Full wwPDB X-ray Structure Validation Report ⓘ

Sep 6, 2023 – 10:16 am BST

PDB ID	:	8OK8
Title	:	Variant Surface Glycoprotein VSG615
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Deposited on	:	2023-03-27
Resolution	:	3.22 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

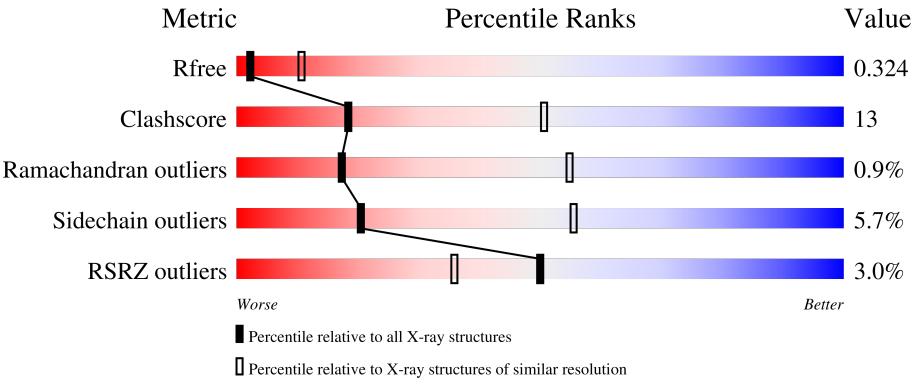
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

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 3.22 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1335 (3.24-3.20)
Clashscore	141614	1460 (3.24-3.20)
Ramachandran outliers	138981	1437 (3.24-3.20)
Sidechain outliers	138945	1436 (3.24-3.20)
RSRZ outliers	127900	1291 (3.24-3.20)

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 <=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	376	5% 54% 21% · 24%
1	C	376	2% 61% 26% · 11%
1	E	376	% 60% 24% · 15%
1	G	376	3% 60% 24% · 14%
1	I	376	2% 59% 23% •• 16%

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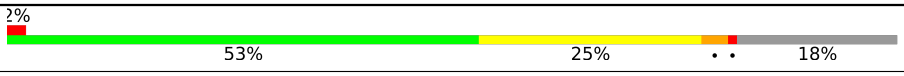
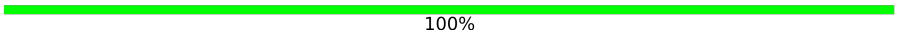
Mol	Chain	Length	Quality of chain
1	K	376	
2	F	2	
2	J	2	

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 14117 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.

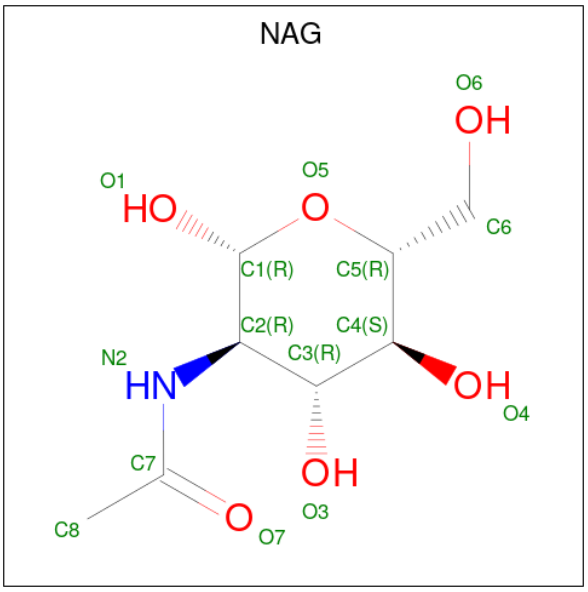
- Molecule 1 is a protein called Variant surface glycoprotein 615.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	286	Total	C	N	O	S	0	0	0
			2123	1302	382	426	13			
1	C	335	Total	C	N	O	S	0	0	0
			2457	1502	438	503	14			
1	E	319	Total	C	N	O	S	0	1	0
			2345	1435	418	478	14			
1	G	325	Total	C	N	O	S	0	0	0
			2379	1452	428	485	14			
1	I	314	Total	C	N	O	S	0	0	0
			2311	1410	417	470	14			
1	K	308	Total	C	N	O	S	0	0	0
			2268	1390	402	462	14			

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

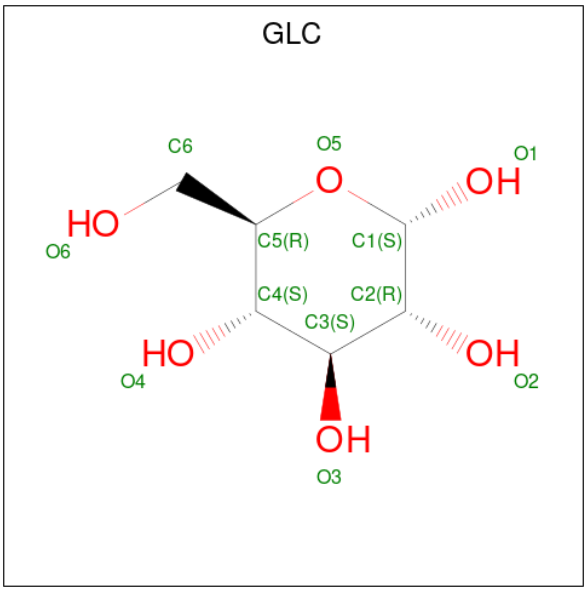
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	J	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	F	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 3 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C N O 14 8 1 5	0	0
3	C	1	Total C N O 14 8 1 5	0	0
3	G	1	Total C N O 14 8 1 5	0	0
3	K	1	Total C N O 14 8 1 5	0	0

- Molecule 4 is alpha-D-glucopyranose (three-letter code: GLC) (formula: $C_6H_{12}O_6$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	C	1	Total C O 11 6 5	0	0
4	C	1	Total C O 11 6 5	0	0
4	E	1	Total C O 11 6 5	0	0
4	E	1	Total C O 11 6 5	0	0
4	G	1	Total C O 11 6 5	0	0
4	G	1	Total C O 11 6 5	0	0
4	I	1	Total C O 11 6 5	0	0
4	I	1	Total C O 11 6 5	0	0
4	K	1	Total C O 11 6 5	0	0
4	K	1	Total C O 11 6 5	0	0

- Molecule 5 is water.

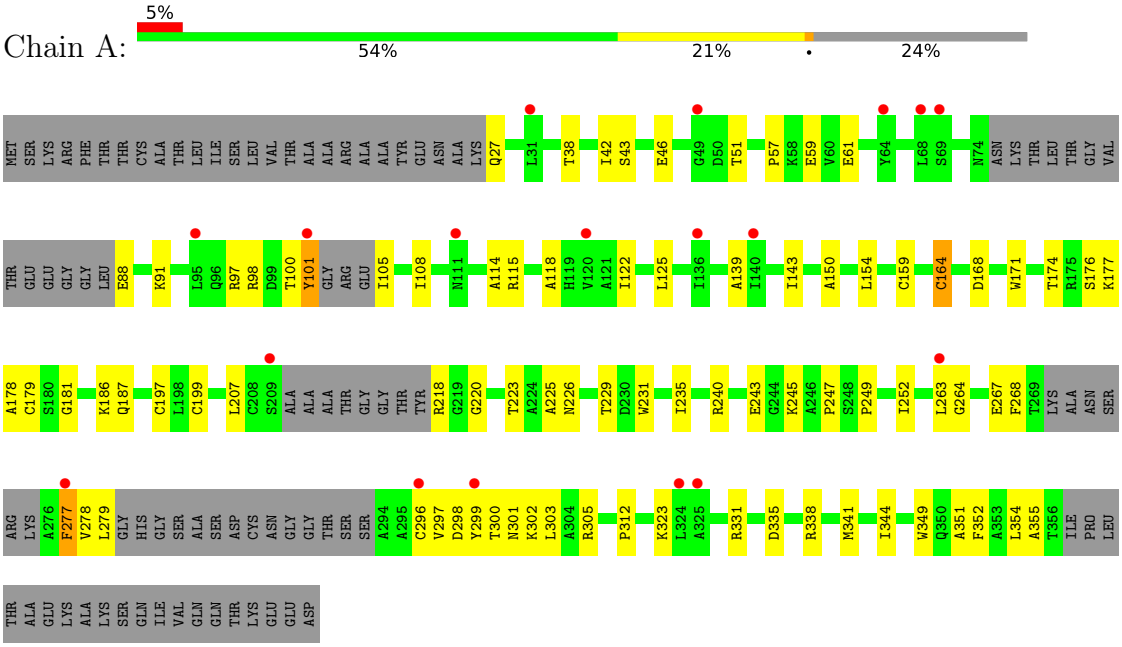
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	C	2	Total O 2 2	0	0
5	E	1	Total O 1 1	0	0
5	G	2	Total O 2 2	0	0
5	I	3	Total O 3 3	0	0
5	K	4	Total O 4 4	0	0

3 Residue-property plots (i)

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

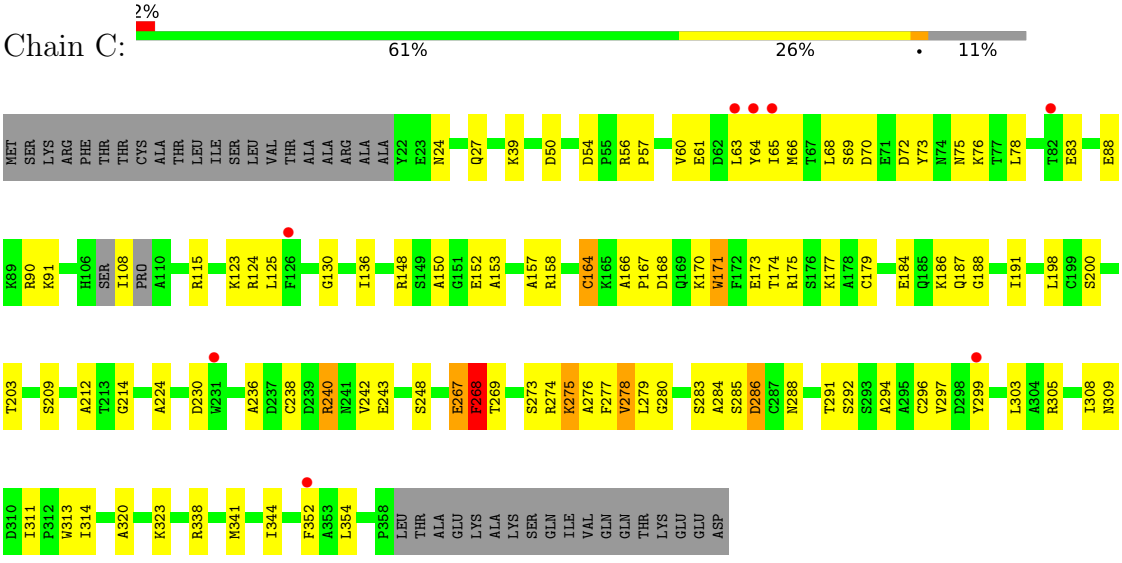
• Molecule 1: Variant surface glycoprotein 615

Chain A:



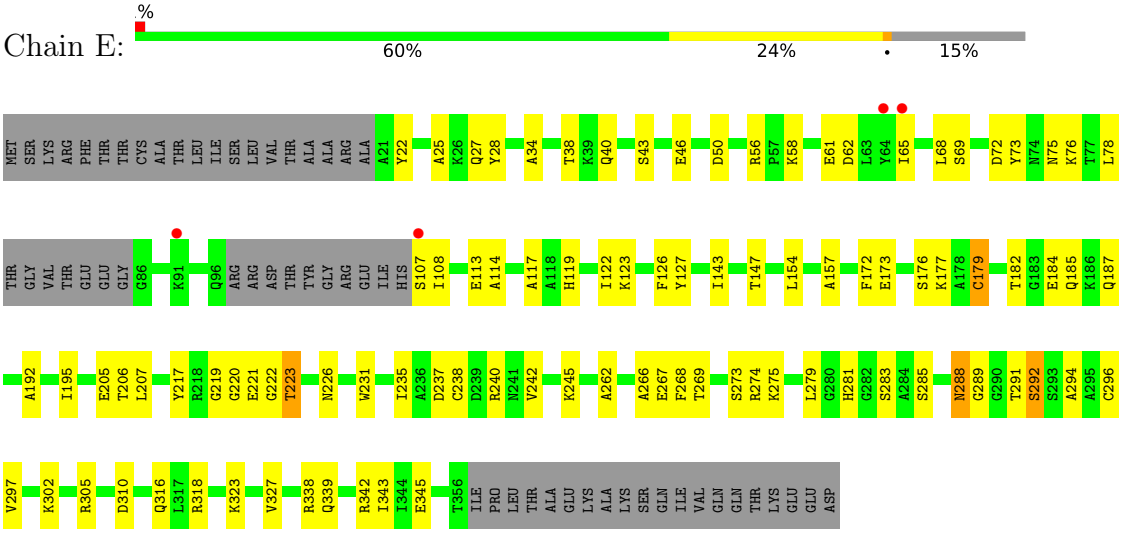
• Molecule 1: Variant surface glycoprotein 615

Chain C:



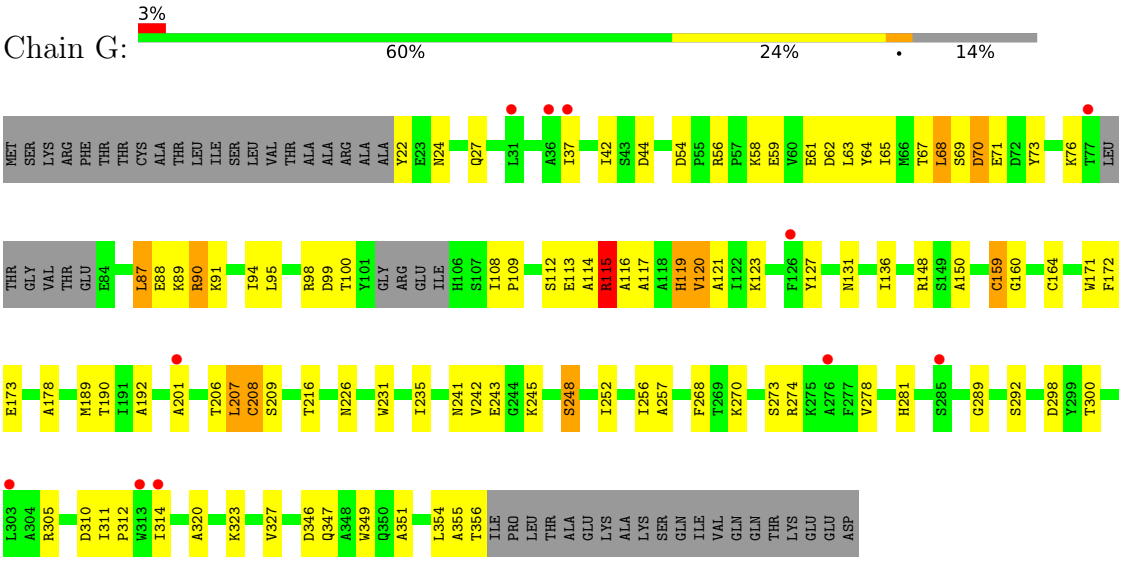
• Molecule 1: Variant surface glycoprotein 615

Chain E:



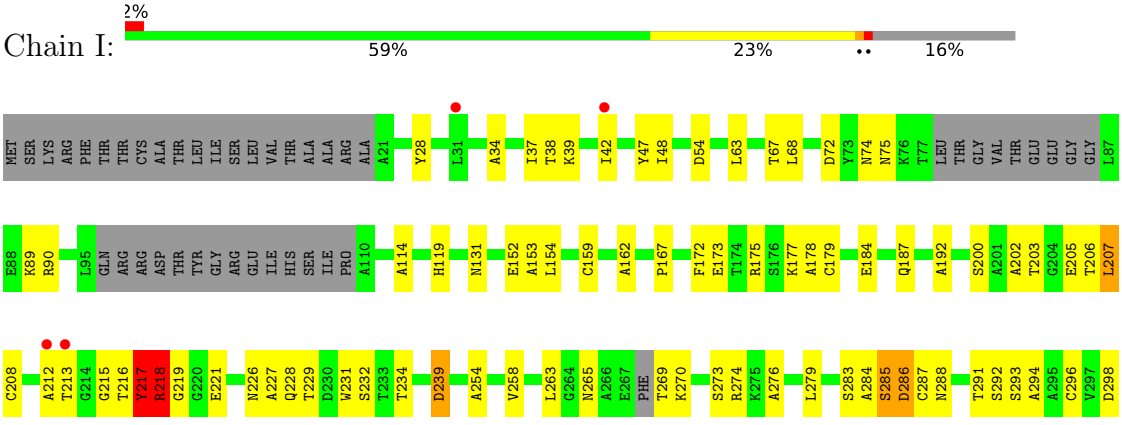
• Molecule 1: Variant surface glycoprotein 615

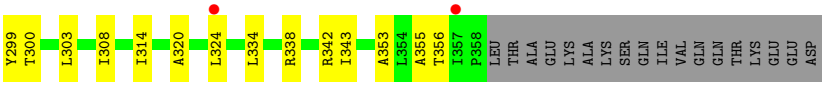
Chain G:



• Molecule 1: Variant surface glycoprotein 615

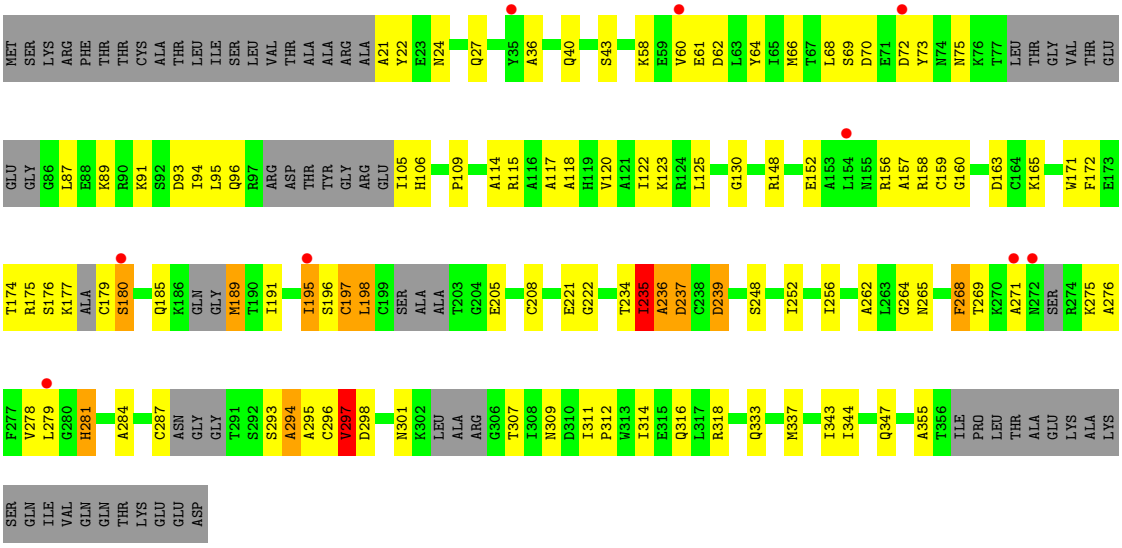
Chain I:





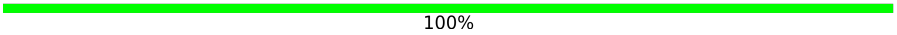
• Molecule 1: Variant surface glycoprotein 615

Chain K:



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

Chain J:



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

Chain F:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	86.28Å 111.23Å 108.59Å 90.00° 91.65° 90.00°	Depositor
Resolution (Å)	77.68 – 3.22 77.68 – 3.22	Depositor EDS
% Data completeness (in resolution range)	92.4 (77.68-3.22) 85.2 (77.68-3.22)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.08 (at 3.19Å)	Xtriage
Refinement program	PHENIX (1.19.2_4158: ???)	Depositor
R, R_{free}	0.307 , 0.325 0.306 , 0.324	Depositor DCC
R_{free} test set	1524 reflections (4.94%)	wwPDB-VP
Wilson B-factor (Å^2)	85.2	Xtriage
Anisotropy	0.098	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 58.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.43$, $< L^2 > = 0.25$	Xtriage
Estimated twinning fraction	0.046 for -h,-l,-k 0.027 for -h,l,k 0.067 for h,-k,-l	Xtriage
F_o,F_c correlation	0.86	EDS
Total number of atoms	14117	wwPDB-VP
Average B, all atoms (Å^2)	88.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.15% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: NAG, GLC

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	0.26	0/2147	0.51	0/2899
1	C	0.32	0/2487	0.53	0/3362
1	E	0.32	0/2374	0.54	0/3209
1	G	0.37	0/2410	0.54	0/3258
1	I	0.33	0/2338	0.56	0/3157
1	K	0.34	0/2292	0.54	0/3091
All	All	0.32	0/14048	0.54	0/18976

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	C	0	1
1	G	0	1
1	I	0	1
All	All	0	3

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	274	ARG	Sidechain
1	G	115	ARG	Sidechain
1	I	218	ARG	Sidechain

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2123	0	2052	55	0
1	C	2457	0	2362	69	0
1	E	2345	0	2266	65	0
1	G	2379	0	2274	66	0
1	I	2311	0	2241	54	0
1	K	2268	0	2171	73	0
2	F	28	0	25	1	0
2	J	28	0	25	0	0
3	A	14	0	13	1	0
3	C	14	0	13	0	0
3	G	14	0	13	1	0
3	K	14	0	13	1	0
4	C	22	0	20	1	0
4	E	22	0	20	0	0
4	G	22	0	20	3	0
4	I	22	0	20	3	0
4	K	22	0	20	0	0
5	C	2	0	0	0	0
5	E	1	0	0	0	0
5	G	2	0	0	0	0
5	I	3	0	0	0	0
5	K	4	0	0	0	0
All	All	14117	0	13568	369	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 13.

All (369) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:217:TYR:H	1:I:226:ASN:HB3	1.41	0.84
1:C:303:LEU:HD21	1:C:311:ILE:HG13	1.59	0.83
1:C:268:PHE:HB3	1:C:273:SER:HB2	1.67	0.76
4:I:401:GLC:H3	4:I:402:GLC:H61	1.66	0.76
1:I:269:THR:N	1:I:285:SER:HG	1.84	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:275:LYS:C	1:C:277:PHE:H	1.92	0.73
1:I:284:ALA:HB3	4:I:402:GLC:H2	1.73	0.71
1:C:291:THR:HG23	1:C:294:ALA:H	1.57	0.70
1:K:120:VAL:HA	1:K:123:LYS:HD3	1.74	0.68
1:K:94:ILE:HG23	1:K:106:HIS:NE2	2.09	0.68
1:C:167:PRO:HD2	1:K:43:SER:HB2	1.76	0.67
1:I:38:THR:HA	1:I:154:LEU:HD12	1.75	0.66
1:I:173:GLU:HB3	1:I:178:ALA:HB2	1.78	0.66
1:K:105:ILE:HD12	1:K:106:HIS:CE1	2.31	0.66
1:A:174:THR:HG21	1:A:177:LYS:HE2	1.78	0.66
1:G:281:HIS:CE1	4:G:403:GLC:HO2	2.14	0.65
1:C:158:ARG:HH21	1:C:164:CYS:HB3	1.60	0.65
1:G:94:ILE:HG22	1:G:95:LEU:HD22	1.78	0.65
1:A:218:ARG:HB2	1:A:223:THR:HG23	1.78	0.65
1:C:200:SER:HA	1:C:214:GLY:HA3	1.78	0.65
1:C:177:LYS:HD3	1:C:184:GLU:HB3	1.79	0.65
1:G:114:ALA:HB1	1:G:355:ALA:HA	1.79	0.64
1:K:125:LEU:HB3	1:K:344:ILE:HG23	1.81	0.63
1:E:173:GLU:HG2	1:E:177:LYS:HD2	1.81	0.63
1:I:343:ILE:HG21	1:K:343:ILE:HD12	1.80	0.63
1:C:158:ARG:NH2	1:C:164:CYS:HB3	2.12	0.62
1:C:173:GLU:HG3	1:C:174:THR:H	1.64	0.62
1:E:219:GLY:HA2	1:E:289:GLY:HA2	1.81	0.62
1:G:201:ALA:HB1	1:G:289:GLY:HA2	1.82	0.62
1:C:179:CYS:HA	1:C:297:VAL:HG13	1.81	0.61
1:A:263:LEU:HD21	1:A:277:PHE:HA	1.82	0.61
1:E:268:PHE:CD2	1:E:269:THR:HG22	2.36	0.61
1:I:175:ARG:HD3	1:I:179:CYS:SG	2.41	0.61
1:K:105:ILE:HG13	1:K:106:HIS:H	1.66	0.61
1:E:65:ILE:HA	1:E:68:LEU:HB2	1.83	0.60
1:K:264:GLY:HA2	1:K:276:ALA:HA	1.83	0.60
1:I:177:LYS:HD2	1:I:184:GLU:HB2	1.83	0.60
1:A:245:LYS:HD3	1:E:318:ARG:HH22	1.66	0.60
1:E:72:ASP:HA	1:E:75:ASN:HB3	1.83	0.60
1:G:208:CYS:SG	1:G:209:SER:N	2.74	0.60
1:C:166:ALA:O	1:C:168:ASP:N	2.31	0.59
1:I:205:GLU:H	1:I:207:LEU:HD23	1.68	0.59
1:A:88:GLU:HG3	1:A:91:LYS:H	1.67	0.59
1:K:158:ARG:HA	1:K:191:ILE:HG12	1.85	0.59
1:E:56:ARG:NH2	1:E:126:PHE:O	2.36	0.58
1:A:264:GLY:N	1:A:278:VAL:O	2.35	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:311:ILE:HG22	1:G:314:ILE:HB	1.84	0.58
1:K:70:ASP:HA	1:K:73:TYR:HD2	1.68	0.58
1:C:275:LYS:C	1:C:277:PHE:N	2.57	0.58
1:E:172:PHE:HE1	1:E:192:ALA:HB1	1.68	0.57
1:I:270:LYS:HG3	1:I:273:SER:HB3	1.86	0.57
1:E:50:ASP:OD1	1:E:338:ARG:NH1	2.37	0.57
1:C:124:ARG:NH2	1:E:345:GLU:OE2	2.37	0.57
1:K:307:THR:HG22	1:K:309:ASN:H	1.68	0.57
1:A:249:PRO:HA	1:A:252:ILE:HD12	1.86	0.57
1:G:65:ILE:HA	1:G:68:LEU:HD12	1.86	0.57
1:G:216:THR:OG1	1:G:226:ASN:O	2.21	0.57
1:E:268:PHE:HD2	1:E:273:SER:HB2	1.69	0.57
1:E:119:HIS:CE1	1:E:123:LYS:HE3	2.40	0.57
1:G:159:CYS:HB2	1:G:171:TRP:CG	2.40	0.56
1:A:243:GLU:HG3	1:E:305:ARG:HH12	1.70	0.56
1:I:167:PRO:O	1:I:228:GLN:NE2	2.38	0.56
1:A:305:ARG:NH2	1:C:243:GLU:OE2	2.38	0.56
1:C:88:GLU:O	1:C:90:ARG:N	2.38	0.56
1:C:175:ARG:HG2	1:C:288:ASN:HA	1.88	0.56
1:K:69:SER:HB2	1:K:72:ASP:HB2	1.87	0.56
1:C:39:LYS:HD2	1:C:158:ARG:NH1	2.21	0.56
1:C:157:ALA:HB1	1:C:313:TRP:HB2	1.88	0.56
1:I:172:PHE:HE1	1:I:192:ALA:HB1	1.71	0.55
1:A:98:ARG:HA	1:A:105:ILE:HG23	1.88	0.55
1:E:56:ARG:NH1	1:E:61:GLU:OE2	2.39	0.55
1:G:119:HIS:O	1:G:123:LYS:N	2.34	0.55
1:C:267:GLU:HB3	1:C:283:SER:HA	1.88	0.54
1:C:275:LYS:HA	1:C:278:VAL:HG22	1.89	0.54
1:K:58:LYS:HA	1:K:61:GLU:HG3	1.89	0.54
1:A:100:THR:O	1:A:101:TYR:HB3	2.07	0.54
1:A:181:GLY:O	1:A:301:ASN:ND2	2.40	0.54
1:I:187:GLN:NE2	1:I:298:ASP:O	2.41	0.54
1:G:173:GLU:HB2	1:G:178:ALA:HB2	1.89	0.54
1:K:198:LEU:HA	1:K:295:ALA:HB1	1.90	0.54
1:A:267:GLU:CD	1:A:268:PHE:H	2.10	0.54
1:A:297:VAL:HG23	1:A:298:ASP:H	1.71	0.54
1:I:153:ALA:HB3	1:I:320:ALA:HB2	1.88	0.54
1:E:269:THR:O	1:E:273:SER:OG	2.25	0.53
1:G:37:ILE:HG21	1:G:252:ILE:HG13	1.90	0.53
1:K:109:PRO:HD2	1:K:115:ARG:HH21	1.72	0.53
1:K:156:ARG:HA	1:K:160:GLY:HA2	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:216:THR:O	1:I:217:TYR:C	2.47	0.53
1:A:176:SER:HB2	1:A:220:GLY:HA2	1.91	0.53
1:A:178:ALA:HA	1:A:186:LYS:O	2.09	0.53
1:C:173:GLU:HG2	1:C:186:LYS:HE2	1.91	0.53
1:C:175:ARG:HG3	1:C:179:CYS:SG	2.49	0.53
1:C:275:LYS:O	1:C:277:PHE:N	2.41	0.53
1:C:187:GLN:HG3	1:C:299:TYR:HA	1.91	0.53
1:E:269:THR:HB	1:E:285:SER:HA	1.91	0.53
1:I:200:SER:HA	1:I:213:THR:HG22	1.91	0.53
1:I:291:THR:HG21	4:I:402:GLC:H3	1.90	0.53
1:E:268:PHE:CD2	1:E:273:SER:HB2	2.45	0.52
1:G:22:TYR:HA	1:G:207:LEU:HD22	1.91	0.52
1:I:338:ARG:HG3	1:I:338:ARG:HH11	1.74	0.52
1:K:185:GLN:HG3	1:K:301:ASN:HB3	1.91	0.52
1:E:176:SER:HB2	1:E:182:THR:O	2.09	0.52
1:E:223:THR:O	1:E:226:ASN:N	2.43	0.52
1:C:305:ARG:HD2	1:E:240:ARG:HD2	1.92	0.52
1:E:222:GLY:O	1:E:223:THR:C	2.47	0.52
1:C:27:GLN:HG2	1:C:279:LEU:HG	1.91	0.52
1:K:36:ALA:O	1:K:40:GLN:HG3	2.10	0.52
1:K:296:CYS:O	1:K:297:VAL:C	2.48	0.52
1:A:88:GLU:HG2	1:A:91:LYS:NZ	2.24	0.51
1:E:231:TRP:CH2	1:E:235:ILE:HG13	2.46	0.51
1:K:294:ALA:O	1:K:295:ALA:C	2.48	0.51
1:C:63:LEU:HD13	1:C:352:PHE:HB2	1.93	0.51
1:E:207:LEU:HD11	1:E:292:SER:HB3	1.92	0.51
1:C:88:GLU:HB3	1:C:91:LYS:HG2	1.93	0.51
1:E:143:ILE:O	1:E:147:THR:HG23	2.11	0.51
1:C:309:ASN:HA	1:C:314:ILE:HG21	1.93	0.51
1:G:274:ARG:H	1:G:300:THR:HG21	1.75	0.51
1:I:215:GLY:O	1:I:218:ARG:HG2	2.11	0.51
1:I:263:LEU:HD23	1:I:279:LEU:HG	1.92	0.51
1:K:114:ALA:HA	1:K:117:ALA:HB3	1.93	0.51
1:E:113:GLU:O	1:E:117:ALA:N	2.43	0.50
1:K:62:ASP:HB2	1:K:106:HIS:CE1	2.46	0.50
1:G:281:HIS:CD2	4:G:403:GLC:C1	2.94	0.50
1:G:356:THR:HG21	1:K:117:ALA:HB2	1.93	0.50
1:K:68:LEU:HD23	1:K:69:SER:N	2.26	0.50
1:A:354:LEU:HD11	1:C:354:LEU:HD23	1.93	0.50
1:K:157:ALA:HB2	1:K:316:GLN:HB2	1.93	0.50
1:K:189:MET:N	1:K:312:PRO:HD2	2.27	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:125:LEU:HB3	1:C:344:ILE:HG23	1.94	0.50
1:I:34:ALA:O	1:I:37:ILE:HG22	2.12	0.50
1:K:94:ILE:HG23	1:K:106:HIS:CD2	2.46	0.50
1:K:93:ASP:OD1	1:K:93:ASP:N	2.45	0.50
1:E:58:LYS:O	1:E:62:ASP:N	2.40	0.49
1:G:59:GLU:O	1:G:63:LEU:HB2	2.12	0.49
1:C:50:ASP:O	1:C:338:ARG:NH1	2.45	0.49
1:C:61:GLU:O	1:C:65:ILE:HD12	2.12	0.49
1:C:170:LYS:HG2	1:C:224:ALA:HB3	1.94	0.49
1:I:67:THR:HG23	1:I:119:HIS:ND1	2.27	0.49
1:K:24:ASN:HB3	1:K:198:LEU:HD21	1.95	0.49
1:K:24:ASN:HA	1:K:27:GLN:HB2	1.94	0.49
1:E:122:ILE:O	1:E:126:PHE:N	2.45	0.49
1:I:47:TYR:O	1:I:48:ILE:HG13	2.12	0.49
1:A:51:THR:H	1:A:338:ARG:NH2	2.11	0.49
1:G:278:VAL:HG22	1:G:298:ASP:HA	1.95	0.49
1:K:118:ALA:O	1:K:122:ILE:HG12	2.13	0.49
1:K:287:CYS:SG	1:K:296:CYS:N	2.86	0.49
1:E:34:ALA:O	1:E:38:THR:HG23	2.13	0.49
1:E:288:ASN:N	1:E:294:ALA:O	2.45	0.49
1:G:172:PHE:HZ	1:G:231:TRP:CG	2.31	0.49
1:K:176:SER:O	1:K:177:LYS:C	2.51	0.49
1:E:172:PHE:CE1	1:E:192:ALA:HB1	2.48	0.49
1:G:245:LYS:NZ	1:K:318:ARG:HE	2.10	0.49
1:K:27:GLN:HG2	1:K:262:ALA:HB1	1.95	0.49
1:G:42:ILE:O	1:G:44:ASP:N	2.44	0.49
1:G:171:TRP:HB2	1:G:190:THR:HG21	1.95	0.48
1:K:235:ILE:O	1:K:237:ASP:N	2.46	0.48
1:K:269:THR:HG22	1:K:271:ALA:H	1.77	0.48
1:A:331:ARG:NH1	1:A:335:ASP:OD1	2.46	0.48
1:G:98:ARG:O	1:G:99:ASP:C	2.52	0.48
1:G:119:HIS:O	1:G:120:VAL:C	2.51	0.48
1:I:274:ARG:HD3	1:I:300:THR:HG23	1.95	0.48
1:K:175:ARG:CB	1:K:222:GLY:HA3	2.43	0.48
1:A:300:THR:HA	1:A:303:LEU:HD12	1.95	0.48
1:C:56:ARG:HH21	1:C:130:GLY:HA3	1.78	0.48
1:G:346:ASP:HA	1:G:349:TRP:HD1	1.79	0.48
1:A:164:CYS:HA	1:A:171:TRP:HZ2	1.78	0.48
1:I:28:TYR:HB2	1:I:208:CYS:SG	2.54	0.48
1:G:248:SER:O	1:G:252:ILE:HD12	2.12	0.48
1:I:68:LEU:HD12	1:I:119:HIS:CE1	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:66:MET:SD	1:K:66:MET:N	2.87	0.48
1:E:114:ALA:HA	1:E:117:ALA:HB3	1.96	0.48
1:K:191:ILE:O	1:K:195:ILE:HG22	2.14	0.48
1:G:62:ASP:HB3	1:G:94:ILE:HG13	1.96	0.48
1:G:108:ILE:HD12	1:G:109:PRO:HD2	1.95	0.48
1:I:175:ARG:HD2	1:I:288:ASN:O	2.13	0.48
1:A:42:ILE:HD13	1:A:247:PRO:HG2	1.96	0.47
1:G:88:GLU:O	1:G:89:LYS:C	2.52	0.47
1:A:88:GLU:HG2	1:A:91:LYS:HZ1	1.79	0.47
1:A:150:ALA:HB2	1:A:323:LYS:HB2	1.95	0.47
1:K:91:LYS:O	1:K:95:LEU:HD23	2.14	0.47
1:K:109:PRO:HB3	1:K:355:ALA:HB1	1.95	0.47
1:C:70:ASP:OD1	1:C:70:ASP:N	2.46	0.47
1:G:69:SER:HA	1:G:115:ARG:HD3	1.97	0.47
1:C:66:MET:HB3	1:C:108:ILE:HD13	1.97	0.47
1:G:76:LYS:NZ	1:G:76:LYS:HB3	2.30	0.47
1:A:164:CYS:HA	1:A:171:TRP:CZ2	2.49	0.47
1:A:278:VAL:HG22	1:A:279:LEU:H	1.80	0.47
1:G:159:CYS:SG	1:G:160:GLY:N	2.88	0.47
1:G:231:TRP:CH2	1:G:235:ILE:HG21	2.49	0.47
1:K:94:ILE:HG22	1:K:95:LEU:HD22	1.95	0.47
1:E:238:CYS:O	1:E:242:VAL:HG13	2.14	0.47
1:C:57:PRO:O	1:C:61:GLU:HG3	2.15	0.47
1:A:174:THR:O	1:A:178:ALA:HB3	2.15	0.47
1:G:90:ARG:HD2	1:G:90:ARG:HA	1.50	0.47
1:K:235:ILE:HB	1:K:236:ALA:H	1.57	0.47
1:E:177:LYS:HG2	1:E:184:GLU:HB3	1.96	0.46
1:C:203:THR:HB	1:C:292:SER:HB3	1.97	0.46
1:C:148:ARG:O	1:C:152:GLU:HG3	2.14	0.46
1:E:25:ALA:HA	1:E:28:TYR:HB3	1.96	0.46
1:E:339:GLN:HA	1:E:342:ARG:HH11	1.80	0.46
1:C:57:PRO:O	1:C:60:VAL:HG22	2.16	0.46
1:C:203:THR:HG21	4:C:402:GLC:O5	2.16	0.46
1:C:56:ARG:NH2	1:C:130:GLY:HA3	2.31	0.46
1:C:299:TYR:HB3	1:C:303:LEU:HG	1.97	0.46
1:E:220:GLY:O	1:E:222:GLY:N	2.48	0.46
1:G:67:THR:HG23	1:G:119:HIS:CD2	2.51	0.46
1:K:96:GLN:O	1:K:105:ILE:HG12	2.14	0.46
1:K:130:GLY:HA3	3:K:401:NAG:H82	1.98	0.46
1:G:159:CYS:HB2	1:G:171:TRP:CD1	2.51	0.46
1:G:347:GLN:HG3	1:K:347:GLN:HE21	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:59:GLU:HG2	1:A:349:TRP:CZ2	2.51	0.46
1:G:54:ASP:HB3	1:G:136:ILE:HG21	1.97	0.46
1:G:305:ARG:NH1	1:G:310:ASP:OD1	2.49	0.46
1:I:299:TYR:HB3	1:I:303:LEU:HB2	1.98	0.46
1:A:100:THR:HG23	1:A:101:TYR:H	1.80	0.46
1:C:69:SER:OG	1:C:70:ASP:N	2.48	0.46
1:E:69:SER:O	1:E:73:TYR:HB2	2.15	0.46
1:A:43:SER:O	1:A:46:GLU:HG2	2.15	0.45
1:C:214:GLY:HA2	1:C:230:ASP:OD2	2.16	0.45
1:I:338:ARG:O	1:I:342:ARG:HG3	2.16	0.45
1:K:159:CYS:HB2	1:K:171:TRP:CG	2.51	0.45
1:C:153:ALA:HB3	1:C:320:ALA:HB2	1.98	0.45
1:C:167:PRO:HA	1:C:171:TRP:CZ2	2.51	0.45
1:E:289:GLY:H	1:E:294:ALA:HB1	1.80	0.45
1:I:63:LEU:O	1:I:67:THR:HG22	2.17	0.45
1:I:152:GLU:HG2	1:I:162:ALA:HB1	1.99	0.45
1:K:333:GLN:O	1:K:337:MET:HG3	2.16	0.45
1:E:43:SER:OG	1:E:46:GLU:HG2	2.17	0.45
1:A:139:ALA:O	1:A:143:ILE:HG13	2.16	0.45
1:C:280:GLY:HA3	1:C:296:CYS:HB3	1.99	0.45
1:G:242:VAL:HG22	1:K:318:ARG:HH22	1.82	0.45
1:E:76:LYS:HG3	1:E:78:LEU:HD22	1.97	0.45
1:K:296:CYS:O	1:K:298:ASP:N	2.50	0.45
1:C:76:LYS:NZ	1:C:78:LEU:HD11	2.31	0.45
1:I:254:ALA:O	1:I:258:VAL:HG23	2.17	0.44
1:K:311:ILE:HD11	1:K:314:ILE:HG13	1.99	0.44
1:C:64:TYR:CE1	1:C:123:LYS:HD3	2.52	0.44
1:C:157:ALA:O	1:C:191:ILE:HG13	2.18	0.44
1:K:72:ASP:HA	1:K:75:ASN:HB2	1.98	0.44
1:K:281:HIS:HE1	1:K:295:ALA:HB3	1.82	0.44
1:A:187:GLN:HG2	1:A:299:TYR:HA	1.99	0.44
1:E:294:ALA:O	1:E:296:CYS:N	2.51	0.44
1:A:38:THR:HA	1:A:154:LEU:HD22	1.99	0.44
1:I:308:ILE:CG2	1:I:314:ILE:HD13	2.47	0.44
1:E:187:GLN:HG3	1:E:302:LYS:HB2	1.99	0.44
1:I:227:ALA:O	1:I:231:TRP:N	2.50	0.44
1:K:265:ASN:HB2	1:K:278:VAL:HB	1.99	0.44
1:A:231:TRP:CH2	1:A:235:ILE:HD11	2.52	0.44
1:E:61:GLU:HG2	1:E:126:PHE:HE1	1.83	0.44
1:E:339:GLN:O	1:E:343:ILE:HG23	2.18	0.44
1:G:189:MET:SD	1:G:312:PRO:HG2	2.57	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:G:402:GLC:O2	4:G:403:GLC:H2	2.17	0.44
1:E:179:CYS:HA	1:E:297:VAL:HG13	1.98	0.44
1:E:205:GLU:O	1:E:206:THR:C	2.55	0.44
1:A:27:GLN:N	1:A:207:LEU:O	2.51	0.43
1:A:302:LYS:HD3	1:A:312:PRO:HD3	2.00	0.43
1:A:351:ALA:O	1:A:354:LEU:HB2	2.18	0.43
1:G:241:ASN:C	1:G:243:GLU:H	2.21	0.43
1:K:70:ASP:HA	1:K:73:TYR:CD2	2.51	0.43
1:A:351:ALA:HA	1:A:354:LEU:HD23	2.01	0.43
1:G:22:TYR:CE2	1:K:275:LYS:HE3	2.54	0.43
1:I:263:LEU:HB3	1:I:276:ALA:O	2.18	0.43
1:I:291:THR:H	1:I:294:ALA:HB3	1.84	0.43
1:C:188:GLY:HA3	1:C:311:ILE:HG23	2.01	0.43
1:E:179:CYS:SG	1:E:288:ASN:HB2	2.58	0.43
1:G:64:TYR:HE1	1:G:123:LYS:HA	1.84	0.43
1:I:270:LYS:HB2	1:I:285:SER:HB2	1.99	0.43
1:I:324:LEU:HD23	1:I:324:LEU:HA	1.83	0.43
1:K:64:TYR:O	1:K:68:LEU:HD12	2.18	0.43
1:K:87:LEU:HD12	1:K:89:LYS:N	2.33	0.43
1:K:275:LYS:HA	1:K:275:LYS:HD3	1.74	0.43
1:C:209:SER:H	1:C:212:ALA:HB2	1.83	0.43
1:G:127:TYR:HB3	3:G:401:NAG:H3	2.00	0.43
1:E:267:GLU:HB2	1:E:283:SER:H	1.83	0.43
1:G:69:SER:C	1:G:71:GLU:N	2.69	0.43
1:G:159:CYS:HB3	1:G:164:CYS:HB3	1.82	0.43
1:E:38:THR:HA	1:E:154:LEU:HB3	2.01	0.43
1:A:114:ALA:HB1	1:A:355:ALA:HA	2.01	0.43
1:C:24:ASN:HB3	1:C:198:LEU:HD11	1.99	0.43
1:E:323:LYS:O	1:E:327:VAL:HG23	2.18	0.43
1:G:24:ASN:H	1:G:27:GLN:HE21	1.67	0.43
1:E:50:ASP:H	1:E:338:ARG:HH22	1.65	0.43
1:E:237:ASP:OD1	1:E:240:ARG:NH1	2.51	0.43
1:I:42:ILE:HG21	1:I:324:LEU:HD21	2.00	0.43
1:C:269:THR:HG22	1:C:285:SER:HA	2.01	0.43
1:E:195:ILE:HG21	1:E:235:ILE:HD11	2.01	0.43
1:G:69:SER:O	1:G:71:GLU:N	2.52	0.43
1:G:70:ASP:HA	1:G:73:TYR:HB2	2.01	0.43
1:K:148:ARG:O	1:K:152:GLU:HG3	2.19	0.43
1:A:108:ILE:HD12	1:A:115:ARG:NH2	2.34	0.42
1:E:27:GLN:HA	1:E:262:ALA:HB1	2.01	0.42
1:E:195:ILE:HD13	1:E:235:ILE:HD11	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:150:ALA:HB1	1:G:320:ALA:HB1	2.02	0.42
1:G:172:PHE:CE1	1:G:192:ALA:HB1	2.54	0.42
1:K:175:ARG:N	1:K:221:GLU:O	2.53	0.42
1:K:197:CYS:HB3	1:K:297:VAL:HG22	2.01	0.42
1:K:239:ASP:OD1	1:K:239:ASP:N	2.52	0.42
1:A:122:ILE:HA	1:A:125:LEU:HB2	2.01	0.42
1:E:157:ALA:HB2	1:E:316:GLN:HB2	2.01	0.42
1:E:302:LYS:NZ	1:E:310:ASP:O	2.50	0.42
1:I:219:GLY:C	1:I:221:GLU:N	2.72	0.42
1:A:118:ALA:O	1:A:122:ILE:HG12	2.19	0.42
1:A:218:ARG:HD2	1:A:218:ARG:HA	1.91	0.42
1:A:245:LYS:H	1:A:245:LYS:HG3	1.63	0.42
1:G:114:ALA:O	1:G:115:ARG:C	2.58	0.42
1:I:48:ILE:HG22	1:I:334:LEU:HD22	2.00	0.42
1:E:68:LEU:HD23	1:E:73:TYR:HA	2.01	0.42
1:I:74:ASN:OD1	1:I:75:ASN:OD1	2.38	0.42
1:I:291:THR:OG1	1:I:292:SER:N	2.53	0.42
1:A:225:ALA:O	1:A:229:THR:HG23	2.19	0.42
1:E:279:LEU:O	1:E:296:CYS:HA	2.19	0.42
1:G:252:ILE:O	1:G:256:ILE:HD12	2.18	0.42
1:G:257:ALA:HB2	1:I:254:ALA:HB1	2.02	0.42
1:K:234:THR:C	1:K:235:ILE:HG13	2.40	0.42
1:K:248:SER:O	1:K:252:ILE:HG13	2.20	0.42
1:A:223:THR:HB	1:A:226:ASN:HB3	2.02	0.42
1:A:300:THR:HA	1:A:303:LEU:HB2	2.01	0.42
1:C:73:TYR:HE1	1:C:91:LYS:HB2	1.84	0.42
1:G:351:ALA:O	1:G:354:LEU:HB2	2.19	0.42
1:I:219:GLY:C	1:I:221:GLU:H	2.23	0.42
1:C:150:ALA:HB2	1:C:323:LYS:HB2	2.01	0.42
1:C:236:ALA:O	1:C:240:ARG:HG3	2.19	0.42
1:I:303:LEU:HD12	1:I:303:LEU:HA	1.77	0.42
1:C:57:PRO:HD3	1:C:341:MET:SD	2.60	0.42
1:G:346:ASP:HA	1:G:349:TRP:CD1	2.55	0.42
1:E:184:GLU:HG2	1:E:185:GLN:H	1.84	0.41
1:I:226:ASN:O	1:I:229:THR:OG1	2.34	0.41
1:I:232:SER:C	1:I:234:THR:H	2.23	0.41
1:C:303:LEU:HD13	1:C:308:ILE:HA	2.02	0.41
1:I:114:ALA:HB1	1:I:355:ALA:HA	2.02	0.41
1:A:277:PHE:CG	1:A:303:LEU:HD11	2.55	0.41
1:C:68:LEU:HG	1:C:72:ASP:HB2	2.01	0.41
1:E:274:ARG:HA	1:E:274:ARG:HD3	1.81	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:120:VAL:HG13	1:G:121:ALA:H	1.84	0.41
1:A:168:ASP:HB3	1:A:171:TRP:CD1	2.55	0.41
1:C:115:ARG:HH11	1:C:115:ARG:HG2	1.85	0.41
1:A:179:CYS:HB3	1:A:296:CYS:O	2.20	0.41
1:A:263:LEU:HD11	1:A:277:PHE:CD1	2.56	0.41
1:G:270:LYS:HE3	1:G:270:LYS:HB3	1.95	0.41
1:A:159:CYS:HB3	1:A:164:CYS:HB3	1.95	0.41
3:A:401:NAG:H61	1:I:221:GLU:HG3	2.01	0.41
1:E:127:TYR:HB2	2:F:1:NAG:H62	2.02	0.41
1:K:165:LYS:H	1:K:165:LYS:HG3	1.67	0.41
1:C:39:LYS:HB3	1:C:242:VAL:HG11	2.01	0.41
1:C:284:ALA:C	1:C:286:ASP:H	2.22	0.41
1:E:266:ALA:HA	1:E:275:LYS:HB3	2.03	0.41
1:G:268:PHE:CZ	1:G:273:SER:HA	2.55	0.41
1:G:323:LYS:O	1:G:327:VAL:HG23	2.21	0.41
1:K:256:ILE:HD13	1:K:314:ILE:HG23	2.02	0.41
1:C:308:ILE:H	1:C:308:ILE:HD12	1.85	0.41
1:G:116:ALA:O	1:G:117:ALA:C	2.59	0.41
1:I:206:THR:H	1:I:212:ALA:HA	1.85	0.41
1:E:107:SER:OG	1:E:108:ILE:N	2.54	0.41
1:E:245:LYS:HA	1:E:245:LYS:HD3	1.76	0.41
1:G:245:LYS:HE3	1:K:318:ARG:HH21	1.85	0.41
1:K:60:VAL:O	1:K:64:TYR:N	2.54	0.41
1:A:341:MET:O	1:A:344:ILE:HG22	2.21	0.40
1:I:285:SER:HB2	1:I:286:ASP:H	1.66	0.40
1:K:268:PHE:HA	1:K:284:ALA:O	2.20	0.40
1:G:56:ARG:HH12	1:G:61:GLU:CG	2.35	0.40
1:I:353:ALA:O	1:I:356:THR:OG1	2.32	0.40
1:K:21:ALA:HB3	1:K:205:GLU:HB2	2.03	0.40
1:G:207:LEU:HD22	1:G:207:LEU:HA	1.82	0.40
1:C:75:ASN:ND2	1:C:88:GLU:OE1	2.43	0.40
1:G:88:GLU:H	1:G:91:LYS:HZ3	1.70	0.40
1:A:57:PRO:O	1:A:61:GLU:HG3	2.22	0.40
1:C:54:ASP:HB3	1:C:136:ILE:HG21	2.02	0.40
1:I:39:LYS:HE3	1:I:239:ASP:OD2	2.22	0.40
1:K:176:SER:HA	1:K:180:SER:H	1.86	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	274/376 (73%)	233 (85%)	41 (15%)	0	100	100
1	C	330/376 (88%)	279 (84%)	49 (15%)	2 (1%)	25	63
1	E	314/376 (84%)	269 (86%)	42 (13%)	3 (1%)	15	52
1	G	319/376 (85%)	268 (84%)	48 (15%)	3 (1%)	17	55
1	I	306/376 (81%)	253 (83%)	49 (16%)	4 (1%)	12	46
1	K	290/376 (77%)	246 (85%)	39 (13%)	5 (2%)	9	40
All	All	1833/2256 (81%)	1548 (84%)	268 (15%)	17 (1%)	17	55

All (17) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	I	202	ALA
1	K	279	LEU
1	K	297	VAL
1	C	268	PHE
1	C	276	ALA
1	E	221	GLU
1	G	87	LEU
1	G	112	SER
1	I	203	THR
1	K	235	ILE
1	K	236	ALA
1	K	294	ALA
1	E	22	TYR
1	E	223	THR
1	I	265	ASN
1	I	217	TYR
1	G	120	VAL

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	210/281 (75%)	202 (96%)	8 (4%)	33	66
1	C	242/281 (86%)	231 (96%)	11 (4%)	27	62
1	E	232/281 (83%)	225 (97%)	7 (3%)	41	72
1	G	233/281 (83%)	216 (93%)	17 (7%)	14	46
1	I	229/281 (82%)	213 (93%)	16 (7%)	15	47
1	K	225/281 (80%)	206 (92%)	19 (8%)	11	38
All	All	1371/1686 (81%)	1293 (94%)	78 (6%)	20	55

All (78) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	97	ARG
1	A	101	TYR
1	A	164	CYS
1	A	197	CYS
1	A	199	CYS
1	A	240	ARG
1	A	277	PHE
1	A	352	PHE
1	C	83	GLU
1	C	164	CYS
1	C	171	TRP
1	C	238	CYS
1	C	240	ARG
1	C	248	SER
1	C	267	GLU
1	C	268	PHE
1	C	275	LYS
1	C	278	VAL
1	C	286	ASP
1	E	40	GLN
1	E	179	CYS
1	E	217	TYR

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Mol	Chain	Res	Type
1	E	281	HIS
1	E	288	ASN
1	E	291	THR
1	E	292	SER
1	G	58	LYS
1	G	68	LEU
1	G	70	ASP
1	G	87	LEU
1	G	90	ARG
1	G	100	THR
1	G	113	GLU
1	G	115	ARG
1	G	119	HIS
1	G	131	ASN
1	G	148	ARG
1	G	159	CYS
1	G	206	THR
1	G	207	LEU
1	G	208	CYS
1	G	248	SER
1	G	292	SER
1	I	54	ASP
1	I	72	ASP
1	I	89	LYS
1	I	90	ARG
1	I	131	ASN
1	I	159	CYS
1	I	207	LEU
1	I	217	TYR
1	I	218	ARG
1	I	239	ASP
1	I	283	SER
1	I	285	SER
1	I	286	ASP
1	I	287	CYS
1	I	293	SER
1	I	296	CYS
1	K	22	TYR
1	K	163	ASP
1	K	172	PHE
1	K	174	THR
1	K	179	CYS

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Mol	Chain	Res	Type
1	K	180	SER
1	K	189	MET
1	K	195	ILE
1	K	196	SER
1	K	197	CYS
1	K	198	LEU
1	K	208	CYS
1	K	235	ILE
1	K	237	ASP
1	K	239	ASP
1	K	268	PHE
1	K	281	HIS
1	K	293	SER
1	K	297	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	G	119	HIS
1	I	187	GLN
1	I	301	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

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	$\#\|Z\| > 2$
2	NAG	F	1	2,1	14,14,15	0.28	0	17,19,21	0.57	0
2	NAG	F	2	2	14,14,15	0.41	0	17,19,21	0.52	0
2	NAG	J	1	2,1	14,14,15	0.28	0	17,19,21	0.60	0
2	NAG	J	2	2	14,14,15	0.35	0	17,19,21	0.50	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	F	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	F	2	2	-	1/6/23/26	0/1/1/1
2	NAG	J	1	2,1	-	3/6/23/26	0/1/1/1
2	NAG	J	2	2	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	J	1	NAG	O5-C5-C6-O6
2	J	2	NAG	C8-C7-N2-C2
2	J	2	NAG	O7-C7-N2-C2
2	J	1	NAG	C4-C5-C6-O6
2	F	2	NAG	O5-C5-C6-O6
2	F	1	NAG	O5-C5-C6-O6
2	J	1	NAG	C3-C2-N2-C7
2	F	1	NAG	C3-C2-N2-C7

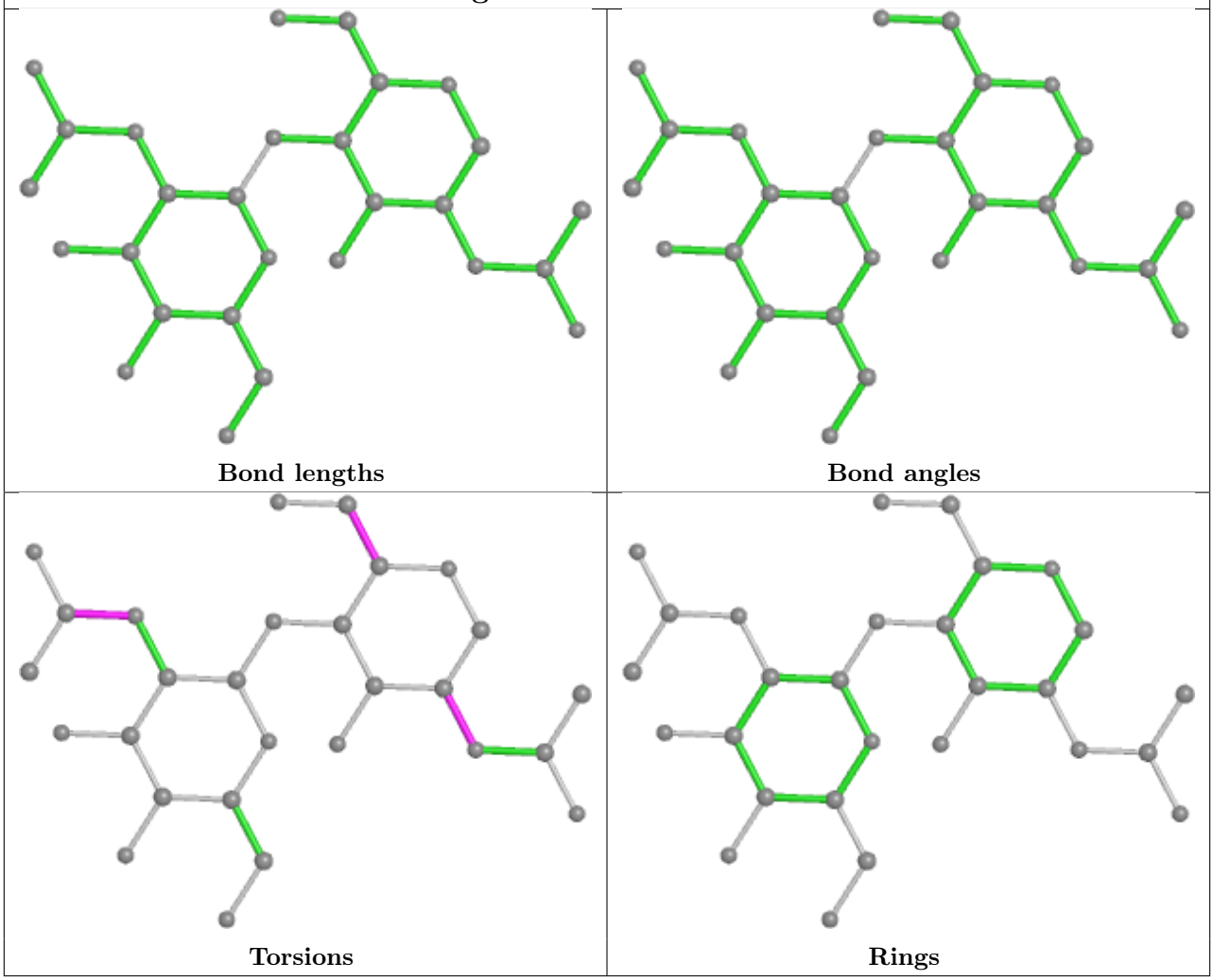
There are no ring outliers.

1 monomer is involved in 1 short contact:

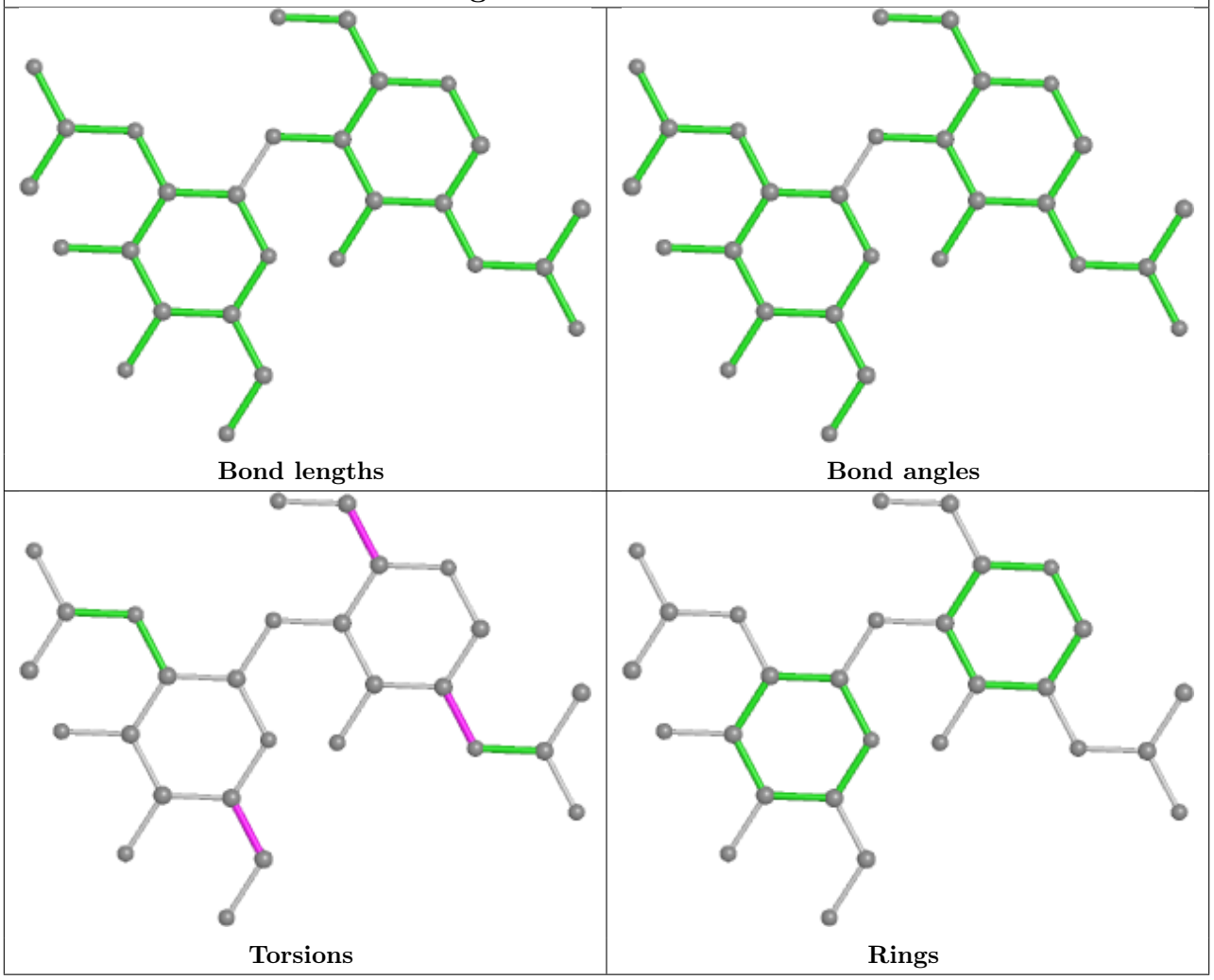
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	F	1	NAG	1	0

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

Oligosaccharide Chain J



Oligosaccharide Chain F



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	$\#\|Z\| > 2$
4	GLC	G	402	1	11,11,12	0.83	0	15,15,17	0.64	0
4	GLC	I	402	1	11,11,12	0.82	0	15,15,17	0.64	0
3	NAG	G	401	1	14,14,15	0.45	0	17,19,21	0.56	0
3	NAG	A	401	1	14,14,15	0.37	0	17,19,21	0.42	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
4	GLC	E	402	1	11,11,12	0.38	0	15,15,17	0.70	0
3	NAG	C	401	1	14,14,15	0.41	0	17,19,21	0.44	0
4	GLC	K	403	1	11,11,12	0.80	0	15,15,17	0.67	0
4	GLC	C	402	1	11,11,12	0.76	0	15,15,17	0.62	0
4	GLC	E	401	1	11,11,12	0.43	0	15,15,17	0.83	1 (6%)
4	GLC	G	403	1	11,11,12	0.89	0	15,15,17	0.62	0
4	GLC	K	402	1	11,11,12	0.85	0	15,15,17	0.62	0
3	NAG	K	401	1	14,14,15	0.28	0	17,19,21	0.44	0
4	GLC	I	401	1	11,11,12	0.80	0	15,15,17	0.62	0
4	GLC	C	403	1	11,11,12	0.76	0	15,15,17	0.65	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	GLC	G	402	1	-	0/2/19/22	0/1/1/1
4	GLC	I	402	1	-	1/2/19/22	0/1/1/1
3	NAG	G	401	1	-	0/6/23/26	0/1/1/1
3	NAG	A	401	1	-	0/6/23/26	0/1/1/1
4	GLC	E	402	1	-	1/2/19/22	0/1/1/1
3	NAG	C	401	1	-	1/6/23/26	0/1/1/1
4	GLC	K	403	1	-	0/2/19/22	0/1/1/1
4	GLC	C	402	1	-	0/2/19/22	0/1/1/1
4	GLC	E	401	1	-	2/2/19/22	0/1/1/1
4	GLC	G	403	1	-	0/2/19/22	0/1/1/1
4	GLC	K	402	1	-	0/2/19/22	0/1/1/1
3	NAG	K	401	1	-	0/6/23/26	0/1/1/1
4	GLC	I	401	1	-	1/2/19/22	0/1/1/1
4	GLC	C	403	1	-	0/2/19/22	0/1/1/1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	E	401	GLC	O5-C1-C2	-2.26	107.28	110.77

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	E	401	GLC	O5-C5-C6-O6
4	E	401	GLC	C4-C5-C6-O6
3	C	401	NAG	O5-C5-C6-O6
4	I	402	GLC	O5-C5-C6-O6
4	I	401	GLC	O5-C5-C6-O6
4	E	402	GLC	O5-C5-C6-O6

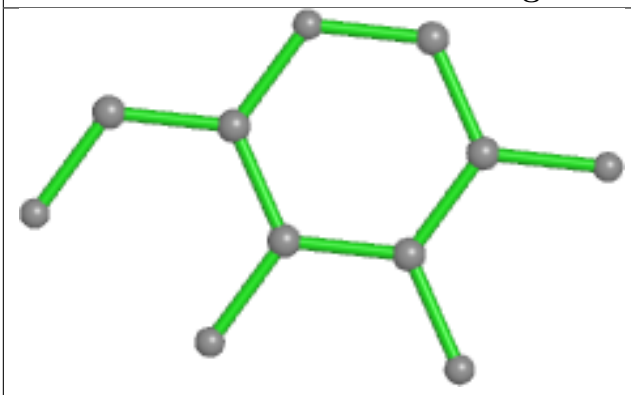
There are no ring outliers.

8 monomers are involved in 10 short contacts:

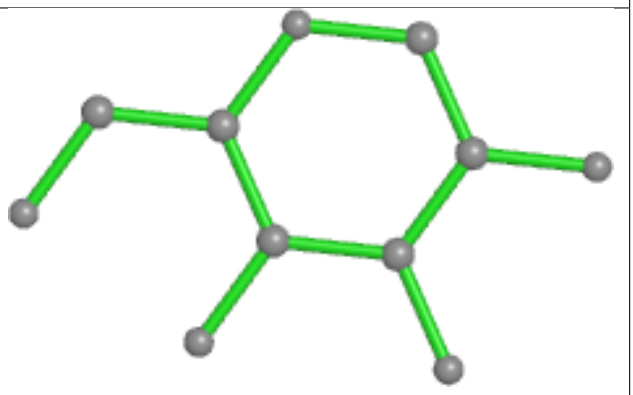
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	G	402	GLC	1	0
4	I	402	GLC	3	0
3	G	401	NAG	1	0
3	A	401	NAG	1	0
4	C	402	GLC	1	0
4	G	403	GLC	3	0
3	K	401	NAG	1	0
4	I	401	GLC	1	0

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 then 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.

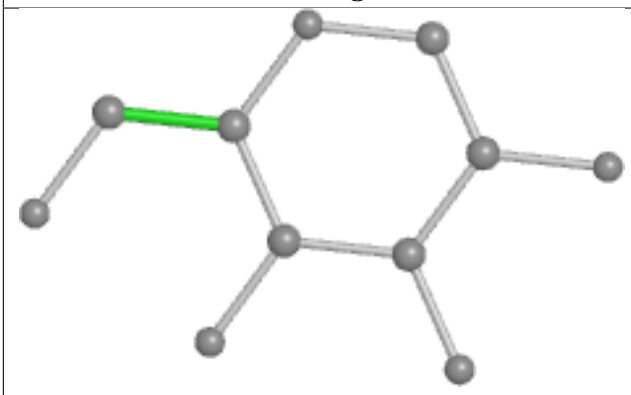
Ligand GLC G 402



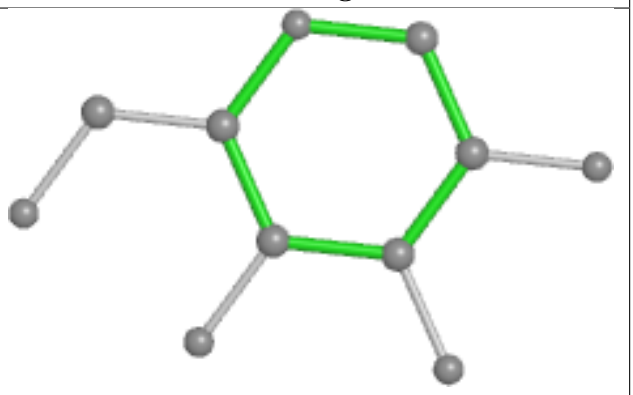
Bond lengths



Bond angles

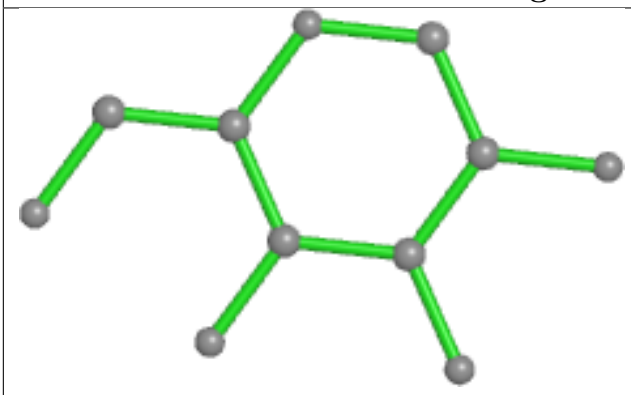


Torsions

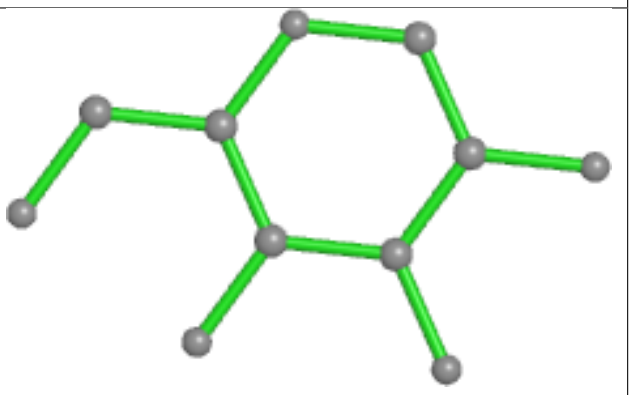


Rings

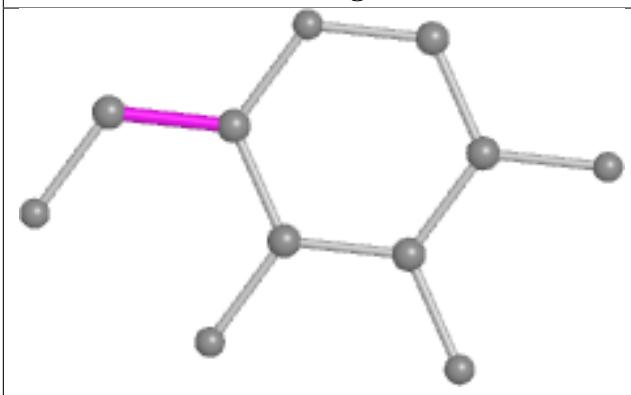
Ligand GLC I 402



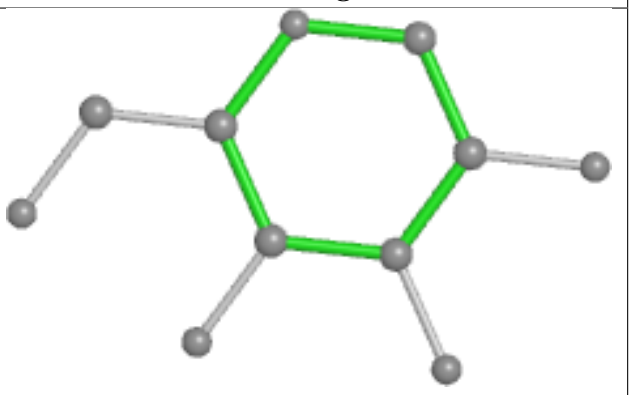
Bond lengths



Bond angles

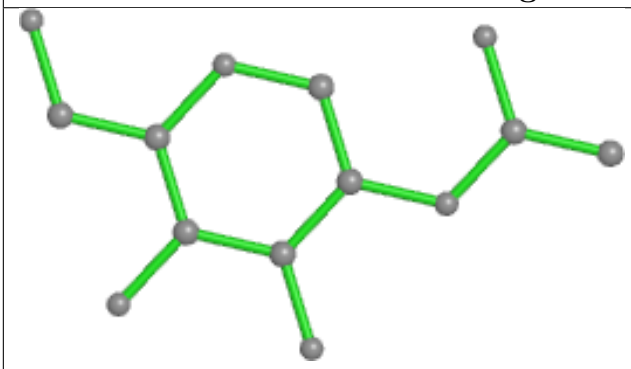


Torsions

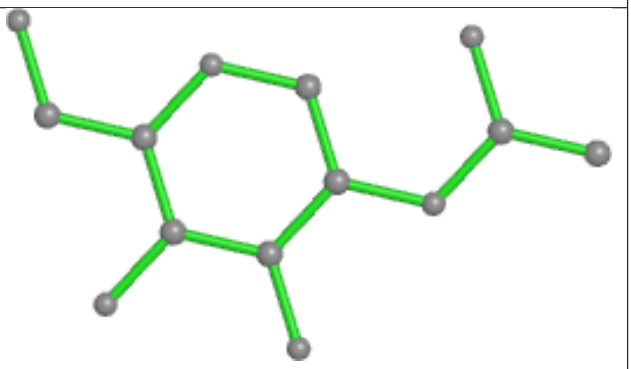


Rings

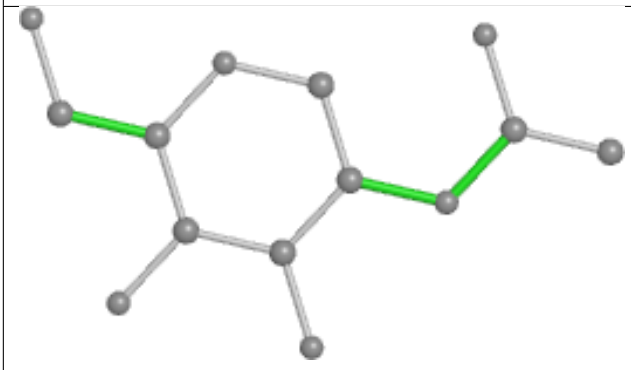
Ligand NAG G 401



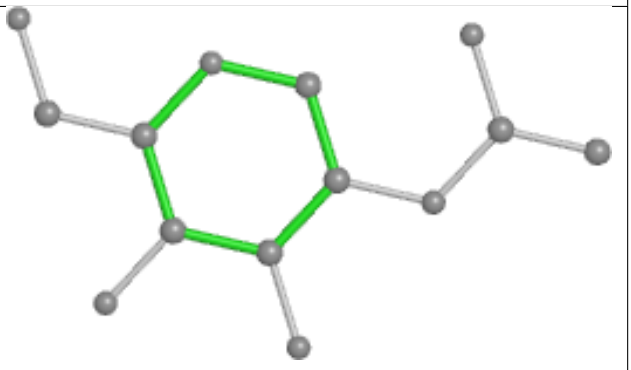
Bond lengths



Bond angles

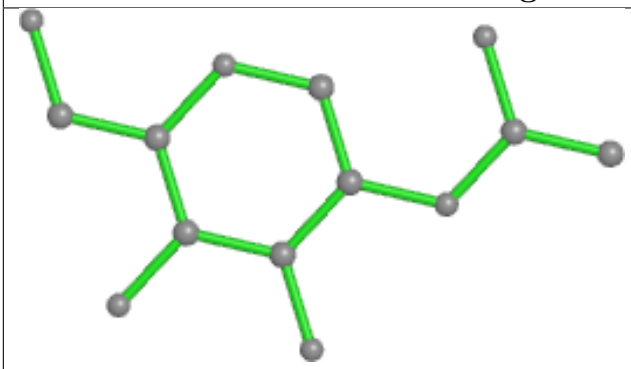


Torsions



Rings

Ligand NAG A 401



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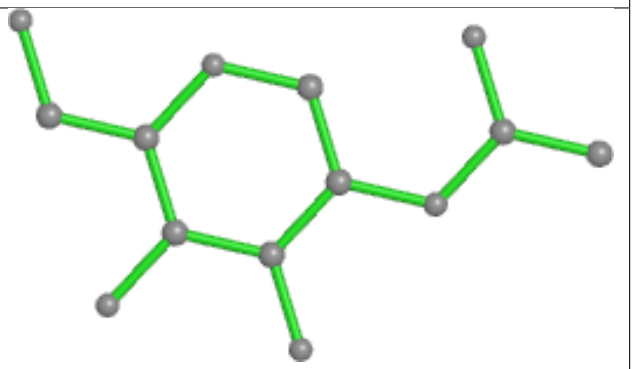
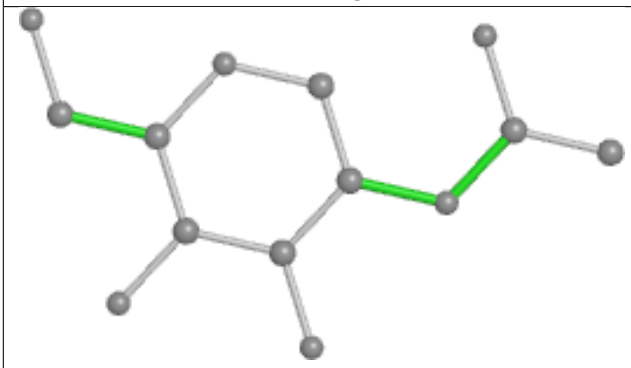


Bond angles



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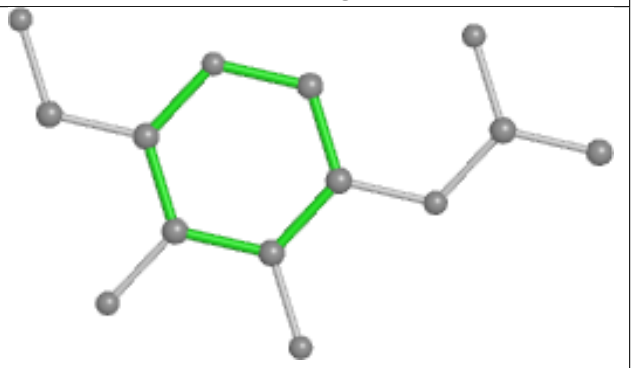
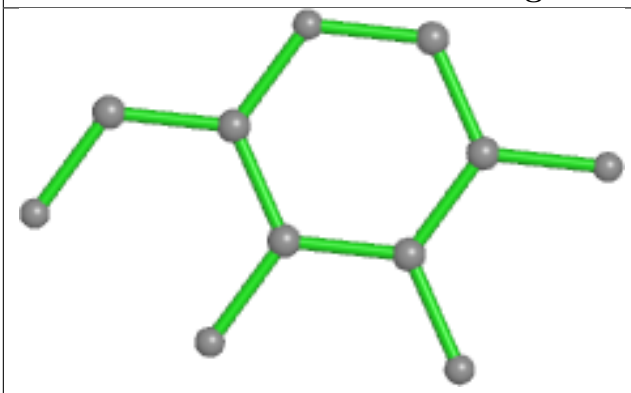


Rings

Ligand GLC E 402



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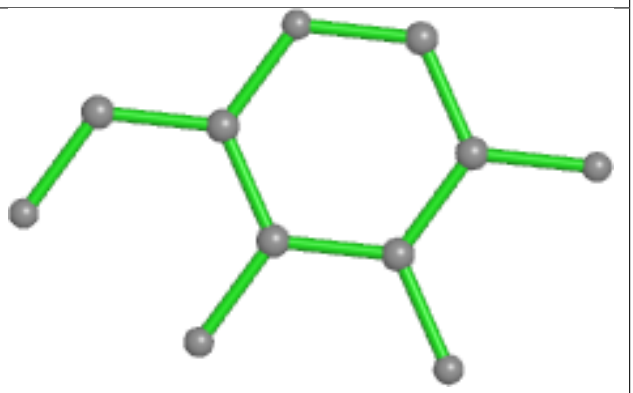

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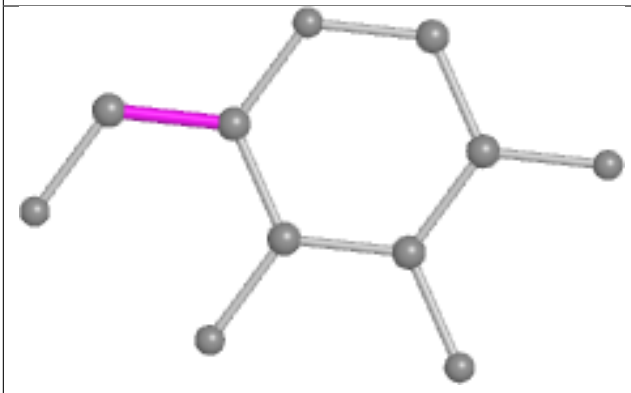

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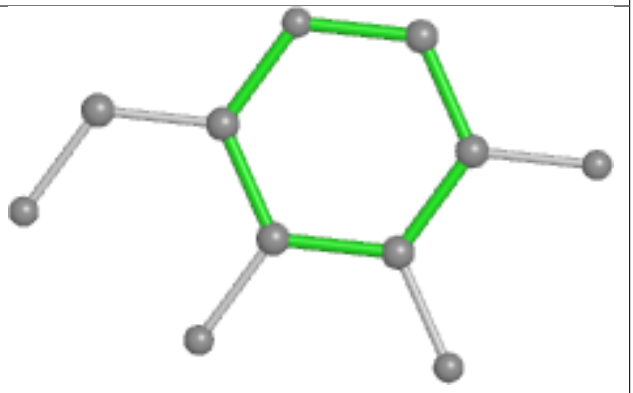
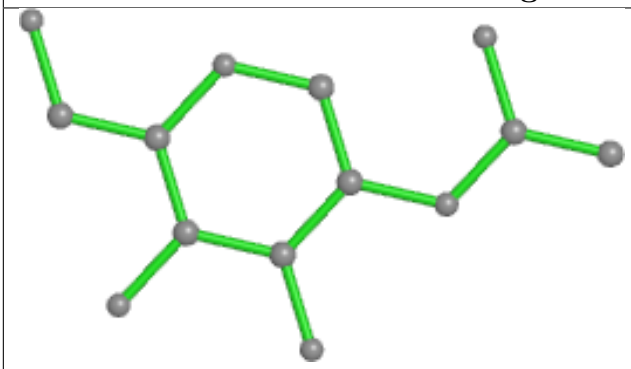


Rings

Ligand NAG C 401



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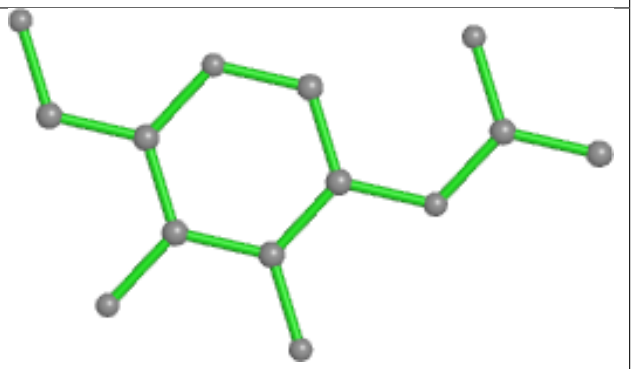
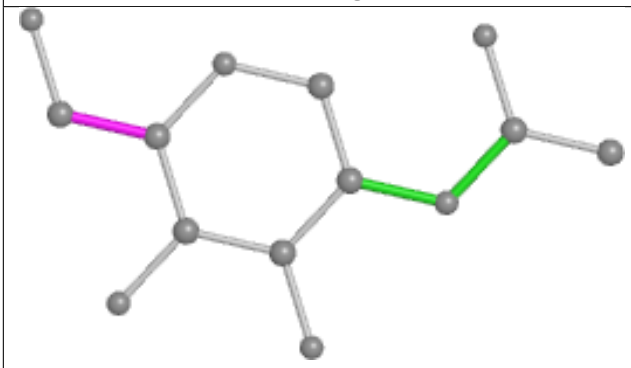


Bond angles



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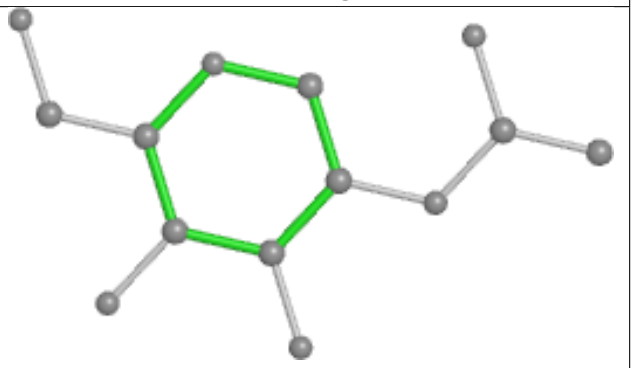
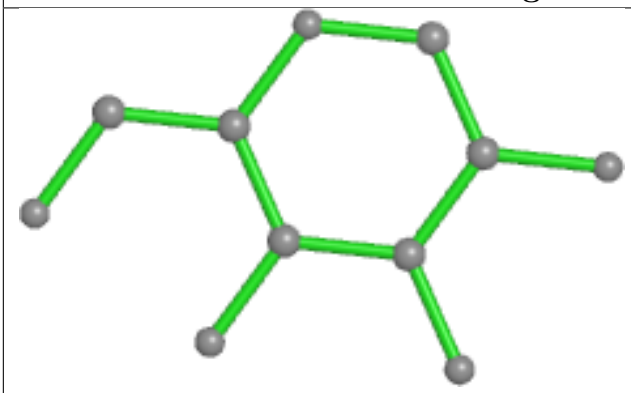


Rings

Ligand GLC K 403



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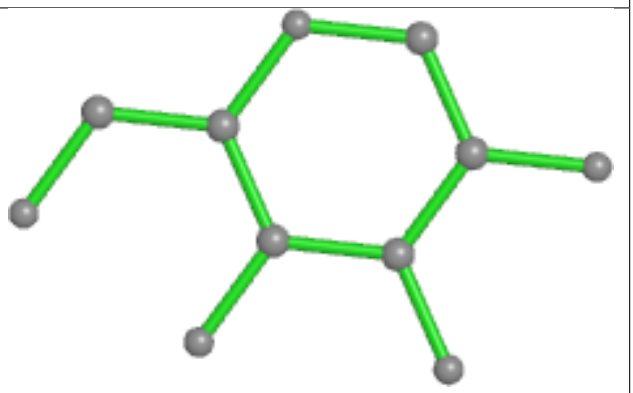

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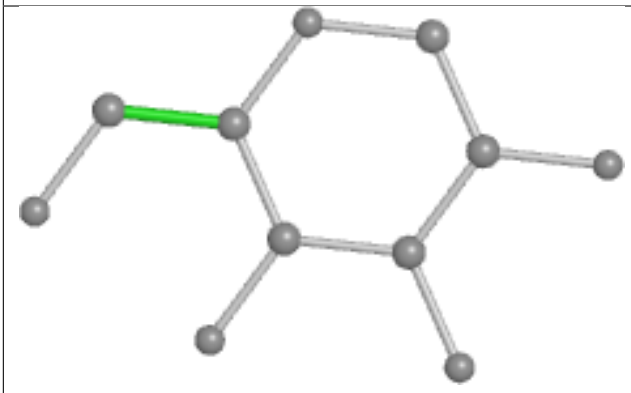
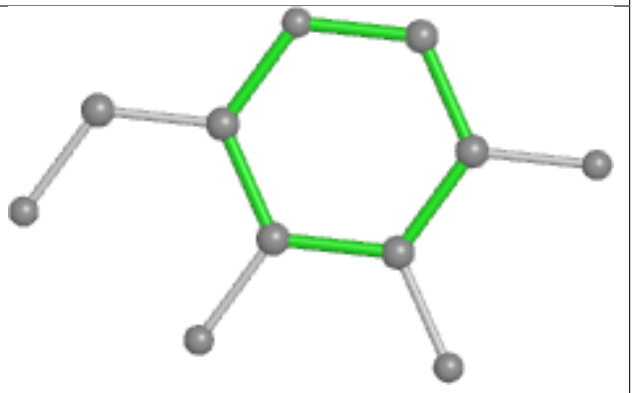
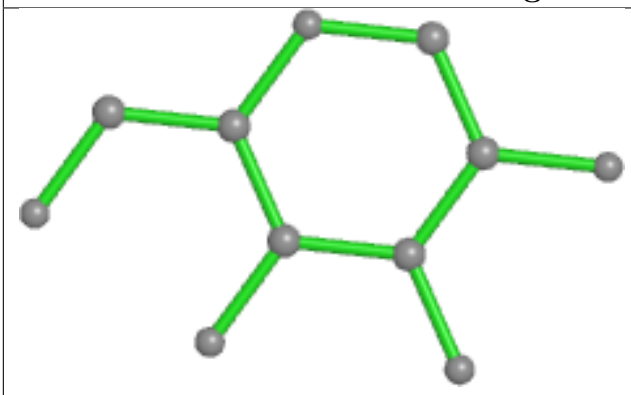


Torsions



Rings

Ligand GLC C 402



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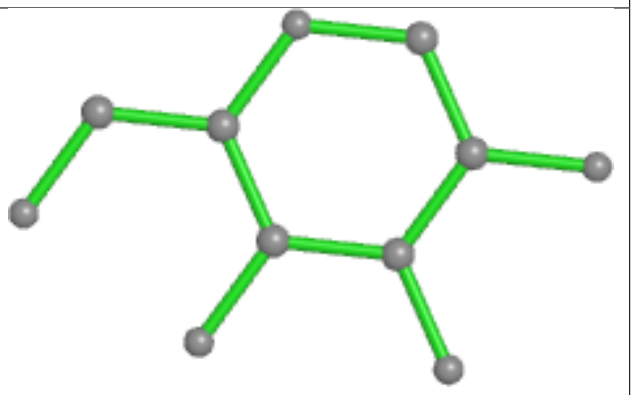
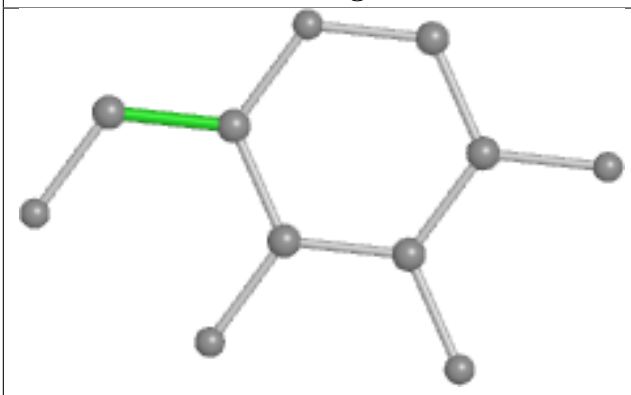


Bond angles



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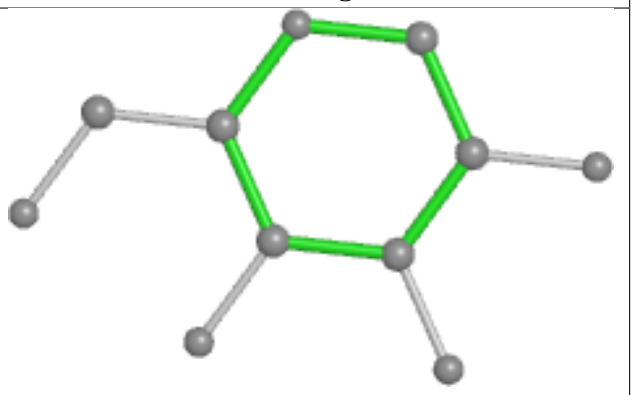
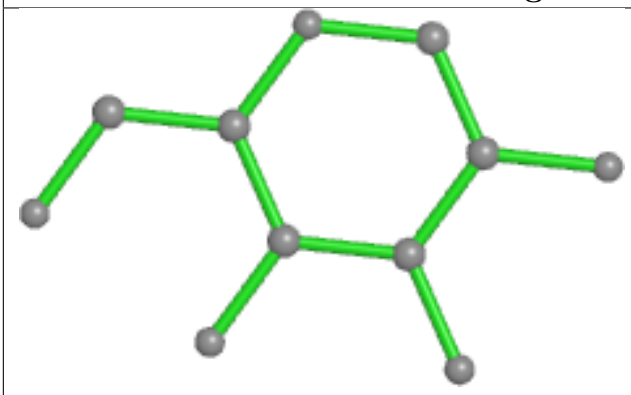


Rings

Ligand GLC E 401



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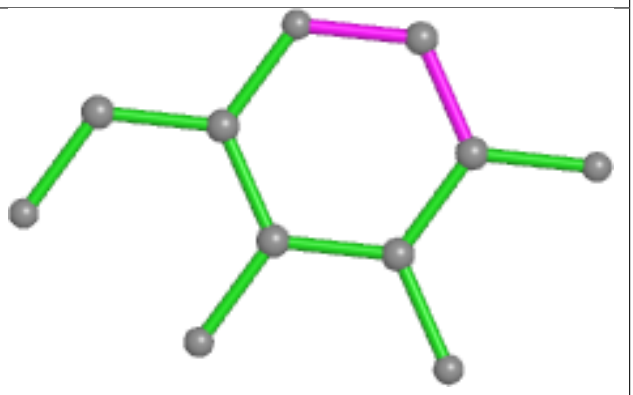

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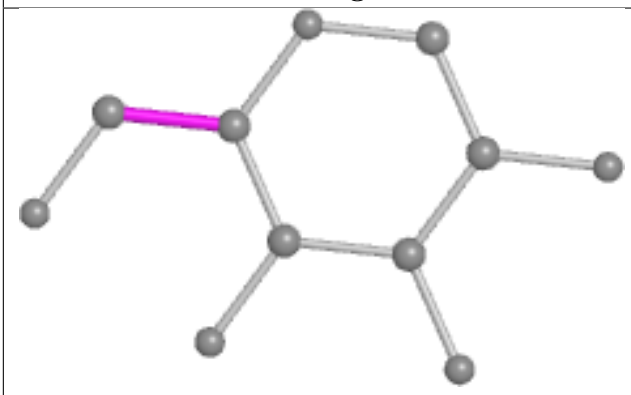

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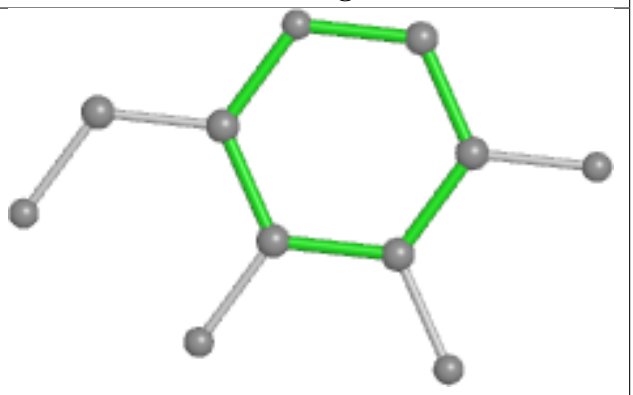
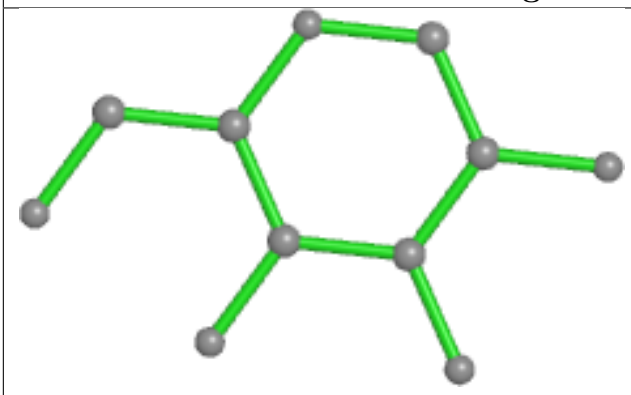


Rings

Ligand GLC G 403



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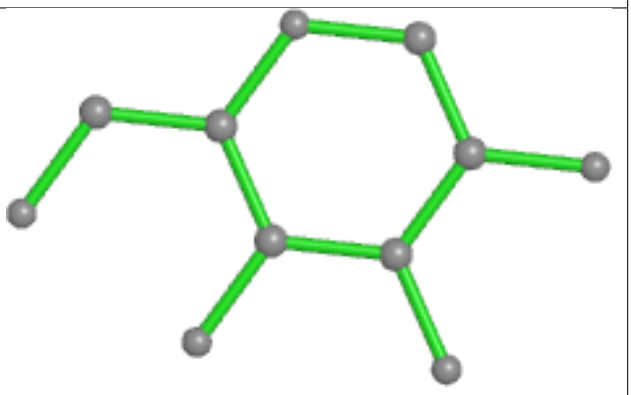
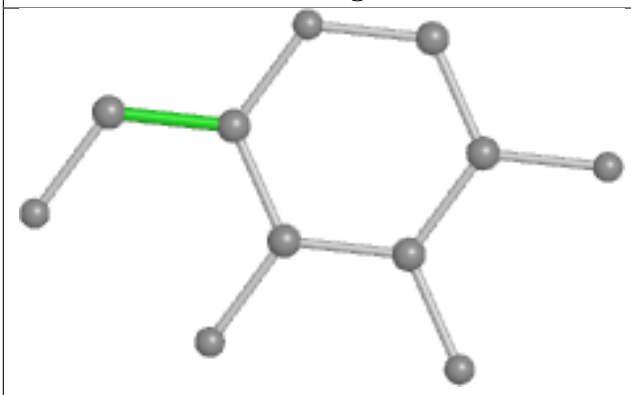


Bond angles



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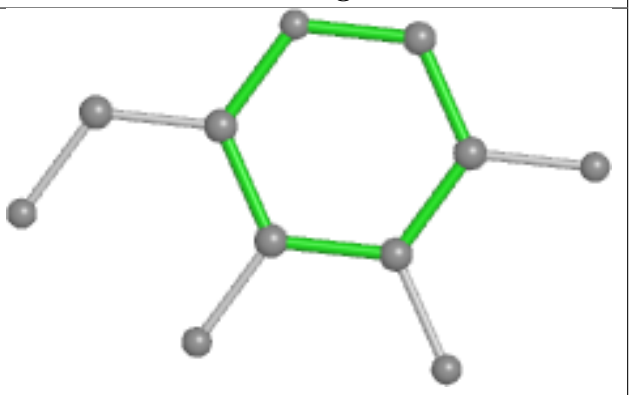

Rings

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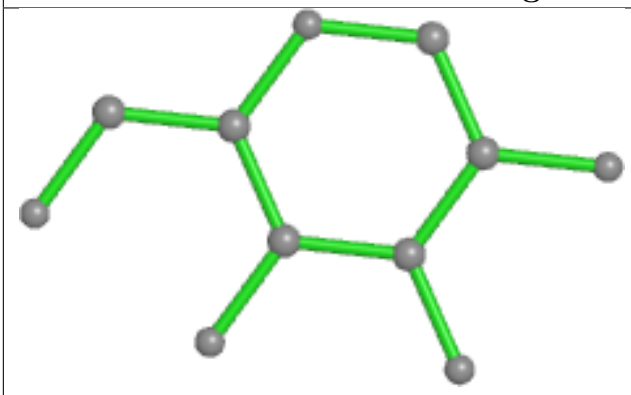

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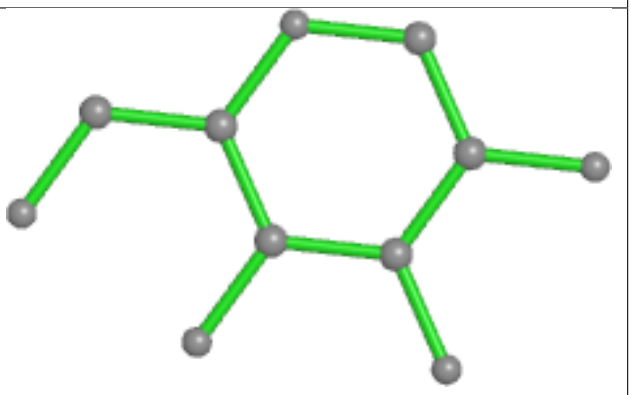

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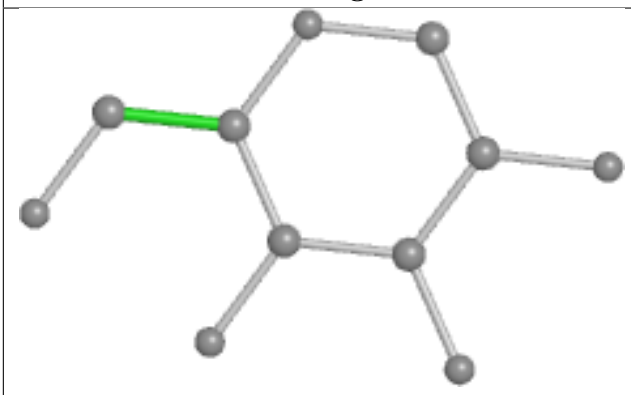

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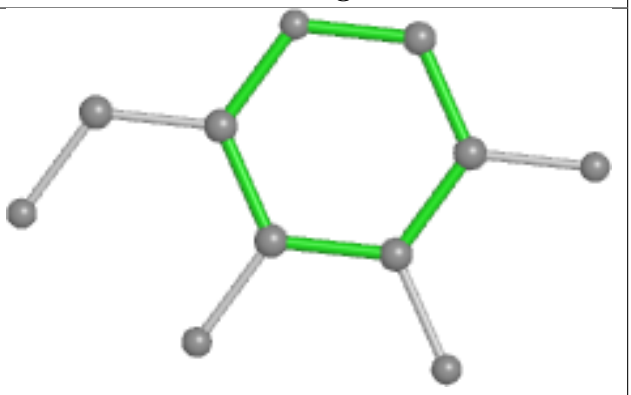
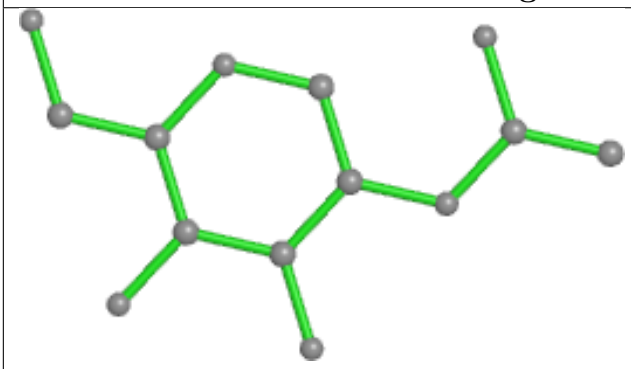


Rings

Ligand NAG K 401



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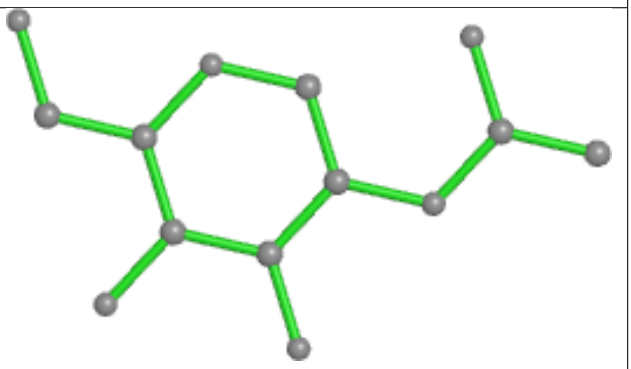
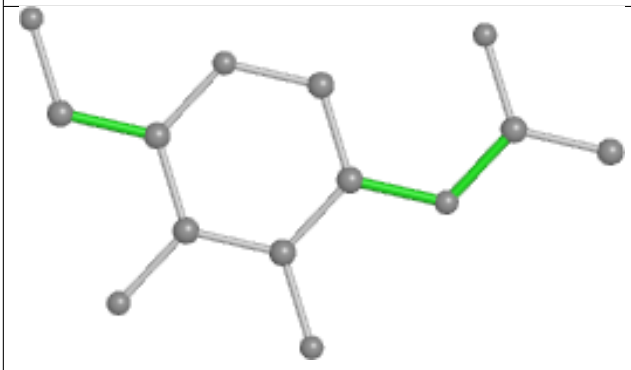
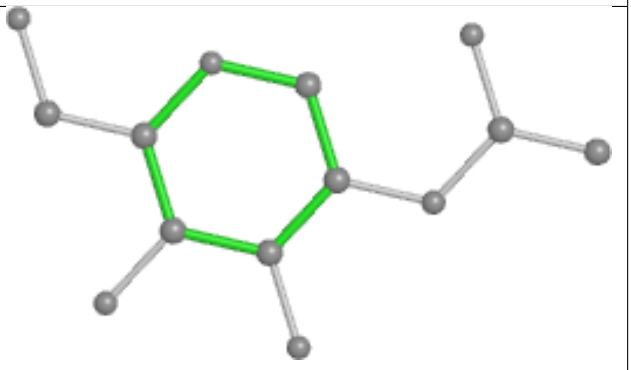


Bond angles

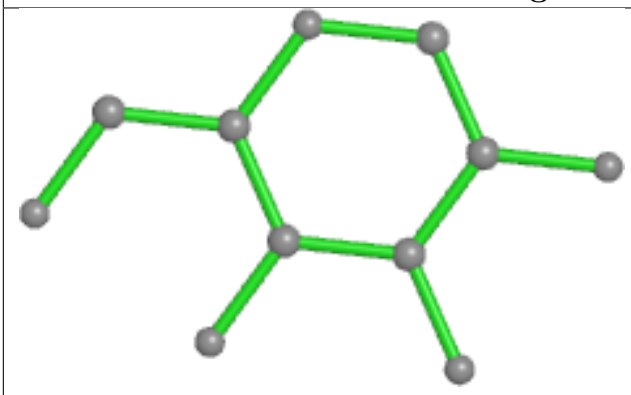


Torsions



Rings

Ligand GLC I 401



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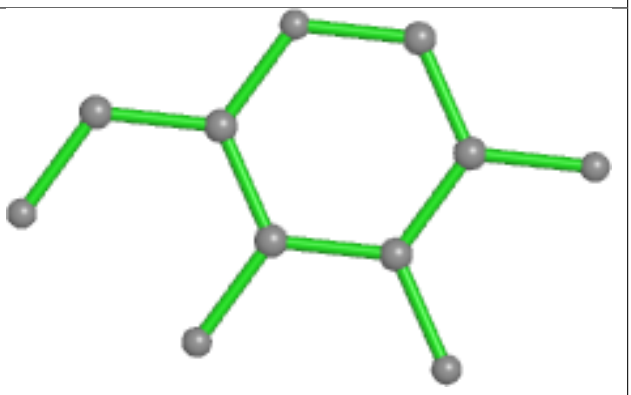
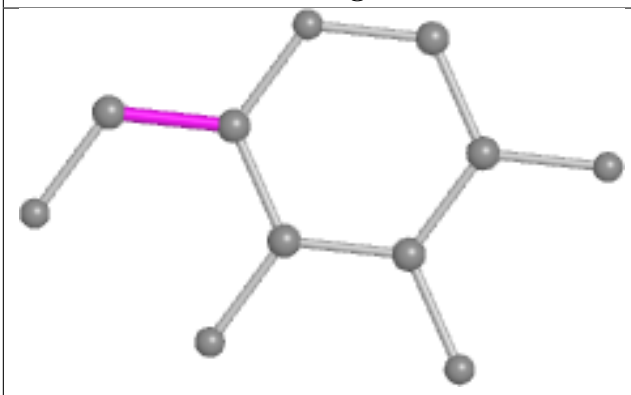


Bond angles



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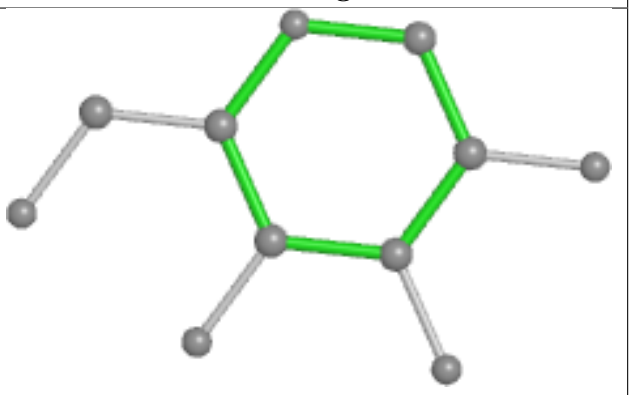
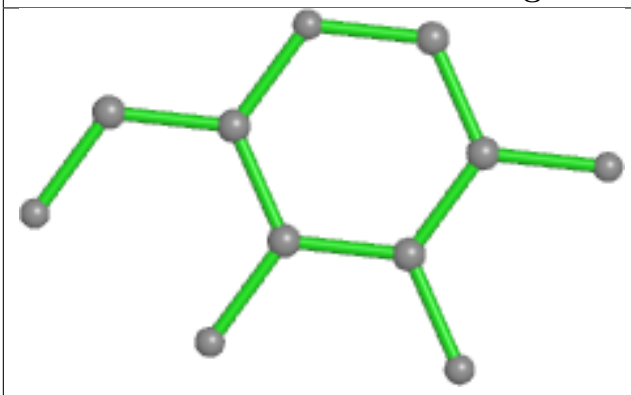
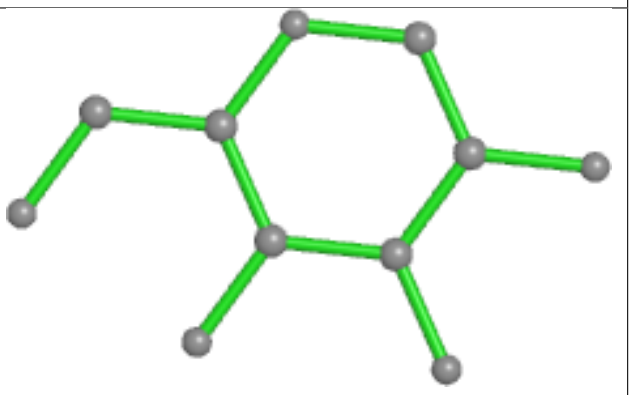


Rings

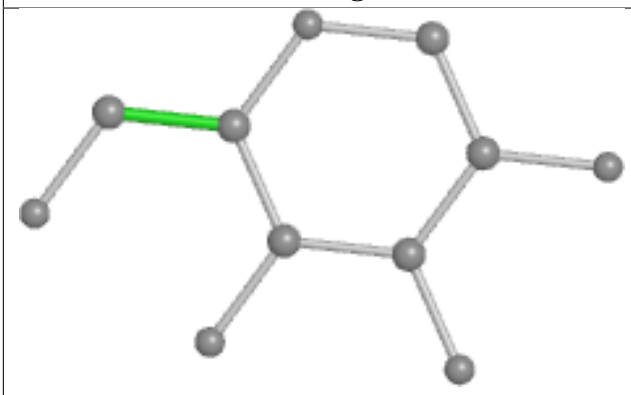
Ligand GLC C 403



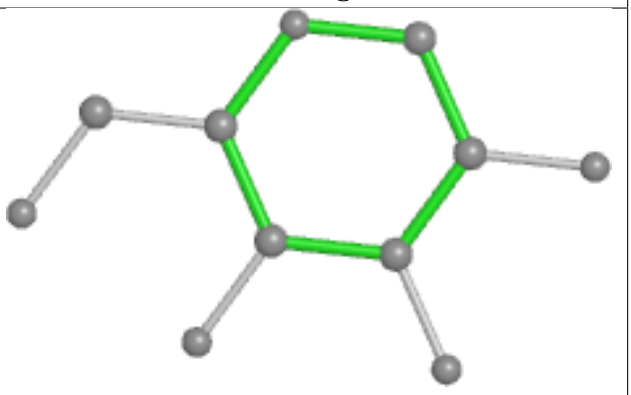
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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, 95^{th} 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	286/376 (76%)	0.35	18 (6%)	20	11	83, 100, 113, 114	0
1	C	335/376 (89%)	0.13	8 (2%)	59	45	62, 77, 116, 118	0
1	E	319/376 (84%)	0.10	4 (1%)	77	66	63, 75, 112, 116	0
1	G	325/376 (86%)	0.13	11 (3%)	45	31	75, 91, 109, 118	0
1	I	314/376 (83%)	0.01	6 (1%)	66	54	64, 74, 105, 111	0
1	K	308/376 (81%)	0.24	9 (2%)	51	37	80, 98, 109, 111	0
All	All	1887/2256 (83%)	0.16	56 (2%)	50	36	62, 88, 111, 118	0

All (56) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	126	PHE	3.8
1	A	69	SER	3.5
1	K	279	LEU	3.2
1	G	201	ALA	3.1
1	A	31	LEU	2.9
1	A	64	TYR	2.9
1	A	324	LEU	2.9
1	K	72	ASP	2.9
1	K	271	ALA	2.9
1	K	35	TYR	2.8
1	C	126	PHE	2.8
1	K	180	SER	2.8
1	K	60	VAL	2.8
1	A	120	VAL	2.8
1	G	77	THR	2.7
1	K	272	ASN	2.7
1	A	95	LEU	2.7
1	A	263	LEU	2.7
1	A	296	CYS	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	49	GLY	2.7
1	C	65	ILE	2.7
1	I	324	LEU	2.6
1	G	276	ALA	2.6
1	A	136	ILE	2.6
1	A	277	PHE	2.5
1	G	313	TRP	2.5
1	A	209	SER	2.5
1	K	154	LEU	2.5
1	A	140	ILE	2.5
1	I	213	THR	2.5
1	E	91	LYS	2.5
1	C	299	TYR	2.4
1	G	285	SER	2.4
1	E	64	TYR	2.4
1	C	231	TRP	2.4
1	I	212	ALA	2.3
1	C	64	TYR	2.3
1	I	42	ILE	2.3
1	G	314	ILE	2.3
1	G	37	ILE	2.3
1	A	299	TYR	2.3
1	E	65	ILE	2.2
1	E	107	SER	2.2
1	C	63	LEU	2.2
1	G	36	ALA	2.2
1	G	31	LEU	2.2
1	A	68	LEU	2.2
1	K	195	ILE	2.1
1	A	101	TYR	2.1
1	C	82	THR	2.1
1	G	303	LEU	2.0
1	I	357	ILE	2.0
1	I	31	LEU	2.0
1	C	352	PHE	2.0
1	A	325	ALA	2.0
1	A	111	ASN	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)

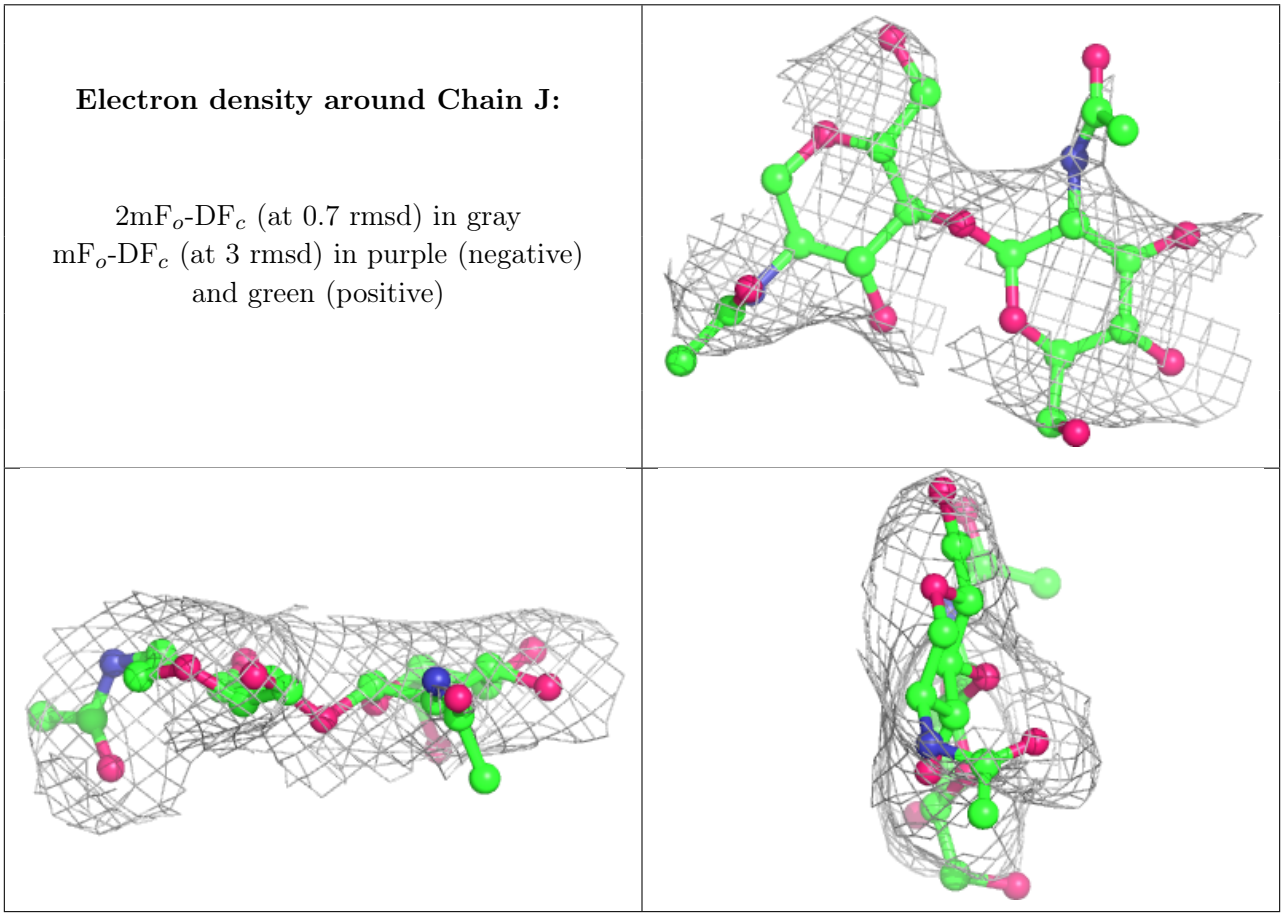
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	NAG	F	2	14/15	0.66	0.24	99,99,99,99	0
2	NAG	J	2	14/15	0.69	0.34	97,97,97,97	0
2	NAG	F	1	14/15	0.84	0.25	98,98,98,98	0
2	NAG	J	1	14/15	0.86	0.20	95,95,95,95	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.

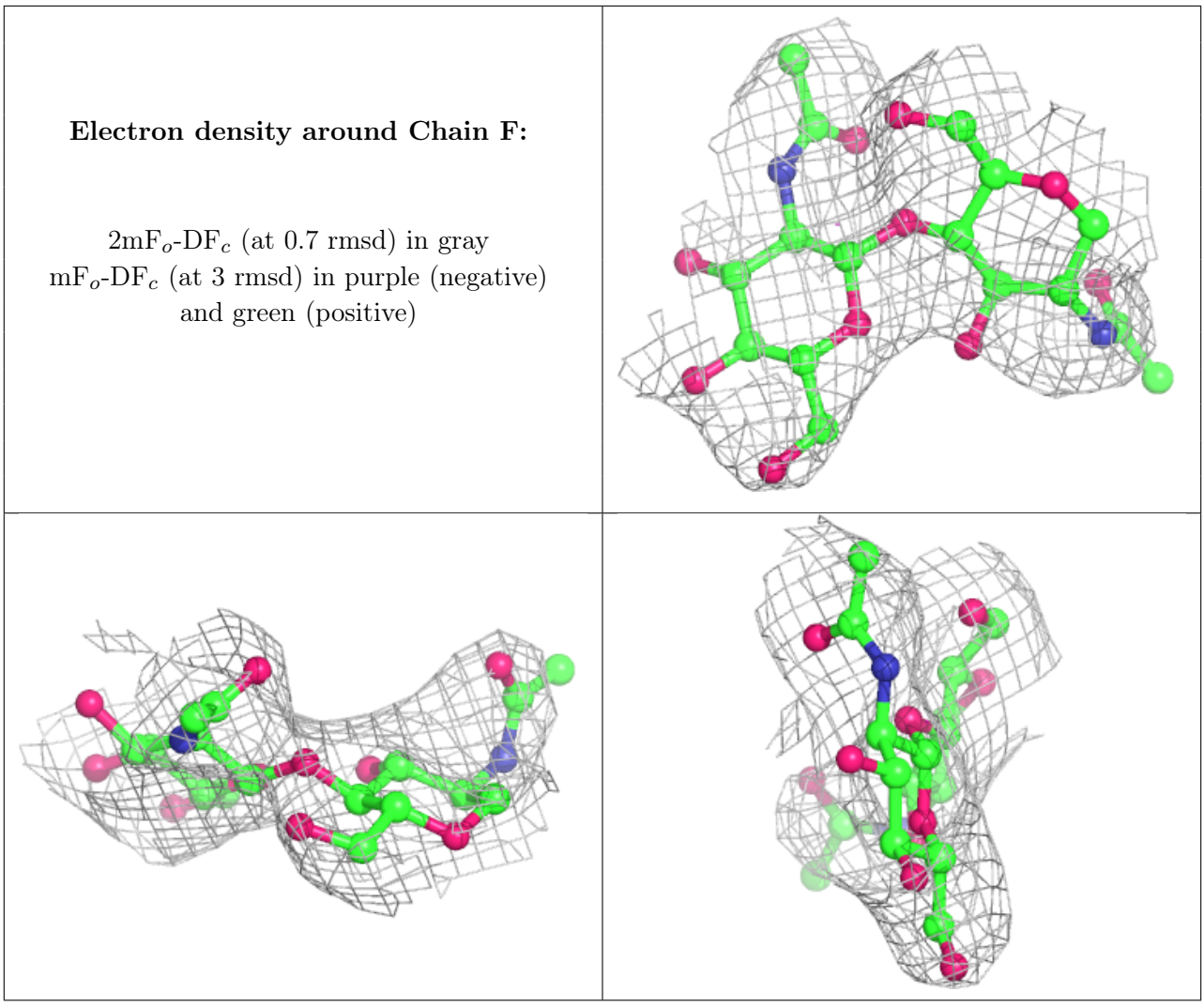
Electron density around Chain J:

$2mF_o$-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 F:

$2mF_o$-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, 95^{th} 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	GLC	K	403	11/12	0.51	0.36	108,108,108,108	0
3	NAG	G	401	14/15	0.70	0.32	97,97,97,97	0
4	GLC	G	403	11/12	0.71	0.24	95,95,95,95	0
3	NAG	C	401	14/15	0.77	0.27	94,94,94,94	0
4	GLC	K	402	11/12	0.77	0.22	107,107,107,107	0
4	GLC	C	403	11/12	0.77	0.28	74,74,74,74	0
4	GLC	E	402	11/12	0.83	0.22	80,80,80,80	0
3	NAG	K	401	14/15	0.83	0.26	94,94,94,94	0

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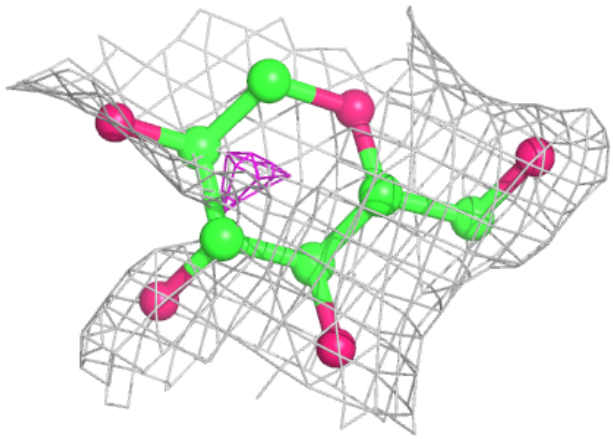
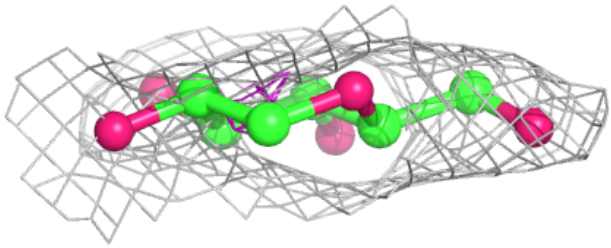
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	GLC	I	402	11/12	0.84	0.27	77,77,77,77	0
4	GLC	G	402	11/12	0.84	0.16	98,98,98,98	0
4	GLC	I	401	11/12	0.84	0.35	77,77,77,77	0
3	NAG	A	401	14/15	0.85	0.21	88,88,88,88	0
4	GLC	C	402	11/12	0.86	0.21	75,75,75,75	0
4	GLC	E	401	11/12	0.90	0.19	76,76,76,76	0

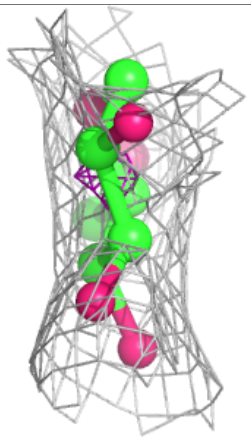
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around GLC K 403:

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

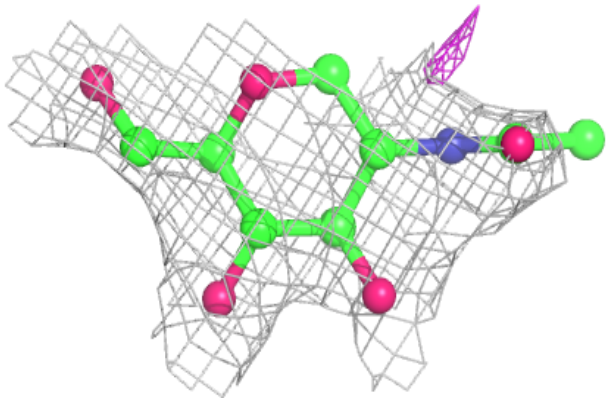


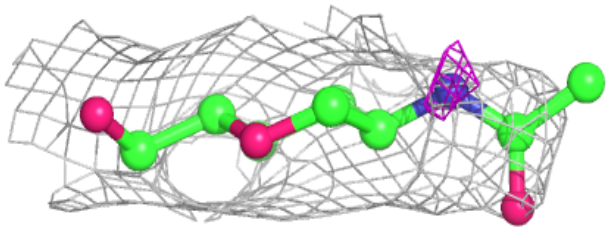


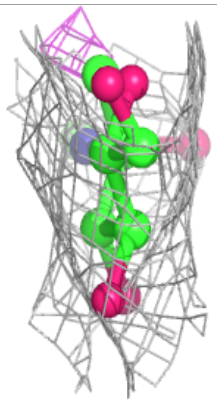


Electron density around NAG G 401:

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

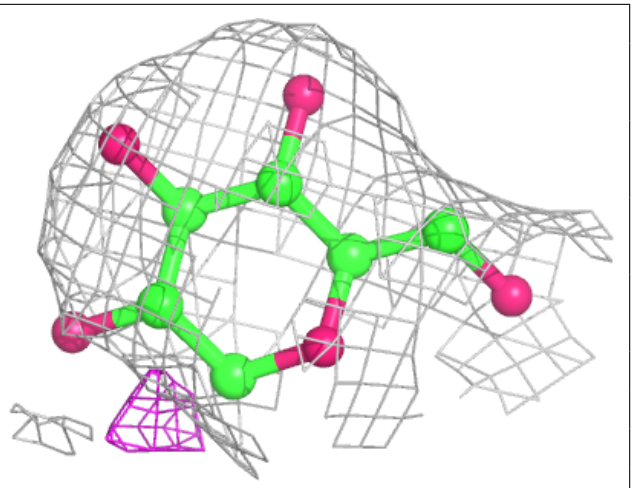


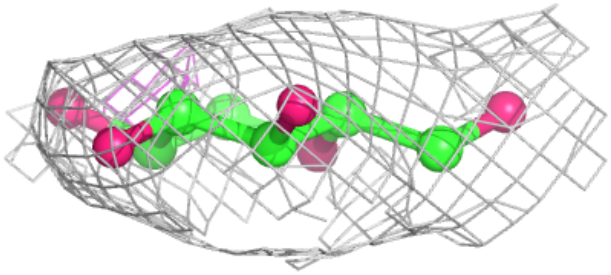


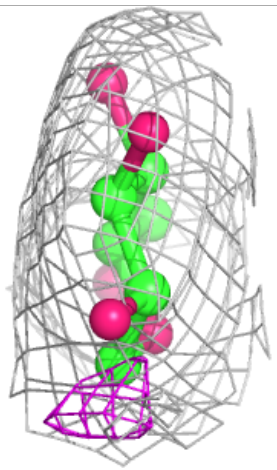


Electron density around GLC G 403:

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

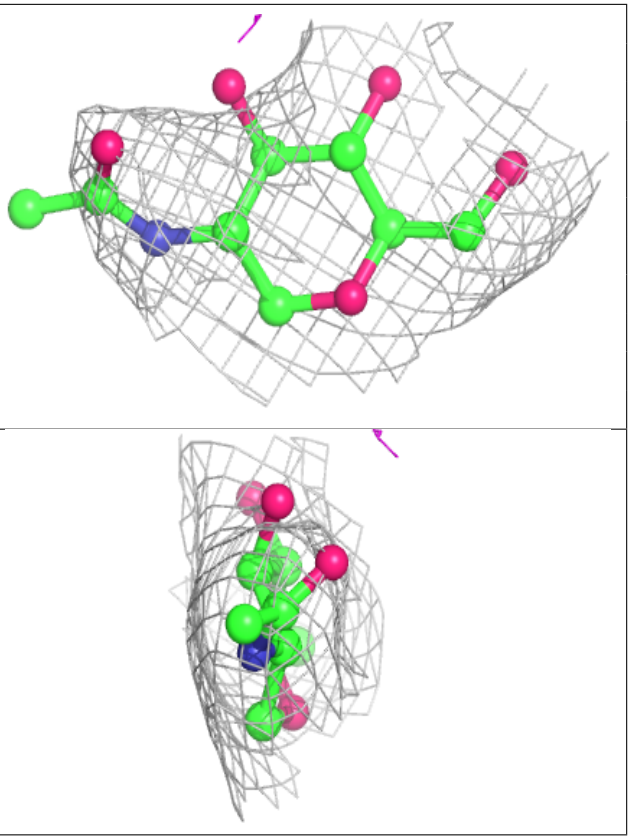


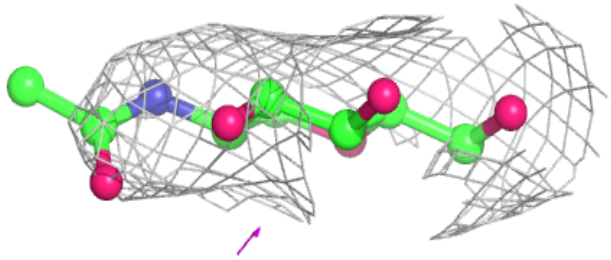




Electron density around NAG C 401:

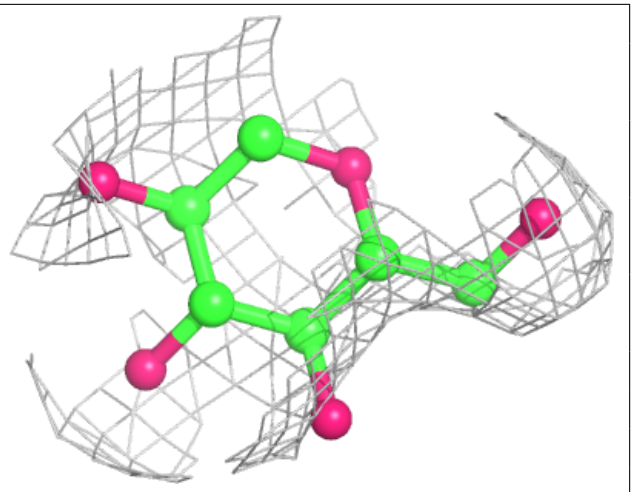
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

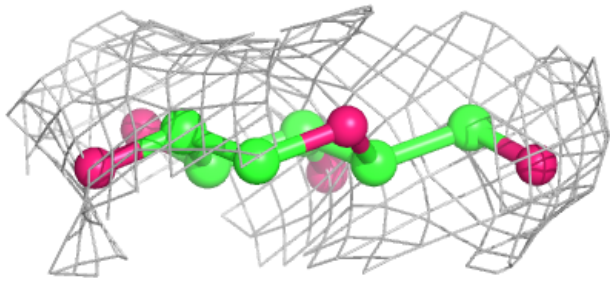


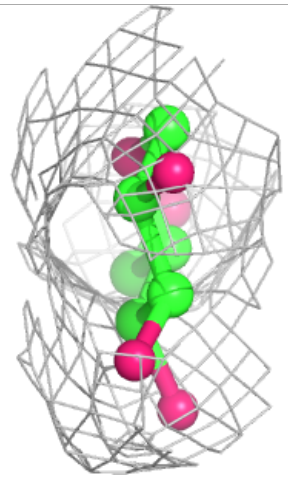


Electron density around GLC K 402:

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

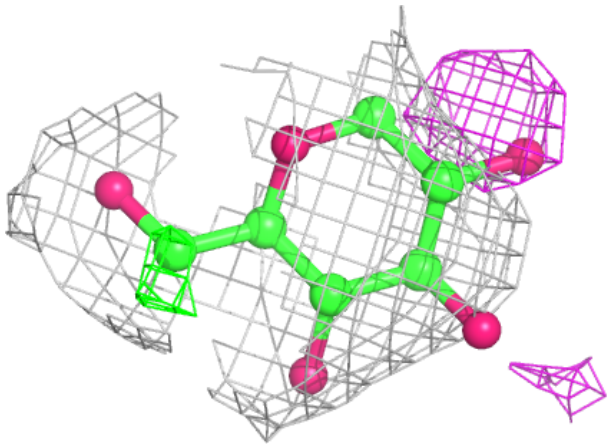


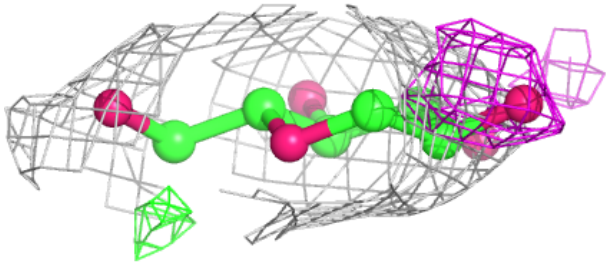


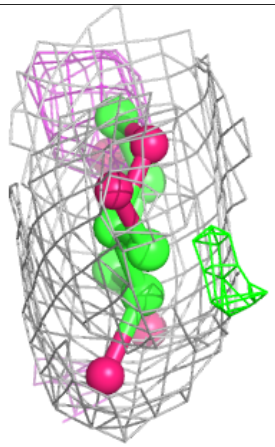


Electron density around GLC C 403:

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

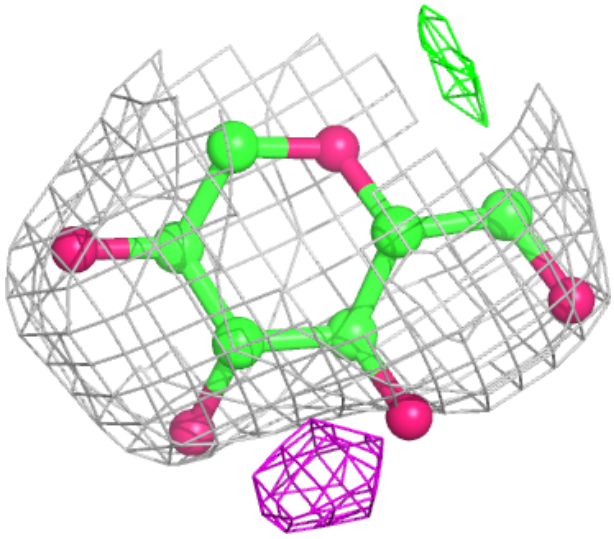


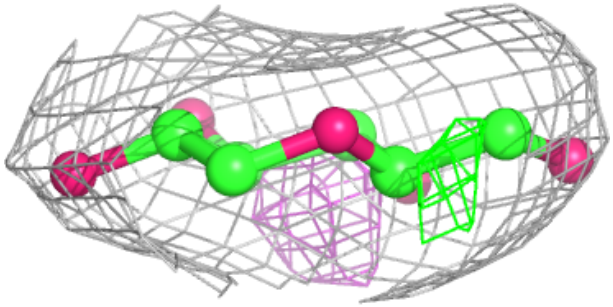


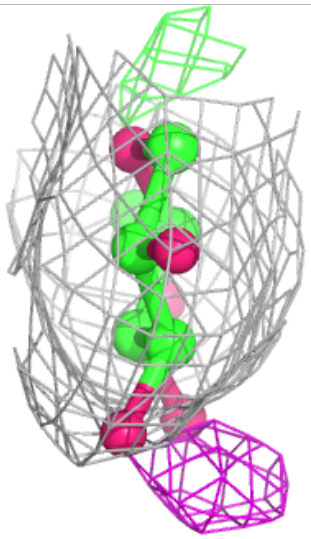


Electron density around GLC E 402:

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

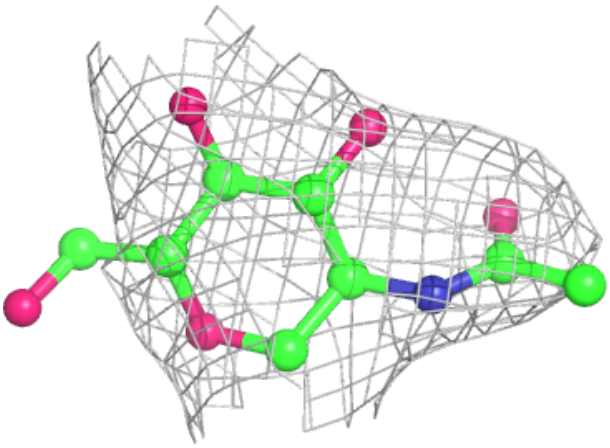


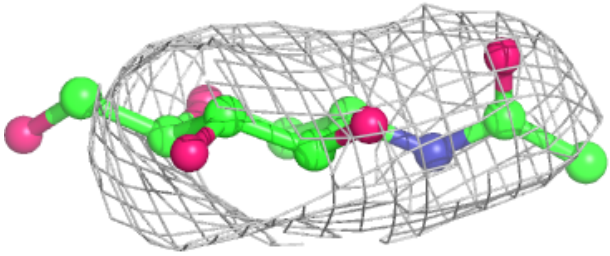


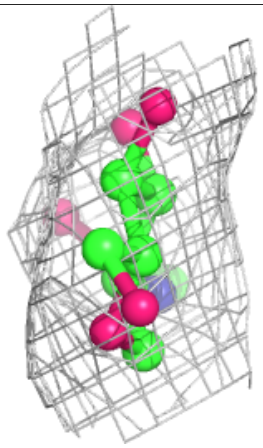


Electron density around NAG K 401:

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

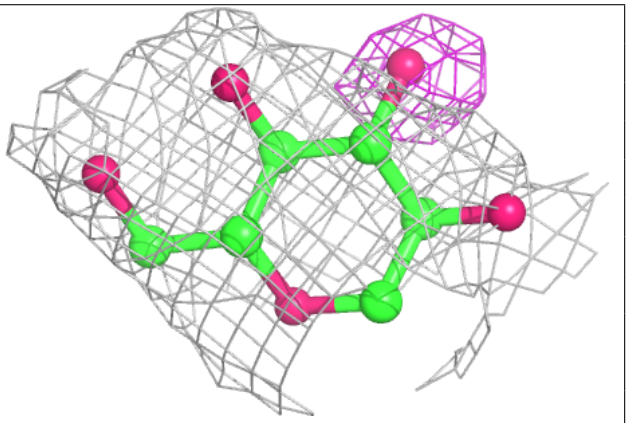


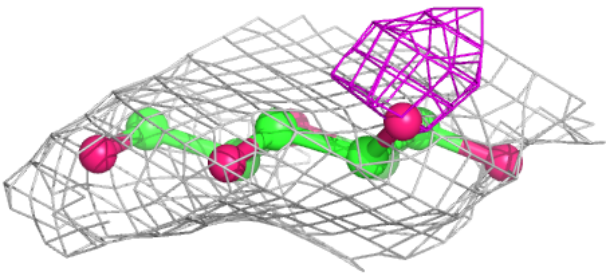


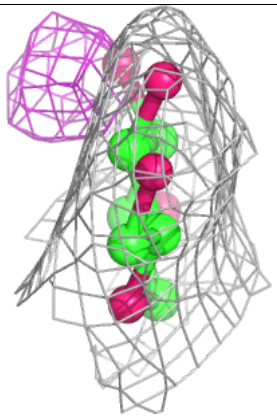


Electron density around GLC I 402:

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

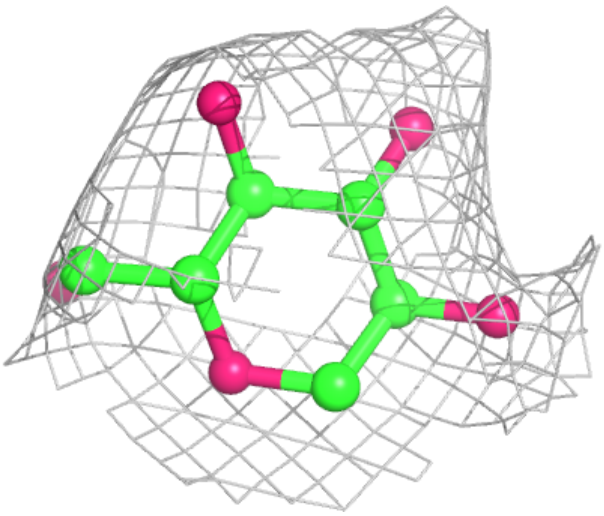


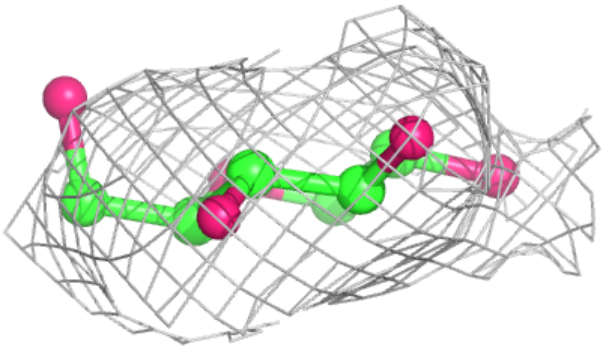


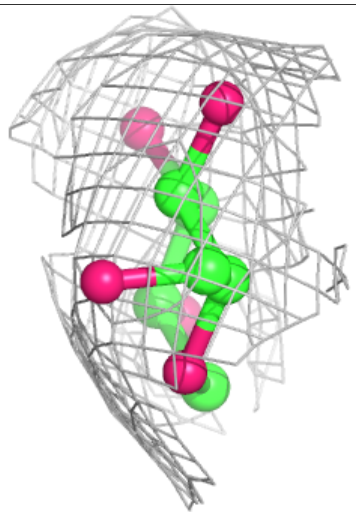


Electron density around GLC G 402:

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

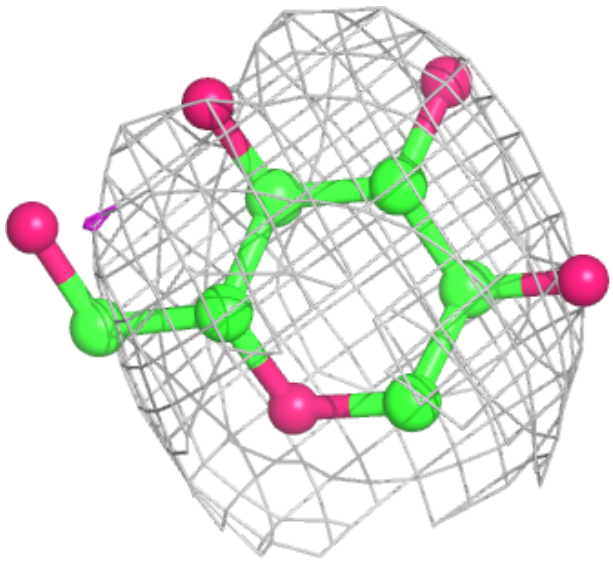


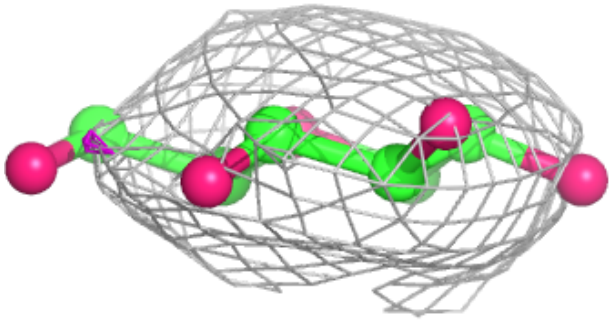


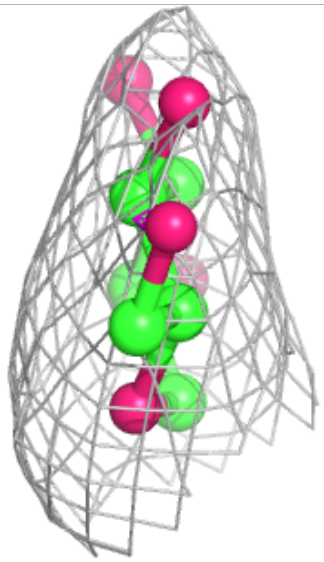


Electron density around GLC I 401:

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

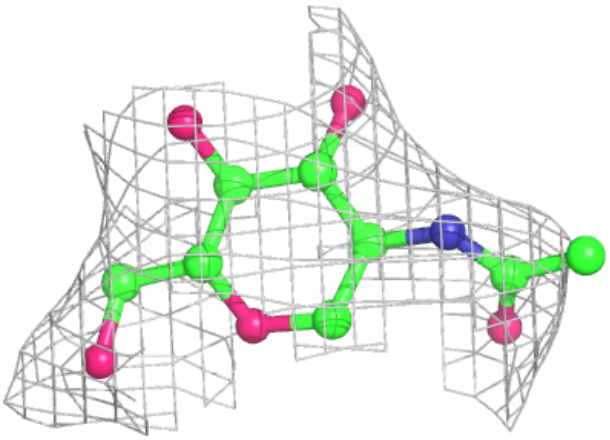


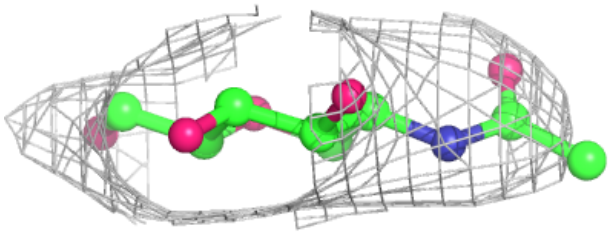


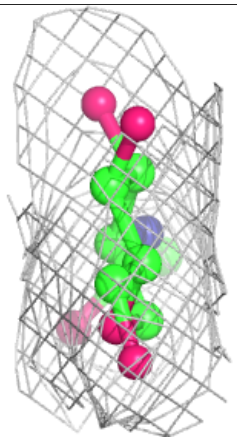


Electron density around NAG A 401:

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

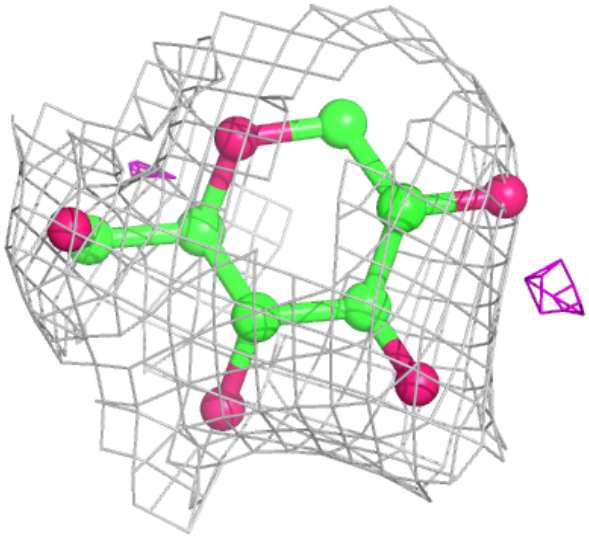


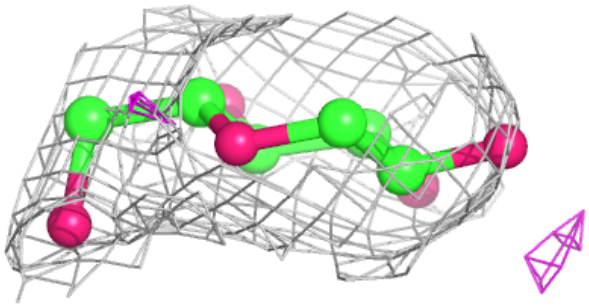


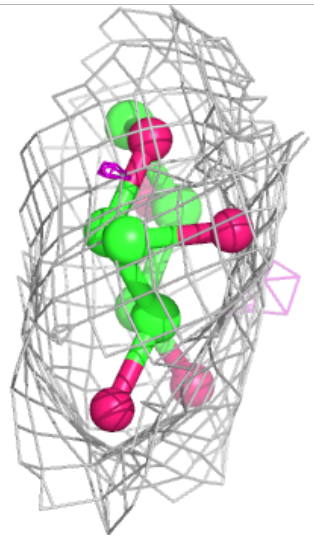


Electron density around GLC C 402:

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

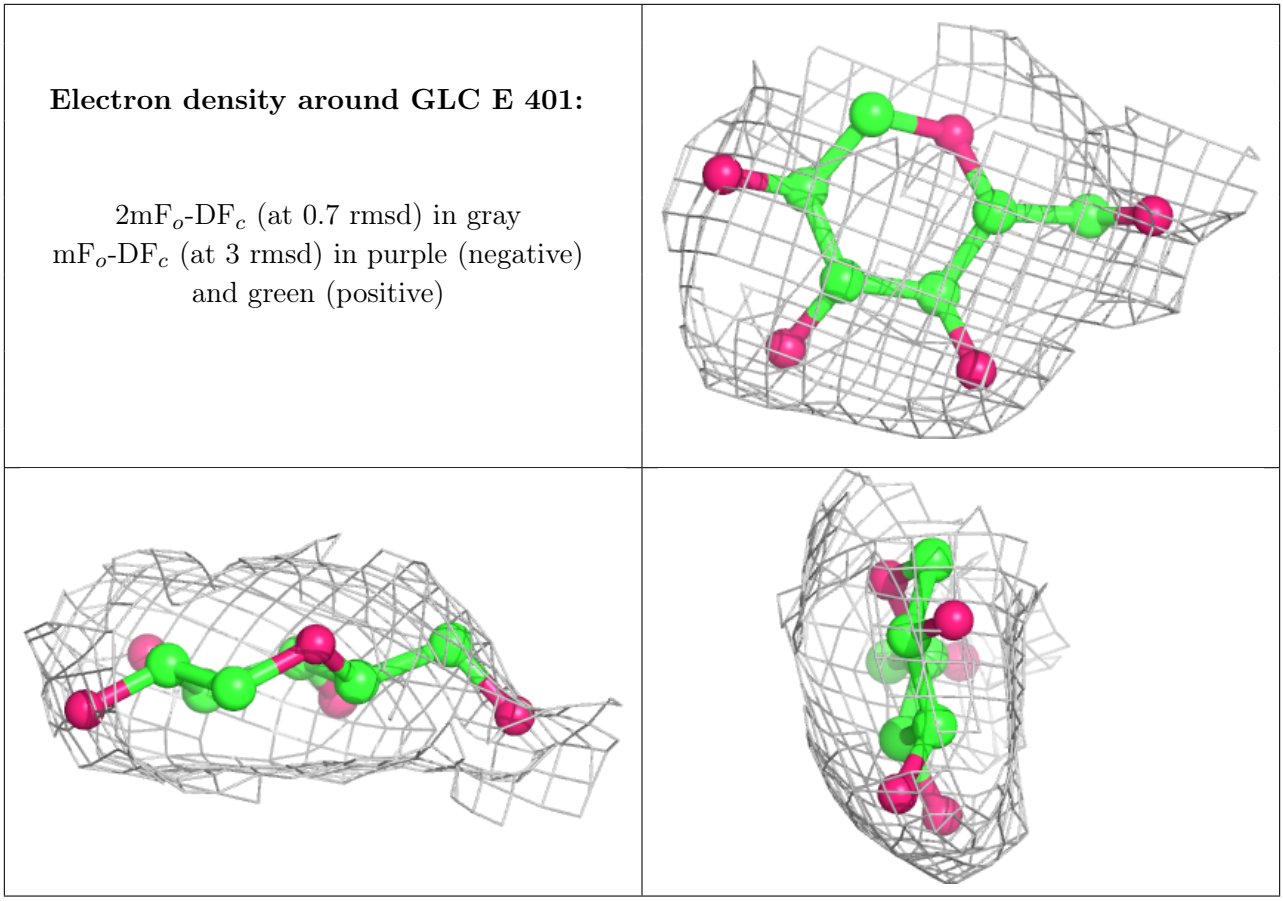






Electron density around GLC E 401:

$2mF_o$-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

There are no such residues in this entry.