



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 04:45 PM UTC

PDB ID : 7UIA / pdb_00007uia
Title : Crystal structure of BoNT/E receptor binding domain in complex with SV2 and VHH
Authors : Liu, Z.; Jin, R.; Chen, P.
Deposited on : 2022-03-28
Resolution : 2.59 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

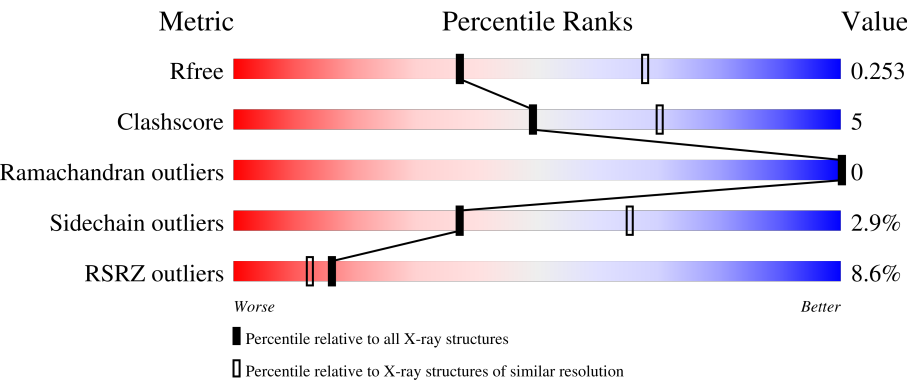
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.59 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.



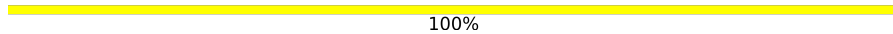
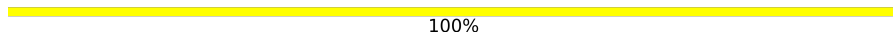
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R _{free}	180053	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (2.60-2.60)

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	B	129	29% 78%22%
1	E	129	30% 85%13%
2	C	105	2% 73%16%10%
2	F	105	4% 76%13%10%
3	A	407	4% 82%17%

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Mol	Chain	Length	Quality of chain
3	D	407	 2% 87% 12%
4	G	2	 100%
4	H	2	 100%

2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 10510 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 VHH-G6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	128	Total	C	N	O	S	0	0	0
			967	611	159	193	4			
1	E	129	Total	C	N	O	S	0	0	0
			983	622	158	199	4			

- Molecule 2 is a protein called SV2Ac.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	95	Total	C	N	O	S	0	0	0
			796	513	127	152	4			
2	F	94	Total	C	N	O	S	0	0	0
			787	508	126	149	4			

- Molecule 3 is a protein called Neurotoxin type E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	406	Total	C	N	O	S	0	0	0
			3320	2099	573	639	9			
3	A	406	Total	C	N	O	S	0	0	0
			3316	2101	573	633	9			

- Molecule 4 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



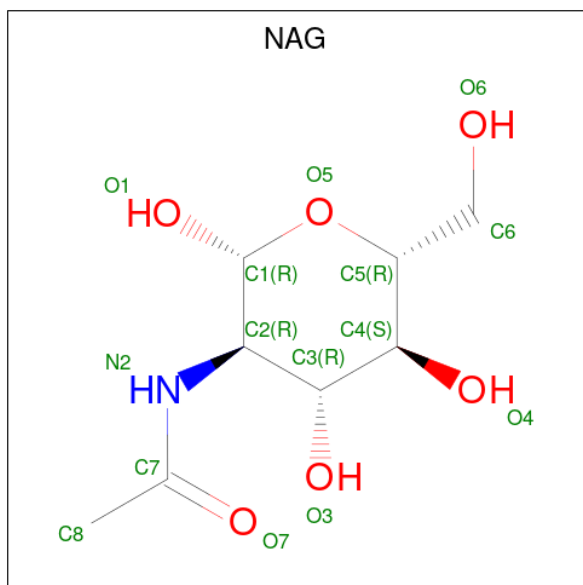
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	G	2	Total	C	N	O	0	0	0
			28	16	2	10			

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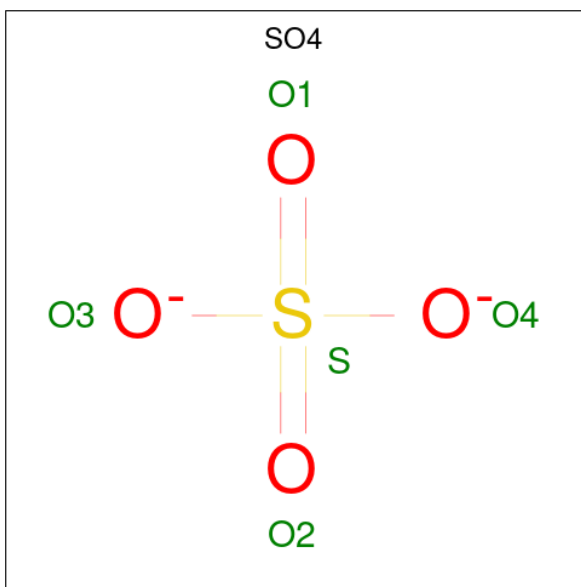
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	H	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$) (labeled as "Ligand of Interest" by depositor).



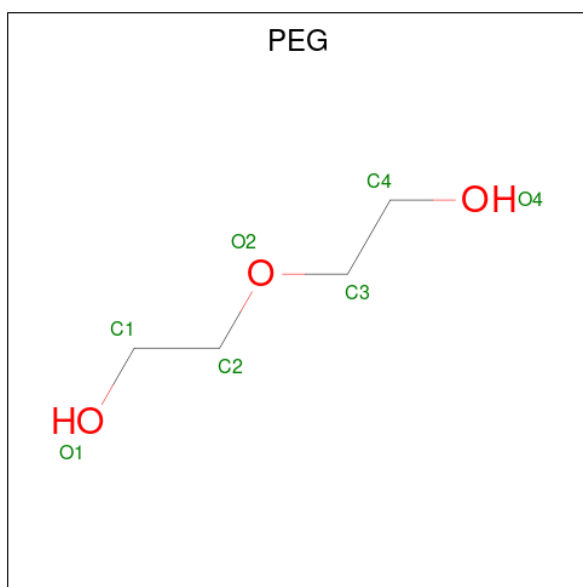
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	C	1	Total	C	N	O	0	0
			14	8	1	5		
5	C	1	Total	C	N	O	0	0
			14	8	1	5		
5	F	1	Total	C	N	O	0	0
			14	8	1	5		
5	F	1	Total	C	N	O	0	0
			14	8	1	5		
5	F	1	Total	C	N	O	0	0
			14	8	1	5		
5	F	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 6 is SULFATE ION (CCD ID: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	C	1	Total	O	S	0	0
			5	4	1		
6	C	1	Total	O	S	0	0
			5	4	1		
6	F	1	Total	O	S	0	0
			5	4	1		
6	D	1	Total	O	S	0	0
			5	4	1		
6	D	1	Total	O	S	0	0
			5	4	1		
6	A	1	Total	O	S	0	0
			5	4	1		
6	A	1	Total	O	S	0	0
			5	4	1		

- Molecule 7 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: C₄H₁₀O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	C	O	0	0
			7	4	3		

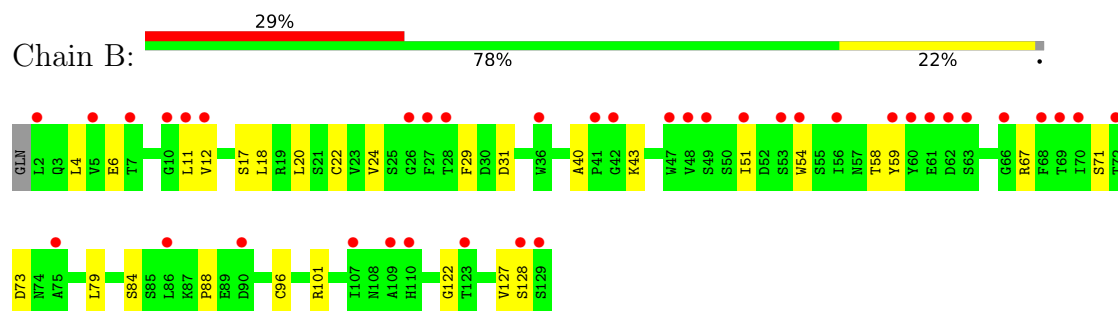
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	B	1	Total	O	0	0
			1	1		
8	C	8	Total	O	0	0
			8	8		
8	E	11	Total	O	0	0
			11	11		
8	F	8	Total	O	0	0
			8	8		
8	D	79	Total	O	0	0
			79	79		
8	A	52	Total	O	0	0
			52	52		

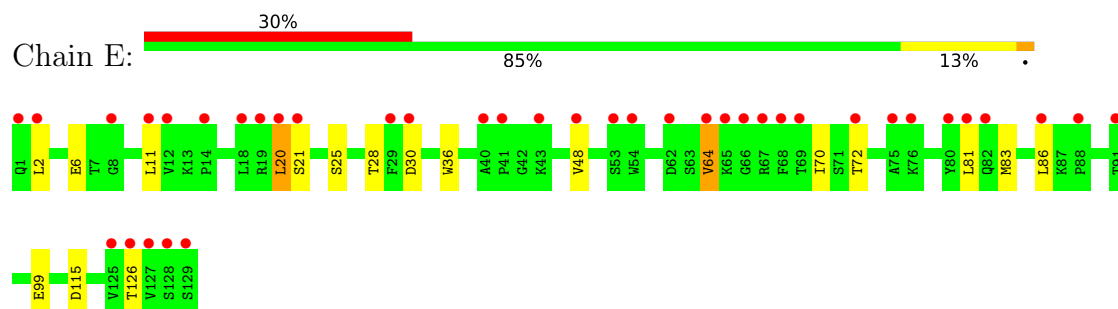
3 Residue-property plots [i](#)

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.

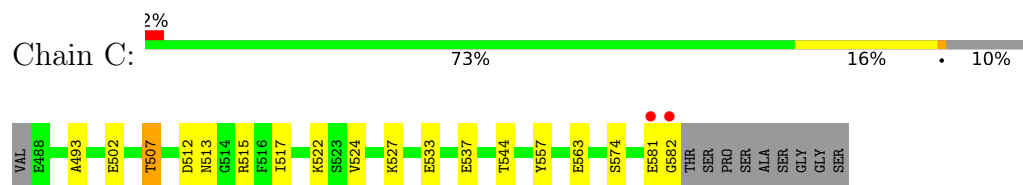
• Molecule 1: VHH-G6



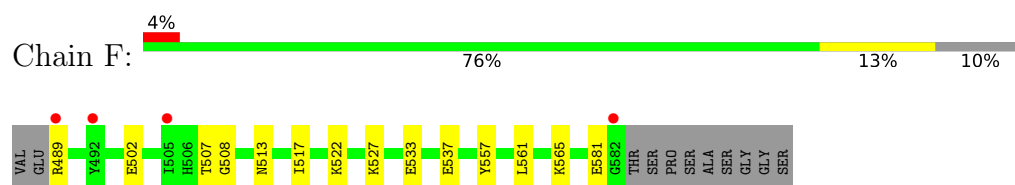
• Molecule 1: VHH-G6



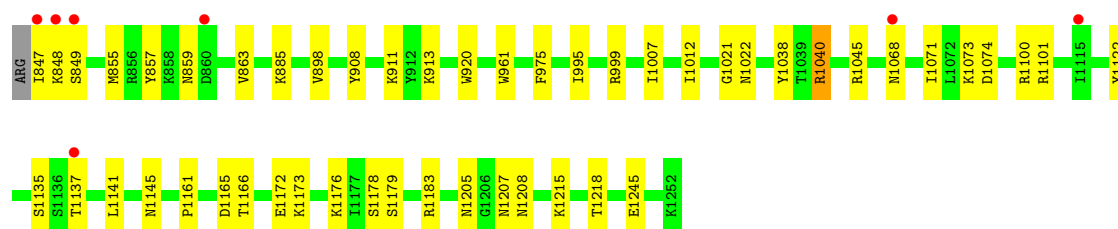
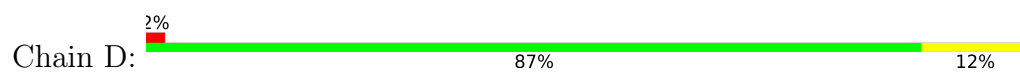
• Molecule 2: SV2Ac



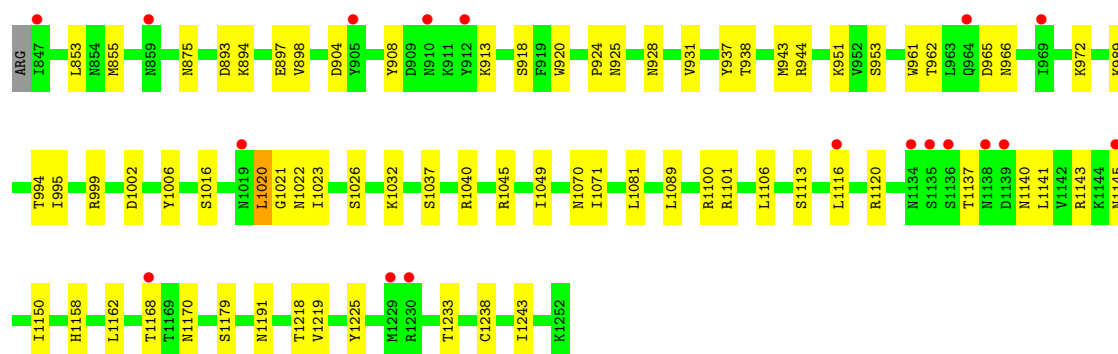
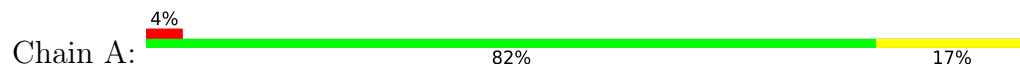
• Molecule 2: SV2Ac



• Molecule 3: Neurotoxin type E



• Molecule 3: Neurotoxin type E



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



NAG1
NAG2

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



NAG1
NAG2

4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	140.74Å 172.34Å 137.16Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	109.01 – 2.59 109.01 – 2.59	Depositor EDS
% Data completeness (in resolution range)	99.9 (109.01-2.59) 100.0 (109.01-2.59)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.45 (at 2.58Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.226 , 0.249 0.229 , 0.253	Depositor DCC
R_{free} test set	2660 reflections (5.11%)	wwPDB-VP
Wilson B-factor (Å ²)	56.7	Xtriage
Anisotropy	0.051	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 25.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	10510	wwPDB-VP
Average B, all atoms (Å ²)	57.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.32% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: SO4, NAG, PEG

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	B	0.98	0/992	1.18	0/1356
1	E	0.91	0/1008	1.10	0/1380
2	C	0.82	0/816	0.98	0/1098
2	F	0.81	0/807	1.00	0/1086
3	A	0.87	0/3386	1.07	0/4592
3	D	0.86	0/3390	1.05	0/4598
All	All	0.88	0/10399	1.07	0/14110

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	967	0	875	16	0
1	E	983	0	901	8	0
2	C	796	0	735	15	0
2	F	787	0	729	9	0
3	A	3316	0	3208	43	0
3	D	3320	0	3201	28	0
4	G	28	0	25	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	H	28	0	25	0	0
5	C	28	0	26	0	0
5	F	56	0	52	0	0
6	A	10	0	0	0	0
6	C	10	0	0	0	0
6	D	10	0	0	0	0
6	F	5	0	0	0	0
7	A	7	0	10	0	0
8	A	52	0	0	1	0
8	B	1	0	0	0	0
8	C	8	0	0	0	0
8	D	79	0	0	0	0
8	E	11	0	0	0	0
8	F	8	0	0	0	0
All	All	10510	0	9787	108	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 (108) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:920:TRP:HB2	3:D:1045:ARG:HG2	1.64	0.80
2:C:515:ARG:HE	3:A:1158:HIS:HD2	1.37	0.72
3:A:924:PRO:O	3:A:1040:ARG:NH2	2.24	0.70
1:B:4:LEU:HD23	1:B:24:VAL:HG12	1.73	0.69
3:A:1168:THR:HG22	3:A:1170:ASN:H	1.58	0.69
3:A:920:TRP:HB2	3:A:1045:ARG:HG2	1.75	0.67
1:B:40:ALA:HB3	1:B:43:LYS:HD3	1.76	0.66
2:C:557:TYR:CZ	3:A:1100:ARG:HD3	2.34	0.62
1:E:83:MET:HE2	1:E:86:LEU:HD22	1.81	0.62
3:A:1101:ARG:NH2	3:A:1218:THR:OG1	2.33	0.61
3:A:875:ASN:HB2	3:A:897:GLU:HG2	1.82	0.60
1:B:88:PRO:HA	1:B:127:VAL:HB	1.84	0.59
1:B:73:ASP:HA	3:D:848:LYS:HD2	1.85	0.58
3:D:961:TRP:CE2	3:D:995:ILE:HG21	2.40	0.56
3:D:1101:ARG:NH2	3:D:1218:THR:OG1	2.39	0.56
3:A:1143:ARG:HH11	3:A:1143:ARG:HG3	1.71	0.56
2:F:502:GLU:HG2	2:F:522:LYS:HB2	1.89	0.55
3:D:1161:PRO:HG2	3:D:1178:SER:HB3	1.88	0.55
3:D:1135:SER:HG	3:D:1137:THR:HG1	1.52	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:22:CYS:HB3	1:B:79:LEU:HD23	1.90	0.54
3:A:1116:LEU:O	3:A:1116:LEU:HG	2.08	0.54
3:D:908:TYR:OH	3:D:913:LYS:O	2.25	0.54
2:C:537:GLU:HA	2:C:557:TYR:O	2.08	0.53
2:C:563:GLU:OE2	3:D:1173:LYS:HE3	2.09	0.52
3:D:1038:TYR:CE2	3:D:1040:ARG:HG2	2.45	0.52
3:D:999:ARG:NH2	3:D:1021:GLY:O	2.38	0.52
2:F:517:ILE:HG21	3:D:1179:SER:HB2	1.91	0.52
2:F:557:TYR:CZ	3:D:1100:ARG:HD3	2.45	0.52
2:F:561:LEU:HA	2:F:565:LYS:HD2	1.92	0.52
3:A:1002:ASP:HA	3:A:1016:SER:HA	1.91	0.52
2:F:537:GLU:HA	2:F:557:TYR:O	2.11	0.51
2:C:582:GLY:HA3	3:D:1208:ASN:HD21	1.76	0.51
3:D:1122:TYR:CE1	3:D:1245:GLU:HA	2.45	0.51
3:D:855:MET:HE1	3:D:898:VAL:HG11	1.92	0.51
2:C:502:GLU:HG3	2:C:522:LYS:HB2	1.93	0.50
2:F:507:THR:HG23	2:F:527:LYS:HB3	1.93	0.50
3:D:1161:PRO:HB3	3:D:1183:ARG:NH1	2.27	0.50
2:C:533:GLU:O	3:A:1158:HIS:HE1	1.94	0.49
2:C:493:ALA:HA	2:C:512:ASP:O	2.12	0.49
3:A:855:MET:HE1	3:A:898:VAL:HG11	1.95	0.49
3:A:937:TYR:OH	3:A:1040:ARG:NH1	2.46	0.49
3:D:1166:THR:HA	3:D:1173:LYS:HD2	1.95	0.49
1:E:20:LEU:HD23	1:E:81:LEU:HD23	1.95	0.48
3:D:1071:ILE:HD13	3:D:1141:LEU:HD13	1.96	0.48
1:E:20:LEU:HD21	1:E:83:MET:SD	2.53	0.48
1:B:54:TRP:CH2	1:B:101:ARG:HB3	2.49	0.47
3:A:961:TRP:CE2	3:A:995:ILE:HG21	2.49	0.47
3:A:1113:SER:HB2	3:A:1120:ARG:HD2	1.96	0.47
3:A:913:LYS:HA	3:A:913:LYS:HD2	1.71	0.47
3:A:962:THR:HG23	3:A:972:LYS:HG2	1.95	0.47
2:C:581:GLU:OE2	2:C:581:GLU:HA	2.13	0.47
1:E:83:MET:HB3	1:E:86:LEU:HD21	1.97	0.47
1:B:4:LEU:HB3	1:B:22:CYS:SG	2.55	0.46
3:A:966:ASN:HD22	3:A:1022:ASN:HD22	1.63	0.46
3:A:908:TYR:CE1	3:A:913:LYS:HB3	2.51	0.46
2:C:507:THR:HG23	2:C:527:LYS:HB3	1.98	0.46
1:B:67:ARG:HB3	1:B:84:SER:O	2.15	0.45
1:B:6:GLU:CD	1:B:122:GLY:H	2.24	0.45
3:A:1106:LEU:HB2	3:A:1219:VAL:HB	1.99	0.45
1:E:36:TRP:HD1	1:E:70:ILE:HD12	1.80	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:6:GLU:N	1:E:6:GLU:OE1	2.50	0.45
3:A:938:THR:HA	3:A:953:SER:HA	1.97	0.45
3:A:1081:LEU:HA	3:A:1140:ASN:O	2.17	0.45
2:C:537:GLU:HG3	2:C:557:TYR:HD2	1.82	0.44
1:B:11:LEU:HD11	1:B:128:SER:HB2	1.98	0.44
2:C:513:ASN:HA	2:C:533:GLU:O	2.17	0.44
3:A:999:ARG:NH2	3:A:1021:GLY:O	2.48	0.44
3:D:1165:ASP:HB2	3:D:1176:LYS:HG3	1.98	0.44
3:D:857:TYR:CZ	3:D:885:LYS:HD3	2.53	0.43
2:F:513:ASN:HA	2:F:533:GLU:O	2.18	0.43
3:A:944:ARG:NH2	3:A:966:ASN:OD1	2.51	0.43
1:E:48:VAL:HG13	1:E:64:VAL:HG21	2.01	0.43
3:D:1068:ASN:O	3:D:1073:LYS:NZ	2.50	0.43
3:A:1070:ASN:ND2	3:A:1143:ARG:HD3	2.33	0.43
1:B:59:TYR:CD1	1:B:59:TYR:N	2.86	0.43
1:B:24:VAL:HG11	1:B:29:PHE:HE1	1.84	0.43
3:A:944:ARG:HG2	3:A:1026:SER:HA	2.00	0.43
1:B:51:ILE:HG13	1:B:58:THR:HG22	2.01	0.42
3:A:966:ASN:ND2	3:A:1022:ASN:HD22	2.16	0.42
3:A:943:MET:HE2	3:A:951:LYS:HD3	2.02	0.42
3:A:994:THR:HB	3:A:1006:TYR:HB2	2.01	0.42
3:A:1089:LEU:HB2	3:A:1243:ILE:HD11	2.02	0.42
3:A:1225:TYR:CG	3:A:1238:CYS:HB3	2.55	0.42
2:C:524:VAL:O	2:C:544:THR:HA	2.20	0.42
3:D:1038:TYR:HE2	3:D:1040:ARG:NH1	2.17	0.42
3:A:893:ASP:OD1	3:A:893:ASP:N	2.49	0.42
3:A:897:GLU:OE1	3:A:1032:LYS:HE2	2.19	0.42
2:F:489:ARG:N	2:F:508:GLY:O	2.53	0.42
3:A:1145:ASN:ND2	3:A:1191:ASN:HD22	2.18	0.41
2:C:517:ILE:HG21	3:A:1179:SER:HB2	2.03	0.41
3:A:938:THR:HG21	3:A:951:LYS:HD2	2.02	0.41
3:D:911:LYS:HG3	3:D:1022:ASN:HD22	1.85	0.41
1:B:4:LEU:HB3	1:B:96:CYS:SG	2.61	0.41
1:B:20:LEU:CD1	1:B:20:LEU:N	2.83	0.41
3:A:989:LYS:NZ	8:A:1411:HOH:O	2.52	0.41
3:A:1150:ILE:HG22	3:A:1162:LEU:HD12	2.01	0.41
1:E:99:GLU:OE1	3:D:1215:LYS:NZ	2.48	0.41
2:F:517:ILE:HA	2:F:537:GLU:O	2.21	0.41
3:A:853:LEU:HB3	3:A:1049:ILE:HB	2.01	0.41
2:C:574:SER:O	3:D:1205:ASN:HB2	2.21	0.41
3:A:965:ASP:HB3	3:A:1020:LEU:HD23	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:847:ILE:C	3:D:849:SER:H	2.29	0.41
3:A:925:ASN:HA	3:A:931:VAL:HG11	2.03	0.41
1:B:40:ALA:CB	1:B:43:LYS:HD3	2.48	0.41
3:D:1074:ASP:OD1	3:D:1074:ASP:C	2.64	0.41
3:A:965:ASP:HA	3:A:1023:ILE:HG13	2.03	0.40
3:A:1071:ILE:HD13	3:A:1141:LEU:HD13	2.03	0.40
3:D:975:PHE:CD2	3:D:1007:ILE:HG13	2.56	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	B	126/129 (98%)	119 (94%)	7 (6%)	0	100	100
1	E	127/129 (98%)	122 (96%)	5 (4%)	0	100	100
2	C	93/105 (89%)	92 (99%)	1 (1%)	0	100	100
2	F	92/105 (88%)	90 (98%)	2 (2%)	0	100	100
3	A	404/407 (99%)	375 (93%)	29 (7%)	0	100	100
3	D	404/407 (99%)	387 (96%)	17 (4%)	0	100	100
All	All	1246/1282 (97%)	1185 (95%)	61 (5%)	0	100	100

There are no Ramachandran outliers to report.

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	B	99/111 (89%)	94 (95%)	5 (5%)	21	45
1	E	104/111 (94%)	93 (89%)	11 (11%)	6	14
2	C	89/97 (92%)	88 (99%)	1 (1%)	65	84
2	F	88/97 (91%)	87 (99%)	1 (1%)	65	84
3	A	371/378 (98%)	363 (98%)	8 (2%)	45	72
3	D	373/378 (99%)	366 (98%)	7 (2%)	50	75
All	All	1124/1172 (96%)	1091 (97%)	33 (3%)	37	65

All (33) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	12	VAL
1	B	17	SER
1	B	18	LEU
1	B	31	ASP
1	B	71	SER
2	C	507	THR
1	E	2	LEU
1	E	11	LEU
1	E	20	LEU
1	E	21	SER
1	E	25	SER
1	E	28	THR
1	E	30	ASP
1	E	64	VAL
1	E	72	THR
1	E	115	ASP
1	E	126	THR
2	F	581	GLU
3	D	859	ASN
3	D	863	VAL
3	D	1012	ILE
3	D	1040	ARG
3	D	1145	ASN
3	D	1172	GLU
3	D	1207	ASN
3	A	894	LYS
3	A	904	ASP
3	A	918	SER

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Mol	Chain	Res	Type
3	A	928	ASN
3	A	1020	LEU
3	A	1037	SER
3	A	1137	THR
3	A	1233	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	57	ASN
1	B	74	ASN
1	B	124	GLN
2	C	568	ASN
1	E	57	ASN
2	F	543	ASN
3	D	859	ASN
3	D	976	ASN
3	D	1022	ASN
3	D	1024	HIS
3	D	1070	ASN
3	D	1195	ASN
3	D	1207	ASN
3	A	859	ASN
3	A	875	ASN
3	A	935	ASN
3	A	941	ASN
3	A	964	GLN
3	A	981	ASN
3	A	1022	ASN
3	A	1145	ASN
3	A	1158	HIS
3	A	1207	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

4 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	NAG	G	1	4,2	14,14,15	0.38	0	17,19,21	1.11	1 (5%)
4	NAG	G	2	4	14,14,15	0.38	0	17,19,21	1.00	1 (5%)
4	NAG	H	1	4,2	14,14,15	0.53	0	17,19,21	0.84	1 (5%)
4	NAG	H	2	4	14,14,15	0.60	0	17,19,21	1.12	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
4	NAG	G	1	4,2	-	4/6/23/26	0/1/1/1
4	NAG	G	2	4	-	2/6/23/26	0/1/1/1
4	NAG	H	1	4,2	-	1/6/23/26	0/1/1/1
4	NAG	H	2	4	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	G	2	NAG	C1-O5-C5	3.67	117.11	112.19
4	G	1	NAG	O5-C5-C6	2.27	112.08	107.66
4	H	2	NAG	C6-C5-C4	-2.18	107.66	113.02
4	H	1	NAG	C2-N2-C7	-2.09	120.10	122.90

There are no chirality outliers.

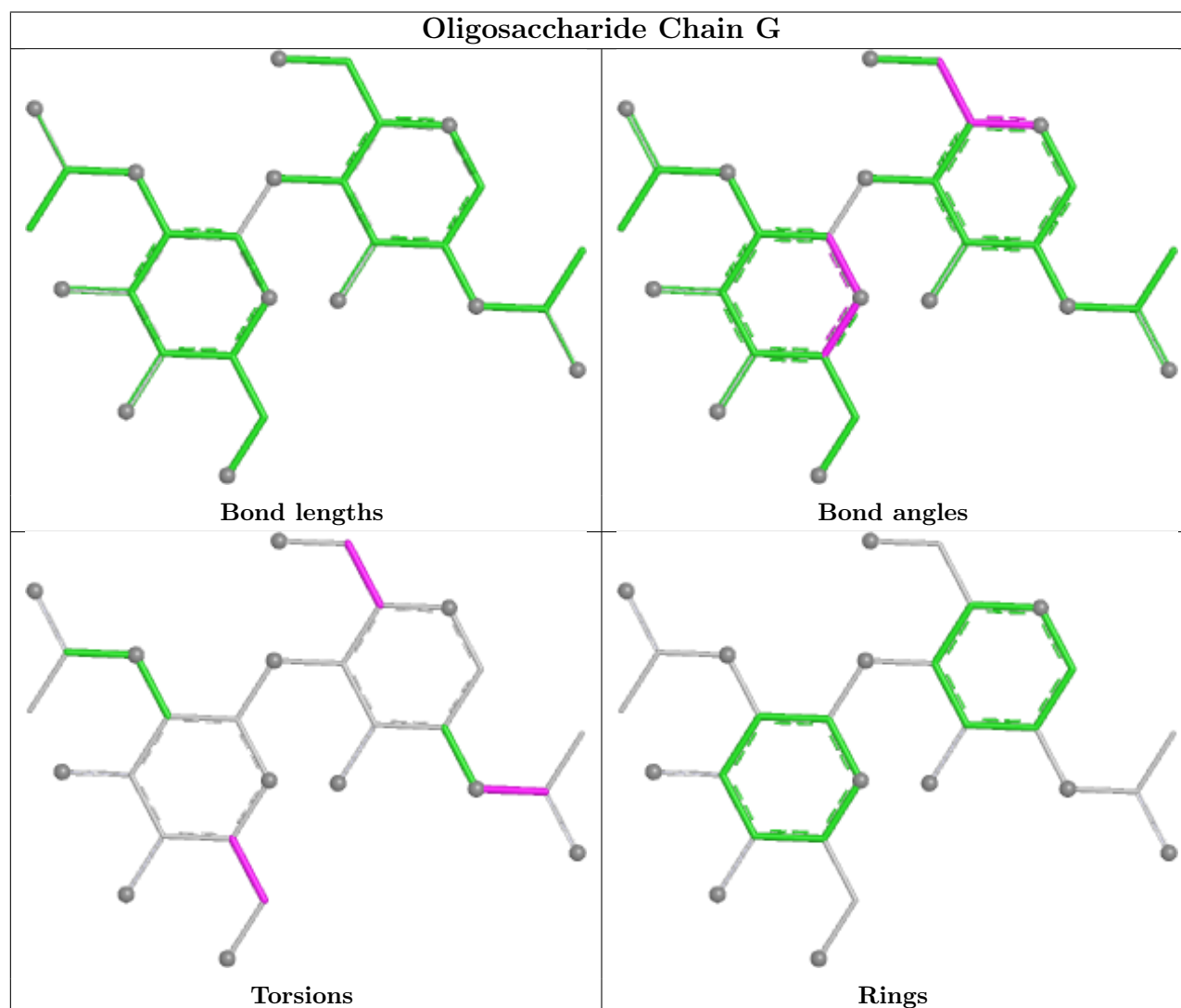
All (7) torsion outliers are listed below:

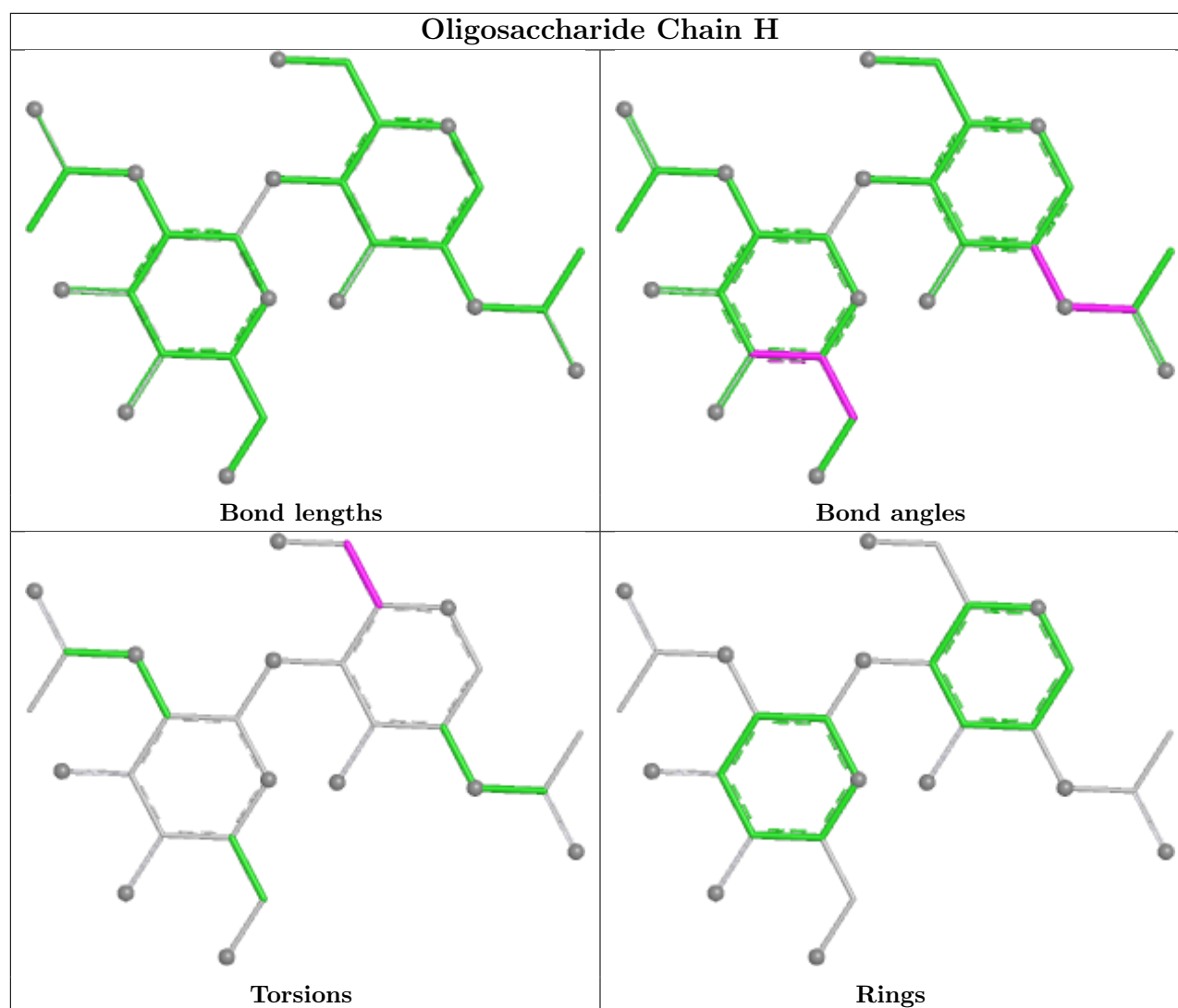
Mol	Chain	Res	Type	Atoms
4	G	1	NAG	O5-C5-C6-O6
4	G	2	NAG	O5-C5-C6-O6
4	G	1	NAG	C4-C5-C6-O6
4	G	2	NAG	C4-C5-C6-O6
4	G	1	NAG	C8-C7-N2-C2
4	G	1	NAG	O7-C7-N2-C2
4	H	1	NAG	C4-C5-C6-O6

There are no ring outliers.

No monomer is involved in short contacts.

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





5.6 Ligand geometry [i](#)

14 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	$\# Z > 2$
5	NAG	F	604	2	14,14,15	0.40	0	17,19,21	0.70	0
5	NAG	F	602	2	14,14,15	0.45	0	17,19,21	0.72	0
6	SO4	F	605	-	4,4,4	0.33	0	6,6,6	0.12	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	SO4	A	1303	-	4,4,4	0.30	0	6,6,6	0.06	0
7	PEG	A	1301	-	6,6,6	0.50	0	5,5,5	0.17	0
5	NAG	C	601	2	14,14,15	0.54	0	17,19,21	0.75	1 (5%)
6	SO4	D	1302	-	4,4,4	0.31	0	6,6,6	0.08	0
5	NAG	F	601	2	14,14,15	0.47	0	17,19,21	0.87	0
6	SO4	D	1301	-	4,4,4	0.30	0	6,6,6	0.09	0
6	SO4	A	1302	-	4,4,4	0.30	0	6,6,6	0.08	0
6	SO4	C	604	-	4,4,4	0.31	0	6,6,6	0.06	0
5	NAG	C	602	2	14,14,15	0.32	0	17,19,21	0.59	0
6	SO4	C	603	-	4,4,4	0.31	0	6,6,6	0.07	0
5	NAG	F	603	2	14,14,15	0.51	0	17,19,21	1.04	1 (5%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	F	604	2	-	2/6/23/26	0/1/1/1
5	NAG	F	602	2	-	2/6/23/26	0/1/1/1
7	PEG	A	1301	-	-	1/4/4/4	-
5	NAG	C	601	2	-	0/6/23/26	0/1/1/1
5	NAG	F	601	2	-	4/6/23/26	0/1/1/1
5	NAG	C	602	2	-	0/6/23/26	0/1/1/1
5	NAG	F	603	2	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	F	603	NAG	C1-O5-C5	3.40	116.74	112.19
5	C	601	NAG	C1-O5-C5	2.34	115.33	112.19

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	F	604	NAG	C4-C5-C6-O6
5	F	601	NAG	C4-C5-C6-O6
5	F	604	NAG	O5-C5-C6-O6

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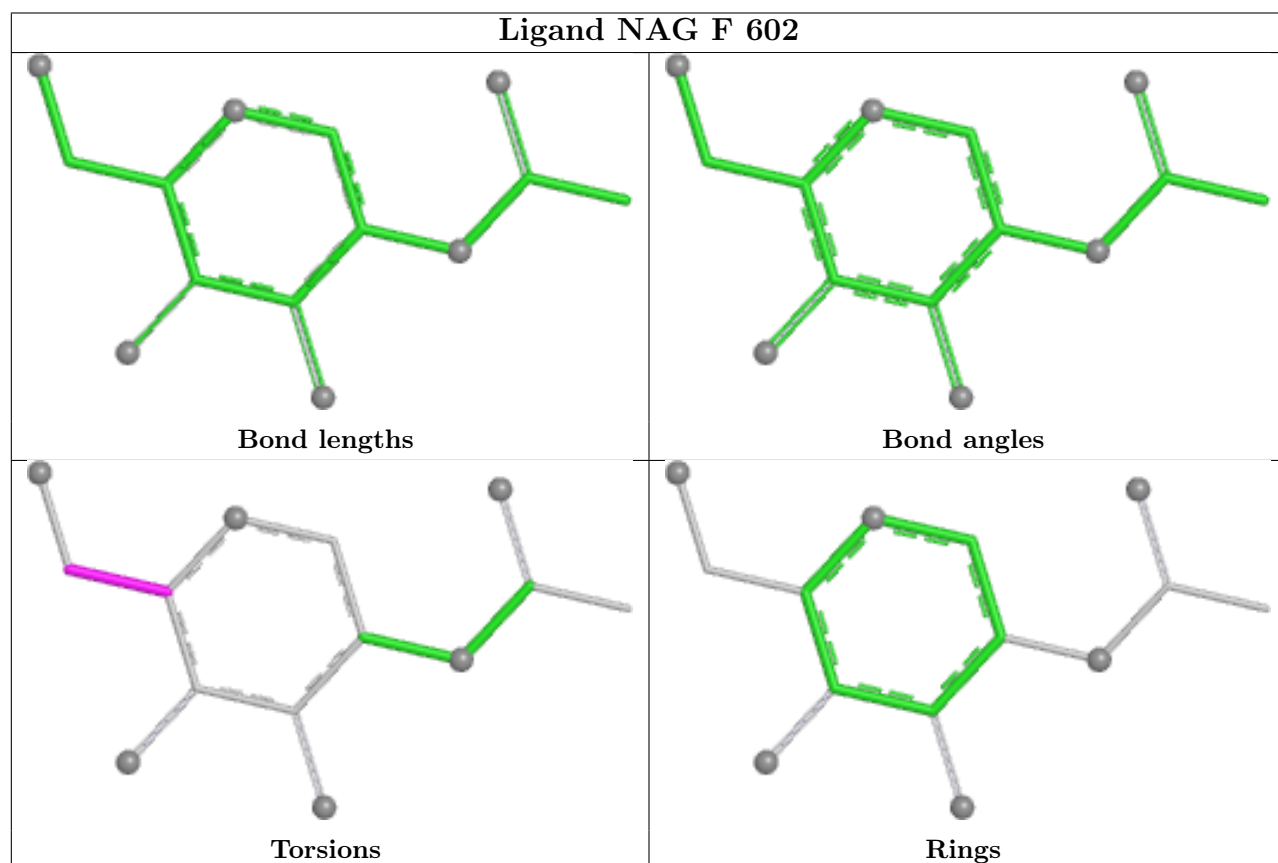
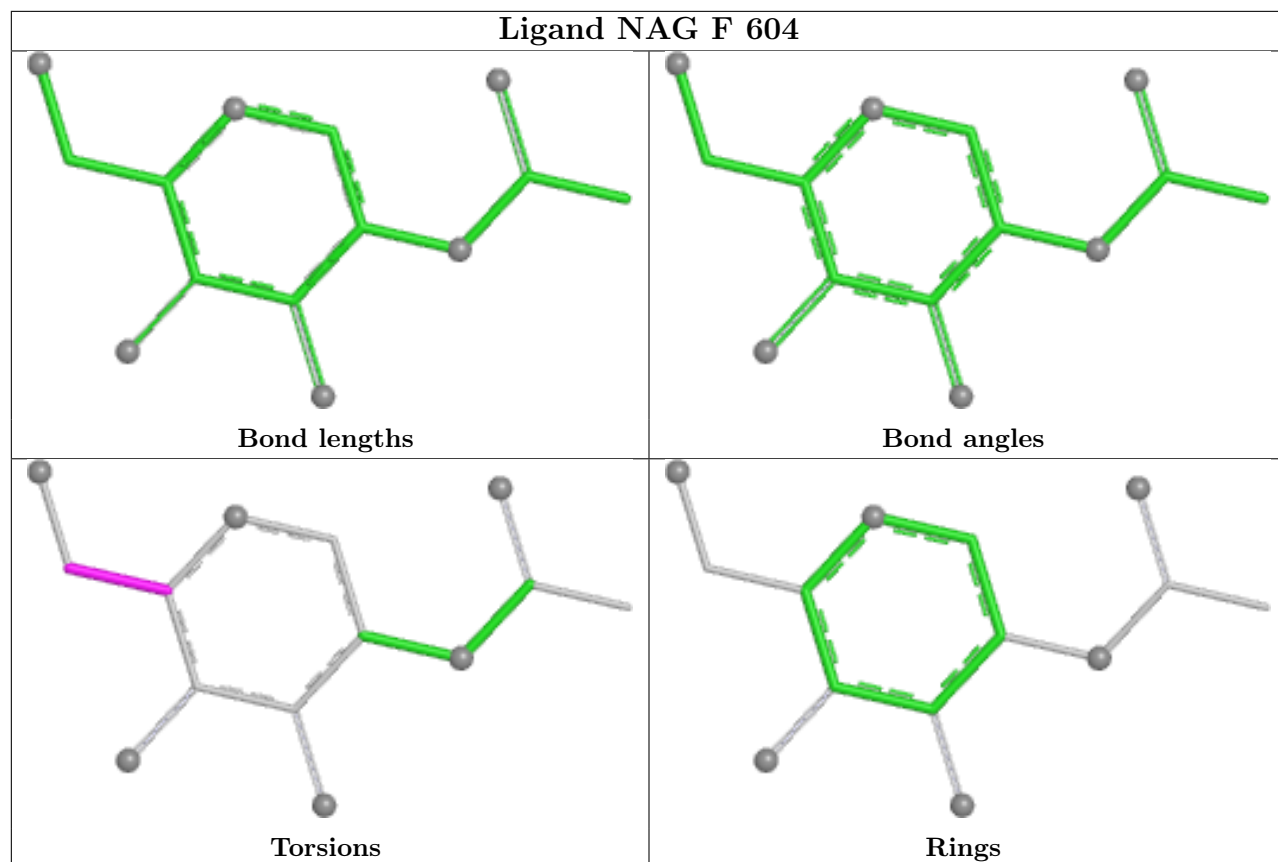
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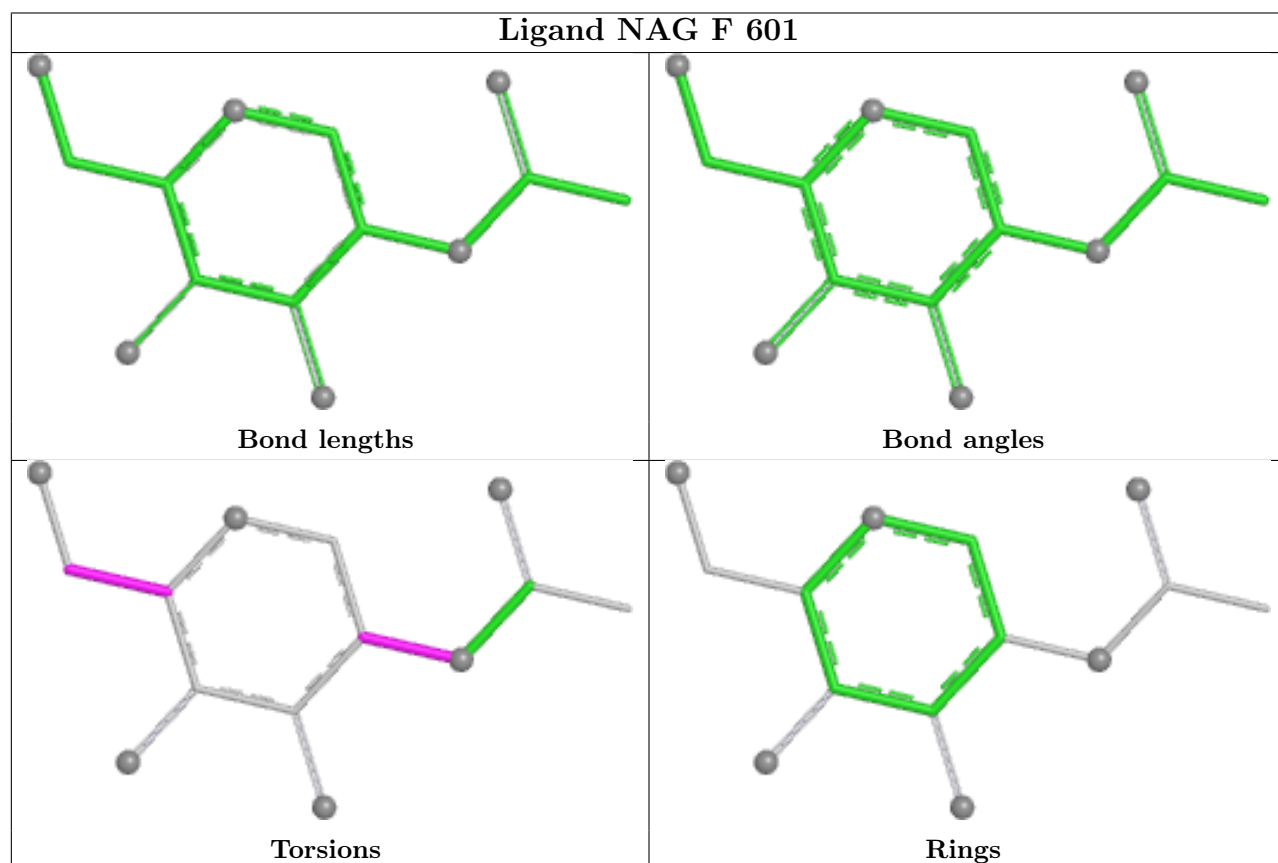
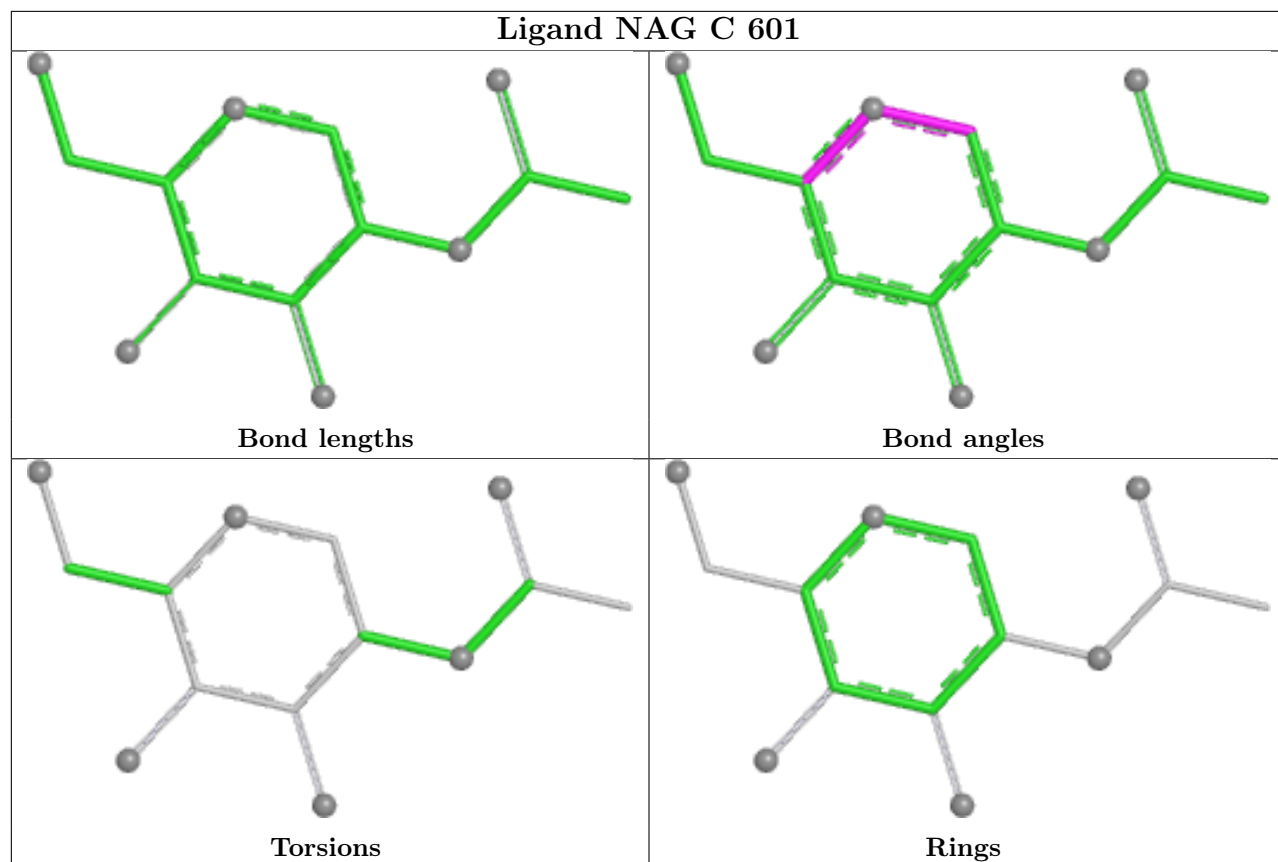
Mol	Chain	Res	Type	Atoms
5	F	601	NAG	O5-C5-C6-O6
7	A	1301	PEG	O1-C1-C2-O2
5	F	601	NAG	C3-C2-N2-C7
5	F	601	NAG	C1-C2-N2-C7
5	F	602	NAG	C4-C5-C6-O6
5	F	602	NAG	O5-C5-C6-O6

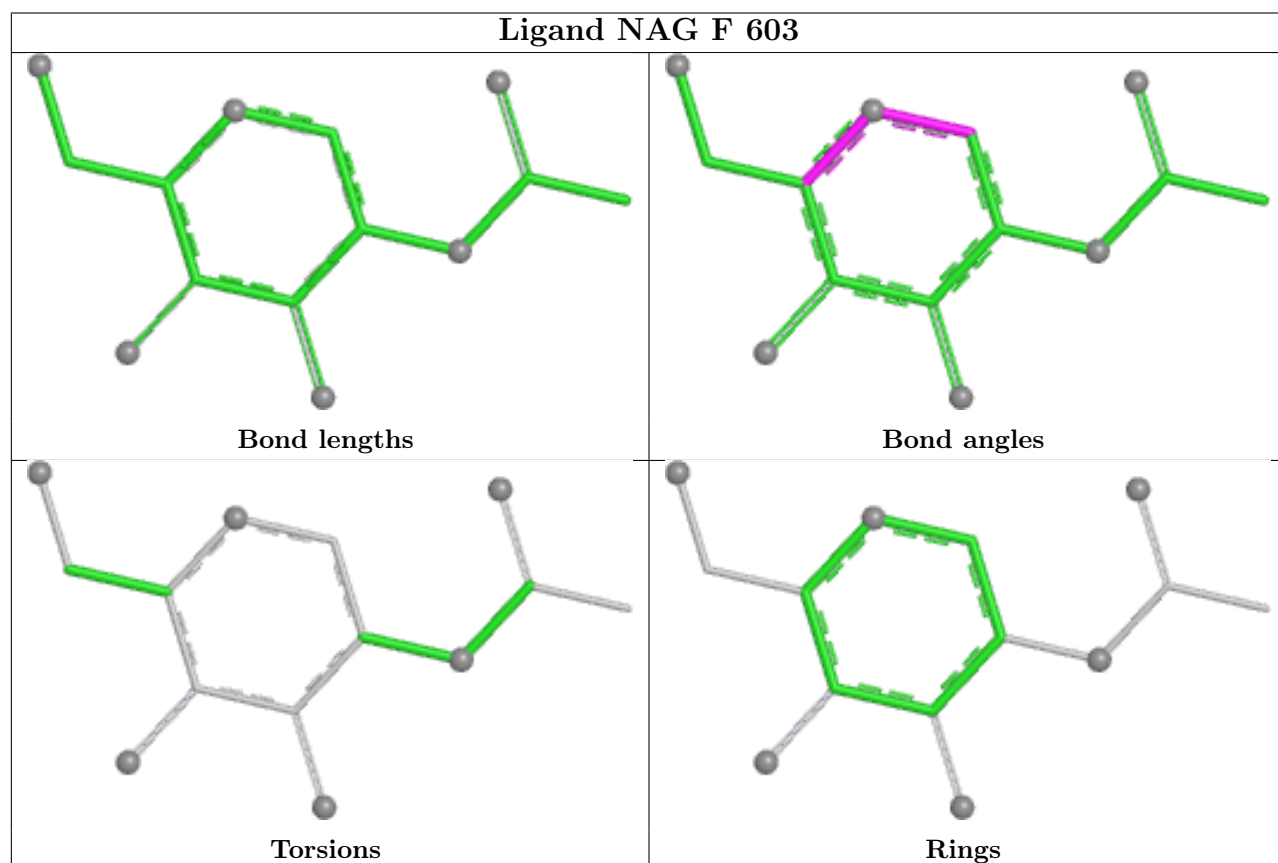
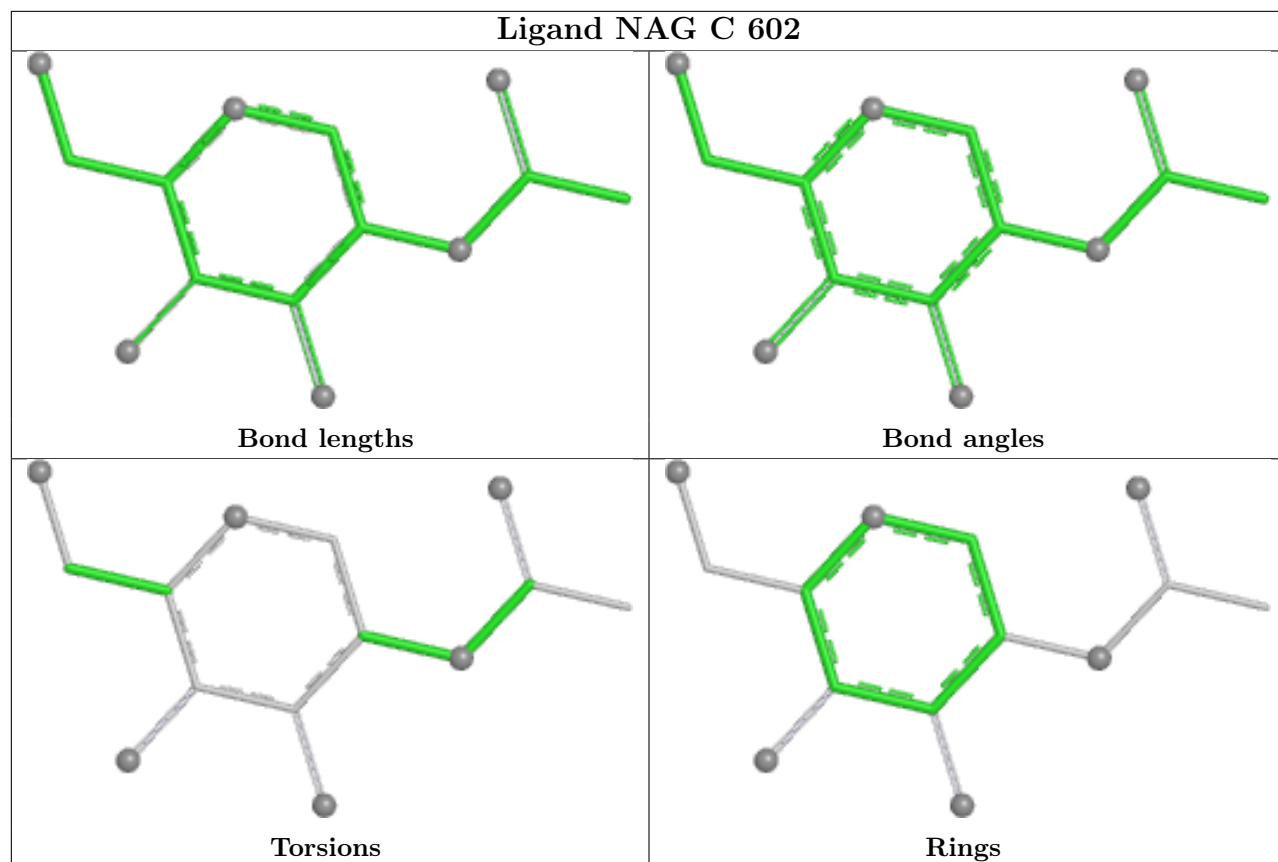
There are no ring outliers.

No monomer is involved in short contacts.

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

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	B	128/129 (99%)	1.50	38 (29%) 1 1	49, 79, 96, 105	0
1	E	129/129 (100%)	1.41	39 (30%) 1 1	42, 79, 105, 129	0
2	C	95/105 (90%)	0.23	2 (2%) 63 58	40, 52, 73, 93	0
2	F	94/105 (89%)	0.57	4 (4%) 40 34	45, 63, 83, 91	0
3	A	406/407 (99%)	0.33	18 (4%) 39 33	37, 52, 78, 94	0
3	D	406/407 (99%)	0.02	7 (1%) 69 64	34, 45, 62, 102	0
All	All	1258/1282 (98%)	0.47	108 (8%) 16 12	34, 53, 91, 129	0

All (108) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	A	847	ILE	5.6
3	D	847	ILE	5.3
3	A	1138	ASN	5.1
1	B	62	ASP	4.9
1	E	75	ALA	4.4
3	A	1019	ASN	4.1
1	B	51	ILE	4.0
1	B	59	TYR	3.9
1	E	2	LEU	3.7
3	A	1136	SER	3.4
1	B	86	LEU	3.4
1	E	40	ALA	3.4
1	E	128	SER	3.4
1	E	41	PRO	3.3
1	E	88	PRO	3.3
1	B	66	GLY	3.2
1	B	49	SER	3.2
1	B	42	GLY	3.1
1	E	12	VAL	3.1

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Mol	Chain	Res	Type	RSRZ
1	E	65	LYS	3.0
1	B	69	THR	3.0
1	E	129	SER	3.0
1	B	129	SER	3.0
1	B	72	THR	2.9
1	E	14	PRO	2.9
1	E	127	VAL	2.9
2	F	489	ARG	2.9
1	B	36	TRP	2.9
3	D	1137	THR	2.8
1	E	76	LYS	2.8
1	B	2	LEU	2.8
1	E	18	LEU	2.8
3	A	1230	ARG	2.8
1	E	19	ARG	2.7
3	D	860	ASP	2.7
1	B	48	VAL	2.7
2	F	492	TYR	2.7
1	E	69	THR	2.7
1	B	53	SER	2.7
1	E	80	TYR	2.7
1	B	75	ALA	2.6
1	E	1	GLN	2.6
2	F	505	ILE	2.6
1	E	20	LEU	2.6
3	A	1116	LEU	2.6
1	B	12	VAL	2.6
1	B	107	ILE	2.6
1	E	11	LEU	2.6
1	E	86	LEU	2.6
1	E	8	GLY	2.5
1	E	82	GLN	2.5
1	E	48	VAL	2.5
1	E	64	VAL	2.5
1	B	63	SER	2.5
1	B	11	LEU	2.5
3	D	848	LYS	2.5
2	C	581	GLU	2.5
3	D	849	SER	2.5
1	E	66	GLY	2.4
1	E	21	SER	2.4
1	E	29	PHE	2.4

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Mol	Chain	Res	Type	RSRZ
1	E	43	LYS	2.4
1	B	47	TRP	2.4
3	A	969	ILE	2.4
1	E	30	ASP	2.4
1	E	68	PHE	2.4
3	A	1134	ASN	2.4
1	B	109	ALA	2.4
1	B	10	GLY	2.3
1	B	60	TYR	2.3
1	B	61	GLU	2.3
1	E	91	THR	2.3
1	B	128	SER	2.3
2	C	582	GLY	2.3
2	F	582	GLY	2.3
1	B	56	ILE	2.3
3	A	1139	ASP	2.3
3	A	1145	ASN	2.3
1	B	28	THR	2.3
1	E	53	SER	2.3
1	B	27	PHE	2.3
1	B	41	PRO	2.3
3	A	964	GLN	2.2
1	B	26	GLY	2.2
1	B	70	ILE	2.2
1	E	125	VAL	2.2
3	D	1068	ASN	2.2
3	A	859	ASN	2.2
3	A	1135	SER	2.2
1	B	5	VAL	2.2
1	B	123	THR	2.2
3	A	910	ASN	2.1
3	A	1229	MET	2.1
3	A	1168	THR	2.1
1	B	54	TRP	2.1
1	E	54	TRP	2.1
1	B	7	THR	2.1
1	B	68	PHE	2.1
1	E	81	LEU	2.1
1	E	67	ARG	2.1
1	E	62	ASP	2.1
1	E	72	THR	2.1
3	D	1115	ILE	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	110	HIS	2.1
1	E	126	THR	2.0
1	B	90	ASP	2.0
3	A	912	TYR	2.0
3	A	905	TYR	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](#)

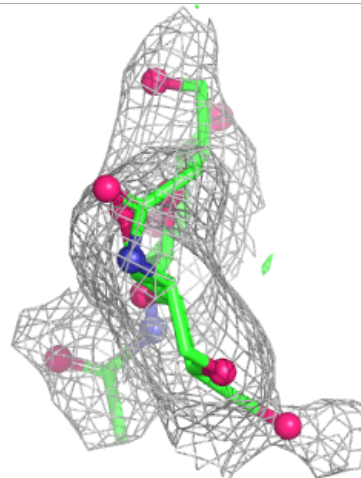
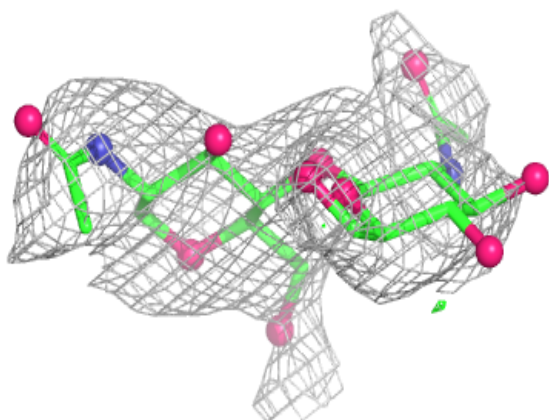
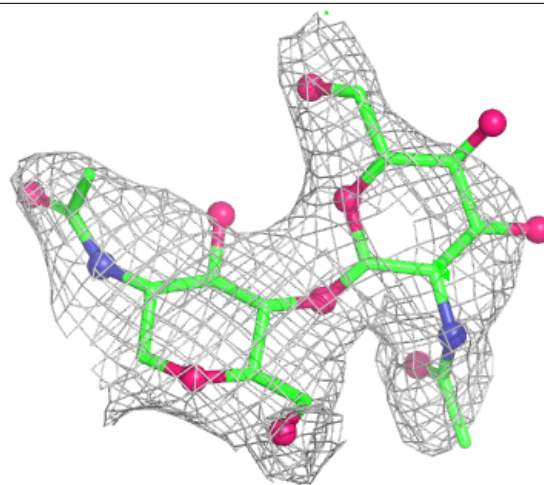
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

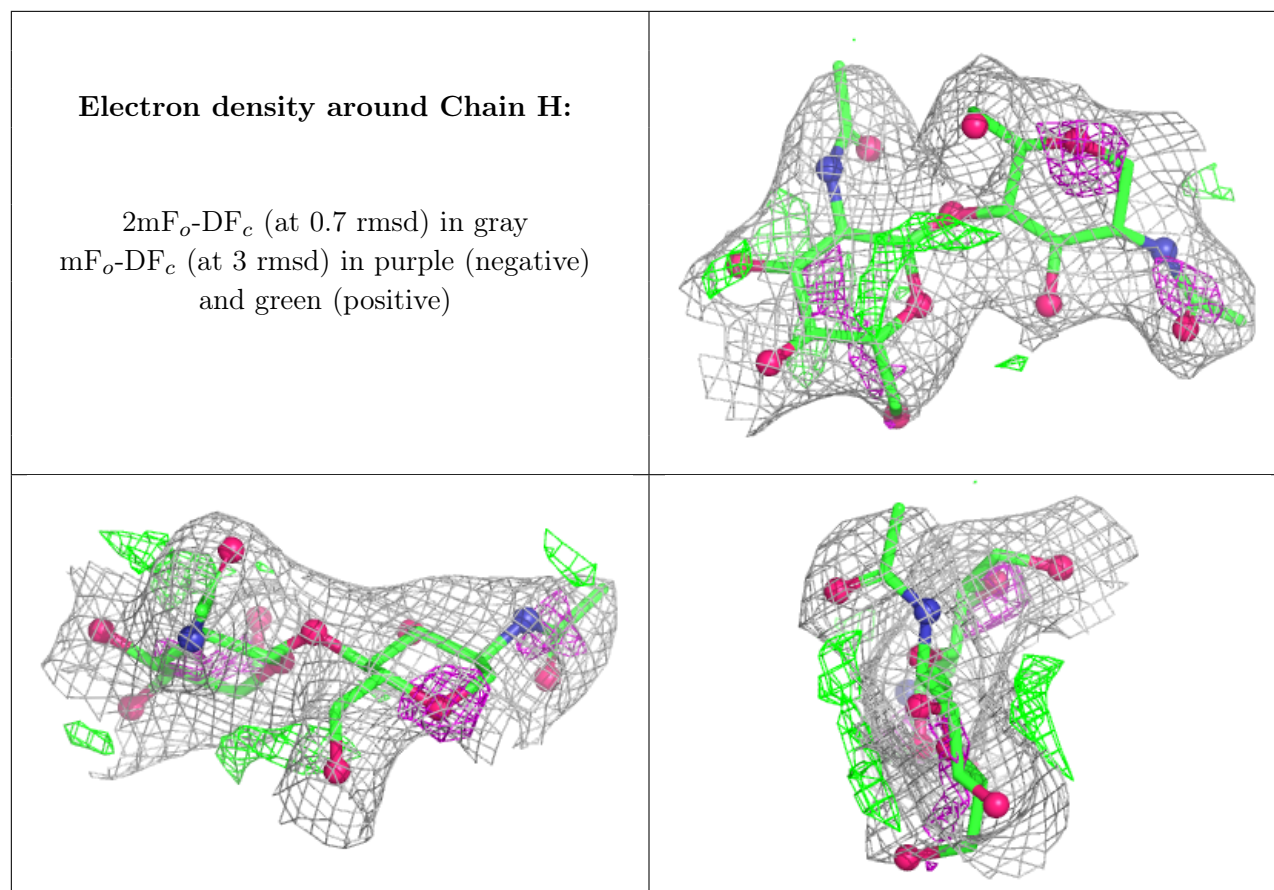
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	NAG	G	2	14/15	0.66	0.15	88,96,98,98	0
4	NAG	H	2	14/15	0.67	0.16	41,45,48,49	0
4	NAG	G	1	14/15	0.73	0.14	80,83,87,92	0
4	NAG	H	1	14/15	0.81	0.12	40,43,45,46	0

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.

Electron density around Chain G:

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





6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	NAG	C	602	14/15	0.55	0.17	92,98,102,102	0
5	NAG	C	601	14/15	0.64	0.17	93,99,101,104	0
5	NAG	F	601	14/15	0.64	0.17	80,90,96,100	0
5	NAG	F	604	14/15	0.68	0.15	89,93,96,97	0
5	NAG	F	603	14/15	0.69	0.15	82,88,91,95	0
5	NAG	F	602	14/15	0.69	0.16	87,92,103,105	0
7	PEG	A	1301	7/7	0.79	0.13	31,33,35,35	0
6	SO4	A	1303	5/5	0.86	0.14	78,79,84,87	0
6	SO4	D	1302	5/5	0.91	0.13	75,81,82,83	0
6	SO4	C	603	5/5	0.91	0.16	67,68,69,73	0
6	SO4	C	604	5/5	0.91	0.14	70,75,79,79	0
6	SO4	A	1302	5/5	0.92	0.13	71,72,76,77	0
6	SO4	D	1301	5/5	0.92	0.11	73,73,74,77	0

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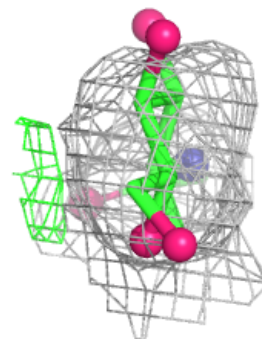
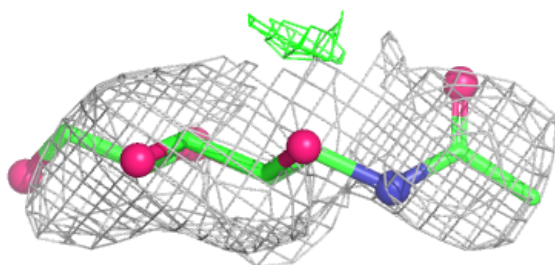
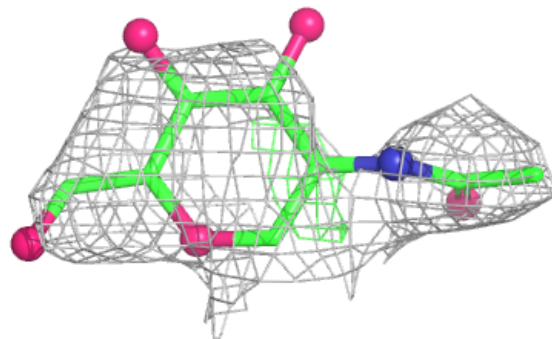
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
6	SO4	F	605	5/5	0.92	0.09	73,77,81,82	0

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

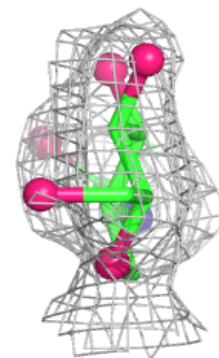
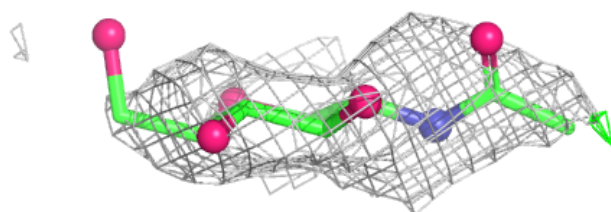
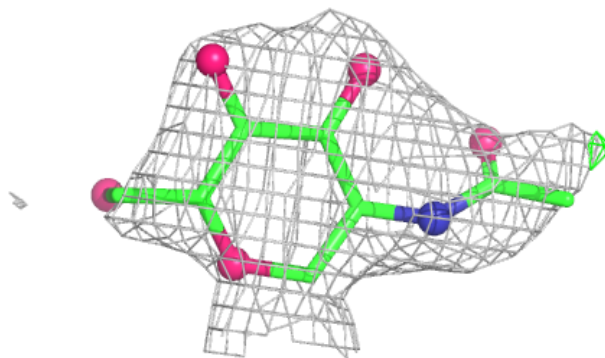
Electron density around NAG C 602:

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

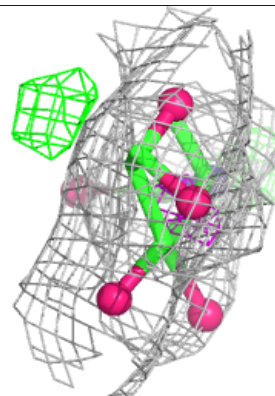
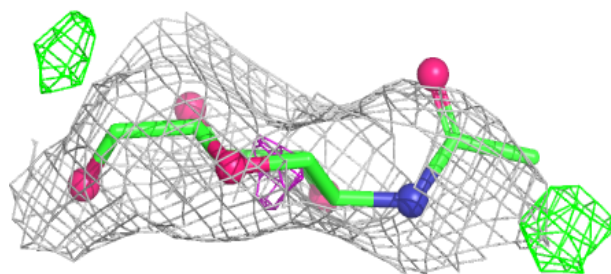
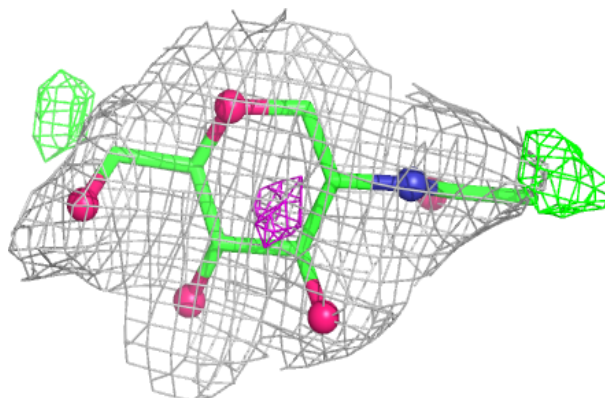


Electron density around NAG C 601:

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

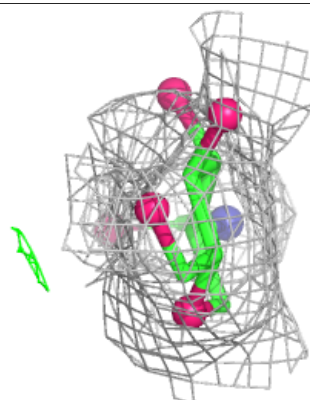
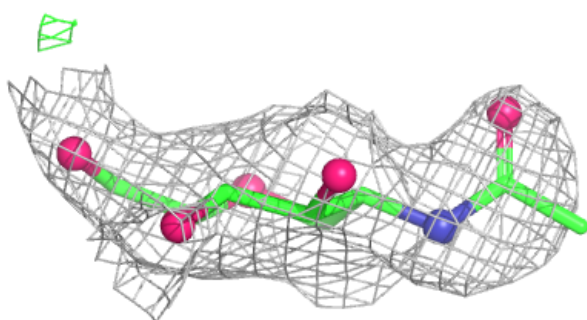
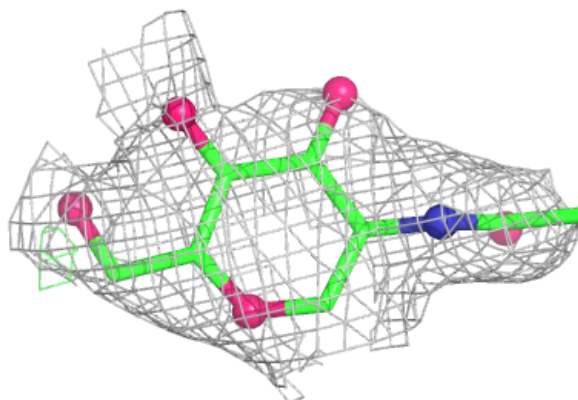
**Electron density around NAG F 601:**

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

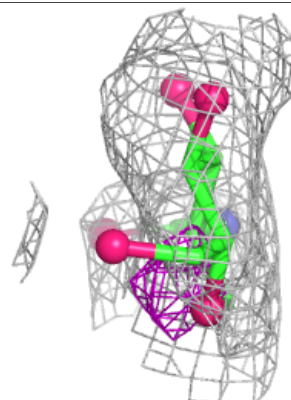
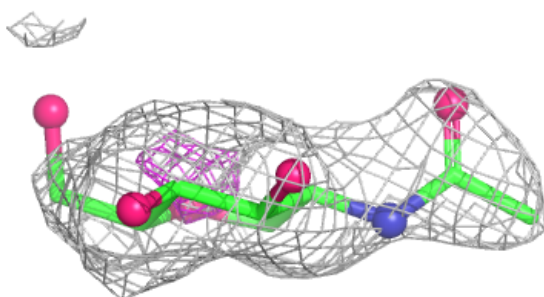
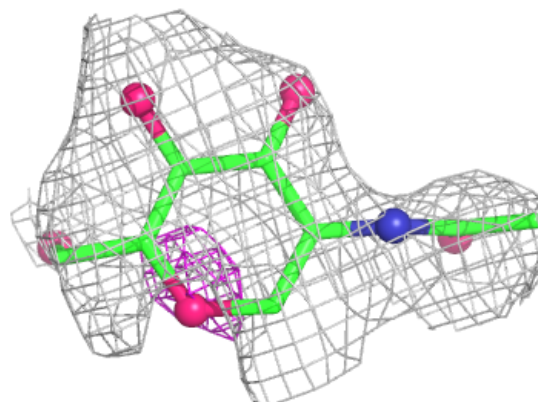


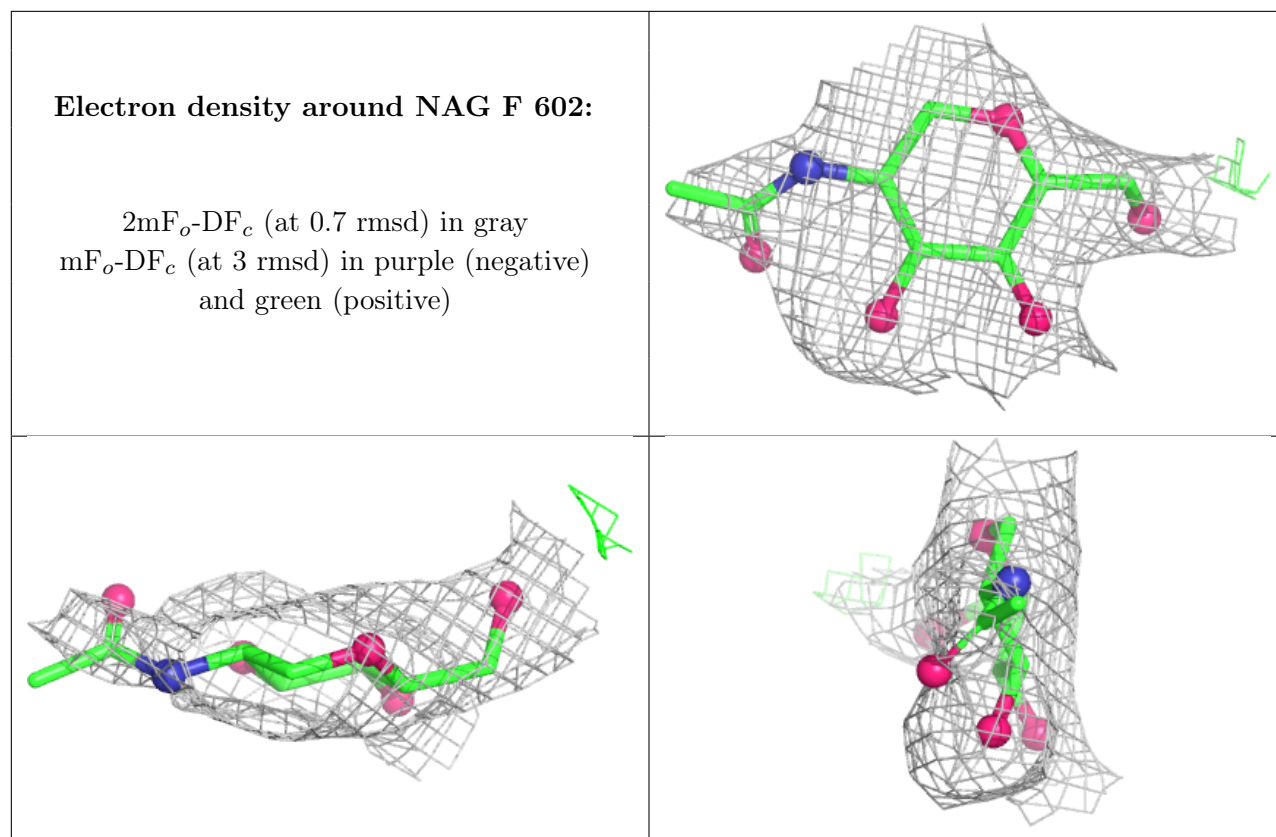
Electron density around NAG F 604:

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

**Electron density around NAG F 603:**

$2mF_o-DF_c$ (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.