



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 27, 2022 – 06:06 PM JST

PDB ID : 7XAZ
Title : Crystal structure of Omicron BA.1.1 RBD complexed with hACE2
Authors : Liao, H.; Meng, Y.; Li, W.
Deposited on : 2022-03-19
Resolution : 3.00 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 : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.29
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) : 2.29

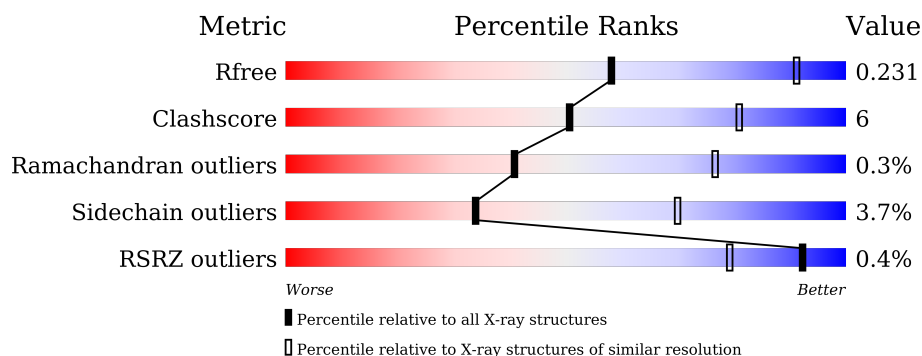
1 Overall quality at a glance

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	596	<div> <div>84%</div> <div>15%</div> </div>
1	C	596	<div> <div>%</div> <div>84%</div> <div>16%</div> </div>
2	B	195	<div> <div>78%</div> <div>20%</div> <div>•</div> </div>
2	D	195	<div> <div>%</div> <div>77%</div> <div>21%</div> <div>•</div> </div>
3	E	2	<div> <div>50%</div> <div>50%</div> </div>

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 13048 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 Angiotensin-converting enzyme 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	596	Total	C	N	O	S	0	1	0
			4869	3116	807	917	29			
1	C	596	Total	C	N	O	S	0	1	0
			4869	3116	807	917	29			

- Molecule 2 is a protein called Spike protein S1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	195	Total	C	N	O	S	0	0	0
			1563	1009	262	284	8			
2	D	195	Total	C	N	O	S	0	0	0
			1563	1009	262	284	8			

There are 32 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	339	ASP	GLY	variant	UNP P0DTC2
B	346	LYS	ARG	variant	UNP P0DTC2
B	371	LEU	SER	variant	UNP P0DTC2
B	373	PRO	SER	variant	UNP P0DTC2
B	375	PHE	SER	variant	UNP P0DTC2
B	417	ASN	LYS	variant	UNP P0DTC2
B	440	LYS	ASN	variant	UNP P0DTC2
B	446	SER	GLY	variant	UNP P0DTC2
B	477	ASN	SER	variant	UNP P0DTC2
B	478	LYS	THR	variant	UNP P0DTC2
B	484	ALA	GLU	variant	UNP P0DTC2
B	493	ARG	GLN	variant	UNP P0DTC2
B	496	SER	GLY	variant	UNP P0DTC2
B	498	ARG	GLN	variant	UNP P0DTC2
B	501	TYR	ASN	variant	UNP P0DTC2
B	505	HIS	TYR	variant	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
D	339	ASP	GLY	variant	UNP P0DTC2
D	346	LYS	ARG	variant	UNP P0DTC2
D	371	LEU	SER	variant	UNP P0DTC2
D	373	PRO	SER	variant	UNP P0DTC2
D	375	PHE	SER	variant	UNP P0DTC2
D	417	ASN	LYS	variant	UNP P0DTC2
D	440	LYS	ASN	variant	UNP P0DTC2
D	446	SER	GLY	variant	UNP P0DTC2
D	477	ASN	SER	variant	UNP P0DTC2
D	478	LYS	THR	variant	UNP P0DTC2
D	484	ALA	GLU	variant	UNP P0DTC2
D	493	ARG	GLN	variant	UNP P0DTC2
D	496	SER	GLY	variant	UNP P0DTC2
D	498	ARG	GLN	variant	UNP P0DTC2
D	501	TYR	ASN	variant	UNP P0DTC2
D	505	HIS	TYR	variant	UNP P0DTC2

- Molecule 3 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
3	E	2	Total	C	N	O	0	0	0
			28	16	2	10			

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

- Molecule 5 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	Zn	0	0
			1	1		

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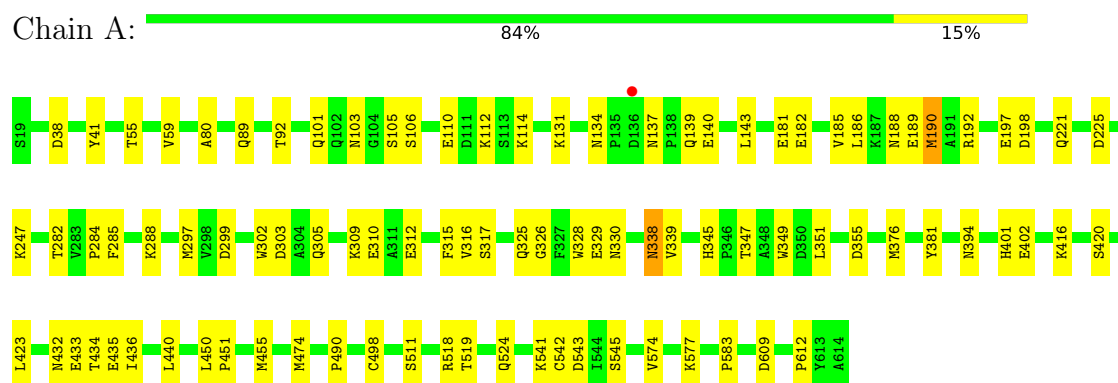
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	C	1	Total	Zn	0	0
			1	1		

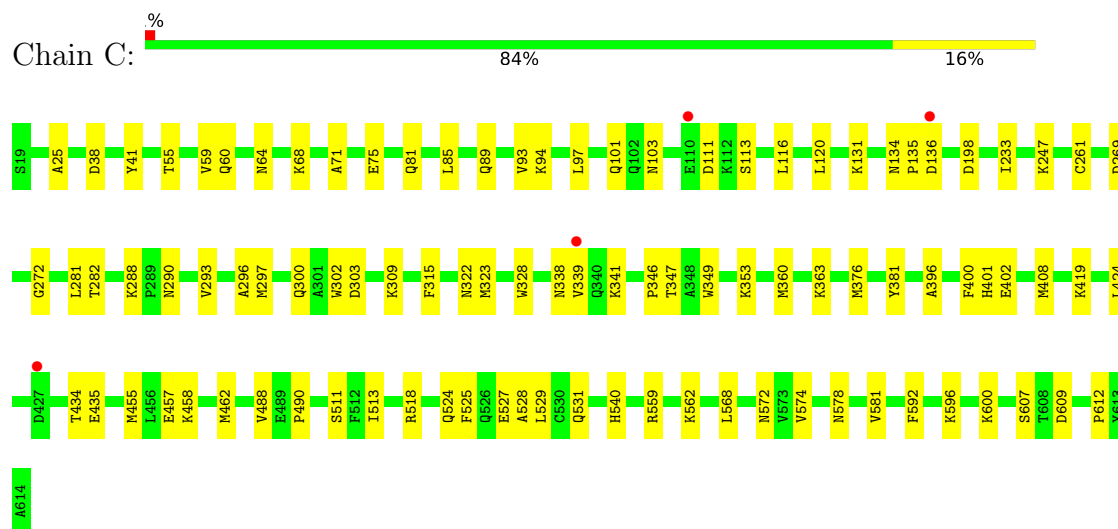
3 Residue-property plots

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

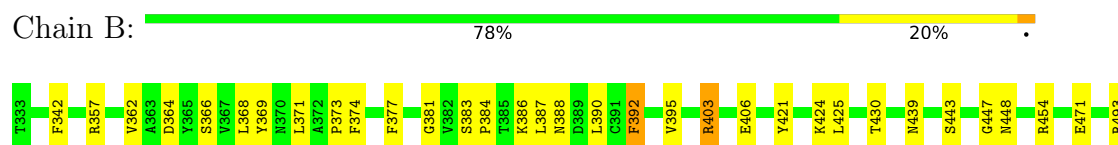
• Molecule 1: Angiotensin-converting enzyme 2



• Molecule 1: Angiotensin-converting enzyme 2

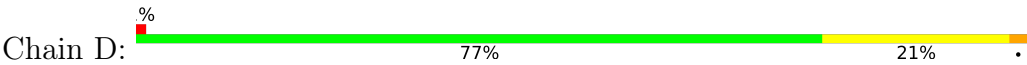


• Molecule 2: Spike protein S1





• Molecule 2: Spike protein S1



• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



4 Data and refinement statistics

Property	Value	Source
Space group	P 41	Depositor
Cell constants a, b, c, α , β , γ	129.52Å 129.52Å 189.20Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	37.59 – 3.00 37.59 – 3.00	Depositor EDS
% Data completeness (in resolution range)	87.4 (37.59-3.00) 87.5 (37.59-3.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.01 (at 3.01Å)	Xtriage
Refinement program	PHENIX 1.20_4459	Depositor
R, R_{free}	0.198 , 0.230 0.197 , 0.231	Depositor DCC
R_{free} test set	2725 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	57.9	Xtriage
Anisotropy	0.182	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 31.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.036 for h,-k,-l	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	13048	wwPDB-VP
Average B, all atoms (Å ²)	57.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.39% 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: ZN, 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	0.25	0/5010	0.44	0/6807
1	C	0.24	0/5010	0.45	0/6807
2	B	0.27	0/1610	0.53	0/2192
2	D	0.26	0/1610	0.52	0/2192
All	All	0.25	0/13240	0.46	0/17998

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	4869	0	4641	48	0
1	C	4869	0	4641	51	1
2	B	1563	0	1493	24	1
2	D	1563	0	1493	26	0
3	E	28	0	25	0	0
4	A	70	0	65	2	0
4	B	14	0	13	1	0
4	C	56	0	52	0	0
4	D	14	0	13	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	A	1	0	0	0	0
5	C	1	0	0	0	0
All	All	13048	0	12436	145	1

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 6.

All (145) 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)
2:D:362:VAL:HG13	2:D:526:GLY:HA2	1.63	0.79
2:B:403:ARG:HG3	2:B:406:GLU:HG3	1.63	0.79
2:D:357:ARG:HH21	2:D:394:ASN:HD21	1.33	0.77
1:A:134:ASN:OD1	1:A:137:ASN:HB3	1.85	0.76
1:A:134:ASN:OD1	1:A:137:ASN:CB	2.36	0.74
1:A:137:ASN:ND2	1:A:140:GLU:HG2	2.01	0.74
1:A:41:TYR:OH	2:B:500:THR:OG1	2.10	0.68
2:B:362:VAL:HG13	2:B:526:GLY:HA2	1.76	0.67
1:A:347:THR:OG1	1:A:349:TRP:NE1	2.29	0.65
1:A:131:LYS:HB3	1:A:143:LEU:HD23	1.78	0.65
1:A:490:PRO:HA	1:A:612:PRO:HG2	1.79	0.65
2:B:520:ALA:HB1	2:B:521:PRO:HD2	1.80	0.64
1:C:85:LEU:HD22	1:C:94:LYS:HG2	1.80	0.64
2:B:421:TYR:HB3	2:B:454:ARG:HG2	1.80	0.63
1:C:71:ALA:O	1:C:75:GLU:HG3	1.98	0.63
2:B:364:ASP:OD1	2:B:366:SER:OG	2.15	0.63
1:C:89:GLN:N	1:C:89:GLN:OE1	2.31	0.63
1:A:416:LYS:HD3	1:A:543:ASP:HB3	1.81	0.63
1:C:81:GLN:NE2	1:C:101:GLN:O	2.28	0.62
1:A:103:ASN:O	1:A:106:SER:OG	2.17	0.61
1:A:315:PHE:CE2	1:A:376:MET:HG2	2.36	0.61
2:D:439:ASN:OD1	2:D:443:SER:OG	2.14	0.61
2:D:342:PHE:HB2	4:D:601:NAG:H82	1.84	0.60
2:D:376:THR:HG23	2:D:378:LYS:HD2	1.85	0.58
1:C:347:THR:OG1	1:C:349:TRP:NE1	2.35	0.58
2:D:403:ARG:HG3	2:D:504:GLY:O	2.02	0.58
1:A:110:GLU:O	1:A:114:LYS:HG3	2.05	0.57
1:C:247:LYS:HB2	1:C:282:THR:HG22	1.87	0.56
1:A:435:GLU:OE2	1:A:541:LYS:NZ	2.22	0.56
1:C:64:ASN:O	1:C:68:LYS:HG2	2.06	0.56
1:C:400:PHE:CE1	1:C:525:PHE:HZ	2.25	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:293:VAL:O	1:C:297:MET:HG3	2.07	0.54
2:B:371:LEU:HB2	2:B:374:PHE:HB3	1.88	0.54
1:A:112:LYS:NZ	1:A:189:GLU:OE1	2.36	0.54
1:A:433:GLU:HG2	4:A:705:NAG:H82	1.89	0.54
2:B:448:ASN:HB3	2:B:497:PHE:HB2	1.89	0.54
1:A:80:ALA:O	1:A:101:GLN:NE2	2.35	0.53
1:A:188:ASN:O	1:A:192:ARG:HG3	2.08	0.53
1:A:55:THR:O	1:A:59:VAL:HG23	2.09	0.53
2:B:520:ALA:HB1	2:B:521:PRO:CD	2.38	0.53
1:C:435:GLU:OE1	1:C:540:HIS:NE2	2.42	0.53
1:C:288:LYS:HB3	1:C:434:THR:HG22	1.90	0.53
1:C:528:ALA:HB2	1:C:574:VAL:HG12	1.92	0.52
2:D:379:CYS:HB2	2:D:384:PRO:HD3	1.91	0.52
2:D:388:ASN:HB2	2:D:527:PRO:HD2	1.91	0.52
2:D:357:ARG:HH21	2:D:394:ASN:ND2	2.05	0.51
1:C:396:ALA:HB3	1:C:400:PHE:CD2	2.45	0.51
1:A:181:GLU:O	1:A:185:VAL:HG13	2.10	0.51
2:B:424:LYS:HD2	2:B:425:LEU:N	2.26	0.51
1:C:261:CYS:HB2	1:C:488:VAL:HB	1.92	0.50
1:A:402:GLU:HB3	1:A:518:ARG:HD2	1.93	0.50
1:C:435:GLU:OE1	1:C:540:HIS:CE1	2.65	0.50
1:A:105:SER:HA	1:A:190:MET:HG3	1.93	0.50
1:A:312:GLU:O	1:A:316:VAL:HG23	2.11	0.49
1:A:297:MET:HG2	1:A:423:LEU:HD22	1.94	0.49
2:B:381:GLY:HA3	2:B:430:THR:HG23	1.94	0.49
1:C:524:GLN:HB3	1:C:574:VAL:HG11	1.95	0.49
2:B:342:PHE:HB2	4:B:601:NAG:H82	1.94	0.49
1:C:315:PHE:CZ	1:C:408:MET:HG3	2.48	0.49
1:C:300:GLN:HB2	1:C:302:TRP:CD1	2.47	0.49
2:B:498:ARG:HB2	2:B:501:TYR:CE1	2.47	0.49
1:C:25:ALA:HB1	1:C:97:LEU:HD11	1.94	0.49
1:C:490:PRO:HA	1:C:612:PRO:HG2	1.94	0.49
1:A:524:GLN:HB3	1:A:574:VAL:HG11	1.94	0.48
2:B:369:TYR:HA	2:B:374:PHE:CE1	2.48	0.48
2:D:496:SER:O	2:D:496:SER:OG	2.32	0.48
1:A:524:GLN:HG2	1:A:583:PRO:HG2	1.96	0.48
1:A:182:GLU:O	1:A:185:VAL:HG22	2.13	0.48
1:A:325:GLN:NE2	1:A:329:GLU:OE2	2.47	0.48
1:C:134:ASN:ND2	1:C:135:PRO:O	2.46	0.48
2:B:392:PHE:HD2	2:B:517:LEU:HD12	1.79	0.48
1:A:351:LEU:HB2	1:A:355:ASP:HB3	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:116:LEU:HG	1:C:120:LEU:HD21	1.96	0.47
1:C:338:ASN:O	1:C:341:LYS:NZ	2.47	0.47
1:C:93:VAL:HG12	1:C:97:LEU:HD12	1.97	0.47
1:C:303:ASP:N	1:C:303:ASP:OD1	2.46	0.47
1:A:545:SER:HB2	4:A:706:NAG:H82	1.97	0.47
1:A:221:GLN:NE2	1:A:225:ASP:OD1	2.47	0.47
1:C:131:LYS:HB3	1:C:131:LYS:HE2	1.69	0.47
1:C:527:GLU:O	1:C:531:GLN:HG3	2.15	0.47
1:A:338:ASN:CG	1:A:339:VAL:H	2.18	0.46
1:C:41:TYR:OH	2:D:500:THR:OG1	2.15	0.46
1:C:568:LEU:O	1:C:572:ASN:ND2	2.44	0.46
1:A:182:GLU:O	1:A:186:LEU:HD12	2.15	0.46
1:A:192:ARG:NH1	1:A:197:GLU:O	2.48	0.46
2:D:357:ARG:NH2	2:D:394:ASN:HD21	2.07	0.46
1:A:432:ASN:OD1	1:A:432:ASN:N	2.49	0.45
2:B:386:LYS:O	2:B:390:LEU:HD12	2.16	0.45
1:C:233:ILE:HG12	1:C:581:VAL:HG21	1.99	0.45
1:A:284:PRO:HB2	1:A:285:PHE:CD2	2.52	0.45
1:C:346:PRO:HB3	1:C:360:MET:HG3	1.99	0.45
1:C:562:LYS:HB3	1:C:562:LYS:HE3	1.68	0.45
1:C:269:ASP:OD1	1:C:272:GLY:N	2.48	0.44
1:C:116:LEU:HG	1:C:120:LEU:CD2	2.47	0.44
1:C:68:LYS:HG2	1:C:68:LYS:H	1.67	0.44
2:D:442:ASP:C	2:D:448:ASN:HD22	2.19	0.44
1:A:137:ASN:CG	1:A:140:GLU:HG2	2.38	0.44
1:C:85:LEU:HG	1:C:101:GLN:NE2	2.31	0.44
1:A:302:TRP:CH2	1:A:310:GLU:HG3	2.53	0.44
2:B:383:SER:HB2	2:B:386:LYS:HD3	2.00	0.44
1:A:326:GLY:O	1:A:330:ASN:ND2	2.51	0.43
1:C:525:PHE:O	1:C:529:LEU:HG	2.18	0.43
1:A:288:LYS:HB3	1:A:434:THR:HG23	2.00	0.43
2:B:342:PHE:CZ	2:B:368:LEU:HD23	2.53	0.43
1:C:309:LYS:HD2	1:C:328:TRP:CH2	2.53	0.43
1:C:458:LYS:O	1:C:462:MET:HG3	2.18	0.43
1:C:353:LYS:HD3	2:D:501:TYR:CZ	2.54	0.43
2:D:360:ASN:H	2:D:523:THR:HB	1.82	0.43
2:B:447:GLY:HA2	2:B:498:ARG:HG3	2.00	0.43
2:B:384:PRO:HA	2:B:387:LEU:HG	2.01	0.43
1:A:247:LYS:HB2	1:A:282:THR:HG22	2.00	0.43
2:D:520:ALA:HB1	2:D:521:PRO:HD2	2.01	0.43
2:D:369:TYR:HA	2:D:374:PHE:CE1	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:419:LYS:HG3	1:C:424:LEU:HB3	2.01	0.42
1:C:457:GLU:HG2	1:C:513:ILE:HB	2.00	0.42
2:B:439:ASN:O	2:B:443:SER:HB2	2.18	0.42
1:C:323:MET:HE3	1:C:376:MET:HG2	2.00	0.42
2:D:479:PRO:HB2	2:D:481:ASN:OD1	2.19	0.42
2:D:399:SER:HA	2:D:510:VAL:O	2.19	0.42
1:A:338:ASN:CG	1:A:339:VAL:N	2.73	0.42
2:D:411:ALA:HB3	2:D:414:GLN:HG3	2.01	0.42
1:A:303:ASP:OD1	1:A:303:ASP:N	2.53	0.41
1:C:64:ASN:N	1:C:64:ASN:HD22	2.18	0.41
1:C:402:GLU:HB3	1:C:518:ARG:HD2	2.02	0.41
1:A:450:LEU:HD21	1:A:519:THR:HG21	2.03	0.41
1:C:322:ASN:OD1	1:C:322:ASN:N	2.53	0.41
1:C:338:ASN:HB3	1:C:339:VAL:H	1.50	0.41
1:A:474:MET:HE1	1:A:498:CYS:HA	2.02	0.41
1:C:296:ALA:O	1:C:300:GLN:HG3	2.19	0.41
1:C:596:LYS:HE2	1:C:596:LYS:HB2	1.74	0.41
1:C:600:LYS:HB2	1:C:600:LYS:HE3	1.70	0.41
1:A:450:LEU:HB2	1:A:451:PRO:HD3	2.02	0.41
2:D:406:GLU:OE1	2:D:495:TYR:OH	2.31	0.41
2:B:395:VAL:HG22	2:B:515:PHE:HB3	2.03	0.41
1:A:577:LYS:HE2	1:A:577:LYS:HB2	1.91	0.41
1:A:309:LYS:HD2	1:A:328:TRP:CH2	2.55	0.41
2:B:387:LEU:HD23	2:B:387:LEU:HA	1.87	0.41
2:D:375:PHE:CD1	2:D:375:PHE:N	2.89	0.41
2:D:384:PRO:HA	2:D:387:LEU:HD22	2.03	0.41
1:C:55:THR:O	1:C:59:VAL:HG23	2.21	0.40
1:A:38:ASP:OD2	2:B:493:ARG:NH2	2.54	0.40
1:A:345:HIS:O	1:A:347:THR:HG23	2.22	0.40
2:D:342:PHE:HZ	2:D:434:ILE:HD12	1.86	0.40
2:D:490:PHE:CE2	2:D:492:LEU:HB2	2.56	0.40
2:D:517:LEU:HD12	2:D:517:LEU:HA	1.96	0.40

All (1) 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)
2:B:386:LYS:NZ	1:C:609:ASP:OD2[3_545]	2.05	0.15

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	595/596 (100%)	584 (98%)	10 (2%)	1 (0%)	47	82
1	C	595/596 (100%)	583 (98%)	12 (2%)	0	100	100
2	B	193/195 (99%)	178 (92%)	13 (7%)	2 (1%)	15	53
2	D	193/195 (99%)	180 (93%)	12 (6%)	1 (0%)	29	68
All	All	1576/1582 (100%)	1525 (97%)	47 (3%)	4 (0%)	41	76

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	338	ASN
2	B	373	PRO
2	D	373	PRO
2	B	520	ALA

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	527/526 (100%)	509 (97%)	18 (3%)	37	72
1	C	527/526 (100%)	509 (97%)	18 (3%)	37	72
2	B	170/170 (100%)	162 (95%)	8 (5%)	26	63
2	D	170/170 (100%)	162 (95%)	8 (5%)	26	63
All	All	1394/1392 (100%)	1342 (96%)	52 (4%)	34	70

All (52) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	89	GLN
1	A	92	THR
1	A	139	GLN
1	A	190	MET
1	A	198	ASP
1	A	299	ASP
1	A	305	GLN
1	A	317	SER
1	A	381	TYR
1	A	394	ASN
1	A	401	HIS
1	A	420	SER
1	A	436	ILE
1	A	440	LEU
1	A	455	MET
1	A	511	SER
1	A	542	CYS
1	A	609	ASP
2	B	357	ARG
2	B	377	PHE
2	B	388	ASN
2	B	392	PHE
2	B	403	ARG
2	B	471	GLU
2	B	514	SER
2	B	515	PHE
1	C	38	ASP
1	C	60	GLN
1	C	103	ASN
1	C	111	ASP
1	C	113	SER
1	C	136	ASP
1	C	198	ASP
1	C	281	LEU
1	C	290	ASN
1	C	363	LYS
1	C	381	TYR
1	C	401	HIS
1	C	455	MET
1	C	511	SER
1	C	559	ARG
1	C	578	ASN

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Mol	Chain	Res	Type
1	C	592	PHE
1	C	607	SER
2	D	351	TYR
2	D	374	PHE
2	D	377	PHE
2	D	388	ASN
2	D	394	ASN
2	D	469	SER
2	D	496	SER
2	D	514	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	103	ASN
1	A	195	HIS
1	C	64	ASN
1	C	121	ASN
2	D	474	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 ⓘ

2 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
3	NAG	E	1	1,3	14,14,15	0.24	0	17,19,21	0.61	1 (5%)
3	NAG	E	2	3	14,14,15	0.23	0	17,19,21	0.48	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
3	NAG	E	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	E	2	3	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	1	NAG	C1-O5-C5	2.10	115.04	112.19

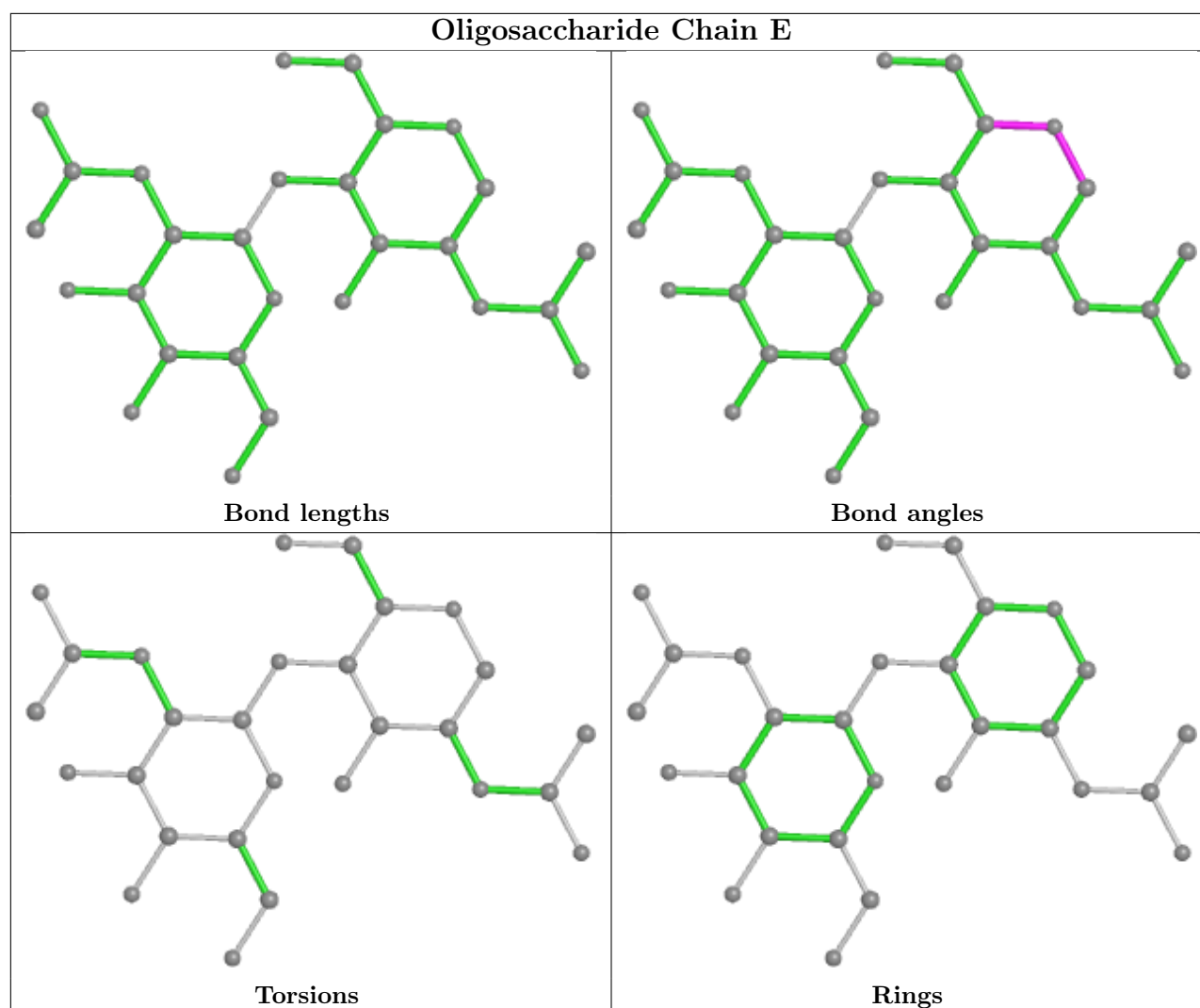
There are no chirality outliers.

There are no torsion outliers.

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 13 ligands modelled in this entry, 2 are monoatomic - leaving 11 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	$\# Z > 2$
4	NAG	A	703	1	14,14,15	0.26	0	17,19,21	0.45	0
4	NAG	A	705	1	14,14,15	0.25	0	17,19,21	1.02	1 (5%)
4	NAG	C	705	1	14,14,15	0.17	0	17,19,21	0.55	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	NAG	C	702	1	14,14,15	0.31	0	17,19,21	0.40	0
4	NAG	C	704	1	14,14,15	0.35	0	17,19,21	0.77	1 (5%)
4	NAG	A	702	1	14,14,15	0.38	0	17,19,21	0.54	0
4	NAG	C	701	1	14,14,15	0.31	0	17,19,21	0.57	0
4	NAG	B	601	2	14,14,15	0.31	0	17,19,21	0.55	0
4	NAG	D	601	2	14,14,15	0.65	1 (7%)	17,19,21	0.84	1 (5%)
4	NAG	A	706	1	14,14,15	0.27	0	17,19,21	0.48	0
4	NAG	A	701	1	14,14,15	0.27	0	17,19,21	0.59	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	A	703	1	-	0/6/23/26	0/1/1/1
4	NAG	A	705	1	-	1/6/23/26	0/1/1/1
4	NAG	C	705	1	-	3/6/23/26	0/1/1/1
4	NAG	C	702	1	-	2/6/23/26	0/1/1/1
4	NAG	C	704	1	-	2/6/23/26	0/1/1/1
4	NAG	A	702	1	-	2/6/23/26	0/1/1/1
4	NAG	C	701	1	-	0/6/23/26	0/1/1/1
4	NAG	B	601	2	-	0/6/23/26	0/1/1/1
4	NAG	D	601	2	-	2/6/23/26	0/1/1/1
4	NAG	A	706	1	-	2/6/23/26	0/1/1/1
4	NAG	A	701	1	-	0/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	601	NAG	O5-C1	2.20	1.47	1.43

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	705	NAG	C1-O5-C5	3.54	116.99	112.19
4	C	704	NAG	C1-O5-C5	2.84	116.04	112.19
4	D	601	NAG	C1-O5-C5	2.61	115.73	112.19

There are no chirality outliers.

All (14) torsion outliers are listed below:

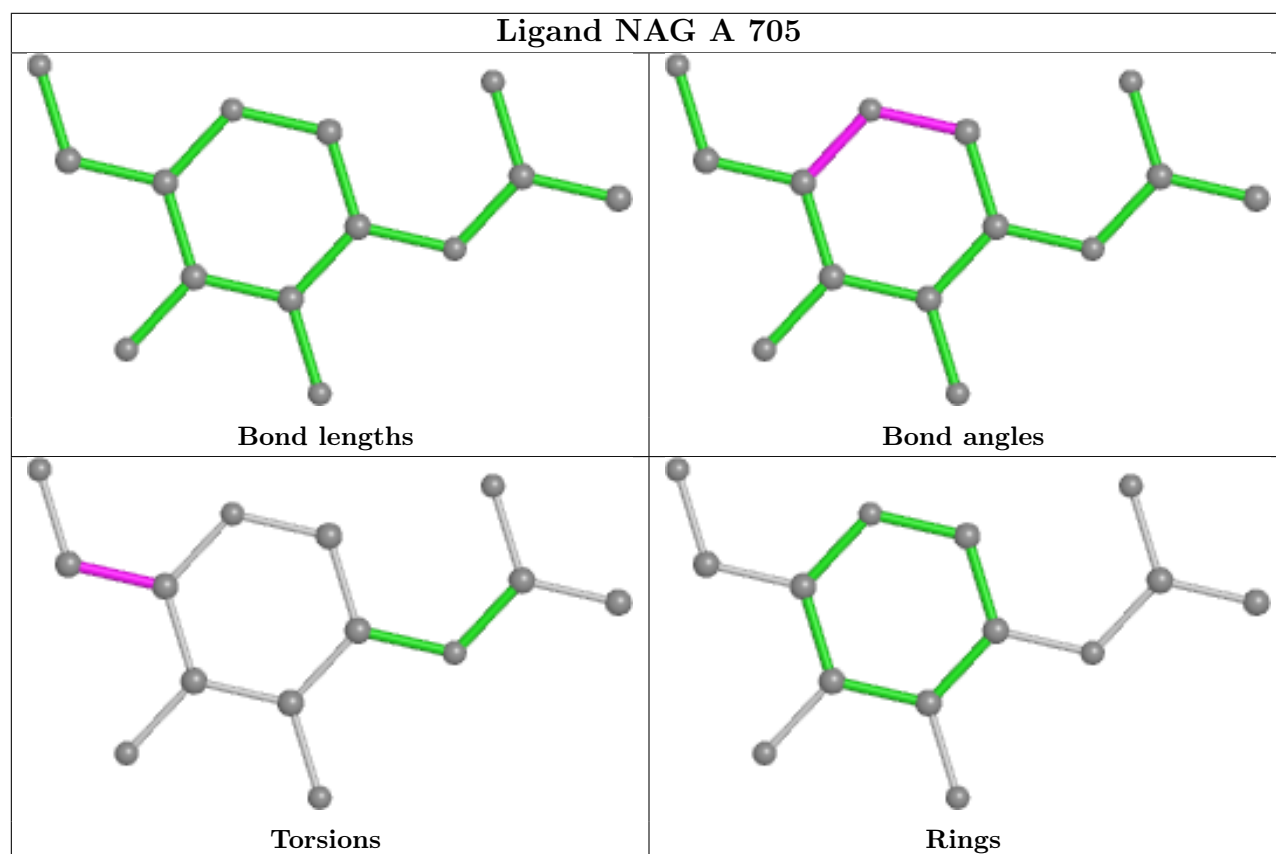
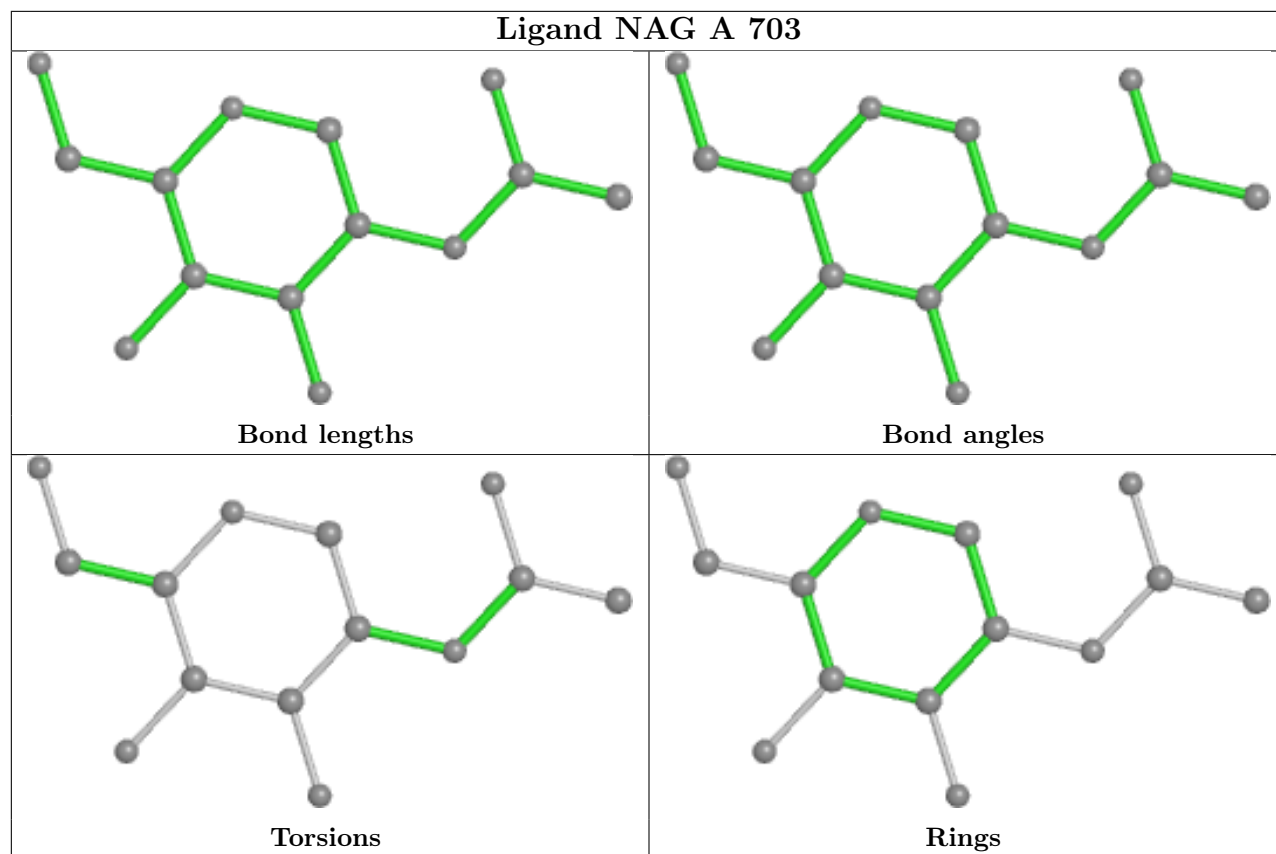
Mol	Chain	Res	Type	Atoms
4	D	601	NAG	O5-C5-C6-O6
4	A	702	NAG	O5-C5-C6-O6
4	A	706	NAG	O5-C5-C6-O6
4	C	704	NAG	C4-C5-C6-O6
4	A	702	NAG	C4-C5-C6-O6
4	D	601	NAG	C4-C5-C6-O6
4	C	704	NAG	O5-C5-C6-O6
4	C	702	NAG	C4-C5-C6-O6
4	A	706	NAG	C4-C5-C6-O6
4	C	705	NAG	O5-C5-C6-O6
4	A	705	NAG	O5-C5-C6-O6
4	C	702	NAG	O5-C5-C6-O6
4	C	705	NAG	C3-C2-N2-C7
4	C	705	NAG	C1-C2-N2-C7

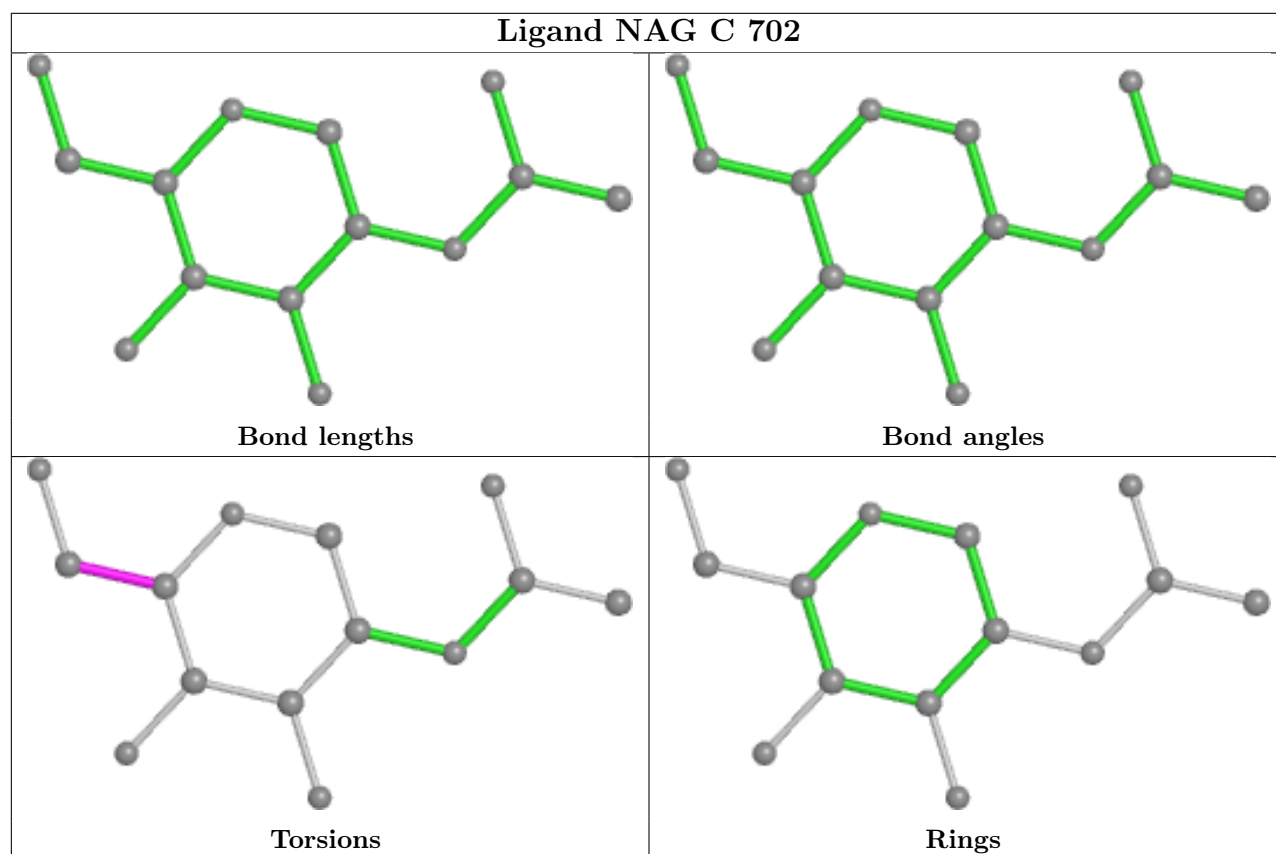
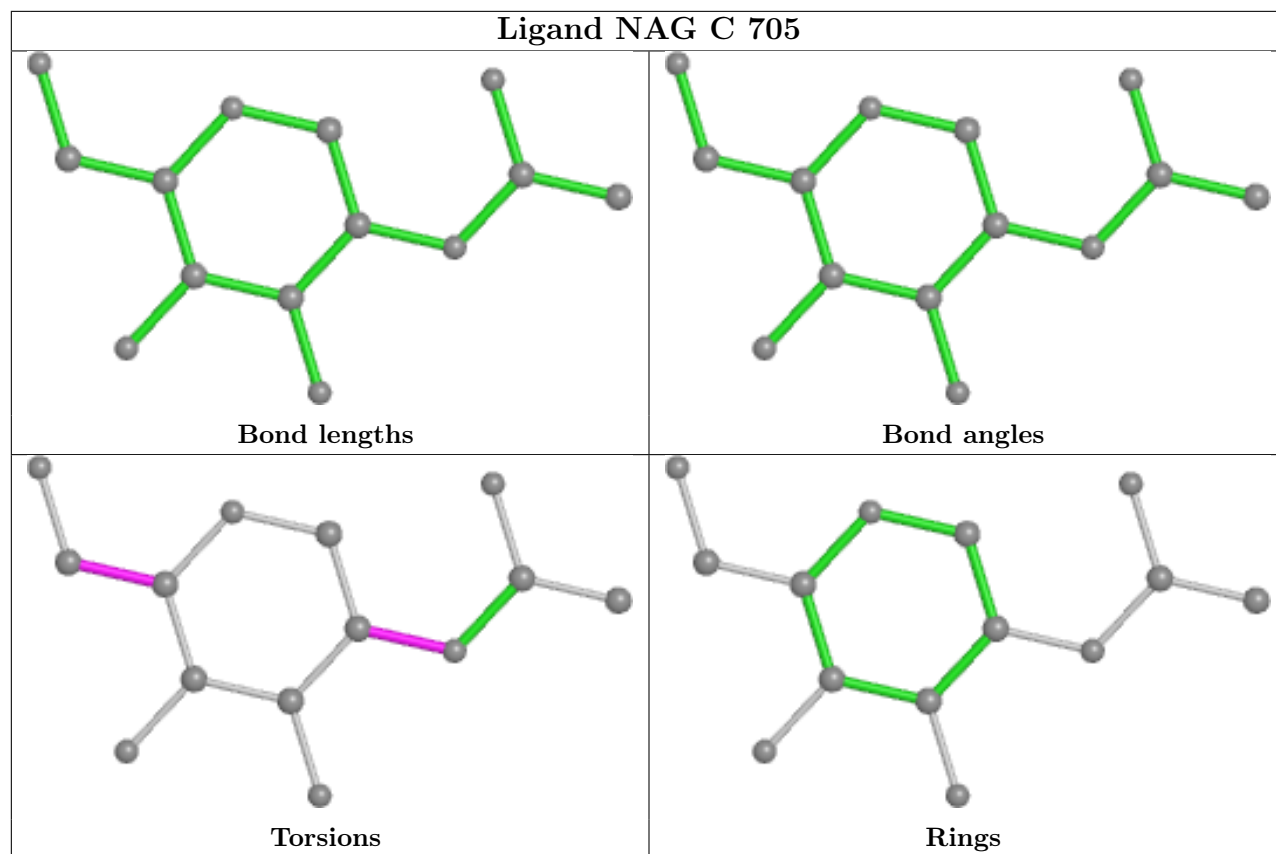
There are no ring outliers.

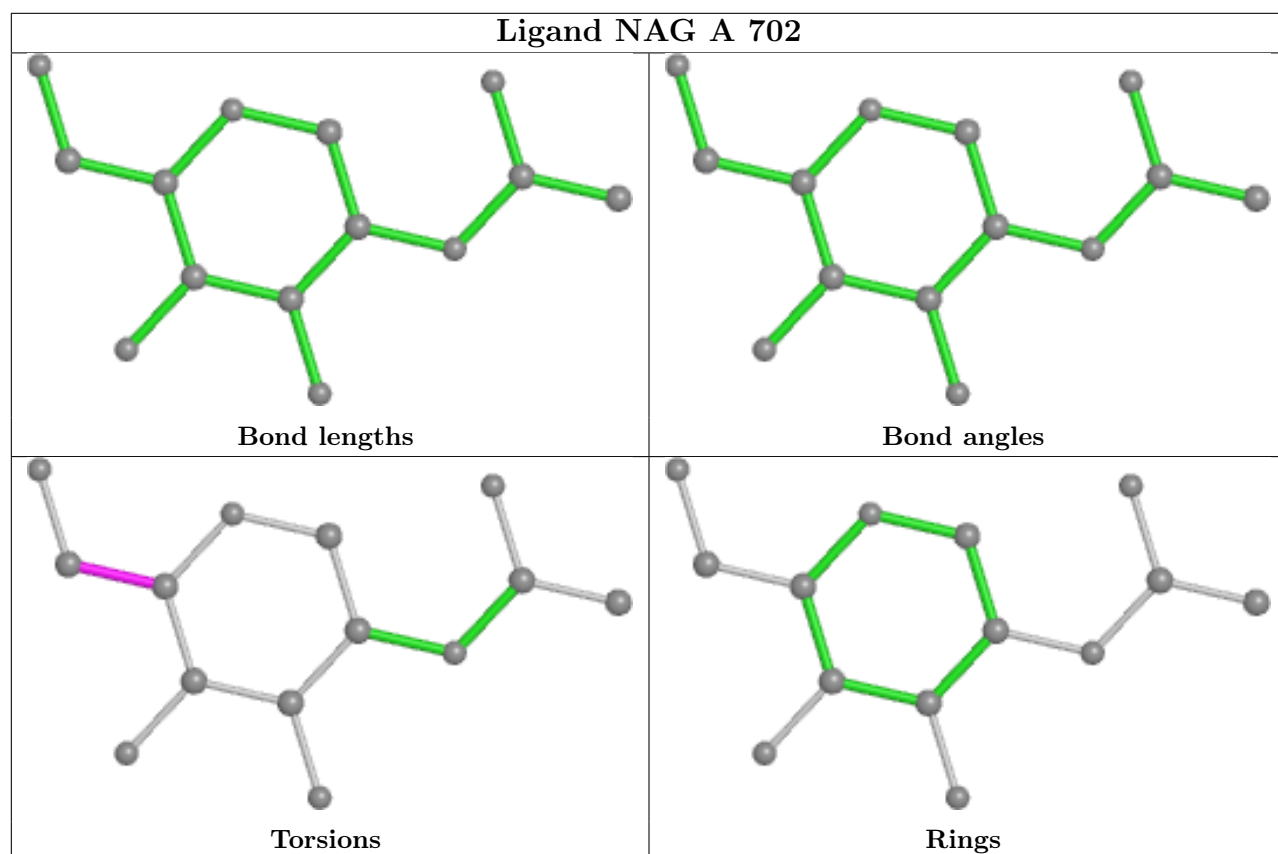
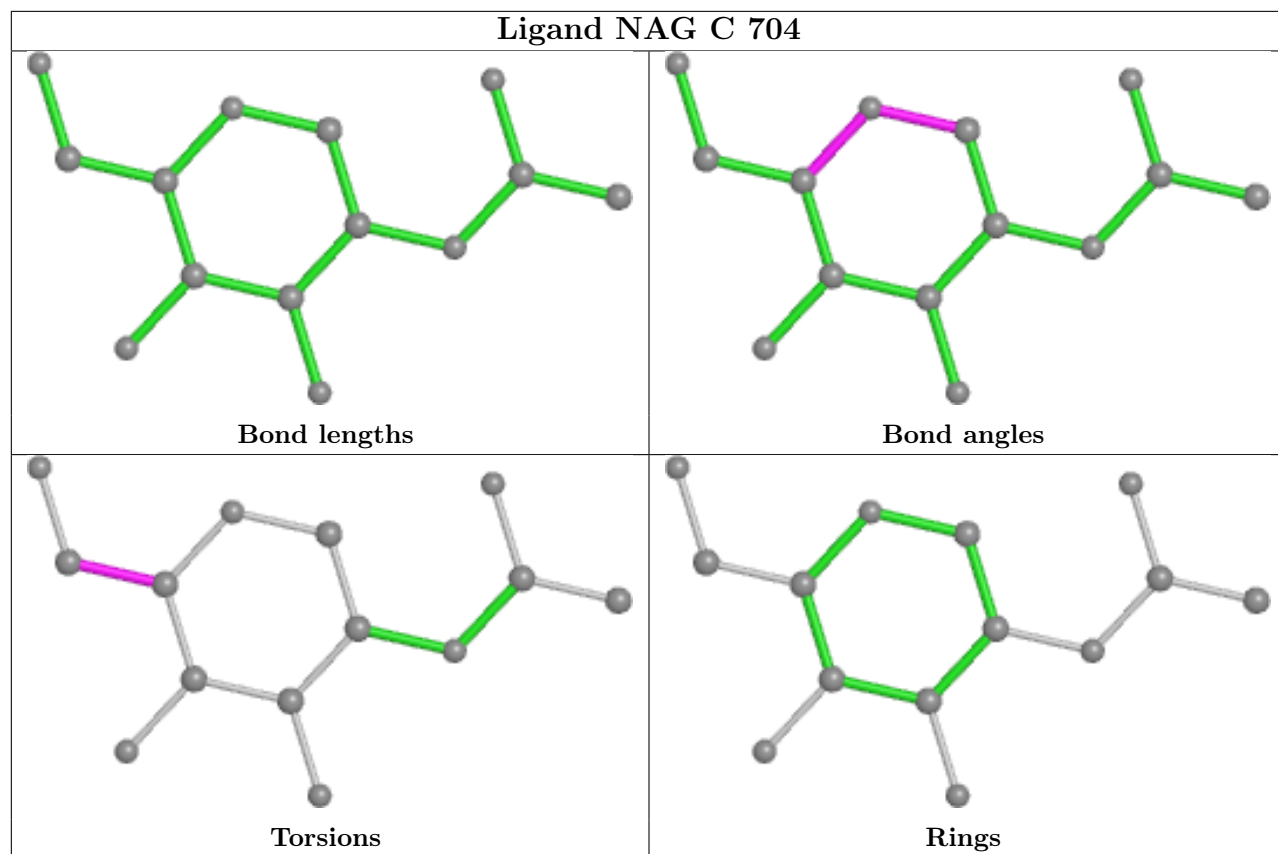
4 monomers are involved in 4 short contacts:

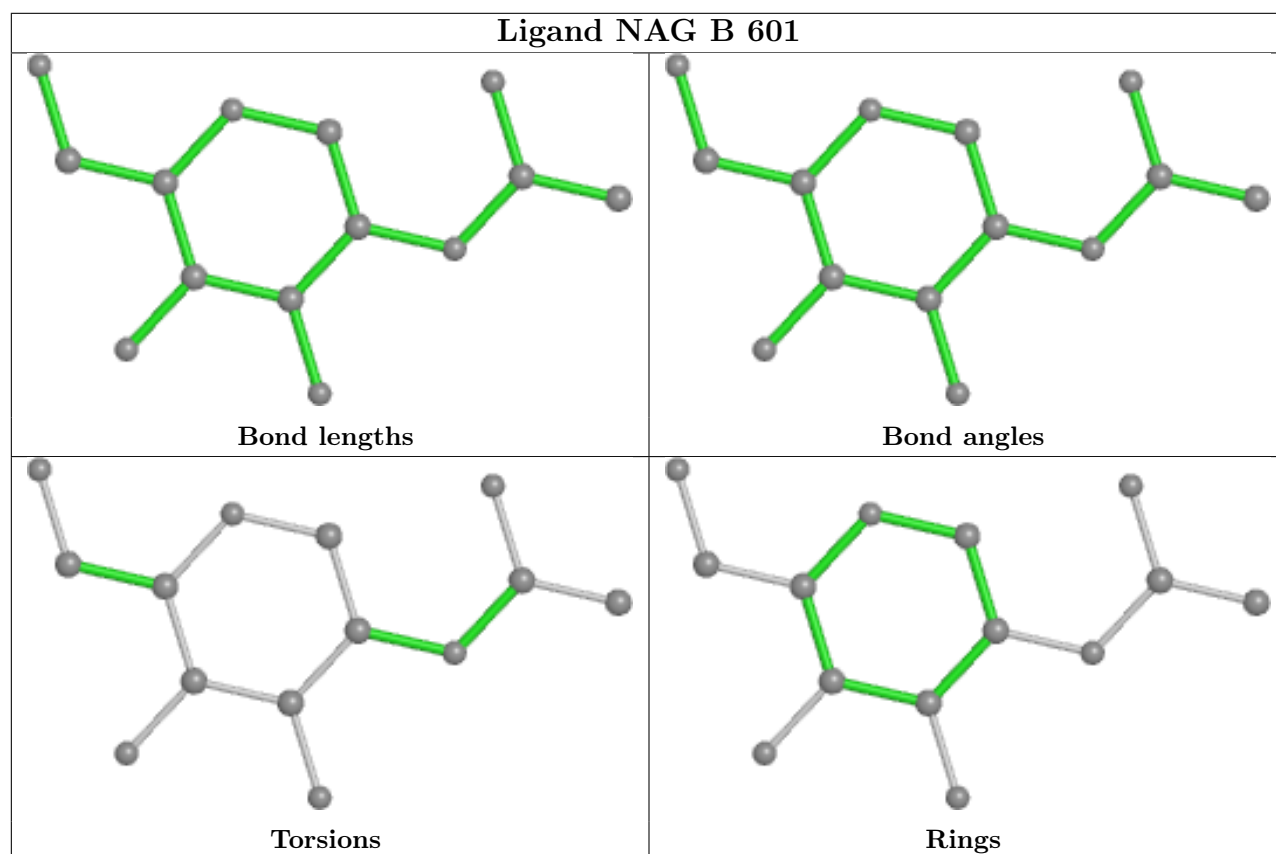
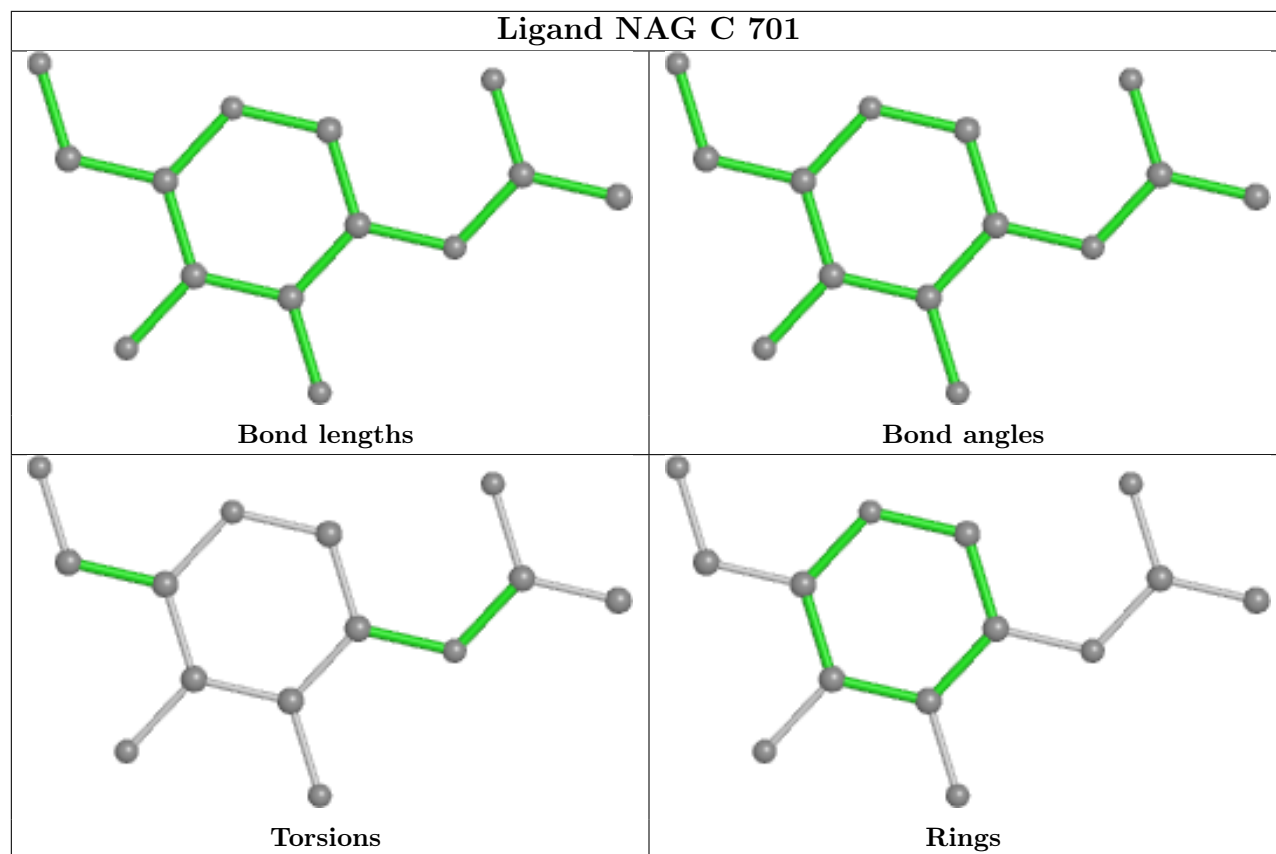
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	705	NAG	1	0
4	B	601	NAG	1	0
4	D	601	NAG	1	0
4	A	706	NAG	1	0

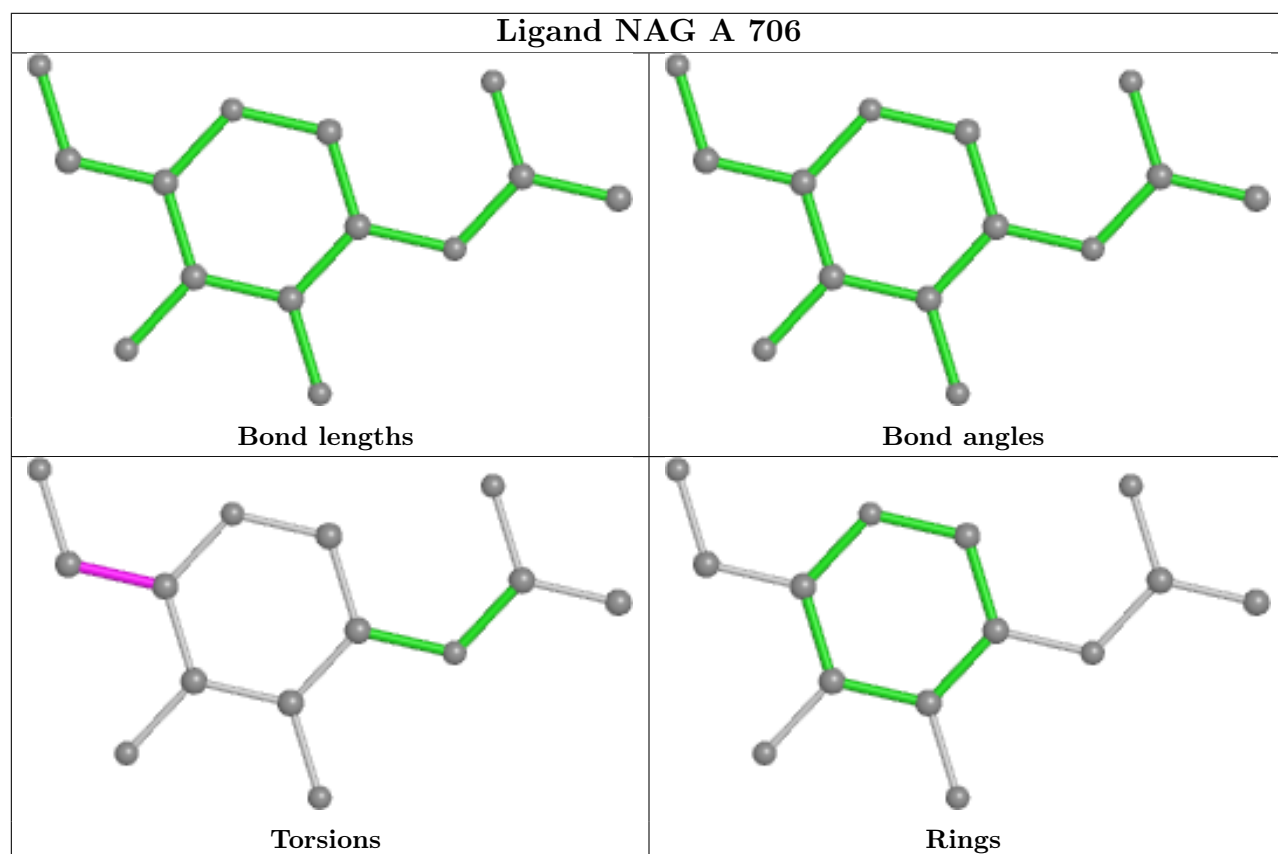
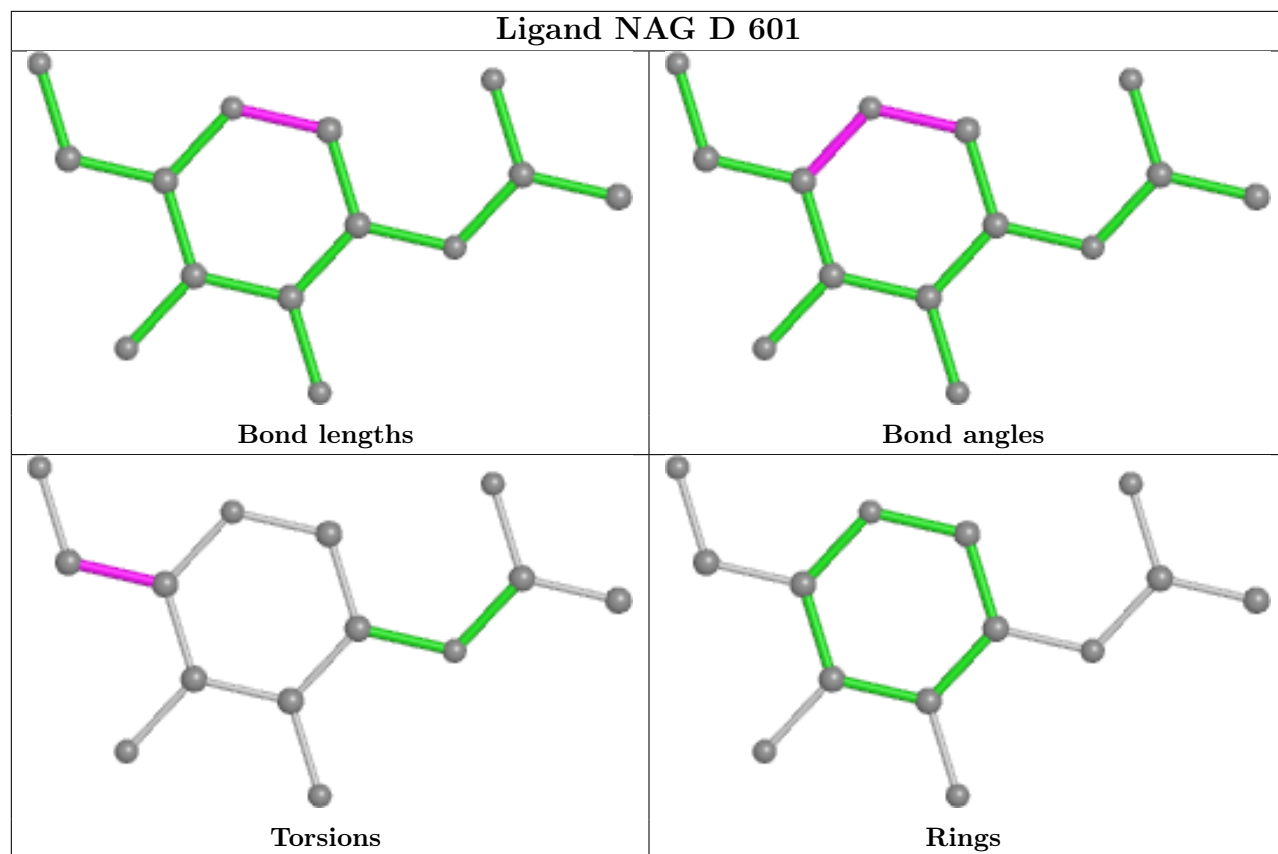
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

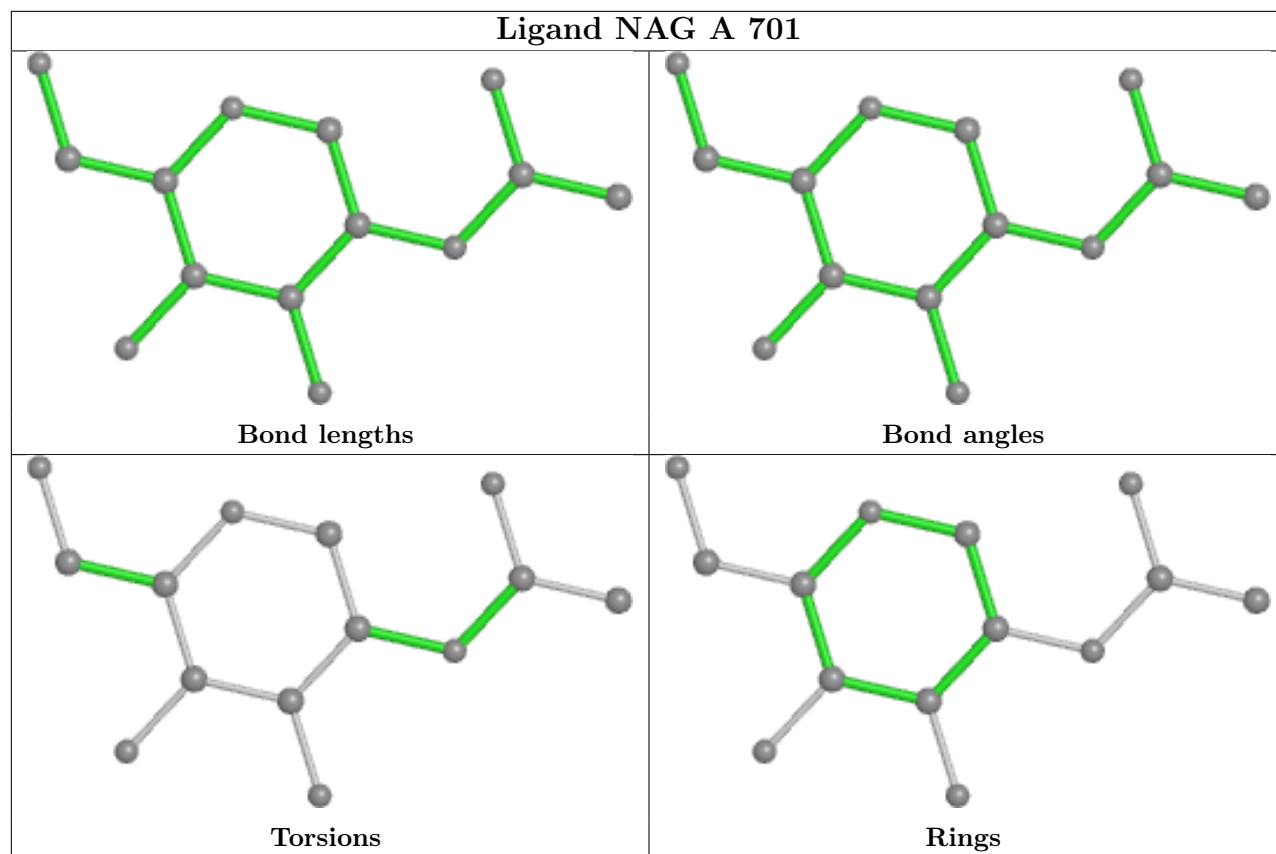












5.7 Other polymers [i](#)

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	596/596 (100%)	-0.53	1 (0%) 95 87	27, 48, 84, 163	0
1	C	596/596 (100%)	-0.42	4 (0%) 87 69	33, 59, 98, 153	0
2	B	195/195 (100%)	-0.51	0 100 100	27, 50, 93, 128	0
2	D	195/195 (100%)	-0.44	1 (0%) 91 75	30, 55, 93, 146	0
All	All	1582/1582 (100%)	-0.48	6 (0%) 92 79	27, 53, 92, 163	0

All (6) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	136	ASP	6.0
1	C	427	ASP	4.7
1	C	136	ASP	2.9
2	D	370	ASN	2.5
1	C	339	VAL	2.4
1	C	110	GLU	2.0

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

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

6.3 Carbohydrates [i](#)

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

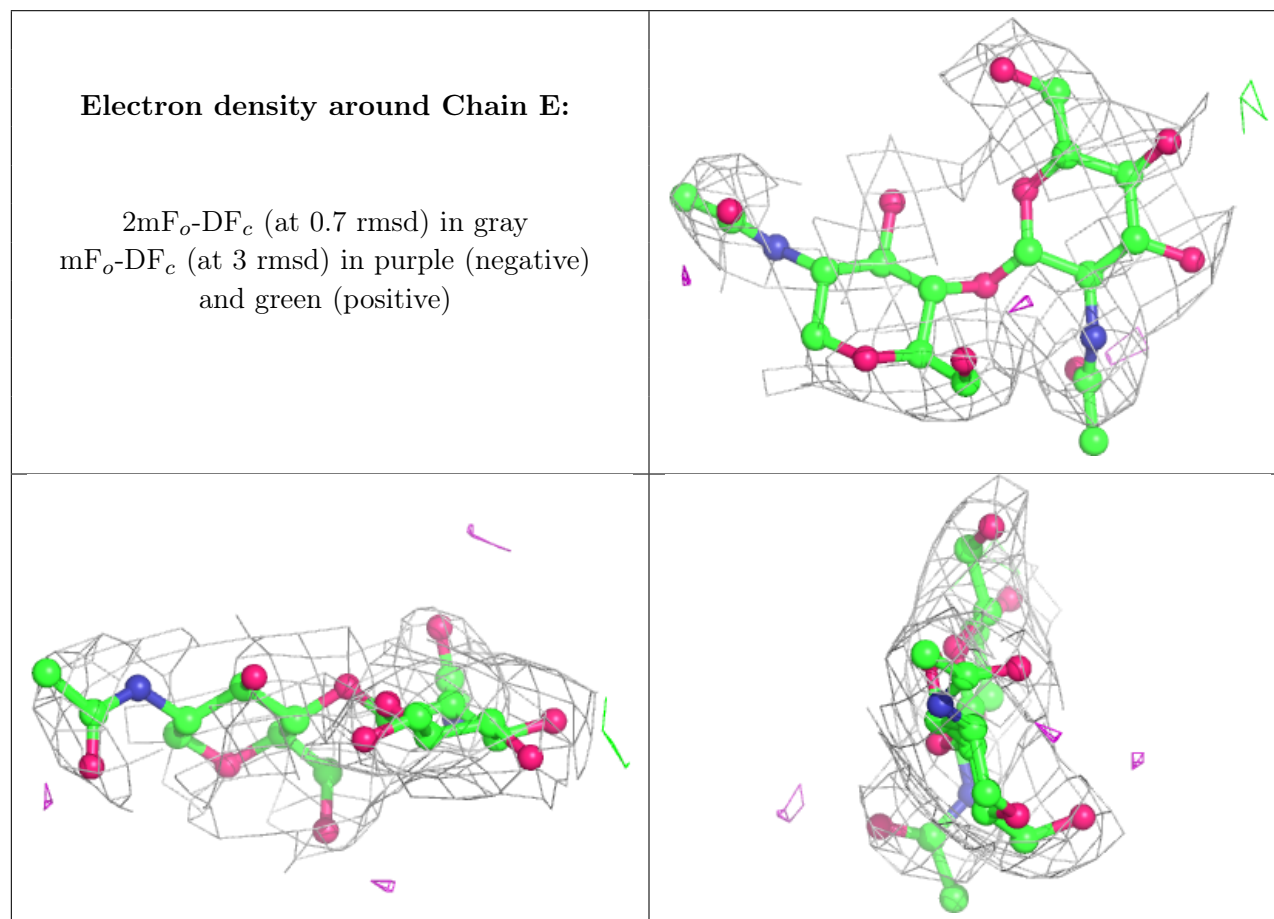
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	NAG	E	2	14/15	0.89	0.23	84,100,108,110	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	NAG	E	1	14/15	0.92	0.18	68,73,80,82	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.

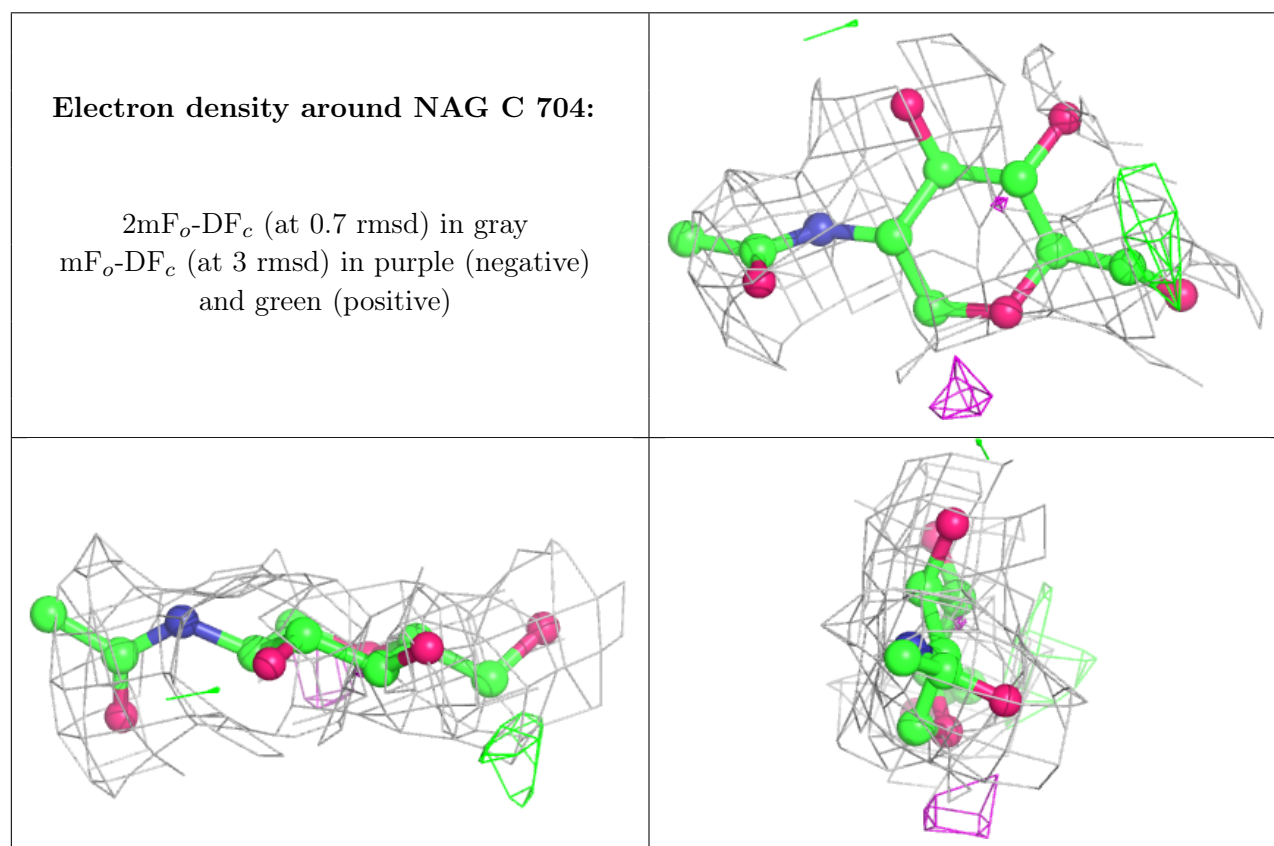
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	NAG	C	704	14/15	0.57	0.39	80,116,128,130	0
4	NAG	A	703	14/15	0.64	0.37	91,116,123,123	0
4	NAG	C	702	14/15	0.72	0.27	87,106,119,122	0
4	NAG	A	701	14/15	0.79	0.26	86,95,109,109	0
4	NAG	A	705	14/15	0.82	0.39	74,102,115,118	0

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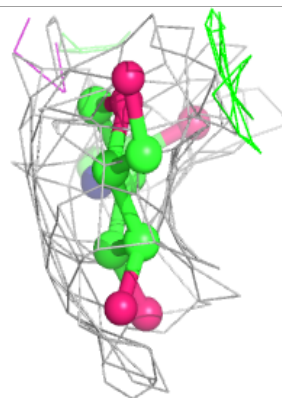
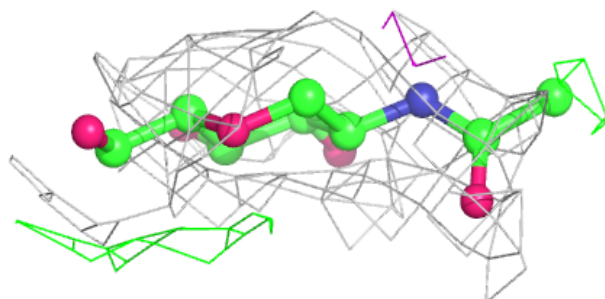
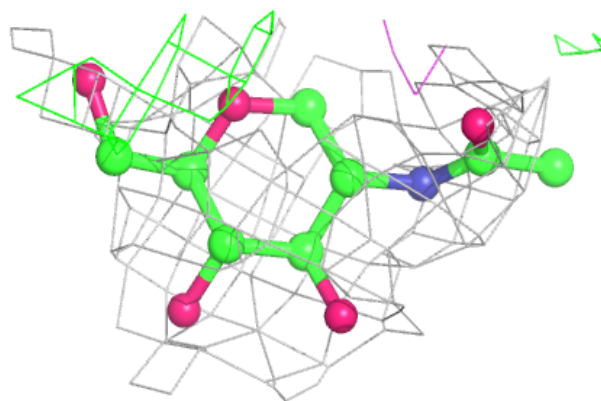
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	NAG	A	702	14/15	0.83	0.20	60,65,69,78	0
4	NAG	D	601	14/15	0.84	0.27	83,100,117,120	0
4	NAG	C	705	14/15	0.85	0.20	97,103,109,110	0
4	NAG	B	601	14/15	0.85	0.26	74,93,103,104	0
4	NAG	C	701	14/15	0.87	0.26	68,82,95,96	0
4	NAG	A	706	14/15	0.88	0.17	77,91,98,100	0
5	ZN	A	704	1/1	0.97	0.14	46,46,46,46	0
5	ZN	C	703	1/1	0.98	0.13	60,60,60,60	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.

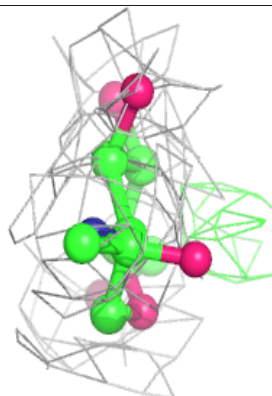
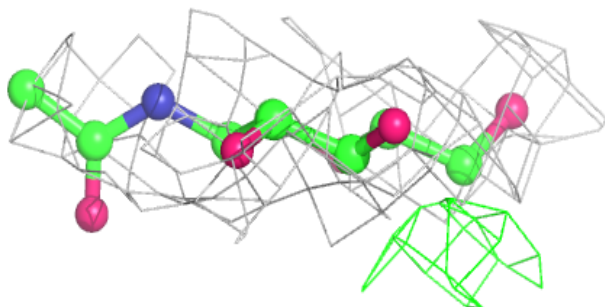
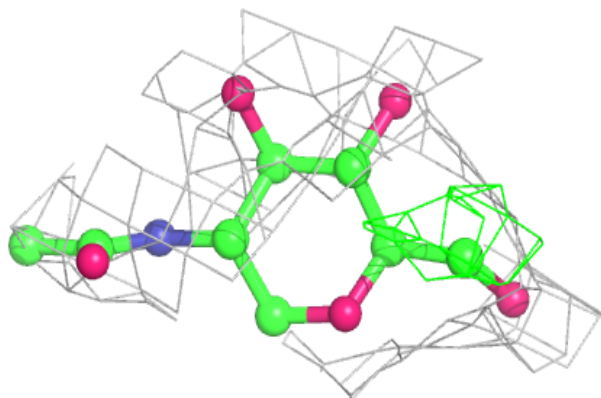


Electron density around NAG A 703:

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

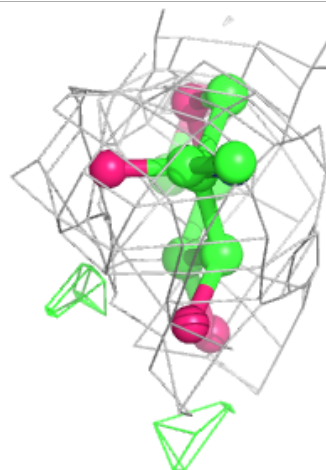
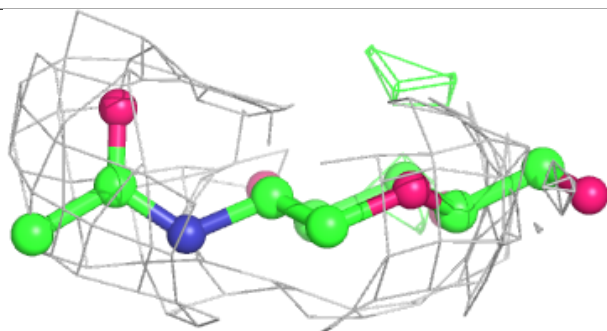
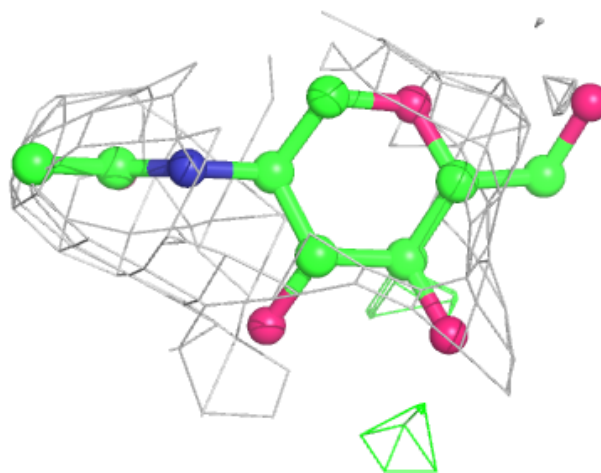
**Electron density around NAG C 702:**

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



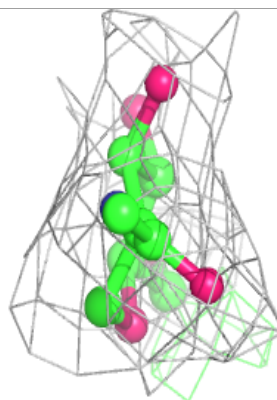
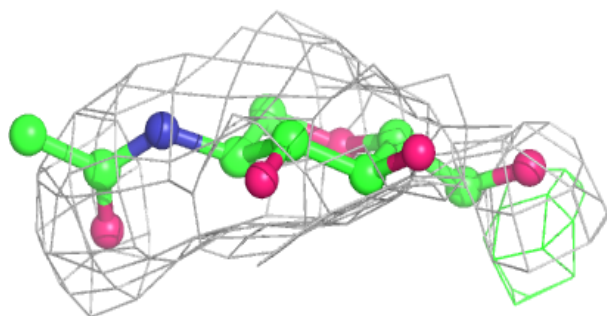
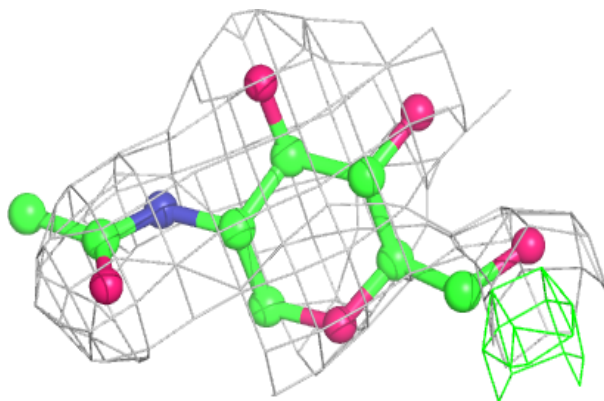
Electron density around NAG A 701:

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

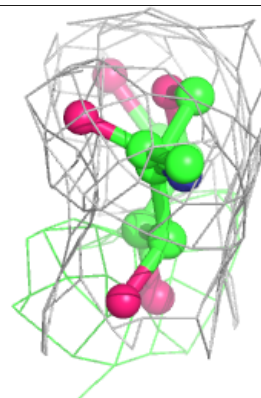
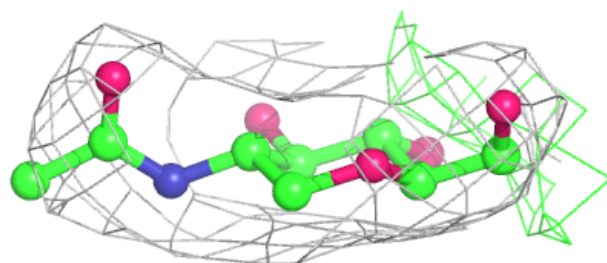
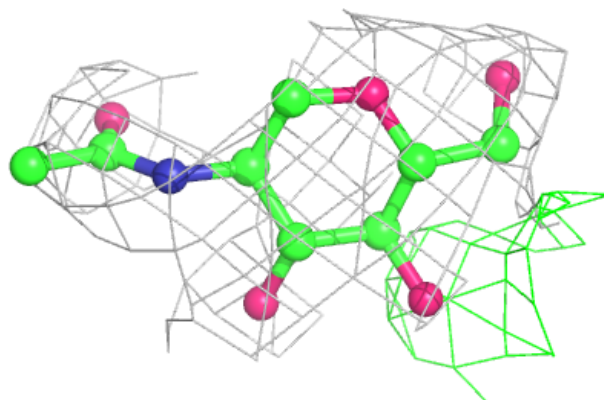


Electron density around NAG A 705:

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

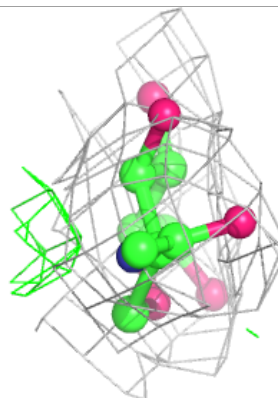
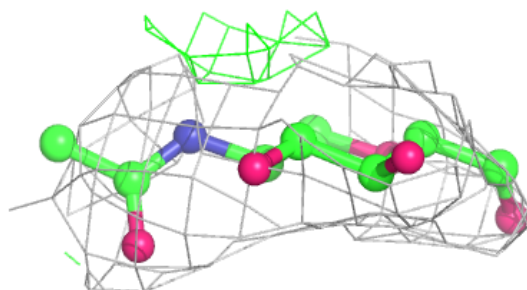
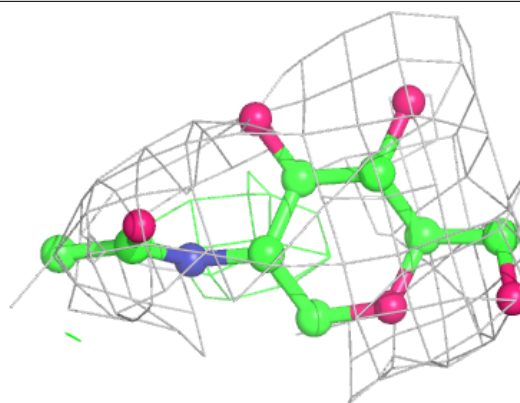
**Electron density around NAG A 702:**

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

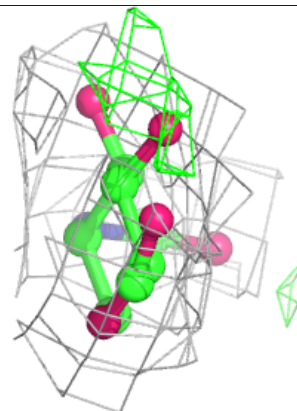
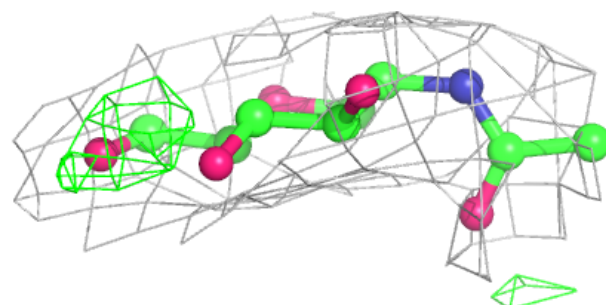
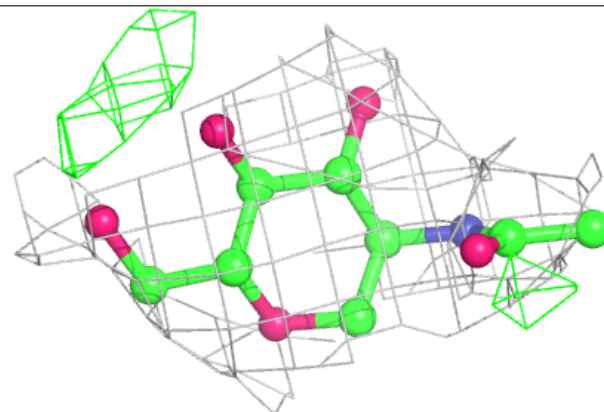


Electron density around NAG D 601:

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

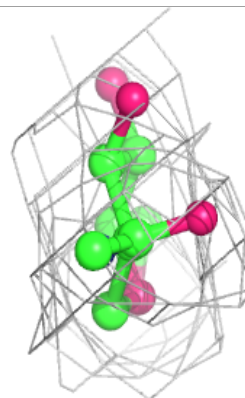
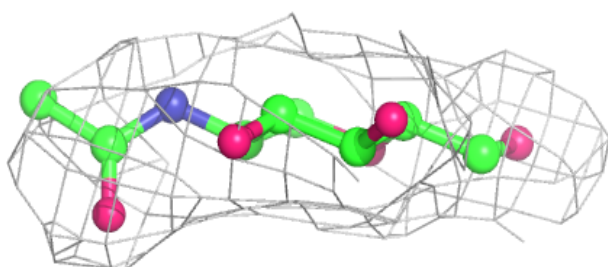
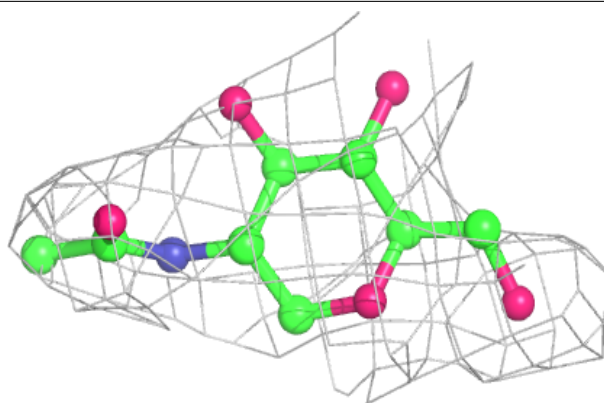
**Electron density around NAG C 705:**

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

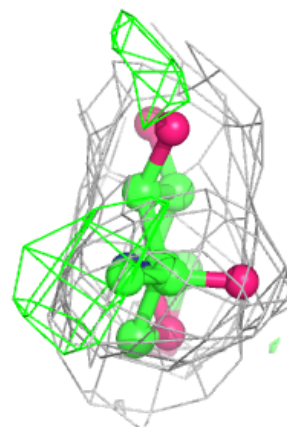
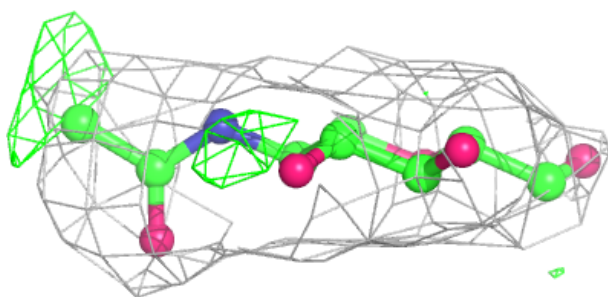
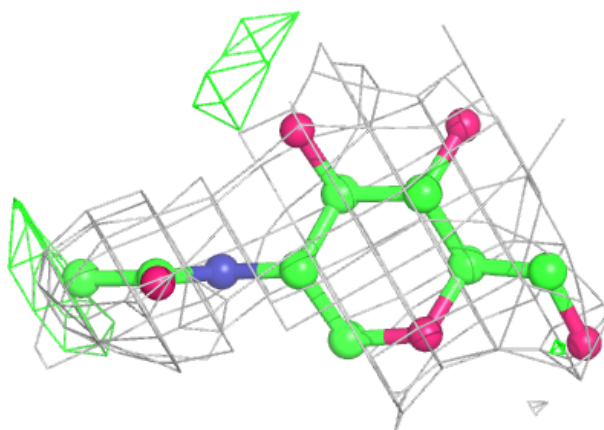


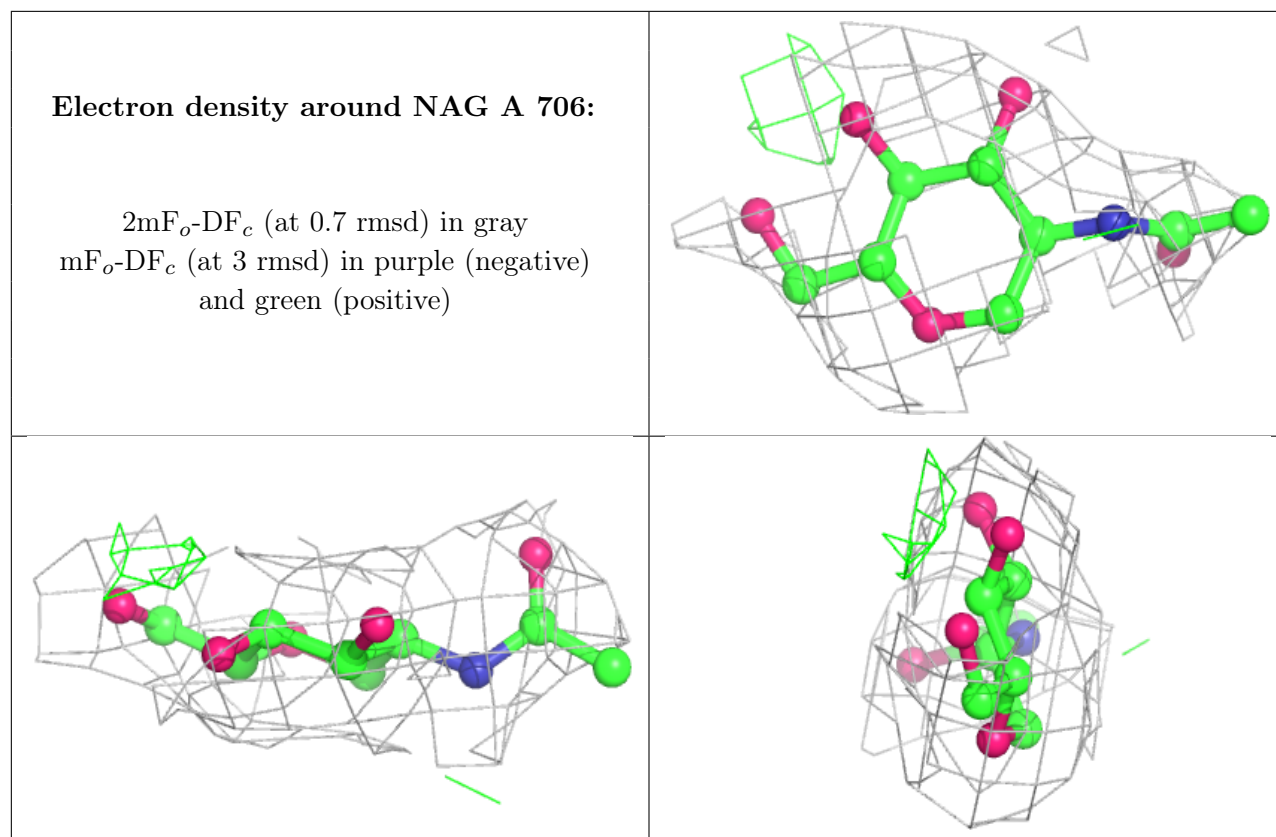
Electron density around NAG B 601:

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

**Electron density around NAG C 701:**

$2mF_o-DF_c$ (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.