



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 02:41 AM UTC

PDB ID : 6TWV / pdb_00006twv
Title : Crystal structure of the haemagglutinin mutant (Gln226Leu) from an H10N7 seal influenza virus isolated in Germany with human receptor analogue, 6'SLN
Authors : Zhang, J.; Xiong, X.; Purkiss, A.; Walker, P.; Gamblin, S.; Skehel, J.J.
Deposited on : 2020-01-13
Resolution : 2.55 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

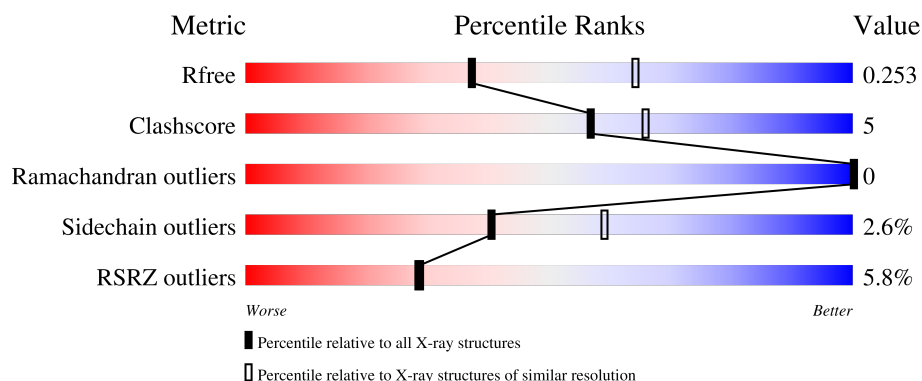
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.55 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1091 (2.54-2.54)
Clashscore	190562	1120 (2.54-2.54)
Ramachandran outliers	187476	1106 (2.54-2.54)
Sidechain outliers	187428	1106 (2.54-2.54)
RSRZ outliers	180081	1091 (2.54-2.54)

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	325	14% 85% 11% ..
1	C	325	2% 90% 7% ..
1	E	325	11% 87% 7% ..
1	G	325	% 89% 8% ..
1	I	325	10% 90% 7% ..

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	K	325	
2	B	177	
2	D	177	
2	F	177	
2	H	177	
2	J	177	
2	L	177	
3	M	3	
3	O	3	
3	P	3	
3	Q	3	
4	N	2	

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 23356 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 Hemagglutinin HA1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	C	318	Total	C	N	O	S	0	1	0
			2429	1508	438	467	16			
1	E	313	Total	C	N	O	S	0	1	0
			2399	1485	436	462	16			
1	K	319	Total	C	N	O	S	0	0	0
			2434	1511	441	466	16			
1	A	315	Total	C	N	O	S	0	1	0
			2399	1492	430	461	16			
1	G	318	Total	C	N	O	S	0	1	0
			2432	1509	440	467	16			
1	I	319	Total	C	N	O	S	0	0	0
			2434	1511	441	466	16			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	-1	ASP	-	expression tag	UNP A0A0A7HR51
C	0	PRO	-	expression tag	UNP A0A0A7HR51
E	-1	ASP	-	expression tag	UNP A0A0A7HR51
E	0	PRO	-	expression tag	UNP A0A0A7HR51
K	-1	ASP	-	expression tag	UNP A0A0A7HR51
K	0	PRO	-	expression tag	UNP A0A0A7HR51
A	-1	ASP	-	expression tag	UNP A0A0A7HR51
A	0	PRO	-	expression tag	UNP A0A0A7HR51
G	-1	ASP	-	expression tag	UNP A0A0A7HR51
G	0	PRO	-	expression tag	UNP A0A0A7HR51
I	-1	ASP	-	expression tag	UNP A0A0A7HR51
I	0	PRO	-	expression tag	UNP A0A0A7HR51

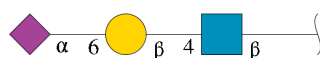
- Molecule 2 is a protein called Hemagglutinin HA2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	172	Total	C	N	O	S	0	0	0
			1386	857	241	280	8			
2	F	172	Total	C	N	O	S	0	0	0
			1386	857	241	280	8			
2	L	172	Total	C	N	O	S	0	0	0
			1383	855	240	280	8			
2	B	172	Total	C	N	O	S	0	0	0
			1383	855	240	280	8			
2	H	172	Total	C	N	O	S	0	0	0
			1383	855	240	280	8			
2	J	172	Total	C	N	O	S	0	0	0
			1383	855	240	280	8			

There are 6 discrepancies between the modelled and reference sequences:

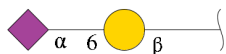
Chain	Residue	Modelled	Actual	Comment	Reference
D	177	LYS	-	expression tag	UNP A0A0A7HR51
F	177	LYS	-	expression tag	UNP A0A0A7HR51
L	177	LYS	-	expression tag	UNP A0A0A7HR51
B	177	LYS	-	expression tag	UNP A0A0A7HR51
H	177	LYS	-	expression tag	UNP A0A0A7HR51
J	177	LYS	-	expression tag	UNP A0A0A7HR51

- Molecule 3 is an oligosaccharide called N-acetyl-alpha-neuraminic acid-(2-6)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	M	3	Total	C	N	O		0	0	0
			46	25	2	19				
3	O	3	Total	C	N	O		0	0	0
			46	25	2	19				
3	P	3	Total	C	N	O		0	0	0
			46	25	2	19				
3	Q	3	Total	C	N	O		0	0	0
			46	25	2	19				

- Molecule 4 is an oligosaccharide called N-acetyl-alpha-neuraminic acid-(2-6)-beta-D-galactopyranose.

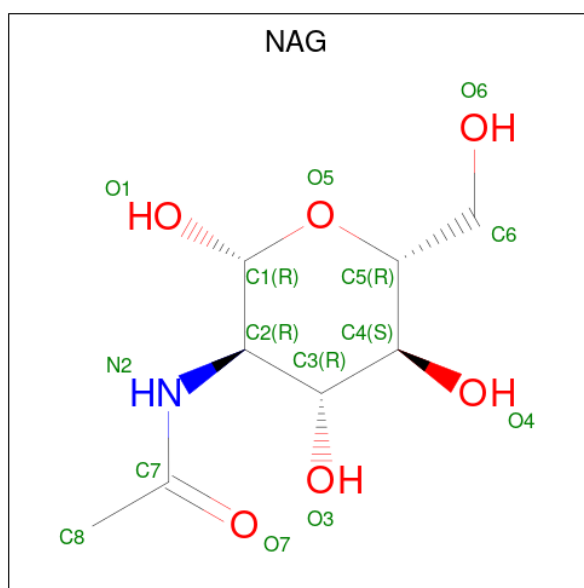


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	N	2	Total	C	N	O	0	0	0
			32	17	1	14			

- Molecule 5 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	C	1	Total	Ca	0	0
			1	1		
5	B	1	Total	Ca	0	0
			1	1		

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



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

Continued on next page...

Continued from previous page...

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

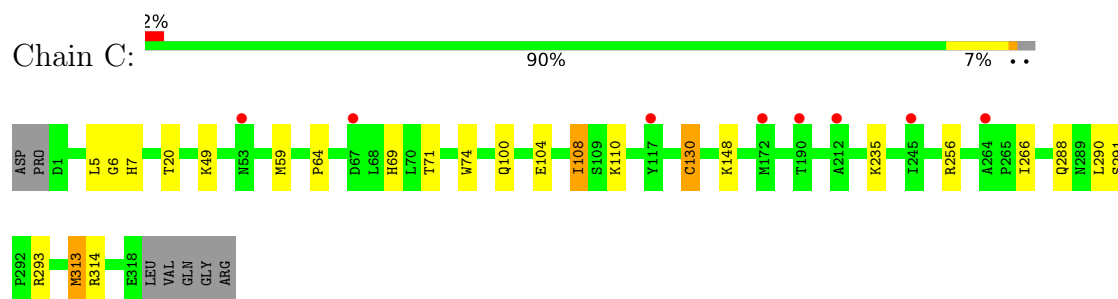
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	C	19	Total	O	0	0
			19	19		
7	D	21	Total	O	0	0
			21	21		
7	E	8	Total	O	0	0
			8	8		
7	F	11	Total	O	0	0
			11	11		
7	K	24	Total	O	0	0
			24	24		
7	L	15	Total	O	0	0
			15	15		
7	A	5	Total	O	0	0
			5	5		
7	B	12	Total	O	0	0
			12	12		
7	G	27	Total	O	0	0
			27	27		
7	H	11	Total	O	0	0
			11	11		
7	I	6	Total	O	0	0
			6	6		
7	J	8	Total	O	0	0
			8	8		

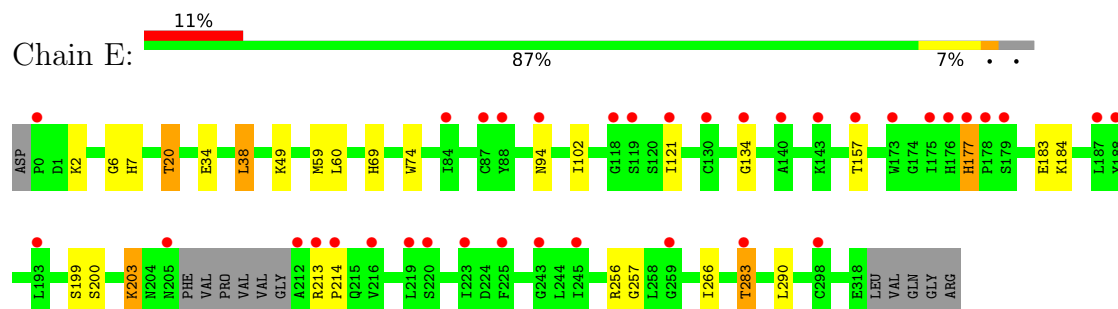
3 Residue-property plots

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.

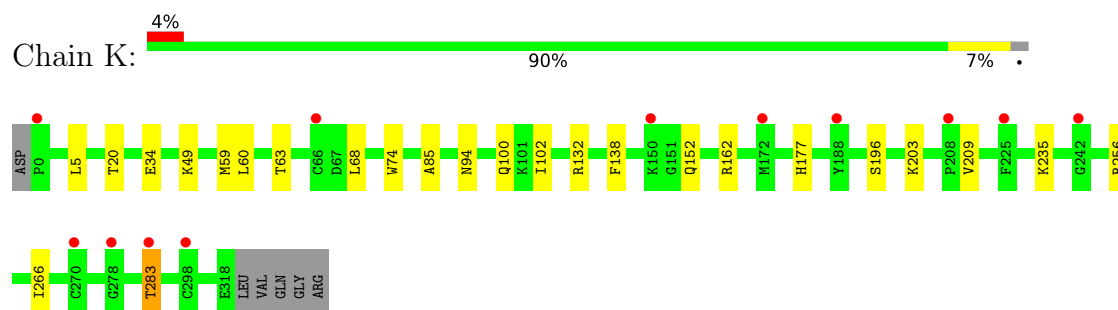
• Molecule 1: Hemagglutinin HA1



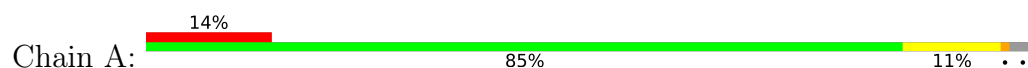
• Molecule 1: Hemagglutinin HA1

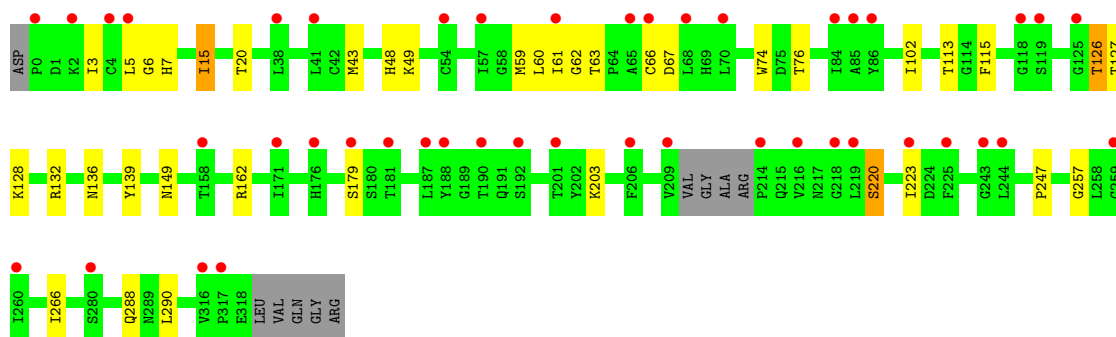


• Molecule 1: Hemagglutinin HA1

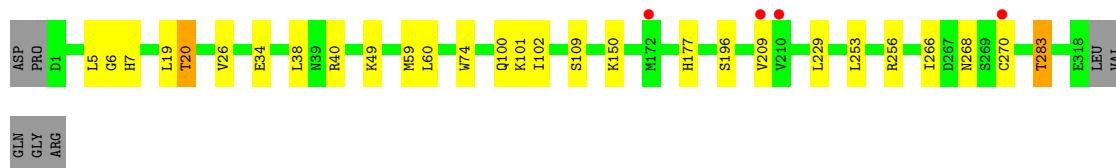


• Molecule 1: Hemagglutinin HA1

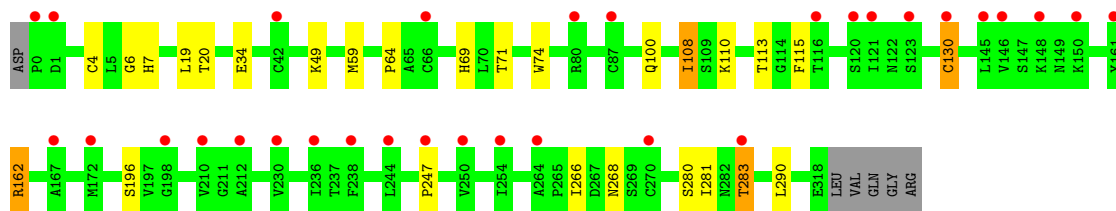
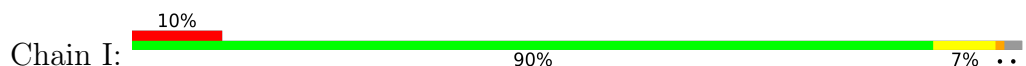




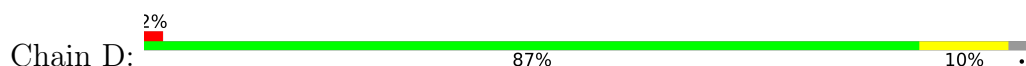
• Molecule 1: Hemagglutinin HA1



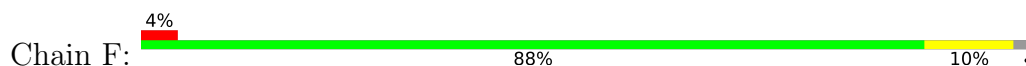
• Molecule 1: Hemagglutinin HA1



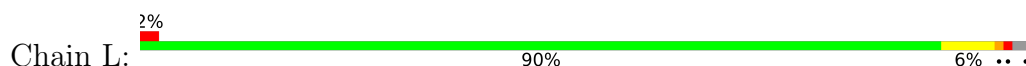
• Molecule 2: Hemagglutinin HA2



• Molecule 2: Hemagglutinin HA2

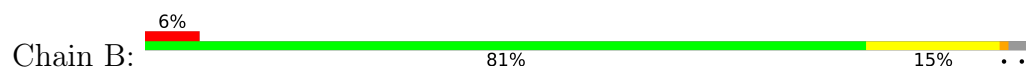


• Molecule 2: Hemagglutinin HA2

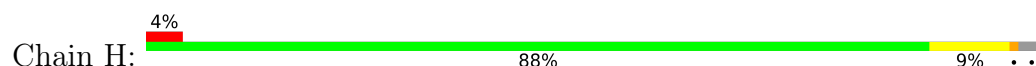




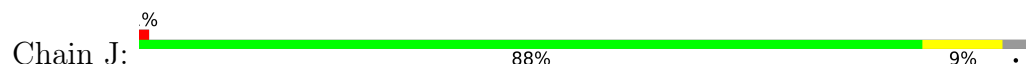
• Molecule 2: Hemagglutinin HA2



• Molecule 2: Hemagglutinin HA2



• Molecule 2: Hemagglutinin HA2



• Molecule 3: N-acetyl-alpha-neuraminic acid-(2-6)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



• Molecule 3: N-acetyl-alpha-neuraminic acid-(2-6)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



• Molecule 3: N-acetyl-alpha-neuraminic acid-(2-6)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose





- Molecule 3: N-acetyl-alpha-neuraminic acid-(2-6)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain Q: 33% 67%



- Molecule 4: N-acetyl-alpha-neuraminic acid-(2-6)-beta-D-galactopyranose

Chain N: 50% 50%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	69.53Å 217.74Å 150.30Å 90.00° 101.25° 90.00°	Depositor
Resolution (Å)	65.08 – 2.55 65.08 – 2.55	Depositor EDS
% Data completeness (in resolution range)	99.0 (65.08-2.55) 99.0 (65.08-2.55)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.77 (at 2.55Å)	Xtriage
Refinement program	REFMAC 5.8.0158	Depositor
R, R_{free}	0.236 , 0.256 0.234 , 0.253	Depositor DCC
R_{free} test set	6995 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å ²)	59.6	Xtriage
Anisotropy	0.574	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 25.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.029 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	23356	wwPDB-VP
Average B, all atoms (Å ²)	76.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 12.85% 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: GAL, CA, NAG, SIA

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	1.04	1/2451 (0.0%)	1.30	2/3320 (0.1%)
1	C	1.01	0/2481	1.31	0/3361
1	E	1.04	1/2449 (0.0%)	1.30	1/3313 (0.0%)
1	G	1.00	0/2484	1.30	0/3365
1	I	1.01	0/2484	1.31	0/3365
1	K	1.00	0/2484	1.29	0/3365
2	B	0.99	0/1408	1.50	1/1900 (0.1%)
2	D	0.98	0/1411	1.49	0/1903
2	F	0.97	0/1411	1.49	1/1903 (0.1%)
2	H	0.98	0/1408	1.48	0/1900
2	J	0.97	0/1408	1.48	0/1900
2	L	0.97	0/1408	1.51	2/1900 (0.1%)
All	All	1.00	2/23287 (0.0%)	1.38	7/31495 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	257	GLY	C-O	6.19	1.29	1.23
1	A	257	GLY	C-O	5.03	1.28	1.23

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	133	ASP	CA-CB-CG	10.60	123.20	112.60
2	L	133	ASP	CA-C-O	-8.17	111.56	121.36
2	L	133	ASP	N-CA-C	-7.62	98.20	110.32
1	A	220	SER	CA-C-N	6.10	125.90	120.10
1	A	220	SER	C-N-CA	6.10	125.90	120.10
1	E	177	HIS	CB-CG-CD2	5.30	138.09	131.20
2	F	112	ASP	CA-CB-CG	5.04	117.64	112.60

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	2399	0	2349	43	0
1	C	2429	0	2389	22	0
1	E	2399	0	2361	26	0
1	G	2432	0	2391	22	0
1	I	2434	0	2395	21	0
1	K	2434	0	2394	20	0
2	B	1383	0	1282	32	0
2	D	1386	0	1291	20	0
2	F	1386	0	1291	17	0
2	H	1383	0	1282	17	0
2	J	1383	0	1282	15	0
2	L	1383	0	1282	12	0
3	M	46	0	40	0	0
3	O	46	0	40	0	0
3	P	46	0	40	1	0
3	Q	46	0	40	0	0
4	N	32	0	28	2	0
5	B	1	0	0	0	0
5	C	1	0	0	0	0
6	A	14	0	13	1	0
6	B	14	0	13	0	0
6	C	14	0	13	0	0
6	D	14	0	13	0	0
6	F	14	0	13	0	0
6	G	14	0	13	0	0
6	H	14	0	13	0	0
6	J	14	0	13	0	0
6	K	14	0	13	0	0
6	L	14	0	13	0	0
7	A	5	0	0	0	0
7	B	12	0	0	1	0
7	C	19	0	0	0	0
7	D	21	0	0	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	E	8	0	0	0	0
7	F	11	0	0	0	0
7	G	27	0	0	1	0
7	H	11	0	0	0	0
7	I	6	0	0	0	0
7	J	8	0	0	0	0
7	K	24	0	0	0	0
7	L	15	0	0	0	0
All	All	23356	0	22307	207	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 5.

All (207) 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:95:GLN:NE2	2:F:95:GLN:HE21	1.59	0.99
2:B:144:CYS:C	2:B:148:CYS:SG	2.52	0.93
2:D:95:GLN:HE22	2:F:95:GLN:HE21	0.96	0.90
1:A:126:THR:CG2	1:A:136:ASN:HB3	2.03	0.89
2:B:145:ASP:O	2:B:148:CYS:SG	2.32	0.88
2:D:95:GLN:HE22	2:F:95:GLN:NE2	1.74	0.85
1:A:113:THR:HG23	1:A:115:PHE:H	1.49	0.78
2:B:145:ASP:N	2:B:148:CYS:SG	2.57	0.78
1:I:113:THR:HG23	1:I:115:PHE:H	1.48	0.78
1:A:61:ILE:HD13	1:A:139:TYR:CD1	2.20	0.76
1:C:288:GLN:NE2	1:C:291:SER:H	1.85	0.75
1:K:63:THR:HG21	1:K:85:ALA:O	1.89	0.73
2:H:17:MET:HE1	2:H:23:GLY:HA3	1.73	0.71
1:I:6:GLY:C	2:J:115:MET:HE1	2.17	0.70
2:F:17:MET:HE1	2:F:23:GLY:HA3	1.74	0.70
2:B:17:MET:HE1	2:B:23:GLY:HA3	1.73	0.70
1:A:43:MET:HE2	1:A:48:HIS:CB	2.23	0.68
1:A:126:THR:HG23	1:A:136:ASN:HB3	1.75	0.68
2:B:95:GLN:OE1	2:J:95:GLN:NE2	2.27	0.68
1:C:6:GLY:C	2:D:115:MET:HE1	2.18	0.68
2:B:161:GLN:HG2	2:B:162:TYR:CD2	2.32	0.65
1:E:6:GLY:C	2:F:115:MET:HE1	2.23	0.63
1:A:15:ILE:N	1:A:15:ILE:HD12	2.13	0.63
1:K:177:HIS:ND1	1:K:209:VAL:HG12	2.14	0.63
1:I:281:ILE:HD11	1:I:290:LEU:HD13	1.81	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:43:MET:HE1	1:A:76:THR:HG21	1.81	0.61
1:A:6:GLY:C	2:B:115:MET:HE1	2.26	0.61
1:E:7:HIS:HB3	2:F:115:MET:CE	2.31	0.61
1:A:61:ILE:HD13	1:A:139:TYR:HD1	1.65	0.61
1:G:177:HIS:ND1	1:G:209:VAL:HG12	2.15	0.61
1:C:288:GLN:HE22	1:C:291:SER:H	1.48	0.60
1:A:43:MET:HE2	1:A:48:HIS:HB2	1.81	0.60
1:A:223:ILE:HG13	1:A:223:ILE:O	2.02	0.60
1:C:7:HIS:HB3	2:D:115:MET:CE	2.31	0.60
2:D:99:LEU:HD22	2:F:94:TYR:OH	2.02	0.59
1:G:7:HIS:HB3	2:H:115:MET:CE	2.32	0.59
2:F:99:LEU:HD22	2:L:94:TYR:OH	2.02	0.59
2:H:17:MET:HE1	2:H:36:ALA:HA	1.85	0.59
1:I:7:HIS:HB3	2:J:115:MET:CE	2.33	0.59
1:I:281:ILE:CD1	1:I:290:LEU:HD13	2.34	0.58
1:A:179:SER:OG	1:A:220:SER:C	2.47	0.58
1:C:7:HIS:HB3	2:D:115:MET:HE2	1.84	0.58
2:F:17:MET:HE1	2:F:36:ALA:HA	1.85	0.58
2:B:161:GLN:HG2	2:B:162:TYR:CE2	2.39	0.58
1:A:7:HIS:HB3	2:B:115:MET:CE	2.33	0.57
1:C:5:LEU:CD1	2:D:119:TYR:HA	2.34	0.57
1:K:63:THR:CG2	1:K:85:ALA:O	2.52	0.57
2:B:17:MET:HE1	2:B:36:ALA:HA	1.85	0.57
1:I:280:SER:O	1:I:281:ILE:HD13	2.04	0.57
1:E:60:LEU:CD2	1:E:102:ILE:HD11	2.35	0.57
6:A:401:NAG:H3	6:A:401:NAG:H83	1.88	0.56
1:I:7:HIS:HB3	2:J:115:MET:HE2	1.87	0.56
1:C:71:THR:HA	1:C:108:ILE:HG23	1.87	0.56
1:C:256:ARG:NH1	2:D:64:GLU:OE2	2.39	0.56
1:E:7:HIS:HB3	2:F:115:MET:HE2	1.87	0.56
1:E:134:GLY:O	1:G:109:SER:HB2	2.06	0.56
1:I:71:THR:HA	1:I:108:ILE:HG23	1.87	0.55
2:L:115:MET:HE3	2:L:115:MET:HA	1.88	0.55
1:K:256:ARG:NH2	2:L:64:GLU:OE1	2.39	0.55
1:E:203:LYS:HD2	1:K:209:VAL:HG11	1.89	0.55
1:I:113:THR:HG21	1:I:247:PRO:O	2.07	0.55
1:A:67:ASP:OD1	1:A:132:ARG:NH1	2.40	0.54
1:C:288:GLN:HE21	1:C:290:LEU:HB2	1.72	0.54
1:A:113:THR:HG21	1:A:247:PRO:O	2.08	0.54
1:C:5:LEU:HD13	2:D:119:TYR:HA	1.89	0.53
2:H:17:MET:CE	2:H:36:ALA:HA	2.38	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:7:HIS:HB3	2:B:115:MET:HE2	1.90	0.53
1:K:5:LEU:CD1	2:L:119:TYR:HA	2.38	0.53
1:G:7:HIS:HB3	2:H:115:MET:HE2	1.91	0.53
2:F:17:MET:CE	2:F:36:ALA:HA	2.39	0.53
1:G:6:GLY:C	2:H:115:MET:HE1	2.34	0.52
2:F:50:GLY:HA3	1:K:20:THR:O	2.10	0.52
1:I:281:ILE:HD12	1:I:290:LEU:CD1	2.38	0.52
2:B:17:MET:CE	2:B:36:ALA:HA	2.39	0.52
2:H:171:LEU:C	2:H:171:LEU:HD23	2.34	0.52
1:A:126:THR:CG2	1:A:136:ASN:CB	2.85	0.52
1:K:68:LEU:HD22	1:K:68:LEU:N	2.25	0.52
1:C:293:ARG:HG2	2:D:67:GLU:OE1	2.09	0.51
2:F:73:ILE:CG2	2:F:77:ILE:HD11	2.40	0.51
1:A:3:ILE:HD12	2:B:26:HIS:HB3	1.92	0.51
2:B:148:CYS:SG	2:B:149:MET:N	2.84	0.51
1:E:60:LEU:N	1:E:60:LEU:CD1	2.73	0.51
2:B:12:ASN:C	2:B:12:ASN:HD22	2.19	0.50
1:A:20:THR:O	2:J:50:GLY:HA3	2.11	0.50
1:C:7:HIS:HD2	1:C:313:MET:HE1	1.77	0.50
2:D:94:TYR:OH	2:L:99:LEU:HD22	2.11	0.50
2:B:94:TYR:OH	2:J:99:LEU:HD22	2.11	0.50
1:E:2:LYS:HG3	2:F:27:GLN:HG2	1.94	0.50
2:J:17:MET:HE1	2:J:23:GLY:HA3	1.93	0.50
2:L:12:ASN:HD22	2:L:12:ASN:C	2.20	0.50
1:I:162:ARG:HB2	1:I:162:ARG:CZ	2.42	0.50
1:A:43:MET:CE	1:A:48:HIS:HB3	2.42	0.50
1:C:49:LYS:HE3	1:C:69:HIS:ND1	2.27	0.49
1:E:60:LEU:HD22	1:E:102:ILE:HD11	1.95	0.49
1:I:49:LYS:HE3	1:I:69:HIS:ND1	2.27	0.49
1:A:43:MET:CE	1:A:48:HIS:CB	2.91	0.48
2:B:124:LYS:HD3	2:H:134:GLY:HA2	1.95	0.48
1:G:49:LYS:HD2	1:G:74:TRP:CE3	2.48	0.48
1:A:126:THR:HG23	1:A:127:THR:N	2.28	0.48
2:B:152:ILE:HD11	2:B:157:TYR:CD2	2.47	0.48
1:E:60:LEU:N	1:E:60:LEU:HD12	2.29	0.48
1:A:61:ILE:HD12	1:A:62:GLY:N	2.29	0.48
1:I:281:ILE:CD1	1:I:290:LEU:CD1	2.92	0.48
1:K:59:MET:HE1	1:K:74:TRP:CH2	2.49	0.48
1:K:5:LEU:HD13	2:L:119:TYR:HA	1.96	0.48
1:K:49:LYS:HD2	1:K:74:TRP:CE3	2.49	0.48
1:G:5:LEU:HD21	2:H:24:PHE:CE2	2.49	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:59:MET:HE1	1:G:74:TRP:CH2	2.48	0.47
2:F:99:LEU:HD22	2:L:94:TYR:HH	1.78	0.47
1:C:313:MET:HE3	1:C:314:ARG:O	2.14	0.47
1:G:268:ASN:ND2	7:G:501:HOH:O	2.47	0.47
1:A:59:MET:HE1	1:A:74:TRP:CH2	2.50	0.47
1:G:256:ARG:NH2	2:H:64:GLU:OE2	2.48	0.47
1:C:288:GLN:HE21	1:C:290:LEU:H	1.63	0.47
1:A:288:GLN:HG2	1:A:290:LEU:HD23	1.97	0.47
1:G:5:LEU:CD1	2:H:119:TYR:HA	2.44	0.47
2:D:54:ARG:HD2	7:D:305:HOH:O	2.14	0.47
1:E:203:LYS:HD2	1:K:209:VAL:CG1	2.44	0.47
1:E:59:MET:HE1	1:E:74:TRP:CH2	2.51	0.47
1:A:139:TYR:HE2	1:A:223:ILE:CD1	2.29	0.46
1:A:5:LEU:HD13	2:B:119:TYR:HA	1.96	0.46
1:G:253:LEU:N	1:G:253:LEU:HD12	2.31	0.46
1:A:3:ILE:HD11	2:B:24:PHE:HB3	1.97	0.46
2:B:152:ILE:CD1	2:B:157:TYR:CG	2.99	0.46
1:I:59:MET:HE1	1:I:74:TRP:CH2	2.51	0.46
2:D:73:ILE:CG2	2:D:77:ILE:HD11	2.46	0.46
1:A:49:LYS:HD2	1:A:74:TRP:CE3	2.50	0.46
1:A:126:THR:CG2	1:A:127:THR:N	2.79	0.46
1:C:59:MET:HE1	1:C:74:TRP:CH2	2.51	0.46
1:E:199:SER:OG	1:E:200:SER:N	2.47	0.45
2:H:99:LEU:HD22	2:J:94:TYR:OH	2.16	0.45
1:E:34:GLU:OE1	1:E:283:THR:CG2	2.64	0.45
2:D:134:GLY:HA2	2:L:124:LYS:HD3	1.99	0.45
1:E:60:LEU:HD21	1:E:102:ILE:HD11	1.99	0.45
2:B:99:LEU:HD22	2:H:94:TYR:OH	2.16	0.45
1:I:7:HIS:HD2	2:J:115:MET:HE3	1.81	0.45
1:A:63:THR:HG22	1:A:66:CYS:SG	2.57	0.45
2:D:171:LEU:HD11	2:F:171:LEU:HD22	1.99	0.45
2:B:152:ILE:HD13	2:B:157:TYR:CB	2.47	0.45
1:E:49:LYS:HE3	1:E:69:HIS:ND1	2.32	0.45
1:A:139:TYR:CE2	1:A:223:ILE:HD11	2.52	0.45
1:A:5:LEU:CD1	2:B:119:TYR:HA	2.47	0.44
1:K:34:GLU:OE1	1:K:283:THR:CG2	2.65	0.44
1:G:253:LEU:N	1:G:253:LEU:CD1	2.80	0.44
1:K:34:GLU:OE1	1:K:283:THR:HG21	2.18	0.44
1:I:34:GLU:OE2	1:I:283:THR:CG2	2.65	0.44
1:C:104:GLU:OE2	1:C:256:ARG:NH2	2.51	0.44
1:E:34:GLU:OE1	1:E:283:THR:HG21	2.17	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:183:GLU:OE1	4:N:2:SIA:C9	2.66	0.44
1:G:34:GLU:OE1	1:G:283:THR:HG21	2.18	0.44
2:B:94:TYR:HH	2:J:99:LEU:HD22	1.81	0.43
1:E:38:LEU:N	1:E:38:LEU:CD2	2.82	0.43
1:A:5:LEU:HD21	2:B:24:PHE:CE2	2.54	0.43
1:E:121:ILE:CD1	1:E:157:THR:HG21	2.49	0.43
1:G:34:GLU:OE1	1:G:283:THR:CG2	2.65	0.43
1:C:108:ILE:HD11	1:C:110:LYS:HE3	2.01	0.43
1:I:64:PRO:CD	1:I:130:CYS:SG	3.07	0.43
2:B:152:ILE:HD11	2:B:157:TYR:CG	2.54	0.43
1:C:235:LYS:HE3	1:E:214:PRO:HG3	2.01	0.43
1:A:43:MET:HE1	1:A:76:THR:CG2	2.48	0.43
1:C:7:HIS:ND1	2:D:115:MET:HE3	2.33	0.42
1:K:5:LEU:HD21	2:L:24:PHE:CE2	2.54	0.42
2:B:134:GLY:HA2	2:J:124:LYS:HD3	2.00	0.42
1:G:150:LYS:NZ	3:P:1:NAG:H82	2.35	0.42
1:E:38:LEU:N	1:E:38:LEU:HD22	2.35	0.42
2:B:90:ASP:OD1	2:J:61:THR:HG21	2.19	0.42
1:G:26:VAL:HG11	2:H:108:ILE:HD11	2.02	0.42
1:I:108:ILE:HD11	1:I:110:LYS:HE3	2.01	0.42
2:J:54:ARG:NH2	2:J:103:GLU:OE2	2.53	0.42
1:E:183:GLU:OE1	4:N:2:SIA:H92	2.20	0.42
2:B:141:TYR:O	2:B:166:ALA:HA	2.20	0.42
1:G:38:LEU:HB3	1:G:40:ARG:HG2	2.02	0.41
2:L:141:TYR:O	2:L:166:ALA:HA	2.20	0.41
1:A:179:SER:HG	1:A:220:SER:C	2.29	0.41
2:B:50:GLY:HA3	1:G:20:THR:O	2.20	0.41
1:C:64:PRO:CD	1:C:130:CYS:SG	3.08	0.41
2:H:141:TYR:O	2:H:166:ALA:HA	2.20	0.41
2:J:141:TYR:O	2:J:166:ALA:HA	2.21	0.41
1:K:60:LEU:HD11	1:K:102:ILE:HD11	2.01	0.41
2:F:141:TYR:O	2:F:166:ALA:HA	2.20	0.41
2:L:133:ASP:OD2	2:L:133:ASP:C	2.63	0.41
2:D:47:GLN:HG2	1:E:20:THR:CG2	2.51	0.41
1:A:15:ILE:N	1:A:15:ILE:CD1	2.80	0.41
1:A:60:LEU:HD11	1:A:102:ILE:HD11	2.02	0.41
1:A:61:ILE:HD13	1:A:139:TYR:CE1	2.55	0.41
1:A:63:THR:CG2	1:A:66:CYS:SG	3.08	0.41
2:D:141:TYR:O	2:D:166:ALA:HA	2.21	0.41
2:B:89:THR:HA	7:B:305:HOH:O	2.20	0.41
1:K:132:ARG:NH2	1:K:138:PHE:O	2.54	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:162:ARG:HG3	1:K:235:LYS:HG2	2.03	0.41
1:I:4:CYS:HA	2:J:137:CYS:HA	2.03	0.41
1:I:34:GLU:HG2	1:I:283:THR:OG1	2.20	0.41
2:D:2:LEU:HD23	2:D:2:LEU:HA	1.96	0.41
1:A:113:THR:OG1	1:A:115:PHE:CE1	2.71	0.40
1:A:223:ILE:O	1:A:223:ILE:CG1	2.69	0.40
1:G:101:LYS:HE2	1:G:229:LEU:HD21	2.03	0.40
1:E:34:GLU:HG2	1:E:283:THR:OG1	2.22	0.40
1:K:68:LEU:N	1:K:68:LEU:CD2	2.84	0.40
1:C:7:HIS:CD2	1:C:313:MET:HE1	2.56	0.40
1:E:290:LEU:CD1	1:E:290:LEU:N	2.85	0.40
1:I:34:GLU:OE2	1:I:283:THR:HG21	2.22	0.40
1:G:34:GLU:HG2	1:G:283:THR:OG1	2.21	0.40
2:H:121:ARG:HH11	2:H:121:ARG:HG3	1.85	0.40
1:K:34:GLU:HG2	1:K:283:THR:OG1	2.22	0.40
1:A:139:TYR:HE2	1:A:223:ILE:HD11	1.86	0.40
1:G:60:LEU:HD11	1:G:102:ILE:HD11	2.03	0.40
2:H:108:ILE:HD13	2:H:108:ILE:N	2.37	0.40

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	312/325 (96%)	304 (97%)	8 (3%)	0	100	100
1	C	317/325 (98%)	308 (97%)	9 (3%)	0	100	100
1	E	310/325 (95%)	302 (97%)	8 (3%)	0	100	100
1	G	317/325 (98%)	310 (98%)	7 (2%)	0	100	100
1	I	317/325 (98%)	308 (97%)	9 (3%)	0	100	100
1	K	317/325 (98%)	310 (98%)	7 (2%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	170/177 (96%)	164 (96%)	6 (4%)	0	100	100
2	D	170/177 (96%)	165 (97%)	5 (3%)	0	100	100
2	F	170/177 (96%)	164 (96%)	6 (4%)	0	100	100
2	H	170/177 (96%)	164 (96%)	6 (4%)	0	100	100
2	J	170/177 (96%)	164 (96%)	6 (4%)	0	100	100
2	L	170/177 (96%)	164 (96%)	6 (4%)	0	100	100
All	All	2910/3012 (97%)	2827 (97%)	83 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	265/275 (96%)	258 (97%)	7 (3%)	40	59
1	C	269/275 (98%)	262 (97%)	7 (3%)	40	59
1	E	266/275 (97%)	256 (96%)	10 (4%)	29	44
1	G	269/275 (98%)	262 (97%)	7 (3%)	40	59
1	I	269/275 (98%)	259 (96%)	10 (4%)	30	45
1	K	269/275 (98%)	262 (97%)	7 (3%)	40	59
2	B	145/151 (96%)	141 (97%)	4 (3%)	38	57
2	D	146/151 (97%)	144 (99%)	2 (1%)	59	75
2	F	146/151 (97%)	144 (99%)	2 (1%)	59	75
2	H	145/151 (96%)	142 (98%)	3 (2%)	47	66
2	J	145/151 (96%)	143 (99%)	2 (1%)	59	75
2	L	145/151 (96%)	141 (97%)	4 (3%)	38	57
All	All	2479/2556 (97%)	2414 (97%)	65 (3%)	40	59

All (65) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	20	THR
1	C	100	GLN
1	C	108	ILE
1	C	130	CYS
1	C	148	LYS
1	C	266	ILE
1	C	313	MET
2	D	32	THR
2	D	133	ASP
1	E	20	THR
1	E	38	LEU
1	E	94	ASN
1	E	177	HIS
1	E	184	LYS
1	E	203	LYS
1	E	213	ARG
1	E	256	ARG
1	E	266	ILE
1	E	283	THR
2	F	32	THR
2	F	133	ASP
1	K	94	ASN
1	K	100	GLN
1	K	152	GLN
1	K	196	SER
1	K	203	LYS
1	K	266	ILE
1	K	283	THR
2	L	12	ASN
2	L	32	THR
2	L	95	GLN
2	L	133	ASP
1	A	15	ILE
1	A	126	THR
1	A	128	LYS
1	A	149	ASN
1	A	162	ARG
1	A	203	LYS
1	A	266	ILE
2	B	12	ASN
2	B	32	THR
2	B	58	LYS
2	B	161	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	G	19	LEU
1	G	20	THR
1	G	100	GLN
1	G	196	SER
1	G	266	ILE
1	G	270	CYS
1	G	283	THR
2	H	32	THR
2	H	108	ILE
2	H	133	ASP
1	I	19	LEU
1	I	20	THR
1	I	100	GLN
1	I	108	ILE
1	I	130	CYS
1	I	162	ARG
1	I	196	SER
1	I	266	ILE
1	I	268	ASN
1	I	283	THR
2	J	32	THR
2	J	133	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (59) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	53	ASN
1	C	112	ASN
1	C	159	ASN
1	C	205	ASN
1	C	231	GLN
1	C	240	HIS
1	C	288	GLN
1	C	303	ASN
2	D	95	GLN
2	D	159	HIS
1	E	94	ASN
1	E	112	ASN
1	E	149	ASN
1	E	205	ASN
1	E	231	GLN
1	E	297	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	E	303	ASN
2	F	12	ASN
2	F	47	GLN
2	F	105	GLN
2	F	159	HIS
1	K	53	ASN
1	K	94	ASN
1	K	100	GLN
1	K	112	ASN
1	K	205	ASN
1	K	231	GLN
2	L	12	ASN
2	L	95	GLN
2	L	105	GLN
2	L	125	GLN
1	A	112	ASN
1	A	205	ASN
1	A	231	GLN
2	B	12	ASN
2	B	27	GLN
2	B	76	GLN
2	B	95	GLN
2	B	105	GLN
1	G	12	ASN
1	G	53	ASN
1	G	112	ASN
1	G	231	GLN
1	G	297	GLN
1	I	7	HIS
1	I	48	HIS
1	I	94	ASN
1	I	112	ASN
1	I	153	ASN
1	I	205	ASN
1	I	217	ASN
1	I	240	HIS
1	I	268	ASN
1	I	297	GLN
1	I	303	ASN
2	J	95	GLN
2	J	154	ASN
2	J	159	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	J	169	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

14 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	M	1	3	15,15,15	0.58	0	21,21,21	1.65	5 (23%)
3	GAL	M	2	3	11,11,12	0.41	0	15,15,17	0.63	0
3	SIA	M	3	3	20,20,21	0.63	0	21,28,31	1.42	5 (23%)
4	GAL	N	1	4	12,12,12	0.57	0	17,17,17	0.84	0
4	SIA	N	2	4	20,20,21	0.63	0	21,28,31	1.25	3 (14%)
3	NAG	O	1	3	15,15,15	0.44	0	21,21,21	1.24	2 (9%)
3	GAL	O	2	3	11,11,12	0.37	0	15,15,17	1.03	1 (6%)
3	SIA	O	3	3	20,20,21	0.62	0	21,28,31	1.29	3 (14%)
3	NAG	P	1	3	15,15,15	0.47	0	21,21,21	0.88	1 (4%)
3	GAL	P	2	3	11,11,12	0.43	0	15,15,17	1.17	1 (6%)
3	SIA	P	3	3	20,20,21	0.69	0	21,28,31	1.36	4 (19%)
3	NAG	Q	1	3	15,15,15	0.58	0	21,21,21	1.66	5 (23%)
3	GAL	Q	2	3	11,11,12	0.40	0	15,15,17	0.69	0
3	SIA	Q	3	3	20,20,21	0.62	0	21,28,31	1.37	3 (14%)

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	M	1	3	-	3/6/26/26	0/1/1/1
3	GAL	M	2	3	-	0/2/19/22	0/1/1/1
3	SIA	M	3	3	-	1/18/34/38	0/1/1/1
4	GAL	N	1	4	-	0/2/22/22	0/1/1/1
4	SIA	N	2	4	-	4/18/34/38	0/1/1/1
3	NAG	O	1	3	-	2/6/26/26	0/1/1/1
3	GAL	O	2	3	-	0/2/19/22	0/1/1/1
3	SIA	O	3	3	-	0/18/34/38	0/1/1/1
3	NAG	P	1	3	-	0/6/26/26	0/1/1/1
3	GAL	P	2	3	-	0/2/19/22	0/1/1/1
3	SIA	P	3	3	-	1/18/34/38	0/1/1/1
3	NAG	Q	1	3	-	3/6/26/26	0/1/1/1
3	GAL	Q	2	3	-	0/2/19/22	0/1/1/1
3	SIA	Q	3	3	-	2/18/34/38	0/1/1/1

There are no bond length outliers.

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	Q	1	NAG	O5-C1-C2	3.66	113.19	109.52
3	M	1	NAG	O5-C1-C2	3.45	112.98	109.52
3	P	3	SIA	C6-C5-N5	-3.44	105.42	110.91
3	M	3	SIA	O6-C2-C1	3.42	114.17	107.72
3	P	2	GAL	C1-C2-C3	3.38	114.57	109.64
3	M	1	NAG	C1-O5-C5	3.33	120.10	113.65
3	O	3	SIA	C4-C5-N5	-3.27	104.00	110.44
3	Q	1	NAG	C1-O5-C5	3.19	119.83	113.65
3	M	1	NAG	C3-C2-N2	-3.08	104.94	110.62
3	M	3	SIA	O1B-C1-C2	3.01	120.53	112.71
3	Q	3	SIA	O1B-C1-C2	2.89	120.22	112.71
3	Q	1	NAG	C8-C7-N2	2.73	120.65	116.12
3	Q	3	SIA	C4-C5-N5	-2.69	105.13	110.44
3	Q	3	SIA	O6-C2-C1	2.66	112.73	107.72
3	O	1	NAG	C8-C7-N2	2.65	120.50	116.12
4	N	2	SIA	O6-C2-C1	2.64	112.70	107.72
3	P	3	SIA	C4-C5-N5	-2.60	105.32	110.44
3	M	1	NAG	C8-C7-N2	2.56	120.37	116.12

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	M	3	SIA	C4-C5-N5	-2.55	105.42	110.44
4	N	2	SIA	O1B-C1-C2	2.55	119.33	112.71
3	O	1	NAG	C4-C3-C2	-2.49	106.78	110.40
3	O	3	SIA	O1B-C1-C2	2.38	118.91	112.71
3	M	3	SIA	O1A-C1-C2	-2.36	117.75	122.85
3	O	2	GAL	C1-O5-C5	2.35	115.33	112.19
3	P	3	SIA	O1B-C1-C2	2.35	118.81	112.71
3	P	1	NAG	C3-C2-N2	-2.29	106.40	110.62
3	M	3	SIA	C6-C5-N5	-2.25	107.31	110.91
4	N	2	SIA	O6-C2-C3	-2.24	107.55	110.56
3	Q	1	NAG	C4-C3-C2	-2.23	107.16	110.40
3	M	1	NAG	C2-N2-C7	2.19	128.24	123.11
3	Q	1	NAG	C1-C2-N2	-2.17	108.22	110.73
3	P	3	SIA	O6-C2-C1	2.12	111.73	107.72
3	O	3	SIA	O6-C2-C1	2.06	111.61	107.72

There are no chirality outliers.

All (16) torsion outliers are listed below:

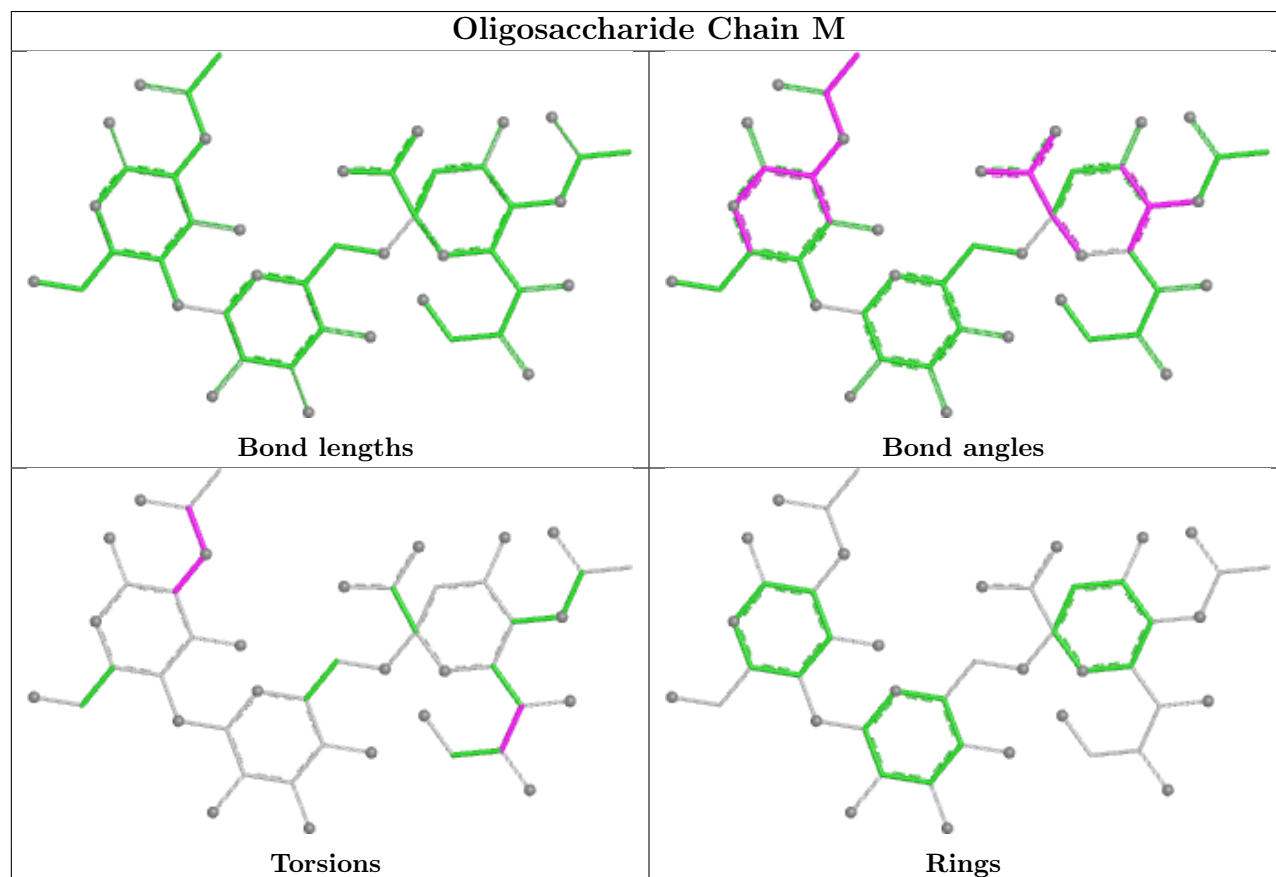
Mol	Chain	Res	Type	Atoms
4	N	2	SIA	O6-C6-C7-O7
3	M	1	NAG	C8-C7-N2-C2
3	M	1	NAG	O7-C7-N2-C2
3	O	1	NAG	C8-C7-N2-C2
3	O	1	NAG	O7-C7-N2-C2
3	Q	1	NAG	C8-C7-N2-C2
3	Q	1	NAG	O7-C7-N2-C2
3	Q	1	NAG	C4-C5-C6-O6
4	N	2	SIA	C5-C6-C7-O7
3	P	3	SIA	C6-C7-C8-O8
4	N	2	SIA	O6-C6-C7-C8
4	N	2	SIA	C5-C6-C7-C8
3	Q	3	SIA	C6-C7-C8-O8
3	M	1	NAG	C3-C2-N2-C7
3	Q	3	SIA	O7-C7-C8-C9
3	M	3	SIA	C6-C7-C8-O8

There are no ring outliers.

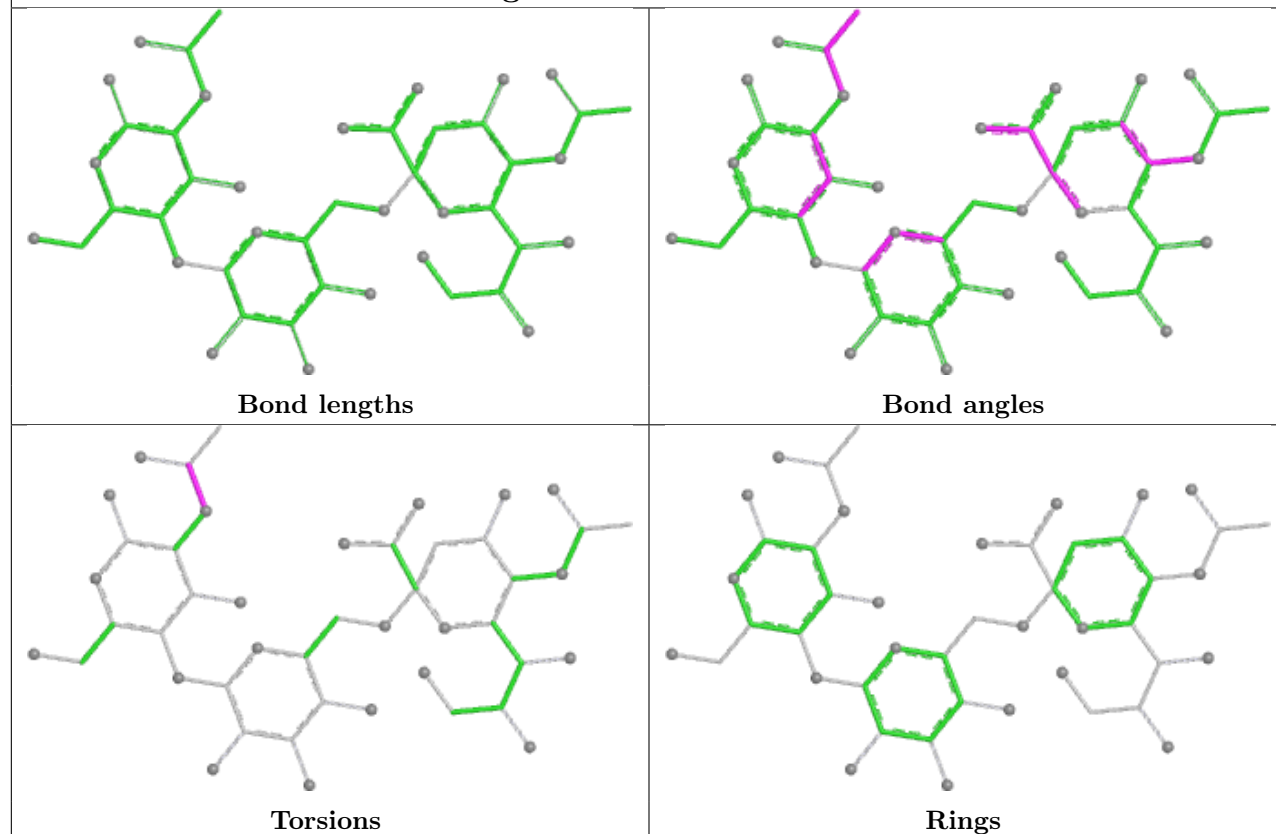
2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	P	1	NAG	1	0
4	N	2	SIA	2	0

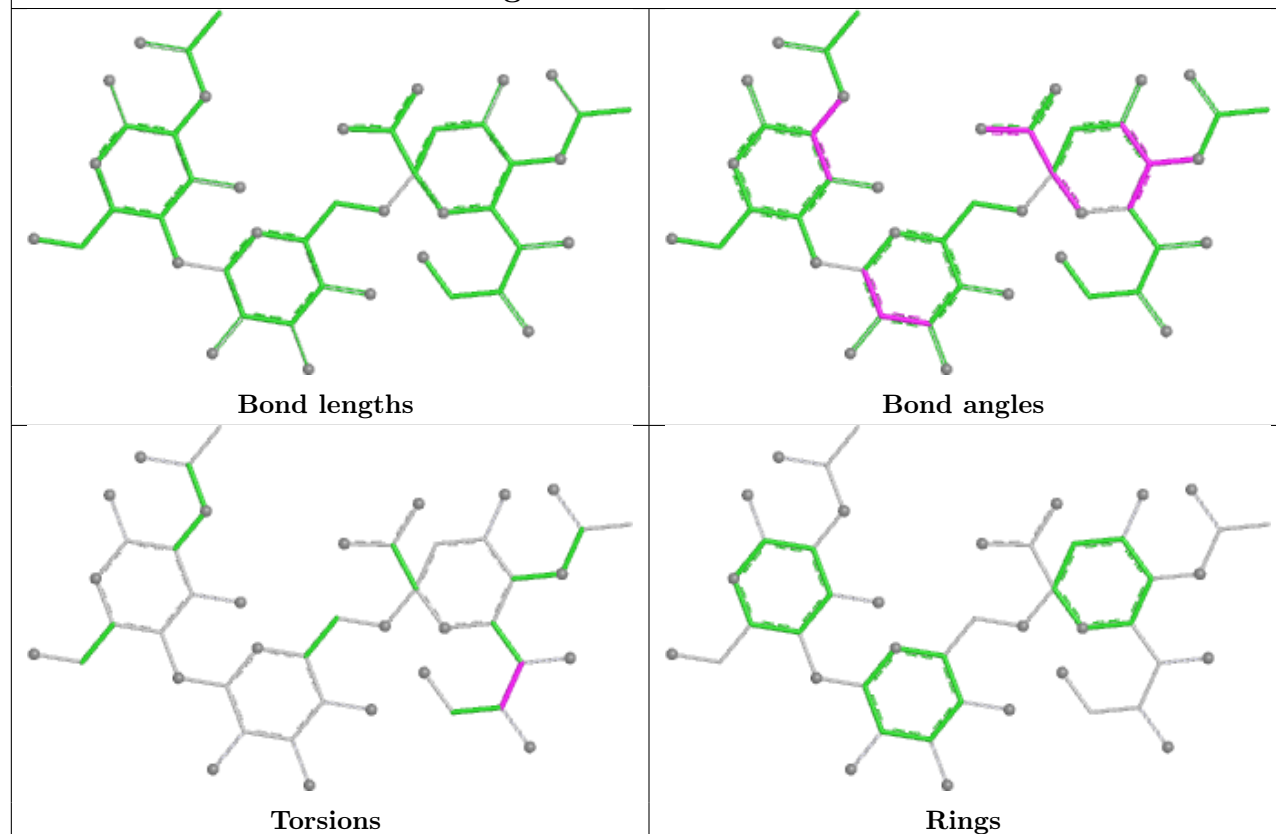
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.



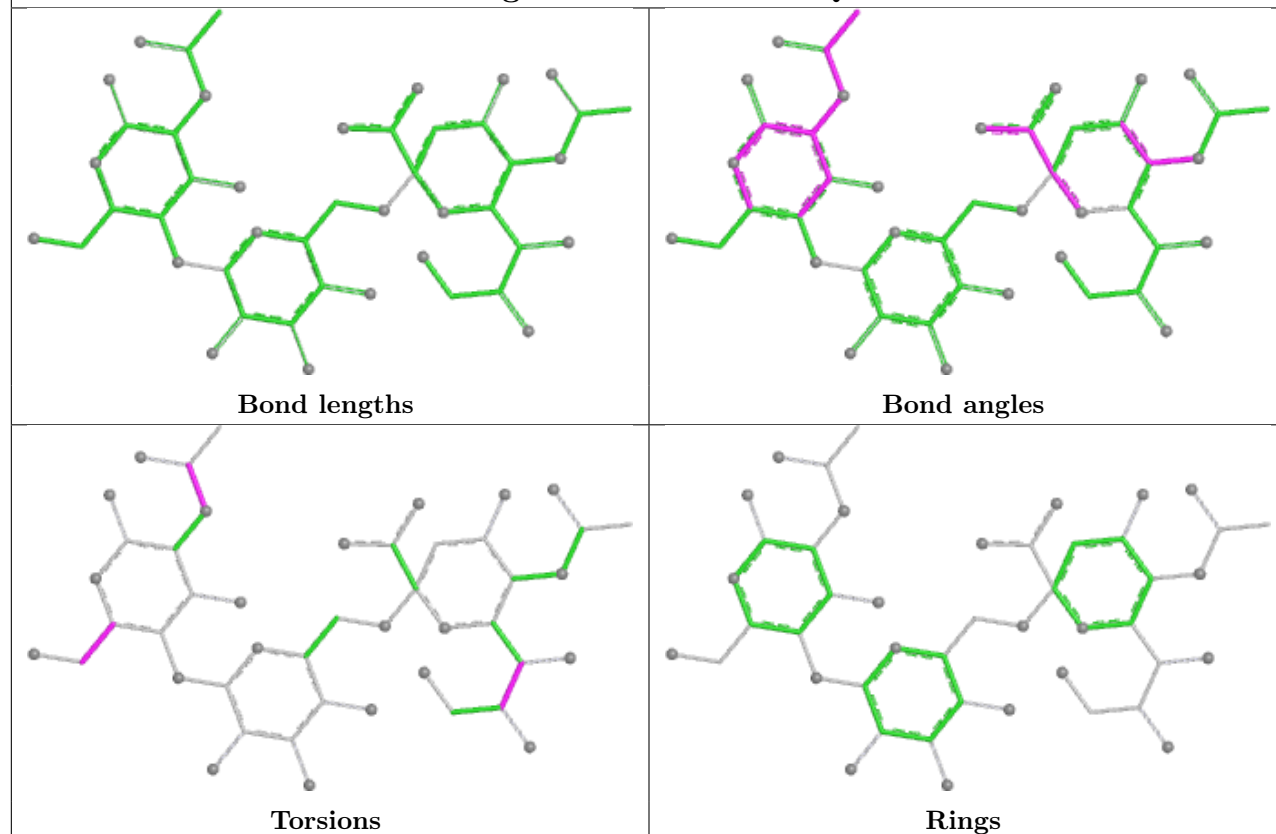
Oligosaccharide Chain O



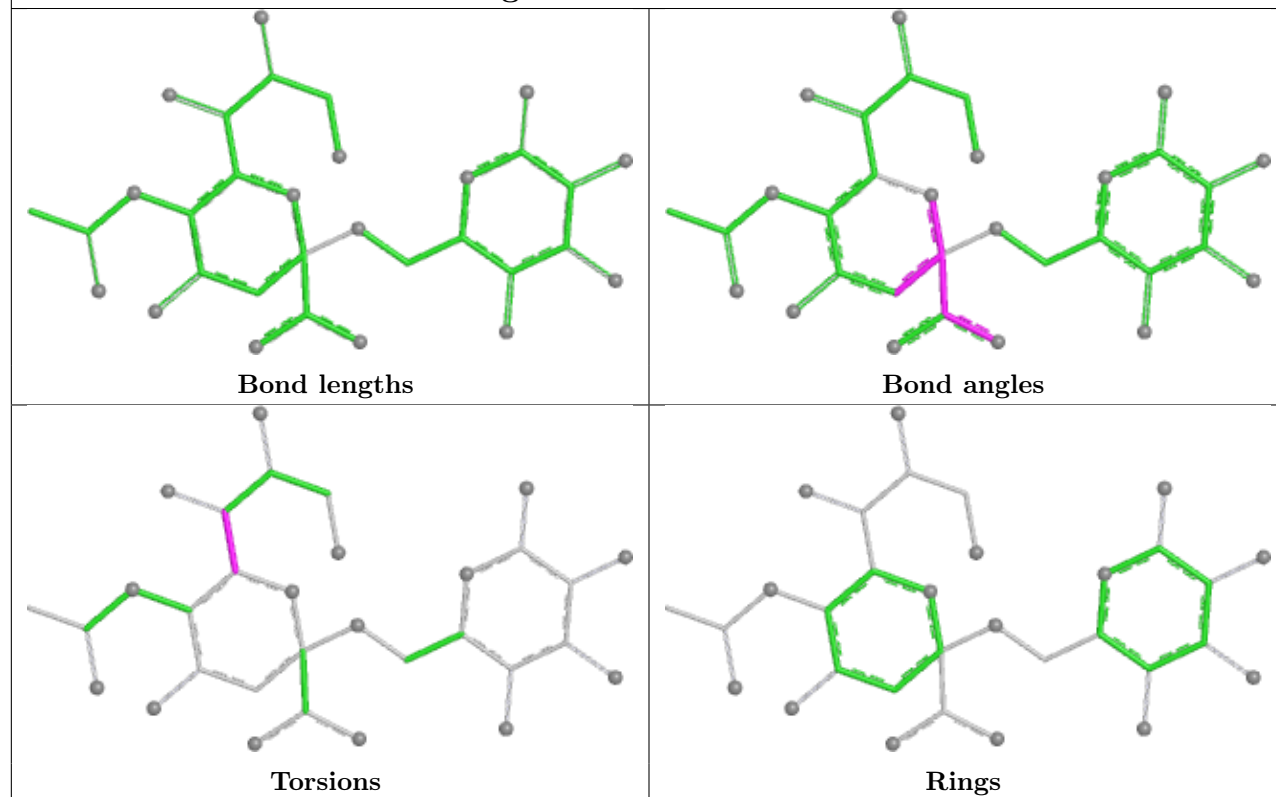
Oligosaccharide Chain P



Oligosaccharide Chain Q



Oligosaccharide Chain N



5.6 Ligand geometry

Of 12 ligands modelled in this entry, 2 are monoatomic - leaving 10 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
6	NAG	B	201	5,2	14,14,15	0.33	0	17,19,21	0.88	1 (5%)
6	NAG	A	401	1	14,14,15	0.63	0	17,19,21	1.96	3 (17%)
6	NAG	K	401	1	14,14,15	0.39	0	17,19,21	0.99	1 (5%)
6	NAG	H	201	2	14,14,15	0.32	0	17,19,21	1.07	1 (5%)
6	NAG	D	201	2	14,14,15	0.36	0	17,19,21	0.89	0
6	NAG	G	401	1	14,14,15	0.40	0	17,19,21	1.07	1 (5%)
6	NAG	L	201	2	14,14,15	0.45	0	17,19,21	1.78	3 (17%)
6	NAG	J	201	2	14,14,15	0.33	0	17,19,21	1.67	1 (5%)
6	NAG	F	201	5,2	14,14,15	0.50	0	17,19,21	1.06	1 (5%)
6	NAG	C	405	1	14,14,15	0.47	0	17,19,21	1.31	1 (5%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	NAG	B	201	5,2	-	2/6/23/26	0/1/1/1
6	NAG	A	401	1	-	4/6/23/26	0/1/1/1
6	NAG	K	401	1	-	0/6/23/26	0/1/1/1
6	NAG	H	201	2	-	0/6/23/26	0/1/1/1
6	NAG	D	201	2	-	2/6/23/26	0/1/1/1
6	NAG	G	401	1	-	2/6/23/26	0/1/1/1
6	NAG	L	201	2	-	2/6/23/26	0/1/1/1
6	NAG	J	201	2	-	0/6/23/26	0/1/1/1
6	NAG	F	201	5,2	-	1/6/23/26	0/1/1/1
6	NAG	C	405	1	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	J	201	NAG	C1-O5-C5	6.08	120.34	112.19
6	L	201	NAG	C1-O5-C5	5.89	120.08	112.19
6	A	401	NAG	C2-N2-C7	4.86	129.41	122.90
6	C	405	NAG	C1-O5-C5	4.51	118.23	112.19
6	A	401	NAG	C8-C7-N2	3.81	122.43	116.12
6	A	401	NAG	C1-O5-C5	3.72	117.17	112.19
6	H	201	NAG	C1-O5-C5	3.39	116.73	112.19
6	F	201	NAG	C1-O5-C5	3.21	116.49	112.19
6	G	401	NAG	C1-O5-C5	2.81	115.96	112.19
6	B	201	NAG	C1-O5-C5	2.64	115.72	112.19
6	K	401	NAG	C1-O5-C5	2.49	115.53	112.19
6	L	201	NAG	O7-C7-N2	2.09	125.68	121.98
6	L	201	NAG	C4-C3-C2	-2.01	108.06	111.02

There are no chirality outliers.

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	L	201	NAG	O5-C5-C6-O6
6	D	201	NAG	O5-C5-C6-O6
6	A	401	NAG	C8-C7-N2-C2
6	A	401	NAG	O7-C7-N2-C2
6	D	201	NAG	C4-C5-C6-O6
6	L	201	NAG	C4-C5-C6-O6
6	B	201	NAG	C4-C5-C6-O6
6	B	201	NAG	O5-C5-C6-O6
6	A	401	NAG	O5-C5-C6-O6
6	F	201	NAG	O5-C5-C6-O6
6	A	401	NAG	C3-C2-N2-C7
6	G	401	NAG	C1-C2-N2-C7
6	G	401	NAG	C3-C2-N2-C7

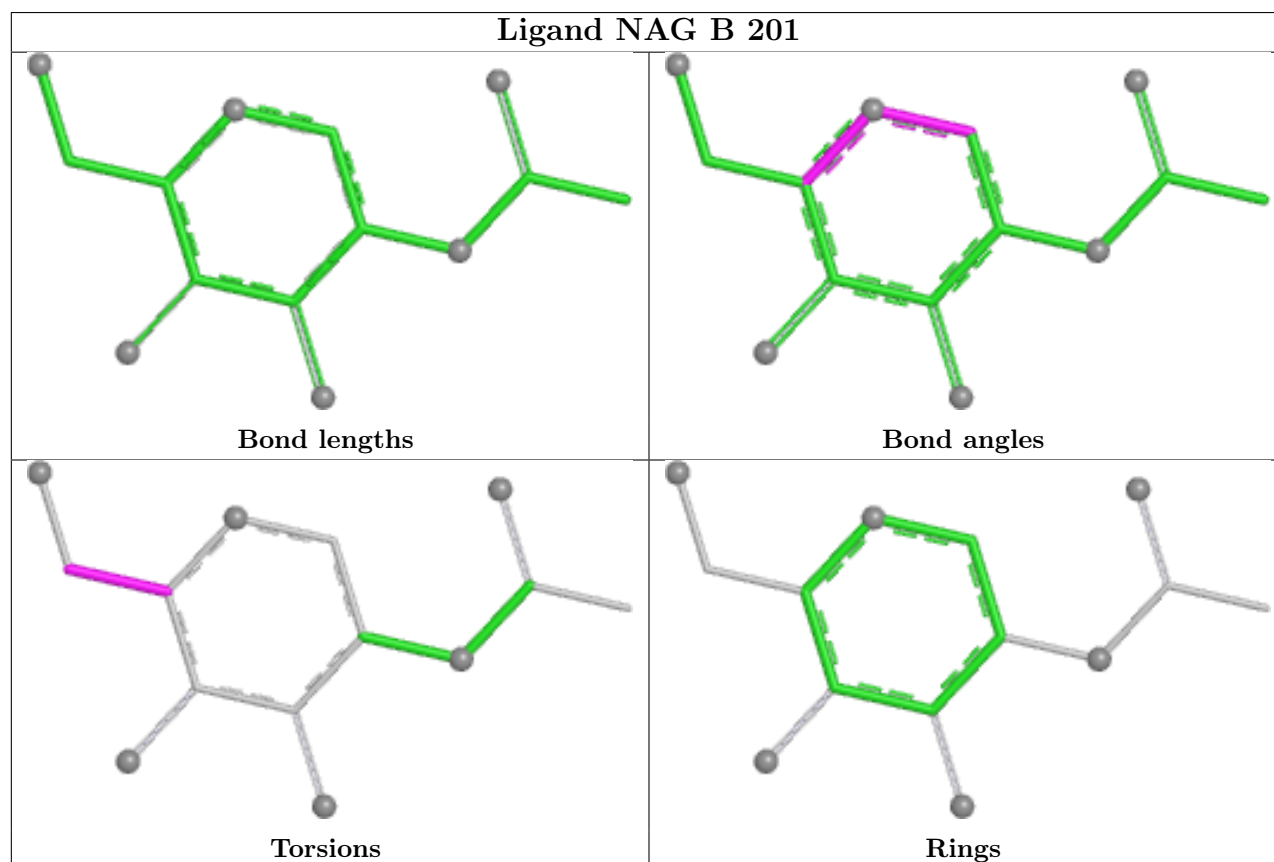
There are no ring outliers.

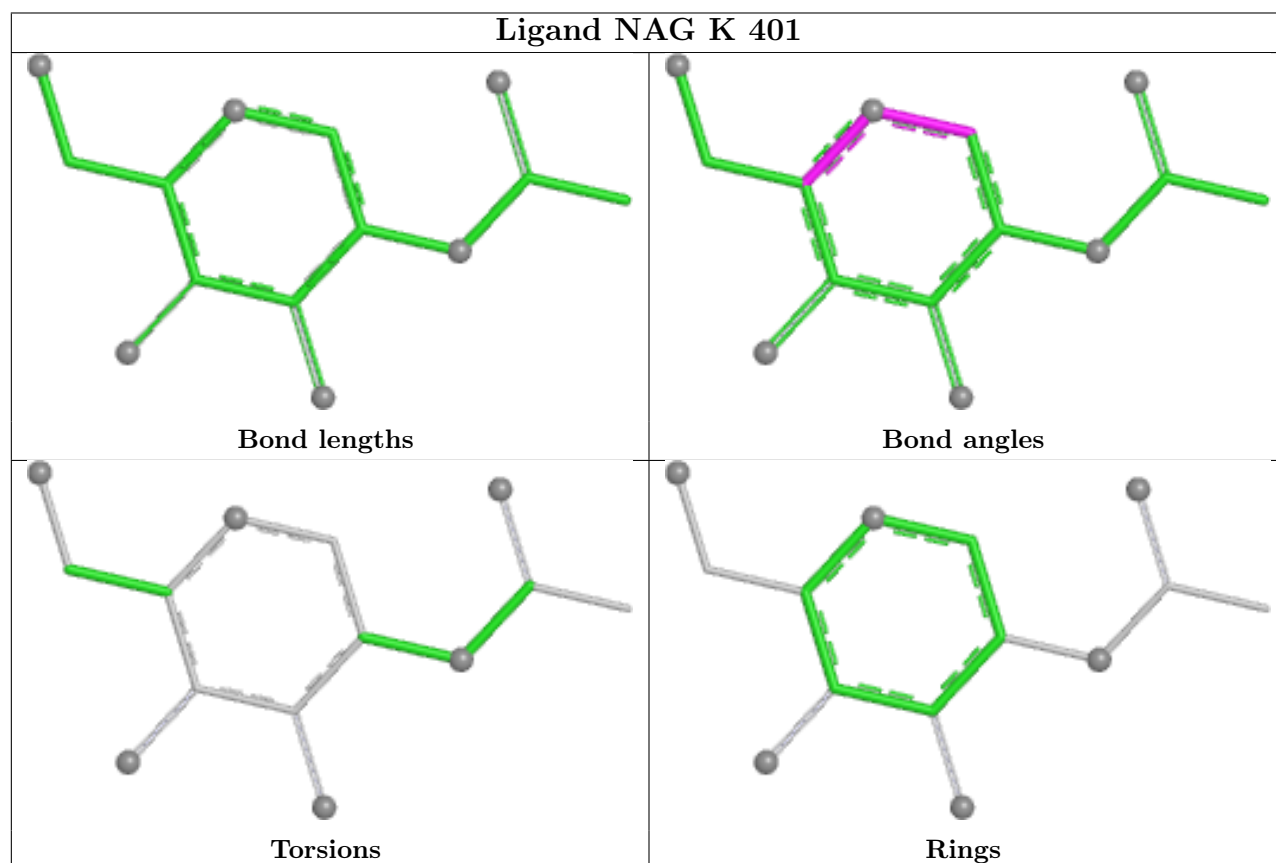
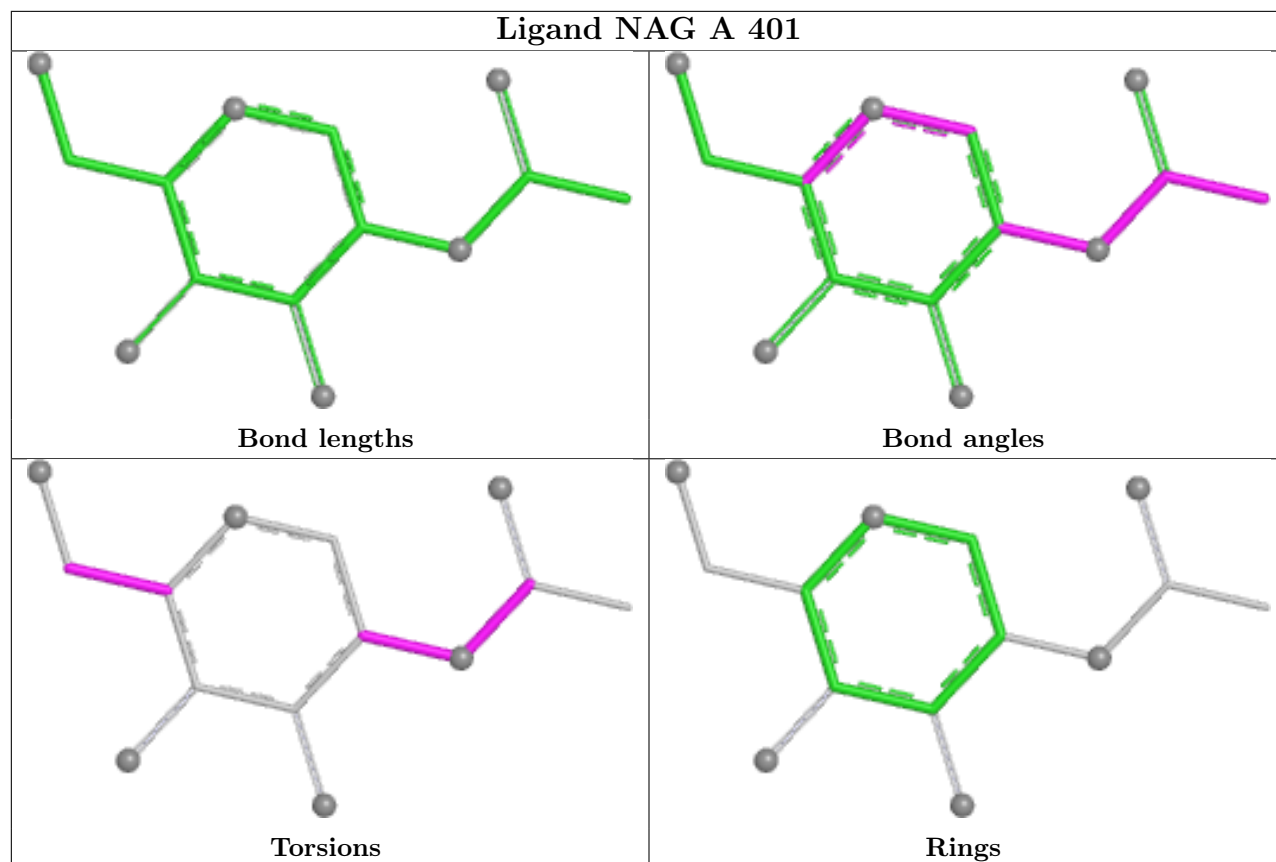
1 monomer is involved in 1 short contact:

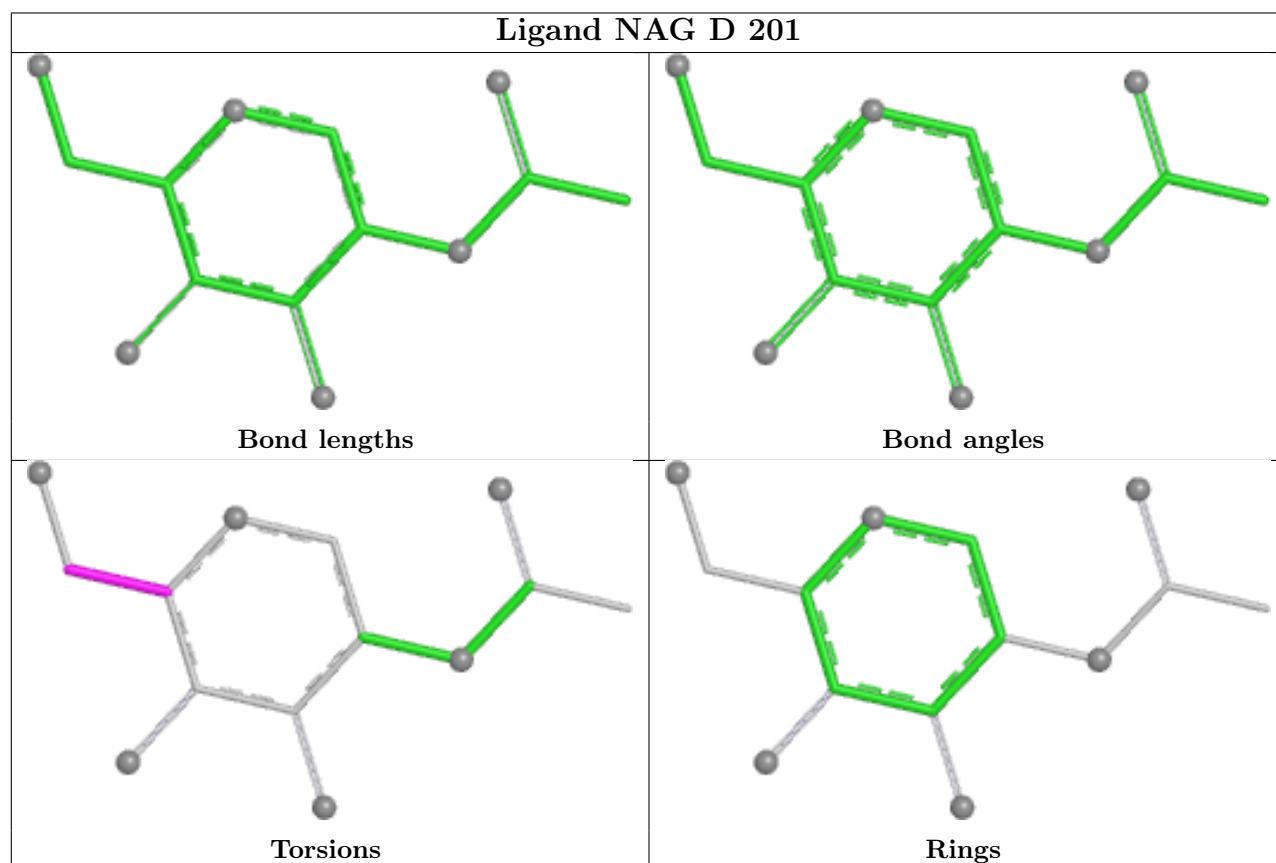
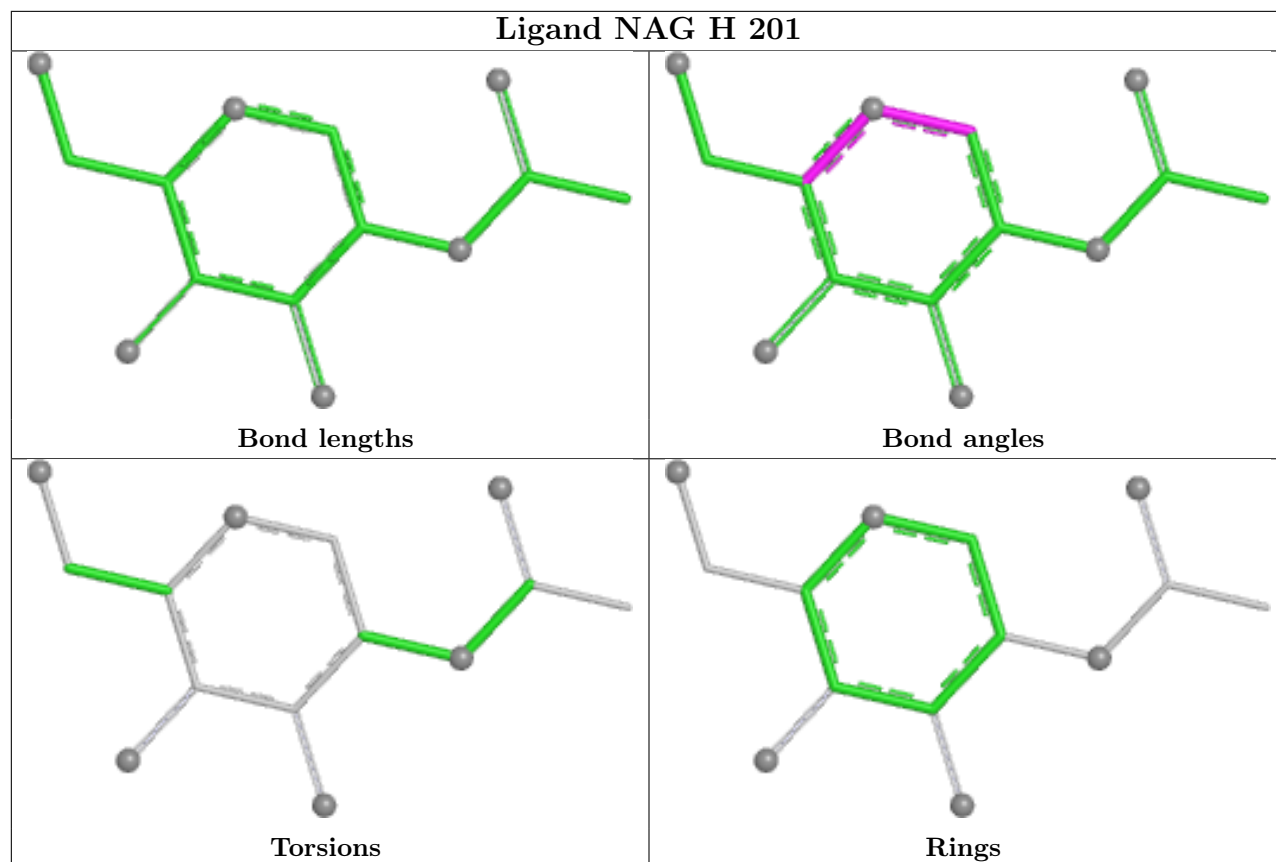
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	401	NAG	1	0

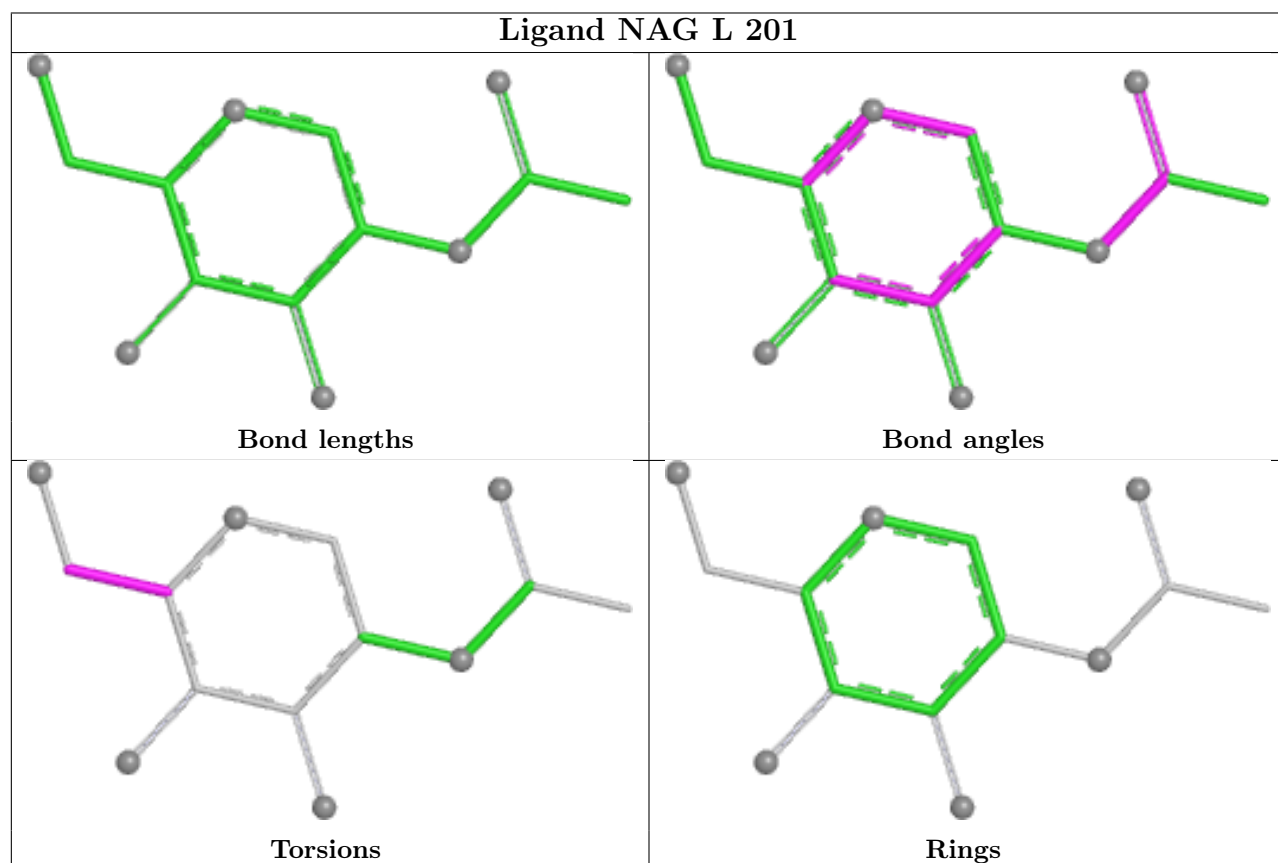
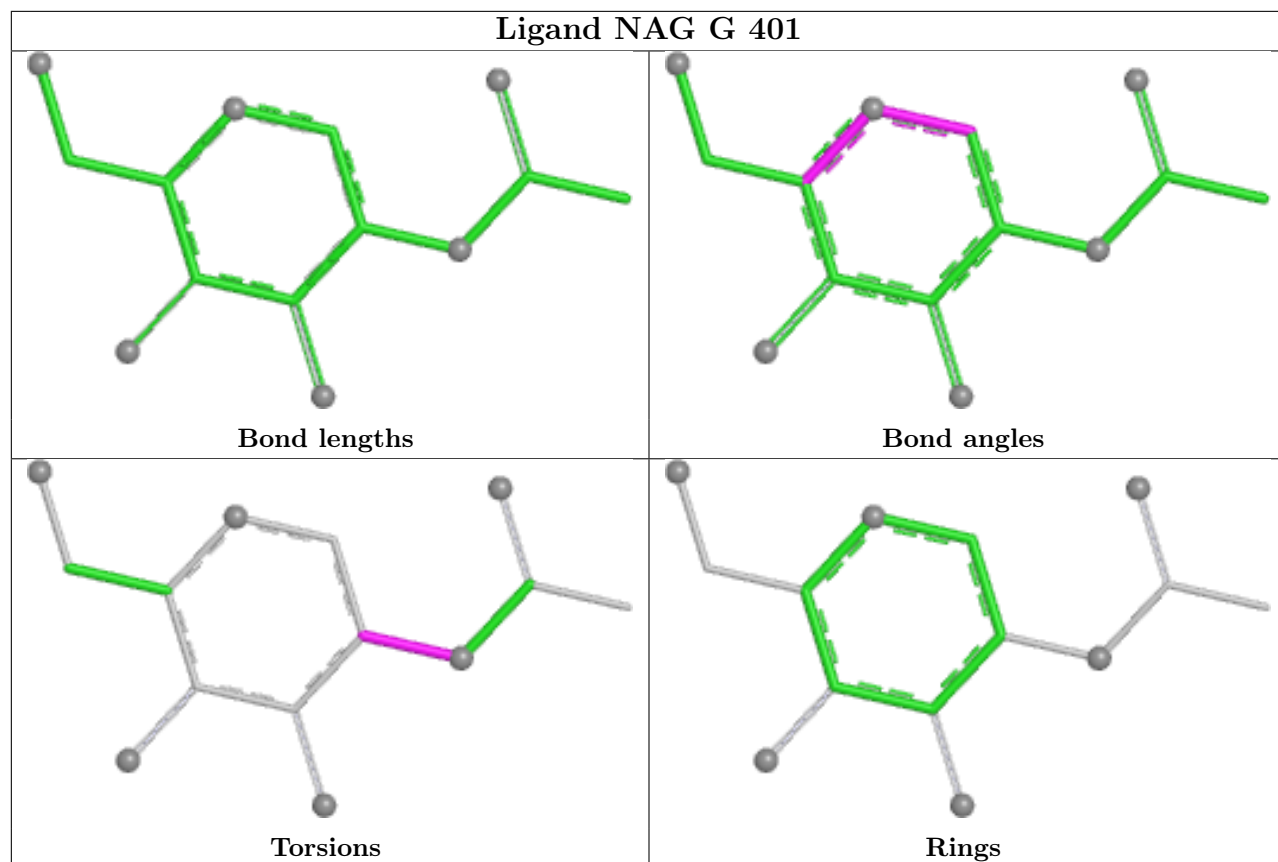
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths,

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.

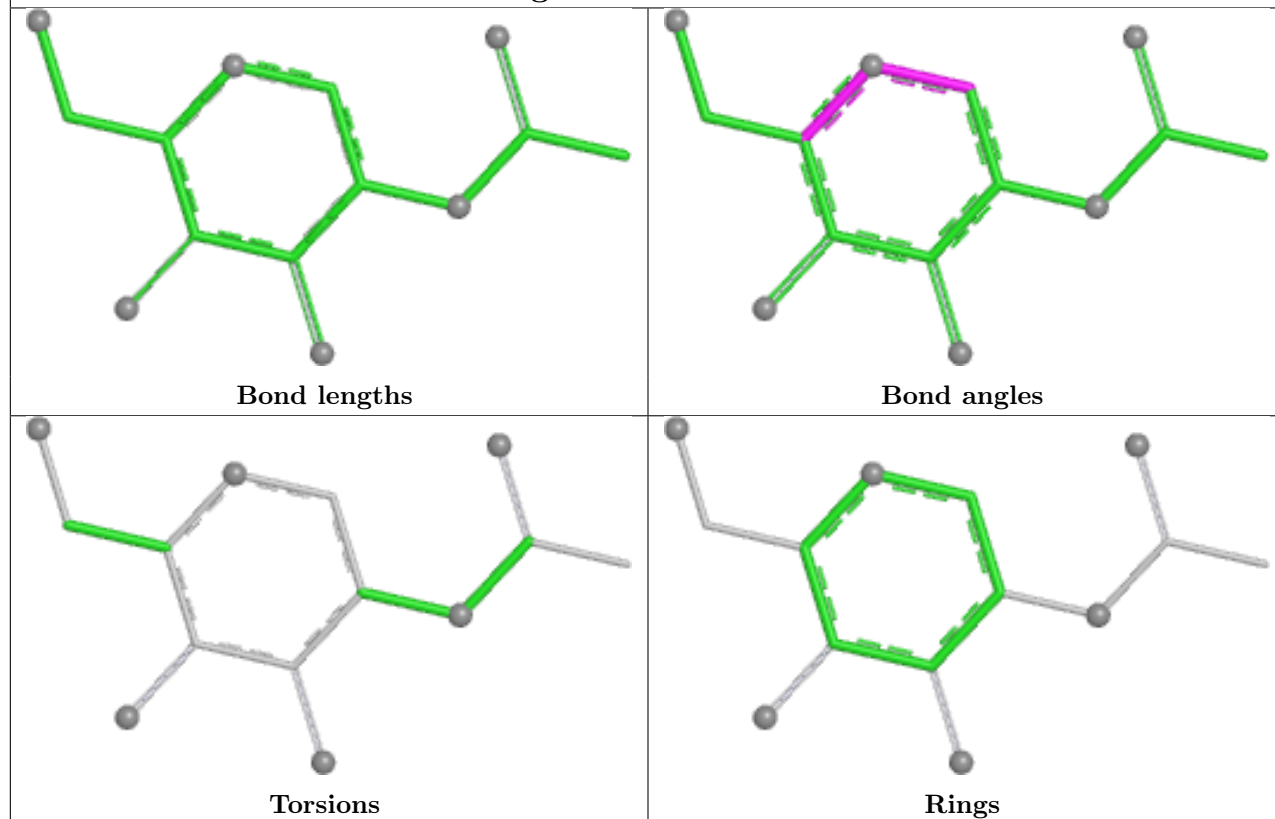




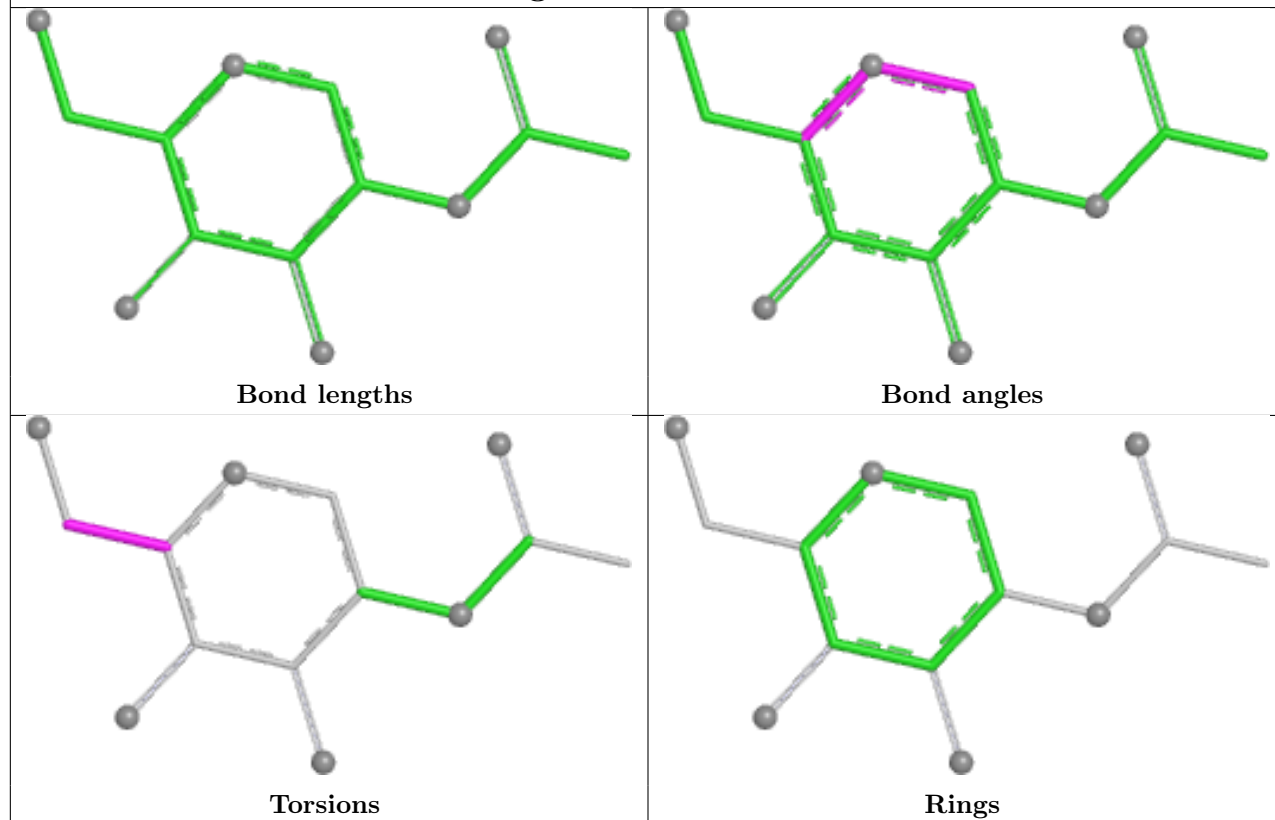


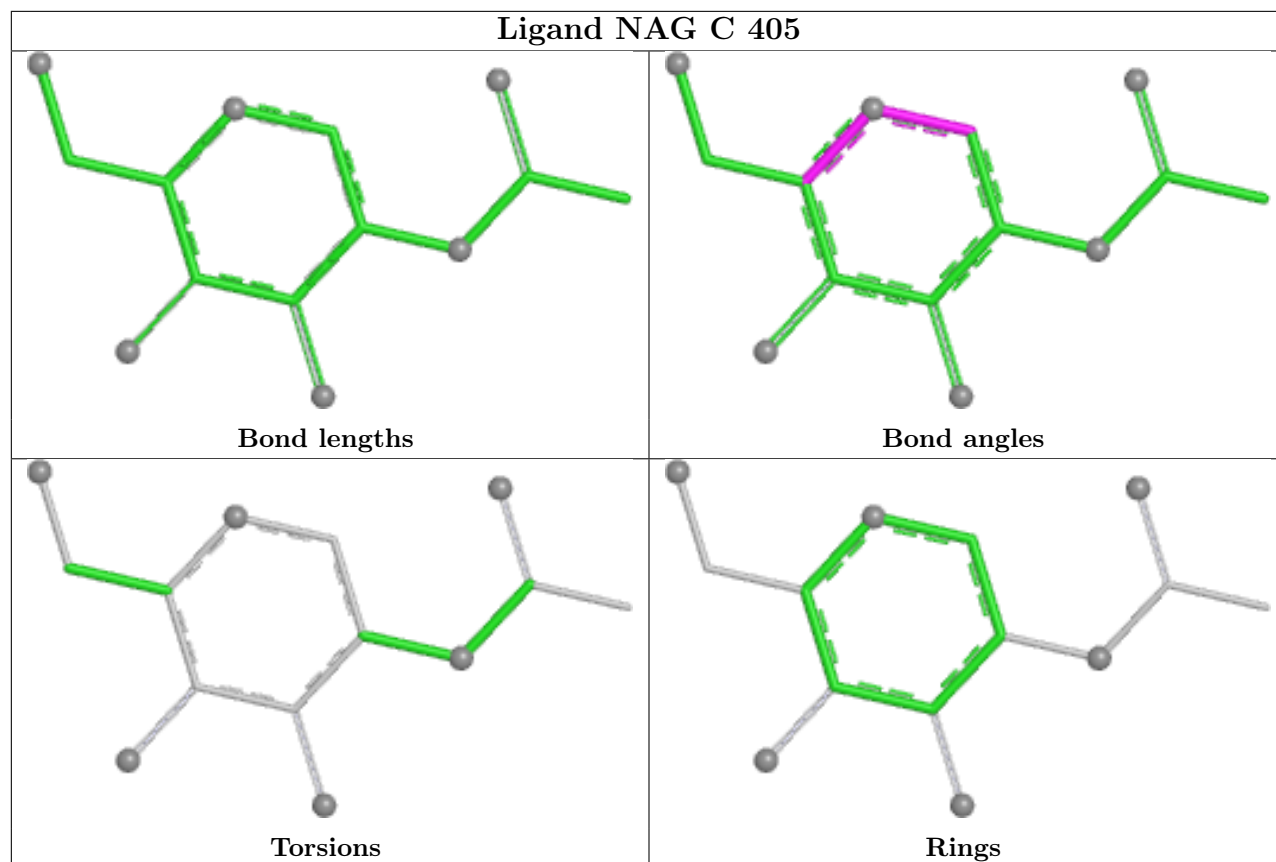


Ligand NAG J 201



Ligand NAG F 201





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	315/325 (96%)	1.19	44 (13%) 6 5	57, 91, 146, 179	1 (0%)
1	C	318/325 (97%)	0.57	8 (2%) 58 59	43, 72, 104, 117	1 (0%)
1	E	313/325 (96%)	0.99	36 (11%) 9 8	50, 83, 136, 184	1 (0%)
1	G	318/325 (97%)	0.36	4 (1%) 75 75	42, 65, 94, 114	1 (0%)
1	I	319/325 (98%)	0.82	31 (9%) 13 12	45, 80, 112, 129	0
1	K	319/325 (98%)	0.44	12 (3%) 44 45	44, 65, 94, 113	0
2	B	172/177 (97%)	0.82	11 (6%) 25 24	51, 80, 107, 119	0
2	D	172/177 (97%)	0.24	4 (2%) 61 62	43, 60, 81, 106	0
2	F	172/177 (97%)	0.70	7 (4%) 41 42	45, 68, 98, 109	0
2	H	172/177 (97%)	0.57	7 (4%) 41 42	42, 71, 103, 127	0
2	J	172/177 (97%)	0.44	2 (1%) 76 77	43, 66, 93, 112	0
2	L	172/177 (97%)	0.30	3 (1%) 69 69	44, 63, 90, 103	0
All	All	2934/3012 (97%)	0.65	169 (5%) 29 28	42, 73, 112, 184	4 (0%)

All (169) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	219	LEU	6.2
1	A	0	PRO	6.1
1	A	225	PHE	5.5
1	A	214	PRO	5.5
1	E	225	PHE	5.1
1	E	212	ALA	5.0
1	A	243	GLY	4.8
1	E	223	ILE	4.7
2	H	171	LEU	4.6
1	E	216	VAL	4.3
1	A	223	ILE	4.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	E	214	PRO	4.1
1	E	176	HIS	4.1
1	K	0	PRO	4.1
2	D	73	ILE	3.9
1	A	176	HIS	3.8
1	A	209	VAL	3.8
1	E	0	PRO	3.7
1	G	210	VAL	3.6
1	A	188	TYR	3.5
2	F	73	ILE	3.4
2	J	76	GLN	3.4
1	G	209	VAL	3.3
2	H	73	ILE	3.3
1	A	38	LEU	3.2
1	I	0	PRO	3.2
2	F	66	ILE	3.2
1	A	118	GLY	3.2
1	A	125	GLY	3.2
1	I	230	VAL	3.2
1	A	4	CYS	3.1
1	E	219	LEU	3.1
1	E	298	CYS	3.1
1	A	187	LEU	3.0
1	A	171	ILE	2.9
1	A	216	VAL	2.9
1	I	264	ALA	2.9
1	K	66	CYS	2.9
1	A	260	ILE	2.9
2	H	168	LEU	2.9
1	C	117	TYR	2.9
2	H	172	ASN	2.9
1	I	244	LEU	2.9
1	A	84	ILE	2.8
1	A	68	LEU	2.8
1	I	161	TYR	2.8
1	E	175	ILE	2.8
2	F	60	ASN	2.8
2	B	32	THR	2.8
1	E	87	CYS	2.8
1	I	145	LEU	2.8
1	I	66	CYS	2.8
1	I	236	ILE	2.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	B	103	GLU	2.8
1	A	259	GLY	2.7
1	C	172	MET	2.7
1	C	212	ALA	2.7
2	B	148	CYS	2.7
1	K	242	GLY	2.7
1	A	57	ILE	2.7
1	K	150	LYS	2.7
1	I	172	MET	2.7
1	E	213	ARG	2.7
2	B	16	GLY	2.7
1	E	220	SER	2.6
1	A	179	SER	2.6
1	E	259	GLY	2.6
1	A	85	ALA	2.6
1	C	67	ASP	2.6
1	A	206	PHE	2.6
1	E	193	LEU	2.6
2	F	103	GLU	2.6
1	I	198	GLY	2.5
1	G	270	CYS	2.5
2	F	144	CYS	2.5
1	E	118	GLY	2.5
2	B	73	ILE	2.5
2	B	35	ALA	2.5
1	E	178	PRO	2.5
1	E	157	THR	2.5
2	L	71	SER	2.5
2	B	33	GLY	2.4
2	L	73	ILE	2.4
2	J	73	ILE	2.4
1	E	243	GLY	2.4
1	E	245	ILE	2.4
1	A	41	LEU	2.4
1	C	190	THR	2.4
1	I	1	ASP	2.4
1	E	173	TRP	2.4
1	A	280	SER	2.3
1	K	172	MET	2.3
2	F	24	PHE	2.3
2	B	24	PHE	2.3
2	B	7	ALA	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	K	208	PRO	2.3
1	I	121	ILE	2.3
2	L	109	ASP	2.3
1	I	210	VAL	2.3
1	A	158	THR	2.3
1	I	283	THR	2.3
2	H	121	ARG	2.3
1	A	190	THR	2.3
1	I	146	VAL	2.3
1	A	86	TYR	2.3
1	I	130	CYS	2.3
1	I	167	ALA	2.2
1	A	181	THR	2.2
1	E	179	SER	2.2
1	E	187	LEU	2.2
1	I	150	LYS	2.2
1	K	270	CYS	2.2
1	A	54	CYS	2.2
1	A	2	LYS	2.2
2	F	168	LEU	2.2
2	H	109	ASP	2.2
1	C	53	ASN	2.2
1	C	264	ALA	2.2
1	E	140	ALA	2.2
1	E	88	TYR	2.2
1	K	188	TYR	2.2
1	I	87	CYS	2.2
1	E	119	SER	2.2
1	A	317	PRO	2.2
1	I	212	ALA	2.2
1	K	278	GLY	2.2
1	I	80	ARG	2.2
1	K	225	PHE	2.2
1	I	250	VAL	2.1
1	E	283	THR	2.1
1	K	283	THR	2.1
1	A	5	LEU	2.1
1	A	201	THR	2.1
1	I	42	CYS	2.1
1	A	192	SER	2.1
1	E	143	LYS	2.1
1	A	70	LEU	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	E	121	ILE	2.1
1	A	61	ILE	2.1
1	I	254	ILE	2.1
1	I	123	SER	2.1
1	G	172	MET	2.1
1	I	238	PHE	2.1
1	E	94	ASN	2.1
1	I	116	THR	2.1
1	I	148	LYS	2.1
2	D	137	CYS	2.1
1	E	177	HIS	2.1
2	D	76	GLN	2.1
1	A	316	VAL	2.1
1	A	65	ALA	2.1
1	A	218	GLY	2.1
2	B	121	ARG	2.1
2	H	74	ASP	2.1
1	E	130	CYS	2.1
1	I	270	CYS	2.1
2	D	75	HIS	2.1
1	E	205	ASN	2.0
1	A	244	LEU	2.0
1	E	134	GLY	2.0
1	C	245	ILE	2.0
1	E	84	ILE	2.0
1	E	188	TYR	2.0
2	B	133	ASP	2.0
1	I	120	SER	2.0
1	I	247	PRO	2.0
1	K	298	CYS	2.0
1	A	66	CYS	2.0
1	A	119	SER	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,

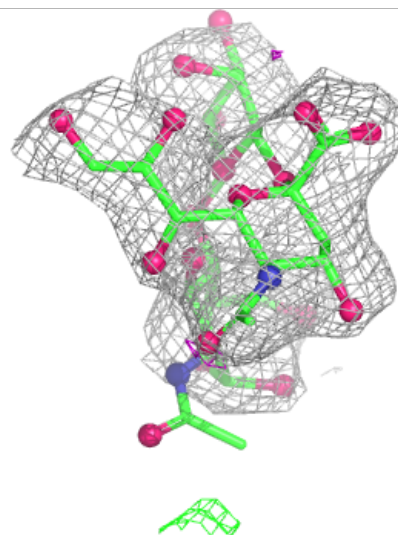
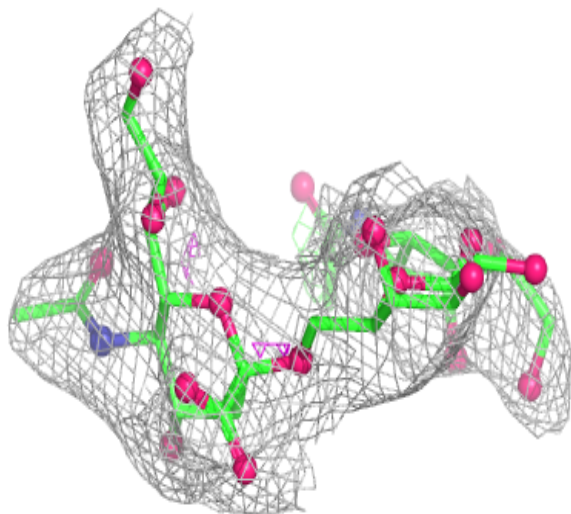
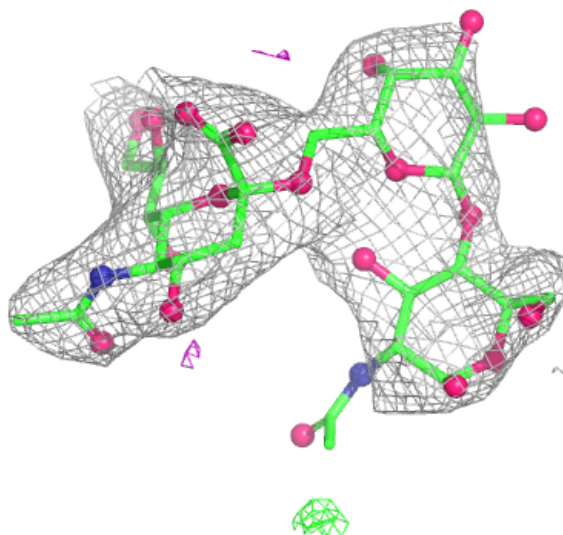
median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	NAG	Q	1	15/15	0.45	0.16	154,163,169,170	0
3	NAG	O	1	15/15	0.53	0.16	144,153,155,156	0
3	NAG	M	1	15/15	0.54	0.16	130,144,153,154	0
3	NAG	P	1	15/15	0.58	0.17	136,152,156,156	0
4	GAL	N	1	12/12	0.66	0.11	123,130,134,134	0
3	GAL	O	2	11/12	0.72	0.12	110,123,130,131	0
3	GAL	P	2	11/12	0.73	0.12	95,114,129,136	0
3	GAL	Q	2	11/12	0.75	0.11	113,130,139,143	0
4	SIA	N	2	20/21	0.76	0.12	101,113,121,126	0
3	GAL	M	2	11/12	0.83	0.09	95,116,132,133	0
3	SIA	Q	3	20/21	0.90	0.10	81,91,104,106	0
3	SIA	O	3	20/21	0.93	0.09	73,78,100,101	0
3	SIA	M	3	20/21	0.93	0.09	68,77,87,88	0
3	SIA	P	3	20/21	0.96	0.09	69,74,82,82	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.

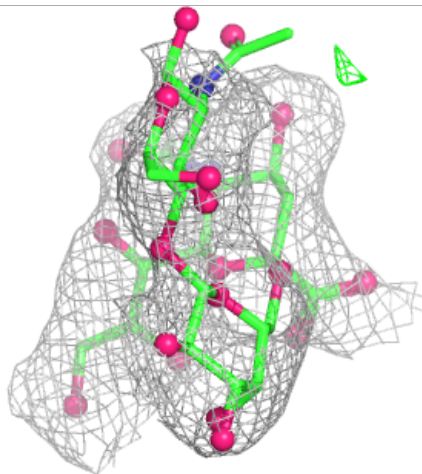
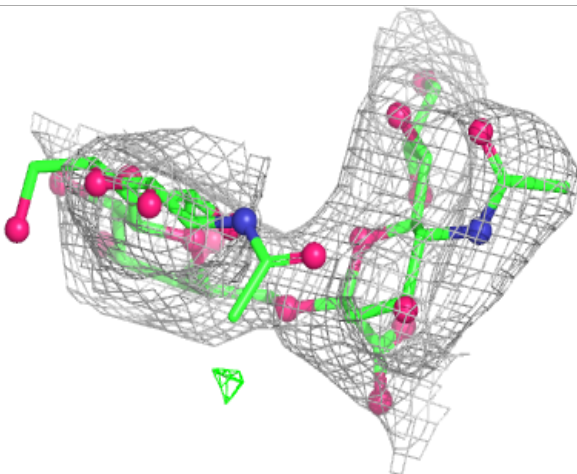
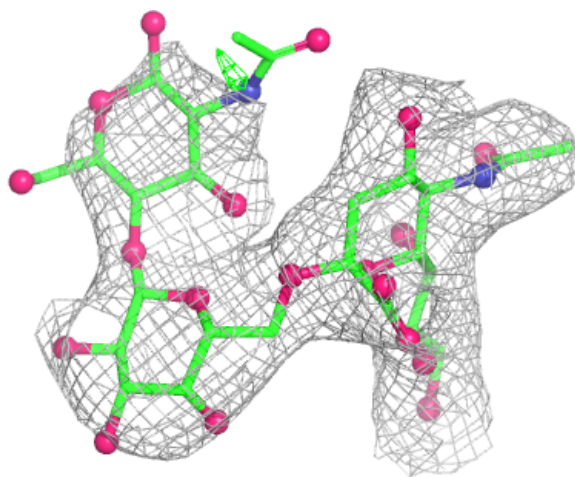
Electron density around Chain M:

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



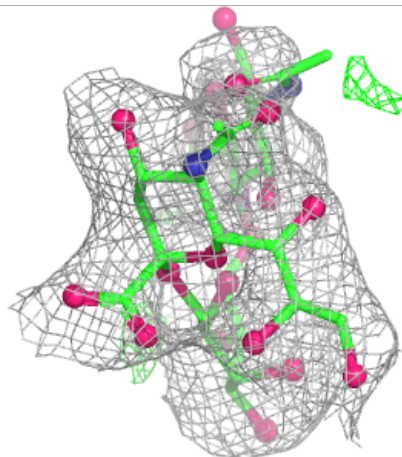
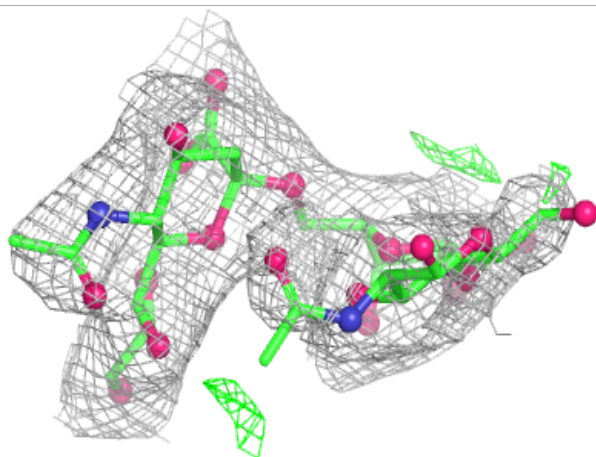
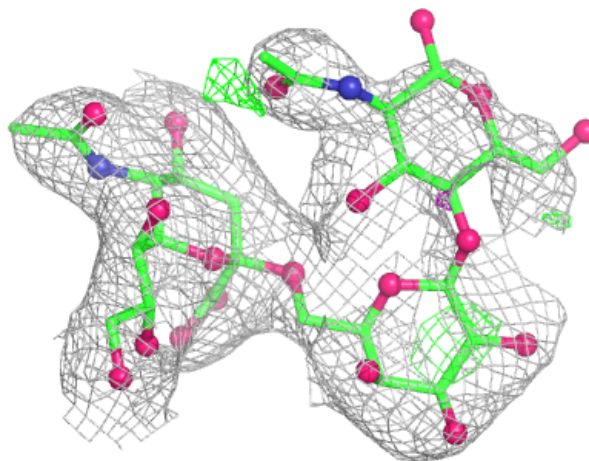
Electron density around Chain O:

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



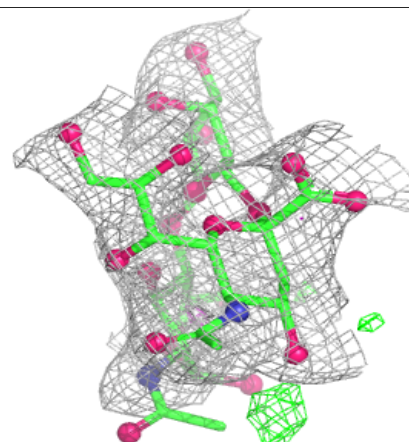
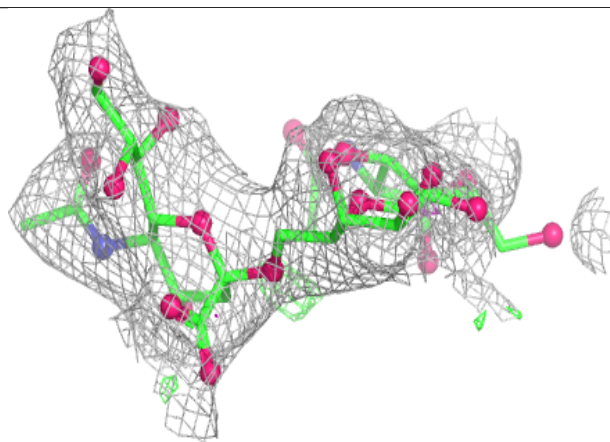
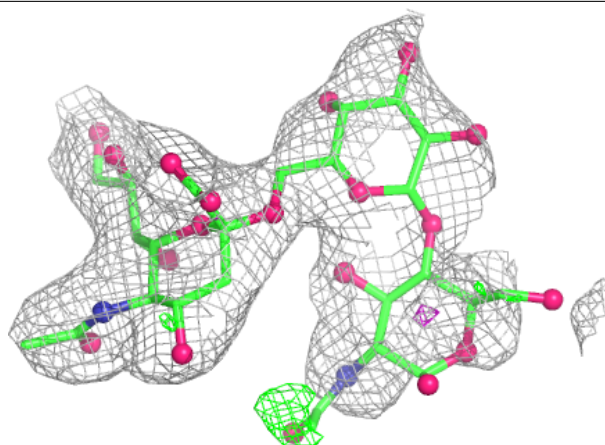
Electron density around Chain P:

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

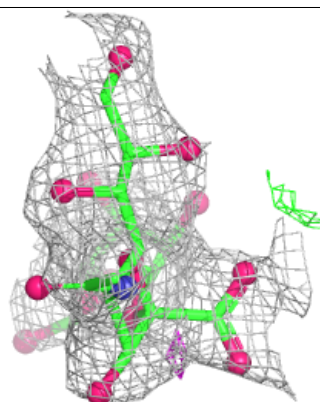
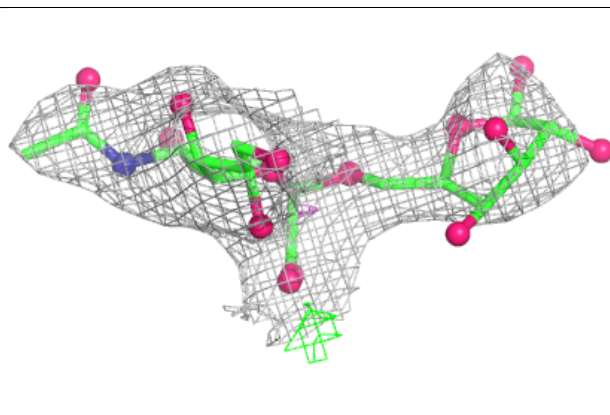
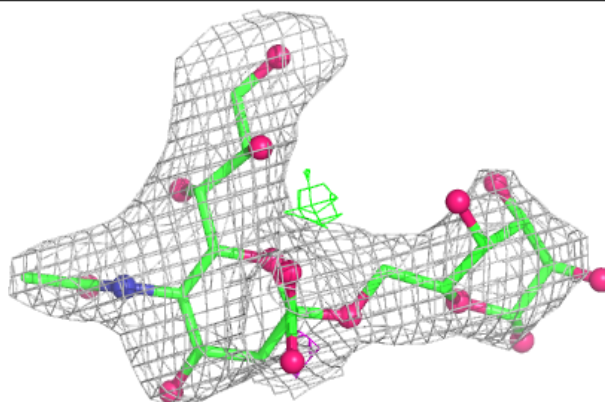


Electron density around Chain Q:

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

**Electron density around Chain N:**

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



6.4 Ligands

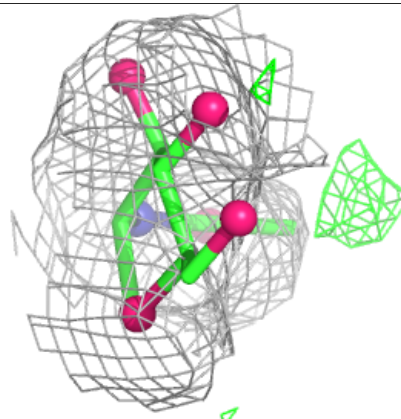
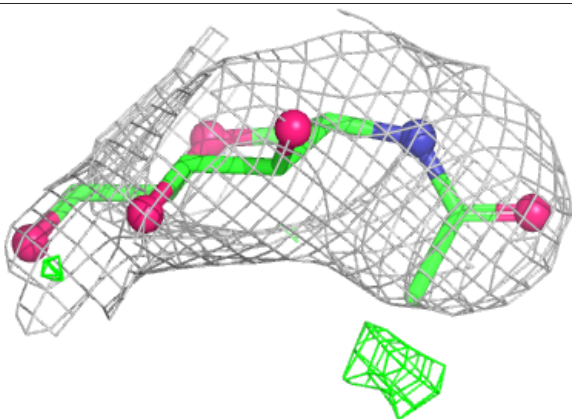
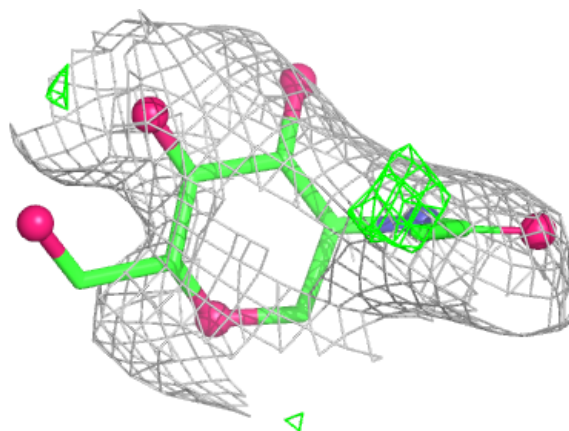
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
6	NAG	A	401	14/15	0.65	0.18	110,116,125,128	0
6	NAG	L	201	14/15	0.69	0.15	90,102,106,115	0
6	NAG	F	201	14/15	0.81	0.12	67,80,96,111	0
6	NAG	C	405	14/15	0.83	0.13	88,99,104,105	0
6	NAG	G	401	14/15	0.84	0.16	95,103,106,106	0
6	NAG	H	201	14/15	0.84	0.11	95,105,111,111	0
6	NAG	D	201	14/15	0.85	0.10	73,78,85,87	0
6	NAG	B	201	14/15	0.86	0.09	85,91,99,104	0
6	NAG	K	401	14/15	0.87	0.14	96,104,108,112	0
6	NAG	J	201	14/15	0.88	0.09	70,77,79,81	0
5	CA	C	404	1/1	0.98	0.03	75,75,75,75	0
5	CA	B	202	1/1	0.98	0.07	88,88,88,88	0

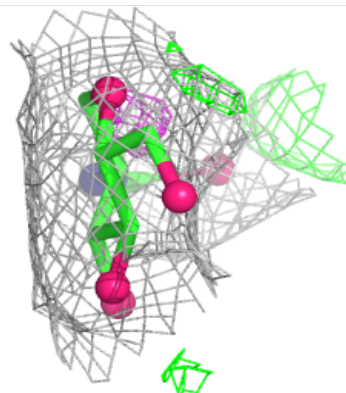
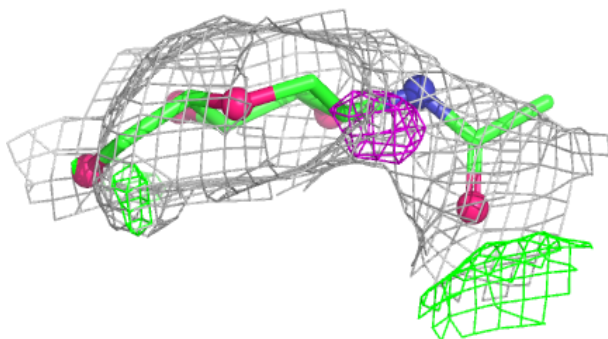
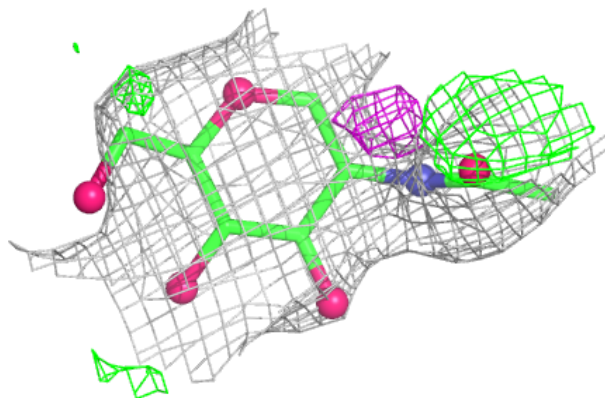
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around NAG A 401:

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

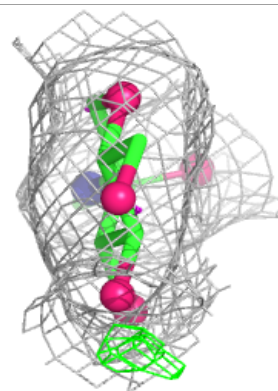
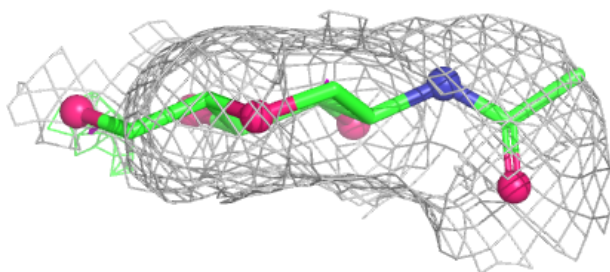
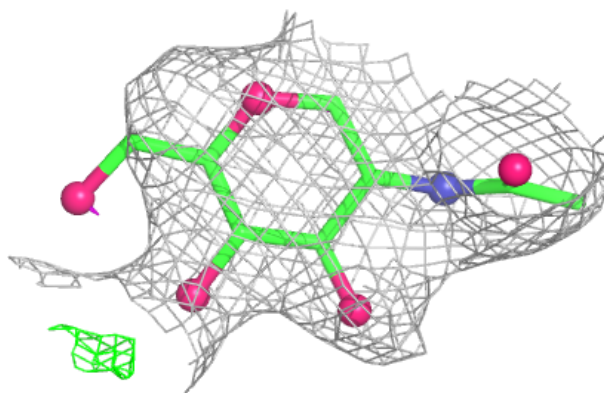
**Electron density around NAG L 201:**

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

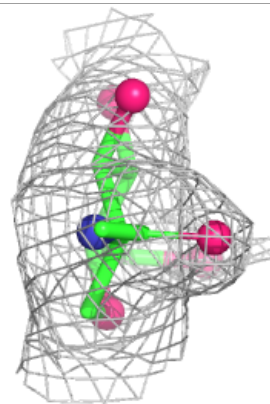
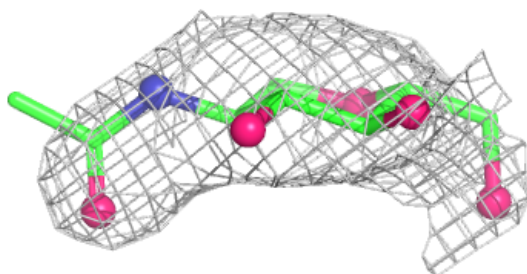
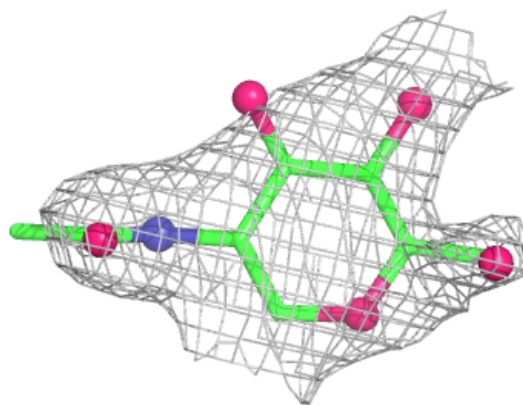


Electron density around NAG F 201:

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

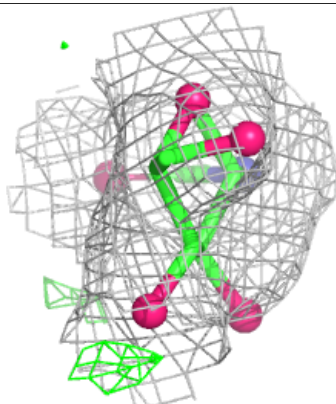
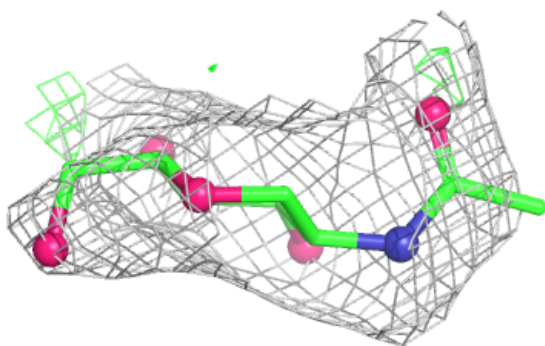
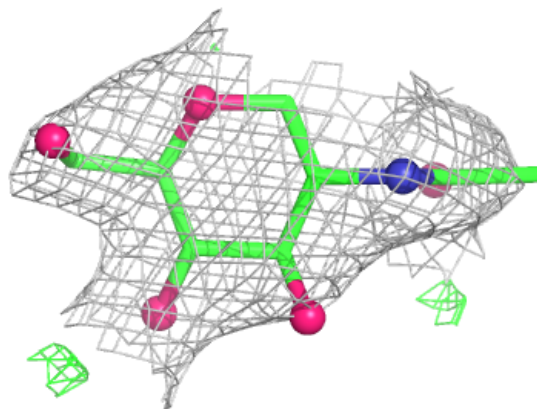
**Electron density around NAG C 405:**

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

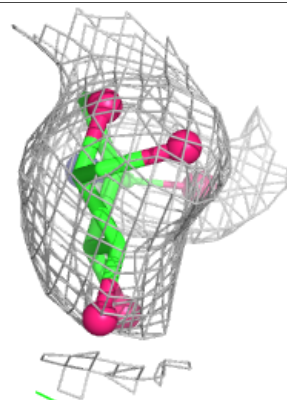
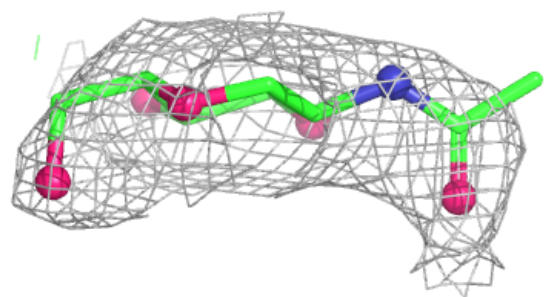
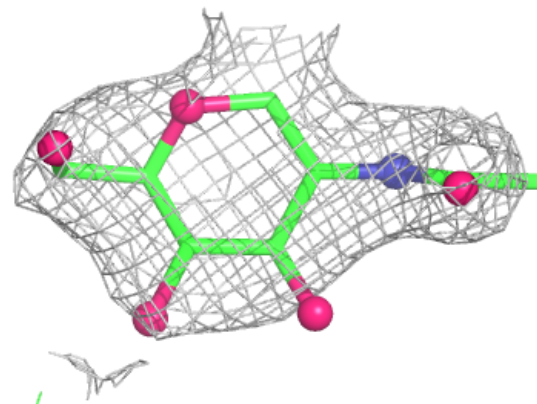


Electron density around NAG G 401:

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

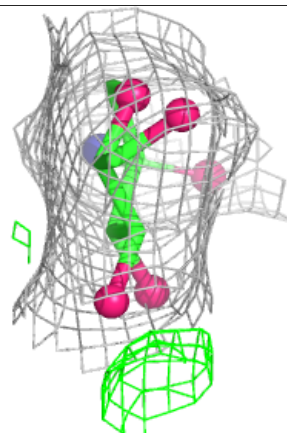
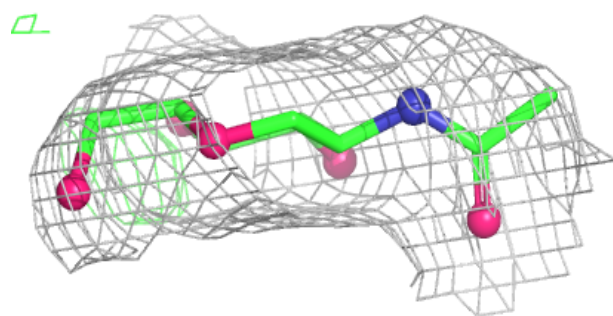
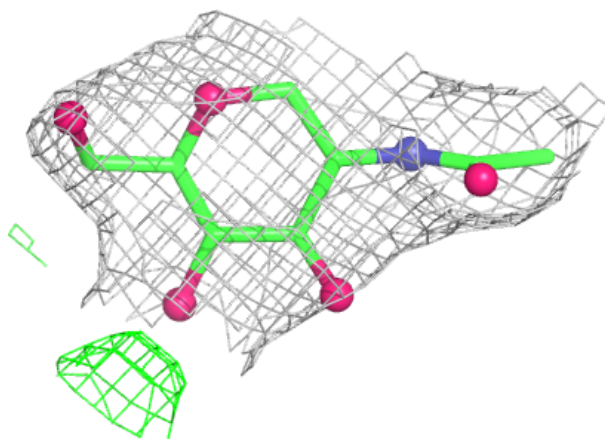
**Electron density around NAG H 201:**

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



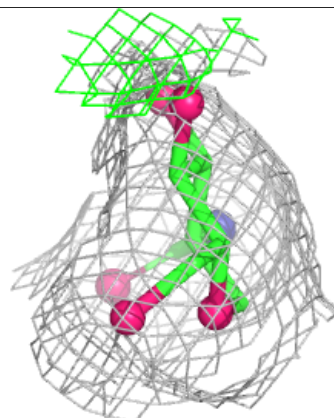
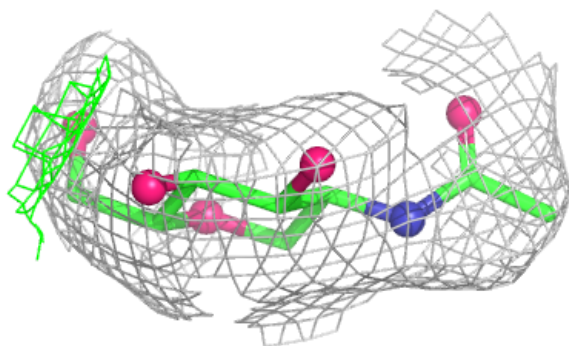
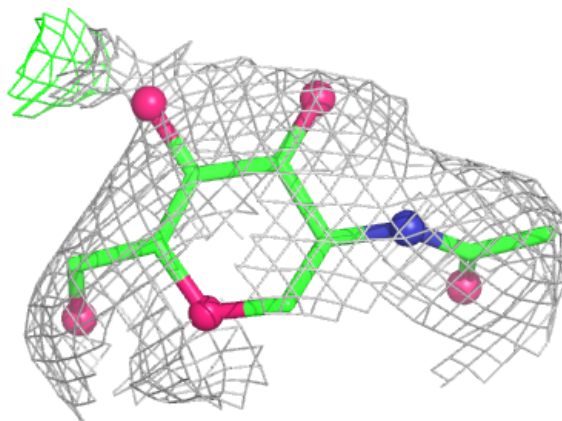
Electron density around NAG D 201:

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



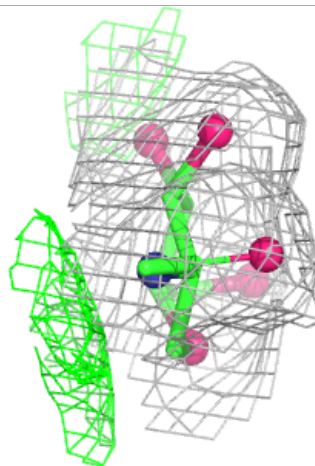
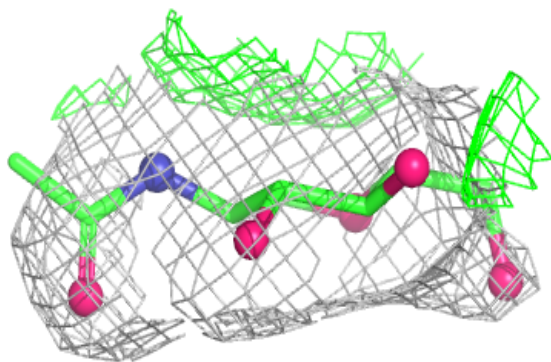
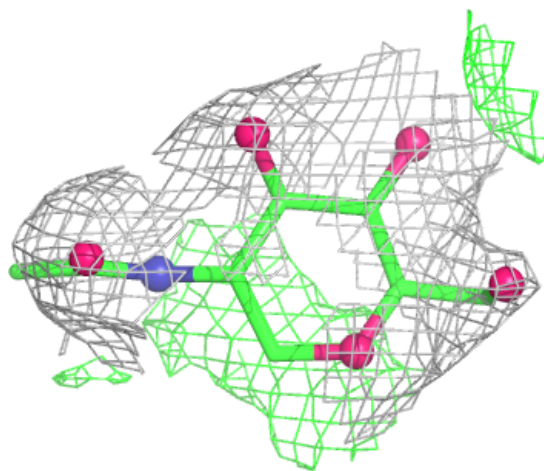
Electron density around NAG B 201:

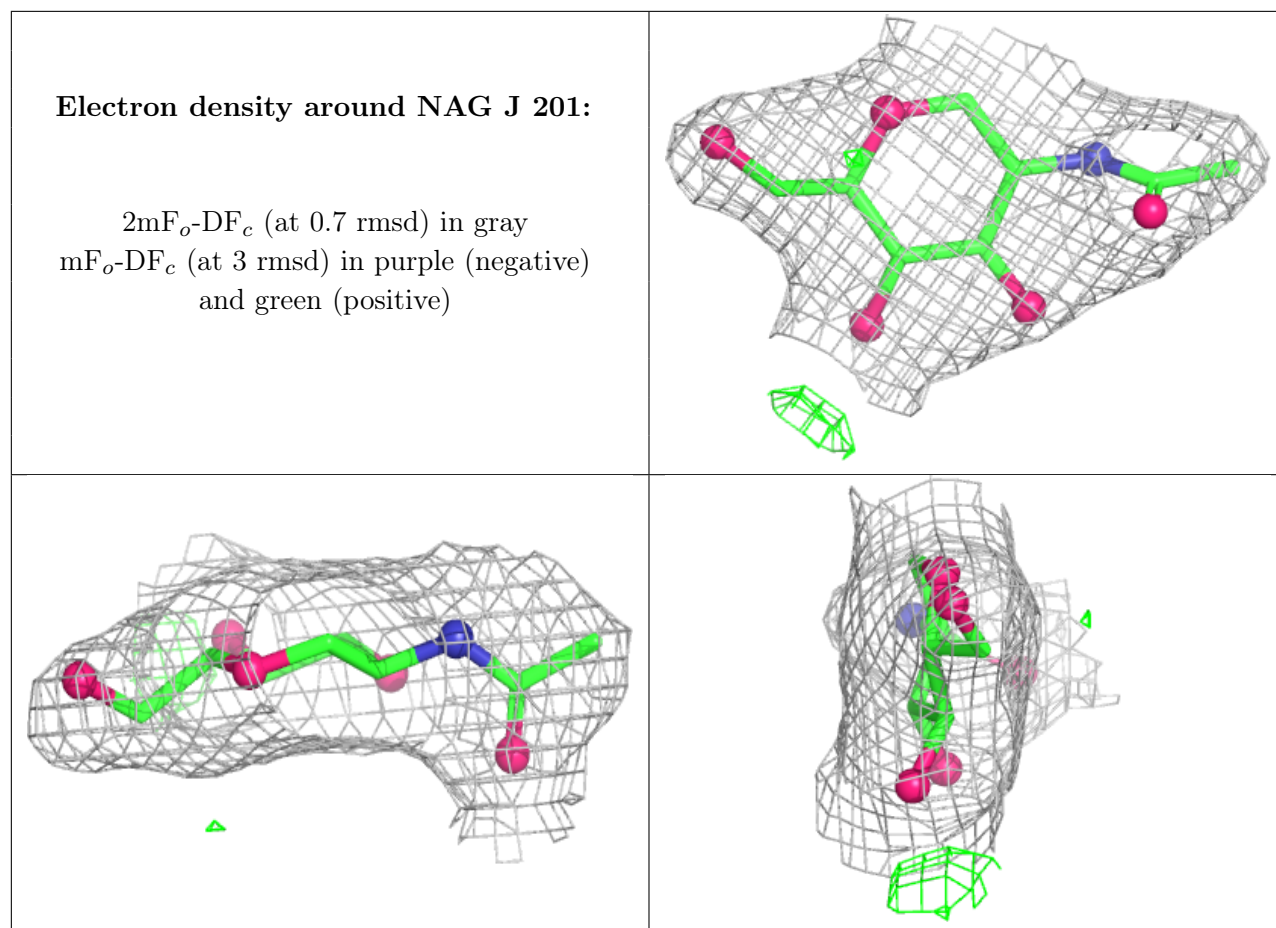
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around NAG K 401:

$2mF_o-DF_c$ (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.