



Full wwPDB X-ray Structure Validation Report ⓘ

Dec 13, 2023 – 05:50 PM JST

PDB ID : 8JPZ
Title : The thermostability mutant Gox_M8 from *Aspergillus niger*
Authors : Tu, T.; Yan, Y.R.
Deposited on : 2023-06-13
Resolution : 2.08 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 : 2.36
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

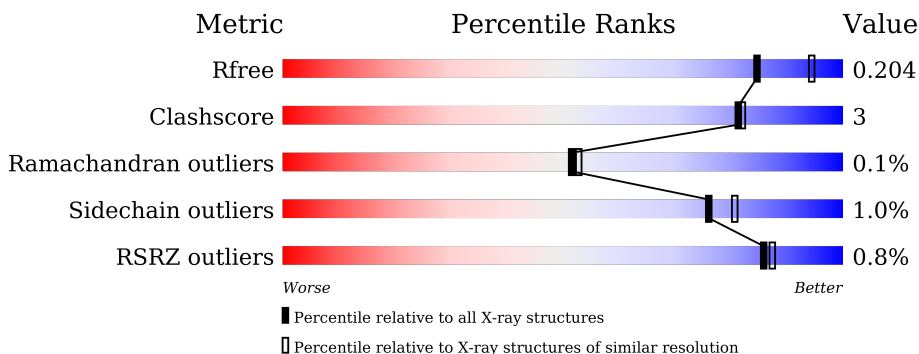
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.08 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	6189 (2.10-2.06)
Clashscore	141614	6738 (2.10-2.06)
Ramachandran outliers	138981	6663 (2.10-2.06)
Sidechain outliers	138945	6664 (2.10-2.06)
RSRZ outliers	127900	6057 (2.10-2.06)

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	581	
1	B	581	
2	C	6	
2	D	6	

2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 10304 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 Glucose oxidase (Fragment).

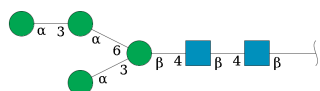
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	581	Total	C	N	O	S	0	6	0
			4504	2837	780	872	15			
1	B	581	Total	C	N	O	S	7	5	0
			4492	2833	776	868	15			

There are 22 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	31	VAL	THR	conflict	UNP Q5Q041
A	32	VAL	THR	conflict	UNP Q5Q041
A	68	LYS	ASP	conflict	UNP Q5Q041
A	82	CYS	GLU	conflict	UNP Q5Q041
A	88	ARG	GLN	conflict	UNP Q5Q041
A	94	ALA	SER	conflict	UNP Q5Q041
A	274	PHE	THR	conflict	UNP Q5Q041
A	278	THR	TYR	conflict	UNP Q5Q041
A	313	LYS	ASP	conflict	UNP Q5Q041
A	418	GLU	VAL	conflict	UNP Q5Q041
A	508	HIS	ASN	conflict	UNP Q5Q041
B	31	VAL	THR	conflict	UNP Q5Q041
B	32	VAL	THR	conflict	UNP Q5Q041
B	68	LYS	ASP	conflict	UNP Q5Q041
B	82	CYS	GLU	conflict	UNP Q5Q041
B	88	ARG	GLN	conflict	UNP Q5Q041
B	94	ALA	SER	conflict	UNP Q5Q041
B	274	PHE	THR	conflict	UNP Q5Q041
B	278	THR	TYR	conflict	UNP Q5Q041
B	313	LYS	ASP	conflict	UNP Q5Q041
B	418	GLU	VAL	conflict	UNP Q5Q041
B	508	HIS	ASN	conflict	UNP Q5Q041

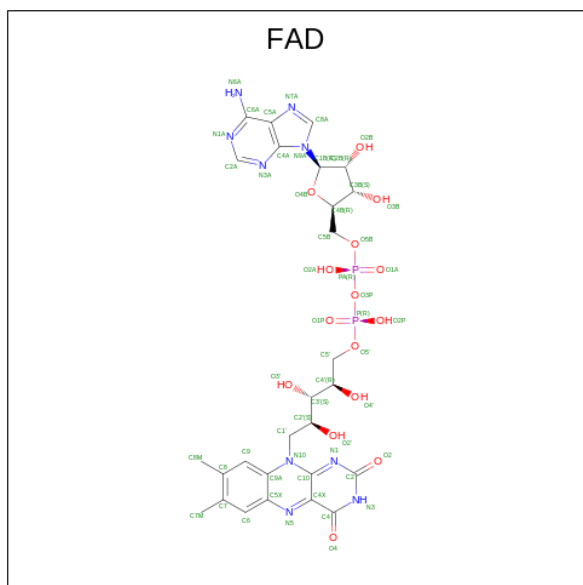
- Molecule 2 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-

beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



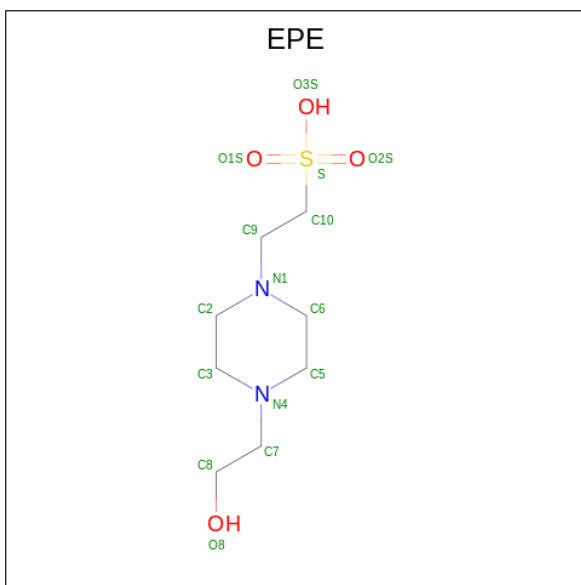
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	C	6	Total	C	N	O	0	0	0
			72	40	2	30			
2	D	6	Total	C	N	O	0	0	0
			72	40	2	30			

- Molecule 3 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula: $C_{27}H_{33}N_9O_{15}P_2$).



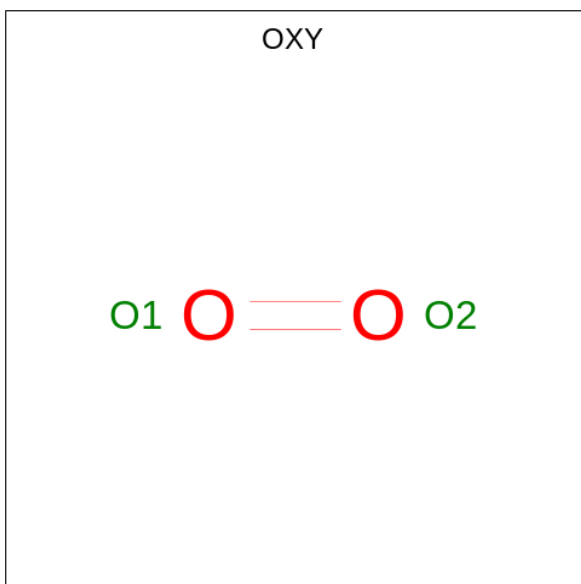
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
3	B	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

- Molecule 4 is 4-(2-HYDROXYETHYL)-1-PIPERAZINE ETHANESULFONIC ACID (three-letter code: EPE) (formula: $C_8H_{18}N_2O_4S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	S		
4	A	1	15	8	2	4	1	0	0
4	B	1	15	8	2	4	1	0	0

- Molecule 5 is OXYGEN MOLECULE (three-letter code: OXY) (formula: O₂) (labeled as "Ligand of Interest" by depositor).



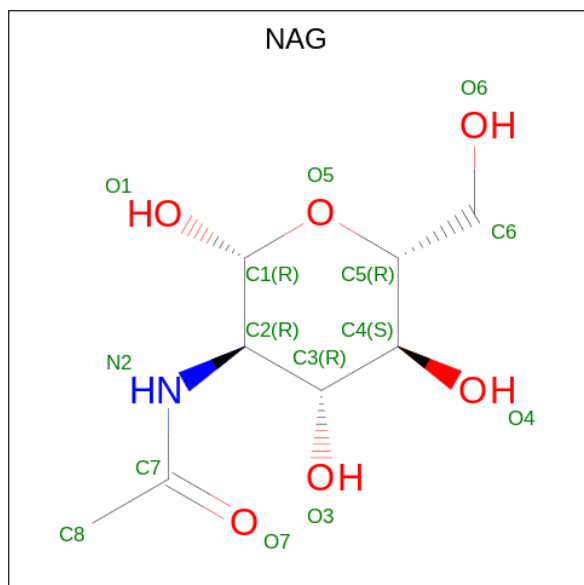
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
5	A	1	2	2	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	1	Total O 2 2	0	0

- Molecule 6 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$) (labeled as "Ligand of Interest" by depositor).



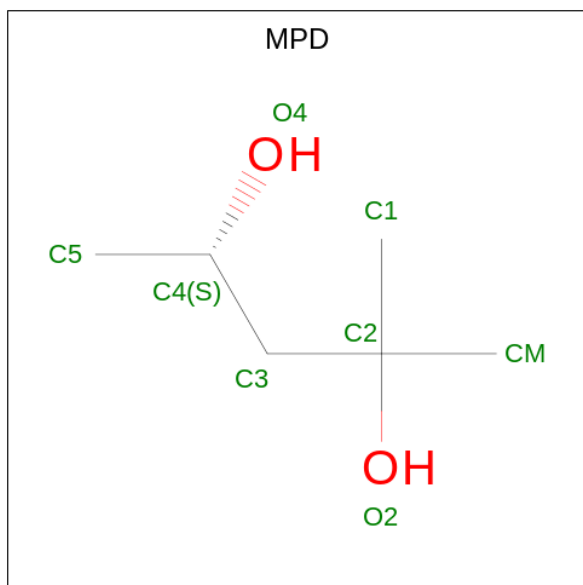
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total C N O 14 8 1 5	0	0
6	A	1	Total C N O 14 8 1 5	0	0
6	A	1	Total C N O 14 8 1 5	0	0
6	A	1	Total C N O 14 8 1 5	0	0
6	A	1	Total C N O 14 8 1 5	0	0
6	B	1	Total C N O 14 8 1 5	0	0
6	B	1	Total C N O 14 8 1 5	0	0
6	B	1	Total C N O 14 8 1 5	0	0
6	B	1	Total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

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

- Molecule 7 is (4S)-2-METHYL-2,4-PENTANEDIOL (three-letter code: MPD) (formula: C₆H₁₄O₂) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
7	A	1	8	6	2	0	0

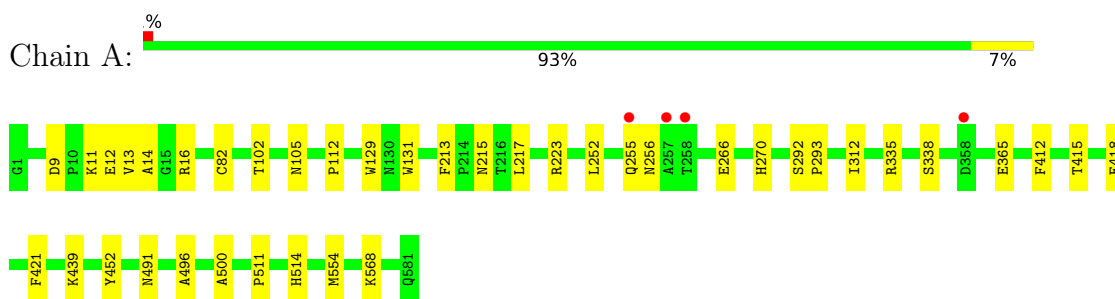
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
8	A	430	430	430	0	0
8	B	432	432	432	0	0

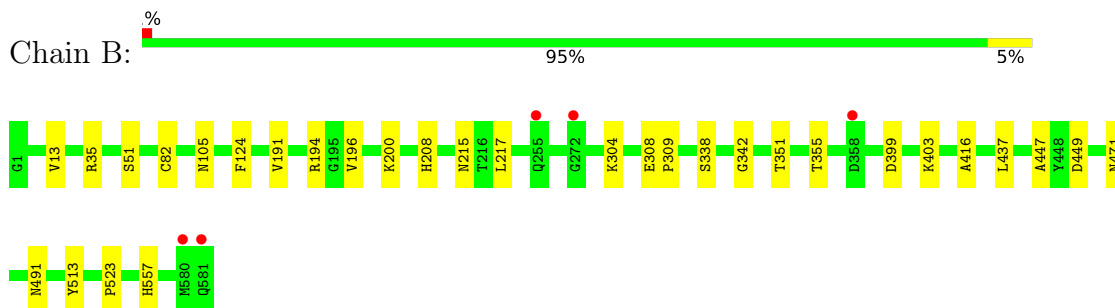
3 Residue-property plots [i](#)

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

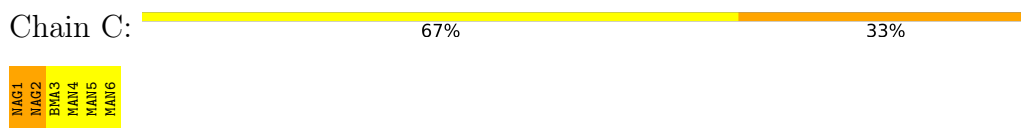
- Molecule 1: Glucose oxidase (Fragment)



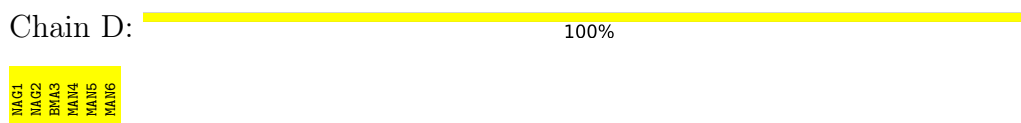
- Molecule 1: Glucose oxidase (Fragment)



- Molecule 2: alpha-D-mannopyranose-(1-3)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 2: alpha-D-mannopyranose-(1-3)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]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	P 41 21 2	Depositor
Cell constants a, b, c, α , β , γ	126.45Å 126.45Å 193.36Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	21.18 – 2.08 21.18 – 2.08	Depositor EDS
% Data completeness (in resolution range)	100.0 (21.18-2.08) 100.0 (21.18-2.08)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.32 (at 2.08Å)	Xtrriage
Refinement program	PHENIX 1.14_3260	Depositor
R, R_{free}	0.166 , 0.204 0.166 , 0.204	Depositor DCC
R_{free} test set	4707 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	36.3	Xtrriage
Anisotropy	0.052	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 49.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	10304	wwPDB-VP
Average B, all atoms (Å ²)	38.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.86% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: FAD, OXY, MPD, EPE, MAN, NAG, BMA

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	0.42	0/4609	0.58	0/6280
1	B	0.44	0/4597	0.58	0/6265
All	All	0.43	0/9206	0.58	0/12545

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

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	4504	0	4332	25	1
1	B	4492	0	4328	19	0
2	C	72	0	61	4	0
2	D	72	0	61	2	0
3	A	53	0	31	2	0
3	B	53	0	31	4	0
4	A	15	0	17	1	0
4	B	15	0	17	1	0
5	A	2	0	0	0	0
5	B	2	0	0	0	0
6	A	70	0	65	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	B	84	0	78	0	0
7	A	8	0	14	1	0
8	A	430	0	0	3	1
8	B	432	0	0	4	0
All	All	10304	0	9035	48	2

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 3.

All (48) 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:B:82:CYS:SG	8:B:1074:HOH:O	2.20	0.98
1:A:82:CYS:SG	8:A:1069:HOH:O	2.22	0.97
1:A:131:TRP:HE1	7:A:609:MPD:HM2	1.46	0.80
1:B:105:ASN:HB2	3:B:601:FAD:C5X	2.13	0.79
1:A:105:ASN:HB2	3:A:601:FAD:C5X	2.13	0.78
1:A:9:ASP:O	1:A:12:GLU:HG2	1.90	0.70
1:B:351:THR:O	1:B:355:THR:HG23	1.94	0.67
1:B:105:ASN:HB2	3:B:601:FAD:N5	2.11	0.65
1:A:105:ASN:HB2	3:A:601:FAD:N5	2.12	0.64
2:C:2:NAG:H3	2:C:2:NAG:H83	1.78	0.64
2:C:1:NAG:H62	2:C:2:NAG:H82	1.82	0.61
8:B:914:HOH:O	2:C:2:NAG:H81	2.02	0.60
1:A:491:ASN:HA	4:B:602:EPE:H82	1.86	0.56
1:A:129:TRP:CE2	1:A:568:LYS:HE3	2.41	0.56
8:A:703:HOH:O	2:C:1:NAG:H81	2.06	0.55
4:A:602:EPE:H72	1:B:491:ASN:HD22	1.70	0.55
1:B:449:ASP:OD2	8:B:701:HOH:O	2.18	0.55
1:A:415:THR:HA	1:A:418:GLU:O	2.07	0.54
1:B:304:LYS:NZ	1:B:308:GLU:OE2	2.43	0.51
1:A:312:ILE:HD11	1:A:439:LYS:HA	1.92	0.51
1:A:252:LEU:HD21	1:A:266[B]:GLU:HG3	1.92	0.50
1:A:365:GLU:OE1	8:A:701:HOH:O	2.20	0.48
1:B:191:VAL:HB	1:B:196:VAL:HB	1.94	0.48
1:A:255:GLN:H	1:A:255:GLN:CD	2.18	0.47
1:A:496:ALA:HB1	1:A:500:ALA:HB3	1.97	0.46
1:A:13:VAL:C	1:A:16:ARG:HE	2.17	0.46
1:A:11:LYS:O	1:A:16:ARG:NH2	2.49	0.46
1:B:194:ARG:NH2	1:B:471:ASN:OD1	2.49	0.46
1:B:437:LEU:HD11	1:B:447:ALA:HB2	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:13:VAL:CA	1:A:16:ARG:HE	2.30	0.45
8:B:743:HOH:O	2:D:1:NAG:H81	2.16	0.45
1:A:452:TYR:OH	1:A:511:PRO:HB3	2.18	0.44
1:A:13:VAL:HA	1:A:16:ARG:HE	1.83	0.44
1:A:270:HIS:CD2	1:B:51[A]:SER:HB2	2.53	0.44
1:A:335[A]:ARG:NH2	2:D:2:NAG:O3	2.44	0.43
1:A:412:PHE:O	1:A:421:PHE:HA	2.18	0.43
1:A:292:SER:N	1:A:293:PRO:HD2	2.33	0.43
1:B:35:ARG:HD2	1:B:35:ARG:HA	1.88	0.42
1:B:342:GLY:O	1:B:416:ALA:HA	2.19	0.42
1:A:112:PRO:HB3	1:A:554:MET:HB2	2.01	0.42
1:B:200:LYS:HD3	1:B:208:HIS:O	2.19	0.42
1:B:124:PHE:O	1:B:523:PRO:HD3	2.19	0.42
1:A:102:THR:O	1:A:223:ARG:HD3	2.20	0.41
1:B:399:ASP:OD1	1:B:403:LYS:HE3	2.20	0.41
1:B:308:GLU:HB3	1:B:309:PRO:HD3	2.02	0.41
1:B:513:TYR:CB	3:B:601:FAD:HM83	2.51	0.41
1:B:557:HIS:HB3	3:B:601:FAD:C2	2.51	0.41
1:A:14:ALA:O	1:A:16:ARG:NH2	2.54	0.40

All (2) 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)
8:A:701:HOH:O	8:A:902:HOH:O[6_554]	1.93	0.27
1:A:16:ARG:NH1	1:A:365:GLU:OE2[6_454]	1.98	0.22

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	585/581 (101%)	565 (97%)	19 (3%)	1 (0%)	47 47

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	584/581 (100%)	564 (97%)	20 (3%)	0	100	100
All	All	1169/1162 (101%)	1129 (97%)	39 (3%)	1 (0%)	51	53

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	256	ASN

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	469/463 (101%)	464 (99%)	5 (1%)	73	78
1	B	468/463 (101%)	463 (99%)	5 (1%)	73	78
All	All	937/926 (101%)	927 (99%)	10 (1%)	76	78

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	213	PHE
1	A	215	ASN
1	A	217	LEU
1	A	338	SER
1	A	514	HIS
1	B	13[A]	VAL
1	B	13[B]	VAL
1	B	215	ASN
1	B	217	LEU
1	B	338	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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](#)

12 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NAG	C	1	2,1	14,14,15	0.72	1 (7%)	17,19,21	0.68	1 (5%)
2	NAG	C	2	2	14,14,15	0.41	0	17,19,21	1.26	1 (5%)
2	BMA	C	3	2	11,11,12	0.98	0	15,15,17	1.09	1 (6%)
2	MAN	C	4	2	11,11,12	0.87	1 (9%)	15,15,17	1.51	3 (20%)
2	MAN	C	5	2	11,11,12	0.70	0	15,15,17	1.10	1 (6%)
2	MAN	C	6	2	11,11,12	1.62	1 (9%)	15,15,17	1.52	5 (33%)
2	NAG	D	1	2,1	14,14,15	0.28	0	17,19,21	0.55	0
2	NAG	D	2	2	14,14,15	0.21	0	17,19,21	0.67	0
2	BMA	D	3	2	11,11,12	0.93	0	15,15,17	1.20	1 (6%)
2	MAN	D	4	2	11,11,12	1.10	1 (9%)	15,15,17	1.59	3 (20%)
2	MAN	D	5	2	11,11,12	0.89	1 (9%)	15,15,17	1.19	2 (13%)
2	MAN	D	6	2	11,11,12	1.31	1 (9%)	15,15,17	1.37	1 (6%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	C	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	C	2	2	-	3/6/23/26	0/1/1/1
2	BMA	C	3	2	-	2/2/19/22	0/1/1/1
2	MAN	C	4	2	-	0/2/19/22	0/1/1/1
2	MAN	C	5	2	-	0/2/19/22	0/1/1/1
2	MAN	C	6	2	-	2/2/19/22	0/1/1/1
2	NAG	D	1	2,1	-	3/6/23/26	0/1/1/1
2	NAG	D	2	2	-	1/6/23/26	0/1/1/1
2	BMA	D	3	2	-	2/2/19/22	0/1/1/1
2	MAN	D	4	2	-	2/2/19/22	0/1/1/1
2	MAN	D	5	2	-	2/2/19/22	0/1/1/1
2	MAN	D	6	2	-	2/2/19/22	0/1/1/1

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	6	MAN	C1-C2	3.96	1.61	1.52
2	D	6	MAN	C1-C2	2.51	1.57	1.52
2	C	1	NAG	O5-C1	-2.46	1.39	1.43
2	D	4	MAN	C2-C3	2.42	1.56	1.52
2	D	5	MAN	C1-C2	2.17	1.57	1.52
2	C	4	MAN	C1-C2	2.04	1.56	1.52

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	4	MAN	C1-O5-C5	4.38	118.13	112.19
2	C	2	NAG	C2-N2-C7	4.09	128.72	122.90
2	D	4	MAN	C1-C2-C3	3.55	114.03	109.67
2	C	5	MAN	C1-O5-C5	3.28	116.63	112.19
2	D	5	MAN	C1-O5-C5	3.27	116.63	112.19
2	C	6	MAN	O5-C1-C2	2.73	114.98	110.77
2	D	4	MAN	C1-O5-C5	2.72	115.88	112.19
2	C	6	MAN	O2-C2-C1	2.70	114.67	109.15
2	C	4	MAN	C1-C2-C3	2.52	112.77	109.67
2	D	6	MAN	C1-O5-C5	2.46	115.53	112.19
2	D	3	BMA	C3-C4-C5	2.43	114.58	110.24
2	C	6	MAN	C1-C2-C3	2.35	112.55	109.67
2	C	4	MAN	O2-C2-C3	-2.33	105.48	110.14
2	D	4	MAN	O5-C1-C2	2.32	114.35	110.77
2	C	3	BMA	C3-C4-C5	2.25	114.26	110.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	6	MAN	O2-C2-C3	-2.24	105.64	110.14
2	C	6	MAN	O5-C5-C6	2.19	110.63	107.20
2	D	5	MAN	O2-C2-C3	-2.10	105.94	110.14
2	C	1	NAG	C1-O5-C5	2.05	114.97	112.19

There are no chirality outliers.

All (21) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	6	MAN	O5-C5-C6-O6
2	D	5	MAN	O5-C5-C6-O6
2	C	6	MAN	C4-C5-C6-O6
2	D	4	MAN	O5-C5-C6-O6
2	D	6	MAN	O5-C5-C6-O6
2	D	4	MAN	C4-C5-C6-O6
2	C	3	BMA	O5-C5-C6-O6
2	D	5	MAN	C4-C5-C6-O6
2	C	1	NAG	C8-C7-N2-C2
2	C	1	NAG	O7-C7-N2-C2
2	C	2	NAG	C8-C7-N2-C2
2	C	2	NAG	O7-C7-N2-C2
2	D	1	NAG	C8-C7-N2-C2
2	D	1	NAG	O7-C7-N2-C2
2	D	6	MAN	C4-C5-C6-O6
2	D	3	BMA	O5-C5-C6-O6
2	C	3	BMA	C4-C5-C6-O6
2	D	1	NAG	O5-C5-C6-O6
2	D	3	BMA	C4-C5-C6-O6
2	C	2	NAG	C3-C2-N2-C7
2	D	2	NAG	C3-C2-N2-C7

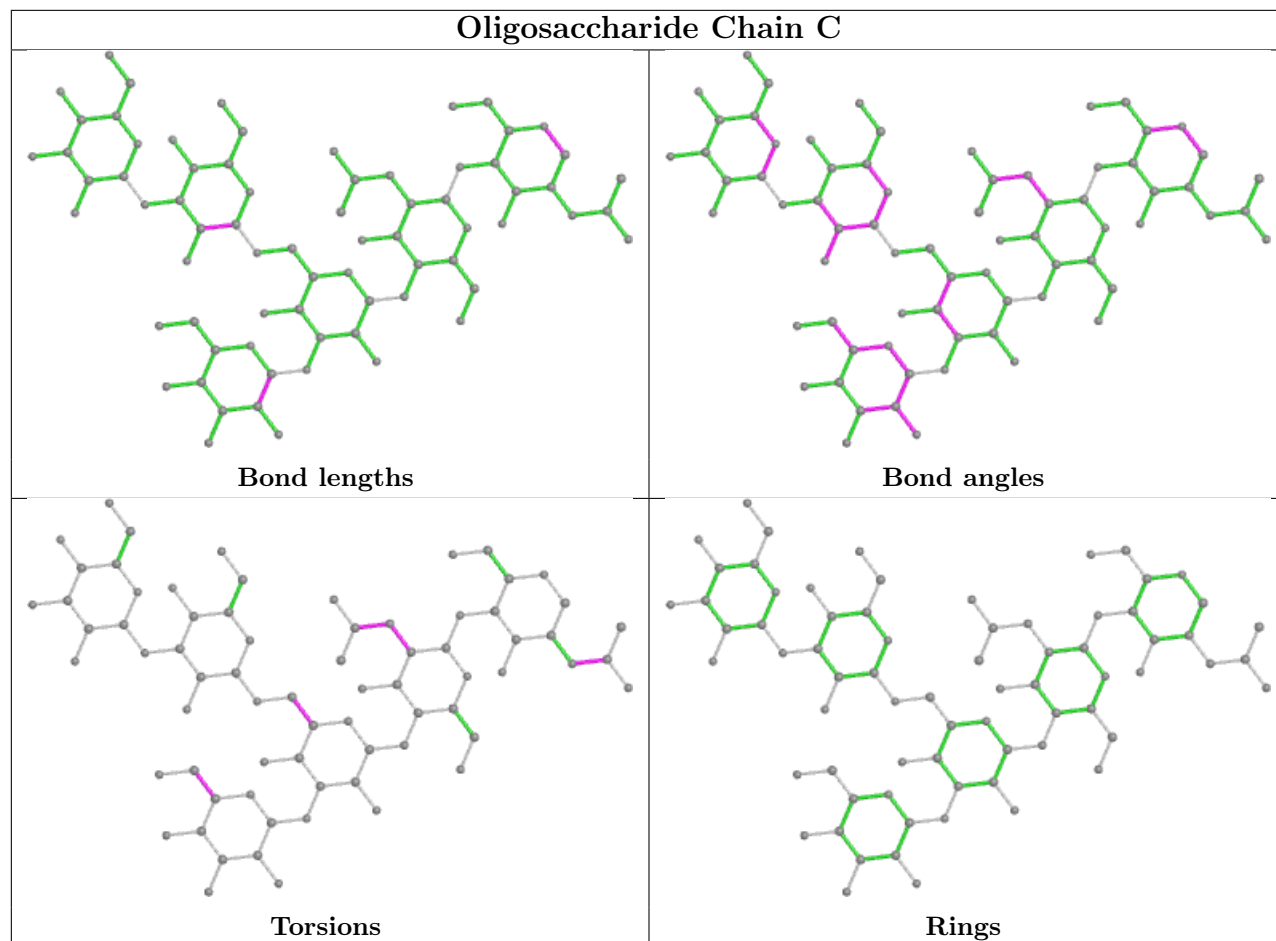
There are no ring outliers.

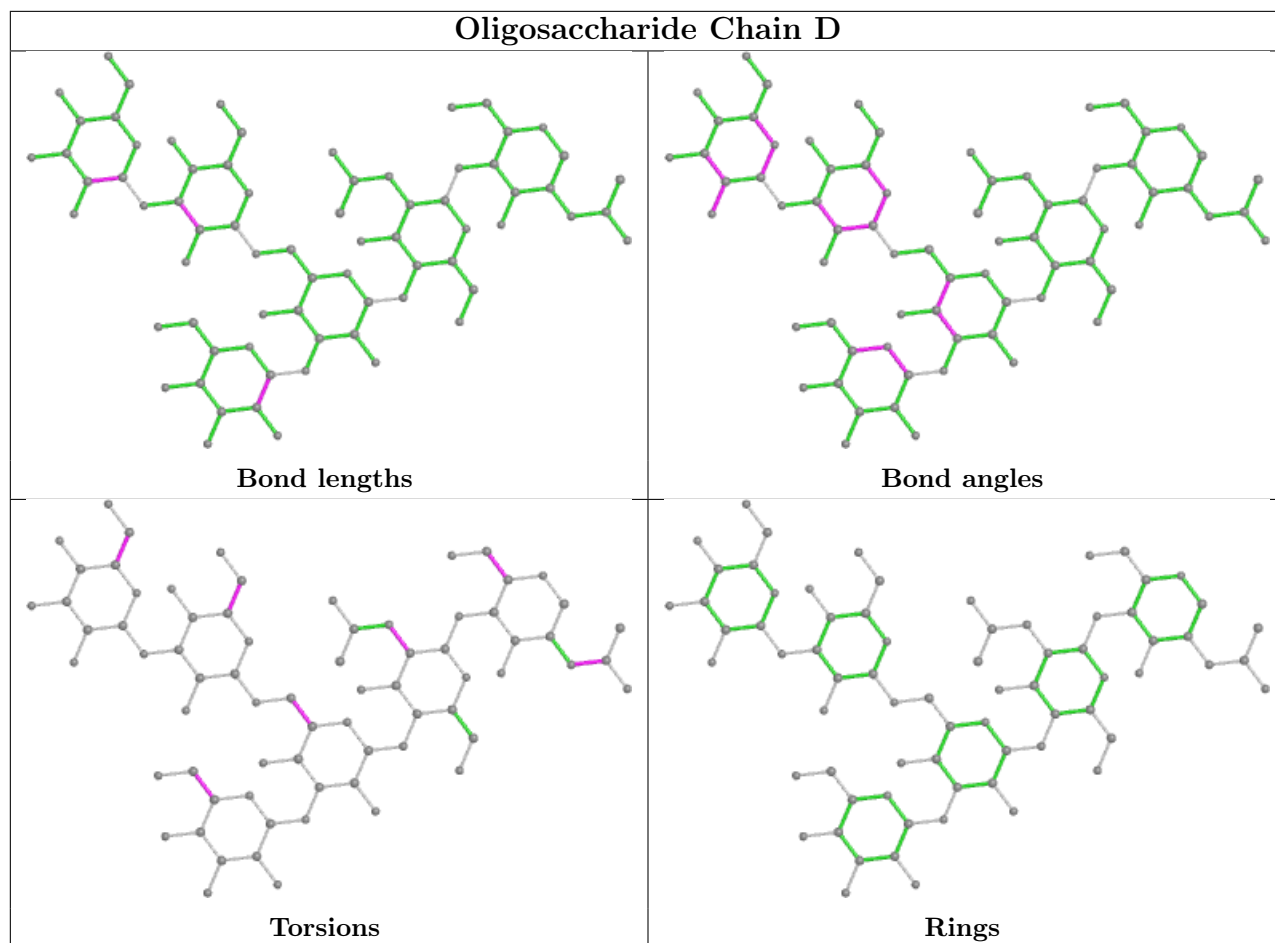
4 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	1	NAG	2	0
2	D	1	NAG	1	0
2	D	2	NAG	1	0
2	C	2	NAG	3	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths,

bond angles, torsion angles, and ring geometry for oligosaccharide.





5.6 Ligand geometry [i](#)

18 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
6	NAG	A	608	1	14,14,15	0.57	0	17,19,21	1.81	2 (11%)
7	MPD	A	609	-	7,7,7	0.31	0	9,10,10	0.79	1 (11%)
6	NAG	A	606	1	14,14,15	0.49	0	17,19,21	1.01	1 (5%)
6	NAG	B	604	1	14,14,15	0.21	0	17,19,21	1.16	1 (5%)
6	NAG	B	609	1	14,14,15	0.52	0	17,19,21	1.03	1 (5%)
6	NAG	A	607	1	14,14,15	0.25	0	17,19,21	0.60	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	OXY	A	603	-	1,1,1	0.21	0	-		
6	NAG	A	605	1	14,14,15	0.41	0	17,19,21	1.22	1 (5%)
3	FAD	A	601	-	53,58,58	0.51	0	68,89,89	0.70	2 (2%)
6	NAG	B	607	1	14,14,15	0.50	0	17,19,21	0.46	0
4	EPE	B	602	-	15,15,15	0.83	1 (6%)	18,20,20	1.87	3 (16%)
6	NAG	B	606	1	14,14,15	0.41	0	17,19,21	0.41	0
6	NAG	A	604	1	14,14,15	0.25	0	17,19,21	0.89	1 (5%)
6	NAG	B	608	1	14,14,15	1.27	1 (7%)	17,19,21	1.47	2 (11%)
3	FAD	B	601	-	53,58,58	0.50	0	68,89,89	0.74	3 (4%)
5	OXY	B	603	-	1,1,1	0.16	0	-		
6	NAG	B	605	1	14,14,15	0.34	0	17,19,21	0.95	0
4	EPE	A	602	-	15,15,15	0.86	1 (6%)	18,20,20	1.76	5 (27%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	NAG	A	608	1	-	4/6/23/26	0/1/1/1
7	MPD	A	609	-	-	2/5/5/5	-
6	NAG	A	606	1	-	4/6/23/26	0/1/1/1
6	NAG	B	604	1	-	2/6/23/26	0/1/1/1
6	NAG	B	609	1	-	1/6/23/26	0/1/1/1
6	NAG	A	607	1	-	3/6/23/26	0/1/1/1
6	NAG	A	605	1	-	2/6/23/26	0/1/1/1
3	FAD	A	601	-	-	4/30/50/50	0/6/6/6
6	NAG	B	607	1	-	0/6/23/26	0/1/1/1
4	EPE	B	602	-	-	2/9/19/19	0/1/1/1
6	NAG	B	606	1	-	0/6/23/26	0/1/1/1
6	NAG	A	604	1	-	0/6/23/26	0/1/1/1
6	NAG	B	608	1	-	3/6/23/26	0/1/1/1
3	FAD	B	601	-	-	6/30/50/50	0/6/6/6
6	NAG	B	605	1	-	1/6/23/26	0/1/1/1
4	EPE	A	602	-	-	2/9/19/19	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	608	NAG	O5-C1	-4.54	1.36	1.43
4	A	602	EPE	C10-S	2.95	1.81	1.77
4	B	602	EPE	C10-S	2.91	1.81	1.77

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	608	NAG	C1-O5-C5	6.20	120.59	112.19
6	B	608	NAG	C3-C4-C5	4.58	118.41	110.24
4	B	602	EPE	C5-N4-C3	4.38	118.69	108.83
4	A	602	EPE	C5-N4-C3	4.01	117.86	108.83
4	B	602	EPE	O1S-S-C10	3.91	111.62	106.92
4	A	602	EPE	O1S-S-C10	3.27	110.85	106.92
6	A	605	NAG	C1-O5-C5	3.20	116.53	112.19
6	B	604	NAG	C1-O5-C5	3.14	116.44	112.19
6	A	604	NAG	C1-O5-C5	3.04	116.32	112.19
4	A	602	EPE	C7-N4-C3	3.04	119.01	111.23
6	A	608	NAG	C3-C4-C5	3.01	115.61	110.24
6	B	608	NAG	C4-C3-C2	2.98	115.39	111.02
6	B	609	NAG	C1-O5-C5	2.82	116.01	112.19
3	B	601	FAD	C5'-C4'-C3'	-2.66	107.06	112.20
3	A	601	FAD	C4'-C3'-C2'	2.51	118.58	113.36
3	B	601	FAD	C4'-C3'-C2'	2.51	118.58	113.36
3	B	601	FAD	C5A-C6A-N6A	2.47	124.10	120.35
4	A	602	EPE	C7-N4-C5	2.38	117.31	111.23
3	A	601	FAD	C5A-C6A-N6A	2.35	123.93	120.35
6	A	606	NAG	C1-O5-C5	2.30	115.31	112.19
4	A	602	EPE	O2S-S-C10	2.12	109.47	106.92
4	B	602	EPE	O3S-S-C10	2.04	109.07	105.77
7	A	609	MPD	CM-C2-C1	-2.00	106.40	110.57

There are no chirality outliers.

All (36) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	601	FAD	N10-C1'-C2'-O2'
3	B	601	FAD	PA-O3P-P-O5'
4	A	602	EPE	C8-C7-N4-C3
7	A	609	MPD	O2-C2-C3-C4
7	A	609	MPD	CM-C2-C3-C4
6	B	608	NAG	O5-C5-C6-O6
6	B	608	NAG	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
6	A	608	NAG	O5-C5-C6-O6
6	A	606	NAG	O5-C5-C6-O6
6	A	606	NAG	C4-C5-C6-O6
6	A	608	NAG	C4-C5-C6-O6
6	A	607	NAG	O5-C5-C6-O6
4	B	602	EPE	C8-C7-N4-C5
6	B	609	NAG	C1-C2-N2-C7
3	B	601	FAD	P-O3P-PA-O1A
3	B	601	FAD	O4B-C4B-C5B-O5B
3	A	601	FAD	PA-O3P-P-O5'
4	B	602	EPE	N4-C7-C8-O8
6	A	607	NAG	C1-C2-N2-C7
3	A	601	FAD	P-O3P-PA-O2A
6	A	606	NAG	C3-C2-N2-C7
6	A	608	NAG	C3-C2-N2-C7
6	B	608	NAG	C3-C2-N2-C7
4	A	602	EPE	C10-C9-N1-C2
6	A	608	NAG	C1-C2-N2-C7
3	A	601	FAD	P-O3P-PA-O1A
3	B	601	FAD	P-O3P-PA-O2A
6	A	605	NAG	C3-C2-N2-C7
6	A	607	NAG	C3-C2-N2-C7
6	B	604	NAG	C3-C2-N2-C7
6	B	605	NAG	C3-C2-N2-C7
3	A	601	FAD	O4B-C4B-C5B-O5B
3	B	601	FAD	C3B-C4B-C5B-O5B
6	A	606	NAG	C1-C2-N2-C7
6	A	605	NAG	C1-C2-N2-C7
6	B	604	NAG	C1-C2-N2-C7

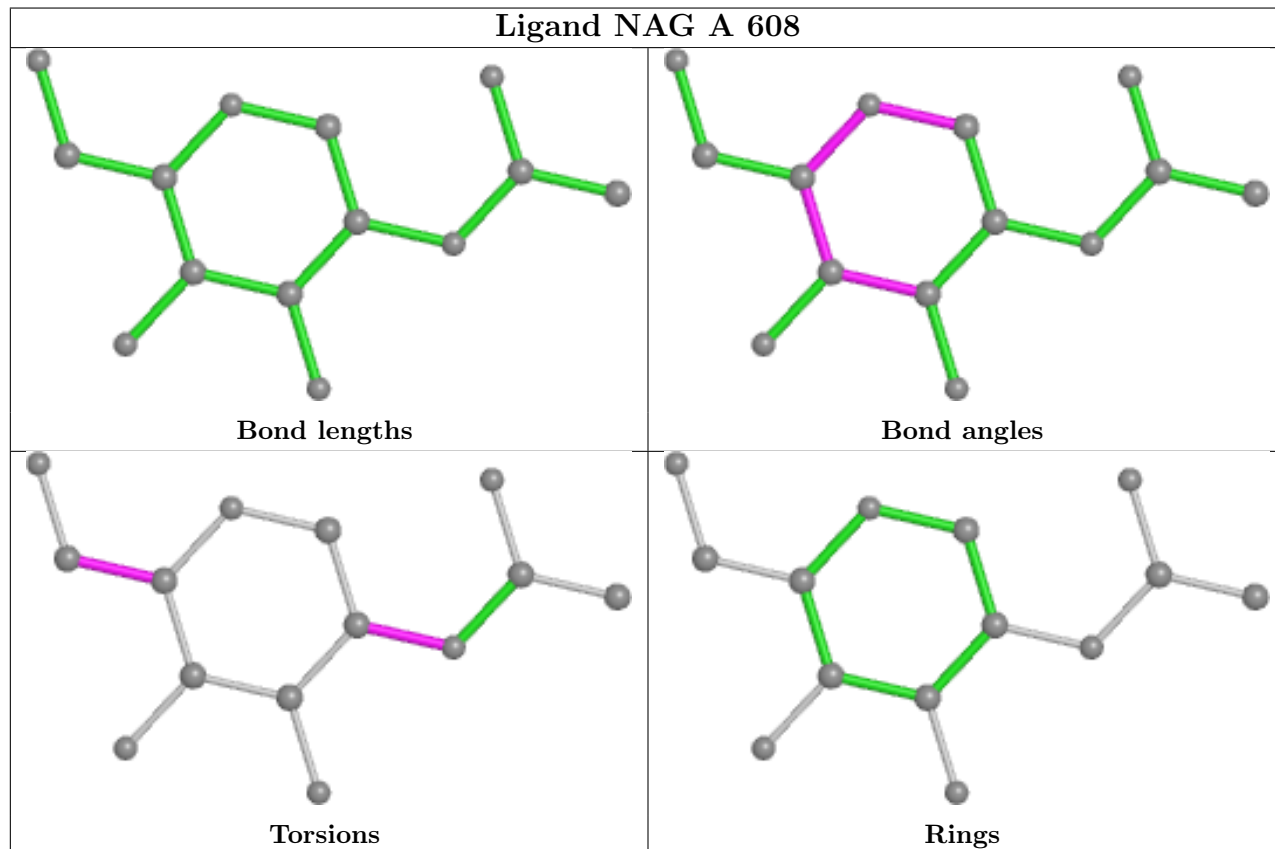
There are no ring outliers.

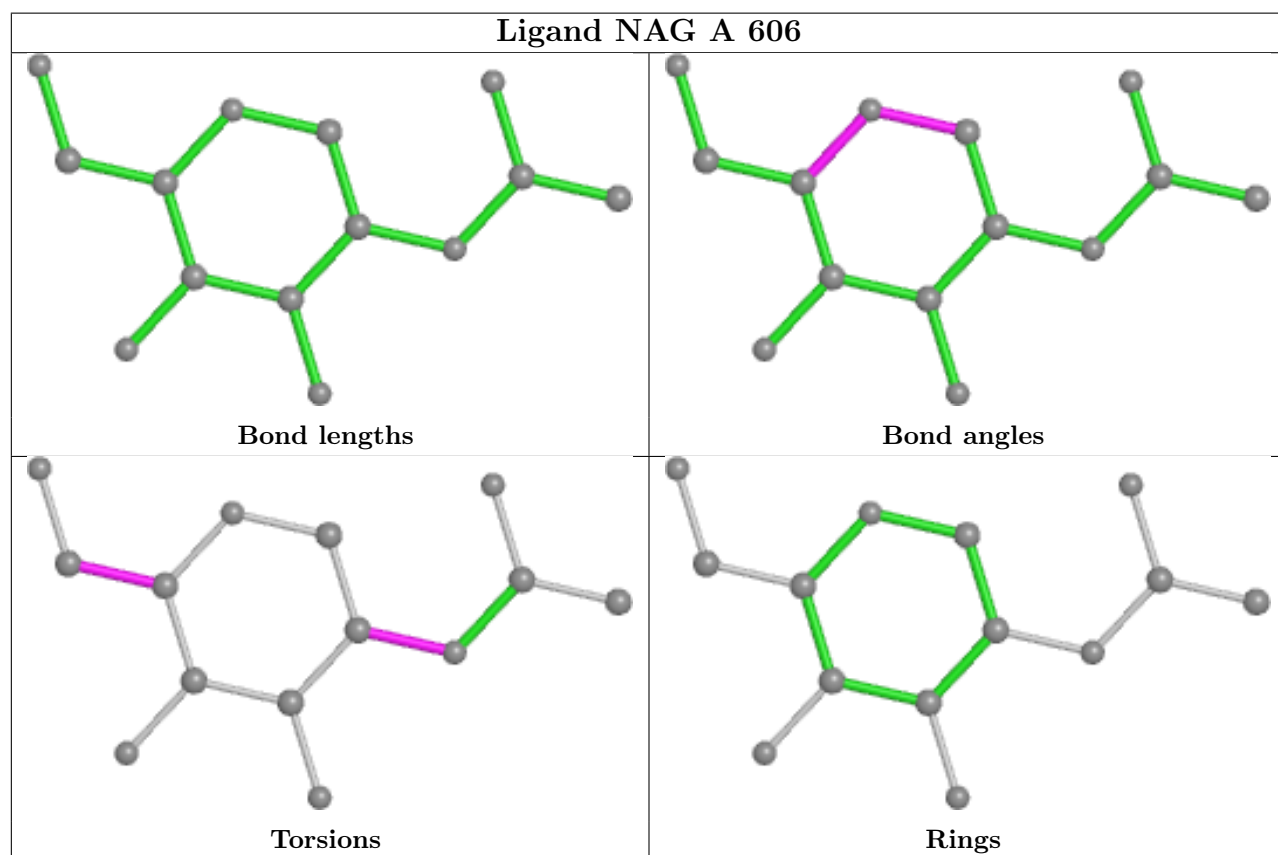
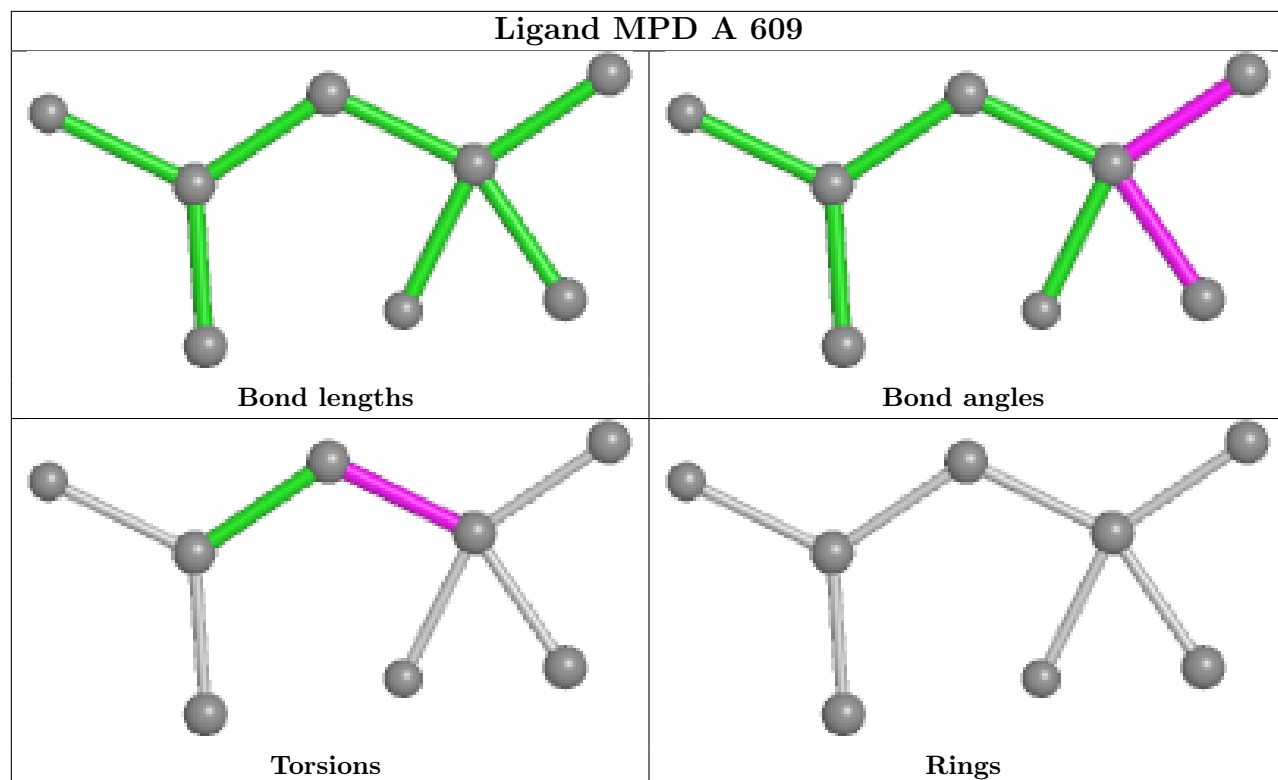
5 monomers are involved in 9 short contacts:

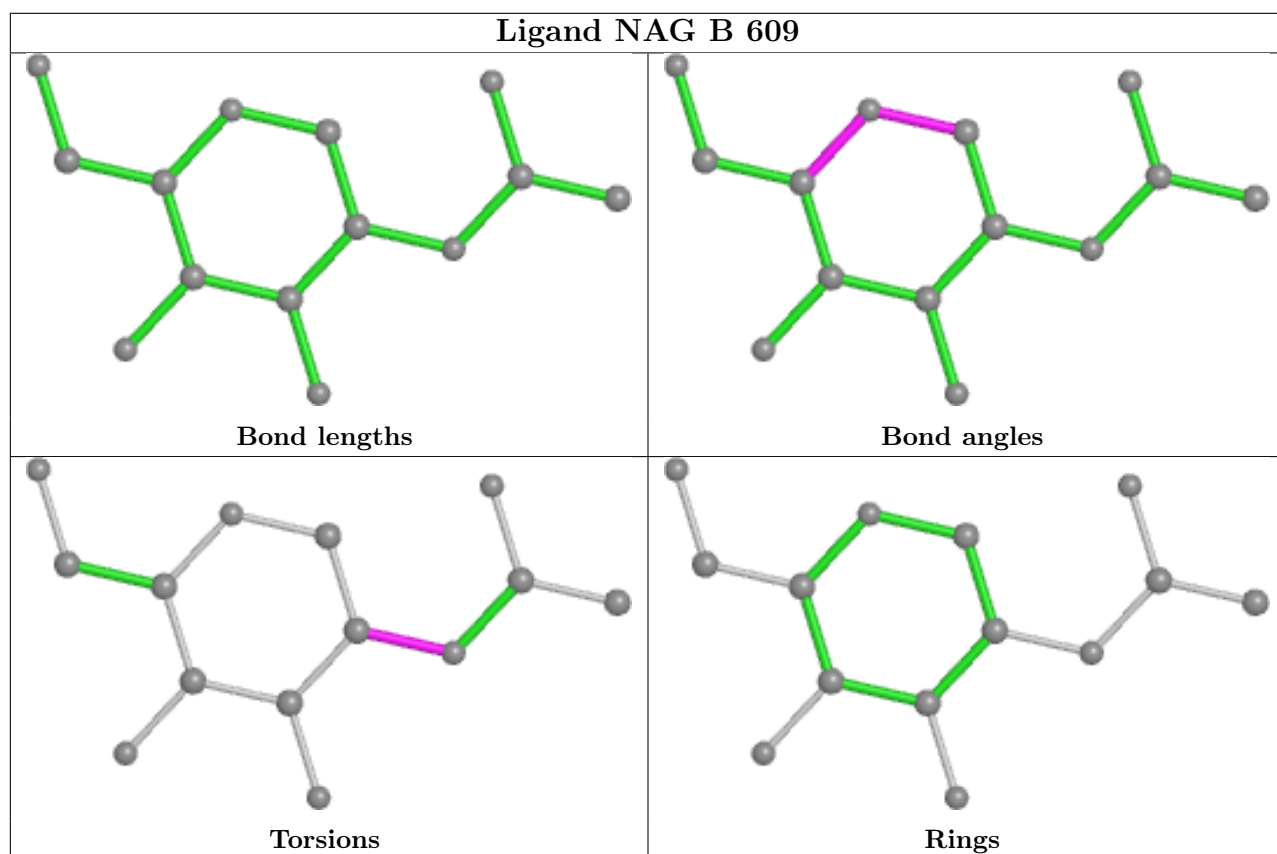
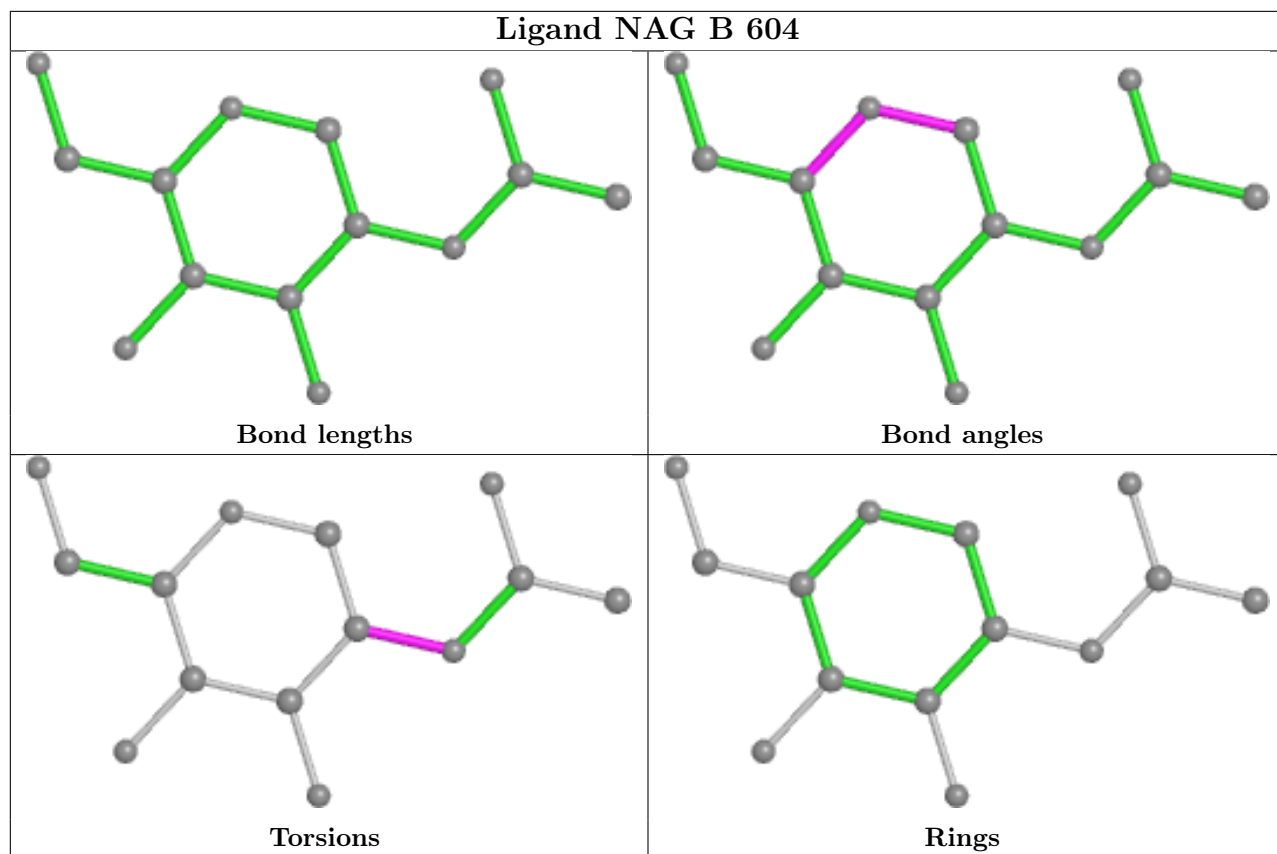
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A	609	MPD	1	0
3	A	601	FAD	2	0
4	B	602	EPE	1	0
3	B	601	FAD	4	0
4	A	602	EPE	1	0

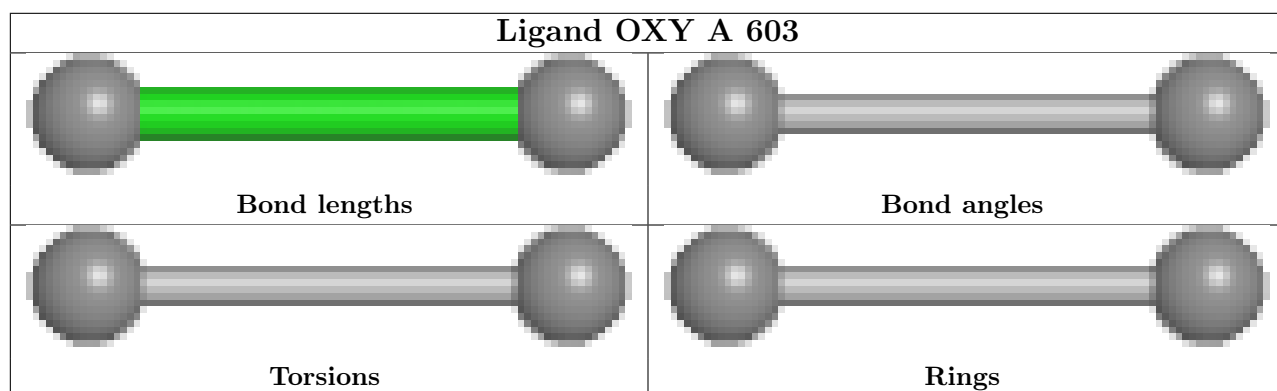
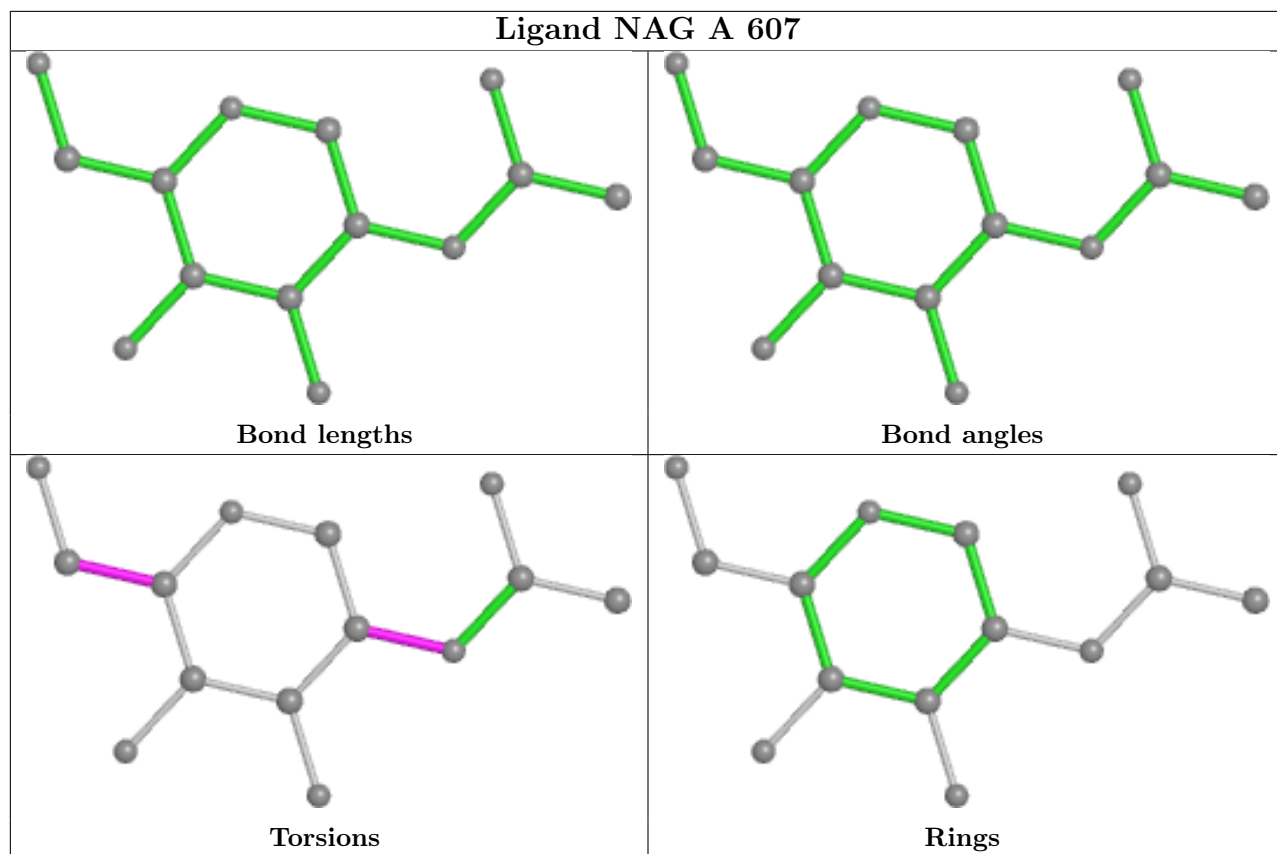
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In

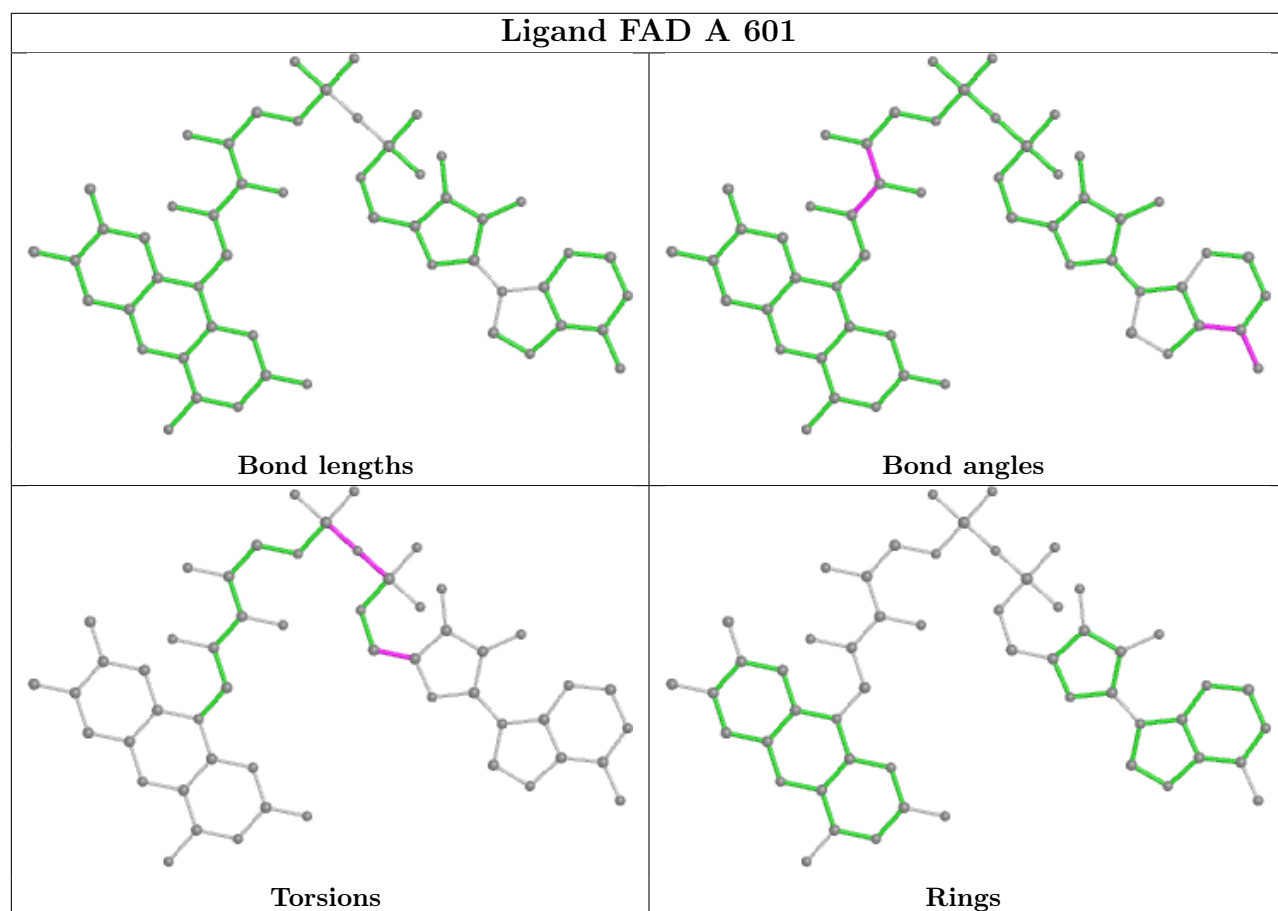
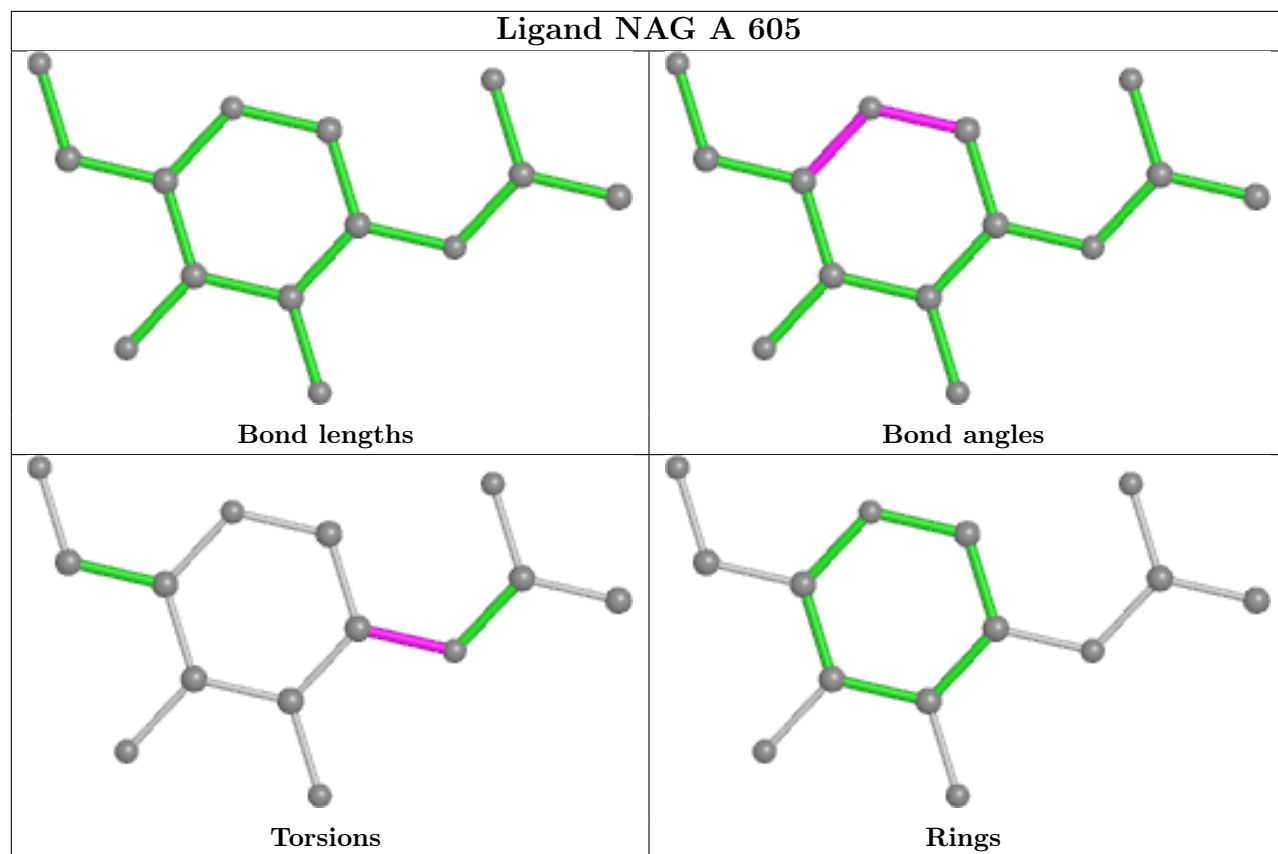
addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. 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.

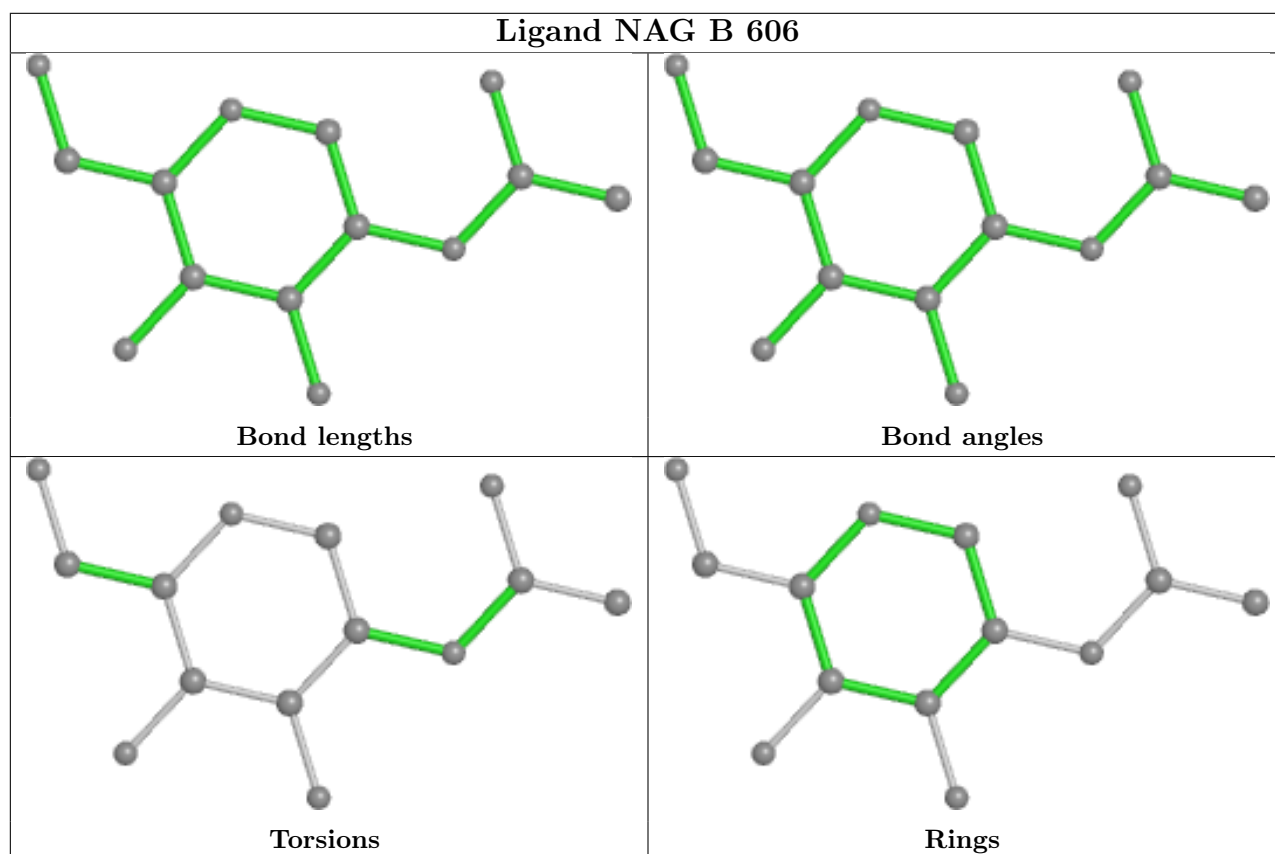
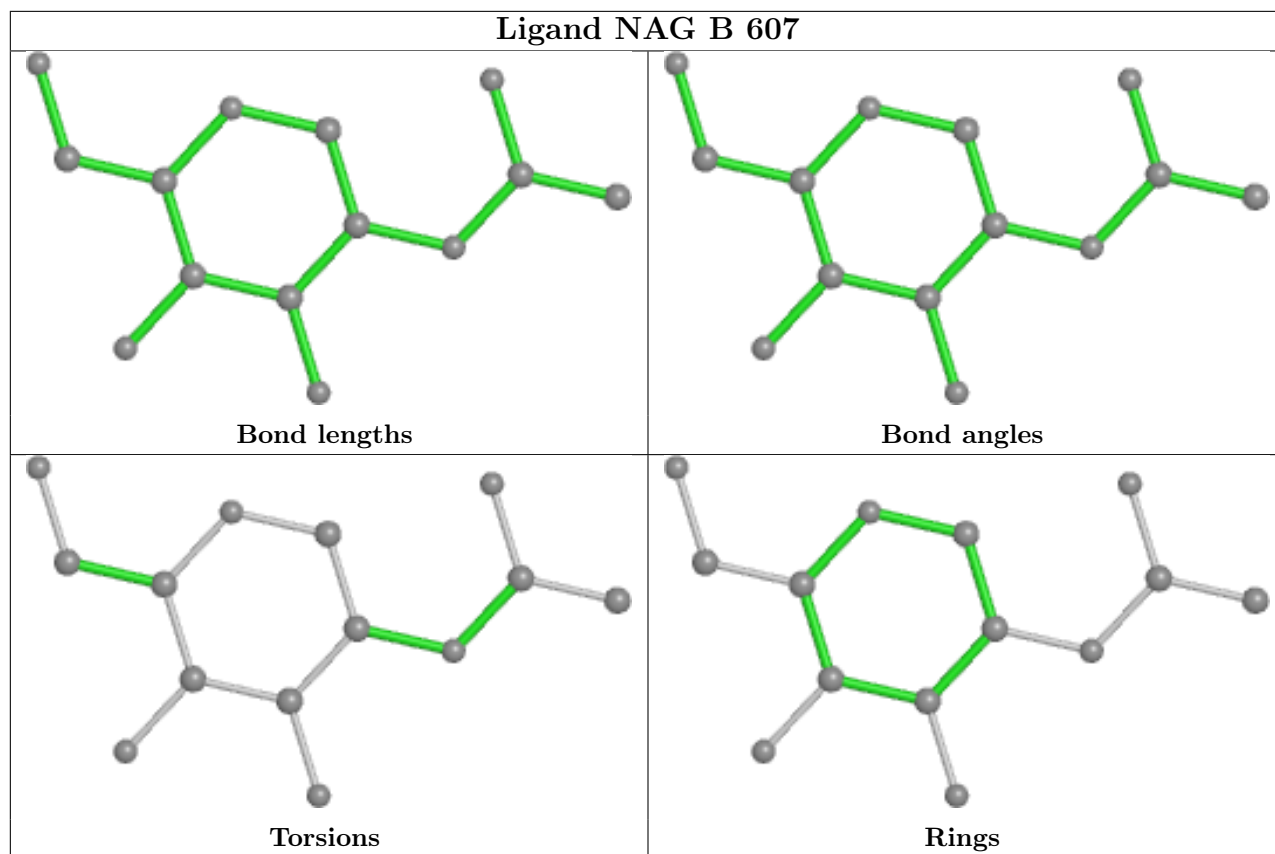


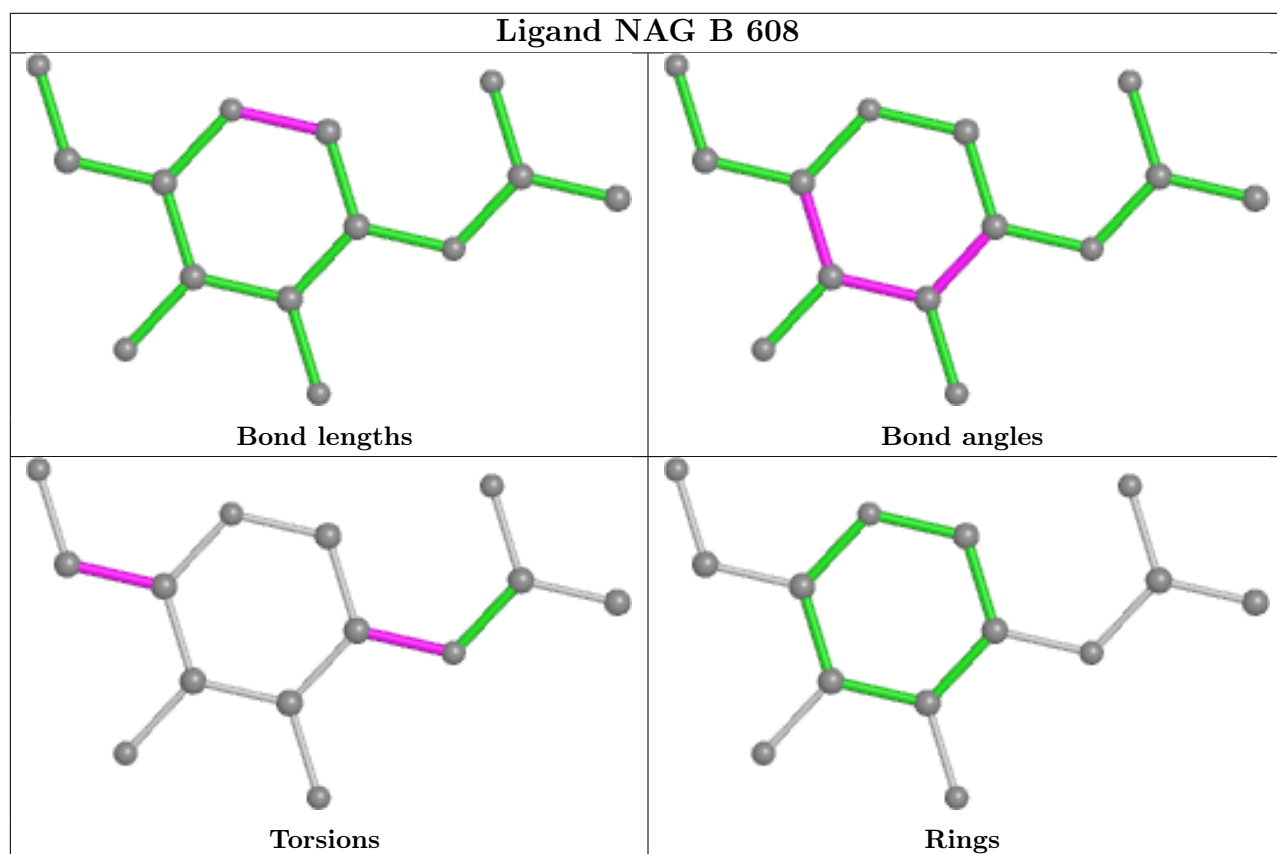
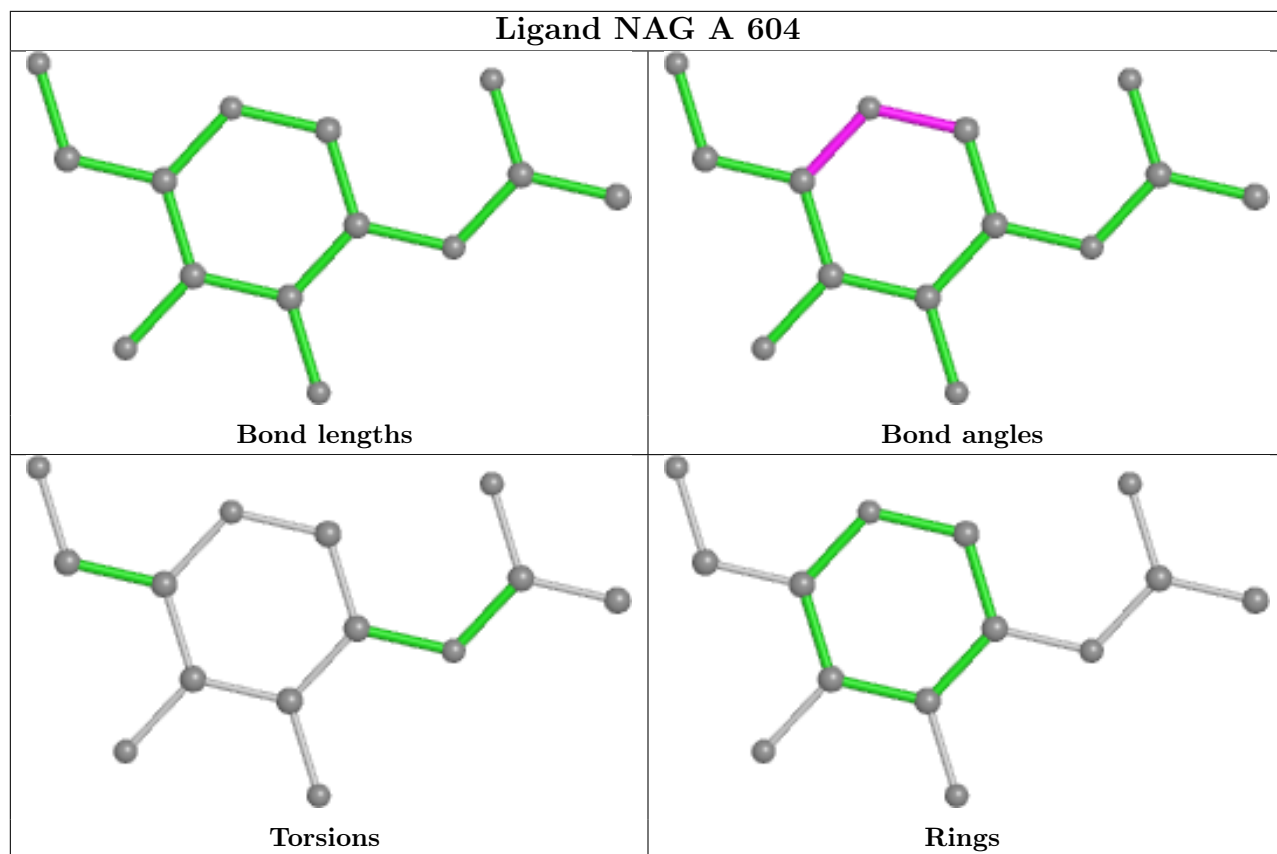


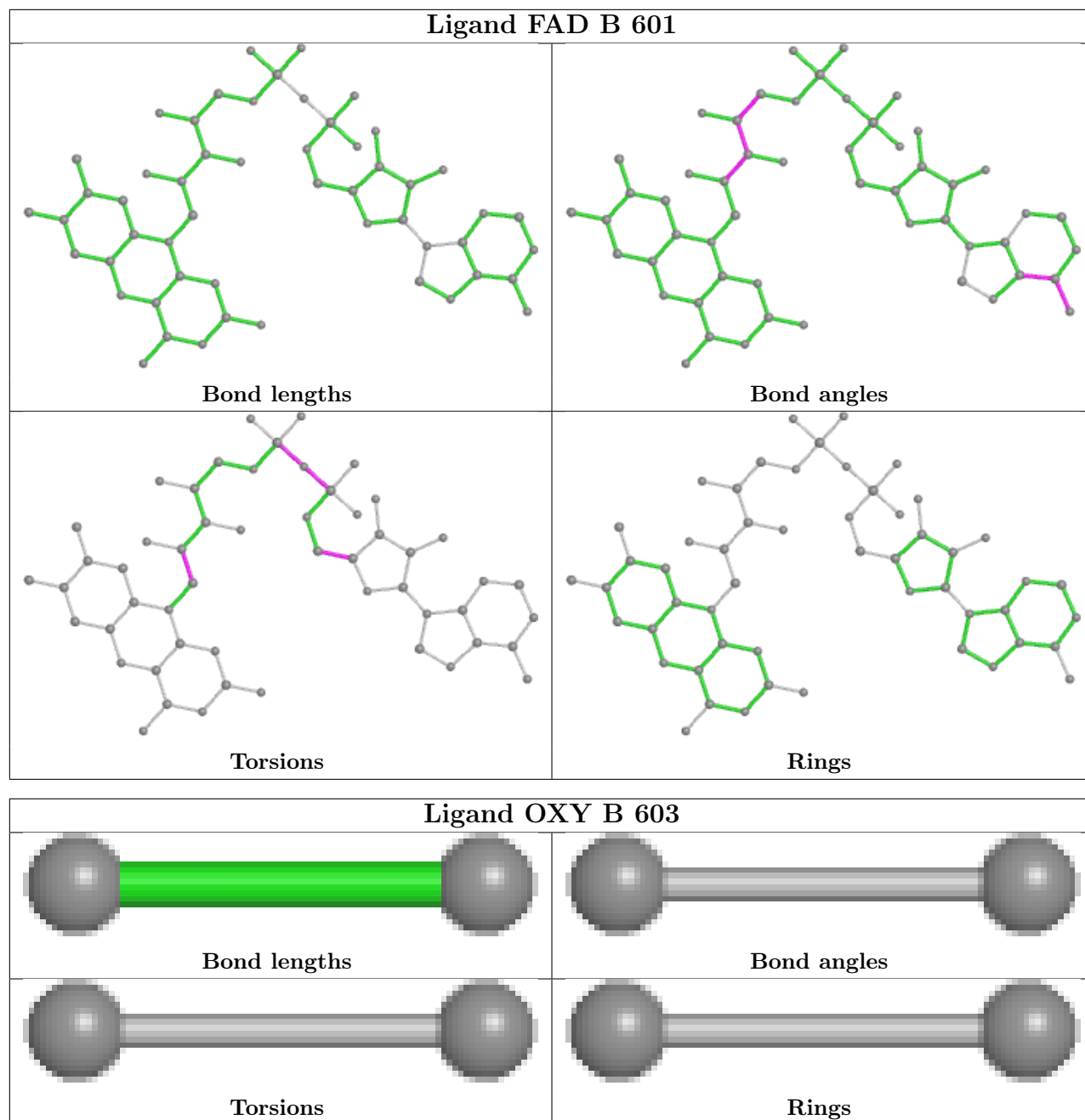


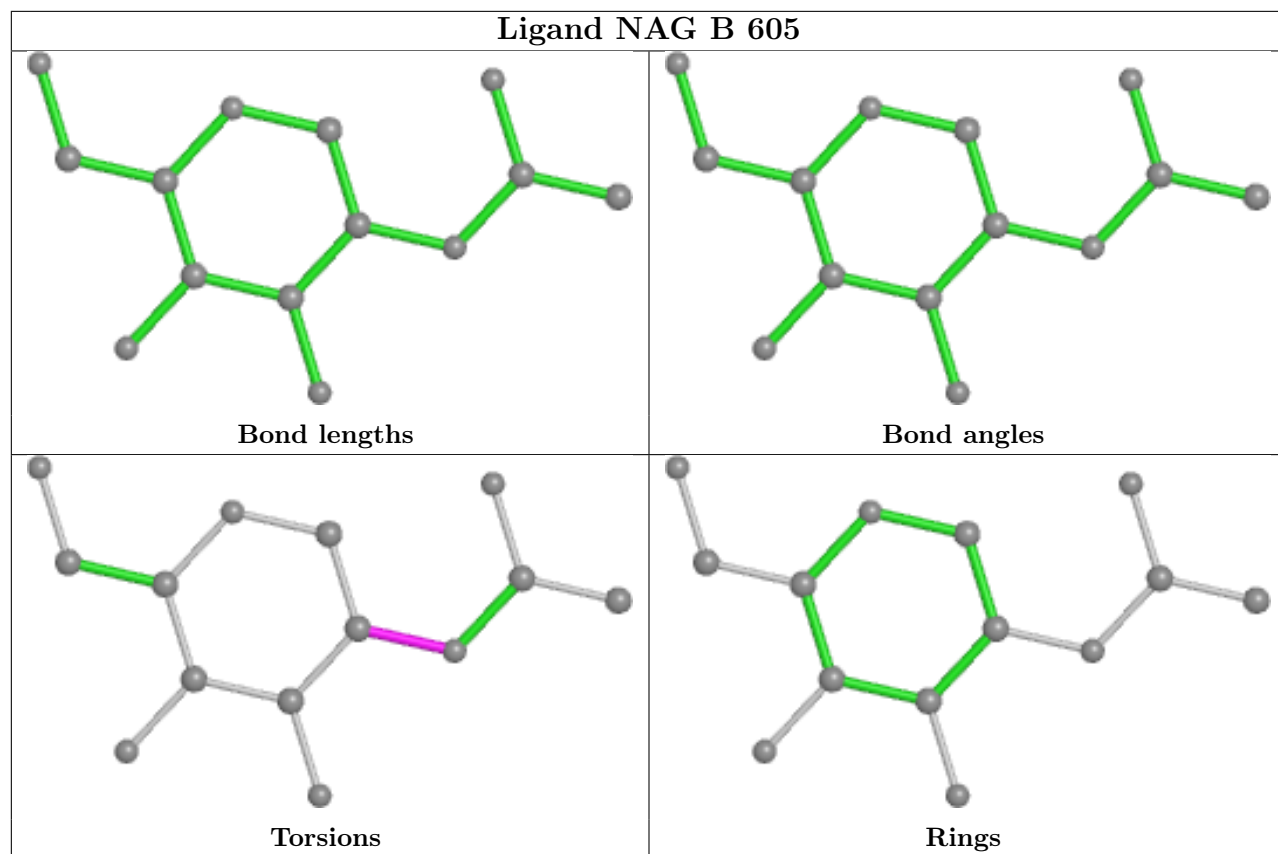












5.7 Other polymers [i](#)

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	581/581 (100%)	-0.53	4 (0%) 87 89	27, 37, 51, 88	0
1	B	581/581 (100%)	-0.52	5 (0%) 84 86	26, 35, 48, 72	0
All	All	1162/1162 (100%)	-0.53	9 (0%) 86 87	26, 36, 49, 88	0

All (9) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	258	THR	4.5
1	A	255	GLN	3.5
1	A	257	ALA	3.3
1	B	581	GLN	3.2
1	B	580	MET	2.9
1	B	358	ASP	2.5
1	A	358	ASP	2.5
1	B	255	GLN	2.4
1	B	272	GLY	2.1

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.

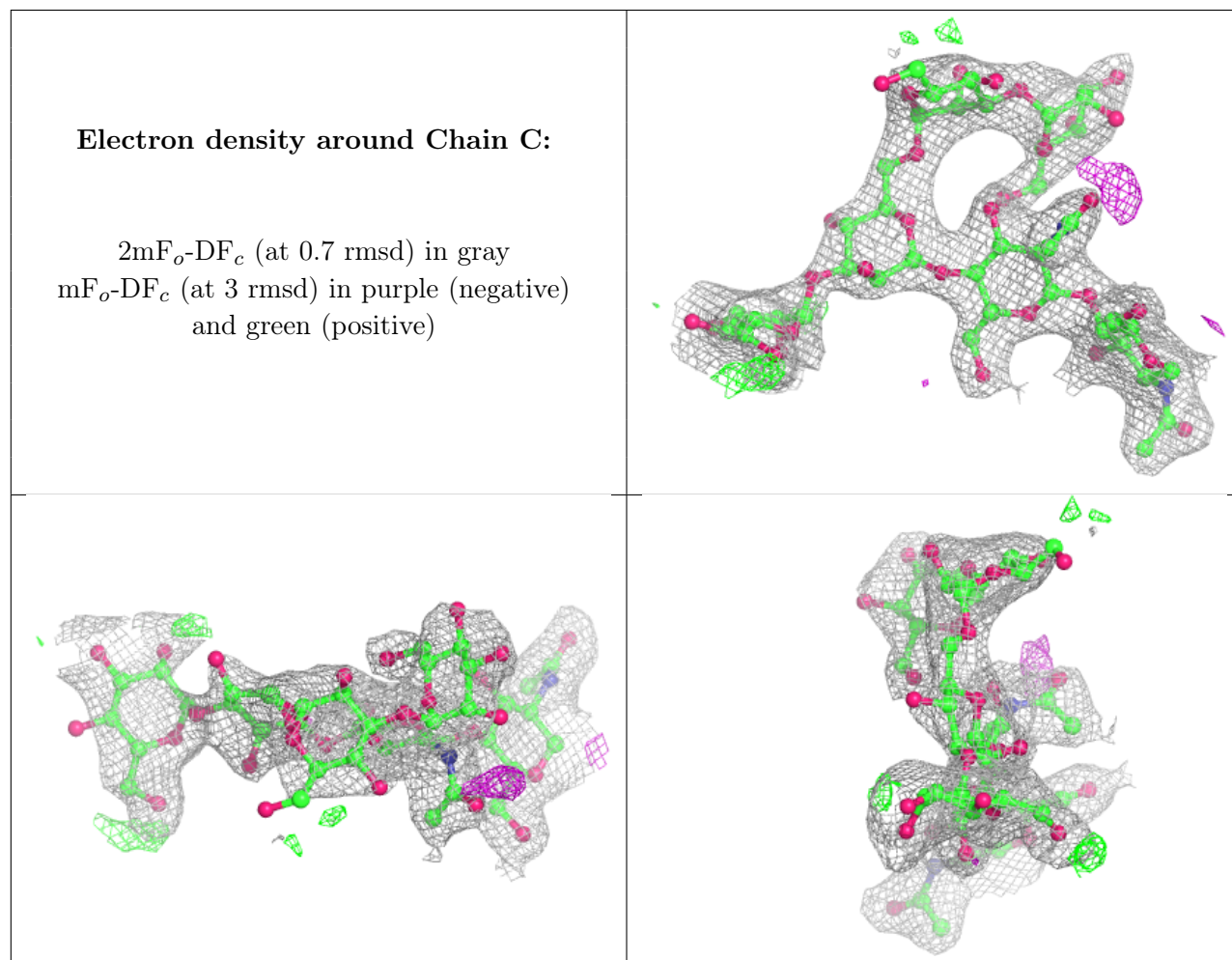
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	MAN	C	6	11/12	0.60	0.25	57,82,89,99	0

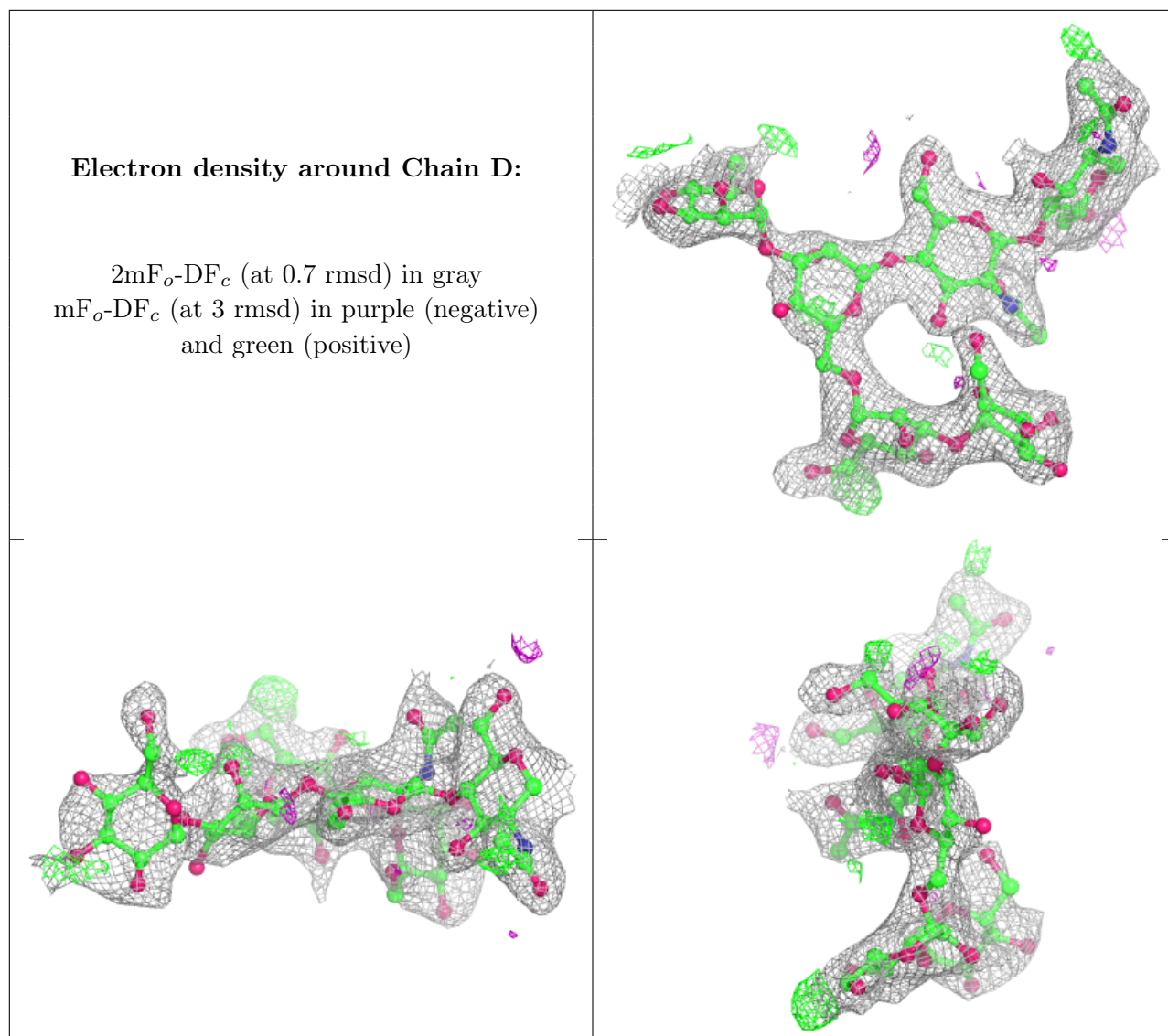
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	MAN	D	6	11/12	0.60	0.31	65,89,95,100	0
2	BMA	D	3	11/12	0.83	0.29	67,75,85,91	0
2	MAN	D	4	11/12	0.84	0.24	67,73,78,82	0
2	BMA	C	3	11/12	0.88	0.24	63,69,80,84	0
2	MAN	C	5	11/12	0.90	0.36	66,79,85,90	0
2	MAN	D	5	11/12	0.91	0.36	76,88,94,95	0
2	MAN	C	4	11/12	0.93	0.27	67,76,81,85	0
2	NAG	D	1	14/15	0.93	0.09	36,42,50,52	0
2	NAG	C	2	14/15	0.94	0.13	40,48,57,63	0
2	NAG	D	2	14/15	0.95	0.14	47,51,58,65	0
2	NAG	C	1	14/15	0.97	0.07	29,40,46,46	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.

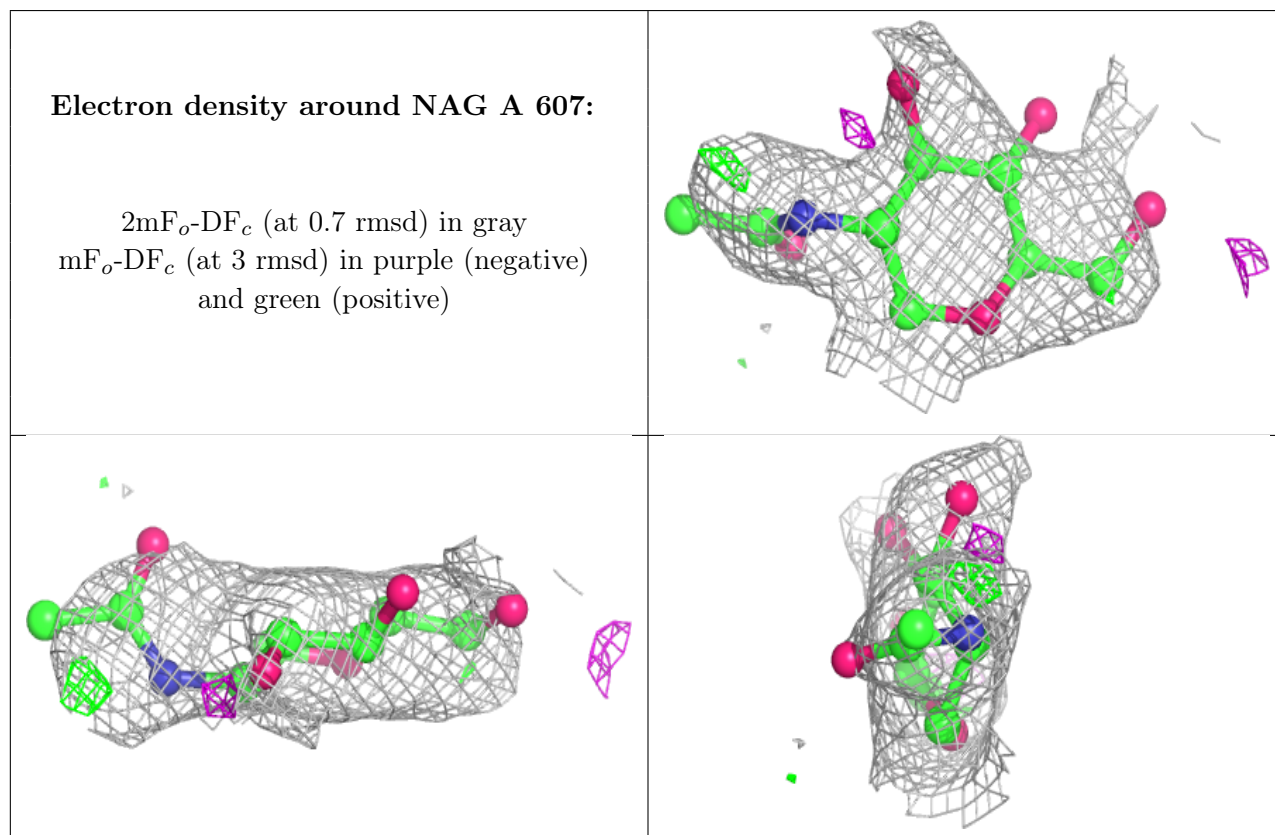
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
6	NAG	A	607	14/15	0.78	0.32	73,83,99,100	0
6	NAG	B	608	14/15	0.79	0.27	71,83,94,102	0
6	NAG	A	608	14/15	0.82	0.28	66,71,84,87	0
6	NAG	B	609	14/15	0.82	0.24	58,72,81,83	0
7	MPD	A	609	8/8	0.84	0.38	48,57,63,67	8
6	NAG	B	604	14/15	0.90	0.24	51,55,64,69	0
6	NAG	A	605	14/15	0.91	0.22	47,56,58,67	0

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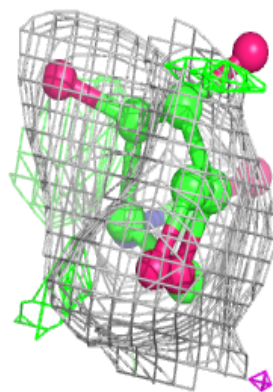
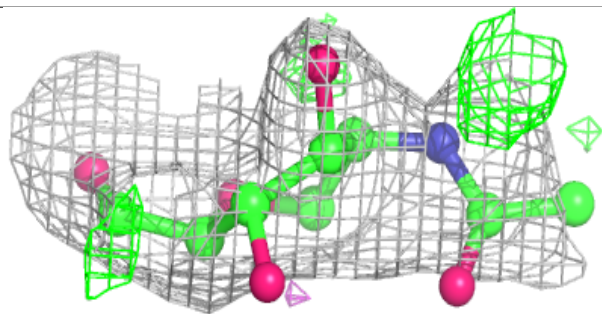
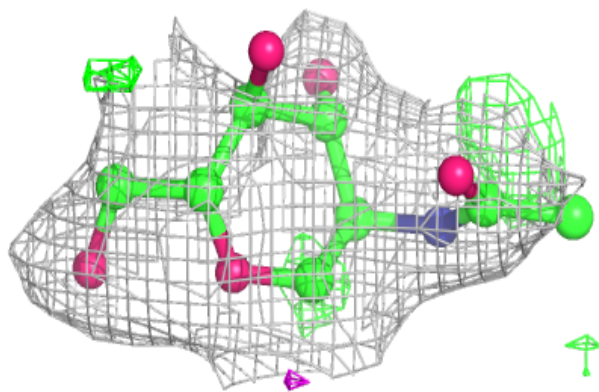
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
6	NAG	A	606	14/15	0.91	0.20	49,59,62,63	0
6	NAG	B	607	14/15	0.92	0.24	49,64,69,73	0
6	NAG	B	605	14/15	0.93	0.23	52,61,70,73	0
6	NAG	A	604	14/15	0.94	0.12	42,50,59,60	0
5	OXY	A	603	2/2	0.96	0.10	40,40,40,41	0
6	NAG	B	606	14/15	0.96	0.12	34,48,60,60	0
3	FAD	B	601	53/53	0.97	0.07	24,32,44,47	0
3	FAD	A	601	53/53	0.97	0.07	25,32,43,46	0
4	EPE	B	602	15/15	0.98	0.08	39,46,49,53	0
4	EPE	A	602	15/15	0.98	0.07	41,44,51,52	0
5	OXY	B	603	2/2	0.98	0.05	37,37,37,43	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.

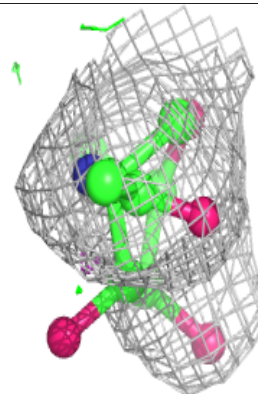
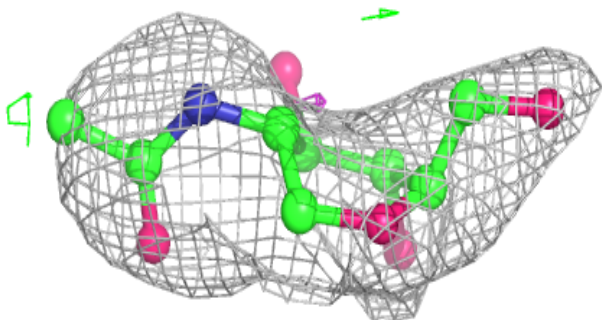
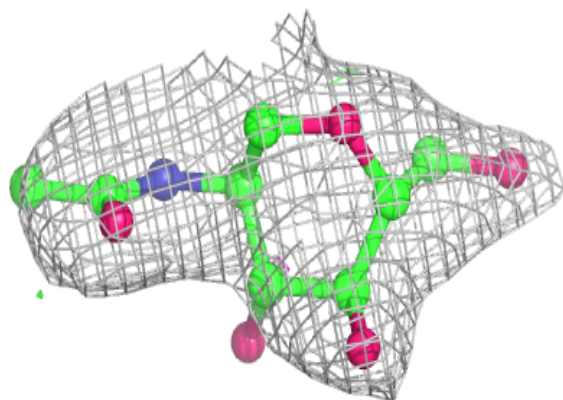


Electron density around NAG B 608:

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

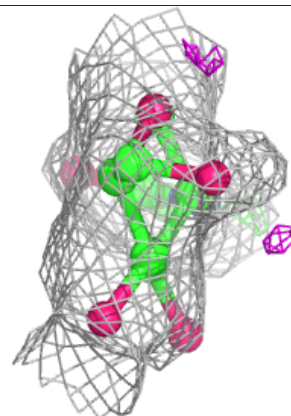
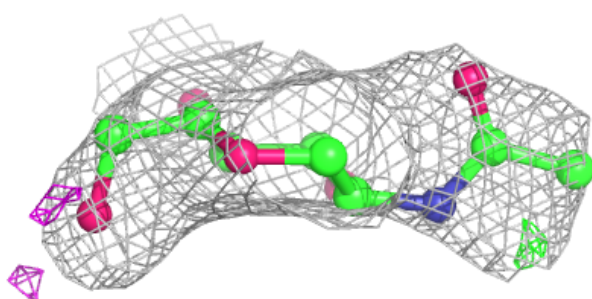
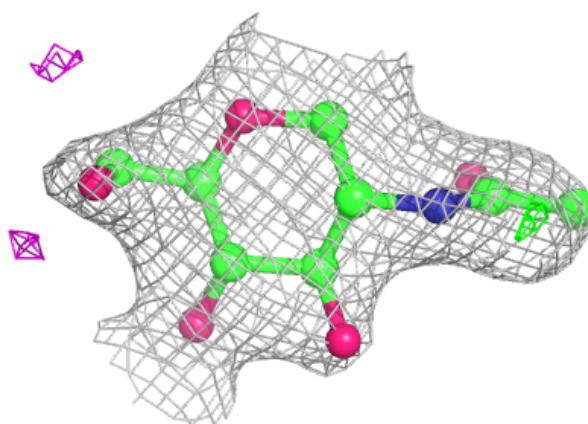
**Electron density around NAG A 608:**

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

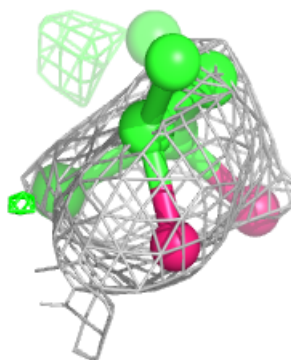
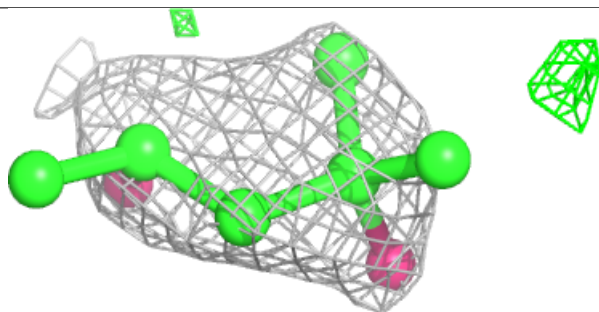
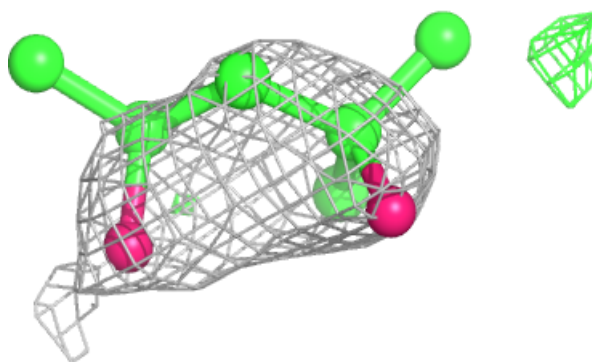


Electron density around NAG B 609:

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

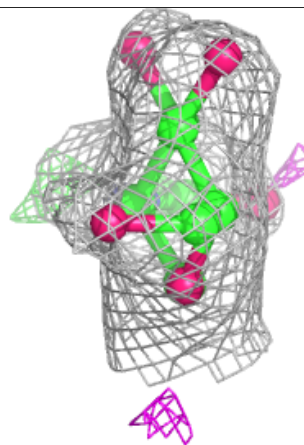
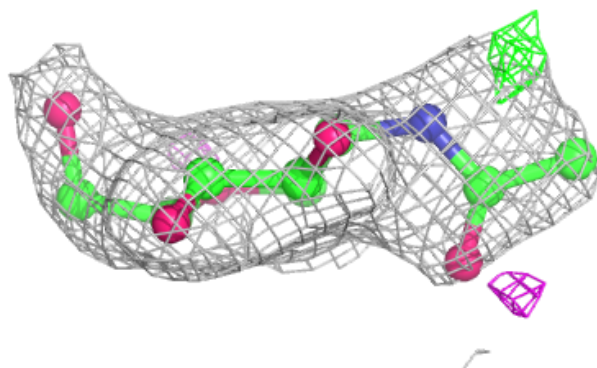
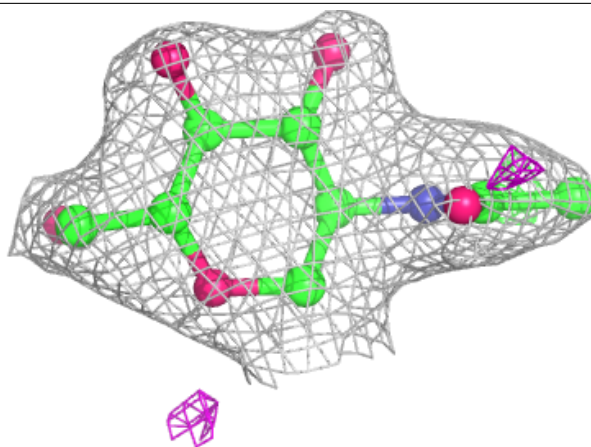
**Electron density around MPD A 609:**

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



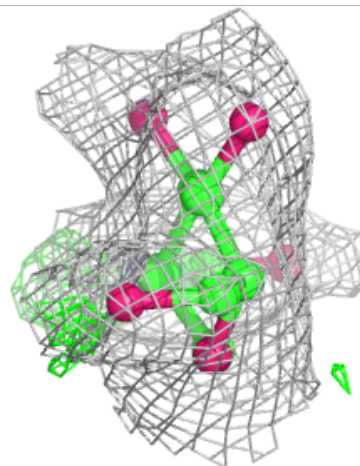
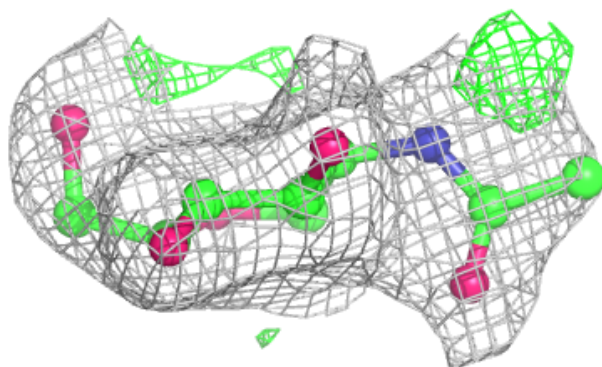
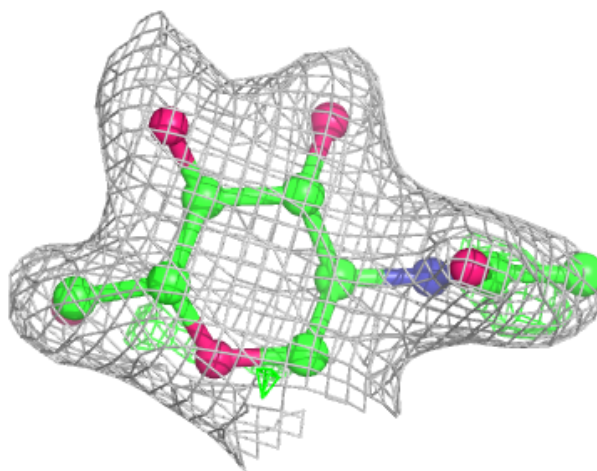
Electron density around NAG B 604:

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



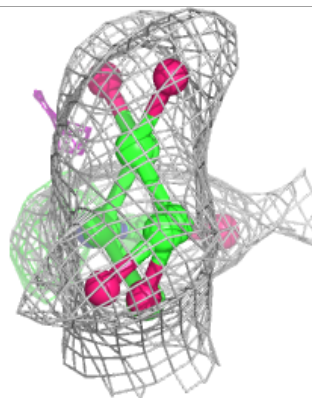
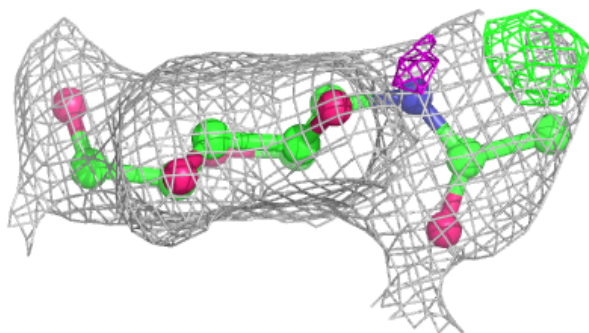
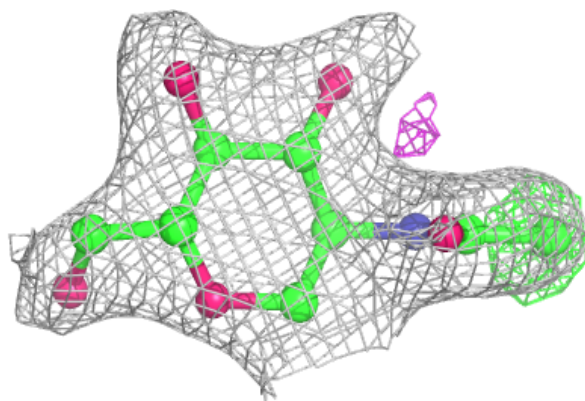
Electron density around NAG A 605:

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

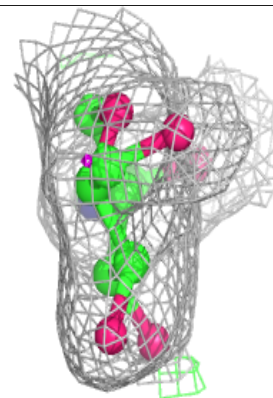
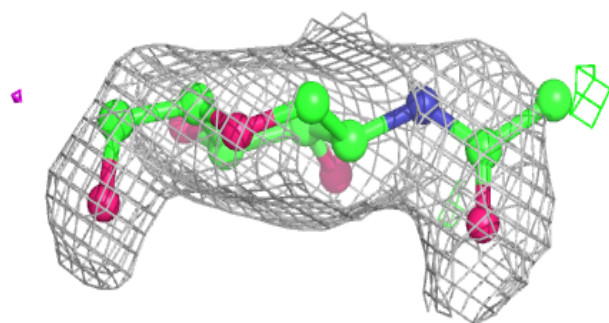
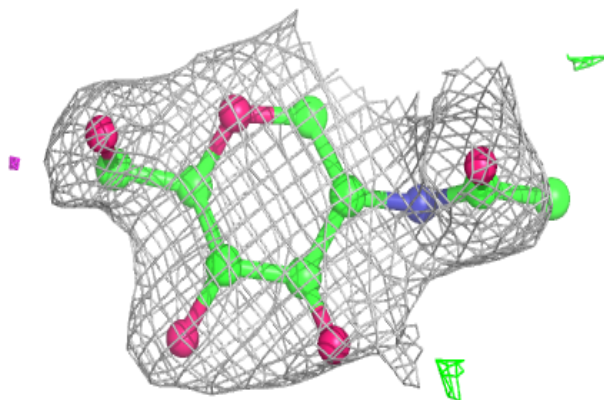


Electron density around NAG A 606:

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

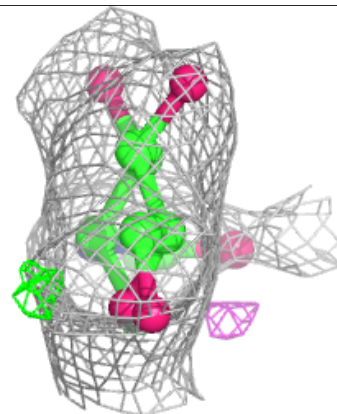
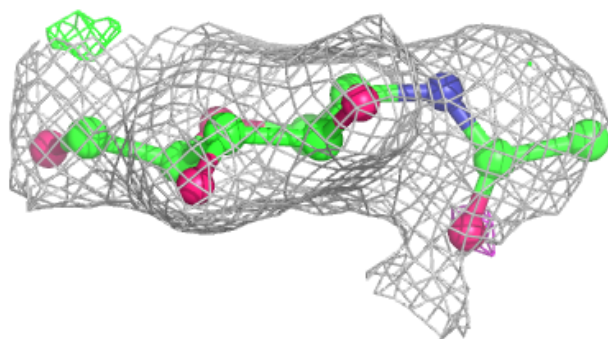
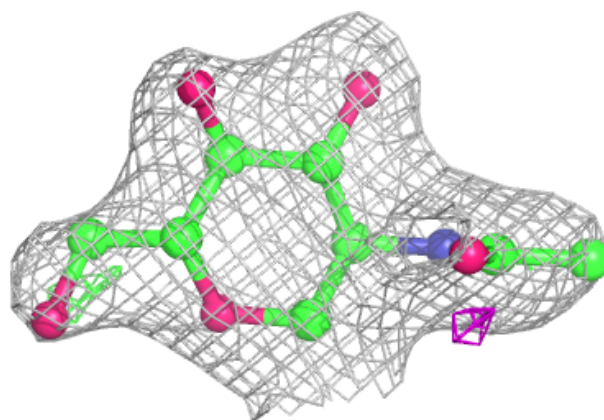
**Electron density around NAG B 607:**

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

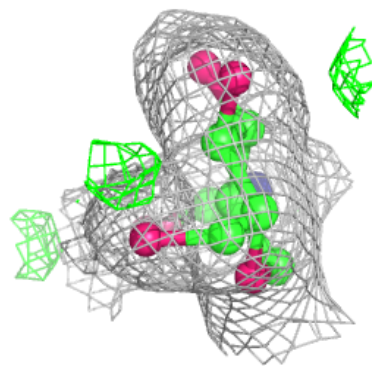
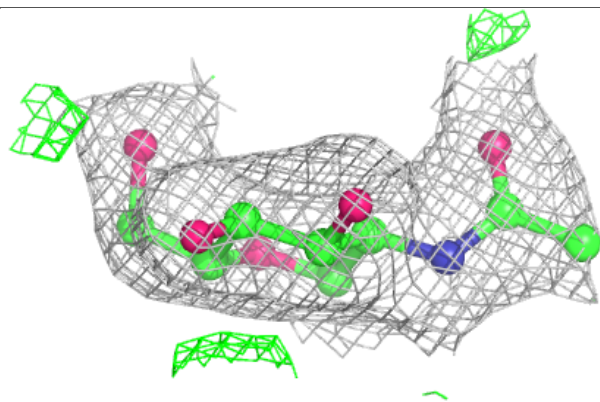
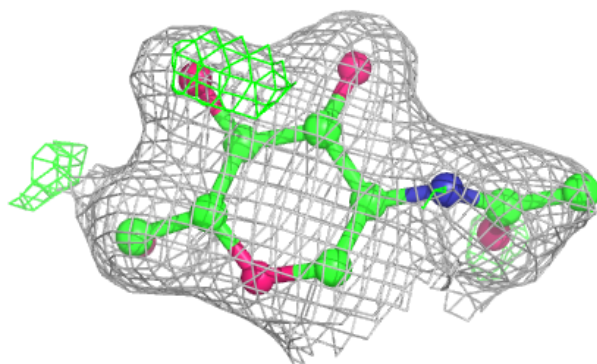


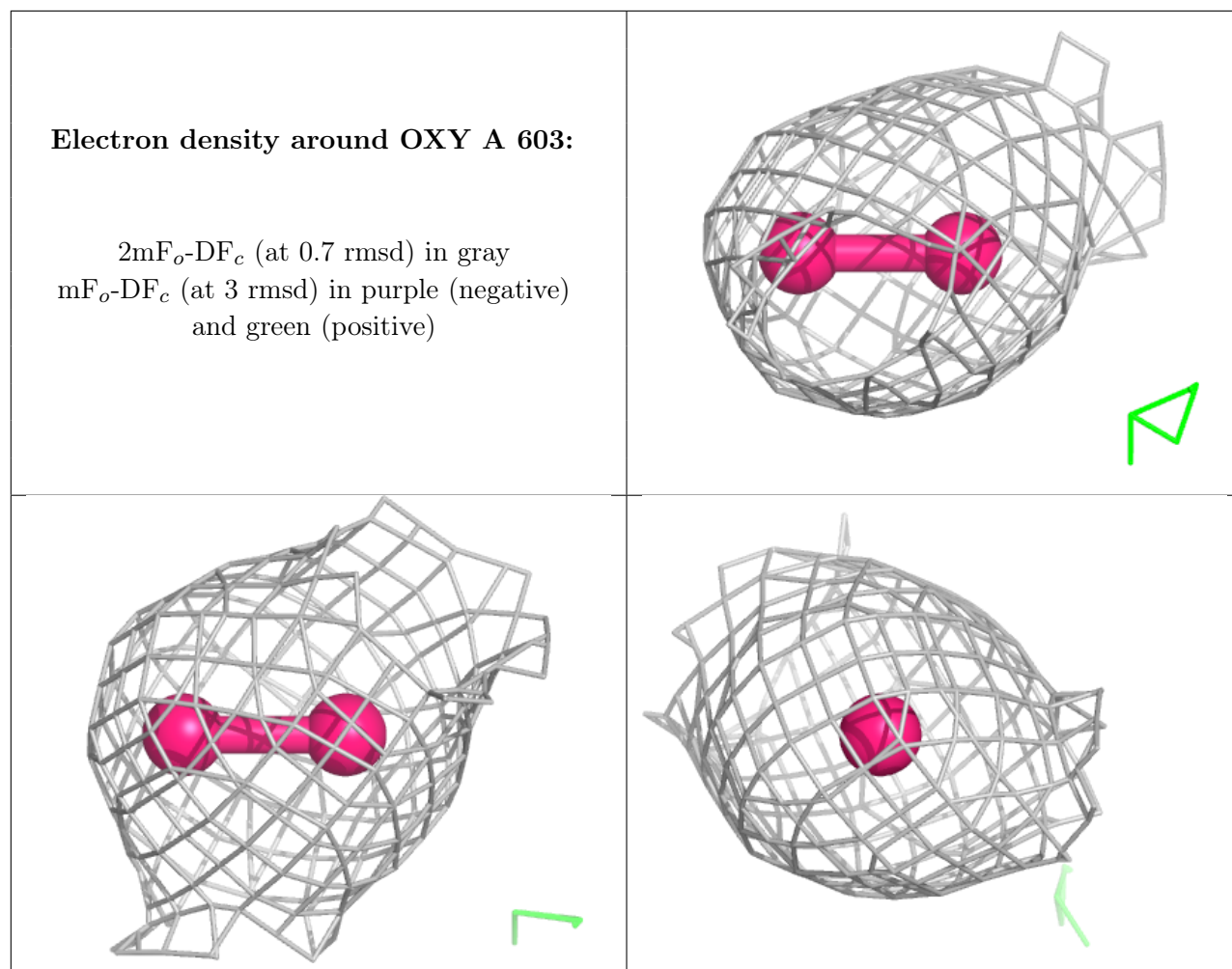
Electron density around NAG B 605:

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

**Electron density around NAG A 604:**

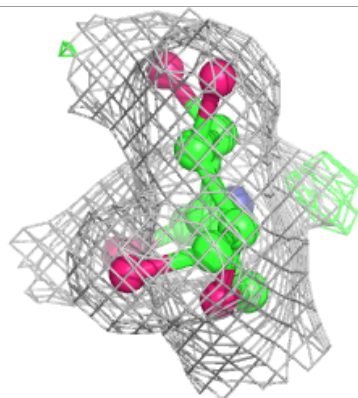
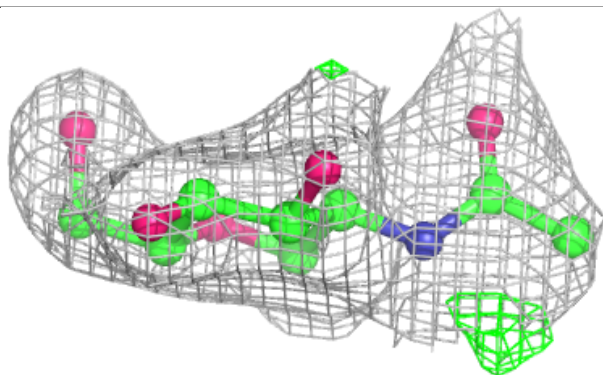
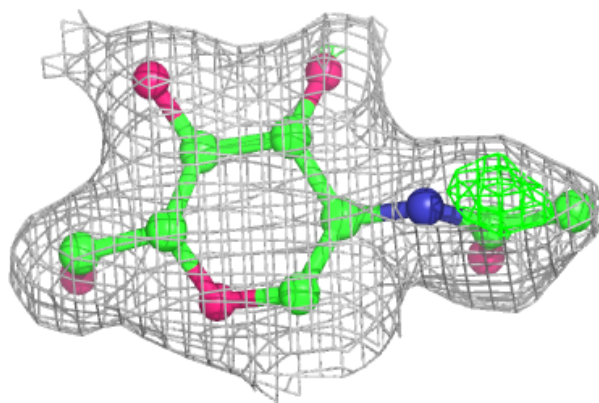
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



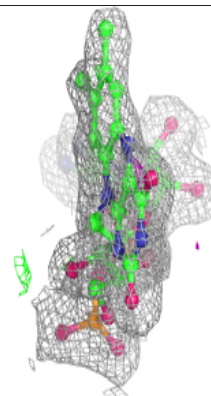
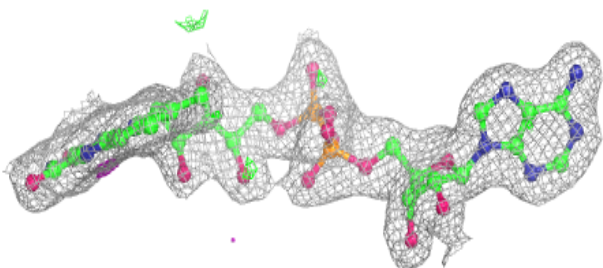
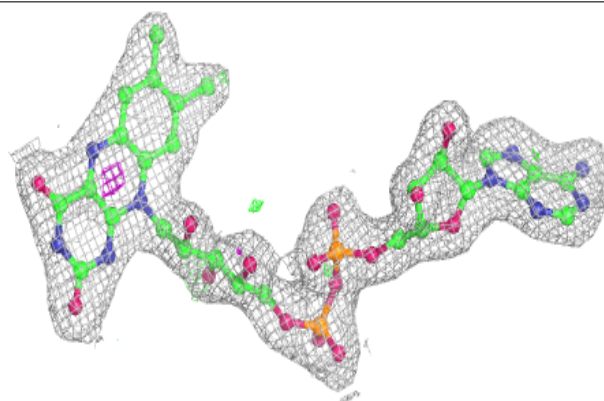


Electron density around NAG B 606:

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

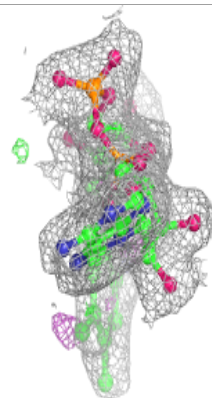
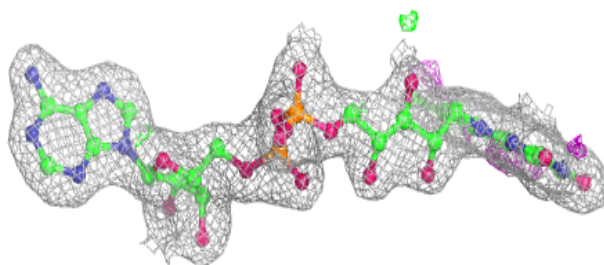
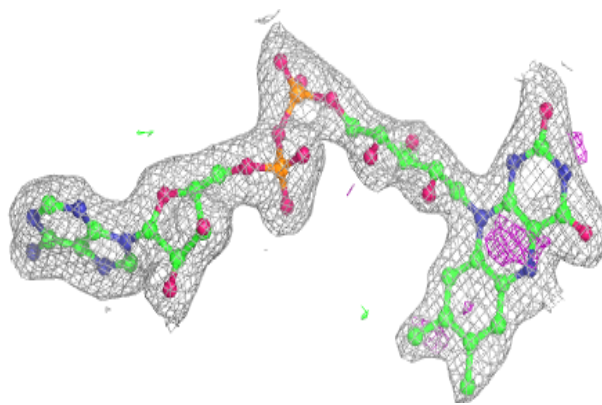
**Electron density around FAD B 601:**

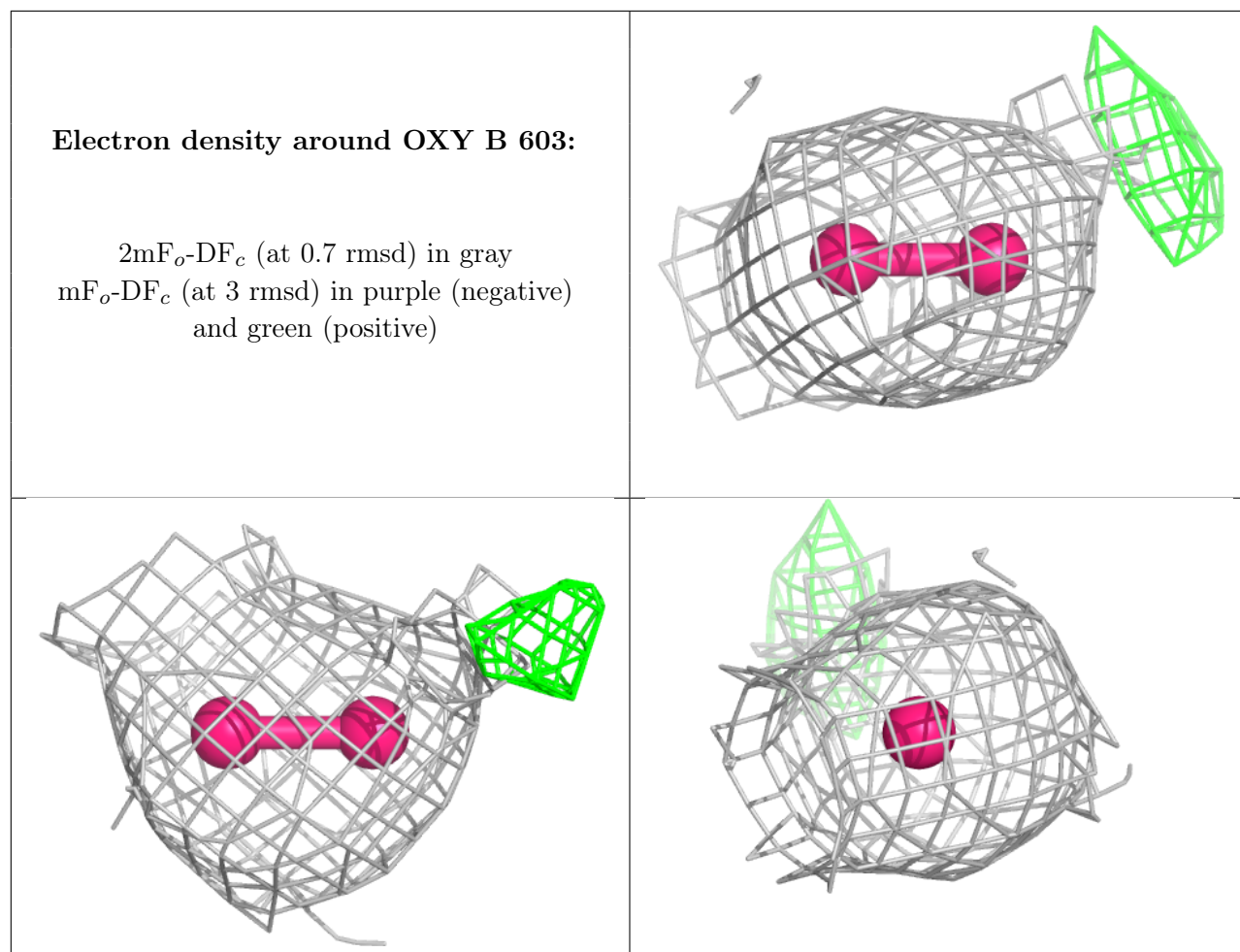
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around FAD A 601:

$2mF_o-DF_c$ (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.