



wwPDB X-ray Structure Validation Summary Report ⓘ

Nov 20, 2023 – 02:26 PM JST

PDB ID : 7CZE
Title : Crystal structure of Epstein-Barr virus (EBV) gHgL and in complex with the ligand binding domain (LBD) of EphA2
Authors : Su, C.; Wu, L.L.; Song, H.; Chai, Y.; Qi, J.X.; Yan, J.H.; Gao, G.F.
Deposited on : 2020-09-08
Resolution : 3.00 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 : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.36
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36

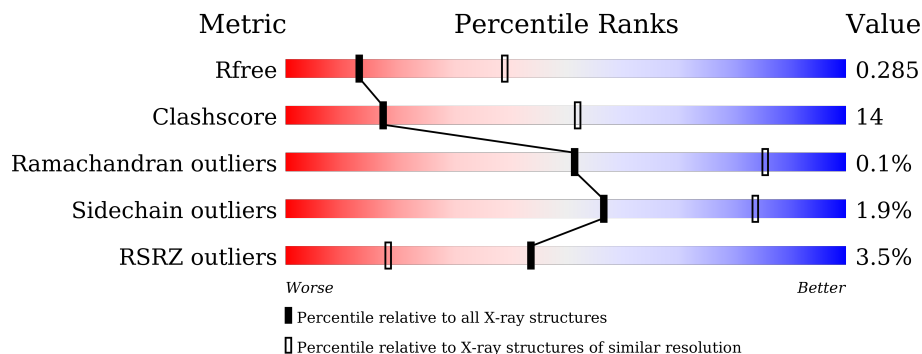
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (3.00-3.00)

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	662	
1	C	662	
1	E	662	
1	G	662	
2	B	114	
2	D	114	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	F	114	<p>2% 56% 35%</p>
2	H	114	<p>4% 60% 32%</p>
3	I	183	<p>% 64% 25% 10%</p>
3	J	183	<p>2% 64% 25% 10%</p>
3	K	183	<p>3% 64% 25% 10%</p>
3	L	183	<p>2% 63% 26% 10%</p>

2 Entry composition i

There are 4 unique types of molecules in this entry. The entry contains 29320 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 Envelope glycoprotein H.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	655	5097	3268	842	956	31	0	0	0
1	C	655	5097	3268	842	956	31	0	0	0
1	E	655	5097	3268	842	956	31	0	0	0
1	G	655	5097	3268	842	956	31	0	0	0

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	675	GLU	-	expression tag	UNP P03231
A	676	GLU	-	expression tag	UNP P03231
A	677	ARG	-	expression tag	UNP P03231
A	678	ALA	-	expression tag	UNP P03231
A	679	HIS	-	expression tag	UNP P03231
C	675	GLU	-	expression tag	UNP P03231
C	676	GLU	-	expression tag	UNP P03231
C	677	ARG	-	expression tag	UNP P03231
C	678	ALA	-	expression tag	UNP P03231
C	679	HIS	-	expression tag	UNP P03231
E	675	GLU	-	expression tag	UNP P03231
E	676	GLU	-	expression tag	UNP P03231
E	677	ARG	-	expression tag	UNP P03231
E	678	ALA	-	expression tag	UNP P03231
E	679	HIS	-	expression tag	UNP P03231
G	675	GLU	-	expression tag	UNP P03231
G	676	GLU	-	expression tag	UNP P03231
G	677	ARG	-	expression tag	UNP P03231
G	678	ALA	-	expression tag	UNP P03231
G	679	HIS	-	expression tag	UNP P03231

- Molecule 2 is a protein called Envelope glycoprotein L.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	109	Total 842	C 532	N 146	O 160	S 4	0	0	0
2	D	109	Total 842	C 532	N 146	O 160	S 4	0	0	0
2	F	109	Total 842	C 532	N 146	O 160	S 4	0	0	0
2	H	109	Total 842	C 532	N 146	O 160	S 4	0	0	0

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	133	TRP	-	expression tag	UNP P03212
B	134	HIS	-	expression tag	UNP P03212
B	135	ARG	-	expression tag	UNP P03212
B	136	GLY	-	expression tag	UNP P03212
B	137	GLY	-	expression tag	UNP P03212
D	133	TRP	-	expression tag	UNP P03212
D	134	HIS	-	expression tag	UNP P03212
D	135	ARG	-	expression tag	UNP P03212
D	136	GLY	-	expression tag	UNP P03212
D	137	GLY	-	expression tag	UNP P03212
F	133	TRP	-	expression tag	UNP P03212
F	134	HIS	-	expression tag	UNP P03212
F	135	ARG	-	expression tag	UNP P03212
F	136	GLY	-	expression tag	UNP P03212
F	137	GLY	-	expression tag	UNP P03212
H	133	TRP	-	expression tag	UNP P03212
H	134	HIS	-	expression tag	UNP P03212
H	135	ARG	-	expression tag	UNP P03212
H	136	GLY	-	expression tag	UNP P03212
H	137	GLY	-	expression tag	UNP P03212

- Molecule 3 is a protein called Ephrin type-A receptor 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	I	165	Total 1335	C 862	N 216	O 248	S 9	0	1	0
3	J	165	Total 1335	C 862	N 216	O 248	S 9	0	1	0
3	K	165	Total 1335	C 862	N 216	O 248	S 9	0	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	L	165	1335	862	216	248	9	0	1	0

There are 32 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
I	201	HIS	-	expression tag	UNP P29317
I	202	HIS	-	expression tag	UNP P29317
I	203	HIS	-	expression tag	UNP P29317
I	204	HIS	-	expression tag	UNP P29317
I	205	HIS	-	expression tag	UNP P29317
I	206	HIS	-	expression tag	UNP P29317
I	207	HIS	-	expression tag	UNP P29317
I	208	HIS	-	expression tag	UNP P29317
J	201	HIS	-	expression tag	UNP P29317
J	202	HIS	-	expression tag	UNP P29317
J	203	HIS	-	expression tag	UNP P29317
J	204	HIS	-	expression tag	UNP P29317
J	205	HIS	-	expression tag	UNP P29317
J	206	HIS	-	expression tag	UNP P29317
J	207	HIS	-	expression tag	UNP P29317
J	208	HIS	-	expression tag	UNP P29317
K	201	HIS	-	expression tag	UNP P29317
K	202	HIS	-	expression tag	UNP P29317
K	203	HIS	-	expression tag	UNP P29317
K	204	HIS	-	expression tag	UNP P29317
K	205	HIS	-	expression tag	UNP P29317
K	206	HIS	-	expression tag	UNP P29317
K	207	HIS	-	expression tag	UNP P29317
K	208	HIS	-	expression tag	UNP P29317
L	201	HIS	-	expression tag	UNP P29317
L	202	HIS	-	expression tag	UNP P29317
L	203	HIS	-	expression tag	UNP P29317
L	204	HIS	-	expression tag	UNP P29317
L	205	HIS	-	expression tag	UNP P29317
L	206	HIS	-	expression tag	UNP P29317
L	207	HIS	-	expression tag	UNP P29317
L	208	HIS	-	expression tag	UNP P29317

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C₈H₁₅NO₆) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
4	A	1	Total 14	8	1	5	0	0
4	A	1	Total 14	8	1	5	0	0
4	B	1	Total 14	8	1	5	0	0
4	B	1	Total 14	8	1	5	0	0
4	C	1	Total 14	8	1	5	0	0
4	C	1	Total 14	8	1	5	0	0
4	D	1	Total 14	8	1	5	0	0
4	D	1	Total 14	8	1	5	0	0
4	E	1	Total 14	8	1	5	0	0
4	E	1	Total 14	8	1	5	0	0
4	F	1	Total 14	8	1	5	0	0
4	F	1	Total 14	8	1	5	0	0
4	G	1	Total 14	8	1	5	0	0
4	G	1	Total 14	8	1	5	0	0

Continued on next page...

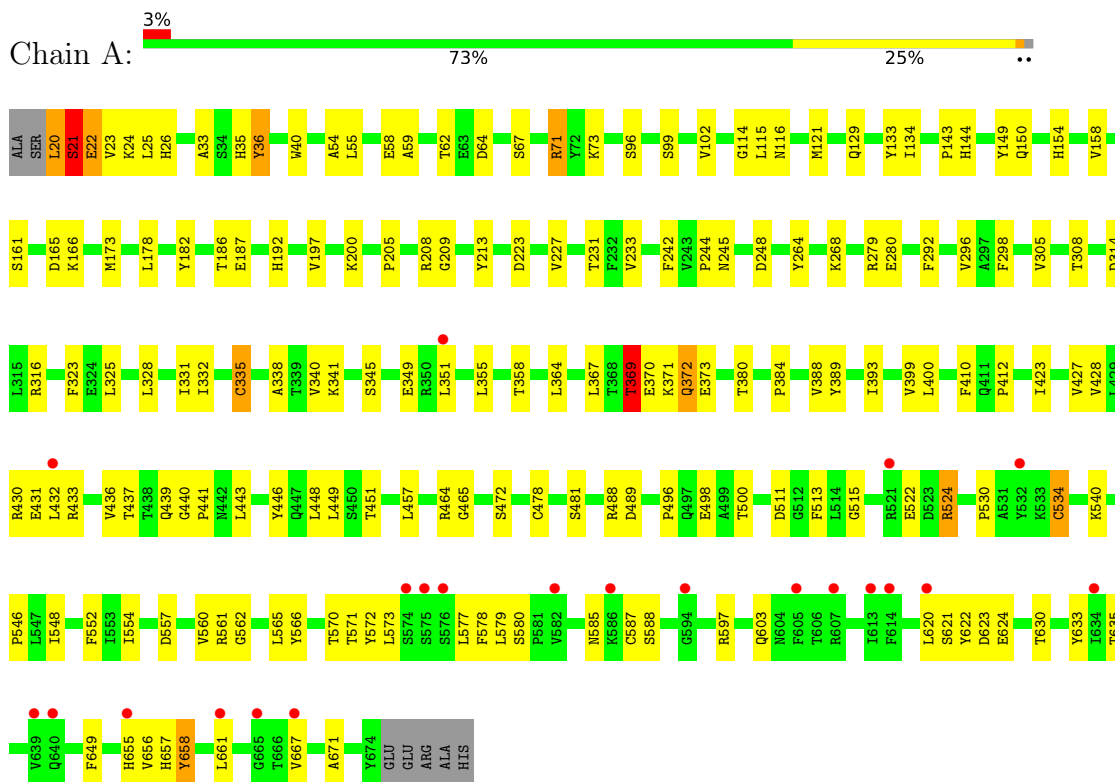
Continued from previous page...

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	H	1	Total	C	N	O	0	0
			14	8	1	5		
4	H	1	Total	C	N	O	0	0
			14	8	1	5		

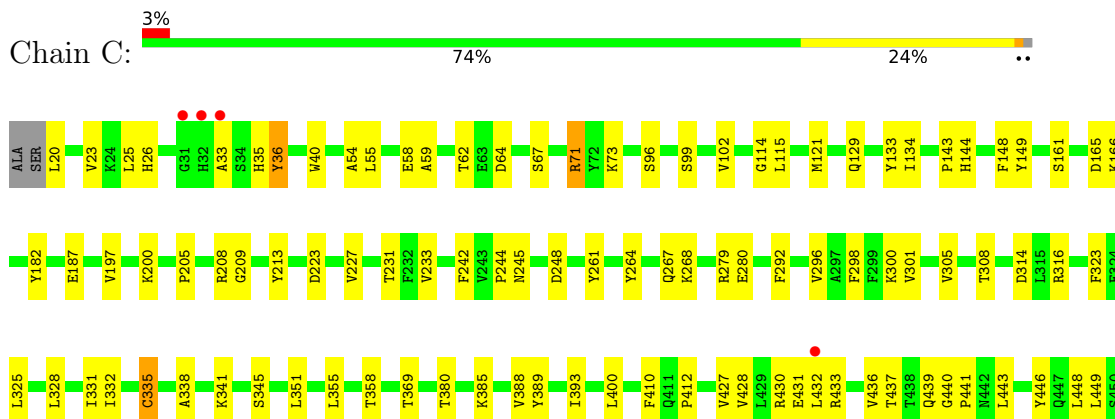
3 Residue-property plots

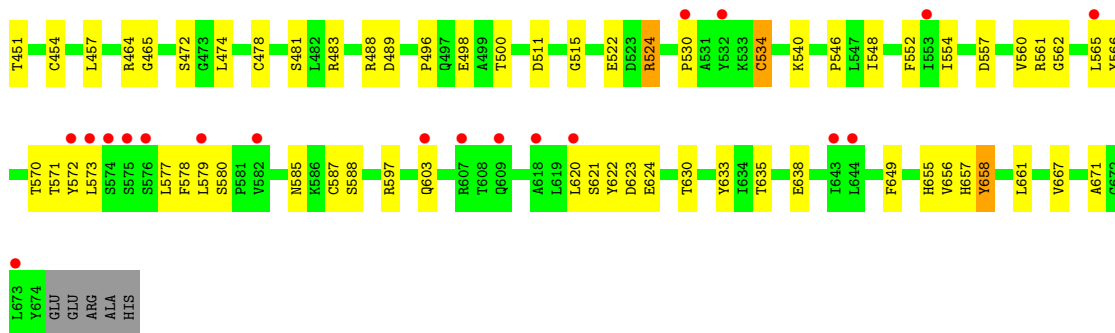
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Envelope glycoprotein H

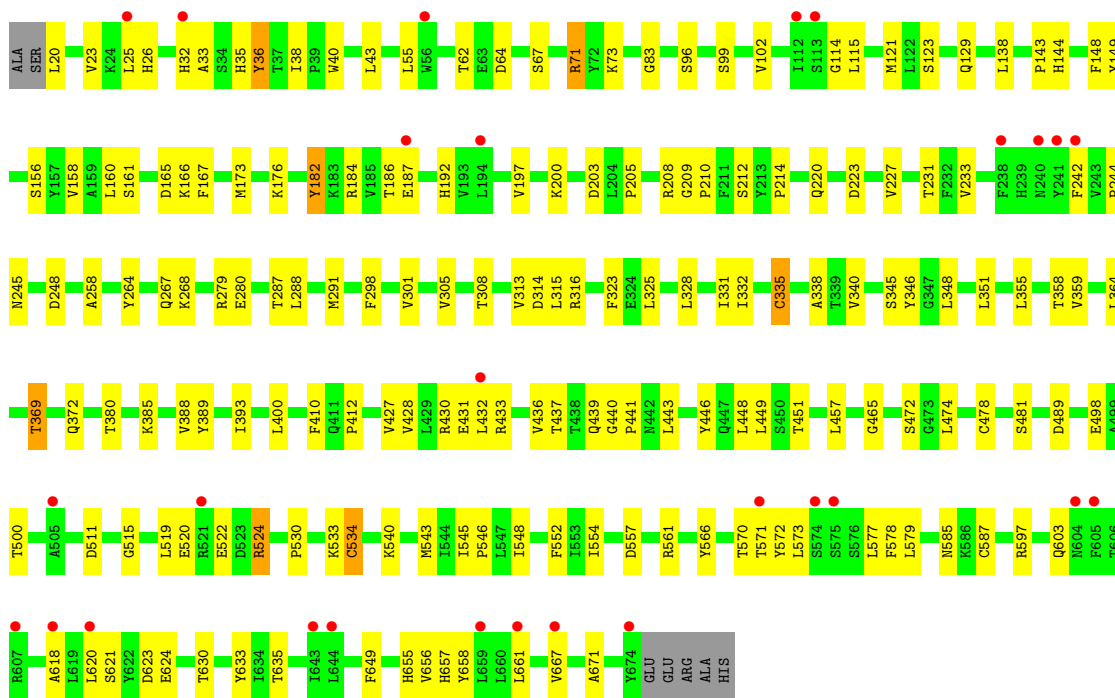


- Molecule 1: Envelope glycoprotein H

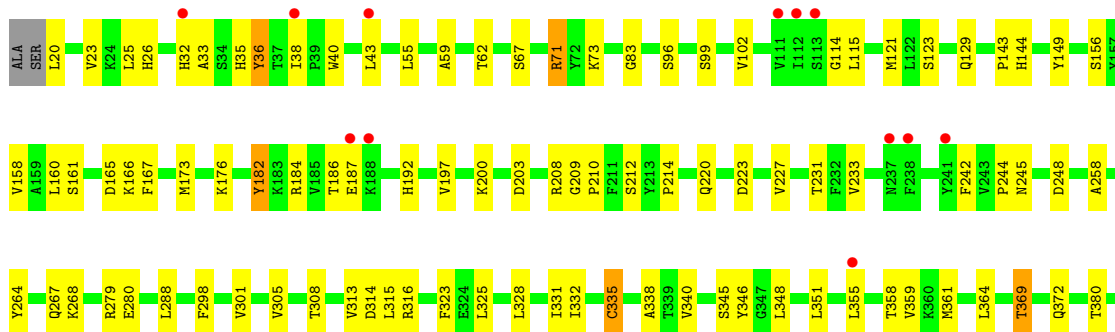
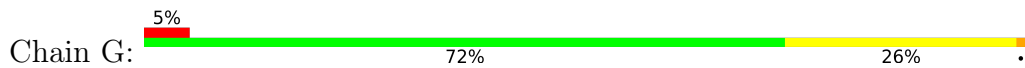


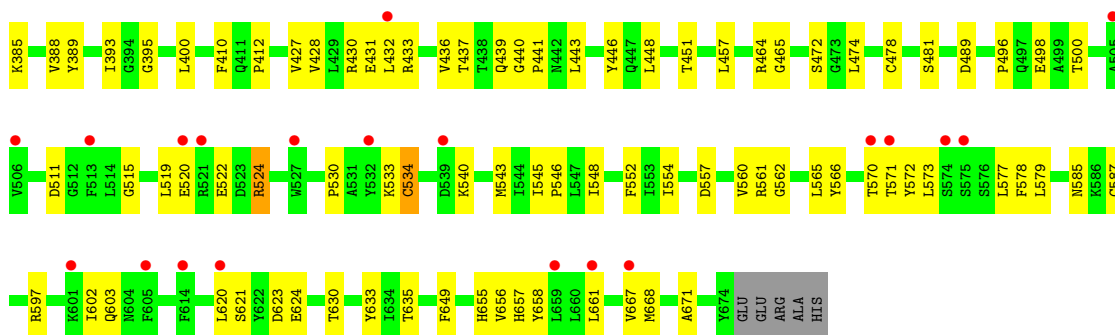


• Molecule 1: Envelope glycoprotein H

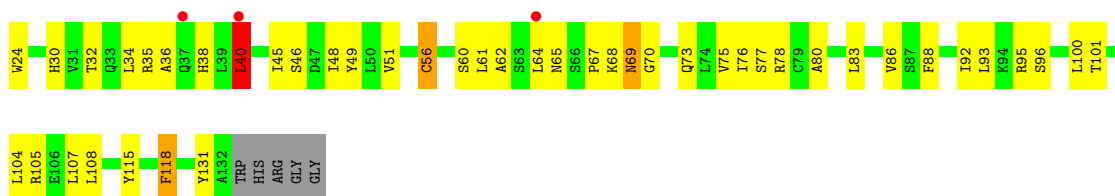


• Molecule 1: Envelope glycoprotein H

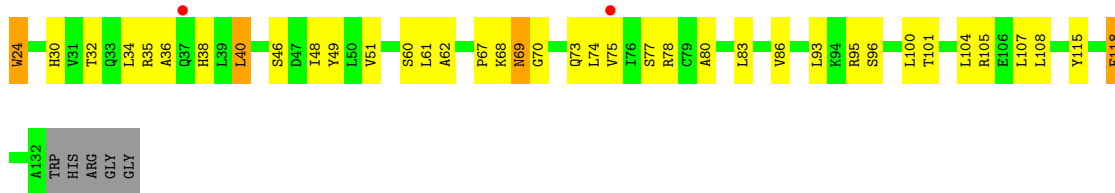




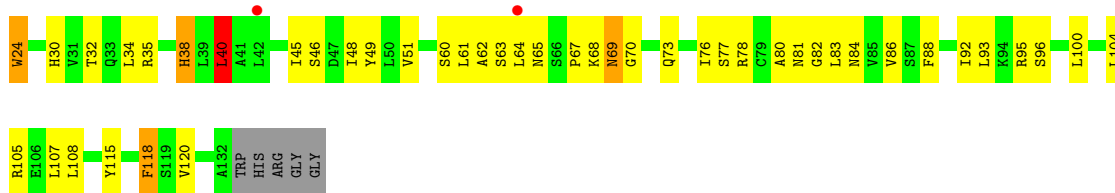
- Molecule 2: Envelope glycoprotein L



- Molecule 2: Envelope glycoprotein L

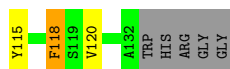


- Molecule 2: Envelope glycoprotein L



- Molecule 2: Envelope glycoprotein L





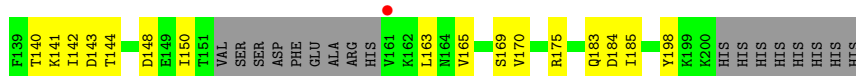
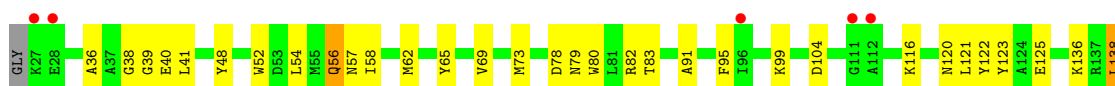
- Molecule 3: Ephrin type-A receptor 2



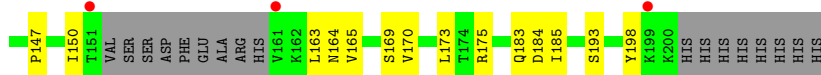
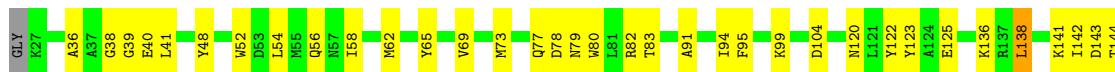
- Molecule 3: Ephrin type-A receptor 2



- Molecule 3: Ephrin type-A receptor 2



- Molecule 3: Ephrin type-A receptor 2



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	94.46Å 113.81Å 119.65Å 90.03° 90.17° 89.89°	Depositor
Resolution (Å)	41.22 – 3.00 41.22 – 3.00	Depositor EDS
% Data completeness (in resolution range)	98.3 (41.22-3.00) 97.9 (41.22-3.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.63 (at 3.01Å)	Xtriage
Refinement program	PHENIX 1.16_3549	Depositor
R, R_{free}	0.257 , 0.285 0.255 , 0.285	Depositor DCC
R_{free} test set	5133 reflections (5.21%)	wwPDB-VP
Wilson B-factor (Å ²)	83.4	Xtriage
Anisotropy	0.760	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 59.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.013 for h,-l,k 0.013 for h,l,-k 0.408 for h,-k,-l 0.145 for -h,k,-l 0.146 for -h,-k,l 0.017 for -h,-l,-k 0.018 for -h,l,k	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	29320	wwPDB-VP
Average B, all atoms (Å ²)	121.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.74% 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: NAG

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	0.31	0/5206	0.57	0/7066
1	C	0.30	0/5206	0.57	0/7066
1	E	0.28	0/5206	0.56	0/7066
1	G	0.28	0/5206	0.56	0/7066
2	B	0.34	0/857	0.69	1/1164 (0.1%)
2	D	0.35	0/857	0.70	1/1164 (0.1%)
2	F	0.33	0/857	0.66	1/1164 (0.1%)
2	H	0.33	0/857	0.66	1/1164 (0.1%)
3	I	0.44	1/1370 (0.1%)	0.66	1/1853 (0.1%)
3	J	0.34	0/1370	0.65	1/1853 (0.1%)
3	K	0.38	1/1370 (0.1%)	0.67	1/1853 (0.1%)
3	L	0.33	0/1370	0.63	1/1853 (0.1%)
All	All	0.32	2/29732 (0.0%)	0.60	8/40332 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	C	0	3
1	E	0	3
1	G	0	3
2	B	0	2
2	D	0	2
2	F	0	1
2	H	0	1
3	I	0	2
3	J	0	2
3	K	0	3

Continued on next page...

Continued from previous page...

Mol	Chain	#Chirality outliers	#Planarity outliers
3	L	0	3
All	All	0	26

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	I	56	GLN	CD-NE2	10.36	1.58	1.32
3	K	56	GLN	CD-NE2	6.96	1.50	1.32

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	J	138	LEU	CA-CB-CG	6.57	130.40	115.30
2	B	40	LEU	CA-CB-CG	6.52	130.30	115.30
2	D	40	LEU	CA-CB-CG	6.48	130.20	115.30
3	I	138	LEU	CA-CB-CG	6.38	129.97	115.30
2	H	40	LEU	CA-CB-CG	6.25	129.69	115.30

There are no chirality outliers.

5 of 26 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	572	TYR	Peptide
2	B	35	ARG	Peptide
2	B	36	ALA	Peptide
1	C	20	LEU	Peptide
1	C	369	THR	Peptide

5.2 Too-close contacts [\(i\)](#)

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	5097	0	5113	154	0
1	C	5097	0	5113	129	0
1	E	5097	0	5113	140	0
1	G	5097	0	5113	136	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	842	0	828	34	0
2	D	842	0	828	35	0
2	F	842	0	828	40	0
2	H	842	0	828	40	0
3	I	1335	0	1293	36	0
3	J	1335	0	1293	39	0
3	K	1335	0	1293	38	0
3	L	1335	0	1293	33	0
4	A	28	0	26	2	0
4	B	28	0	26	1	0
4	C	28	0	26	2	0
4	D	28	0	26	2	0
4	E	28	0	26	2	0
4	F	28	0	26	0	0
4	G	28	0	26	2	0
4	H	28	0	26	1	0
All	All	29320	0	29144	807	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 14.

The worst 5 of 807 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:20:LEU:CD1	1:A:40:TRP:CB	2.14	1.26
1:A:20:LEU:CD1	1:A:40:TRP:HB3	1.68	1.20
3:K:40:GLU:HG3	3:K:41:LEU:H	1.10	1.15
3:L:40:GLU:HG3	3:L:41:LEU:H	1.11	1.13
1:A:20:LEU:HD12	1:A:40:TRP:HB3	1.17	1.12

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	653/662 (99%)	648 (99%)	3 (0%)	2 (0%)	41	76
1	C	653/662 (99%)	651 (100%)	2 (0%)	0	100	100
1	E	653/662 (99%)	651 (100%)	2 (0%)	0	100	100
1	G	653/662 (99%)	651 (100%)	2 (0%)	0	100	100
2	B	107/114 (94%)	105 (98%)	2 (2%)	0	100	100
2	D	107/114 (94%)	104 (97%)	3 (3%)	0	100	100
2	F	107/114 (94%)	105 (98%)	2 (2%)	0	100	100
2	H	107/114 (94%)	104 (97%)	3 (3%)	0	100	100
3	I	162/183 (88%)	162 (100%)	0	0	100	100
3	J	162/183 (88%)	161 (99%)	1 (1%)	0	100	100
3	K	162/183 (88%)	162 (100%)	0	0	100	100
3	L	162/183 (88%)	162 (100%)	0	0	100	100
All	All	3688/3836 (96%)	3666 (99%)	20 (0%)	2 (0%)	51	85

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	21	SER
1	A	369	THR

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	561/566 (99%)	546 (97%)	15 (3%)	44	77
1	C	561/566 (99%)	552 (98%)	9 (2%)	62	86
1	E	561/566 (99%)	553 (99%)	8 (1%)	67	88
1	G	561/566 (99%)	553 (99%)	8 (1%)	67	88

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	B	95/98 (97%)	90 (95%)	5 (5%)	22	58
2	D	95/98 (97%)	91 (96%)	4 (4%)	30	66
2	F	95/98 (97%)	90 (95%)	5 (5%)	22	58
2	H	95/98 (97%)	91 (96%)	4 (4%)	30	66
3	I	142/158 (90%)	140 (99%)	2 (1%)	67	88
3	J	142/158 (90%)	140 (99%)	2 (1%)	67	88
3	K	142/158 (90%)	140 (99%)	2 (1%)	67	88
3	L	142/158 (90%)	140 (99%)	2 (1%)	67	88
All	All	3192/3288 (97%)	3126 (98%)	66 (2%)	57	82

5 of 66 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	H	118	PHE
3	I	48[B]	TYR
3	L	48[B]	TYR
1	C	478	CYS
1	C	454	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 10 such sidechains are listed below:

Mol	Chain	Res	Type
1	E	237	ASN
1	G	237	ASN
3	J	56	GLN
2	B	38	HIS
1	C	35	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

16 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
4	NAG	E	702	1	14,14,15	0.48	0	17,19,21	0.84	1 (5%)
4	NAG	C	701	1	14,14,15	0.42	0	17,19,21	0.50	0
4	NAG	D	202	2	14,14,15	0.36	0	17,19,21	0.48	0
4	NAG	B	202	2	14,14,15	0.28	0	17,19,21	0.52	0
4	NAG	D	201	2	14,14,15	0.34	0	17,19,21	0.60	0
4	NAG	F	201	2	14,14,15	0.44	0	17,19,21	0.64	1 (5%)
4	NAG	G	702	1	14,14,15	0.54	0	17,19,21	0.88	1 (5%)
4	NAG	A	702	1	14,14,15	0.51	0	17,19,21	0.81	1 (5%)
4	NAG	F	202	2	14,14,15	0.31	0	17,19,21	0.40	0
4	NAG	H	202	2	14,14,15	0.38	0	17,19,21	0.41	0
4	NAG	B	201	2	14,14,15	0.33	0	17,19,21	0.79	1 (5%)
4	NAG	E	701	1	14,14,15	0.60	0	17,19,21	0.52	0
4	NAG	G	701	1	14,14,15	0.63	0	17,19,21	0.52	0
4	NAG	A	701	1	14,14,15	0.36	0	17,19,21	0.47	0
4	NAG	C	702	1	14,14,15	0.51	0	17,19,21	0.79	1 (5%)
4	NAG	H	201	2	14,14,15	0.40	0	17,19,21	0.66	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. '2' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	E	702	1	-	2/6/23/26	0/1/1/1
4	NAG	C	701	1	-	0/6/23/26	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	D	202	2	-	2/6/23/26	0/1/1/1
4	NAG	B	202	2	-	2/6/23/26	0/1/1/1
4	NAG	D	201	2	-	0/6/23/26	0/1/1/1
4	NAG	F	201	2	-	1/6/23/26	0/1/1/1
4	NAG	G	702	1	-	2/6/23/26	0/1/1/1
4	NAG	A	702	1	-	2/6/23/26	0/1/1/1
4	NAG	F	202	2	-	2/6/23/26	0/1/1/1
4	NAG	H	202	2	-	2/6/23/26	0/1/1/1
4	NAG	B	201	2	-	1/6/23/26	0/1/1/1
4	NAG	E	701	1	-	0/6/23/26	0/1/1/1
4	NAG	G	701	1	-	0/6/23/26	0/1/1/1
4	NAG	A	701	1	-	0/6/23/26	0/1/1/1
4	NAG	C	702	1	-	2/6/23/26	0/1/1/1
4	NAG	H	201	2	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	G	702	NAG	C1-O5-C5	3.24	116.59	112.19
4	E	702	NAG	C1-O5-C5	2.96	116.20	112.19
4	B	201	NAG	C1-O5-C5	2.91	116.14	112.19
4	A	702	NAG	C1-O5-C5	2.88	116.10	112.19
4	C	702	NAG	C1-O5-C5	2.69	115.84	112.19

There are no chirality outliers.

5 of 18 torsion outliers are listed below:

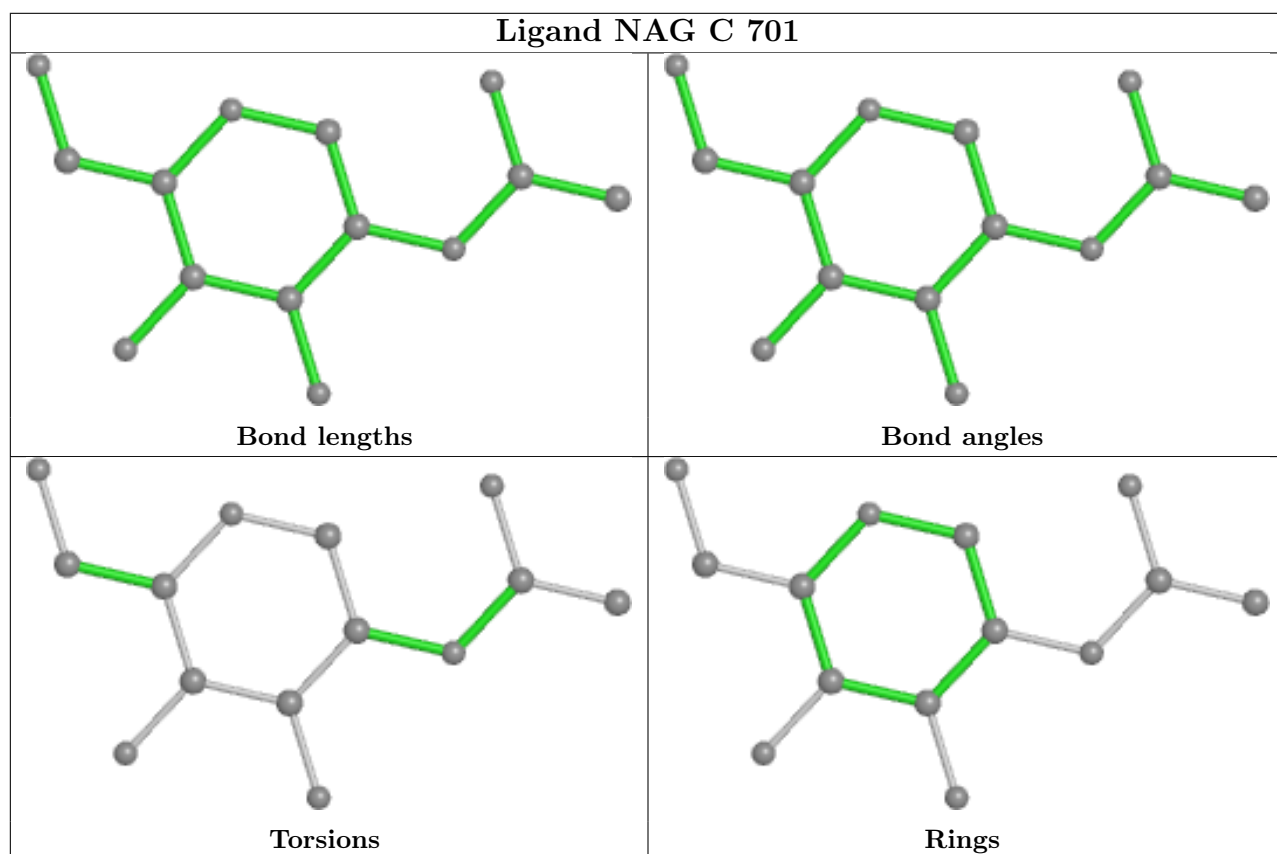
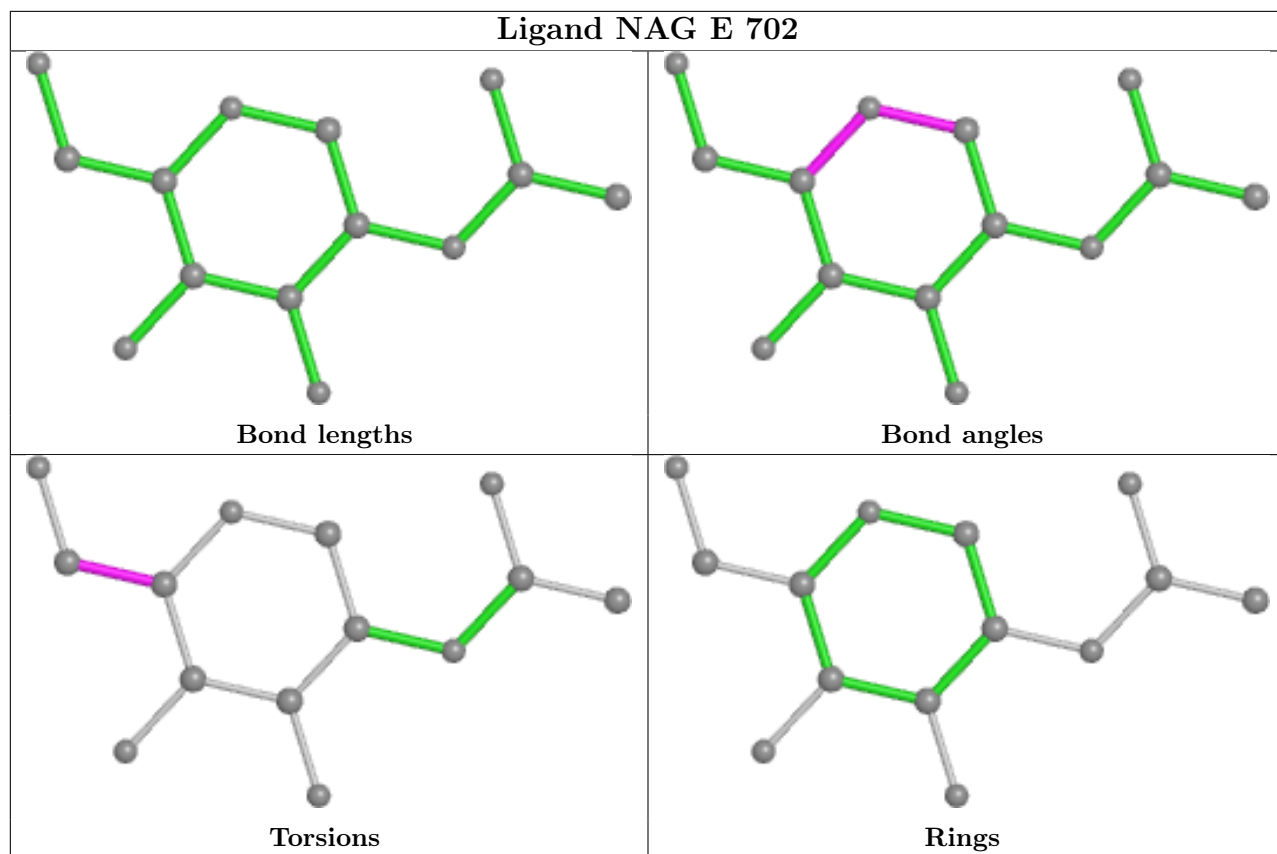
Mol	Chain	Res	Type	Atoms
4	G	702	NAG	O5-C5-C6-O6
4	E	702	NAG	O5-C5-C6-O6
4	A	702	NAG	O5-C5-C6-O6
4	C	702	NAG	O5-C5-C6-O6
4	A	702	NAG	C4-C5-C6-O6

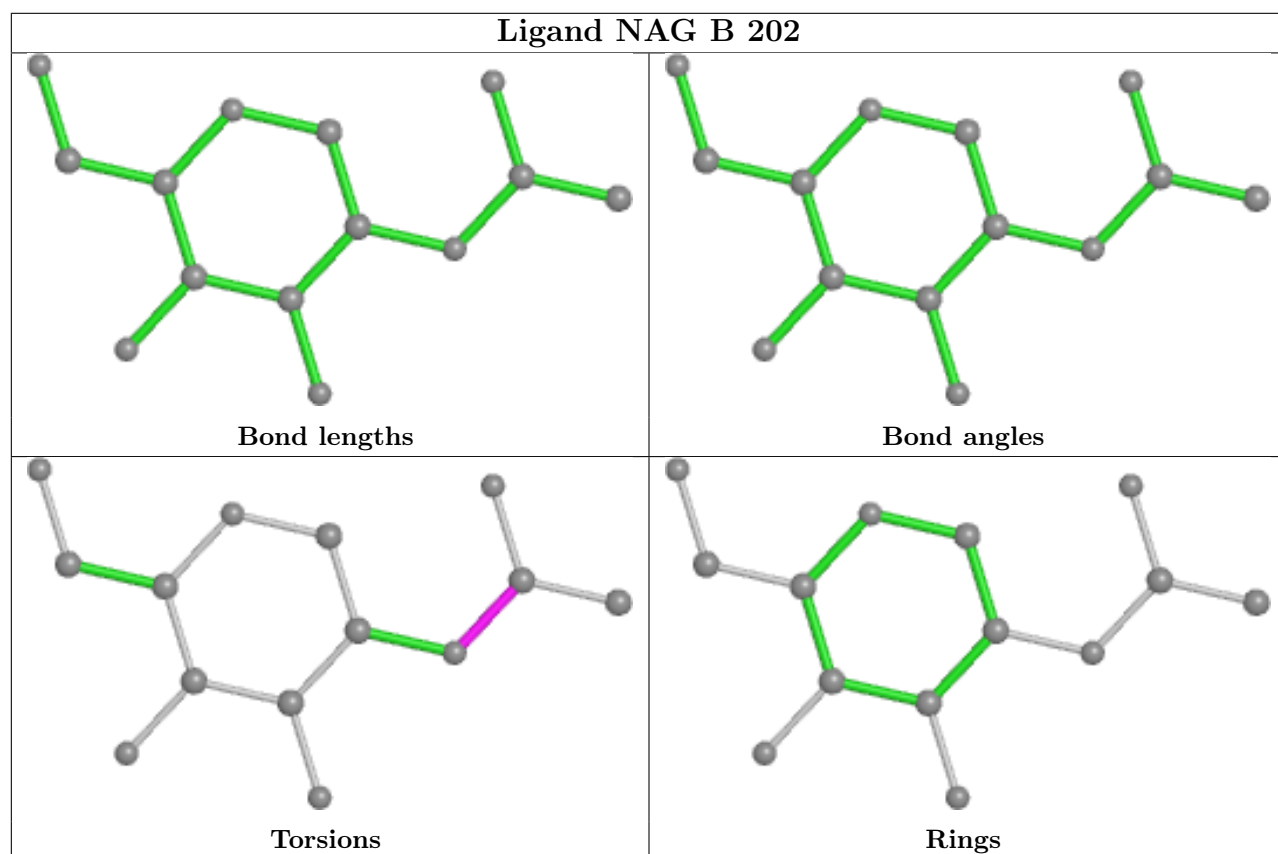
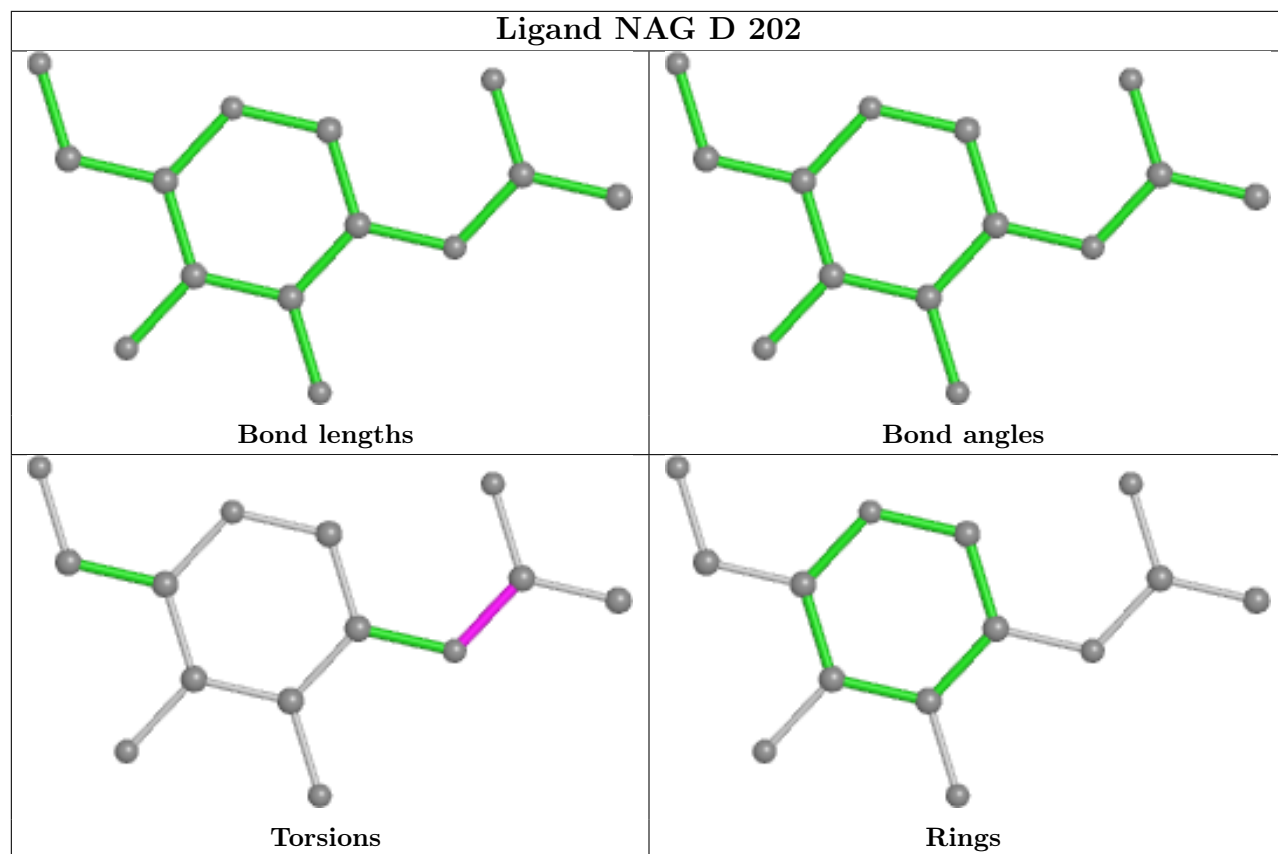
There are no ring outliers.

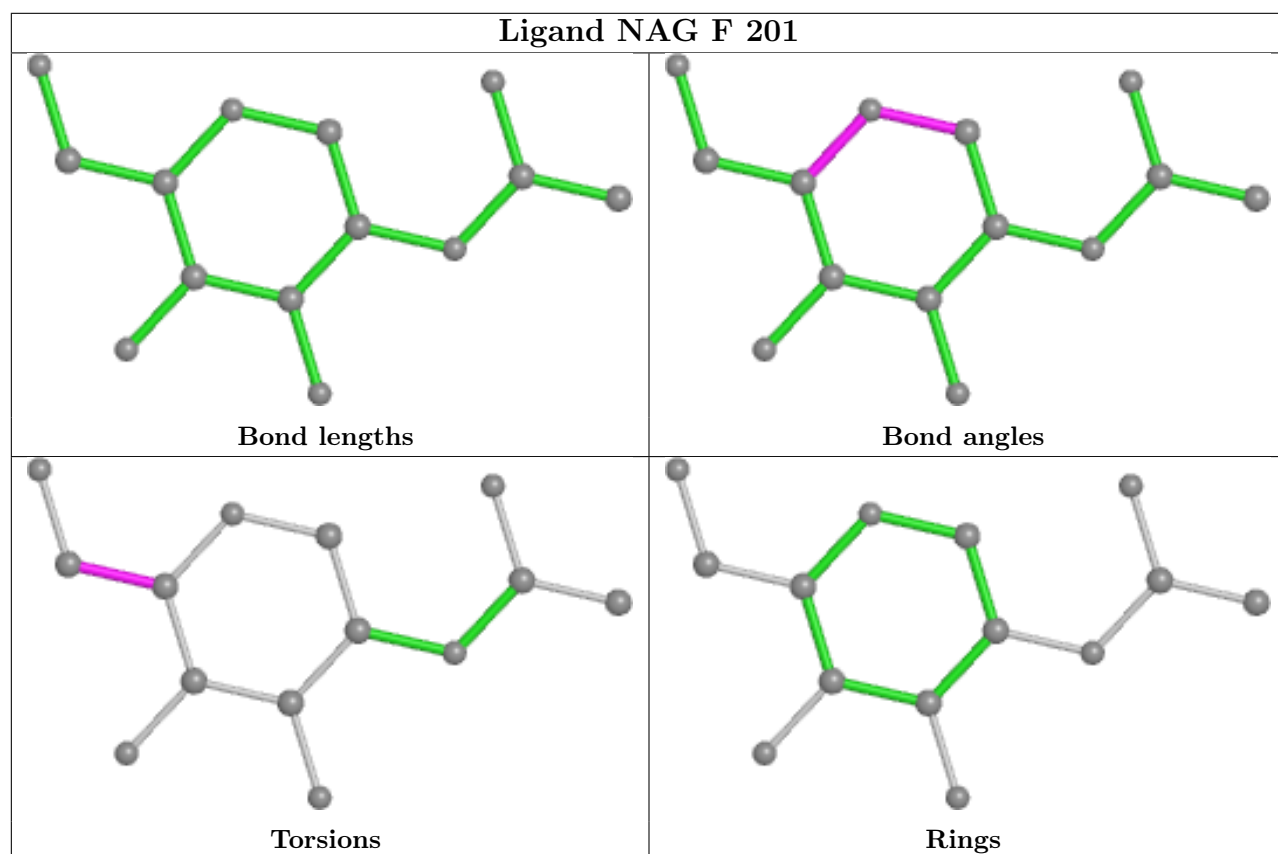
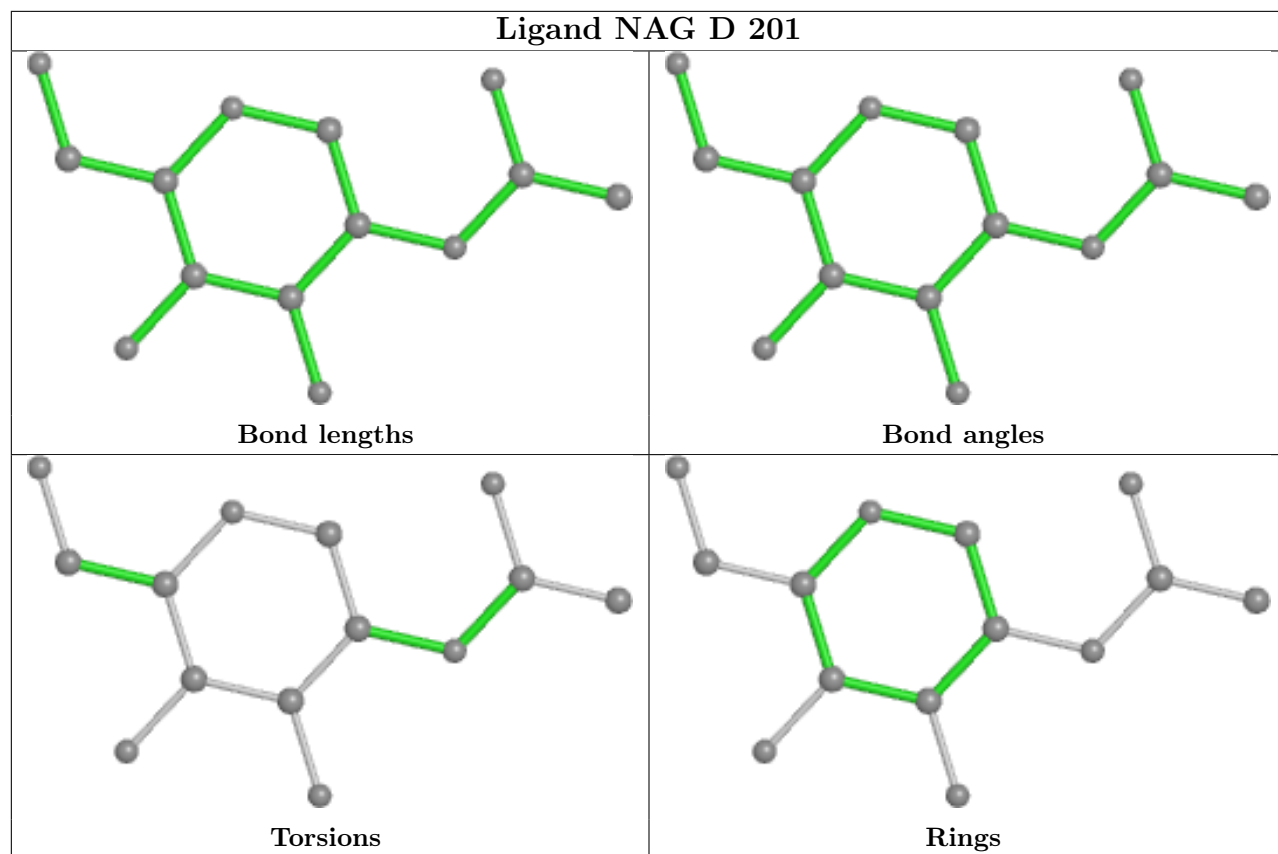
11 monomers are involved in 12 short contacts:

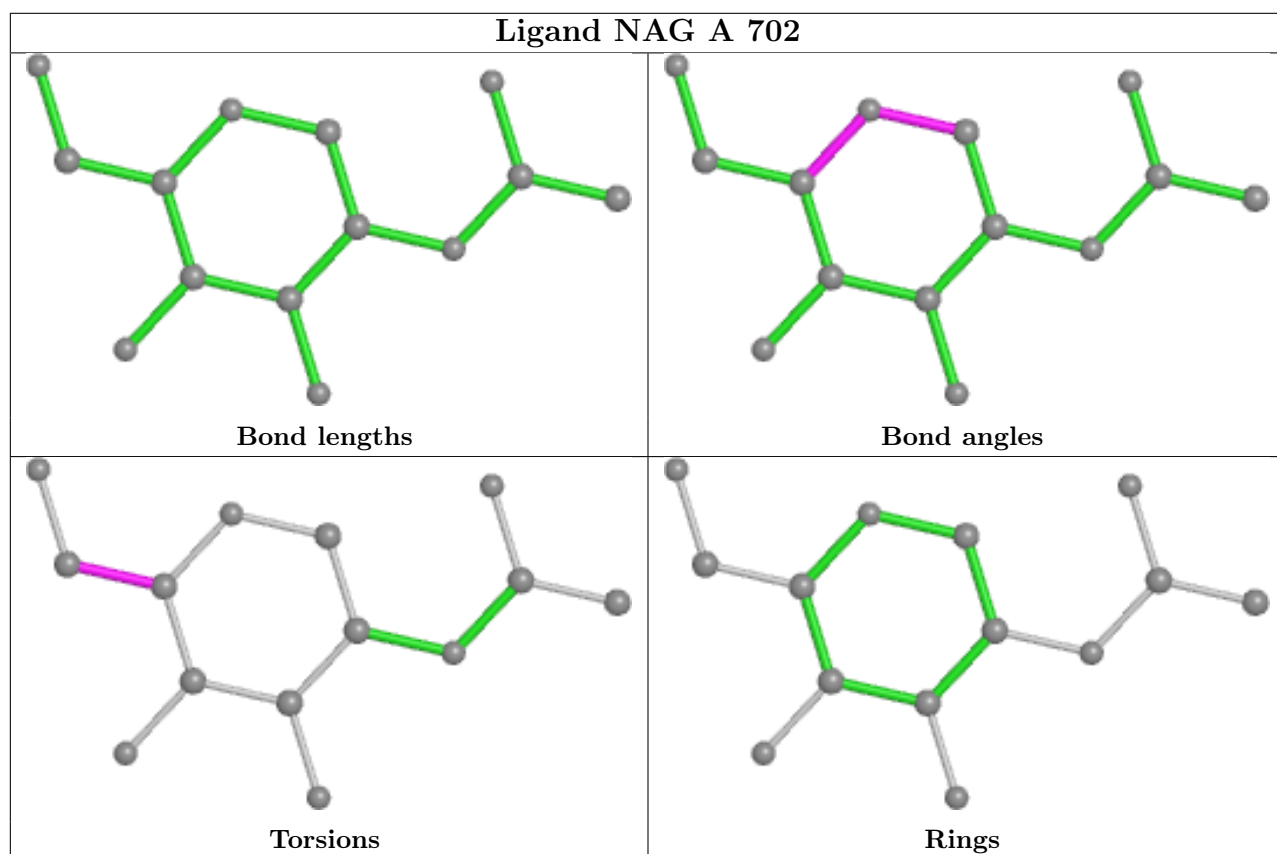
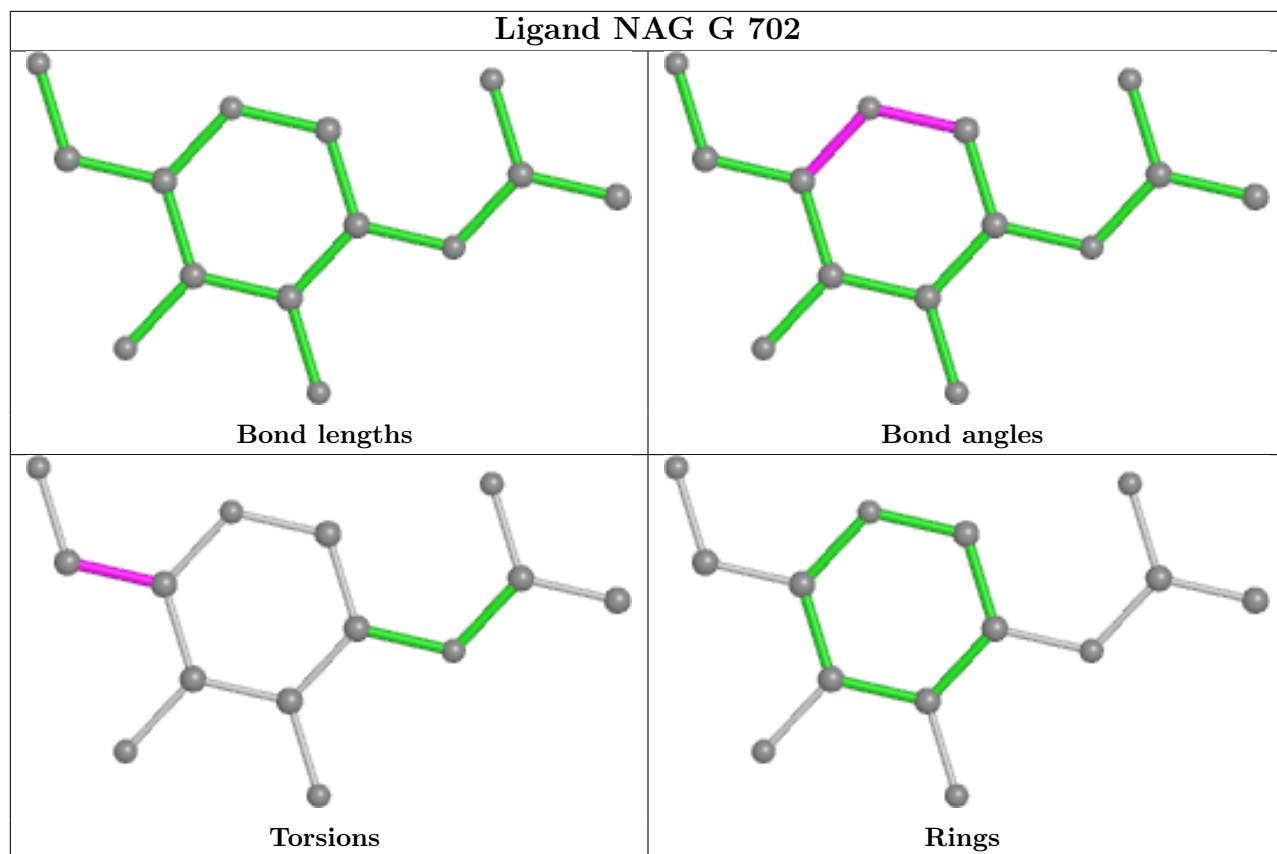
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	E	702	NAG	1	0
4	C	701	NAG	1	0
4	D	202	NAG	2	0
4	B	202	NAG	1	0
4	G	702	NAG	1	0
4	A	702	NAG	1	0
4	H	202	NAG	1	0
4	E	701	NAG	1	0
4	G	701	NAG	1	0
4	A	701	NAG	1	0
4	C	702	NAG	1	0

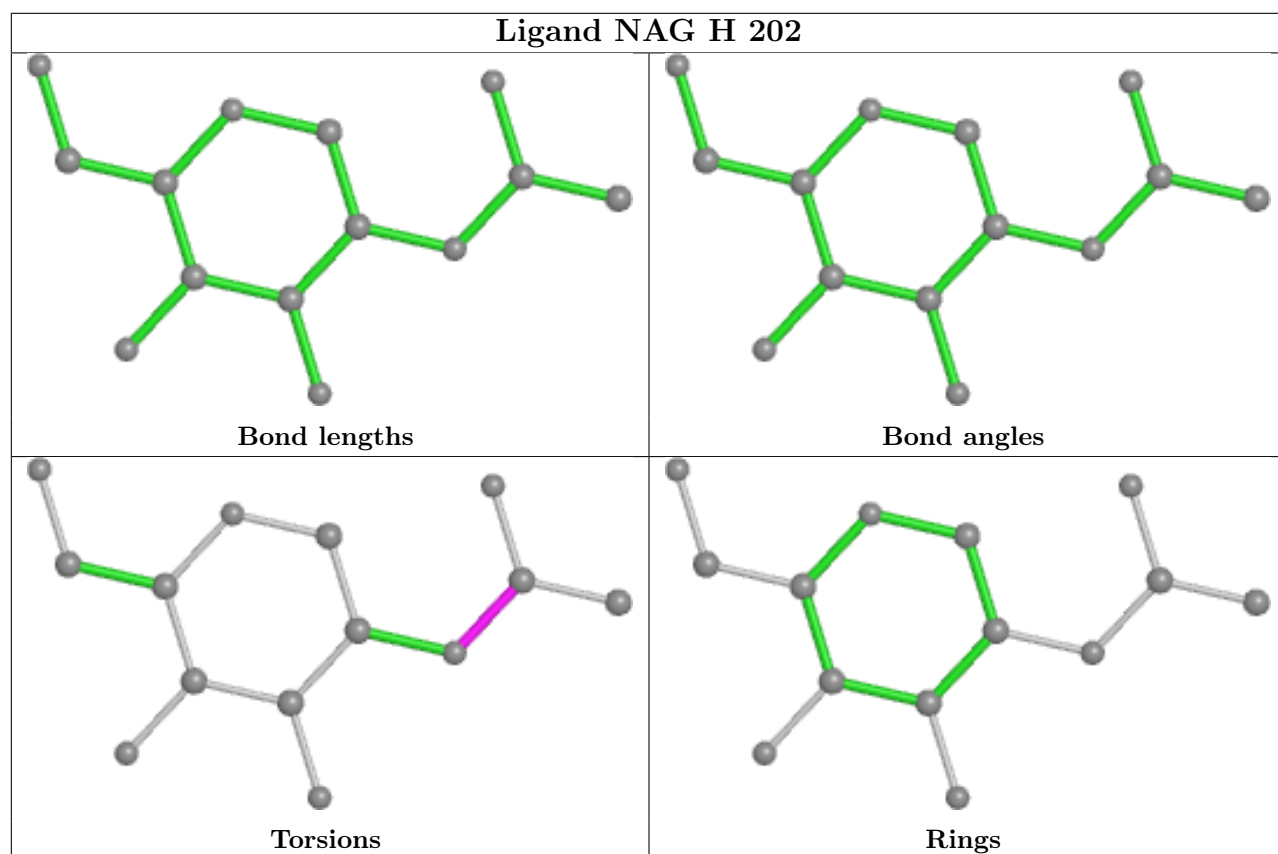
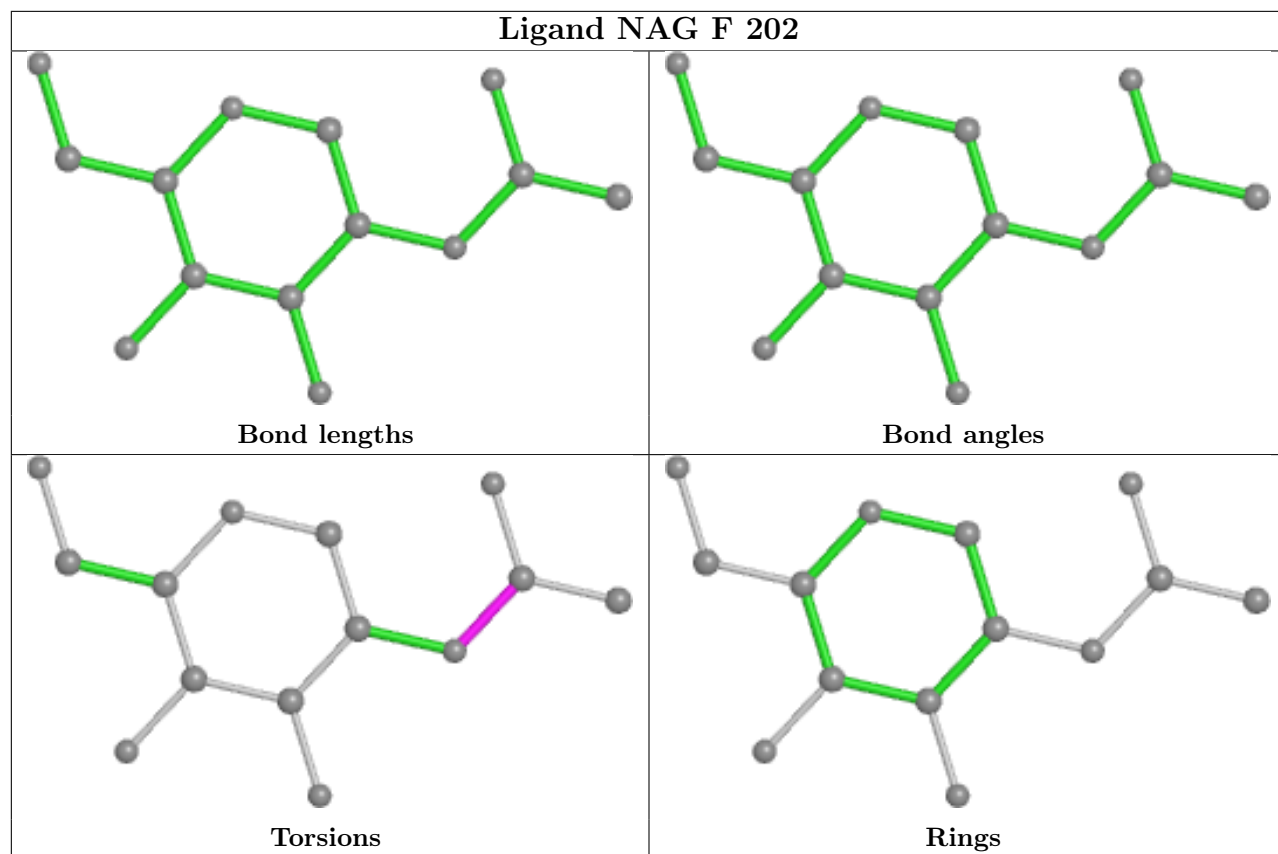
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

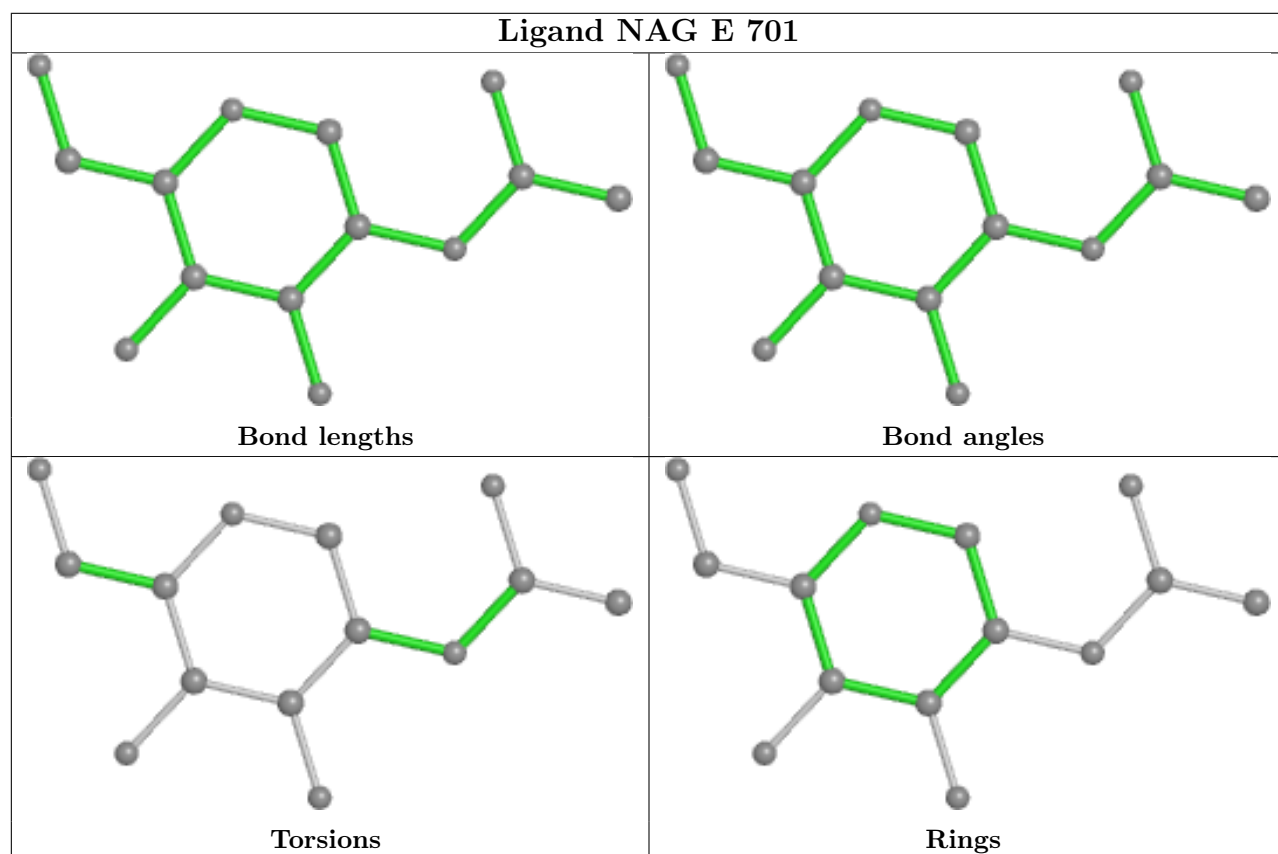
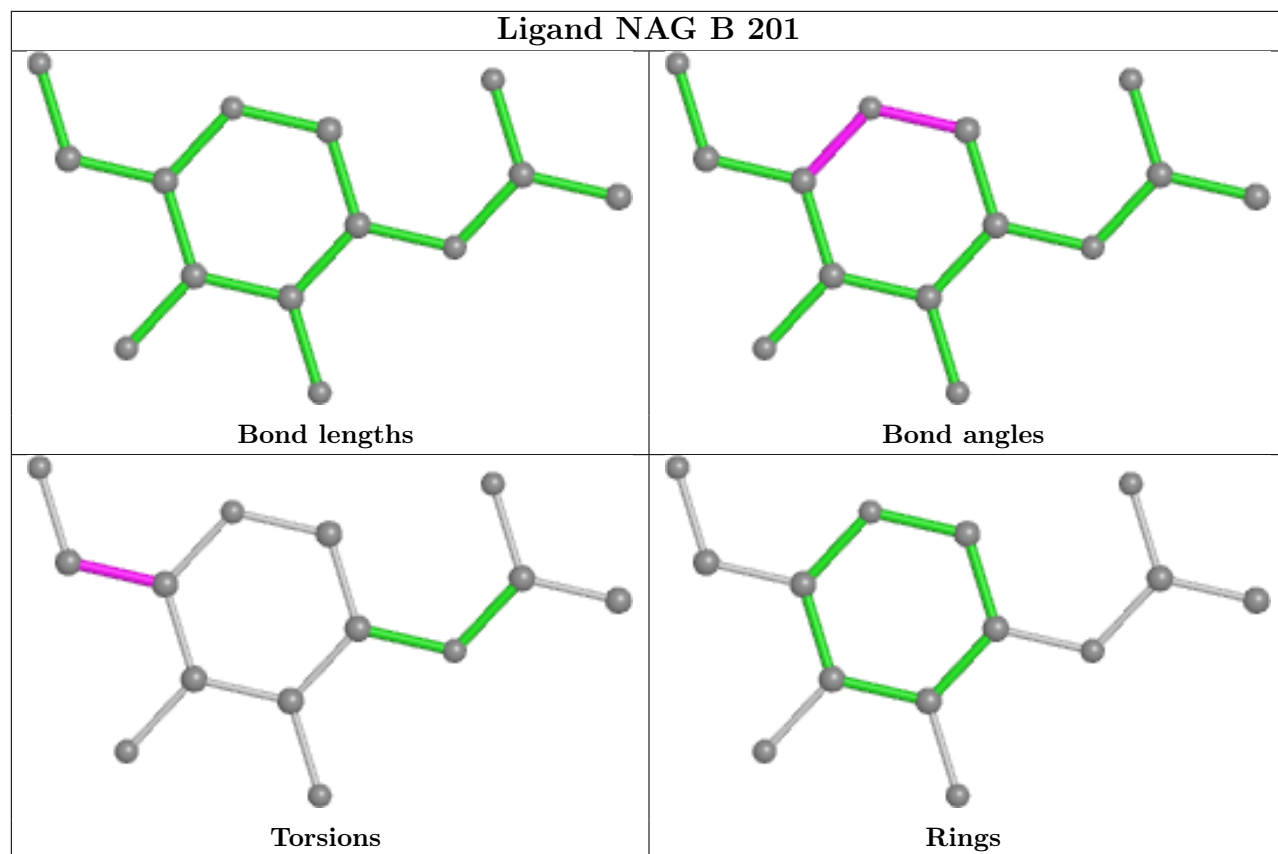


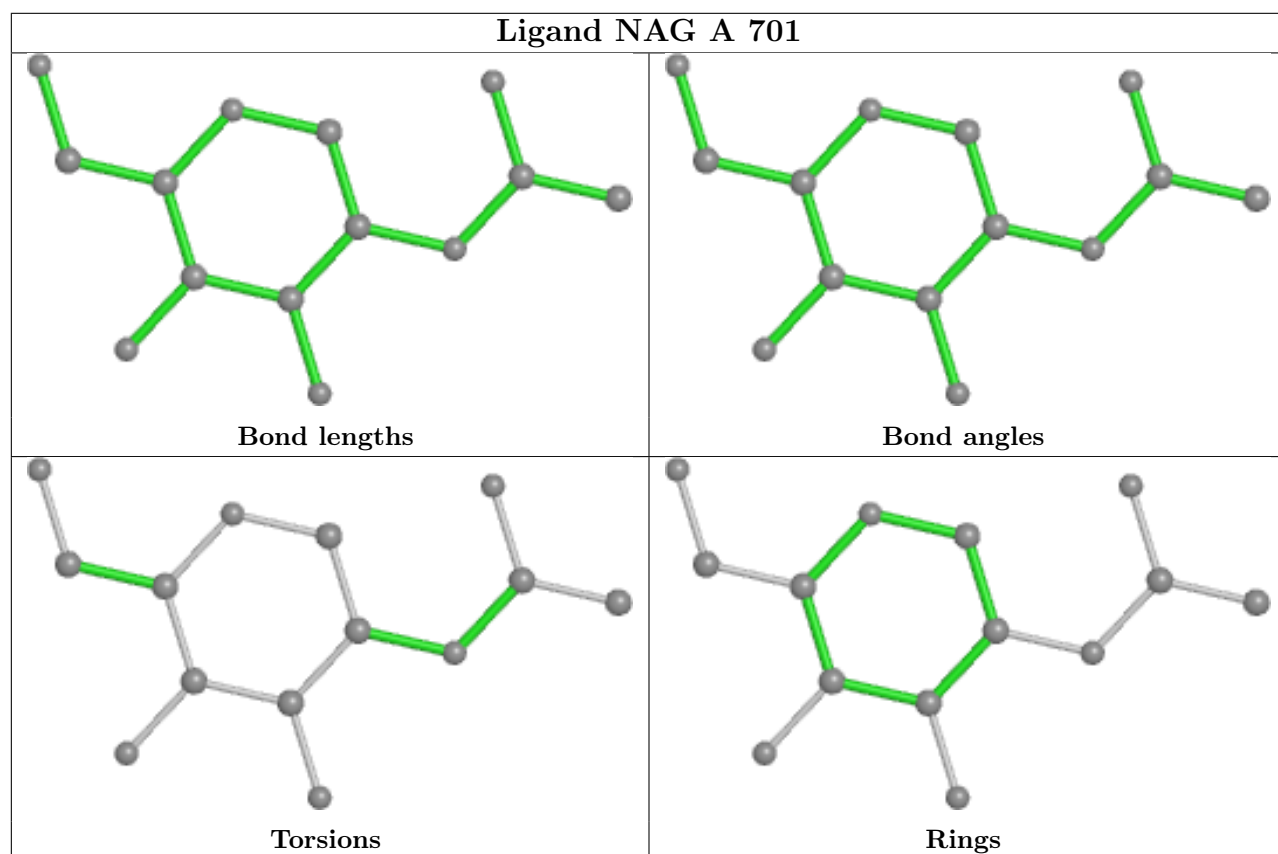
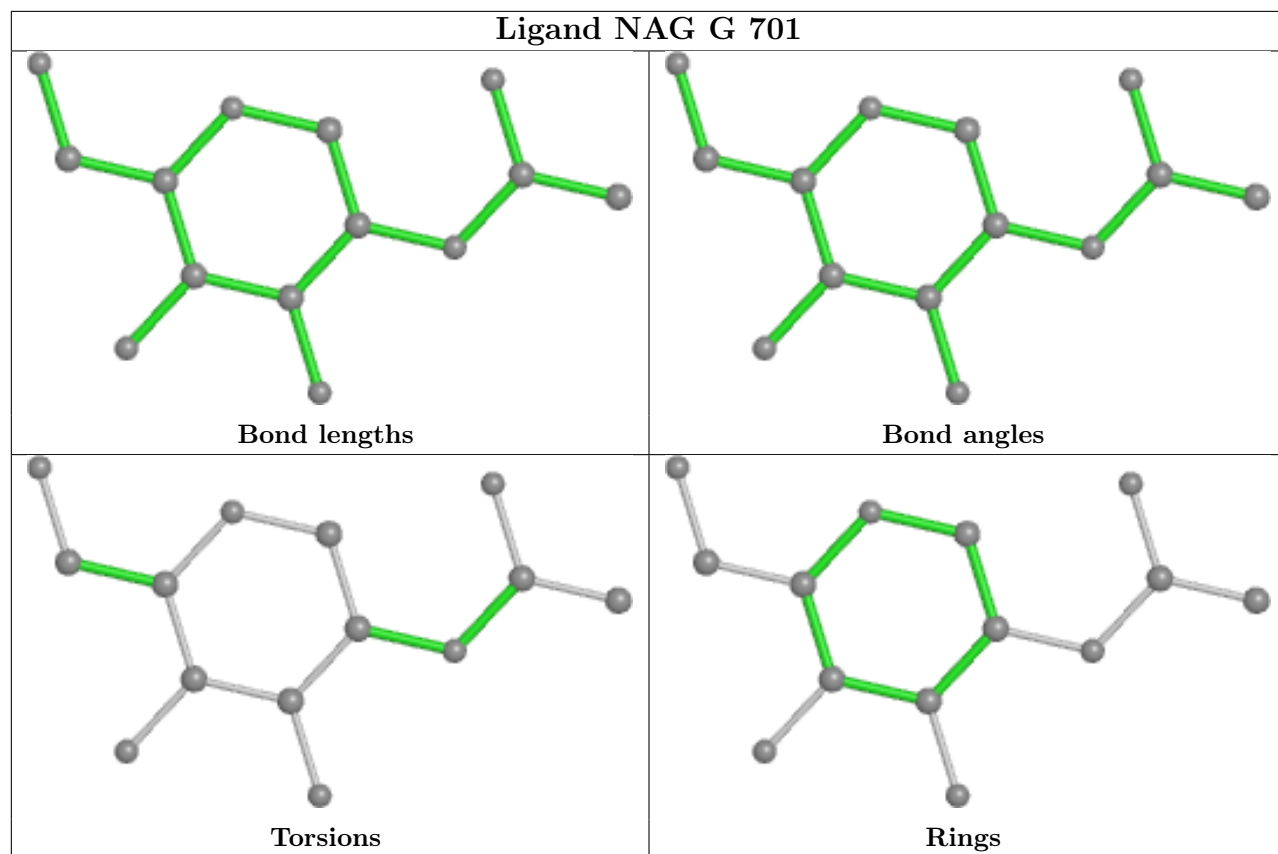


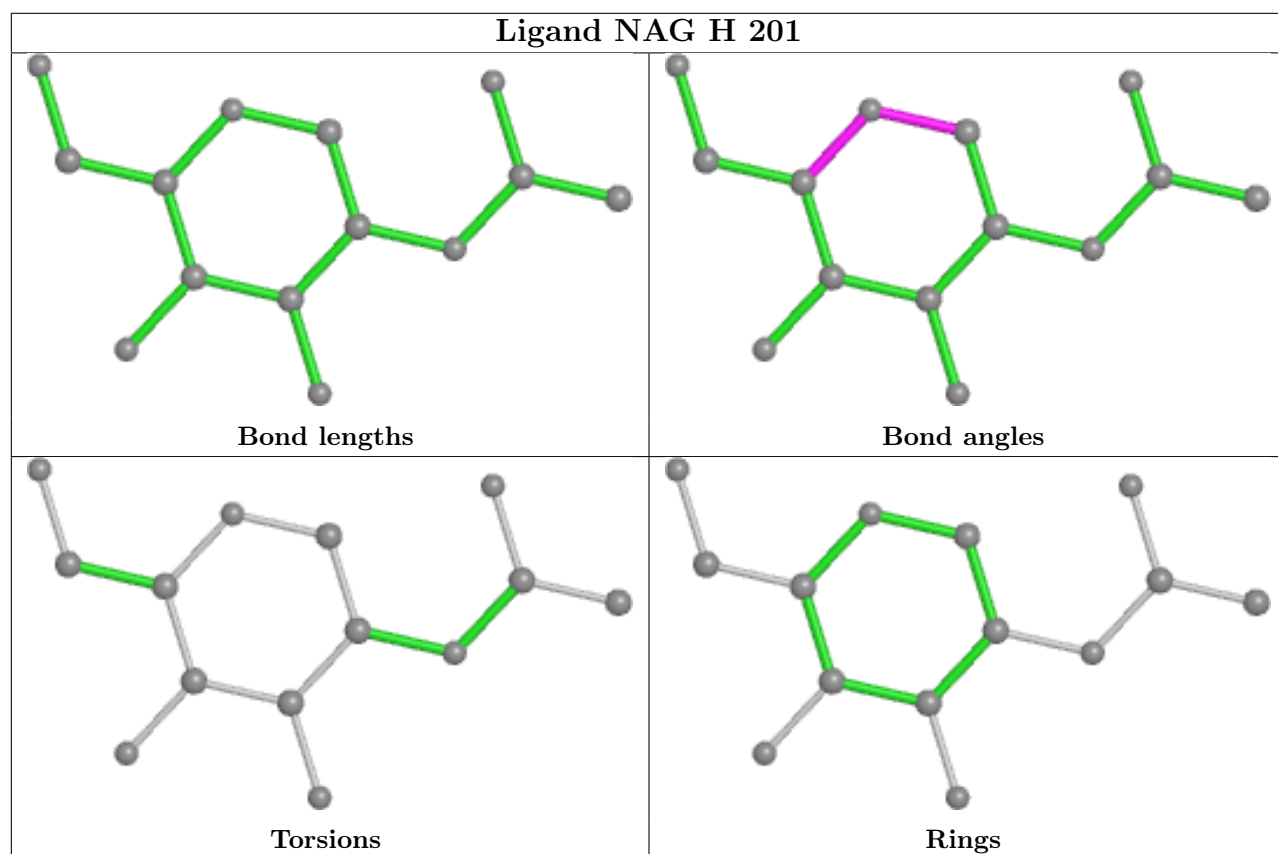
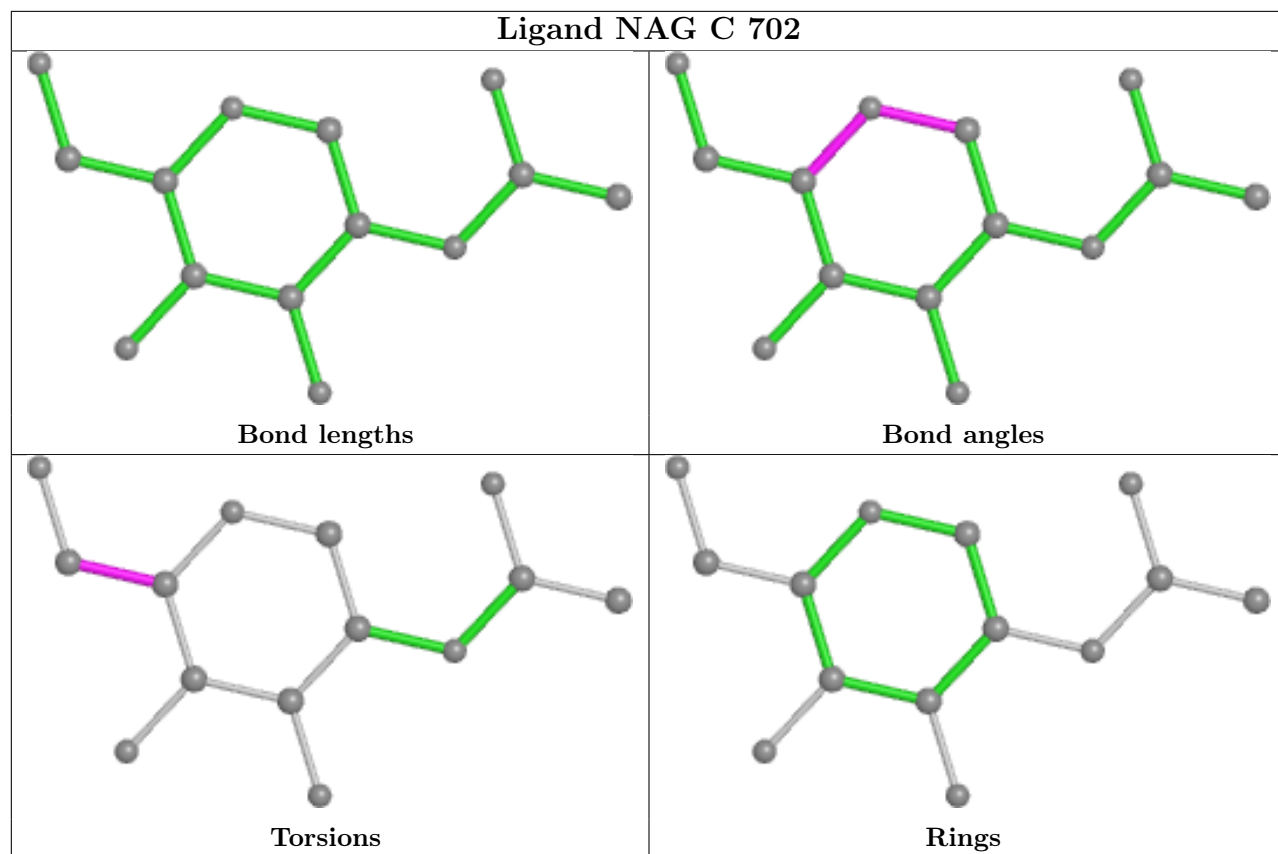












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

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

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

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å ²)	Q<0.9
1	A	655/662 (98%)	-0.03	22 (3%)	45 19	61, 108, 208, 295	0
1	C	655/662 (98%)	-0.04	23 (3%)	44 18	62, 105, 207, 293	0
1	E	655/662 (98%)	0.09	28 (4%)	35 13	66, 115, 214, 305	0
1	G	655/662 (98%)	0.10	32 (4%)	29 11	70, 117, 213, 307	0
2	B	109/114 (95%)	-0.03	3 (2%)	53 25	70, 112, 173, 235	0
2	D	109/114 (95%)	-0.13	2 (1%)	68 40	75, 107, 137, 157	0
2	F	109/114 (95%)	-0.09	2 (1%)	68 40	86, 121, 178, 224	0
2	H	109/114 (95%)	0.14	4 (3%)	41 17	90, 125, 185, 262	0
3	I	165/183 (90%)	-0.15	2 (1%)	79 54	70, 105, 173, 230	0
3	J	165/183 (90%)	-0.12	4 (2%)	59 30	68, 103, 168, 232	0
3	K	165/183 (90%)	-0.14	6 (3%)	42 17	72, 108, 187, 252	0
3	L	165/183 (90%)	-0.02	3 (1%)	68 40	66, 104, 180, 238	0
All	All	3716/3836 (96%)	-0.00	131 (3%)	44 18	61, 111, 203, 307	0

The worst 5 of 131 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	575	SER	22.9
1	A	575	SER	20.4
1	G	521	ARG	13.8
1	E	575	SER	8.9
1	C	574	SER	8.2

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

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

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

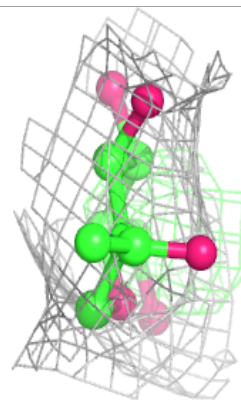
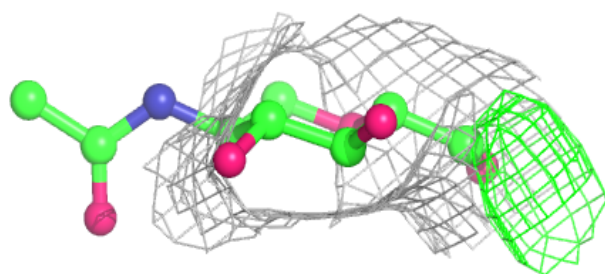
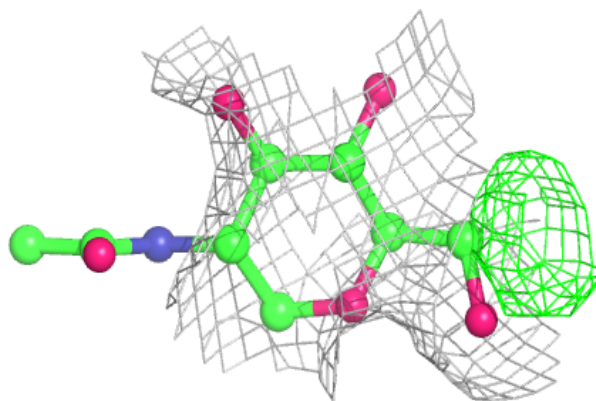
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	NAG	C	702	14/15	0.35	0.40	185,192,196,197	0
4	NAG	A	702	14/15	0.62	0.28	173,179,183,184	0
4	NAG	A	701	14/15	0.67	0.26	148,152,155,156	0
4	NAG	G	702	14/15	0.73	0.27	198,202,205,208	0
4	NAG	E	702	14/15	0.74	0.28	196,202,207,208	0
4	NAG	H	202	14/15	0.76	0.23	114,115,117,117	0
4	NAG	B	202	14/15	0.79	0.18	129,131,135,136	0
4	NAG	C	701	14/15	0.79	0.24	137,140,144,144	0
4	NAG	H	201	14/15	0.81	0.24	149,153,155,155	0
4	NAG	G	701	14/15	0.81	0.22	130,136,141,142	0
4	NAG	E	701	14/15	0.82	0.23	124,132,137,137	0
4	NAG	F	201	14/15	0.84	0.29	140,142,142,143	0
4	NAG	D	201	14/15	0.85	0.15	75,75,75,75	0
4	NAG	B	201	14/15	0.88	0.22	131,134,135,136	0
4	NAG	F	202	14/15	0.89	0.16	117,118,119,119	0
4	NAG	D	202	14/15	0.91	0.10	75,75,75,75	0

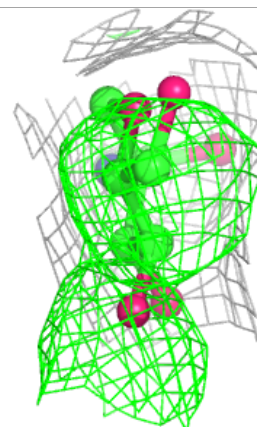
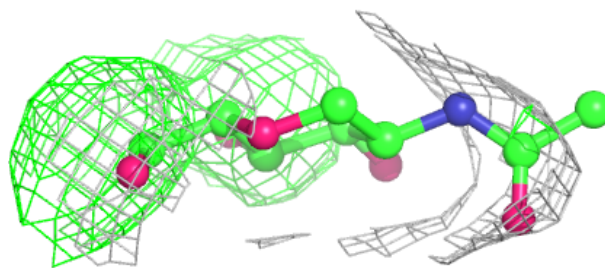
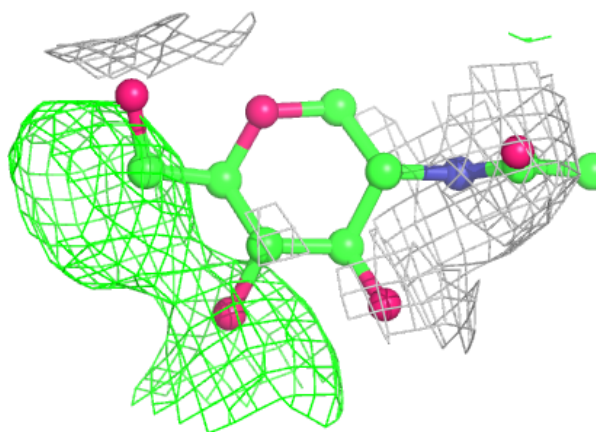
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around NAG C 702:

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

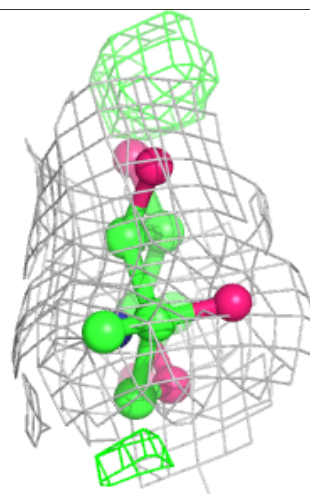
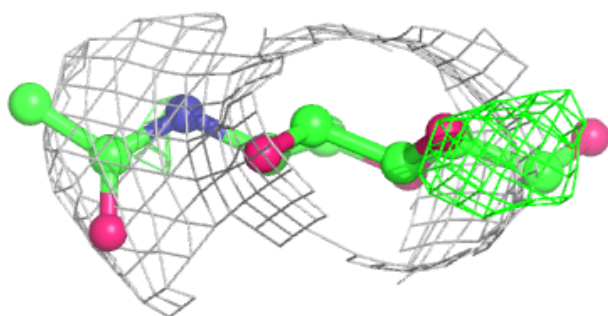
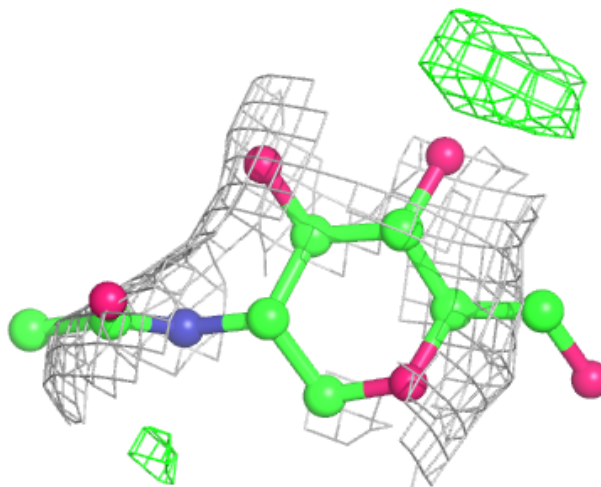
**Electron density around NAG A 702:**

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



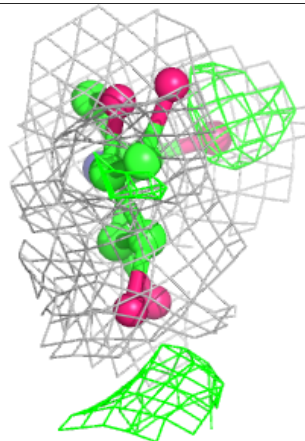
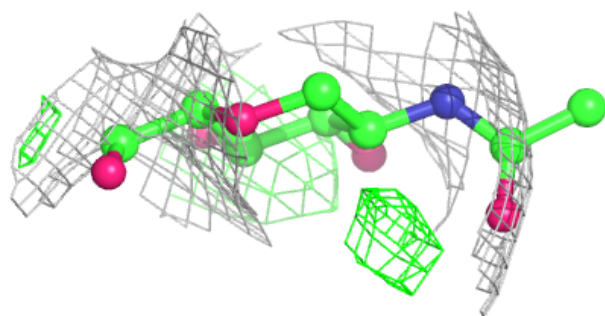
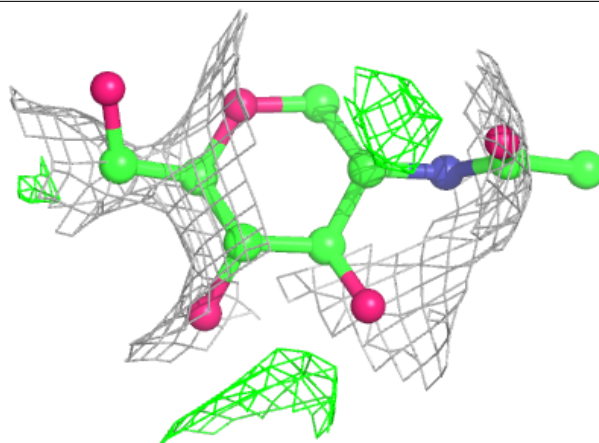
Electron density around NAG A 701:

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

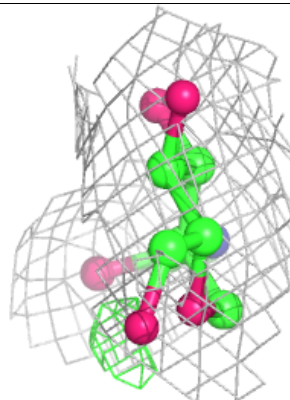
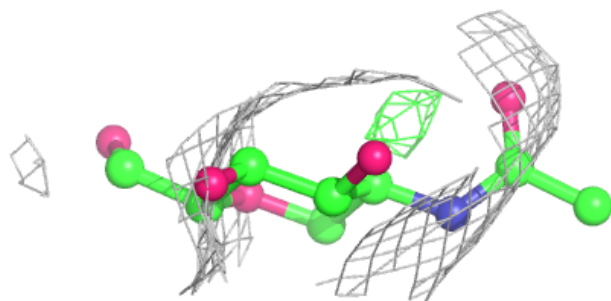
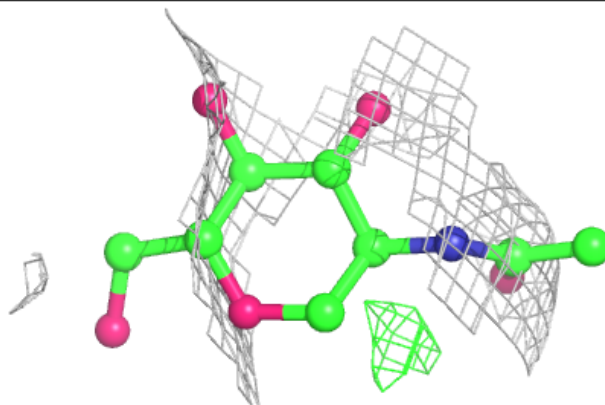


Electron density around NAG G 702:

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

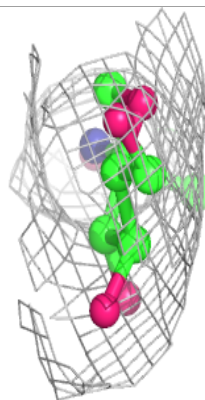
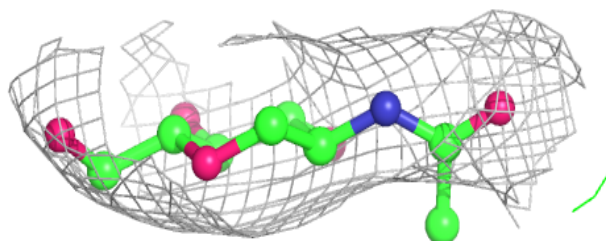
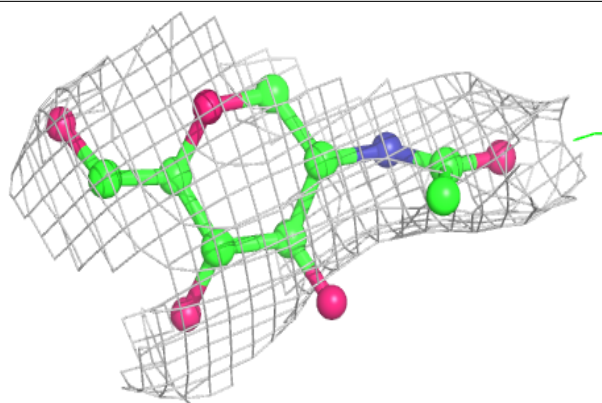
**Electron density around NAG E 702:**

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

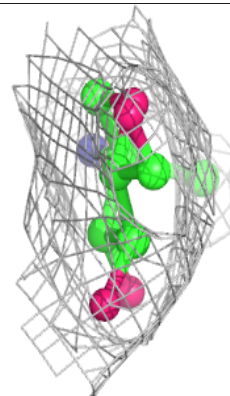
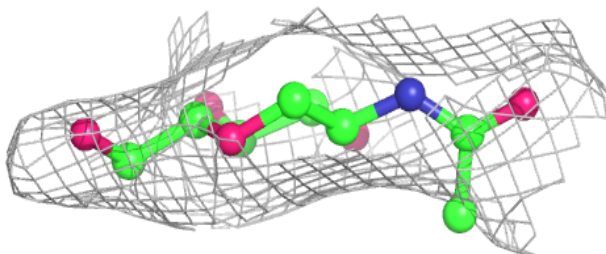
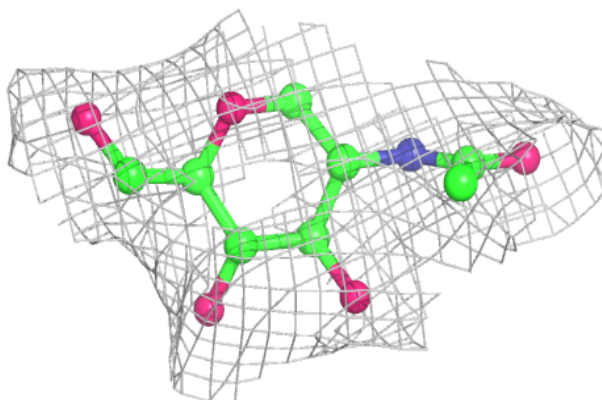


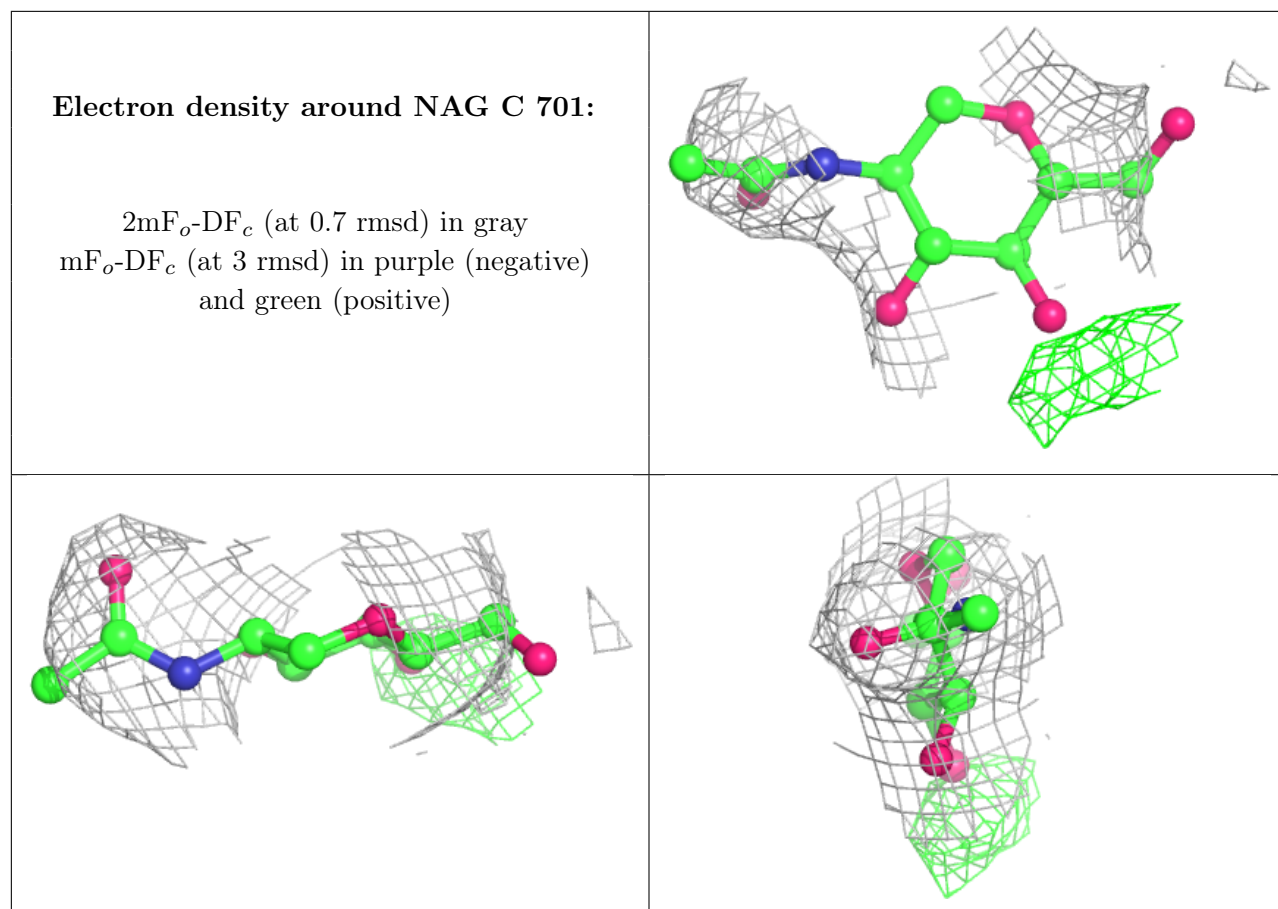
Electron density around NAG H 202:

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

**Electron density around NAG B 202:**

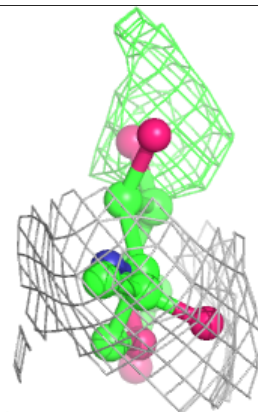
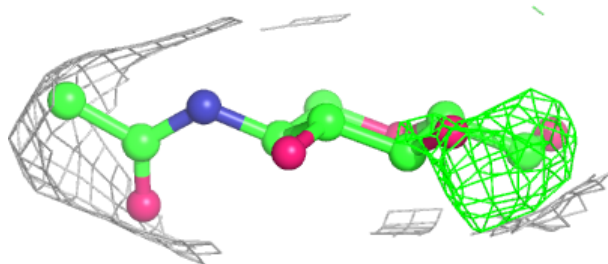
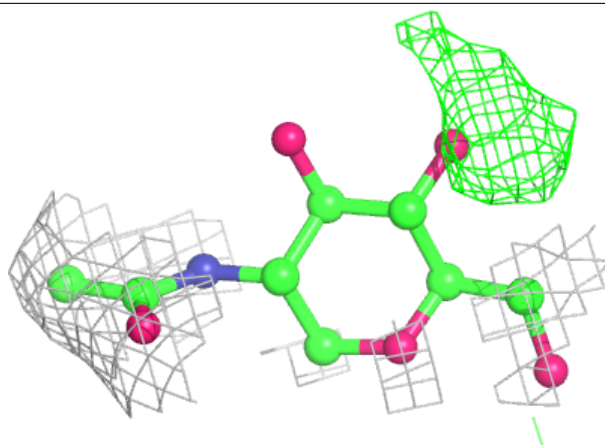
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



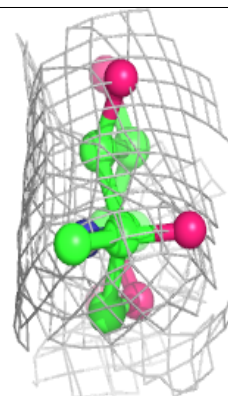
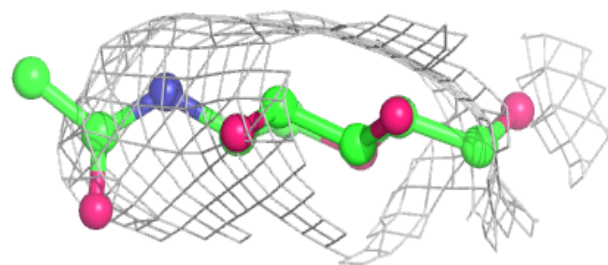
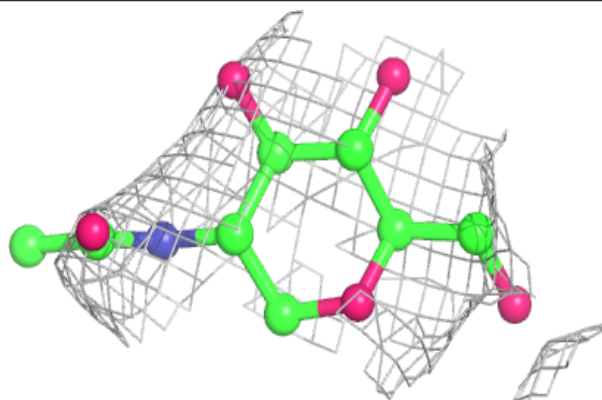


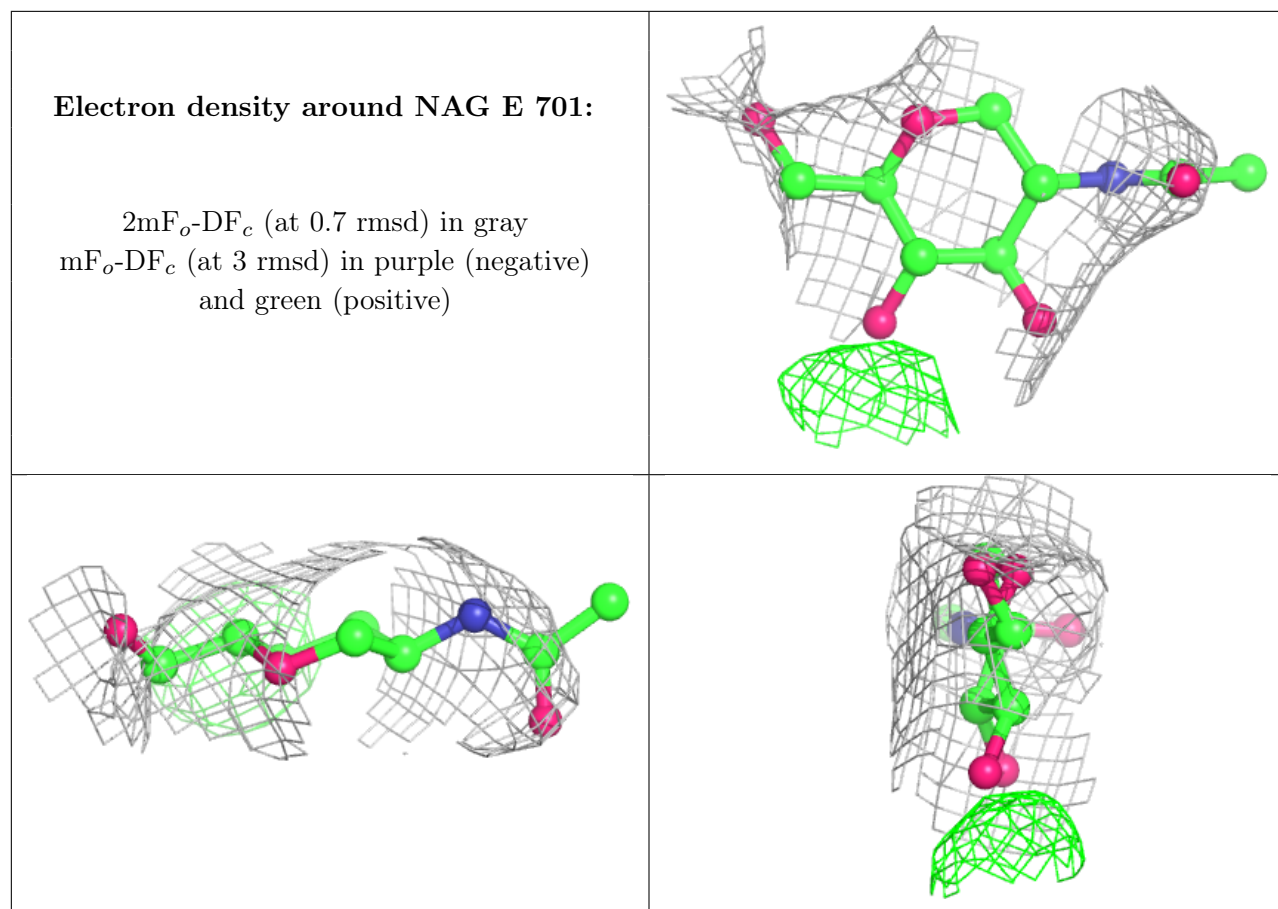
Electron density around NAG H 201:

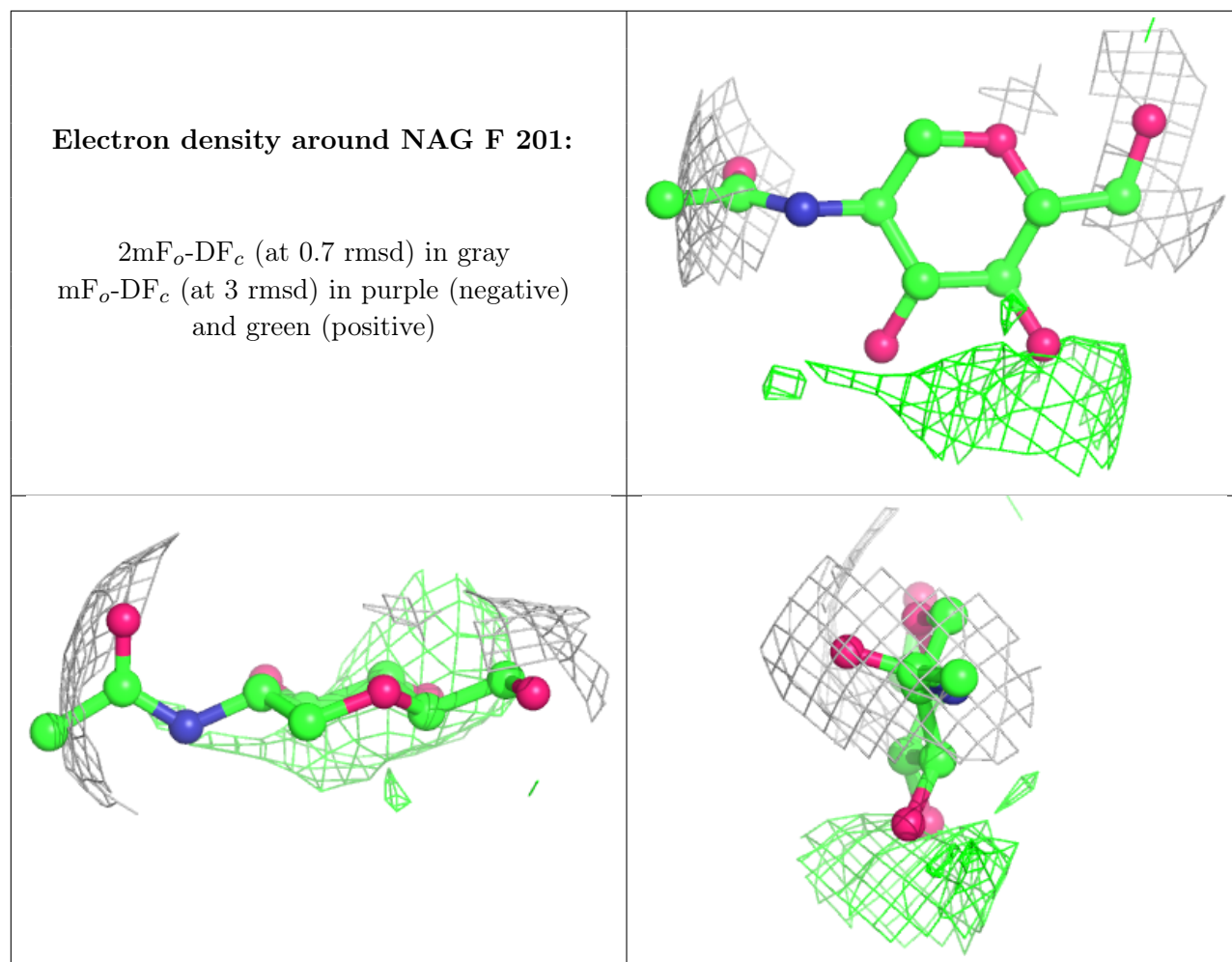
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

**Electron density around NAG G 701:**

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

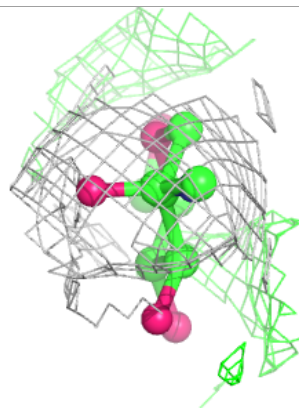
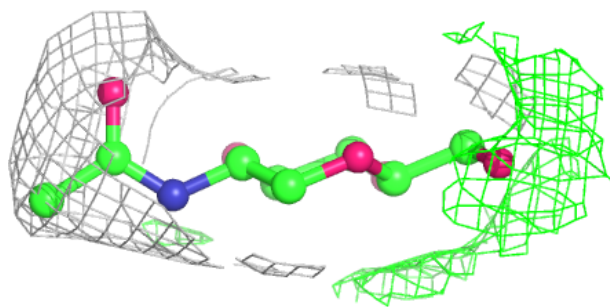
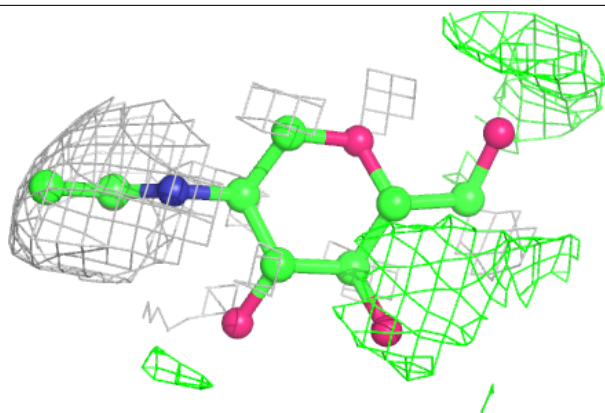




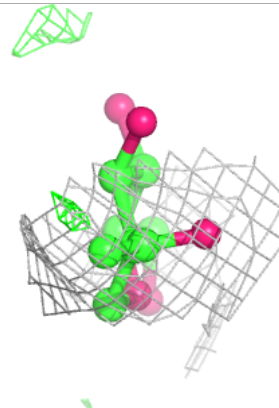
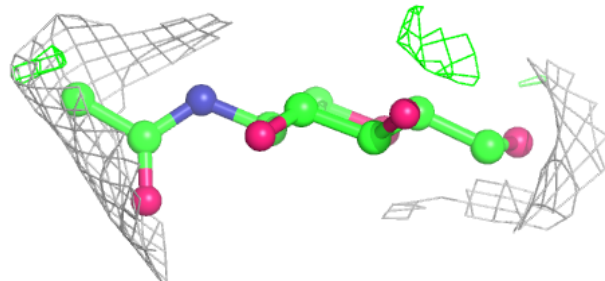
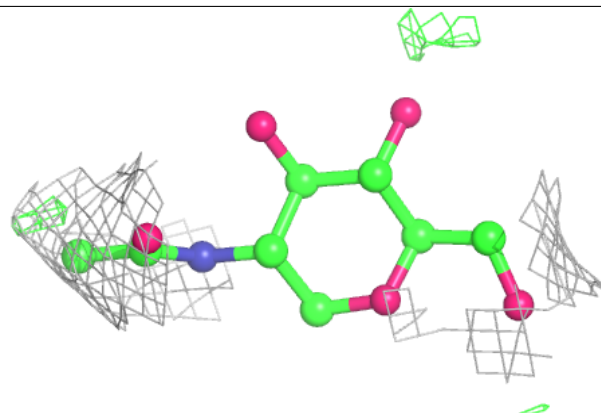


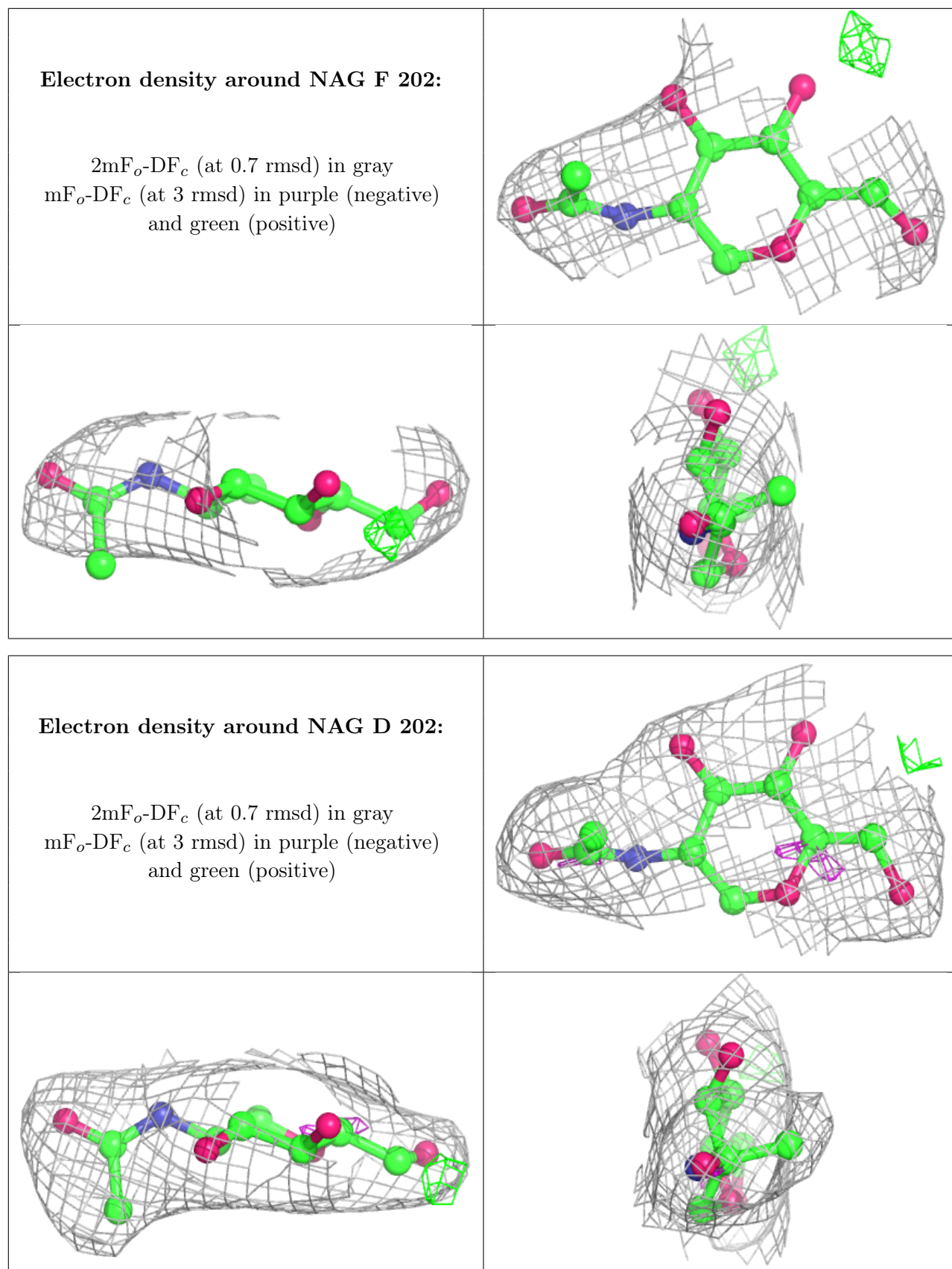
Electron density around NAG D 201:

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

**Electron density around NAG B 201:**

$2mF_o-DF_c$ (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.