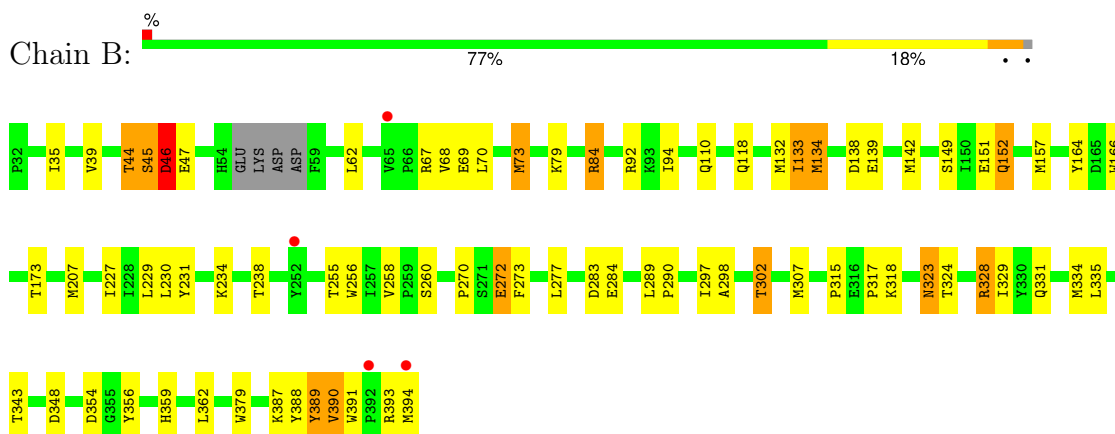
3 Residue-property plots

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.

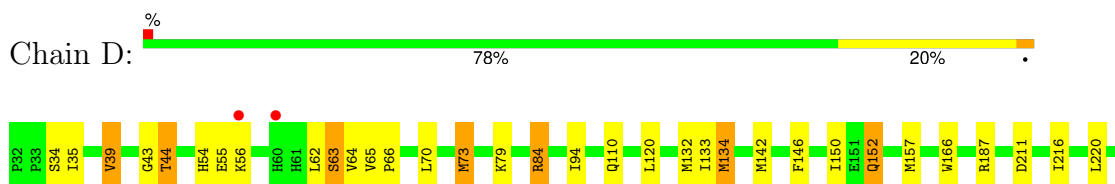
- Molecule 1: Glutamate receptor ionotropic, NMDA 1

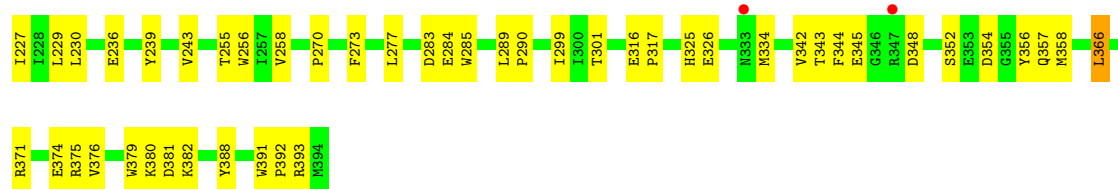


- Molecule 2: Glutamate receptor ionotropic, NMDA 2B

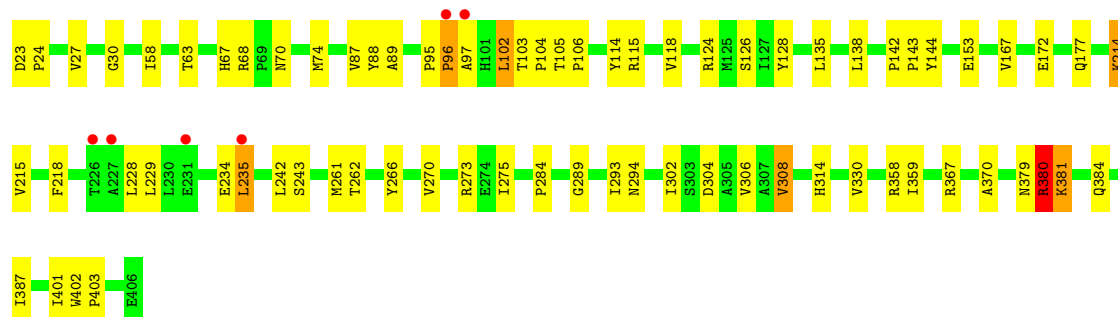
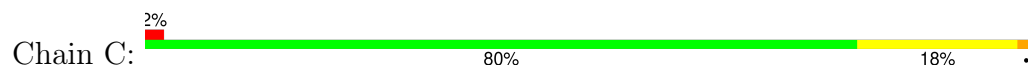


- Molecule 2: Glutamate receptor ionotropic, NMDA 2B





• Molecule 3: Glutamate receptor ionotropic, NMDA 1



• Molecule 4: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-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	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	267.95Å 60.67Å 144.65Å 90.00° 116.23° 90.00°	Depositor
Resolution (Å)	25.00 – 2.74 25.00 – 2.74	Depositor EDS
% Data completeness (in resolution range)	98.4 (25.00-2.74) 98.6 (25.00-2.74)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.87 (at 2.76Å)	Xtriage
Refinement program	REFMAC 5.8.0135	Depositor
R, R_{free}	0.187 , 0.223 0.234 , 0.262	Depositor DCC
R_{free} test set	2653 reflections (4.78%)	wwPDB-VP
Wilson B-factor (Å ²)	68.5	Xtriage
Anisotropy	0.083	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 34.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	11408	wwPDB-VP
Average B, all atoms (Å ²)	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.04% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: MAN, BMA, CL, NAG, NA, A1CNW

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	0.34	0/2822	0.68	0/3834
2	B	0.33	0/2873	0.69	1/3914 (0.0%)
2	D	0.46	0/2818	0.72	0/3850
3	C	0.34	0/2795	0.66	0/3801
All	All	0.37	0/11308	0.69	1/15399 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
3	C	0	1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
2	B	389	TYR	N-CA-C	-10.14	101.47	114.04

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	C	380	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	2765	0	2731	53	0
2	B	2805	0	2684	66	0
2	D	2754	0	2589	69	0
3	C	2739	0	2699	56	0
4	E	61	0	52	0	0
5	A	14	0	13	0	0
5	B	28	0	26	3	0
5	C	28	0	26	0	0
5	D	14	0	13	0	0
6	A	29	0	0	1	0
6	D	29	0	0	2	0
7	A	1	0	0	0	0
7	C	1	0	0	0	0
8	A	2	0	0	1	0
8	B	3	0	0	1	0
8	C	3	0	0	0	0
8	D	1	0	0	1	0
9	A	52	0	0	1	0
9	B	32	0	0	2	0
9	C	26	0	0	0	0
9	D	21	0	0	2	0
All	All	11408	0	10833	245	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 11.

The worst 5 of 245 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)
3:C:229:LEU:HB3	3:C:261:MET:HE1	1.36	1.07
2:B:298:ALA:O	2:B:302:THR:HG23	1.58	1.02
2:D:133:ILE:HD12	2:D:150:ILE:HG12	1.54	0.89
2:B:118:GLN:O	2:B:324:THR:HG21	1.74	0.88
1:A:270:VAL:HG13	1:A:274:GLU:HB2	1.66	0.77

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	353/359 (98%)	337 (96%)	14 (4%)	2 (1%)	21	36
2	B	356/363 (98%)	334 (94%)	19 (5%)	3 (1%)	16	29
2	D	361/363 (99%)	338 (94%)	19 (5%)	4 (1%)	11	20
3	C	352/358 (98%)	335 (95%)	16 (4%)	1 (0%)	36	54
All	All	1422/1443 (98%)	1344 (94%)	68 (5%)	10 (1%)	18	32

5 of 10 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	44	THR
2	B	45	SER
2	D	55	GLU
2	D	63	SER
2	D	284	GLU

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	289/305 (95%)	286 (99%)	3 (1%)	68	80
2	B	302/326 (93%)	288 (95%)	14 (5%)	24	43
2	D	286/326 (88%)	277 (97%)	9 (3%)	35	57

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	C	289/305 (95%)	278 (96%)	11 (4%)	29	51
All	All	1166/1262 (92%)	1129 (97%)	37 (3%)	35	56

5 of 37 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	D	39	VAL
2	D	374	GLU
2	D	73	MET
2	D	152	GLN
2	B	323	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 26 such sidechains are listed below:

Mol	Chain	Res	Type
3	C	67	HIS
3	C	321	ASN
2	D	159	ASN
3	C	291	GLN
3	C	334	ASN

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 ⓘ

5 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	NAG	E	1	4,1	14,14,15	0.33	0	17,19,21	0.90	0
4	NAG	E	2	4	14,14,15	0.31	0	17,19,21	0.81	0
4	BMA	E	3	4	11,11,12	0.23	0	15,15,17	0.78	0
4	MAN	E	4	4	11,11,12	0.33	0	15,15,17	0.68	0
4	MAN	E	5	4	11,11,12	0.25	0	15,15,17	0.49	0

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	NAG	E	1	4,1	-	0/6/23/26	0/1/1/1
4	NAG	E	2	4	-	0/6/23/26	0/1/1/1
4	BMA	E	3	4	-	2/2/19/22	0/1/1/1
4	MAN	E	4	4	-	0/2/19/22	0/1/1/1
4	MAN	E	5	4	-	0/2/19/22	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

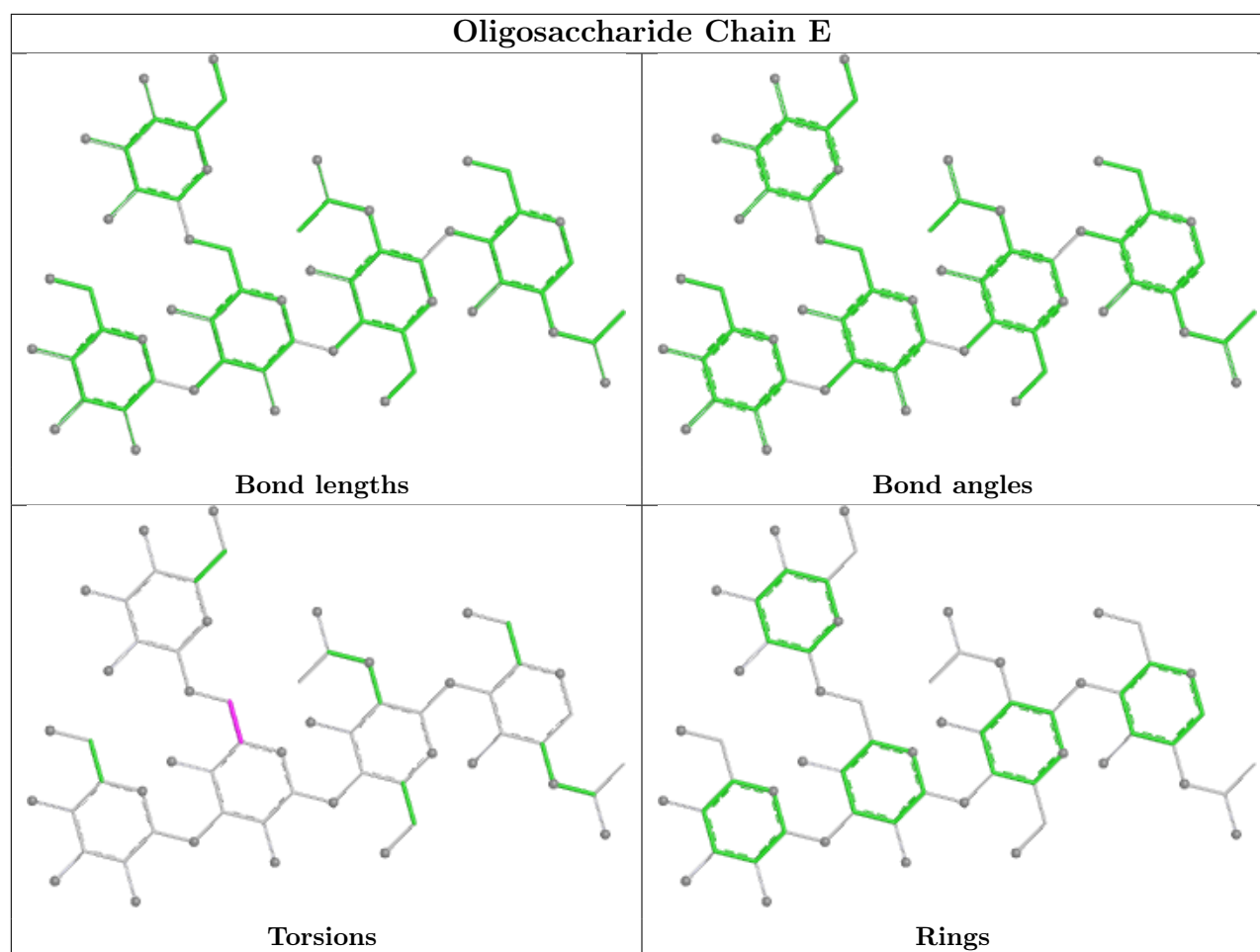
All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	E	3	BMA	O5-C5-C6-O6
4	E	3	BMA	C4-C5-C6-O6

There are no ring outliers.

No monomer is involved in short contacts.

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



5.6 Ligand geometry [i](#)

Of 19 ligands modelled in this entry, 11 are monoatomic - leaving 8 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	$\# Z > 2$
5	NAG	A	501	1	14,14,15	0.29	0	17,19,21	0.66	0
5	NAG	C	502	3	14,14,15	0.31	0	17,19,21	0.50	0
5	NAG	B	502	2	14,14,15	0.31	0	17,19,21	0.85	1 (5%)
5	NAG	B	501	2	14,14,15	0.30	0	17,19,21	0.69	0
5	NAG	D	401	2	14,14,15	0.33	0	17,19,21	0.69	0
6	A1CNW	A	502	-	32,32,32	2.48	8 (25%)	44,45,45	1.83	9 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	A1CNW	D	402	-	32,32,32	2.52	7 (21%)	44,45,45	1.80	9 (20%)
5	NAG	C	501	3	14,14,15	0.38	0	17,19,21	0.71	1 (5%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	A	501	1	-	0/6/23/26	0/1/1/1
5	NAG	C	502	3	-	2/6/23/26	0/1/1/1
5	NAG	B	502	2	-	3/6/23/26	0/1/1/1
5	NAG	B	501	2	-	2/6/23/26	0/1/1/1
5	NAG	D	401	2	-	4/6/23/26	0/1/1/1
6	A1CNW	A	502	-	-	3/16/26/26	0/4/4/4
6	A1CNW	D	402	-	-	3/16/26/26	0/4/4/4
5	NAG	C	501	3	-	2/6/23/26	0/1/1/1

The worst 5 of 15 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	D	402	A1CNW	C27-N29	8.75	1.42	1.35
6	A	502	A1CNW	C27-N29	8.69	1.42	1.35
6	D	402	A1CNW	C09-N10	6.23	1.45	1.34
6	A	502	A1CNW	C09-N10	5.92	1.45	1.34
6	D	402	A1CNW	C08-N07	4.46	1.44	1.35

The worst 5 of 20 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	D	402	A1CNW	C05-N07-C08	-4.99	118.60	127.45
6	A	502	A1CNW	C05-N07-C08	-4.82	118.89	127.45
6	D	402	A1CNW	C09-C08-N07	4.56	120.30	112.28
6	A	502	A1CNW	C09-C08-N07	4.14	119.56	112.28
6	A	502	A1CNW	C17-C16-C13	-4.06	107.01	114.45

There are no chirality outliers.

5 of 19 torsion outliers are listed below:

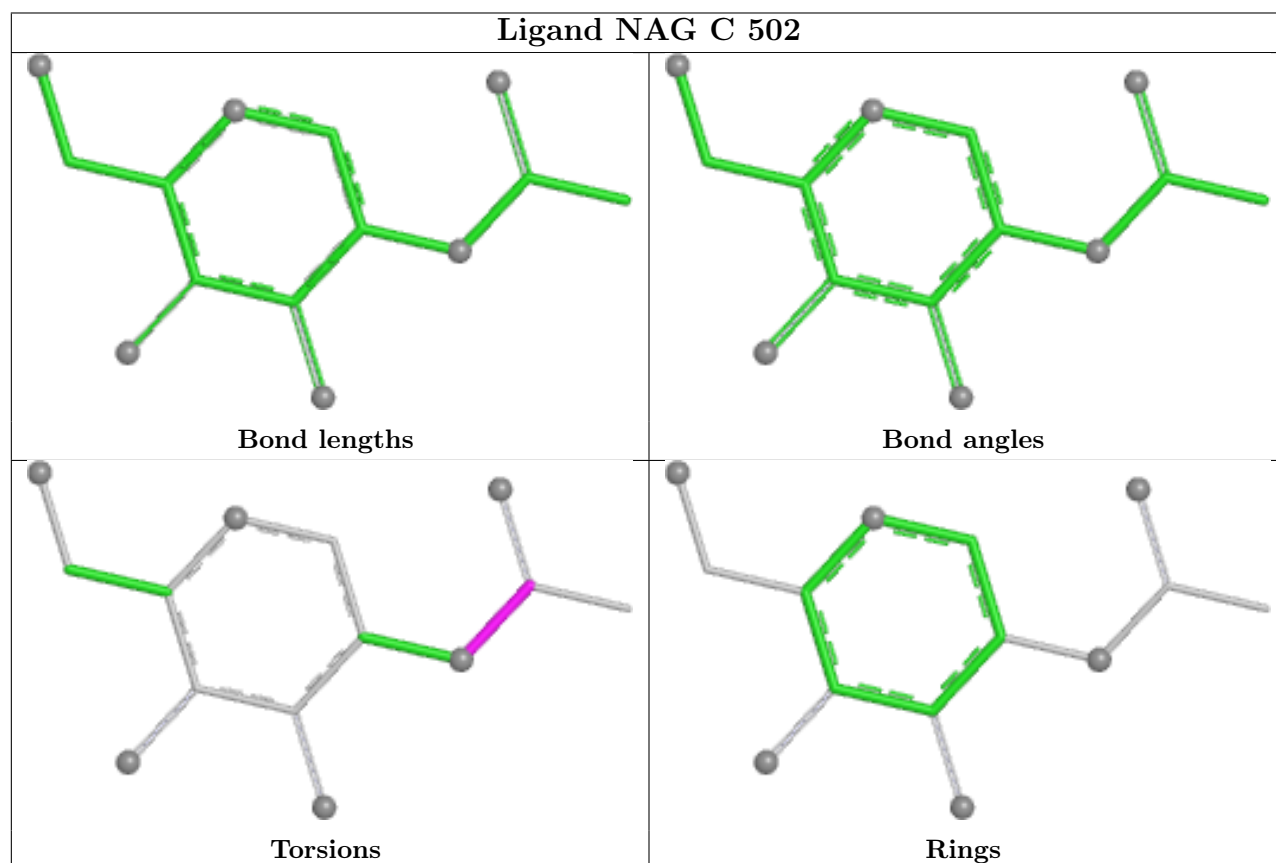
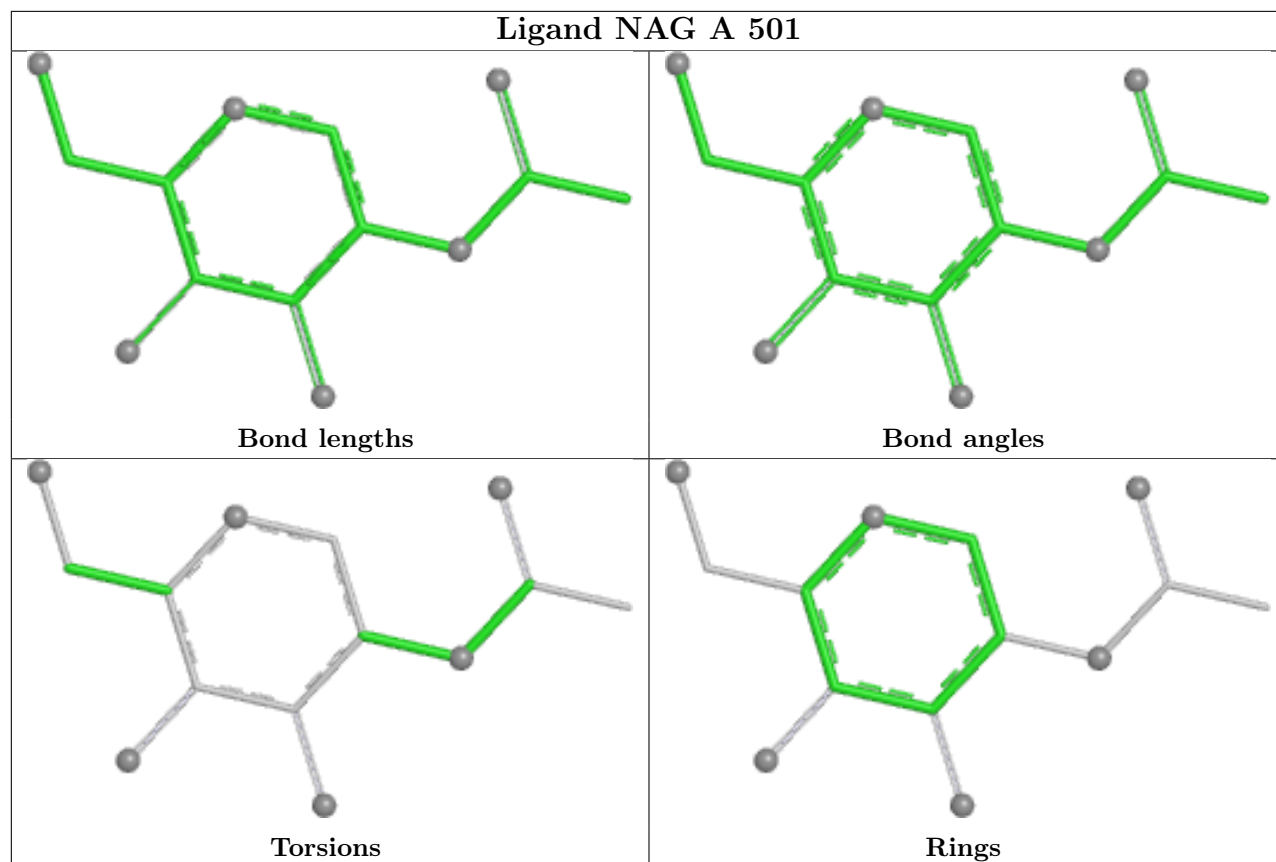
Mol	Chain	Res	Type	Atoms
5	D	401	NAG	C8-C7-N2-C2
5	D	401	NAG	O7-C7-N2-C2
5	B	501	NAG	C4-C5-C6-O6
5	D	401	NAG	O5-C5-C6-O6
5	B	502	NAG	C8-C7-N2-C2

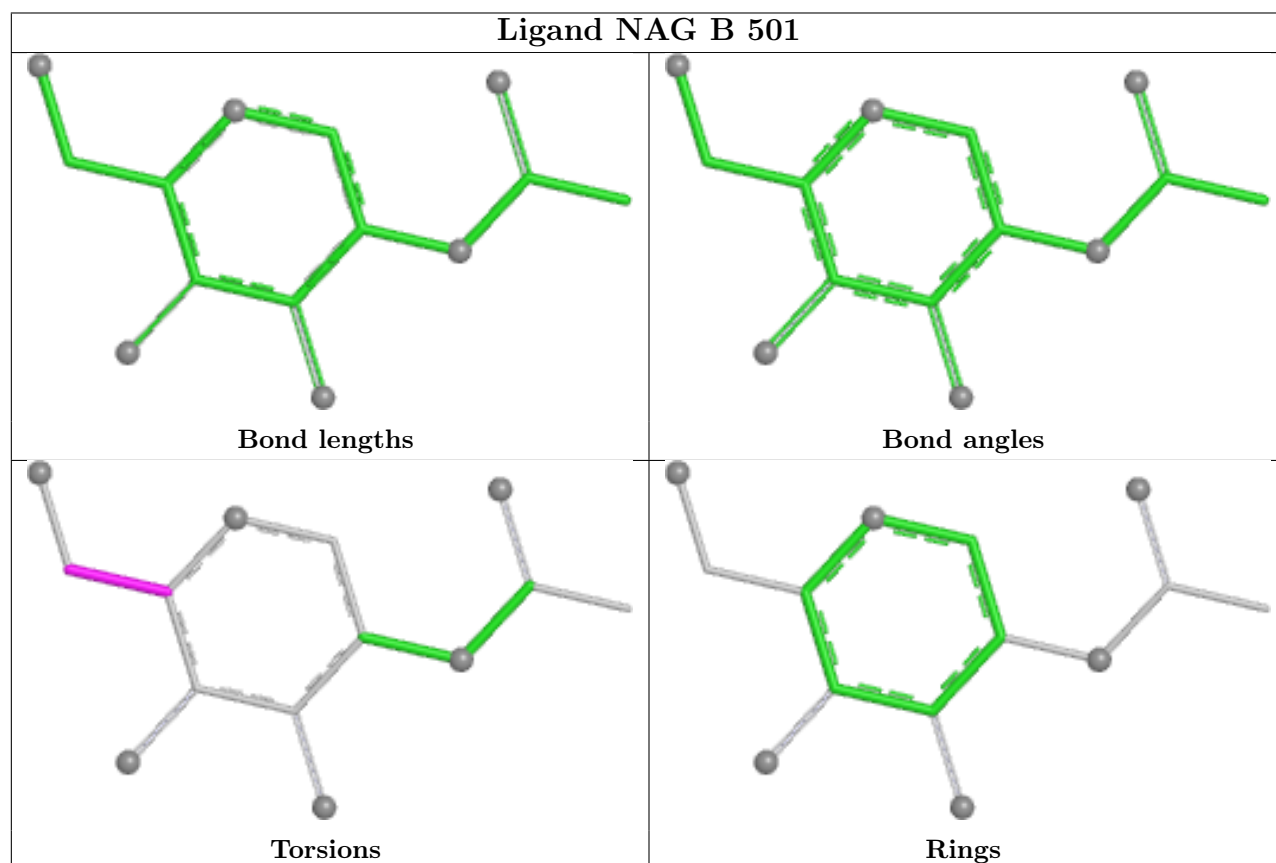
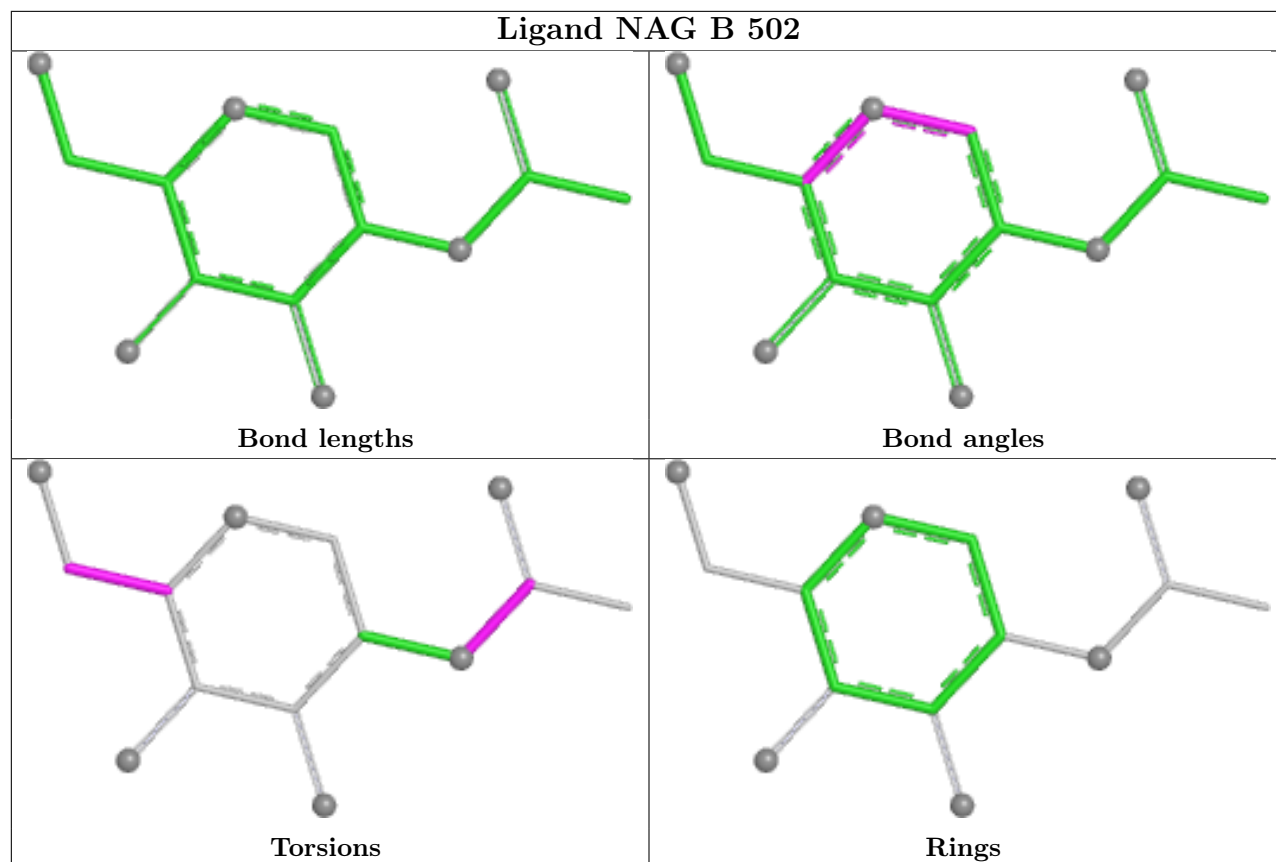
There are no ring outliers.

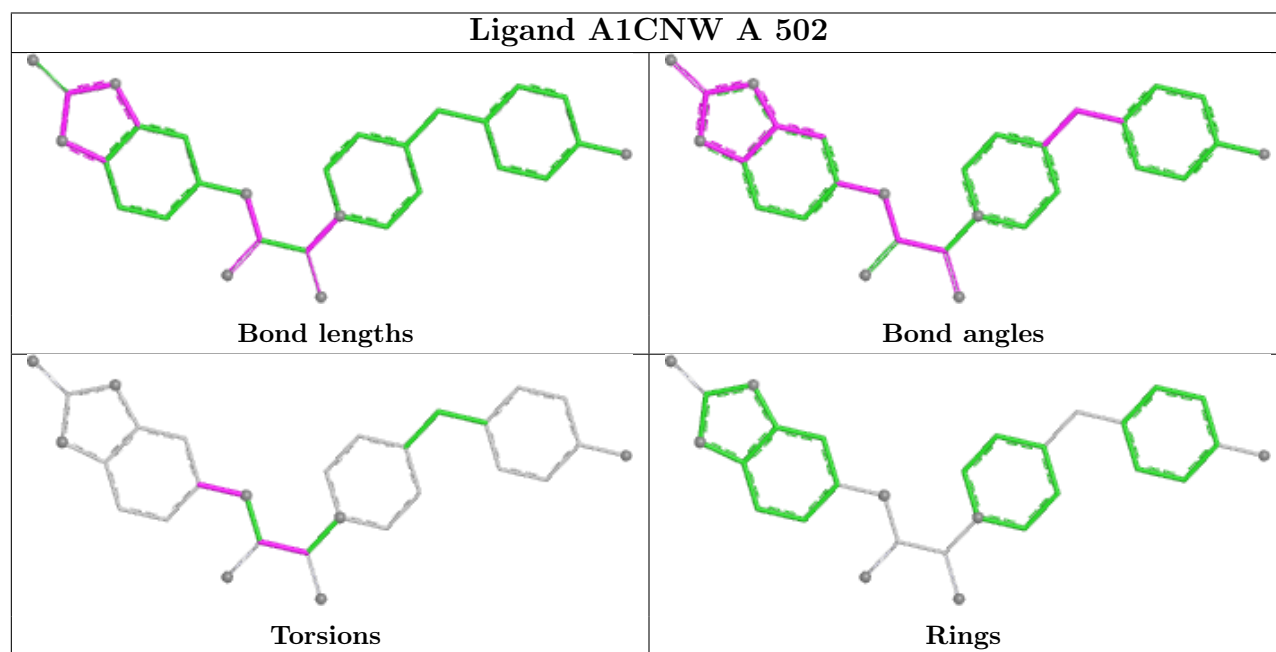
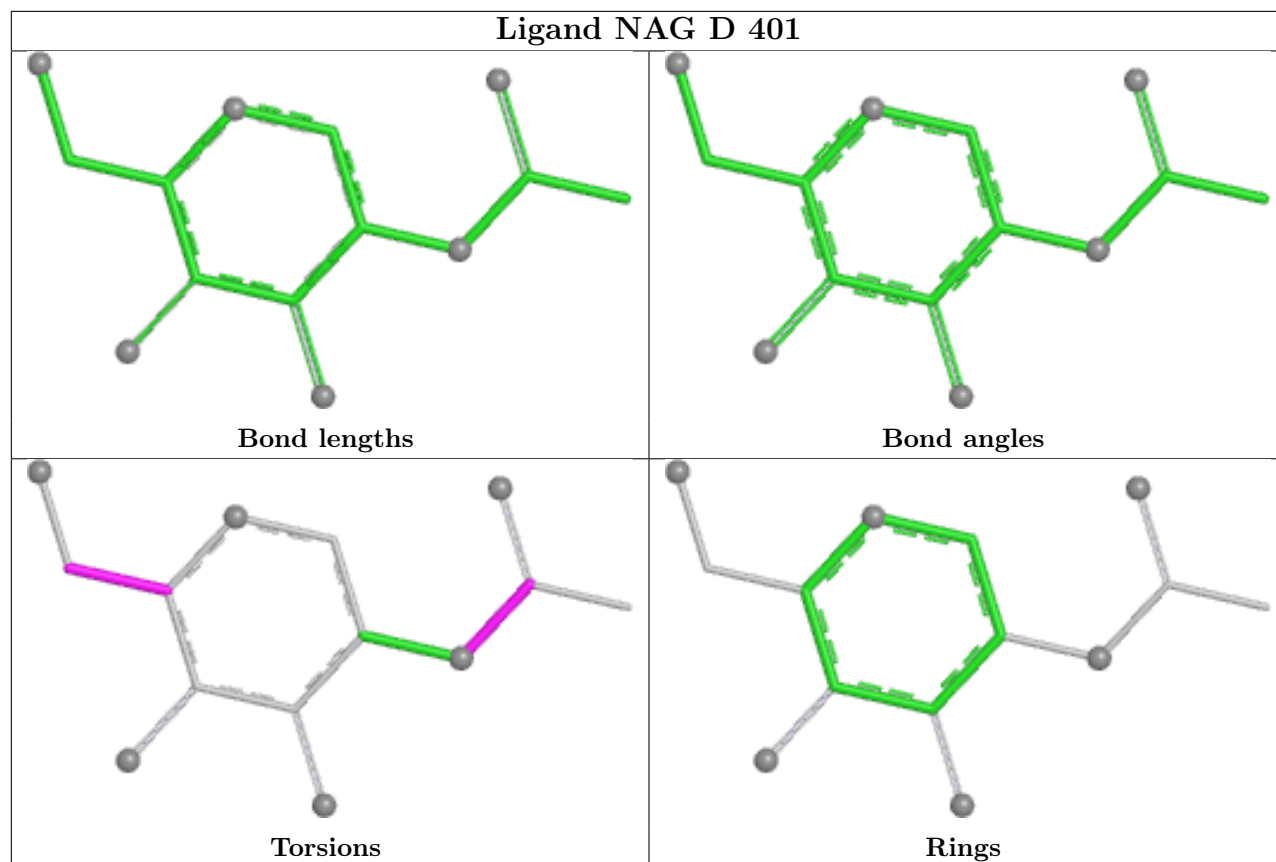
3 monomers are involved in 6 short contacts:

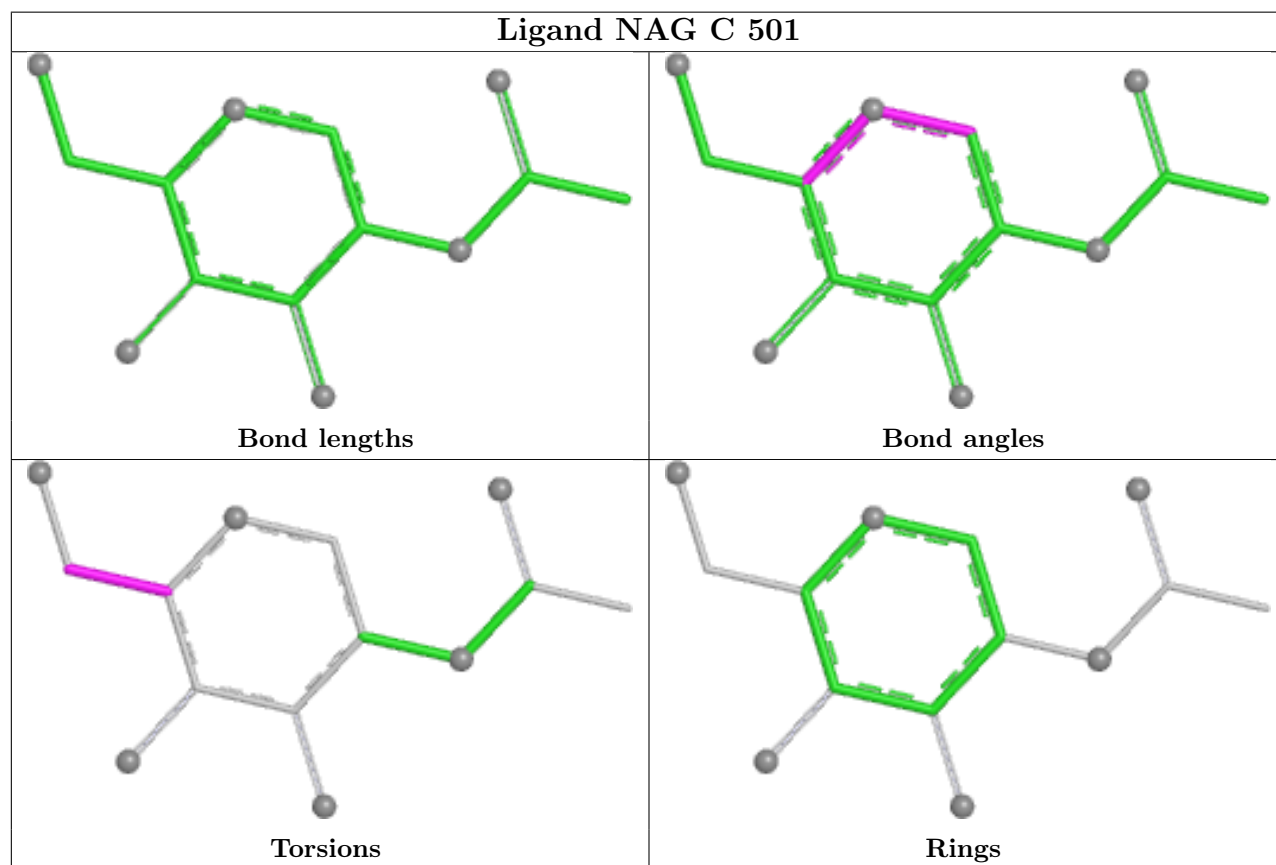
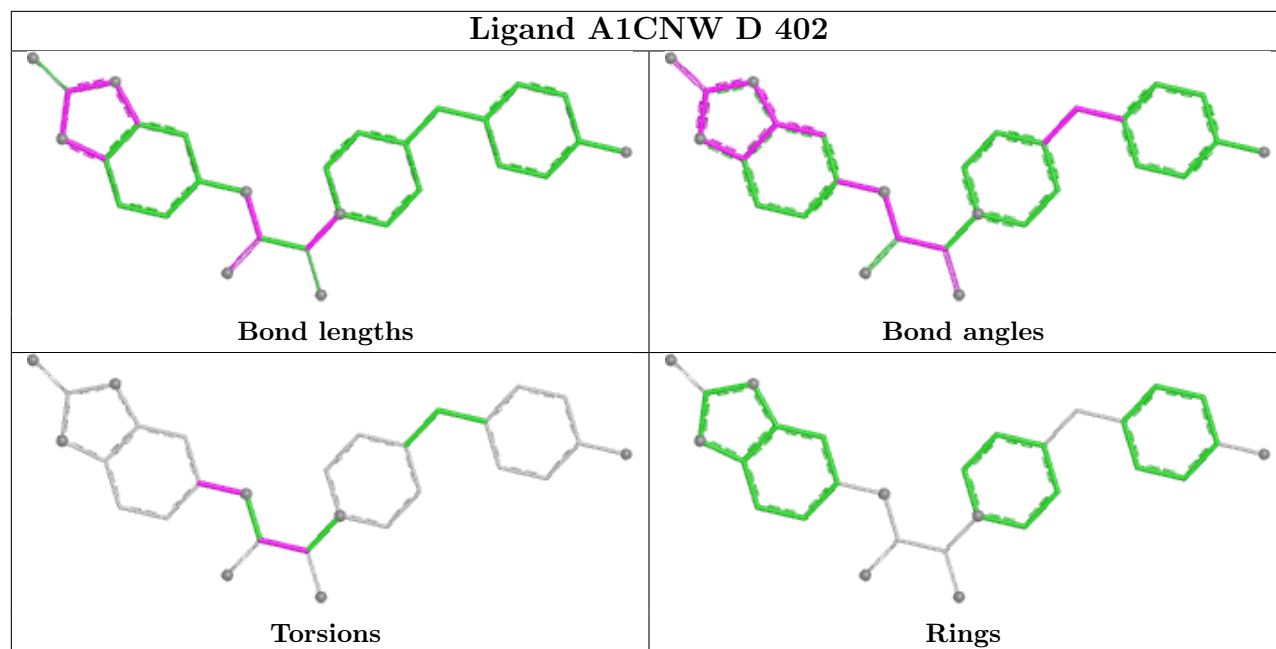
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	502	NAG	3	0
6	A	502	A1CNW	1	0
6	D	402	A1CNW	2	0

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

The following chains have linkage breaks:

Mol	Chain	Number of breaks
3	C	2
1	A	2

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	C	185:GLU	C	209:GLY	N	10.36
1	A	186:GLY	C	209:GLY	N	10.06
1	A	97:ALA	C	102:LEU	N	7.35
1	C	97:ALA	C	101:HIS	N	5.50

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

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

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	359/359 (100%)	0.09	8 (2%) 62 59	25, 39, 60, 99	0
2	B	359/363 (98%)	0.05	4 (1%) 78 77	23, 36, 70, 102	1 (0%)
2	D	363/363 (100%)	-0.01	4 (1%) 78 77	24, 39, 75, 92	0
3	C	358/358 (100%)	-0.06	6 (1%) 69 66	24, 40, 63, 108	0
All	All	1439/1443 (99%)	0.02	22 (1%) 72 69	23, 39, 69, 108	1 (0%)

The worst 5 of 22 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	C	97	ALA	4.9
2	B	394	MET	4.5
2	B	252	TYR	3.3
2	D	347	ARG	3.1
2	D	56	LYS	3.0

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.

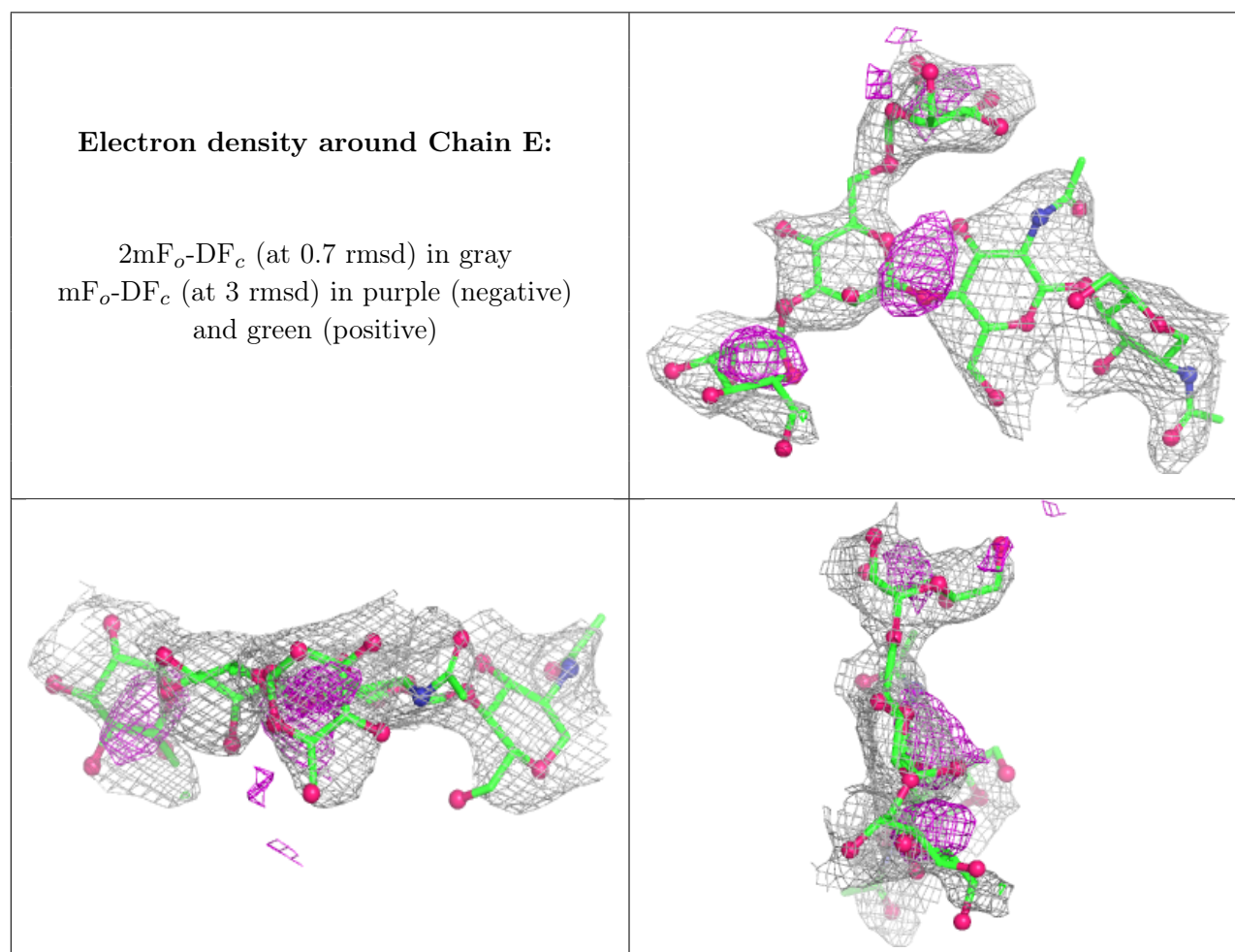
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	MAN	E	4	11/12	0.37	0.16	78,93,107,111	0
4	NAG	E	2	14/15	0.63	0.14	60,76,81,82	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	NAG	E	1	14/15	0.80	0.12	51,62,63,68	0
4	BMA	E	3	11/12	0.84	0.10	56,78,84,99	0
4	MAN	E	5	11/12	0.85	0.10	46,53,61,63	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.



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
5	NAG	B	502	14/15	0.50	0.14	66,83,90,95	0
5	NAG	C	501	14/15	0.64	0.15	61,83,89,90	0

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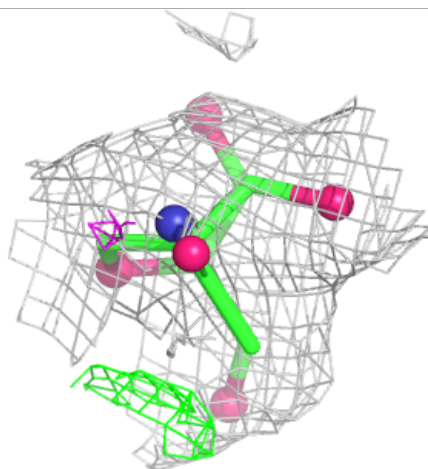
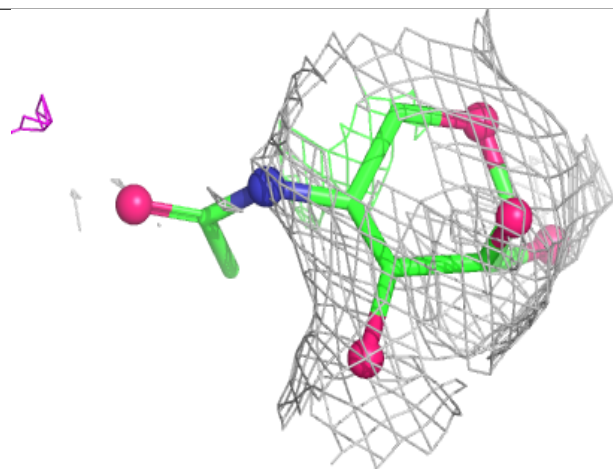
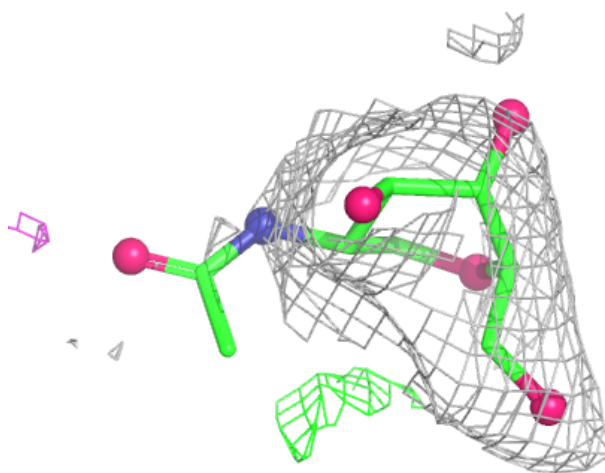
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	NAG	D	401	14/15	0.67	0.11	64,71,81,83	0
8	CL	B	503	1/1	0.73	0.27	100,100,100,100	0
5	NAG	B	501	14/15	0.74	0.12	59,77,95,103	0
8	CL	C	505	1/1	0.79	0.28	86,86,86,86	0
5	NAG	C	502	14/15	0.80	0.11	40,46,49,50	0
8	CL	B	504	1/1	0.82	0.18	90,90,90,90	0
8	CL	B	505	1/1	0.83	0.17	103,103,103,103	0
7	NA	A	503	1/1	0.84	0.16	58,58,58,58	0
7	NA	C	503	1/1	0.84	0.16	65,65,65,65	0
5	NAG	A	501	14/15	0.87	0.10	49,65,72,75	0
8	CL	C	506	1/1	0.90	0.12	103,103,103,103	0
8	CL	A	504	1/1	0.91	0.29	88,88,88,88	0
8	CL	A	505	1/1	0.93	0.18	77,77,77,77	0
8	CL	D	403	1/1	0.93	0.25	97,97,97,97	0
8	CL	C	504	1/1	0.94	0.20	105,105,105,105	0
6	A1CNW	D	402	29/29	0.94	0.18	52,67,78,95	0
6	A1CNW	A	502	29/29	0.96	0.19	38,56,72,78	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.

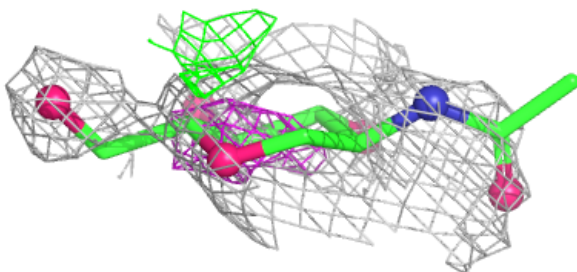
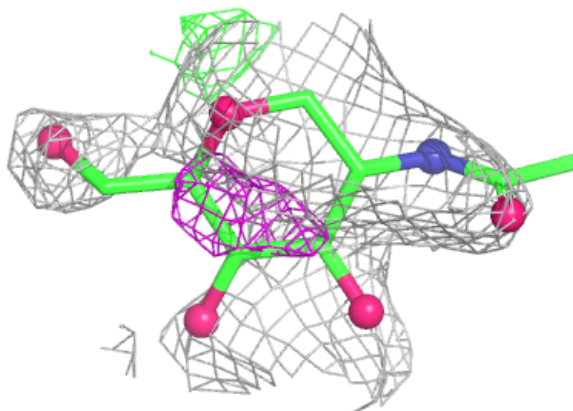
Electron density around NAG B 502:

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



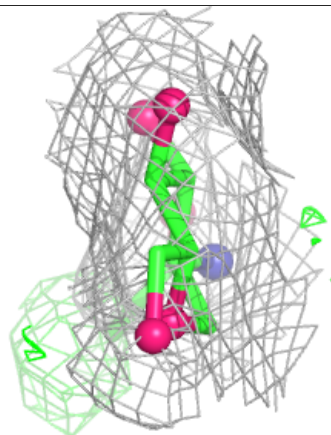
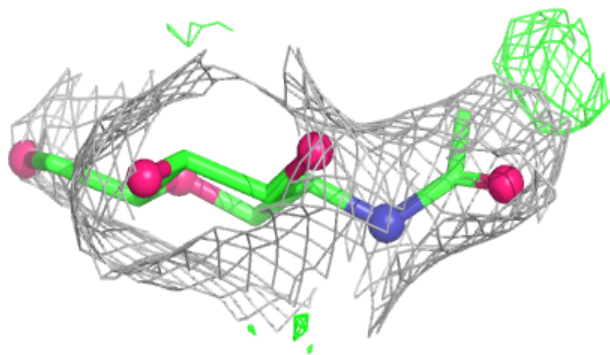
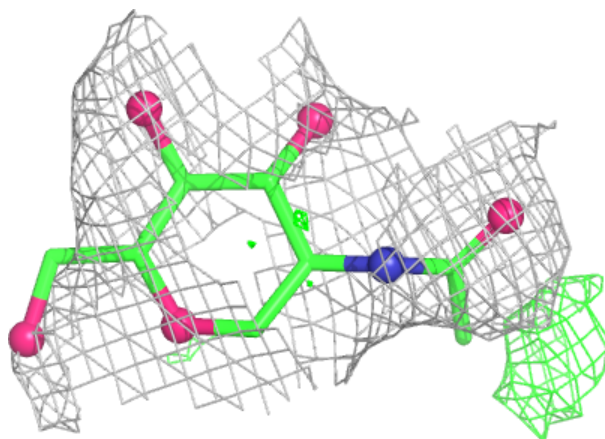
Electron density around NAG C 501:

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and green (positive)



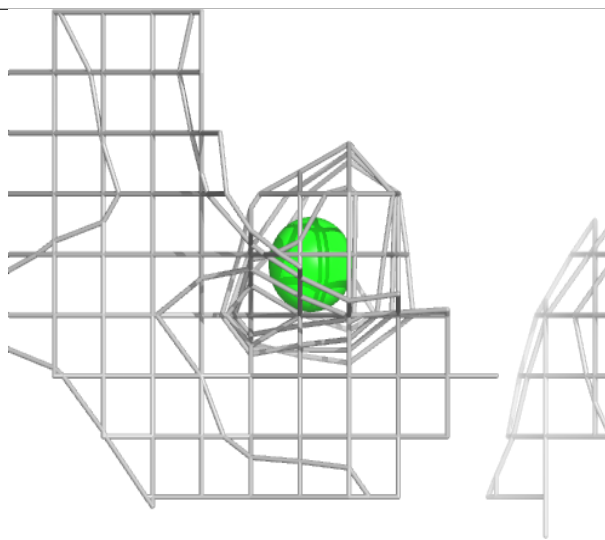
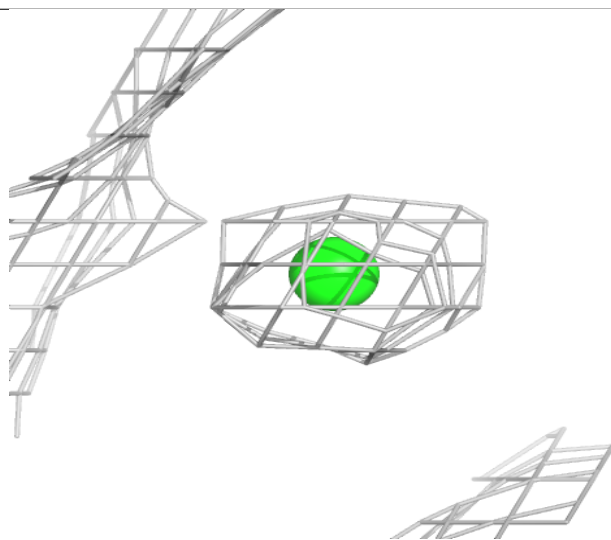
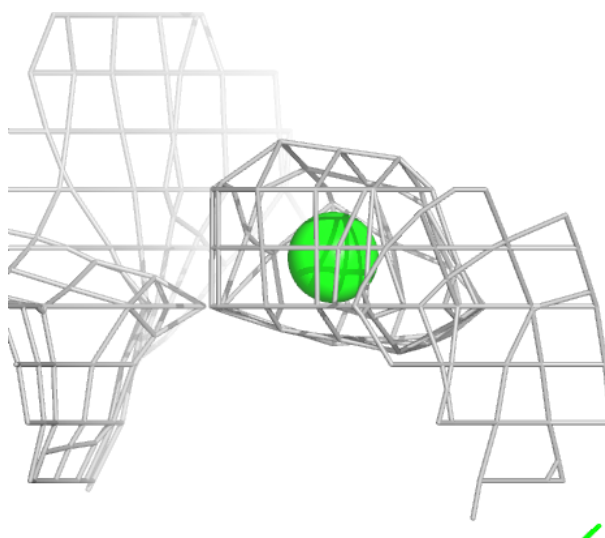
Electron density around NAG D 401:

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and green (positive)



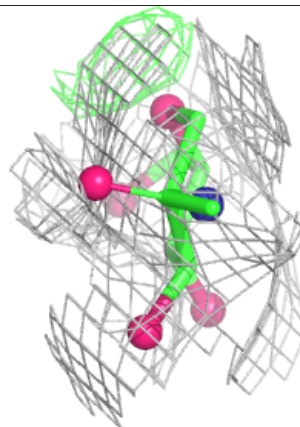
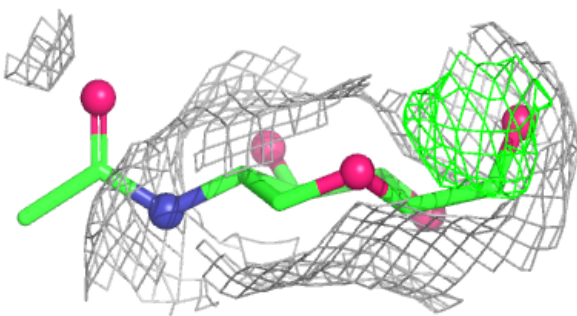
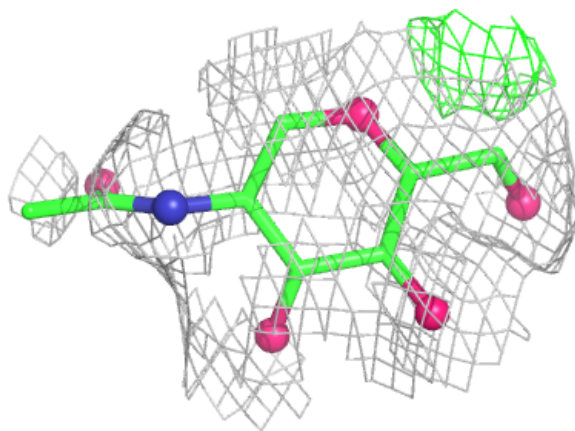
Electron density around CL B 503:

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and green (positive)



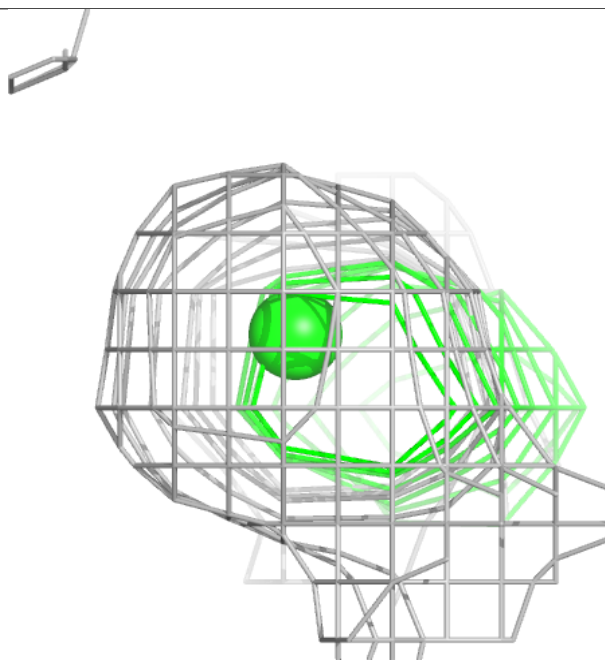
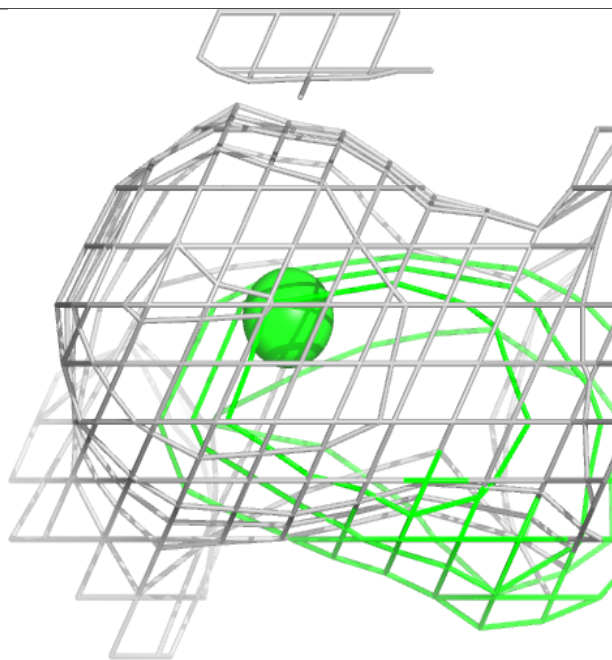
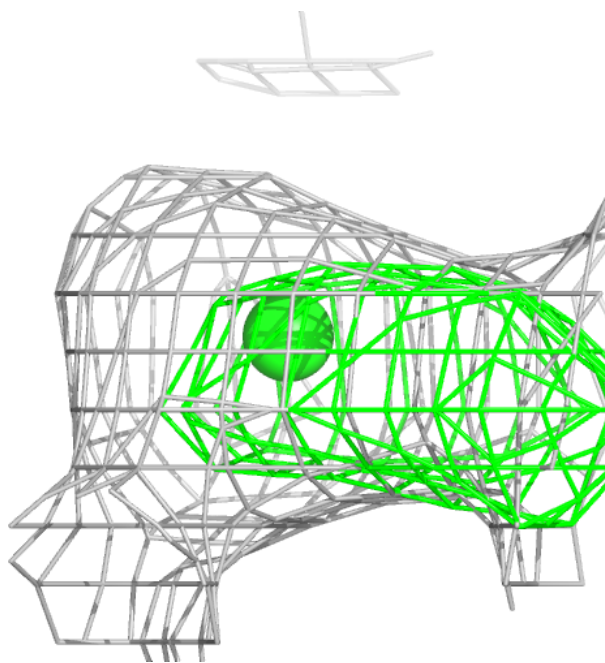
Electron density around NAG B 501:

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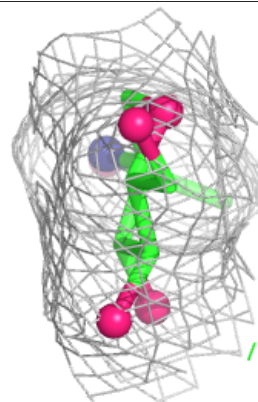
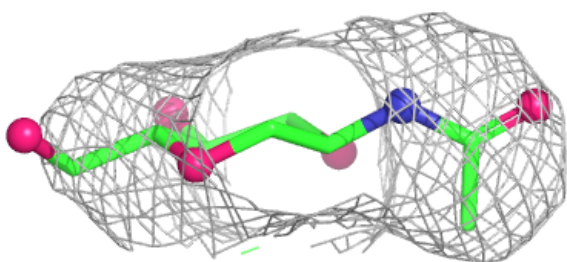
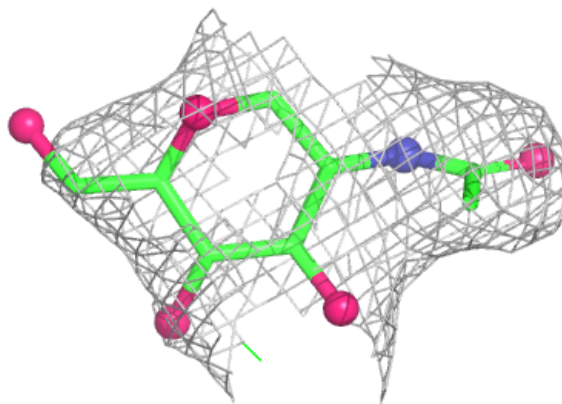
Electron density around CL C 505:

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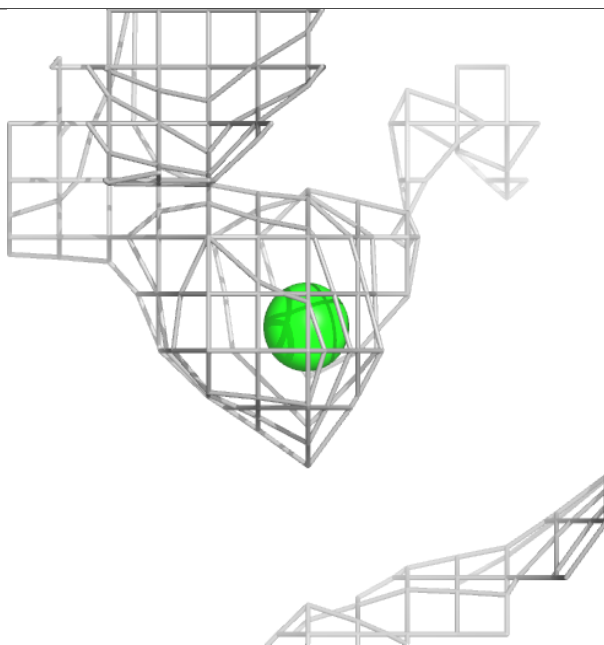
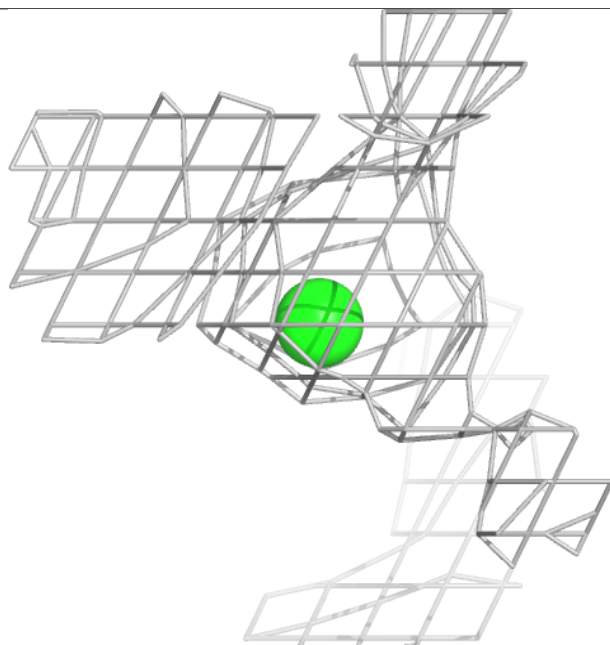
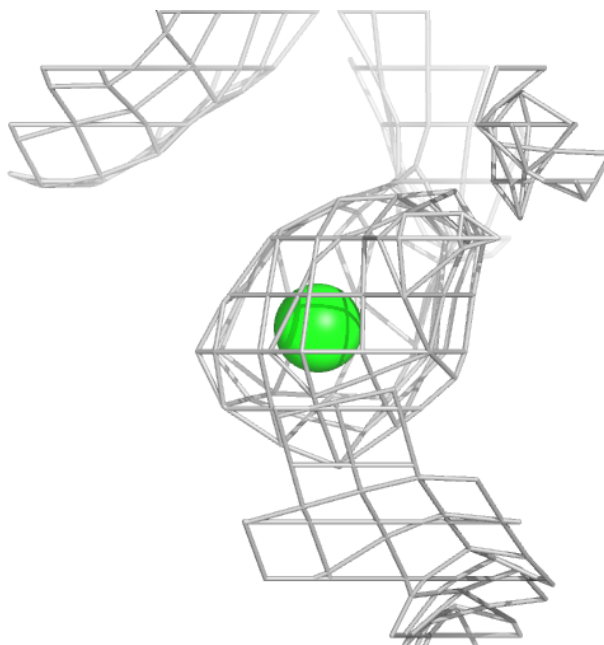
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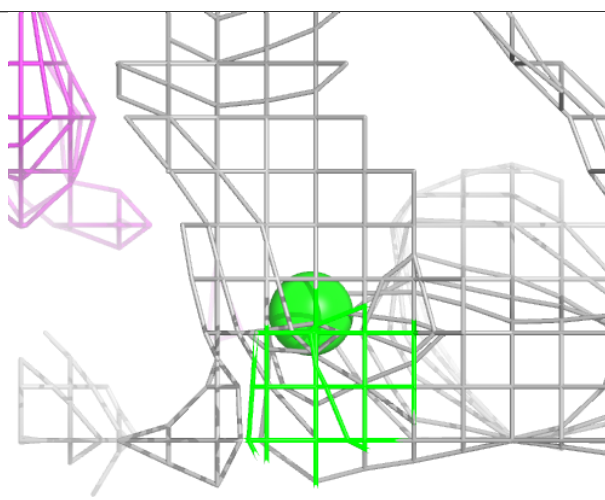
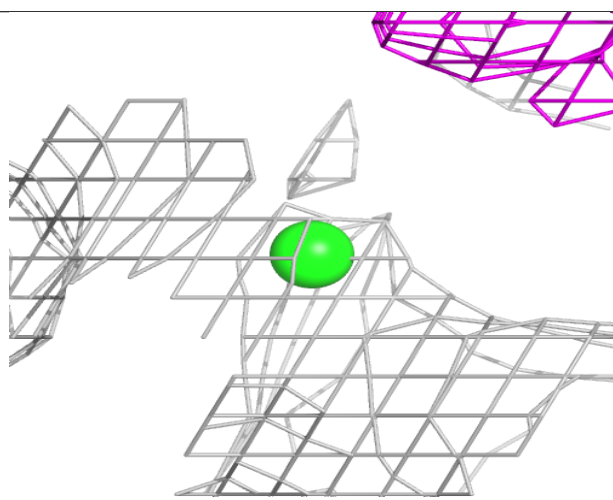
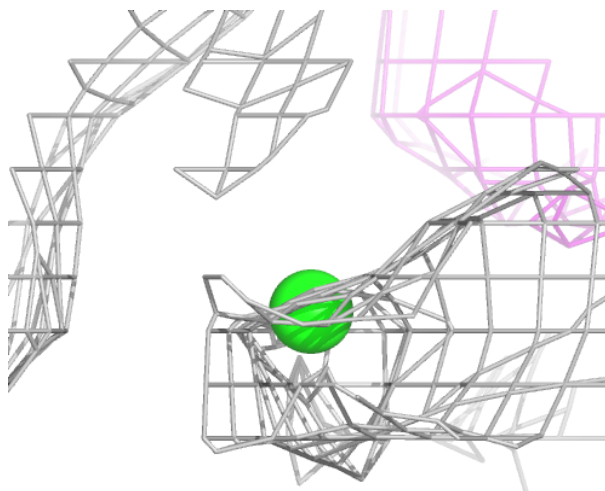
Electron density around CL B 504:

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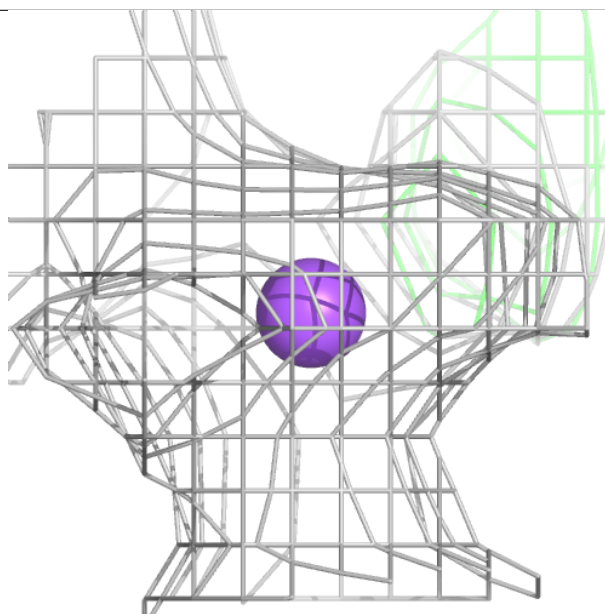
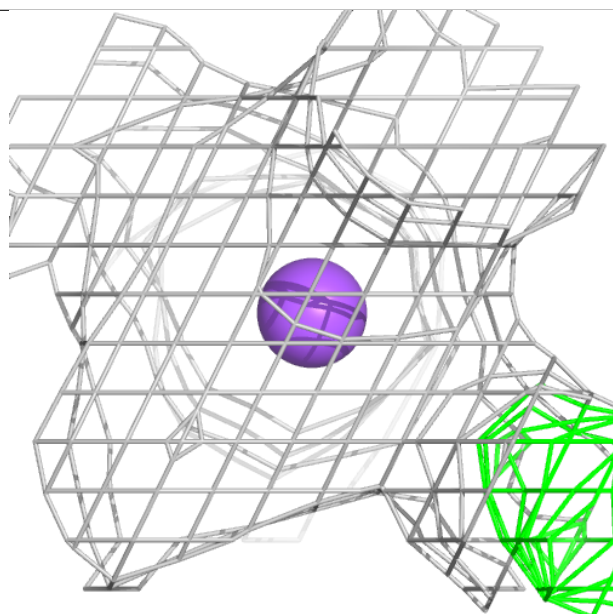
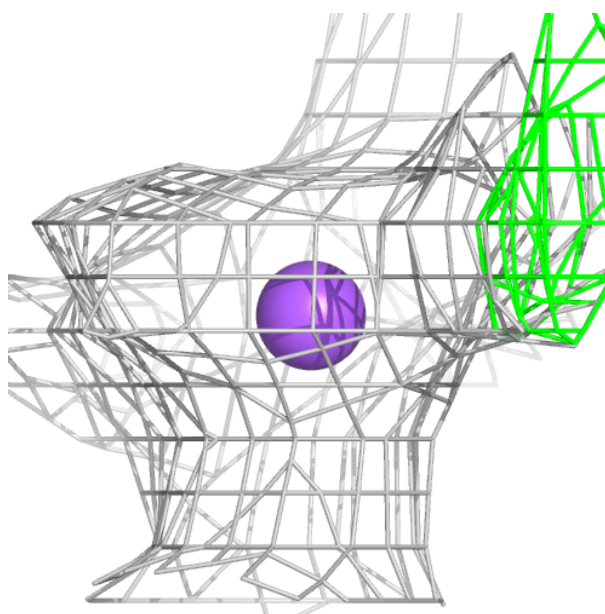
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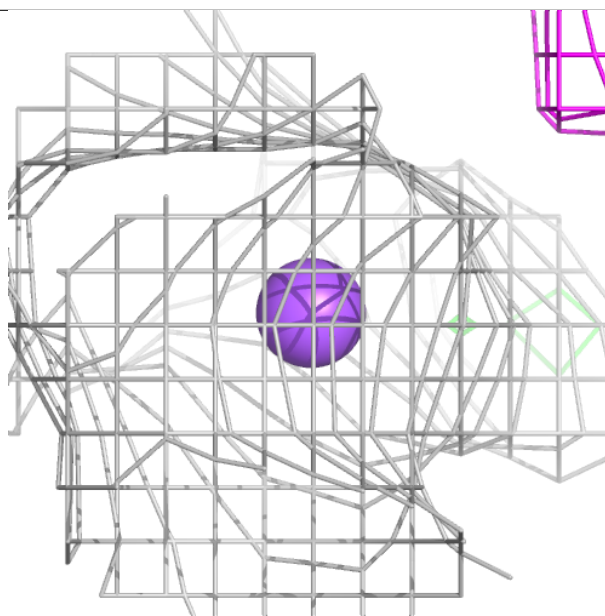
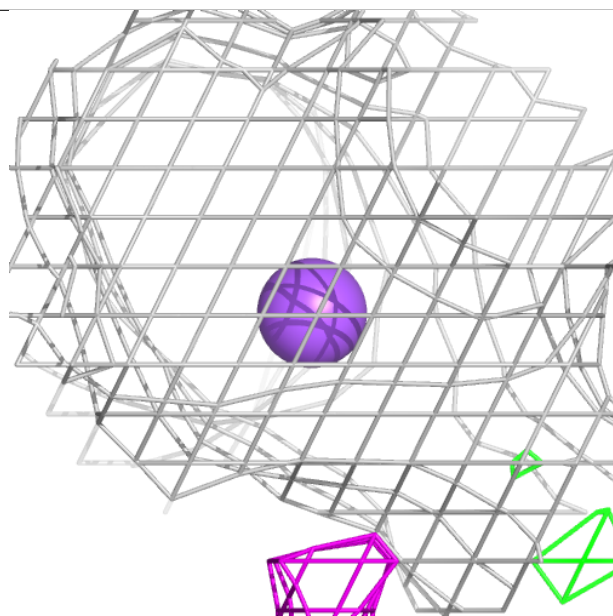
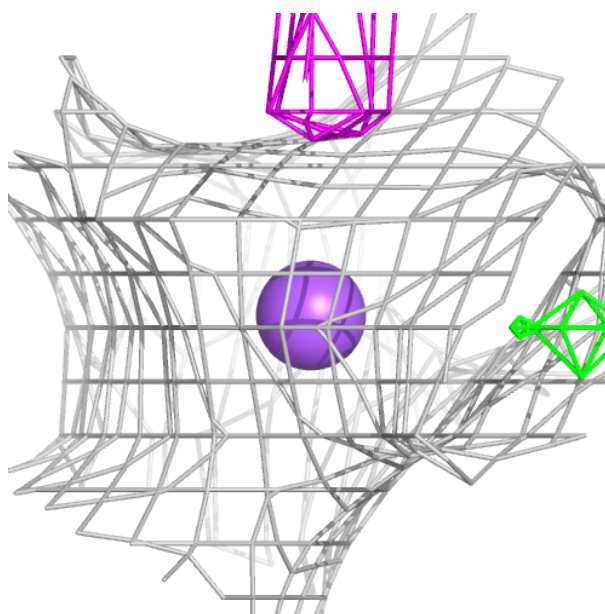
Electron density around NA A 503:

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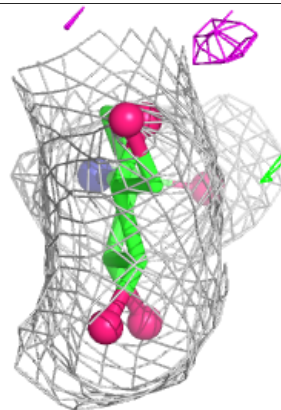
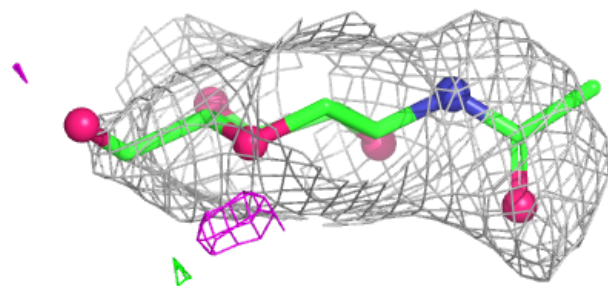
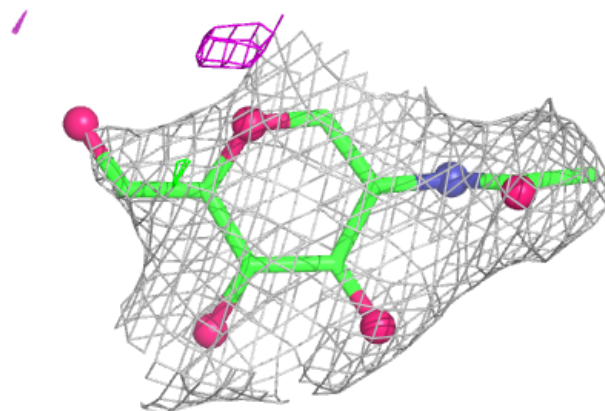
Electron density around NA C 503:

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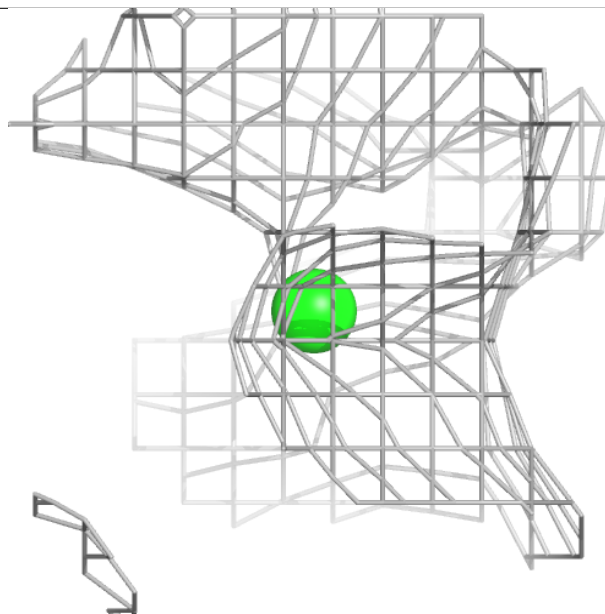
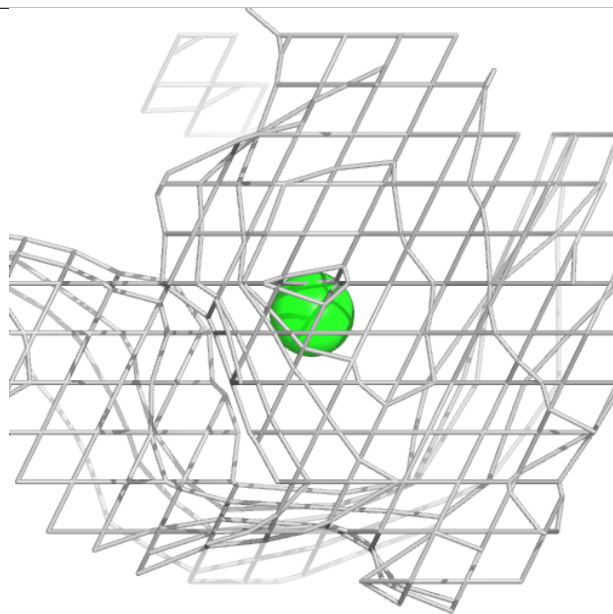
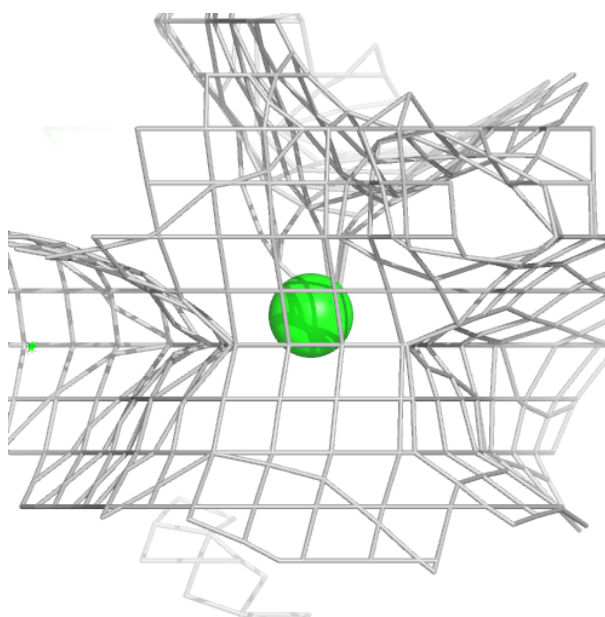
Electron density around NAG A 501:

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and green (positive)



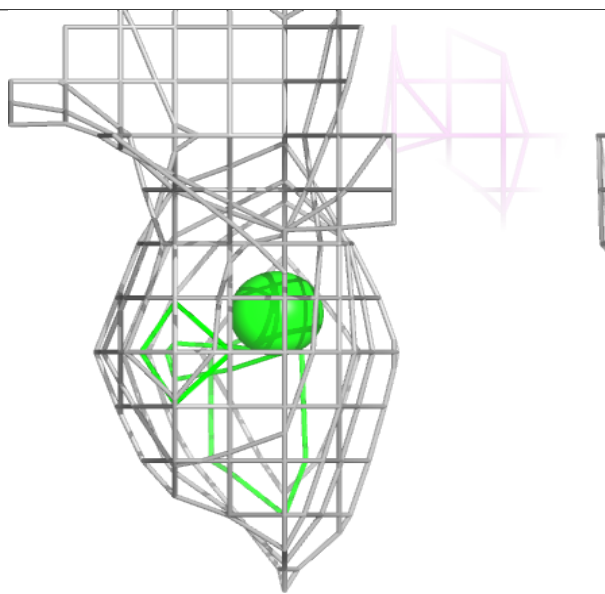
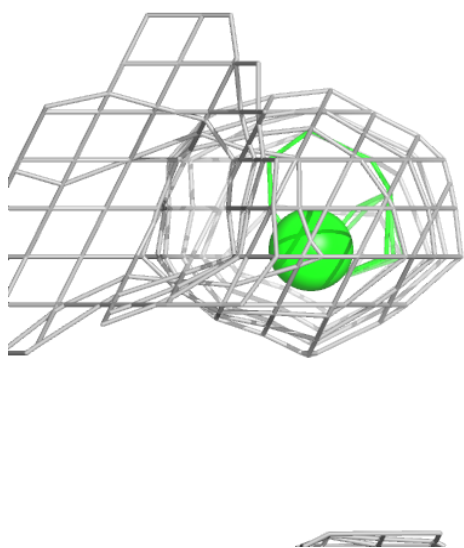
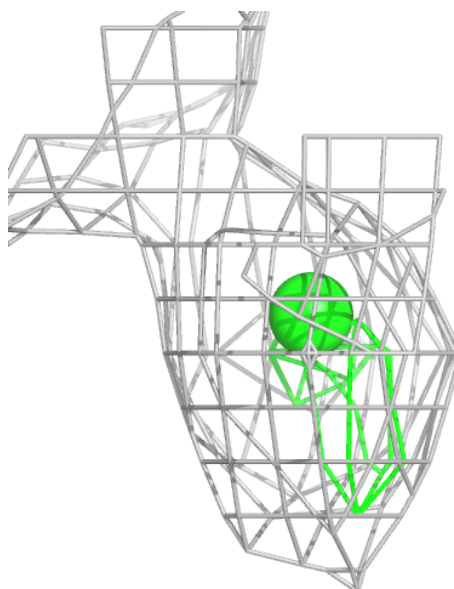
Electron density around CL C 506:

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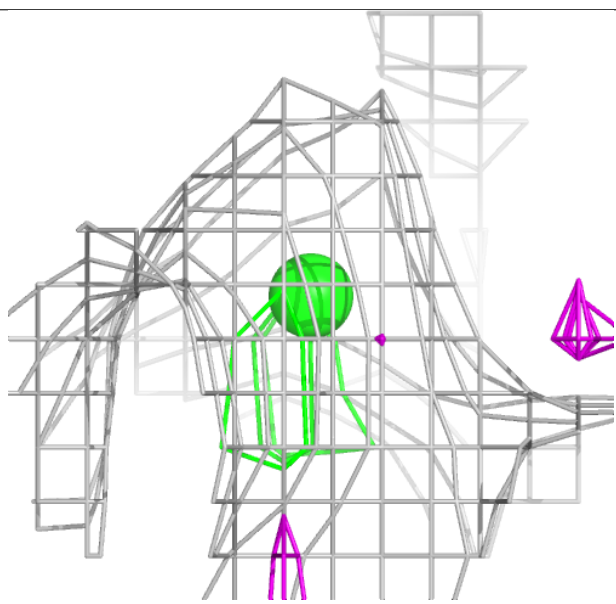
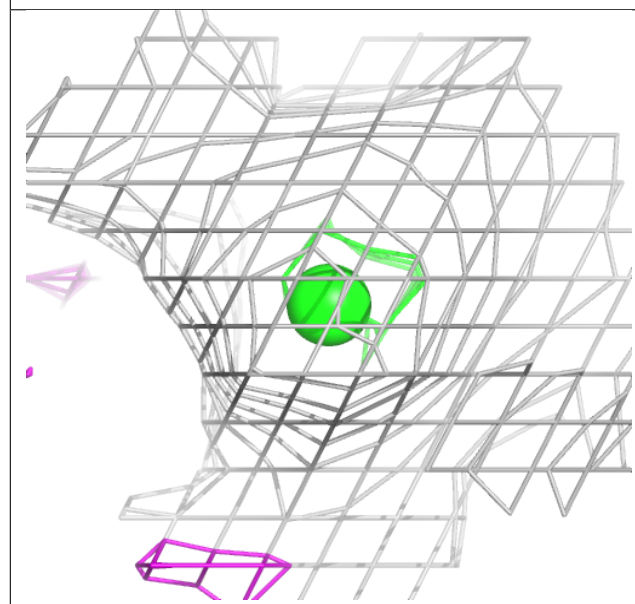
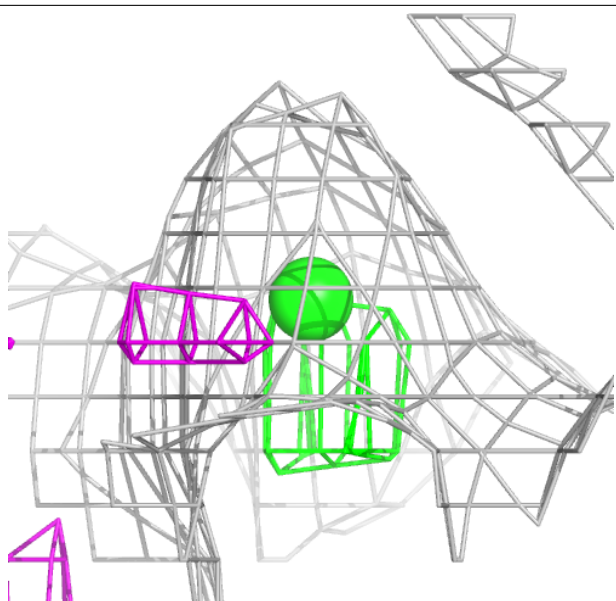
Electron density around CL A 504:

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



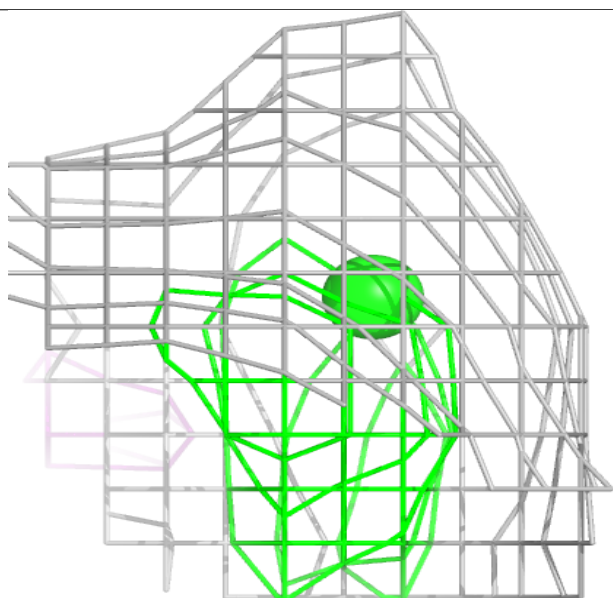
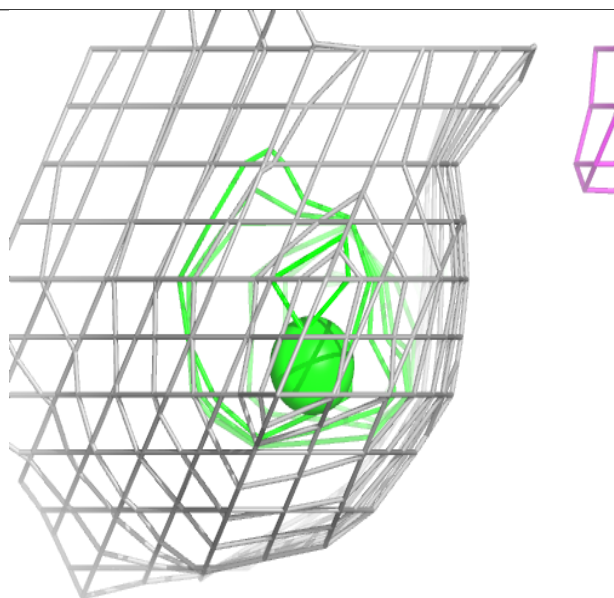
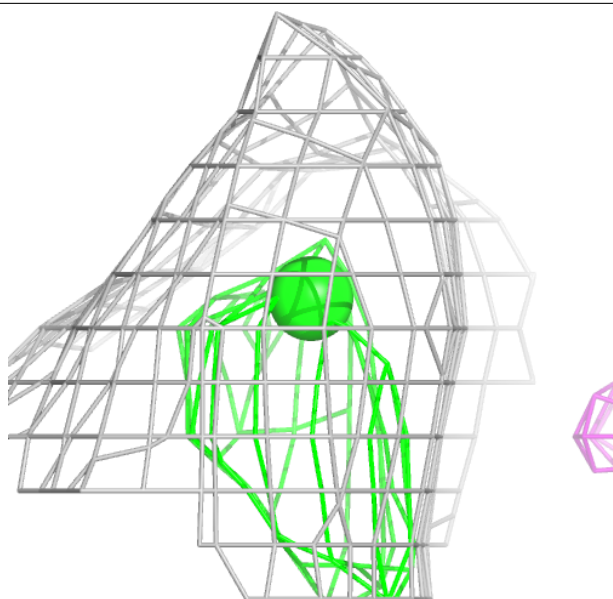
Electron density around CL A 505:

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



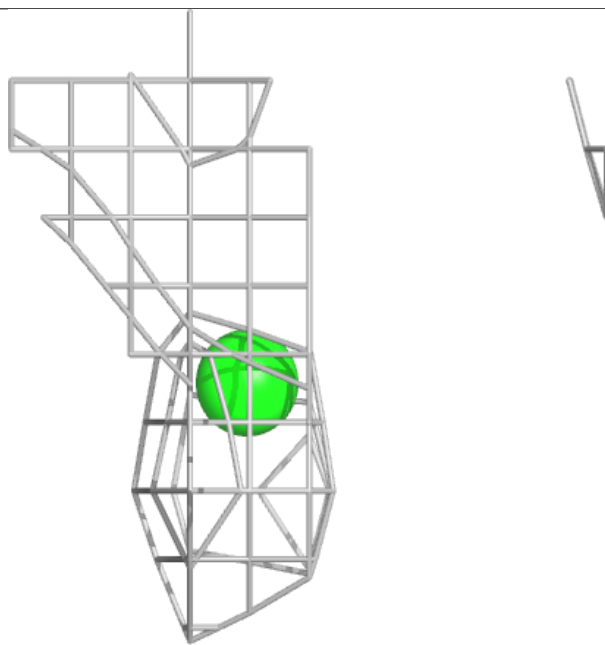
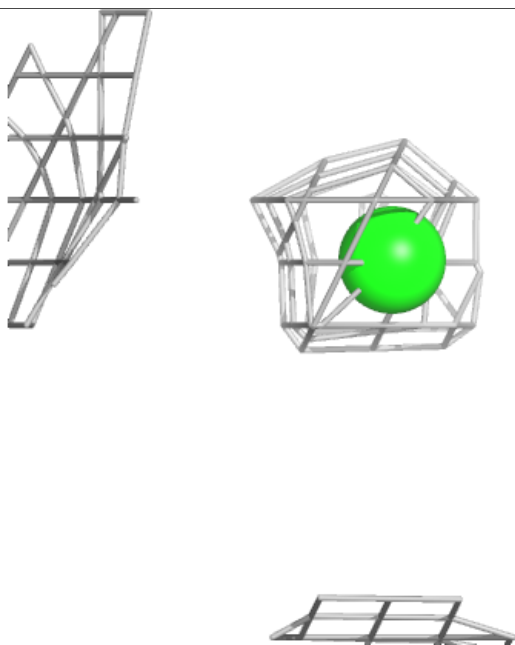
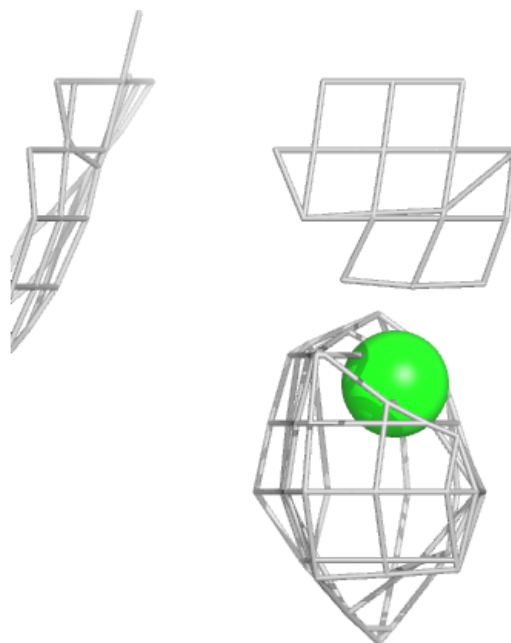
Electron density around CL D 403:

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



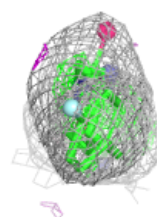
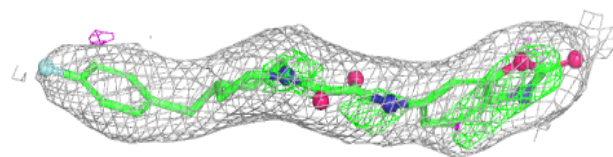
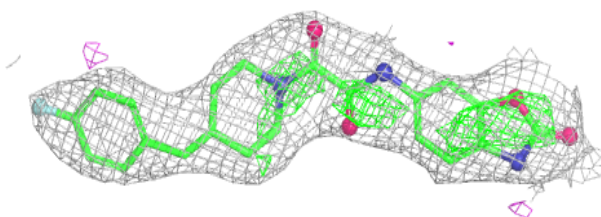
Electron density around CL C 504:

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

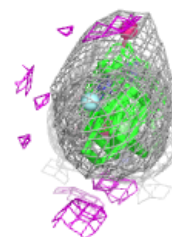
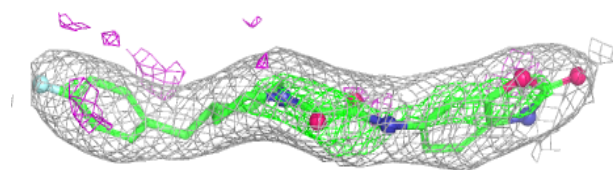
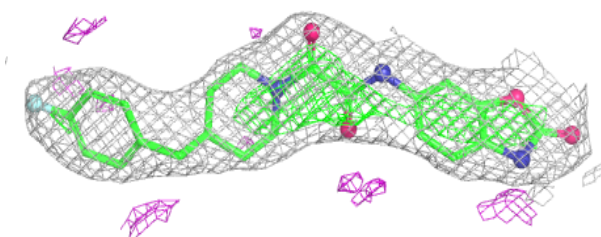


Electron density around A1CNW D 402:

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

**Electron density around A1CNW 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)



6.5 Other polymers [i](#)

There are no such residues in this entry.