



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 10:22 AM UTC

PDB ID : 6MFT / pdb_00006mft
Title : Crystal structure of glycosylated 426c HIV-1 gp120 core G459C in complex with gIVRC01 A60C heavy chain
Authors : Weidle, C.; Pancera, M.; Stamatatos, L.; Gray, M.
Deposited on : 2018-09-12
Resolution : 2.31 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

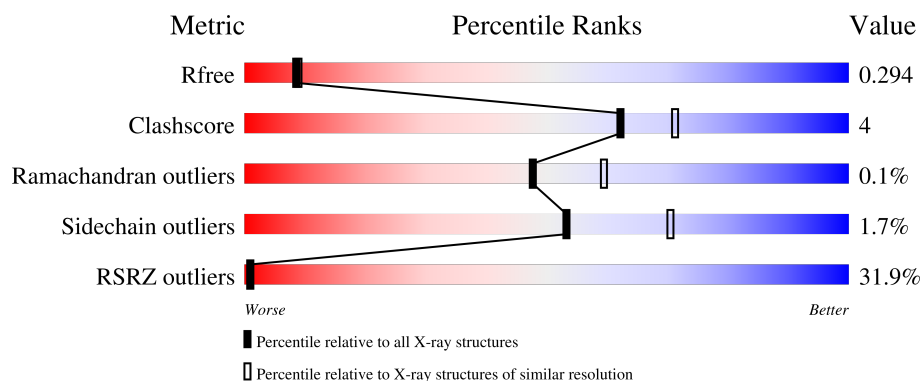
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.31 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	7754 (2.34-2.30)
Clashscore	190562	8383 (2.34-2.30)
Ramachandran outliers	187476	8303 (2.34-2.30)
Sidechain outliers	187428	8303 (2.34-2.30)
RSRZ outliers	180081	7760 (2.34-2.30)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	233	
1	H	233	
2	B	210	
2	L	210	
3	C	347	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	G	347	13% 91% 5%
4	D	2	50% 50%
4	E	2	50% 50%
5	F	6	17% 50% 33%
6	I	5	20% 80%

2 Entry composition [i](#)

There are 11 unique types of molecules in this entry. The entry contains 23916 atoms, of which 11446 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 Heavy Chain glVRC01.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	H	216	Total	C	H	N	O	S	0	0	0
			3223	1034	1582	281	317	9			
1	A	215	Total	C	H	N	O	S	0	0	0
			3216	1032	1579	280	316	9			

- Molecule 2 is a protein called Light chain glVRC01.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	L	208	Total	C	H	N	O	S	0	0	0
			3158	1007	1554	269	324	4			
2	B	209	Total	C	H	N	O	S	0	0	0
			3177	1012	1564	270	327	4			

- Molecule 3 is a protein called Gp120.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
3	G	336	Total	C	H	N	O	S	0	1	0
			5199	1647	2572	454	502	24			
3	C	336	Total	C	H	N	O	S	0	0	0
			5192	1645	2568	454	502	23			

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



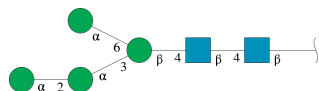
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	D	2	Total	C	N	O	0	0	0
			28	16	2	10			

Continued on next page...

Continued from previous page...

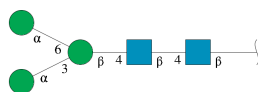
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	E	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 5 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



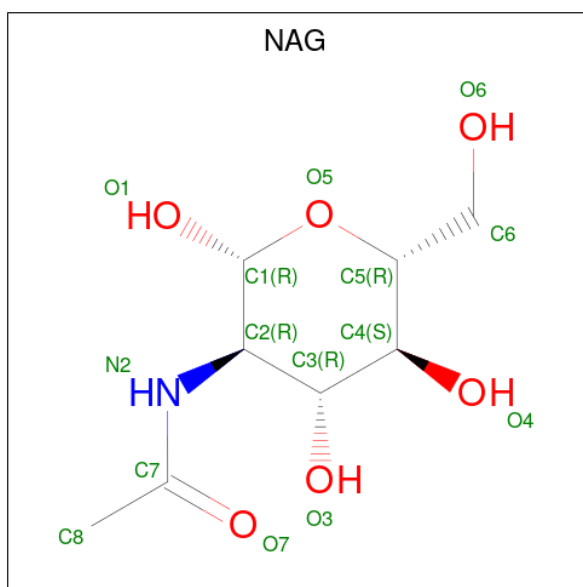
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	F	6	Total	C	N	O	0	0	0
			72	40	2	30			

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



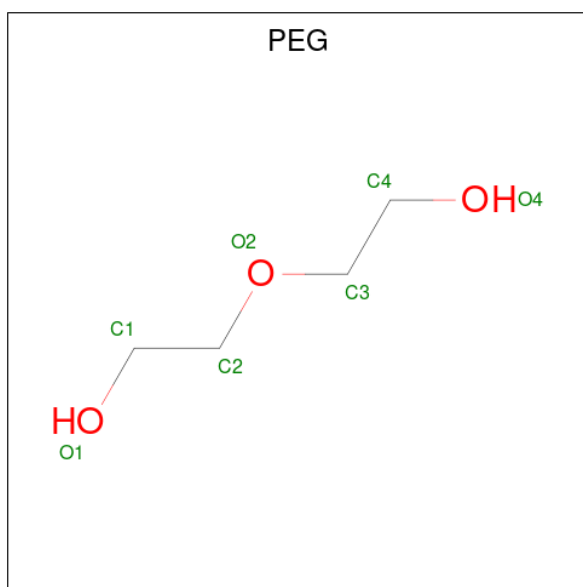
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
6	I	5	Total	C	N	O	0	0	0
			61	34	2	25			

- Molecule 7 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆) (labeled as "Ligand of Interest" by depositor).



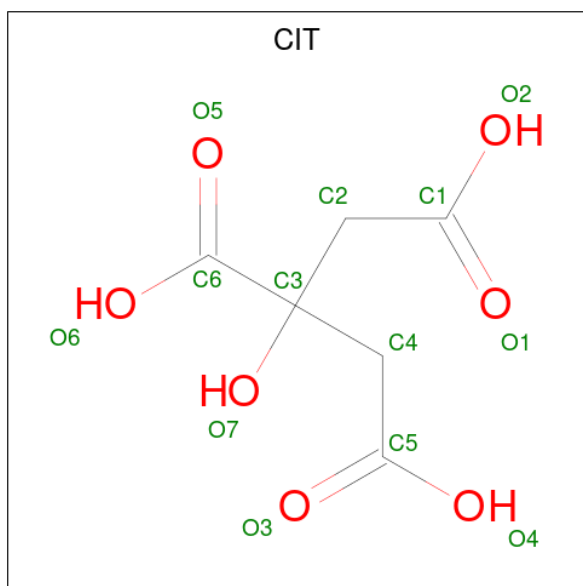
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	G	1	Total	C	N	O	0	0
			14	8	1	5		
7	G	1	Total	C	N	O	0	0
			14	8	1	5		
7	G	1	Total	C	N	O	0	0
			14	8	1	5		
7	G	1	Total	C	N	O	0	0
			14	8	1	5		
7	G	1	Total	C	N	O	0	0
			14	8	1	5		
7	G	1	Total	C	N	O	0	0
			14	8	1	5		
7	C	1	Total	C	N	O	0	0
			14	8	1	5		
7	C	1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

- Molecule 8 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: C₄H₁₀O₃).



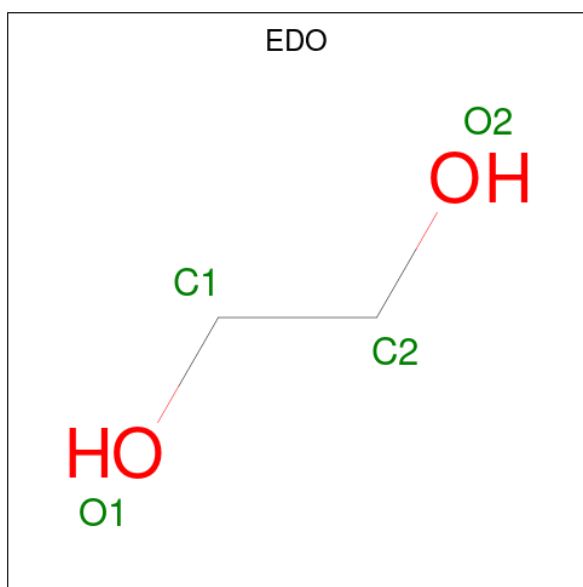
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	G	1	Total	C	H	O	0	0
			17	4	10	3		

- Molecule 9 is CITRIC ACID (CCD ID: CIT) (formula: $C_6H_8O_7$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
9	C	1	Total	C	H	O	0	0
			18	6	5	7		

- Molecule 10 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: $C_2H_6O_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
10	C	1	Total	C	H	O	0	0
			10	2	6	2		
10	C	1	Total	C	H	O	0	0
			10	2	6	2		

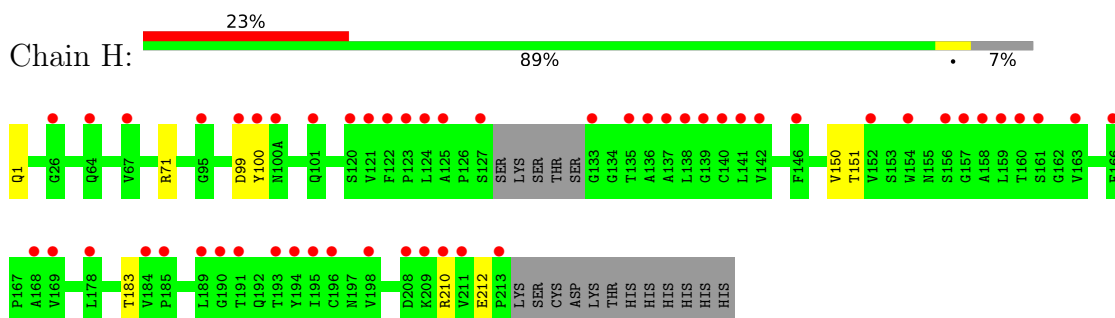
- Molecule 11 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	H	62	Total	O	0	0
			62	62		
11	L	44	Total	O	0	0
			44	44		
11	A	29	Total	O	0	0
			29	29		
11	B	23	Total	O	0	0
			23	23		
11	G	117	Total	O	0	0
			117	117		
11	C	50	Total	O	0	0
			50	50		

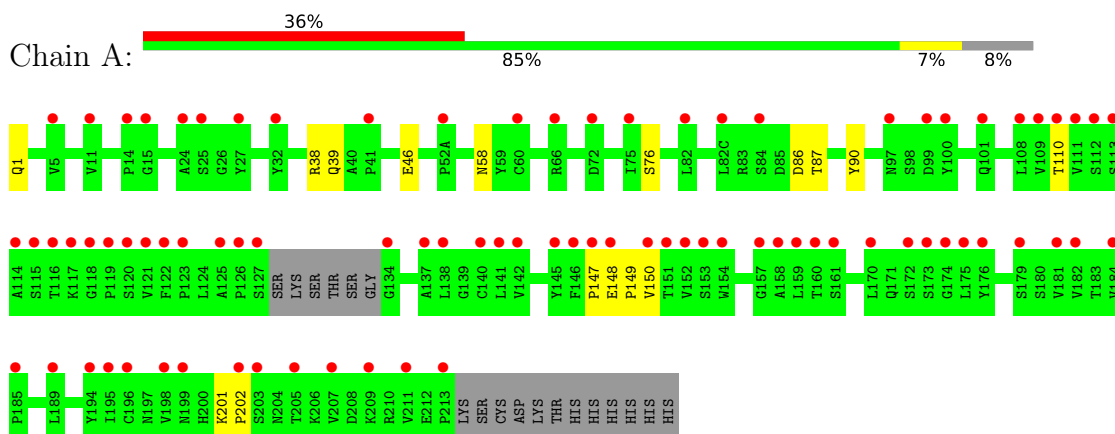
3 Residue-property plots [i](#)

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.

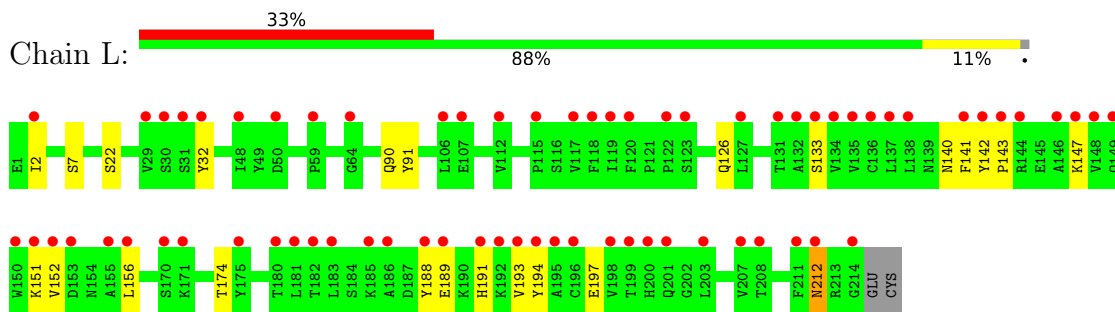
- Molecule 1: Heavy Chain gIVRC01



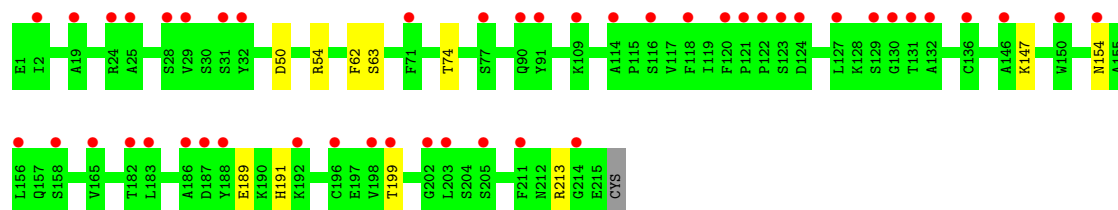
- Molecule 1: Heavy Chain gIVRC01



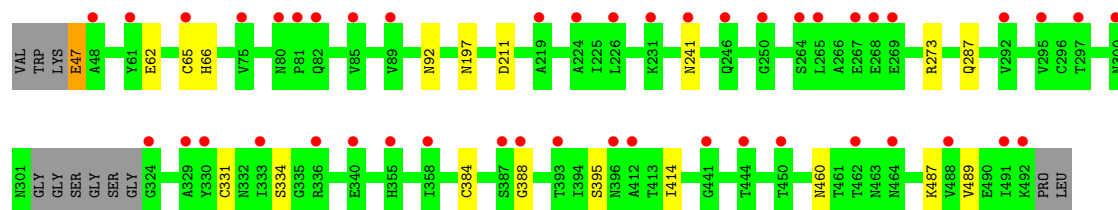
- Molecule 2: Light chain gIVRC01



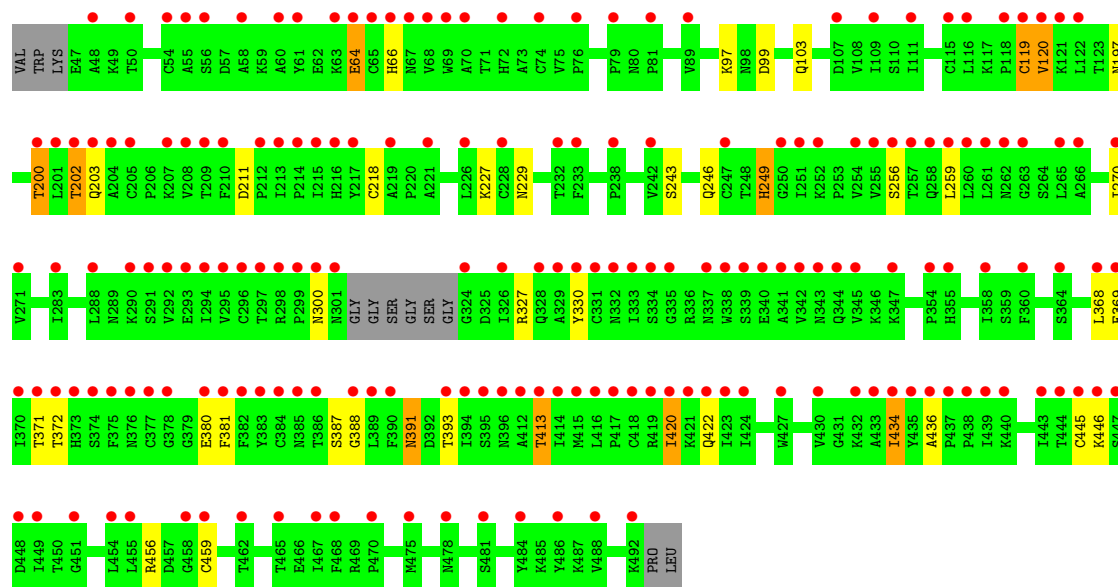
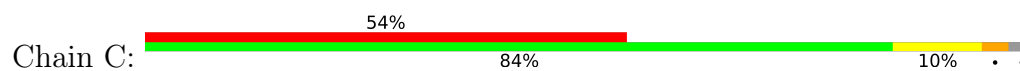
- Molecule 2: Light chain gIVRC01



• Molecule 3: Gp120



• Molecule 3: Gp120



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

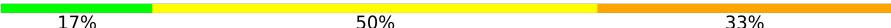


- Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain E:  50% 50%

MAG1
MAG2

- Molecule 5: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain F:  17% 50% 33%

MAG1
MAG2
BMA3
MAN4
MAN5
MAN6

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

Chain I:  20% 80%

MAG1
MAG2
BMA3
MAN4
MAN5

4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	197.08Å 109.00Å 103.22Å 90.00° 114.47° 90.00°	Depositor
Resolution (Å)	49.15 – 2.31 49.15 – 2.31	Depositor EDS
% Data completeness (in resolution range)	96.0 (49.15-2.31) 96.0 (49.15-2.31)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.35 (at 2.32Å)	Xtriage
Refinement program	PHENIX (1.12_2829)	Depositor
R, R_{free}	0.244 , 0.295 0.243 , 0.294	Depositor DCC
R_{free} test set	4263 reflections (4.93%)	wwPDB-VP
Wilson B-factor (Å ²)	49.9	Xtriage
Anisotropy	0.769	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 43.2	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	0.94	EDS
Total number of atoms	23916	wwPDB-VP
Average B, all atoms (Å ²)	81.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.63% 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: EDO, CIT, BMA, PCA, MAN, PEG, NAG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.11	0/1673	0.31	0/2281
1	H	0.11	0/1677	0.29	0/2286
2	B	0.11	0/1648	0.30	0/2238
2	L	0.12	0/1639	0.35	0/2226
3	C	0.12	0/2676	0.32	0/3630
3	G	0.11	0/2682	0.30	0/3638
All	All	0.12	0/11995	0.31	0/16299

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1637	1579	1579	10	0
1	H	1641	1582	1582	3	0
2	B	1613	1564	1564	6	0
2	L	1604	1554	1558	15	0
3	C	2624	2568	2573	33	1
3	G	2627	2572	2574	19	0
4	D	28	0	25	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	E	28	0	25	3	0
5	F	72	0	61	6	0
6	I	61	0	52	4	0
7	C	84	0	78	14	0
7	G	98	0	91	8	0
8	G	7	10	10	0	0
9	C	13	5	5	1	0
10	C	8	12	12	0	0
11	A	29	0	0	1	0
11	B	23	0	0	0	0
11	C	50	0	0	5	0
11	G	117	0	0	1	0
11	H	62	0	0	1	0
11	L	44	0	0	2	0
All	All	12470	11446	11789	97	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

All (97) 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:A:39:GLN:O	11:A:301:HOH:O	1.97	0.81
3:C:372:THR:OG1	11:C:1701:HOH:O	1.97	0.81
3:C:393:THR:CG2	7:C:1609:NAG:H4	2.15	0.76
3:G:197:ASN:OD1	7:G:511:NAG:H61	1.86	0.76
3:G:92:ASN:O	3:G:487:LYS:NZ	2.15	0.75
9:C:1612:CIT:O3	9:C:1612:CIT:O7	2.05	0.74
2:L:32:TYR:O	2:L:90:GLN:NE2	2.22	0.72
1:H:183:THR:O	11:H:301:HOH:O	2.07	0.72
7:C:1602:NAG:O4	11:C:1702:HOH:O	2.07	0.72
6:I:1:NAG:H62	6:I:2:NAG:N2	2.05	0.71
1:A:38:ARG:NH1	1:A:86:ASP:OD1	2.24	0.71
3:C:391:ASN:N	3:C:391:ASN:OD1	2.24	0.70
3:C:436:ALA:O	11:C:1703:HOH:O	2.10	0.69
3:G:47:GLU:N	3:G:47:GLU:OE1	2.26	0.68
3:G:388:GLY:O	7:G:505:NAG:H82	1.94	0.68
3:C:246:GLN:NE2	11:C:1704:HOH:O	2.27	0.68
3:C:227:LYS:NZ	3:C:229:ASN:OD1	2.26	0.68
7:C:1611:NAG:O7	7:C:1611:NAG:O3	2.11	0.67
2:L:151:LYS:NZ	2:L:197:GLU:OE2	2.25	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:189:GLU:OE1	11:L:301:HOH:O	2.13	0.66
3:G:334:SER:OG	7:G:508:NAG:H82	1.96	0.66
3:C:393:THR:HG21	7:C:1609:NAG:H4	1.79	0.64
3:C:327:ARG:NH2	3:C:422:GLN:OE1	2.30	0.63
3:C:391:ASN:HB3	7:C:1609:NAG:O5	1.99	0.62
4:E:1:NAG:O6	4:E:2:NAG:H83	1.98	0.62
5:F:1:NAG:H61	5:F:2:NAG:N2	2.15	0.61
2:L:188:TYR:O	2:L:194:TYR:OH	2.17	0.60
3:G:197:ASN:ND2	7:G:511:NAG:O7	2.34	0.59
2:B:189:GLU:OE1	2:B:213:ARG:NH1	2.36	0.59
2:L:142:TYR:CD2	2:L:143:PRO:HA	2.38	0.59
3:C:256:SER:OG	3:C:259:LEU:O	2.16	0.57
2:L:147:LYS:NZ	11:L:304:HOH:O	2.37	0.57
3:C:270:ILE:H	7:C:1611:NAG:H82	1.70	0.57
1:A:58:ASN:ND2	3:C:456:ARG:O	2.37	0.56
2:B:63:SER:OG	2:B:74:THR:OG1	2.23	0.55
3:G:241:ASN:OD1	7:G:501:NAG:H2	2.07	0.54
4:E:1:NAG:O4	4:E:2:NAG:H61	2.07	0.53
3:G:62:GLU:OE1	5:F:4:MAN:O6	2.26	0.52
1:H:210:ARG:NH2	1:H:212:GLU:OE2	2.38	0.51
3:C:119:CYS:O	3:C:203:GLN:N	2.40	0.51
2:L:126:GLN:OE1	2:L:133:SER:N	2.44	0.51
1:A:86:ASP:OD1	1:A:90:TYR:OH	2.29	0.51
3:C:120:VAL:HG22	3:C:434:ILE:HB	1.92	0.51
6:I:1:NAG:H62	6:I:2:NAG:HN2	1.74	0.50
2:B:54:ARG:NH1	2:B:62:PHE:O	2.41	0.50
3:C:197:ASN:HD21	7:C:1603:NAG:H4	1.76	0.49
2:B:191:HIS:O	2:B:213:ARG:NE	2.43	0.49
3:C:99:ASP:OD2	3:C:103:GLN:NE2	2.41	0.49
3:C:388:GLY:HA2	3:C:391:ASN:HD21	1.77	0.48
1:A:38:ARG:NE	1:A:46:GLU:OE2	2.40	0.48
1:A:76:SER:OG	7:C:1603:NAG:H61	2.14	0.48
5:F:4:MAN:C1	5:F:5:MAN:H5	2.44	0.48
3:C:229:ASN:ND2	7:C:1610:NAG:H61	2.29	0.48
2:L:152:VAL:HA	2:L:193:VAL:O	2.14	0.48
3:C:197:ASN:ND2	7:C:1603:NAG:H4	2.31	0.46
3:G:460:ASN:OD1	11:G:601:HOH:O	2.21	0.46
2:L:212:ASN:OD1	2:L:212:ASN:N	2.49	0.46
3:G:62:GLU:OE2	5:F:4:MAN:H62	2.15	0.46
3:C:300:ASN:OD1	3:C:300:ASN:N	2.49	0.46
3:C:446:LYS:O	6:I:1:NAG:H5	2.16	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:249:HIS:C	3:C:249:HIS:CD2	2.94	0.46
3:C:387:SER:OG	7:C:1602:NAG:H5	2.16	0.45
1:A:201:LYS:N	1:A:202:PRO:HD2	2.31	0.45
1:H:99:ASP:OD1	1:H:100:TYR:N	2.46	0.45
2:L:151:LYS:HA	2:L:156:LEU:HA	1.97	0.45
3:G:241:ASN:OD1	7:G:501:NAG:C2	2.65	0.45
3:G:414:ILE:HG12	7:G:505:NAG:H81	1.99	0.45
2:L:141:PHE:N	2:L:174:THR:OG1	2.50	0.45
1:A:148:GLU:N	1:A:149:PRO:HD2	2.32	0.45
2:B:154:ASN:O	2:B:154:ASN:ND2	2.49	0.45
3:C:393:THR:HG23	7:C:1609:NAG:H4	1.99	0.44
3:C:229:ASN:ND2	3:C:243:SER:OG	2.50	0.44
7:C:1611:NAG:HO3	7:C:1611:NAG:C7	2.18	0.43
3:C:97:LYS:NZ	11:C:1706:HOH:O	2.51	0.43
2:L:91:TYR:OH	4:D:1:NAG:H61	2.19	0.43
3:C:64:GLU:OE1	3:C:66:HIS:N	2.40	0.43
3:C:211:ASP:OD2	6:I:2:NAG:H5	2.19	0.42
2:L:152:VAL:HG11	2:L:191:HIS:HB3	2.02	0.42
1:A:147:PRO:HG2	1:A:202:PRO:HG3	2.02	0.42
3:G:395:SER:N	7:G:505:NAG:O7	2.47	0.42
3:G:211:ASP:OD2	5:F:2:NAG:H5	2.19	0.42
3:C:369:GLU:OE1	3:C:369:GLU:N	2.40	0.42
2:L:7:SER:OG	2:L:22:SER:OG	2.38	0.41
3:C:393:THR:HG23	7:C:1609:NAG:H2	2.02	0.41
3:G:331:CYS:SG	3:G:384:CYS:SG	3.18	0.41
2:B:147:LYS:HB3	2:B:199:THR:OG1	2.20	0.41
3:G:65[B]:CYS:SG	3:G:66:HIS:N	2.93	0.41
3:C:380:GLU:HB3	3:C:420:ILE:HD12	2.02	0.41
3:G:273:ARG:NH2	3:G:287:GLN:OE1	2.43	0.41
3:G:47:GLU:N	3:G:489:VAL:HA	2.36	0.41
2:L:151:LYS:CB	2:L:156:LEU:HA	2.50	0.41
5:F:1:NAG:H61	5:F:2:NAG:C7	2.50	0.41
3:G:47:GLU:N	3:G:489:VAL:HG12	2.35	0.40
3:C:381:PHE:O	3:C:420:ILE:HA	2.22	0.40
1:A:87:THR:HG23	1:A:110:THR:HA	2.04	0.40
3:C:368:LEU:HA	3:C:371:THR:HG22	2.03	0.40
4:E:1:NAG:O3	4:E:2:NAG:C1	2.68	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:200:THR:O	3:C:202:THR:H[2_557]	1.53	0.07

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	211/233 (91%)	201 (95%)	10 (5%)	0	100	100
1	H	212/233 (91%)	200 (94%)	12 (6%)	0	100	100
2	B	207/210 (99%)	193 (93%)	14 (7%)	0	100	100
2	L	206/210 (98%)	185 (90%)	20 (10%)	1 (0%)	24	30
3	C	332/347 (96%)	309 (93%)	22 (7%)	1 (0%)	36	45
3	G	333/347 (96%)	314 (94%)	19 (6%)	0	100	100
All	All	1501/1580 (95%)	1402 (93%)	97 (6%)	2 (0%)	48	59

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	413	THR
2	L	140	ASN

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	181/198 (91%)	180 (99%)	1 (1%)	78	88

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	H	181/198 (91%)	178 (98%)	3 (2%)	53	70
2	B	181/182 (100%)	180 (99%)	1 (1%)	78	88
2	L	180/182 (99%)	178 (99%)	2 (1%)	65	80
3	C	300/307 (98%)	286 (95%)	14 (5%)	23	34
3	G	301/307 (98%)	300 (100%)	1 (0%)	86	92
All	All	1324/1374 (96%)	1302 (98%)	22 (2%)	53	70

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	H	71	ARG
1	H	150	VAL
1	H	151	THR
2	L	2	ILE
2	L	212	ASN
1	A	150	VAL
2	B	50	ASP
3	G	47	GLU
3	C	64	GLU
3	C	119	CYS
3	C	120	VAL
3	C	200	THR
3	C	202	THR
3	C	218	CYS
3	C	249	HIS
3	C	330	TYR
3	C	391	ASN
3	C	413	THR
3	C	420	ILE
3	C	434	ILE
3	C	445	CYS
3	C	459	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	H	164	HIS
1	A	164	HIS
3	G	396	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	C	67	ASN
3	C	332	ASN
3	C	376	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

2 non-standard protein/DNA/RNA residues 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	$\# Z > 2$
1	PCA	H	1	1	7,8,9	2.32	2 (28%)	9,10,12	1.96	4 (44%)
1	PCA	A	1	1	7,8,9	2.31	2 (28%)	9,10,12	2.05	4 (44%)

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
1	PCA	H	1	1	-	0/0/11/13	0/1/1/1
1	PCA	A	1	1	-	0/0/11/13	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1	PCA	CD-N	4.98	1.46	1.34
1	H	1	PCA	CD-N	4.96	1.46	1.34
1	H	1	PCA	CA-N	3.45	1.50	1.46
1	A	1	PCA	CA-N	3.38	1.50	1.46

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1	PCA	CA-N-CD	-3.13	102.85	113.58
1	A	1	PCA	OE-CD-CG	-2.90	121.54	126.72
1	H	1	PCA	CA-N-CD	-2.88	103.71	113.58
1	H	1	PCA	OE-CD-CG	-2.83	121.67	126.72
1	A	1	PCA	CB-CA-N	2.56	110.29	103.24
1	H	1	PCA	CB-CA-N	2.54	110.24	103.24
1	H	1	PCA	CG-CD-N	2.52	114.56	108.39
1	A	1	PCA	CG-CD-N	2.50	114.52	108.39

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

15 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	D	1	4,3	14,14,15	0.19	0	17,19,21	0.45	0
4	NAG	D	2	4	14,14,15	0.25	0	17,19,21	0.46	0
4	NAG	E	1	4,3	14,14,15	0.45	0	17,19,21	0.58	0
4	NAG	E	2	4	14,14,15	0.28	0	17,19,21	0.77	1 (5%)
5	NAG	F	1	5,3	14,14,15	0.40	0	17,19,21	0.60	0
5	NAG	F	2	5	14,14,15	0.22	0	17,19,21	0.43	0
5	BMA	F	3	5	11,11,12	0.60	0	15,15,17	0.75	0
5	MAN	F	4	5	11,11,12	0.72	0	15,15,17	0.96	1 (6%)
5	MAN	F	5	5	11,11,12	0.64	0	15,15,17	0.99	2 (13%)
5	MAN	F	6	5	11,11,12	0.61	0	15,15,17	1.15	2 (13%)
6	NAG	I	1	6,3	14,14,15	0.32	0	17,19,21	0.50	0
6	NAG	I	2	6	14,14,15	0.24	0	17,19,21	0.40	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	BMA	I	3	6	11,11,12	0.64	0	15,15,17	0.73	0
6	MAN	I	4	6	11,11,12	0.69	0	15,15,17	0.98	2 (13%)
6	MAN	I	5	6	11,11,12	1.01	0	15,15,17	1.13	1 (6%)

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

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

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	E	2	NAG	C1-O5-C5	2.84	115.99	112.19
5	F	6	MAN	C1-O5-C5	2.72	115.83	112.19
6	I	4	MAN	C1-O5-C5	2.48	115.50	112.19
5	F	5	MAN	C1-O5-C5	2.40	115.40	112.19
5	F	4	MAN	O2-C2-C3	-2.37	105.23	110.15
5	F	6	MAN	O2-C2-C3	-2.23	105.52	110.15
6	I	4	MAN	O2-C2-C3	-2.16	105.67	110.15
6	I	5	MAN	O2-C2-C3	-2.16	105.67	110.15
5	F	5	MAN	O2-C2-C3	-2.00	106.00	110.15

There are no chirality outliers.

All (18) torsion outliers are listed below:

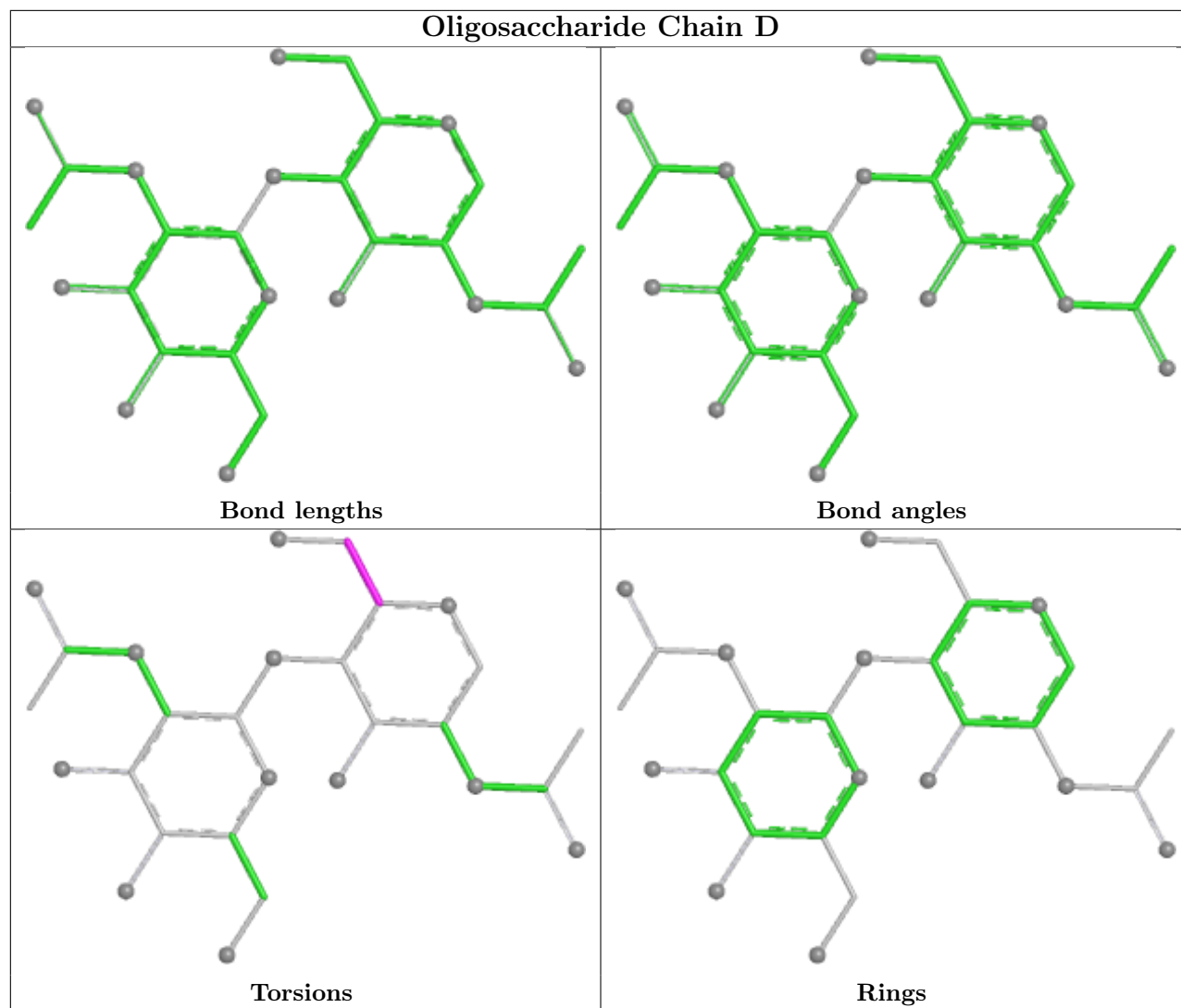
Mol	Chain	Res	Type	Atoms
6	I	3	BMA	O5-C5-C6-O6
4	E	1	NAG	O5-C5-C6-O6
5	F	4	MAN	O5-C5-C6-O6
4	E	1	NAG	C4-C5-C6-O6
4	D	1	NAG	O5-C5-C6-O6
5	F	2	NAG	O5-C5-C6-O6
6	I	5	MAN	O5-C5-C6-O6
4	D	1	NAG	C4-C5-C6-O6
6	I	3	BMA	C4-C5-C6-O6
5	F	2	NAG	C4-C5-C6-O6
4	E	2	NAG	C8-C7-N2-C2
4	E	2	NAG	O7-C7-N2-C2
6	I	4	MAN	O5-C5-C6-O6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

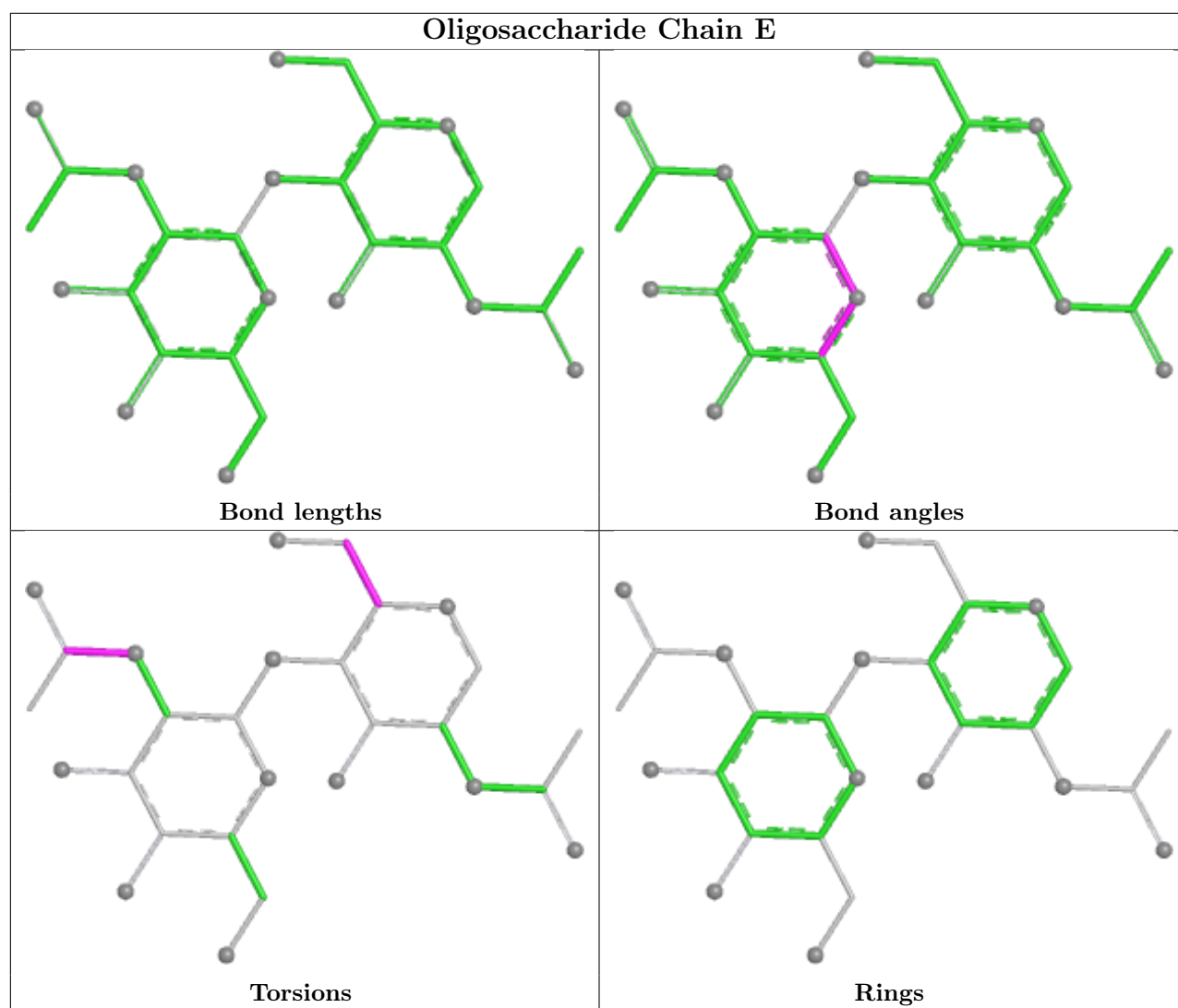
There are no ring outliers.

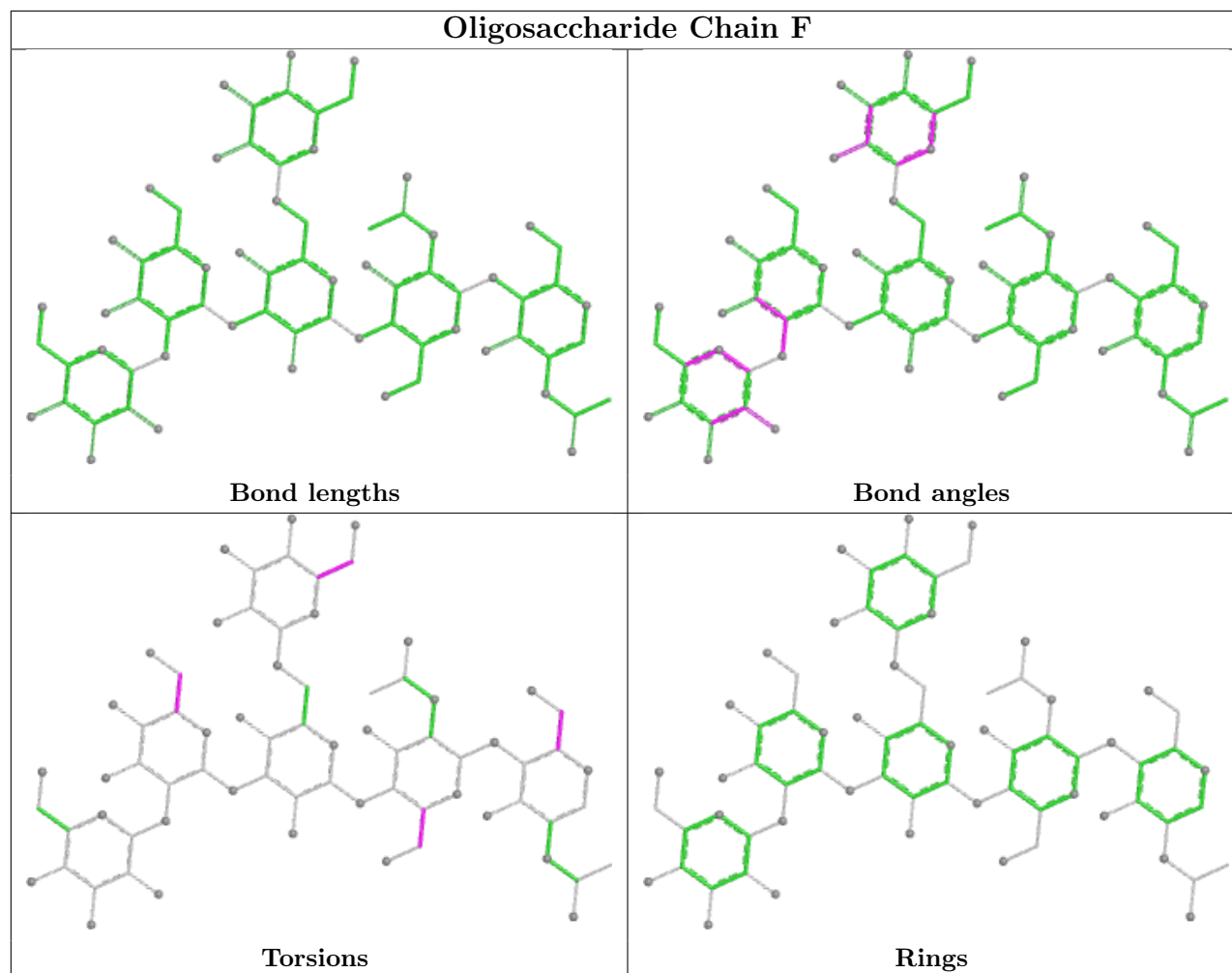
9 monomers are involved in 14 short contacts:

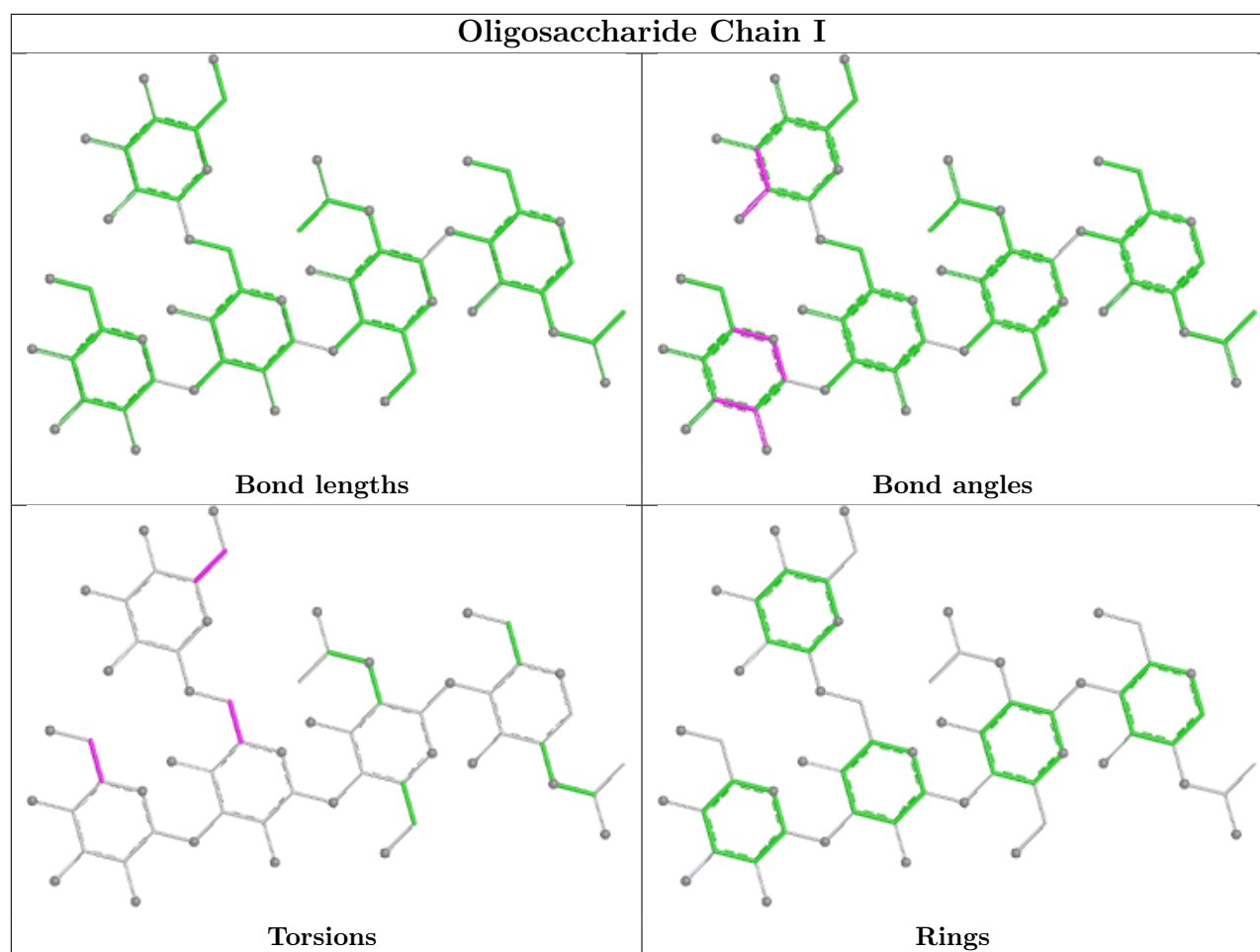
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	E	1	NAG	3	0
5	F	4	MAN	3	0
5	F	1	NAG	2	0
5	F	5	MAN	1	0
4	E	2	NAG	3	0
5	F	2	NAG	3	0
6	I	1	NAG	3	0
6	I	2	NAG	3	0
4	D	1	NAG	1	0

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









5.6 Ligand geometry [i](#)

17 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	$\# Z > 2$
7	NAG	C	1611	3	14,14,15	0.29	0	17,19,21	0.39	0
9	CIT	C	1612	-	12,12,12	1.08	0	17,17,17	1.61	2 (11%)
7	NAG	G	501	3	14,14,15	0.28	0	17,19,21	0.46	0
7	NAG	C	1609	3	14,14,15	0.22	0	17,19,21	0.39	0
7	NAG	G	505	3	14,14,15	0.21	0	17,19,21	0.40	0
7	NAG	C	1610	3	14,14,15	0.28	0	17,19,21	0.52	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	NAG	C	1603	3	14,14,15	0.53	0	17,19,21	0.78	1 (5%)
7	NAG	G	507	3	14,14,15	0.22	0	17,19,21	0.42	0
7	NAG	G	511	3	14,14,15	1.39	1 (7%)	17,19,21	1.67	1 (5%)
10	EDO	C	1614	-	3,3,3	0.42	0	2,2,2	0.35	0
7	NAG	C	1601	3	14,14,15	0.21	0	17,19,21	0.44	0
10	EDO	C	1613	-	3,3,3	0.41	0	2,2,2	0.36	0
7	NAG	C	1602	3	14,14,15	0.24	0	17,19,21	0.40	0
7	NAG	G	506	3	14,14,15	0.23	0	17,19,21	0.45	0
7	NAG	G	504	3	14,14,15	0.19	0	17,19,21	0.47	0
7	NAG	G	508	3	14,14,15	0.26	0	17,19,21	0.46	0
8	PEG	G	518	-	6,6,6	0.49	0	5,5,5	0.21	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
7	NAG	C	1611	3	-	2/6/23/26	0/1/1/1
9	CIT	C	1612	-	-	3/16/16/16	-
7	NAG	G	501	3	-	2/6/23/26	0/1/1/1
7	NAG	C	1609	3	-	0/6/23/26	0/1/1/1
7	NAG	G	505	3	-	2/6/23/26	0/1/1/1
7	NAG	C	1610	3	-	2/6/23/26	0/1/1/1
7	NAG	C	1603	3	-	2/6/23/26	0/1/1/1
7	NAG	G	507	3	-	0/6/23/26	0/1/1/1
7	NAG	G	511	3	-	3/6/23/26	0/1/1/1
10	EDO	C	1614	-	-	0/1/1/1	-
7	NAG	C	1601	3	-	2/6/23/26	0/1/1/1
10	EDO	C	1613	-	-	0/1/1/1	-
7	NAG	C	1602	3	-	2/6/23/26	0/1/1/1
7	NAG	G	506	3	-	4/6/23/26	0/1/1/1
7	NAG	G	504	3	-	2/6/23/26	0/1/1/1
7	NAG	G	508	3	-	0/6/23/26	0/1/1/1
8	PEG	G	518	-	-	0/4/4/4	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	G	511	NAG	O5-C1	5.03	1.52	1.43

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	G	511	NAG	C1-O5-C5	6.63	121.07	112.19
9	C	1612	CIT	O6-C6-C3	4.26	121.31	113.14
7	C	1603	NAG	C1-O5-C5	2.93	116.11	112.19
9	C	1612	CIT	C3-C4-C5	-2.19	107.95	113.92

There are no chirality outliers.

All (26) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	G	511	NAG	C1-C2-N2-C7
9	C	1612	CIT	O7-C3-C4-C5
7	G	506	NAG	C4-C5-C6-O6
7	G	505	NAG	O5-C5-C6-O6
7	G	506	NAG	O5-C5-C6-O6
7	C	1601	NAG	C4-C5-C6-O6
7	C	1602	NAG	O5-C5-C6-O6
7	C	1601	NAG	O5-C5-C6-O6
7	C	1610	NAG	O5-C5-C6-O6
7	G	505	NAG	C4-C5-C6-O6
7	C	1602	NAG	C4-C5-C6-O6
7	G	506	NAG	C8-C7-N2-C2
7	G	506	NAG	O7-C7-N2-C2
7	C	1603	NAG	C8-C7-N2-C2
7	C	1603	NAG	O7-C7-N2-C2
7	G	501	NAG	O5-C5-C6-O6
7	G	504	NAG	C4-C5-C6-O6
7	C	1610	NAG	C4-C5-C6-O6
9	C	1612	CIT	C6-C3-C4-C5
7	G	504	NAG	O5-C5-C6-O6
9	C	1612	CIT	C2-C3-C4-C5
7	G	511	NAG	C4-C5-C6-O6
7	C	1611	NAG	C1-C2-N2-C7
7	G	501	NAG	C4-C5-C6-O6
7	C	1611	NAG	C3-C2-N2-C7
7	G	511	NAG	O5-C5-C6-O6

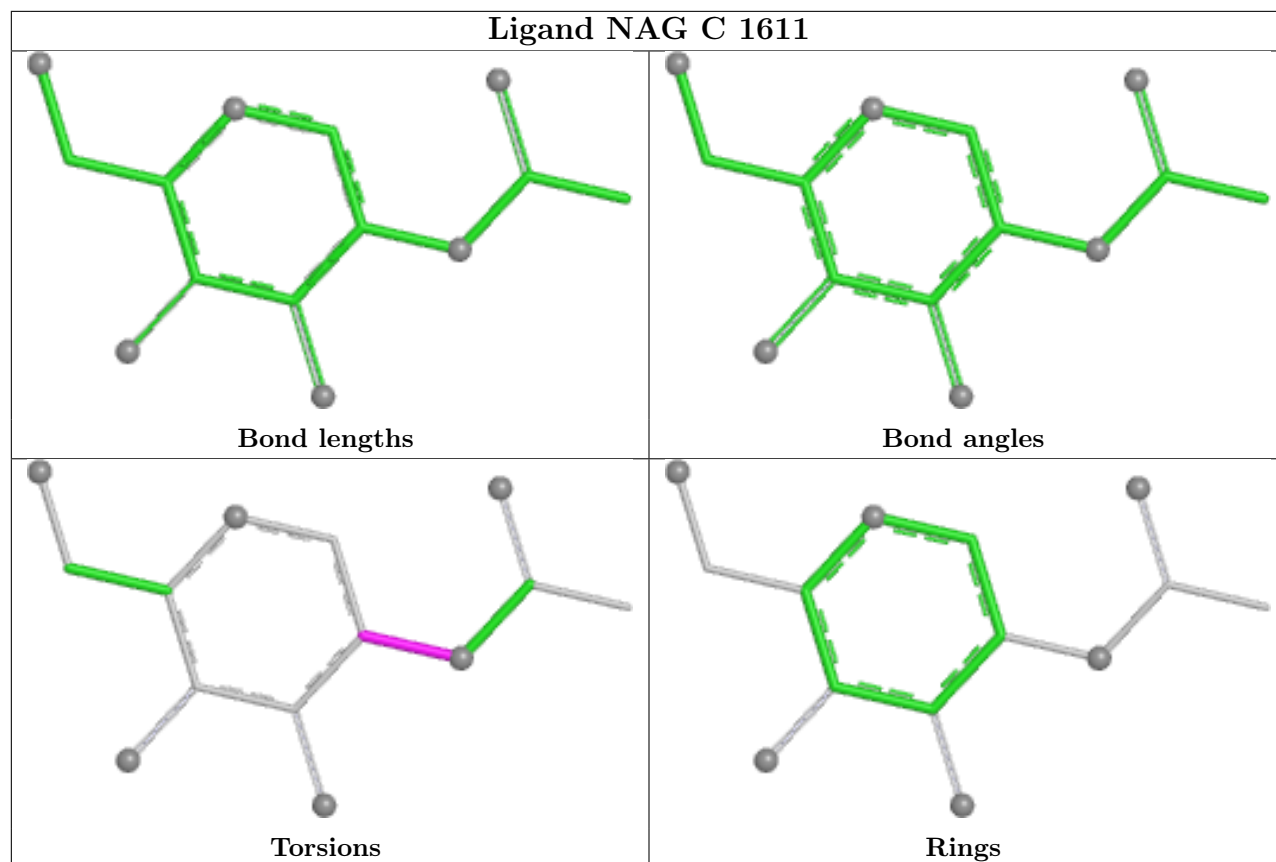
There are no ring outliers.

10 monomers are involved in 23 short contacts:

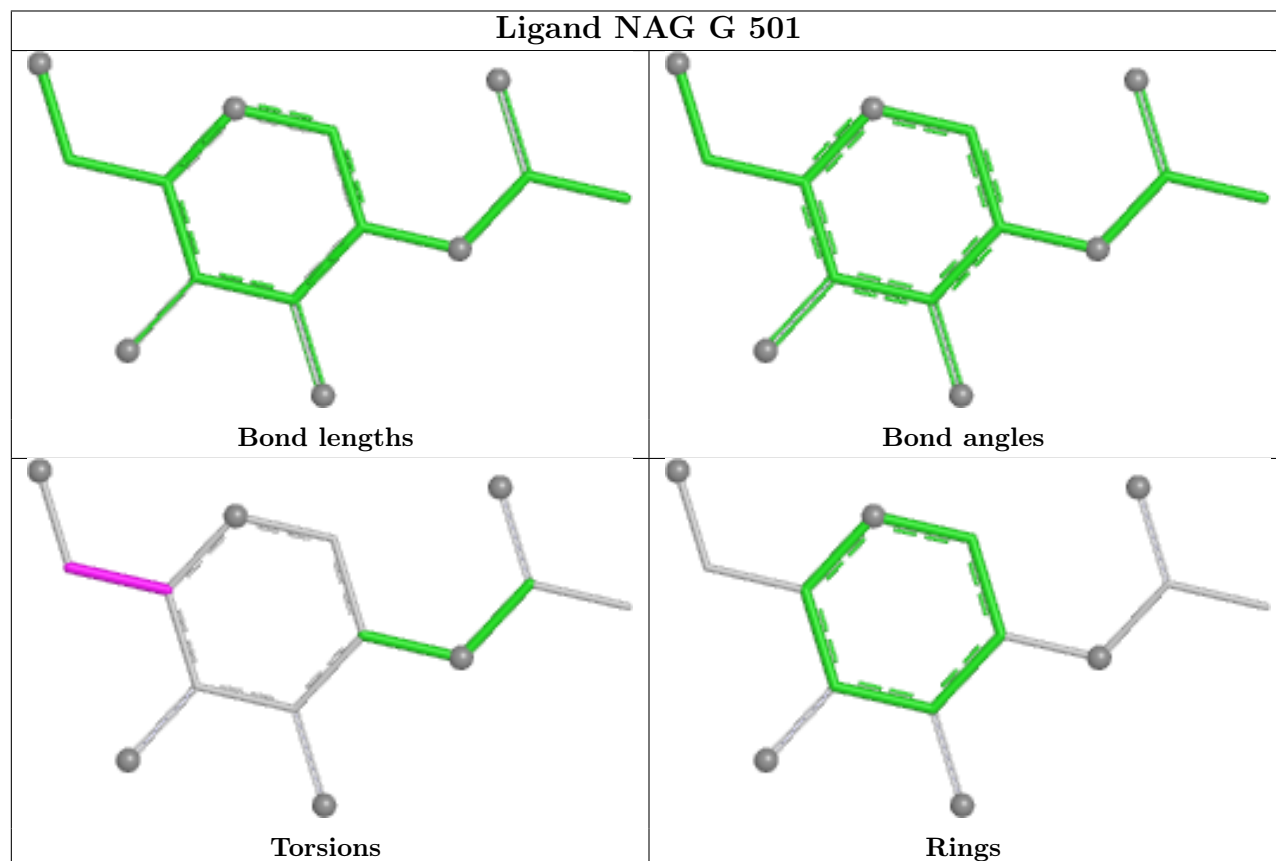
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	C	1611	NAG	3	0
9	C	1612	CIT	1	0
7	G	501	NAG	2	0
7	C	1609	NAG	5	0
7	G	505	NAG	3	0
7	C	1610	NAG	1	0
7	C	1603	NAG	3	0
7	G	511	NAG	2	0
7	C	1602	NAG	2	0
7	G	508	NAG	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

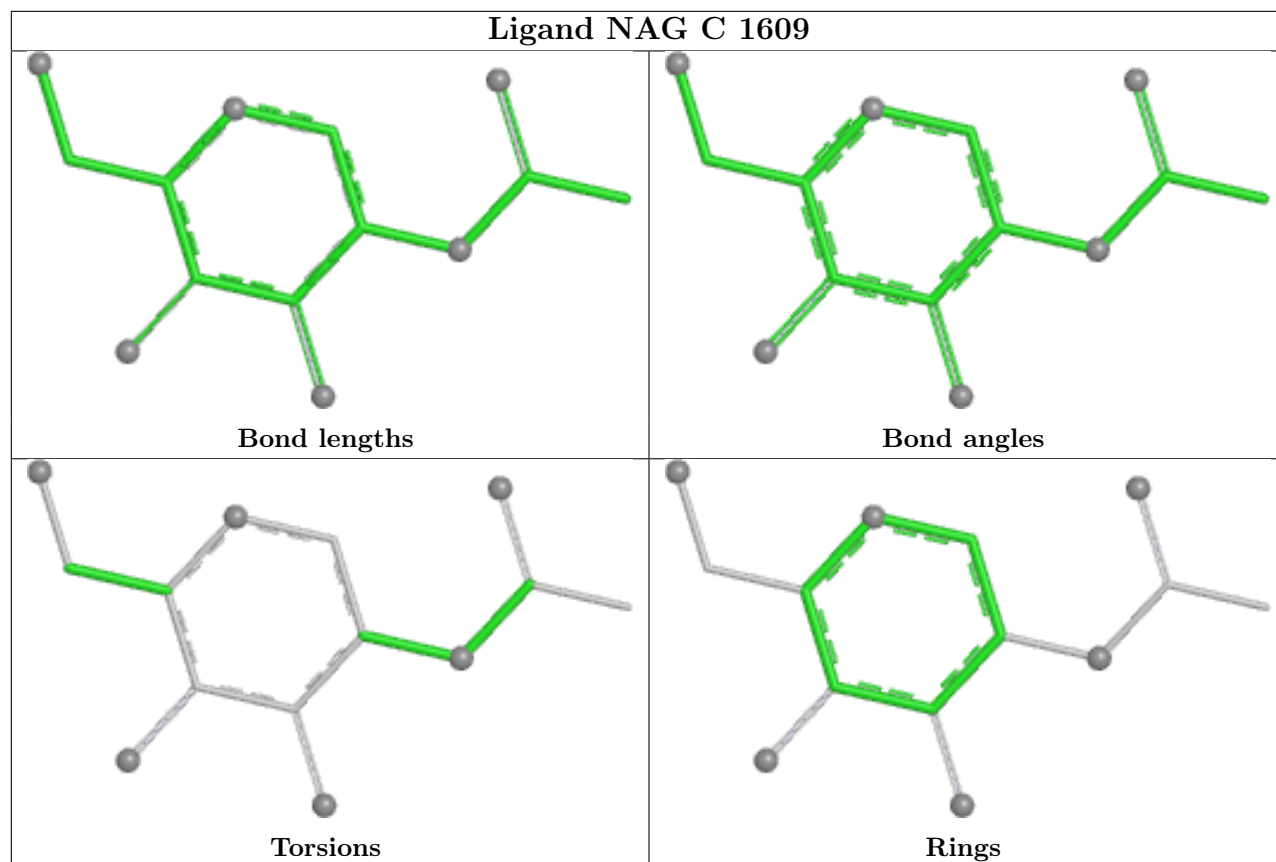
Ligand NAG C 1611



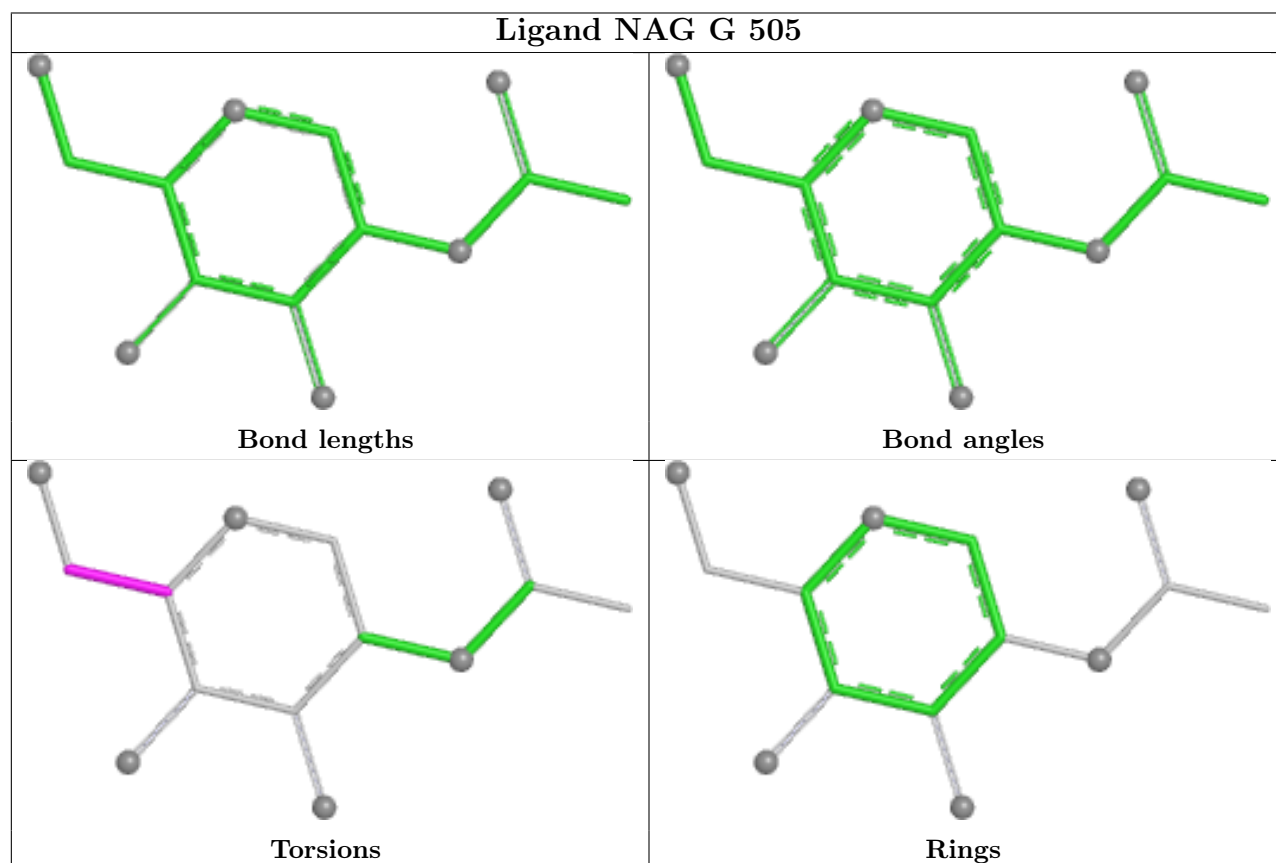
Ligand NAG G 501



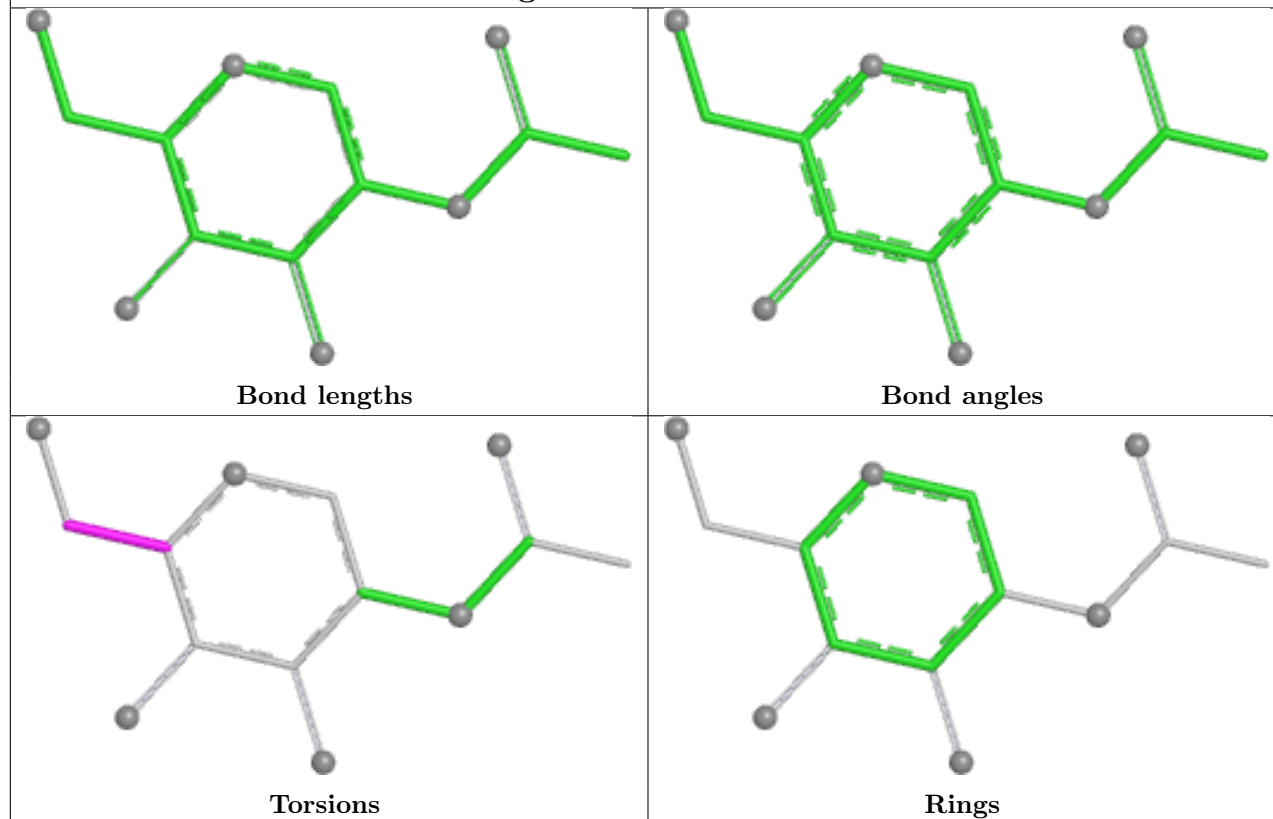
Ligand NAG C 1609



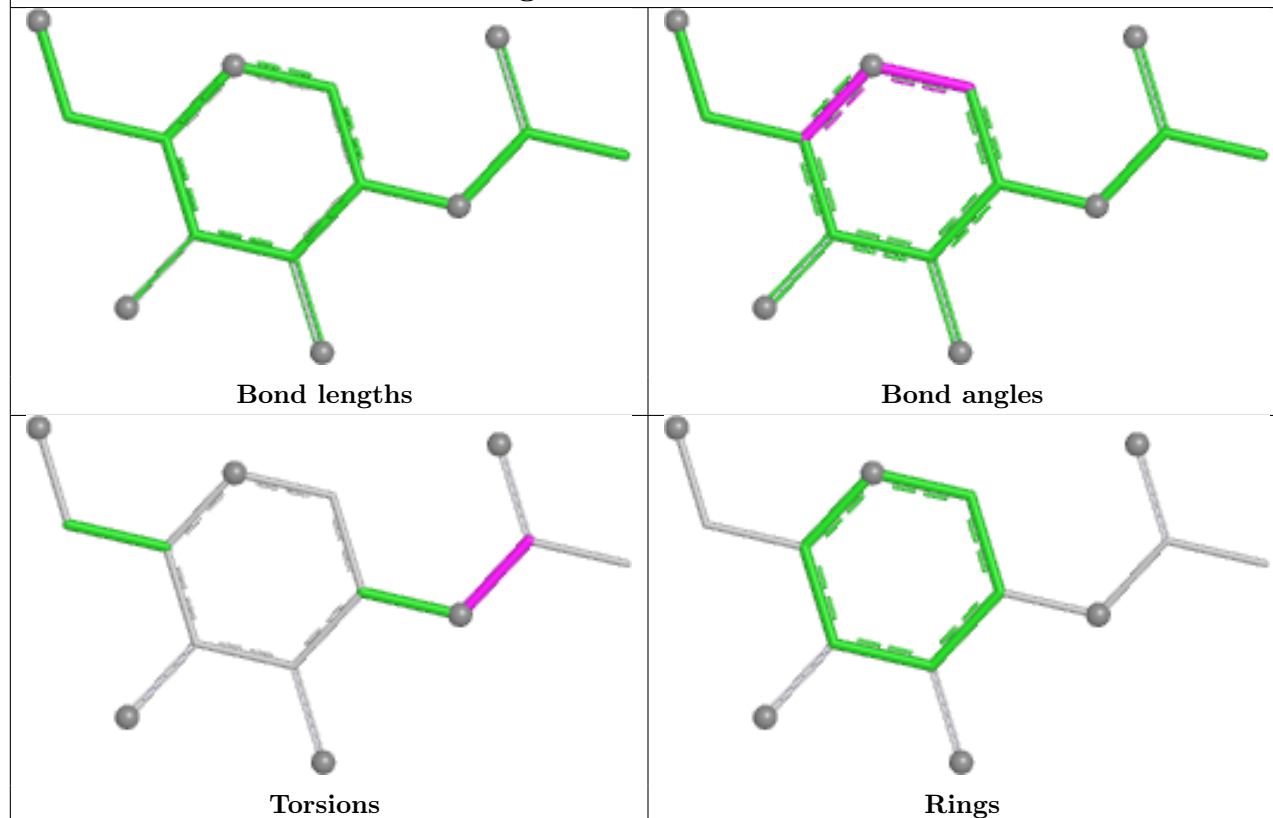
Ligand NAG G 505

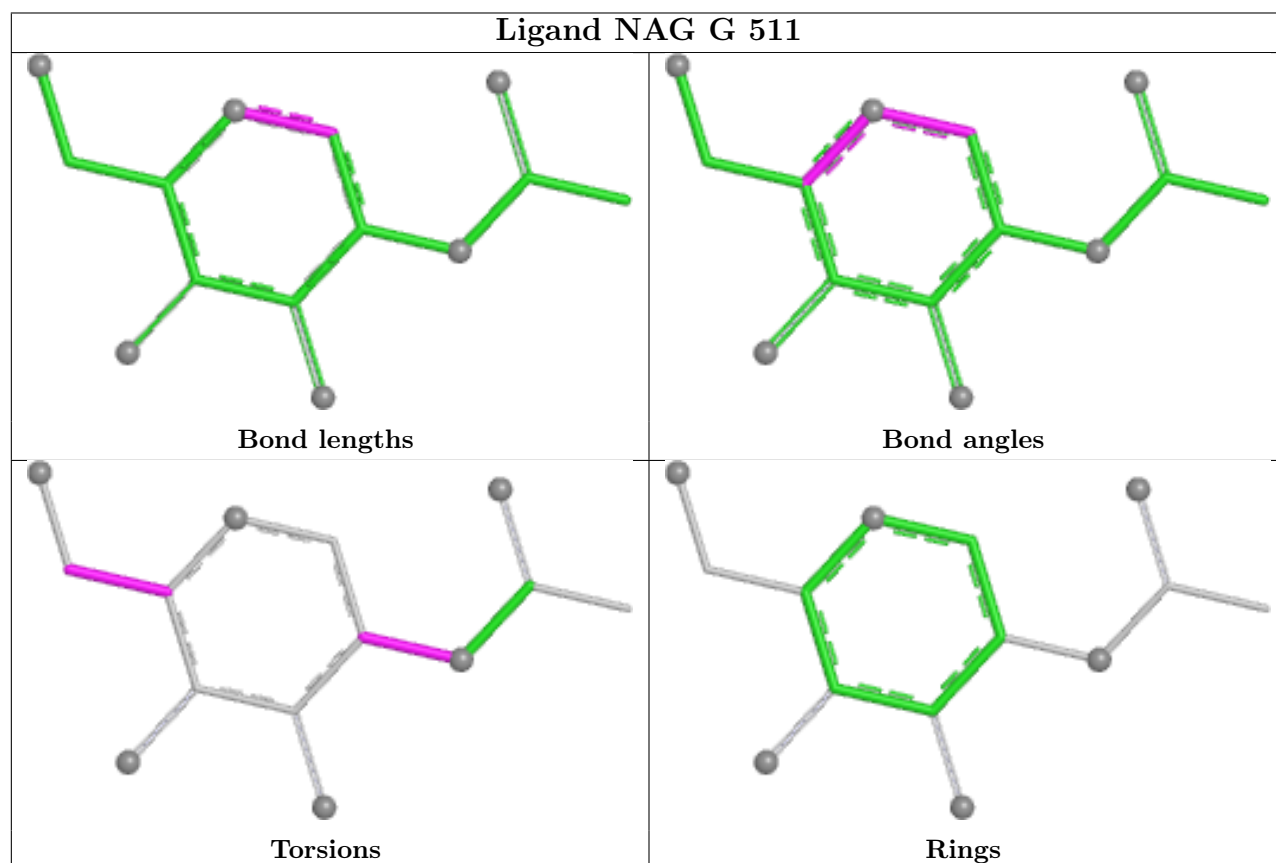
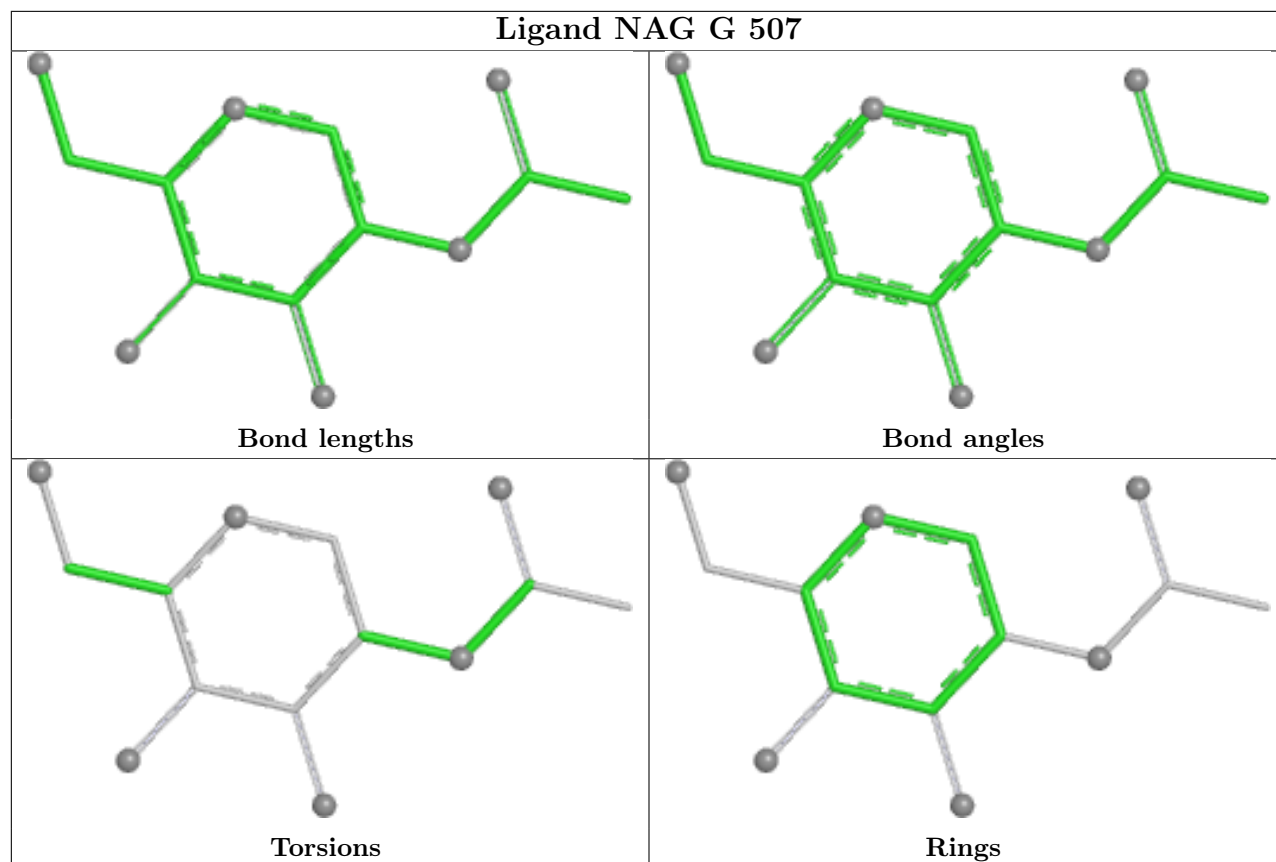


Ligand NAG C 1610

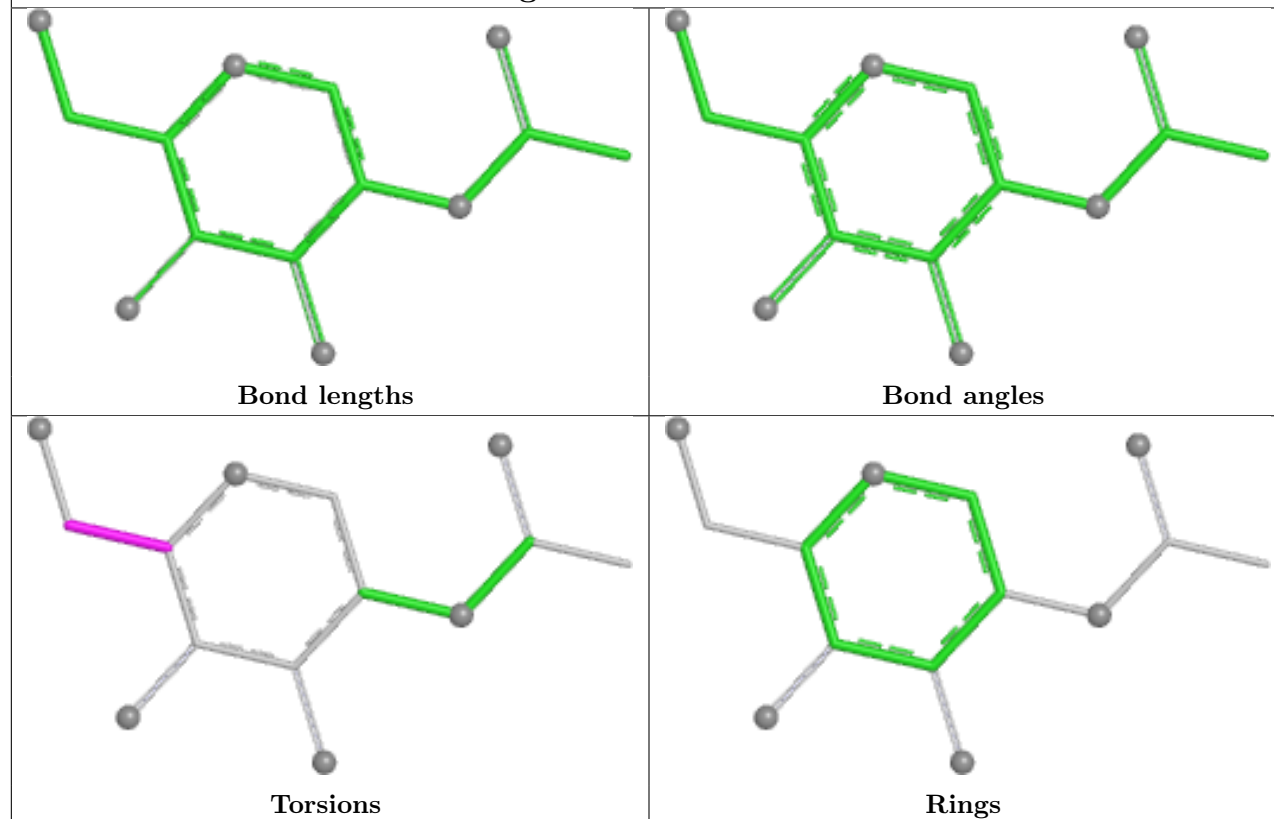


Ligand NAG C 1603

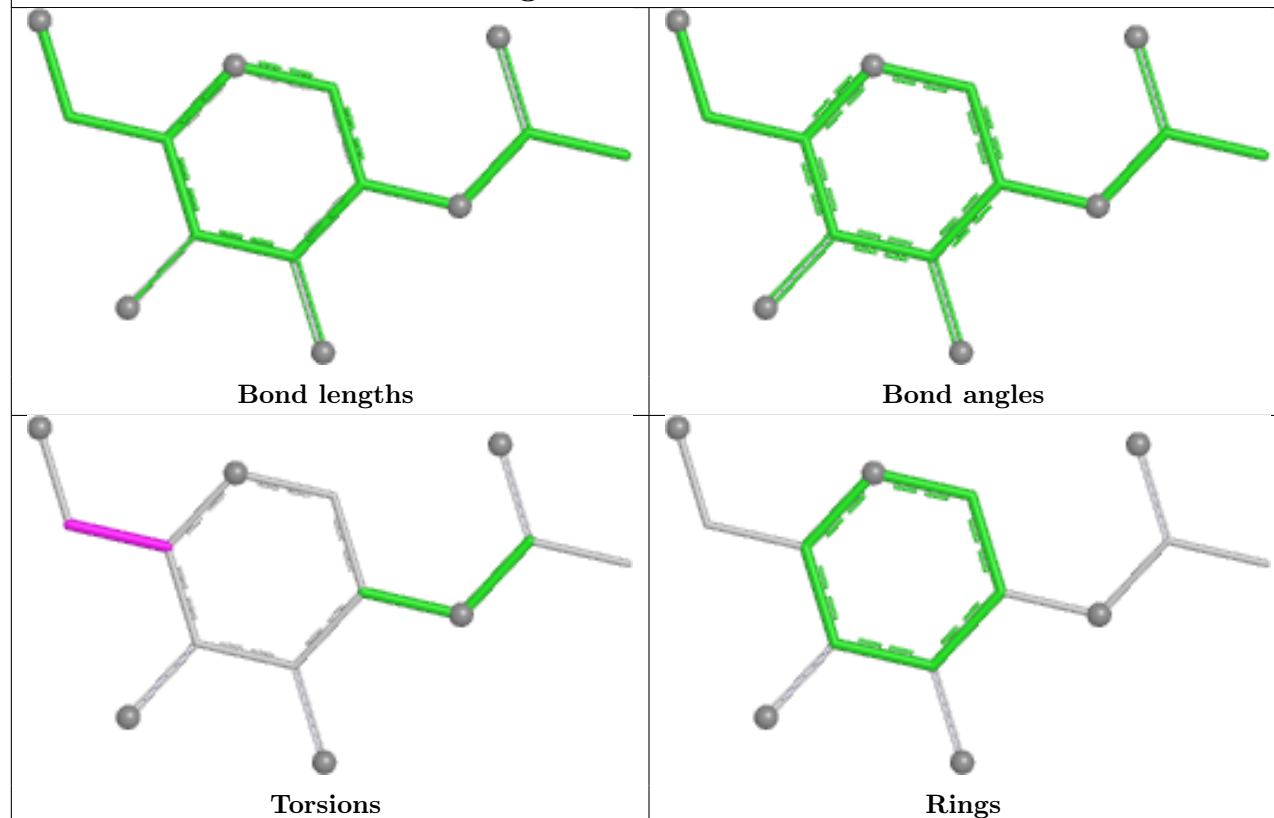


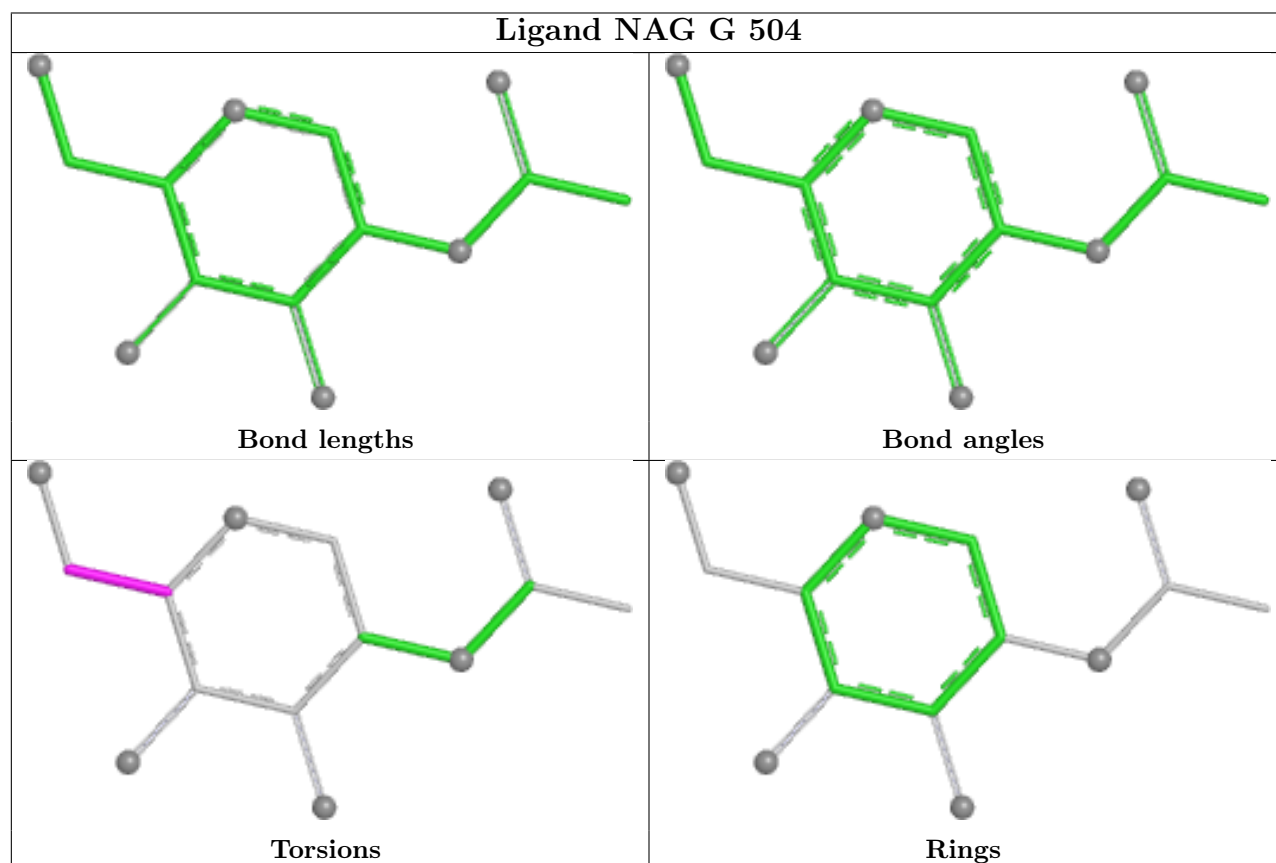
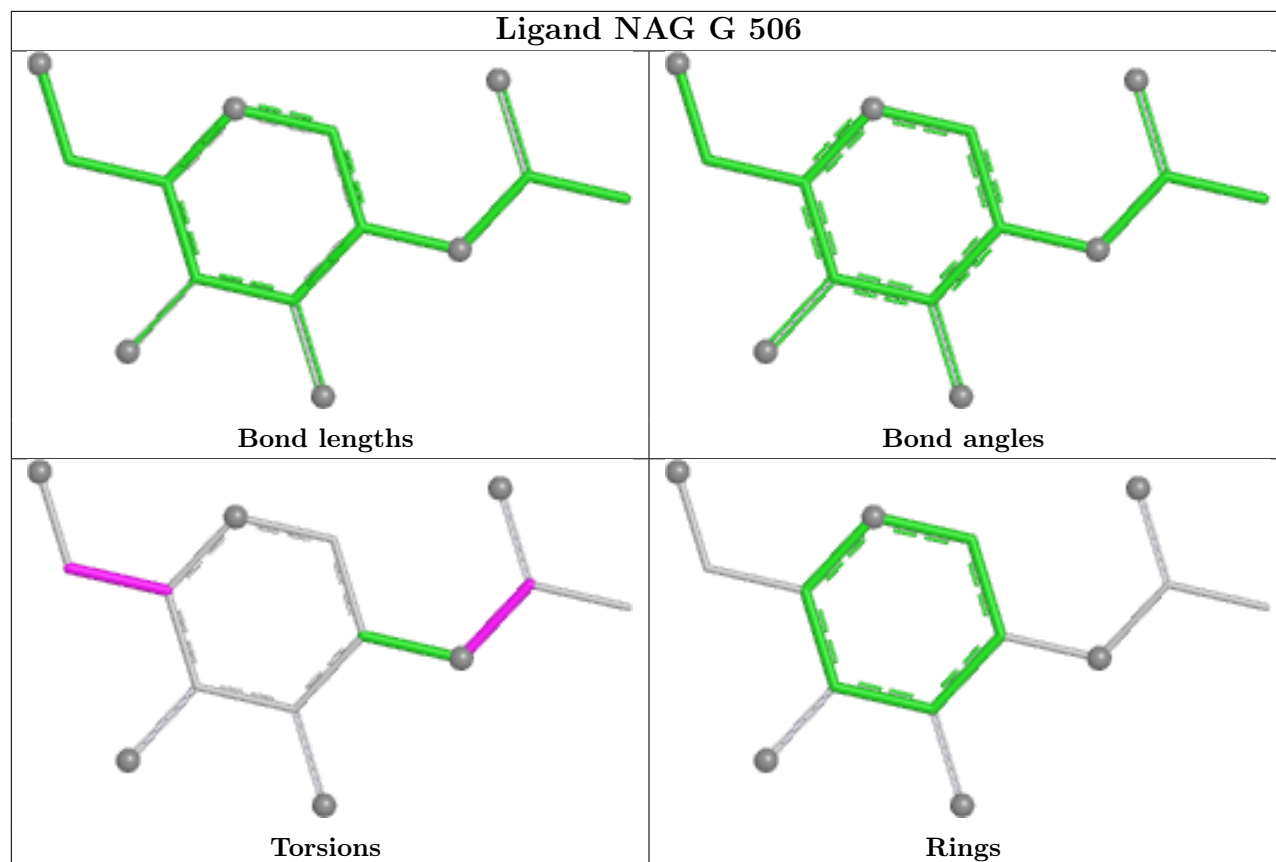


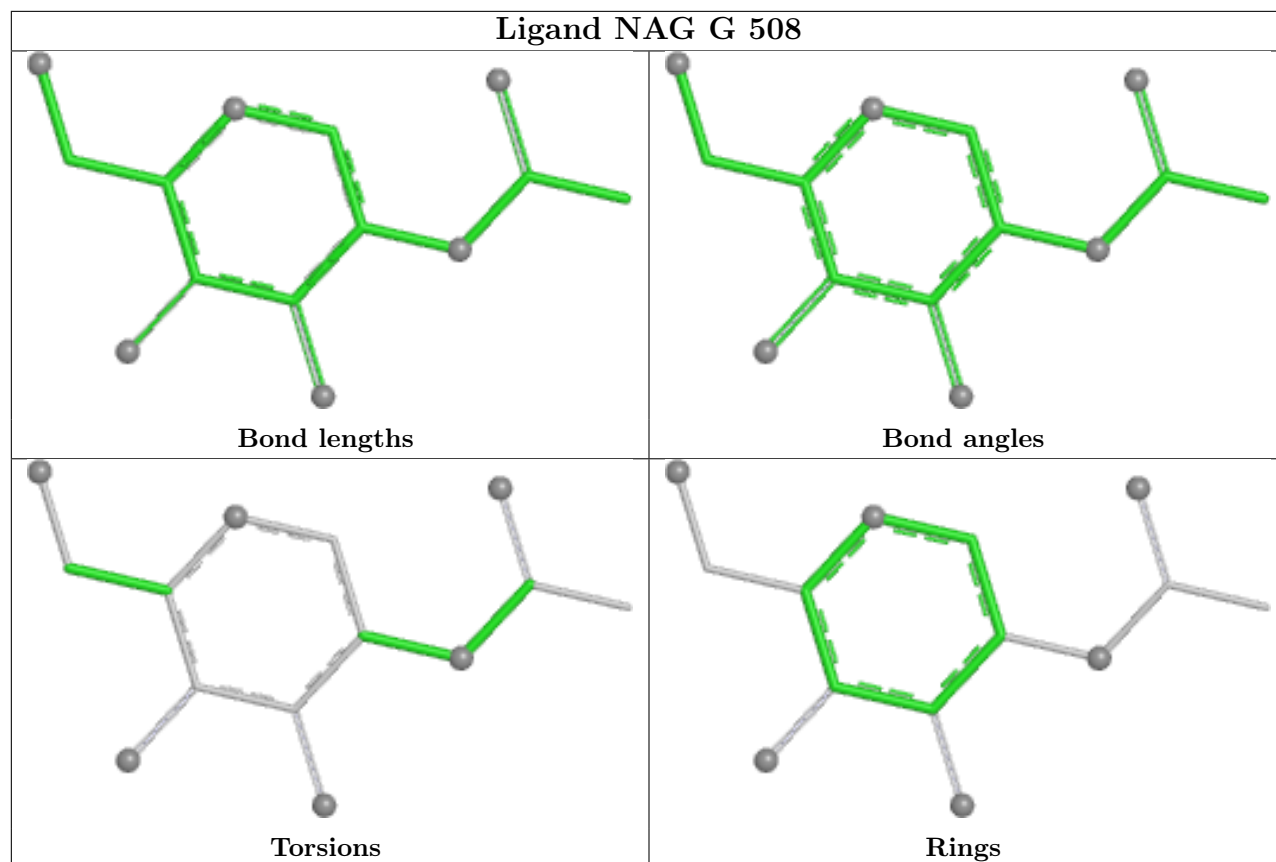
Ligand NAG C 1601



Ligand NAG C 1602







5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	214/233 (91%)	1.82	84 (39%) 1 0	51, 90, 123, 135	0
1	H	215/233 (92%)	1.44	53 (24%) 2 2	45, 73, 115, 134	0
2	B	209/210 (99%)	1.46	47 (22%) 2 2	49, 79, 116, 142	0
2	L	208/210 (99%)	1.76	69 (33%) 1 1	47, 84, 132, 144	0
3	C	336/347 (96%)	2.40	186 (55%) 0 0	56, 86, 116, 134	0
3	G	336/347 (96%)	1.20	46 (13%) 6 7	41, 64, 98, 136	1 (0%)
All	All	1518/1580 (96%)	1.70	485 (31%) 1 1	41, 78, 119, 144	1 (0%)

All (485) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	C	295	VAL	7.1
3	C	375	PHE	6.2
1	H	196	CYS	6.1
3	C	424	ILE	6.1
3	C	296	CYS	6.0
3	C	294	ILE	5.9
3	C	212	PRO	5.9
3	C	388	GLY	5.8
3	C	338	TRP	5.7
3	C	65	CYS	5.7
3	C	382	PHE	5.5
3	C	381	PHE	5.4
3	C	412	ALA	5.2
2	L	214	GLY	5.1
3	C	330	TYR	5.1
2	L	148	VAL	5.1
3	C	394	ILE	5.0
3	C	120	VAL	5.0
3	C	376	ASN	4.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
3	C	254	VAL	4.9
3	C	439	ILE	4.9
3	C	342	VAL	4.9
3	C	423	ILE	4.8
2	L	155	ALA	4.7
3	C	299	PRO	4.7
1	A	122	PHE	4.6
3	G	324	GLY	4.6
3	C	261	LEU	4.6
3	C	418	CYS	4.6
3	C	416	LEU	4.6
1	A	213	PRO	4.6
3	C	331	CYS	4.5
1	H	211	VAL	4.5
3	C	449	ILE	4.5
3	C	201	LEU	4.5
1	A	11	VAL	4.5
3	C	385	ASN	4.5
3	C	288	LEU	4.4
3	C	370	ILE	4.4
2	L	152	VAL	4.4
3	C	378	GLY	4.4
1	A	207	VAL	4.3
3	C	66	HIS	4.3
1	A	138	LEU	4.3
3	C	368	LEU	4.3
3	C	434	ILE	4.3
2	B	29	VAL	4.2
3	C	209	THR	4.2
1	A	194	TYR	4.2
3	C	443	ILE	4.1
2	L	211	PHE	4.1
3	C	414	ILE	4.1
1	A	112	SER	4.1
1	A	127	SER	4.1
3	C	433	ALA	4.1
3	G	396	ASN	4.1
3	C	395	SER	4.1
2	B	127	LEU	4.0
3	C	259	LEU	4.0
3	C	300	ASN	4.0
2	L	150	TRP	4.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	L	143	PRO	4.0
3	C	333	ILE	4.0
3	C	200	THR	4.0
3	C	435	TYR	4.0
2	L	198	VAL	3.9
1	H	141	LEU	3.9
3	C	301	ASN	3.9
2	L	122	PRO	3.9
3	C	326	ILE	3.8
1	A	170	LEU	3.8
3	C	413	THR	3.8
3	C	339	SER	3.8
3	C	420	ILE	3.8
3	G	462	THR	3.8
3	C	341	ALA	3.8
3	C	422	GLN	3.8
1	H	123	PRO	3.8
3	C	445	CYS	3.8
1	H	127	SER	3.8
3	C	427	TRP	3.8
1	A	118	GLY	3.8
1	H	100	TYR	3.7
1	A	176	TYR	3.7
1	H	193	THR	3.7
3	G	412	ALA	3.7
3	C	358	ILE	3.7
3	C	69	TRP	3.7
3	C	297	THR	3.7
2	L	196	CYS	3.7
2	L	193	VAL	3.7
1	A	141	LEU	3.6
3	C	255	VAL	3.6
3	G	444	THR	3.6
3	C	293	GLU	3.6
3	C	263	GLY	3.6
3	C	371	THR	3.6
3	C	430	VAL	3.6
1	A	114	ALA	3.6
3	C	438	PRO	3.6
3	G	441	GLY	3.6
1	A	198	VAL	3.6
2	L	147	LYS	3.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	148	GLU	3.6
1	A	151	THR	3.5
3	G	81	PRO	3.5
2	L	156	LEU	3.5
2	L	149	GLN	3.5
1	H	154	TRP	3.5
3	C	122	LEU	3.5
3	C	332	ASN	3.5
3	G	297	THR	3.4
3	C	202	THR	3.4
3	C	417	PRO	3.4
3	C	432	LYS	3.4
3	C	213	ILE	3.4
2	L	138	LEU	3.4
3	C	337	ASN	3.4
3	C	421	LYS	3.4
3	C	292	VAL	3.4
1	H	194	TYR	3.4
3	C	386	THR	3.4
3	C	364	SER	3.4
2	L	199	THR	3.3
3	C	372	THR	3.3
3	C	221	ALA	3.3
3	C	458	GLY	3.3
3	C	384	CYS	3.3
3	C	415	MET	3.3
3	C	265	LEU	3.3
2	L	208	THR	3.3
2	B	131	THR	3.3
2	B	32	TYR	3.3
1	A	152	VAL	3.3
2	L	137	LEU	3.3
3	C	373	HIS	3.3
2	L	32	TYR	3.3
3	C	324	GLY	3.2
1	A	184	VAL	3.2
2	B	186	ALA	3.2
3	C	451	GLY	3.2
1	H	189	LEU	3.2
1	H	195	ILE	3.2
3	C	208	VAL	3.2
3	C	210	PHE	3.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	145	TYR	3.2
3	C	444	THR	3.2
2	B	205	SER	3.1
2	L	127	LEU	3.1
3	G	491	ILE	3.1
3	C	334	SER	3.1
1	A	123	PRO	3.1
1	A	209	LYS	3.1
2	L	194	TYR	3.1
2	L	2	ILE	3.1
3	C	340	GLU	3.1
1	A	115	SER	3.1
3	G	65[A]	CYS	3.1
1	H	136	ALA	3.1
1	H	163	VAL	3.1
3	C	345	VAL	3.1
2	B	199	THR	3.0
3	C	462	THR	3.0
1	H	161	SER	3.0
3	C	262	ASN	3.0
3	C	329	ALA	3.0
1	A	109	VAL	3.0
1	A	159	LEU	3.0
2	B	198	VAL	3.0
3	C	393	THR	3.0
1	H	124	LEU	3.0
3	C	389	LEU	3.0
2	L	142	TYR	3.0
2	L	201	GLN	3.0
1	H	122	PHE	3.0
1	H	125	ALA	3.0
1	A	111	VAL	3.0
2	B	2	ILE	3.0
3	C	344	GLN	3.0
1	A	147	PRO	3.0
3	C	470	PRO	3.0
3	C	70	ALA	2.9
1	H	159	LEU	2.9
3	C	121	LYS	2.9
3	C	419	ARG	2.9
2	B	28	SER	2.9
3	C	437	PRO	2.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	108	LEU	2.9
1	H	142	VAL	2.9
2	L	151	LYS	2.9
3	G	336	ARG	2.9
3	C	215	ILE	2.9
3	C	251	ILE	2.9
3	G	292	VAL	2.9
2	B	196	CYS	2.9
3	C	377	CYS	2.9
1	H	100(A)	ASN	2.9
3	G	241	ASN	2.9
3	C	56	SER	2.9
3	C	396	ASN	2.9
1	H	209	LYS	2.9
3	C	436	ALA	2.9
2	B	24	ARG	2.8
3	C	48	ALA	2.8
3	G	358	ILE	2.8
3	G	464	ASN	2.8
3	C	355	HIS	2.8
2	L	203	LEU	2.8
2	L	120	PHE	2.8
3	C	54	CYS	2.8
3	G	250	GLY	2.8
1	H	185	PRO	2.8
1	H	158	ALA	2.8
3	C	55	ALA	2.8
3	C	360	PHE	2.8
2	L	134	VAL	2.8
3	C	467	ILE	2.8
2	L	212	ASN	2.8
2	B	129	SER	2.8
2	B	202	GLY	2.8
3	C	119	CYS	2.8
1	A	160	THR	2.7
1	A	15	GLY	2.7
3	C	205	CYS	2.7
1	A	121	VAL	2.7
3	C	328	GLN	2.7
2	B	214	GLY	2.7
1	A	120	SER	2.7
3	C	252	LYS	2.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
3	C	290	LYS	2.7
3	C	298	ARG	2.7
3	G	219	ALA	2.7
3	C	266	ALA	2.7
3	C	383	TYR	2.7
2	L	135	VAL	2.7
3	C	107	ASP	2.7
1	H	156	SER	2.7
1	A	119	PRO	2.7
3	C	118	PRO	2.7
1	A	189	LEU	2.7
2	L	106	LEU	2.7
3	C	390	PHE	2.7
1	A	150	VAL	2.7
2	L	192	LYS	2.7
3	C	492	LYS	2.7
3	G	333	ILE	2.7
1	H	213	PRO	2.7
1	A	202	PRO	2.7
1	A	203	SER	2.7
3	C	228	CYS	2.7
1	H	184	VAL	2.6
1	A	174	GLY	2.6
3	C	115	CYS	2.6
2	B	90	GLN	2.6
3	G	492	LYS	2.6
1	A	24	ALA	2.6
2	L	146	ALA	2.6
2	B	132	ALA	2.6
2	B	120	PHE	2.6
1	A	100	TYR	2.6
1	H	169	VAL	2.6
1	H	198	VAL	2.6
1	A	182	VAL	2.6
3	C	109	ILE	2.6
3	C	291	SER	2.6
1	A	82(C)	LEU	2.6
3	C	58	ALA	2.6
2	B	154	ASN	2.6
3	G	393	THR	2.6
2	B	122	PRO	2.6
2	L	170	SER	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	B	77	SER	2.6
2	L	195	ALA	2.6
1	H	133	GLY	2.6
2	B	118	PHE	2.6
2	B	130	GLY	2.6
1	A	142	VAL	2.6
3	C	68	VAL	2.6
3	C	270	ILE	2.6
2	B	109	LYS	2.6
3	C	116	LEU	2.5
1	H	210	ARG	2.5
1	H	137	ALA	2.5
2	B	114	ALA	2.5
3	C	247	CYS	2.5
1	A	146	PHE	2.5
1	A	25	SER	2.5
2	L	191	HIS	2.5
3	C	203	GLN	2.5
3	C	226	LEU	2.5
1	A	185	PRO	2.5
1	H	135	THR	2.5
2	L	131	THR	2.5
2	B	182	THR	2.5
1	A	161	SER	2.5
2	L	133	SER	2.5
3	C	260	LEU	2.5
2	B	124	ASP	2.5
3	G	231	LYS	2.5
3	C	50	THR	2.5
3	C	447	SER	2.5
3	C	455	LEU	2.5
3	C	475	MET	2.5
2	B	146	ALA	2.5
3	C	204	ALA	2.5
3	C	74	CYS	2.4
3	C	465	THR	2.4
2	L	29	VAL	2.4
2	B	188	TYR	2.4
3	G	226	LEU	2.4
1	H	139	GLY	2.4
1	A	113	SER	2.4
1	A	140	CYS	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	L	123	SER	2.4
2	B	123	SER	2.4
3	G	85	VAL	2.4
3	C	233	PHE	2.4
3	C	446	LYS	2.4
1	H	138	LEU	2.4
3	C	217	TYR	2.4
3	G	246	GLN	2.4
1	H	95	GLY	2.4
1	H	157	GLY	2.4
2	L	186	ALA	2.4
2	B	121	PRO	2.4
3	C	238	PRO	2.4
1	H	160	THR	2.4
2	L	117	VAL	2.4
2	L	183	LEU	2.4
1	A	154	TRP	2.4
2	L	144	ARG	2.4
3	G	61	TYR	2.4
1	A	97	ASN	2.4
1	A	199	ASN	2.4
1	A	125	ALA	2.4
2	L	182	THR	2.4
2	B	31	SER	2.4
1	H	140	CYS	2.4
1	H	146	PHE	2.4
1	A	60	CYS	2.4
2	L	141	PHE	2.4
3	C	111	ILE	2.4
3	C	242	VAL	2.4
1	A	175	LEU	2.4
2	B	156	LEU	2.4
2	L	153	ASP	2.3
1	A	14	PRO	2.3
1	A	126	PRO	2.3
1	H	168	ALA	2.3
2	B	25	ALA	2.3
2	L	31	SER	2.3
1	H	166	PHE	2.3
2	L	119	ILE	2.3
2	B	136	CYS	2.3
3	G	269	GLU	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	27	TYR	2.3
1	A	32	TYR	2.3
3	C	214	PRO	2.3
3	C	347	LYS	2.3
1	A	172	SER	2.3
2	B	158	SER	2.3
3	C	481	SER	2.3
1	A	211	VAL	2.3
2	L	200	HIS	2.3
2	L	181	LEU	2.3
2	B	183	LEU	2.3
1	A	99	ASP	2.3
3	C	67	ASN	2.3
2	L	64	GLY	2.3
2	B	150	TRP	2.3
3	G	48	ALA	2.3
3	C	257	THR	2.3
3	C	374	SER	2.3
3	C	258	GLN	2.3
1	A	195	ILE	2.3
1	H	121	VAL	2.3
3	C	271	VAL	2.3
1	A	72	ASP	2.3
1	H	26	GLY	2.3
3	C	250	GLY	2.3
3	C	64	GLU	2.3
3	G	300	ASN	2.2
3	C	459	CYS	2.2
1	H	191	THR	2.2
1	A	116	THR	2.2
1	A	205	THR	2.2
3	C	369	GLU	2.2
1	A	84	SER	2.2
1	A	153	SER	2.2
2	L	48	ILE	2.2
3	C	89	VAL	2.2
3	C	454	LEU	2.2
3	C	343	ASN	2.2
3	C	79	PRO	2.2
3	C	335	GLY	2.2
2	L	132	ALA	2.2
2	L	180	THR	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	L	207	VAL	2.2
1	A	52(A)	PRO	2.2
3	C	76	PRO	2.2
1	A	157	GLY	2.2
2	L	136	CYS	2.2
3	G	267	GLU	2.2
3	C	207	LYS	2.2
3	C	219	ALA	2.2
2	B	91	TYR	2.2
2	B	187	ASP	2.2
3	G	295	VAL	2.2
3	C	478	ASN	2.2
1	H	190	GLY	2.2
3	G	264	SER	2.2
3	G	330	TYR	2.1
3	C	486	TYR	2.1
3	G	89	VAL	2.1
2	L	107	GLU	2.1
2	B	71	PHE	2.1
2	B	211	PHE	2.1
1	A	101	GLN	2.1
1	A	173	SER	2.1
2	L	30	SER	2.1
3	G	224	ALA	2.1
3	C	60	ALA	2.1
1	A	66	ARG	2.1
2	L	188	TYR	2.1
1	A	117	LYS	2.1
2	B	192	LYS	2.1
1	H	208	ASP	2.1
3	G	80	ASN	2.1
3	C	380	GLU	2.1
1	A	181	VAL	2.1
2	L	59	PRO	2.1
3	C	468	PHE	2.1
1	A	134	GLY	2.1
1	H	120	SER	2.1
2	B	19	ALA	2.1
2	L	171	LYS	2.1
2	L	189	GLU	2.1
1	H	99	ASP	2.1
1	A	75	ILE	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
3	C	81	PRO	2.1
1	A	110	THR	2.1
2	B	116	SER	2.1
3	C	232	THR	2.1
3	G	329	ALA	2.1
2	L	50	ASP	2.1
3	G	82	GLN	2.1
3	C	72	HIS	2.1
2	L	115	PRO	2.1
2	L	175	TYR	2.1
1	H	67	VAL	2.1
1	A	5	VAL	2.1
3	G	75	VAL	2.1
2	L	118	PHE	2.1
2	L	185	LYS	2.0
3	G	387	SER	2.0
3	C	256	SER	2.0
1	A	137	ALA	2.0
3	G	340	GLU	2.0
1	H	64	GLN	2.0
1	A	82	LEU	2.0
2	B	203	LEU	2.0
3	C	283	ILE	2.0
3	C	354	PRO	2.0
3	C	61	TYR	2.0
3	C	484	TYR	2.0
1	H	152	VAL	2.0
2	L	112	VAL	2.0
2	B	165	VAL	2.0
3	G	488	VAL	2.0
3	C	488	VAL	2.0
3	G	388	GLY	2.0
3	C	440	LYS	2.0
1	A	179	SER	2.0
3	G	268	GLU	2.0
3	G	450	THR	2.0
1	A	158	ALA	2.0
1	H	101	GLN	2.0
1	A	196	CYS	2.0
3	G	355	HIS	2.0
3	C	216	HIS	2.0
1	H	178	LEU	2.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
3	G	265	LEU	2.0
3	C	448	ASP	2.0
1	A	41	PRO	2.0
3	C	63	LYS	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [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
1	PCA	H	1	8/9	0.63	0.19	72,94,107,107	0
1	PCA	A	1	8/9	0.69	0.16	75,109,121,130	0

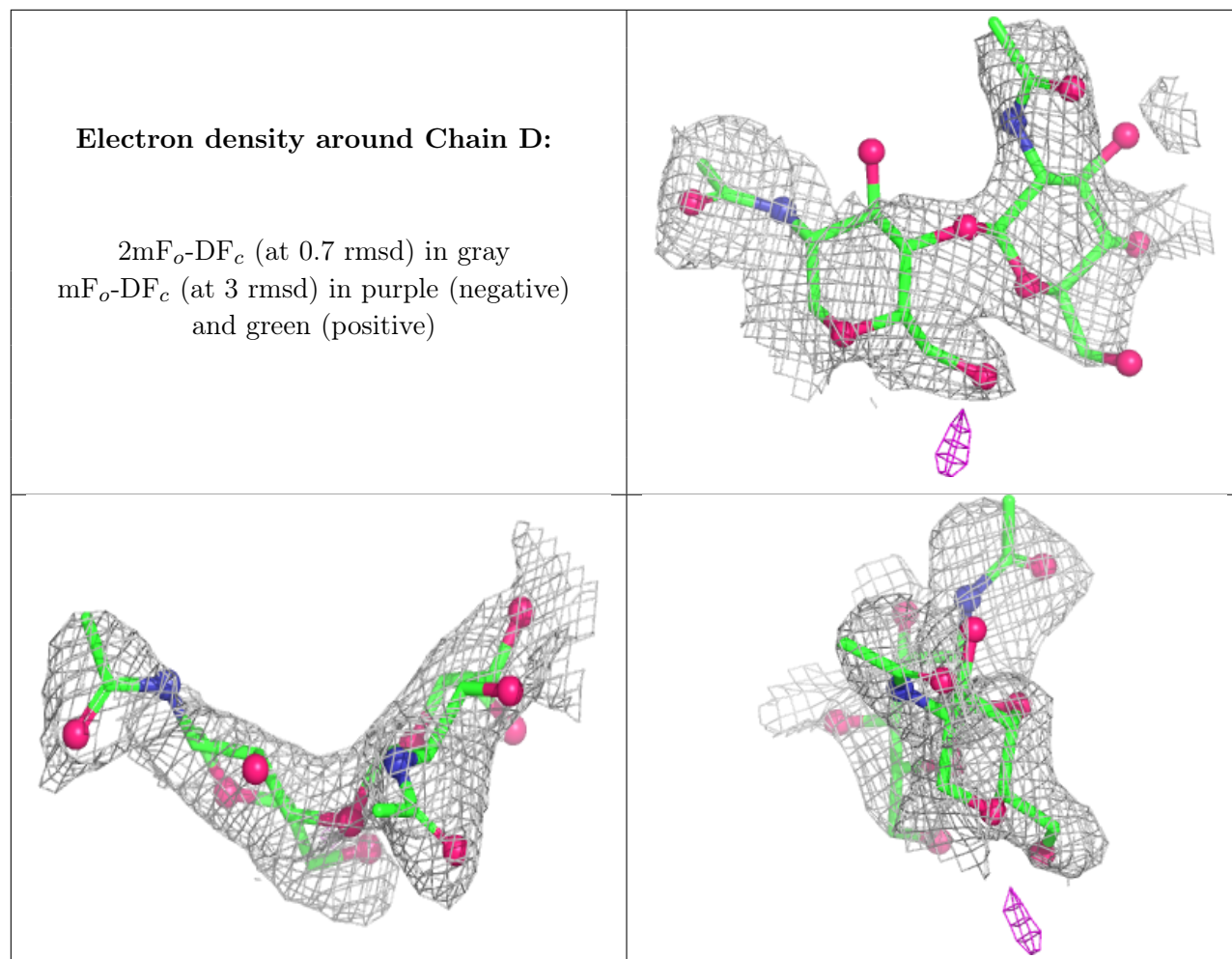
6.3 Carbohydrates [i](#)

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	D	1	14/15	-	-	74,89,101,102	0
4	NAG	D	2	14/15	-	-	91,102,110,110	0
4	NAG	E	1	14/15	-	-	61,69,82,99	0
4	NAG	E	2	14/15	-	-	81,101,113,117	0
5	NAG	F	1	14/15	-	-	45,55,63,69	0
5	NAG	F	2	14/15	-	-	60,72,83,86	0
5	BMA	F	3	11/12	-	-	91,99,108,109	0
5	MAN	F	4	11/12	-	-	94,98,103,106	0
5	MAN	F	5	11/12	-	-	96,102,114,117	0
5	MAN	F	6	11/12	-	-	81,105,111,119	0
6	MAN	I	5	11/12	0.65	0.19	110,120,131,132	0
6	MAN	I	4	11/12	0.70	0.13	99,113,120,121	0
6	BMA	I	3	11/12	0.78	0.14	105,119,122,126	0
6	NAG	I	2	14/15	0.84	0.14	78,100,111,112	0
6	NAG	I	1	14/15	0.92	0.11	71,91,104,107	0

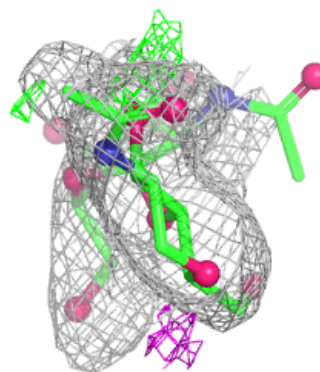
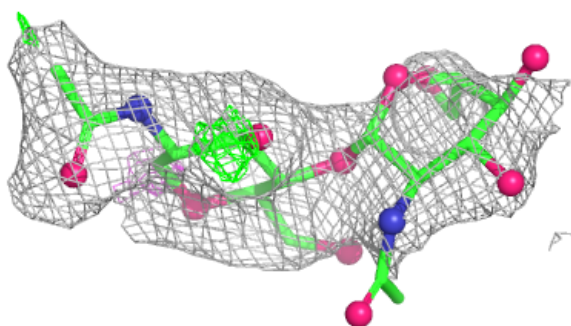
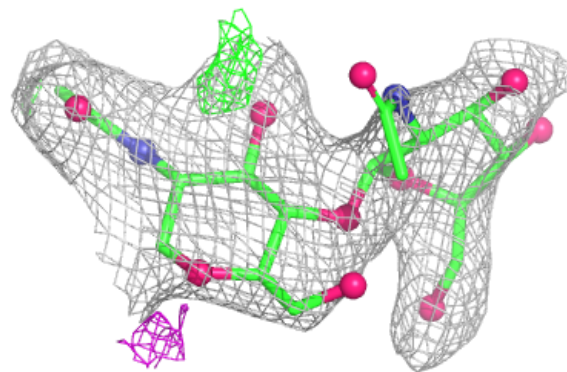
The following is a graphical depiction of the model fit to experimental electron density for oligosac-

charide. Each fit is shown from different orientation to approximate a three-dimensional view.



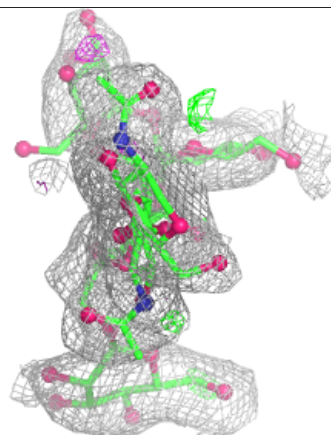
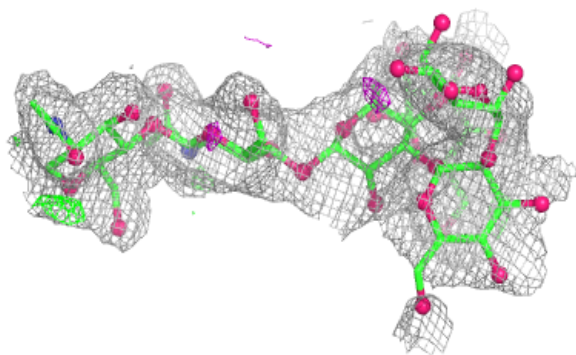
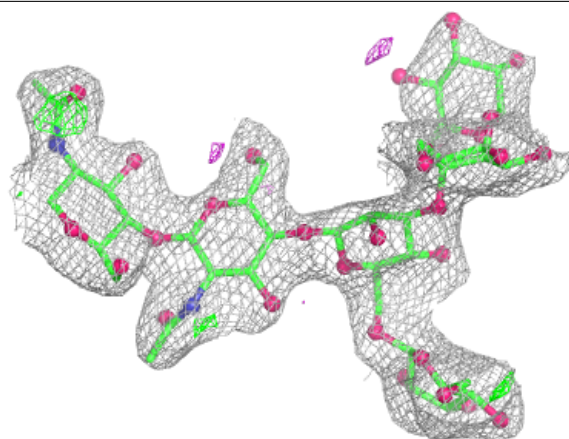
Electron density around Chain E:

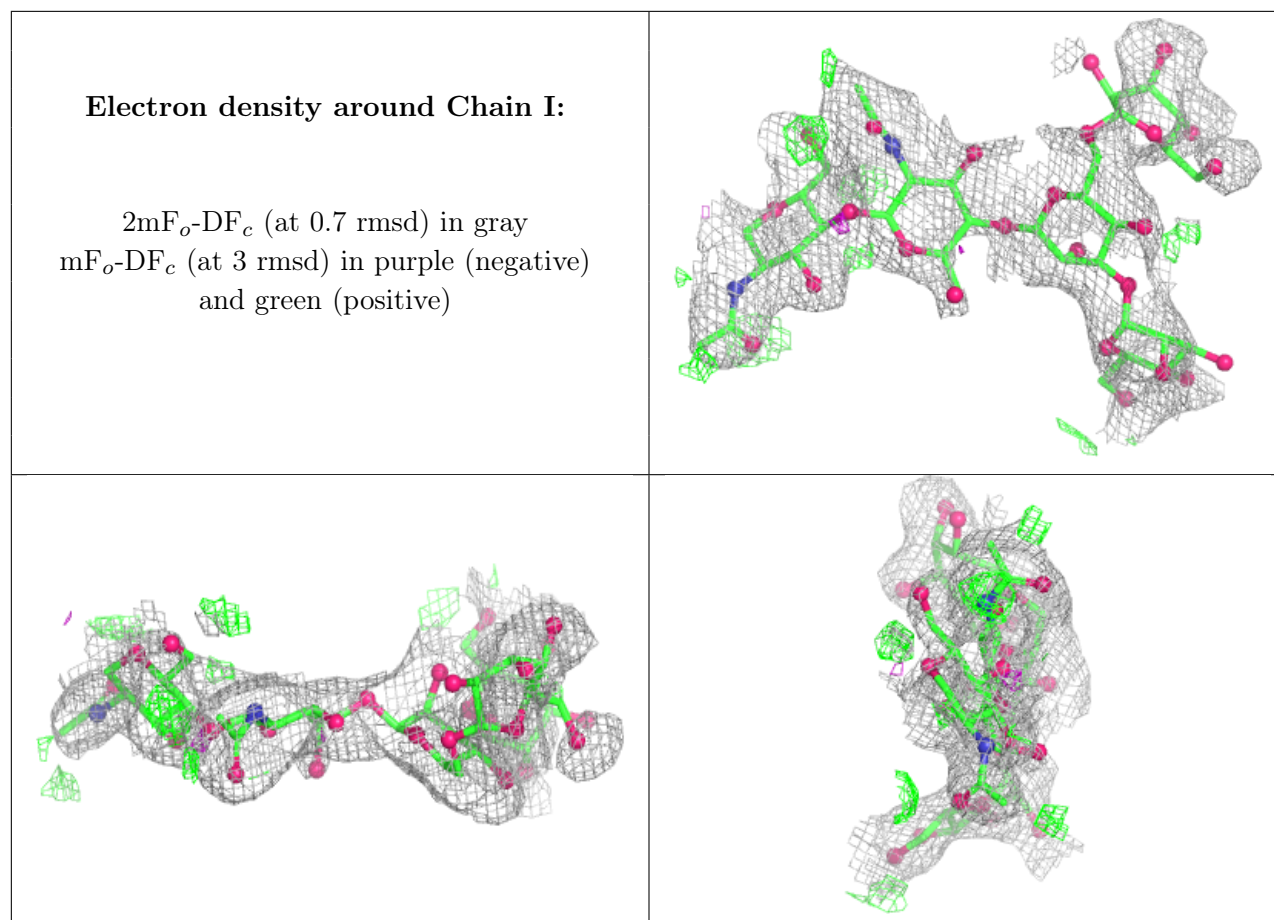
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



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 [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.

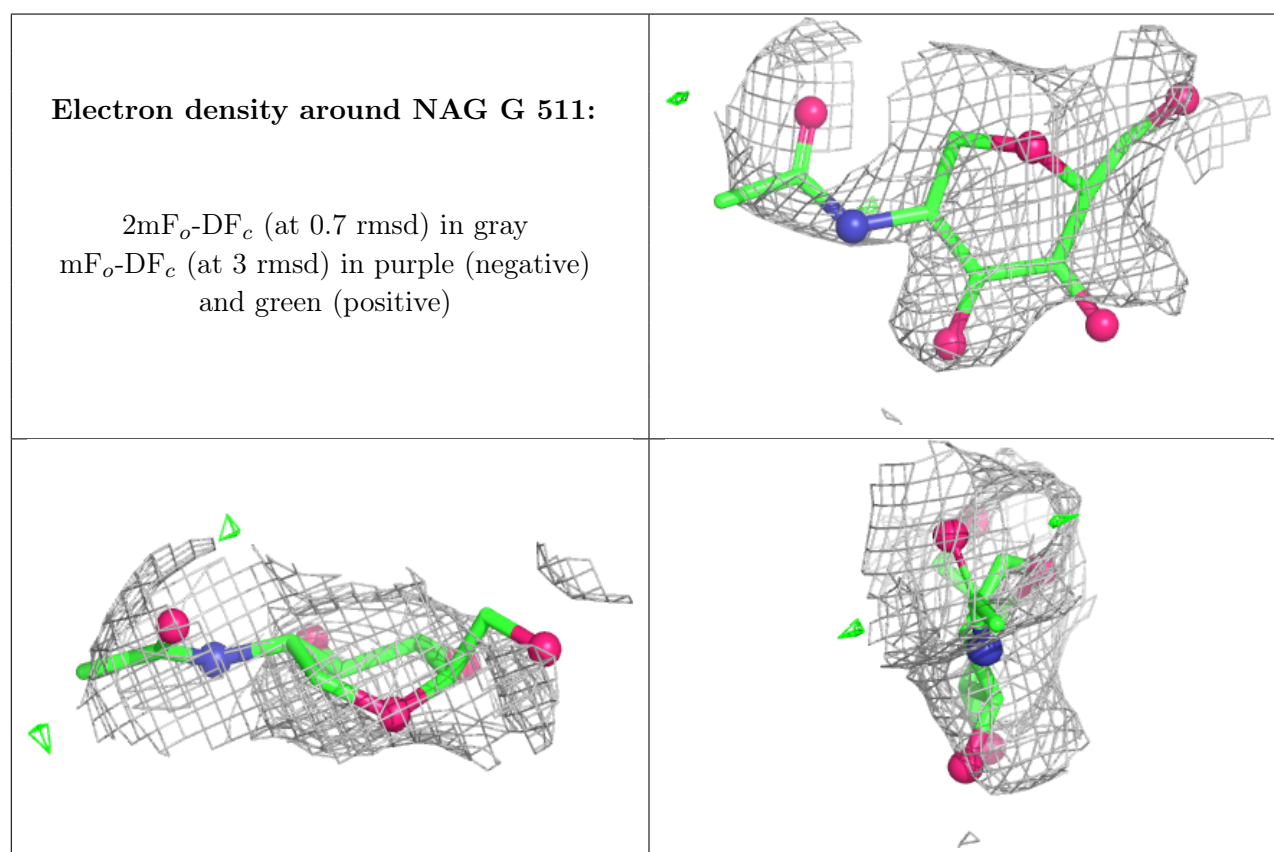
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
7	NAG	G	511	14/15	0.38	0.18	74,113,117,117	0
7	NAG	C	1609	14/15	0.40	0.26	110,118,122,129	0
7	NAG	C	1603	14/15	0.56	0.20	98,110,120,123	0
7	NAG	C	1610	14/15	0.57	0.23	98,106,126,128	0
7	NAG	G	501	14/15	0.64	0.26	83,94,100,104	0
7	NAG	C	1611	14/15	0.64	0.28	98,113,124,125	0
7	NAG	G	507	14/15	0.65	0.21	88,99,110,114	0
7	NAG	G	506	14/15	0.65	0.25	89,98,102,106	0
7	NAG	G	508	14/15	0.67	0.21	100,113,118,123	0
7	NAG	C	1601	14/15	0.70	0.19	108,119,131,132	0
7	NAG	C	1602	14/15	0.74	0.19	70,96,101,102	0
8	PEG	G	518	7/7	0.75	0.28	54,65,77,78	0

Continued on next page...

Continued from previous page...

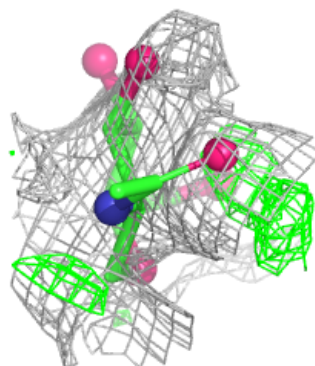
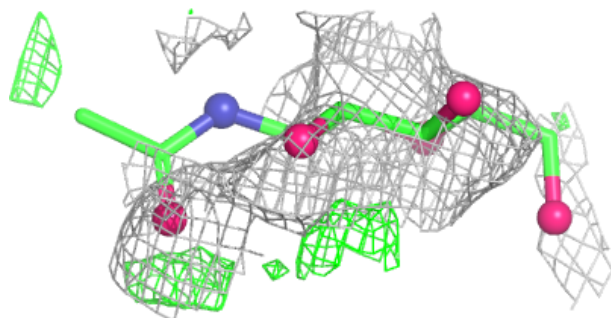
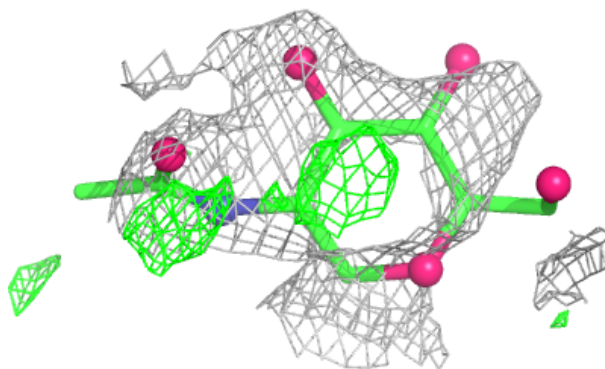
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
9	CIT	C	1612	13/13	0.79	0.20	53,78,102,102	0
7	NAG	G	505	14/15	0.80	0.18	65,75,90,91	0
7	NAG	G	504	14/15	0.83	0.19	70,77,86,94	0
10	EDO	C	1614	4/4	0.85	0.28	72,86,104,104	0
10	EDO	C	1613	4/4	0.87	0.21	61,76,92,95	0

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.

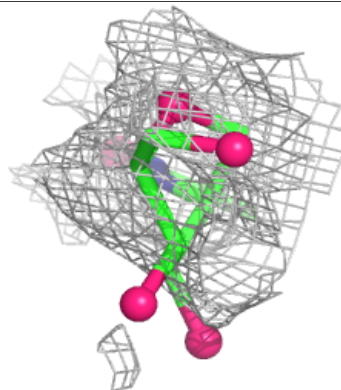
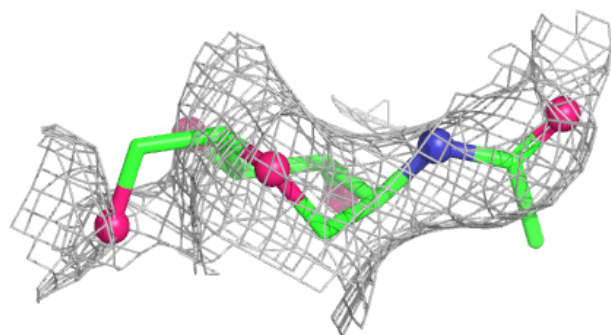
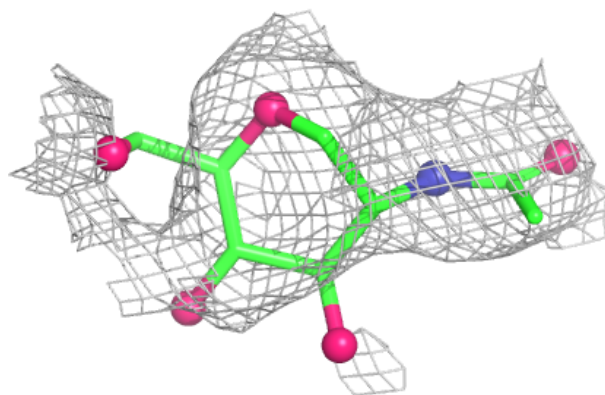


Electron density around NAG C 1609:

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

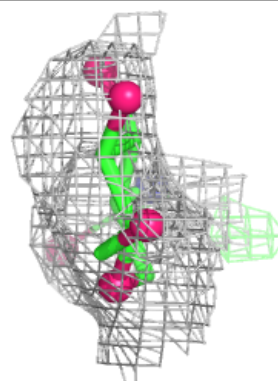
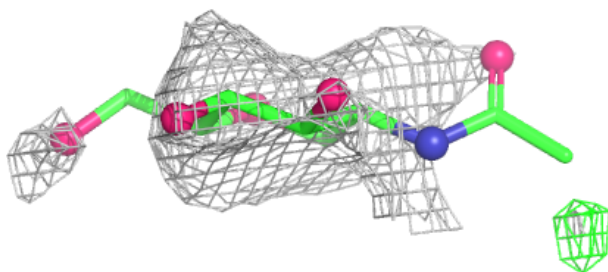
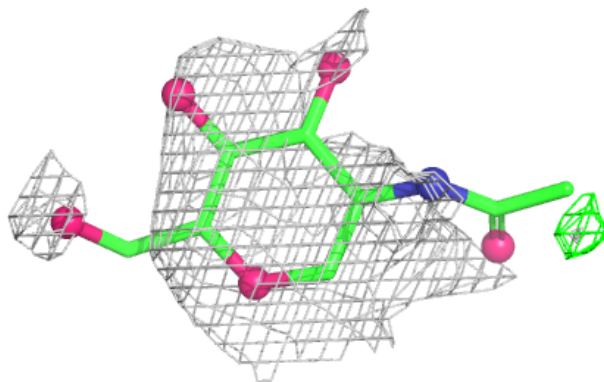
**Electron density around NAG C 1603:**

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

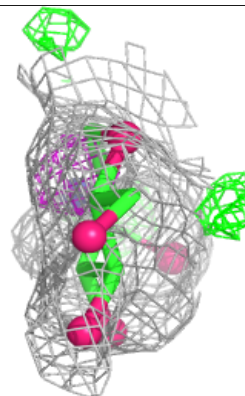
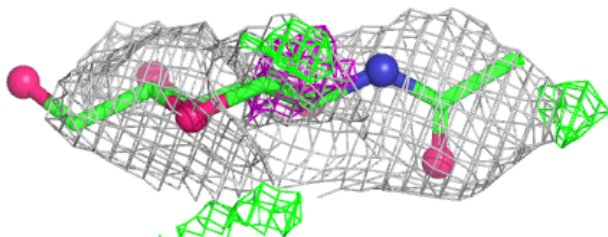
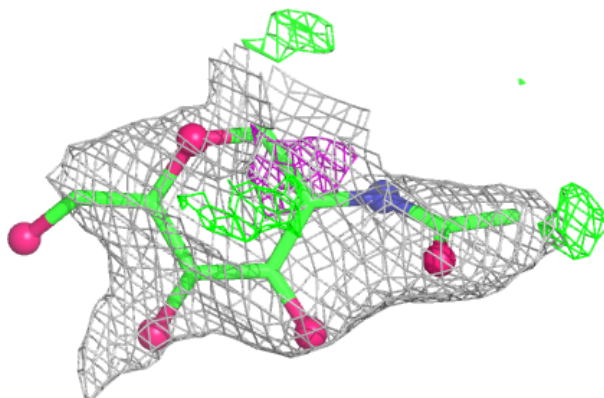


Electron density around NAG C 1610:

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

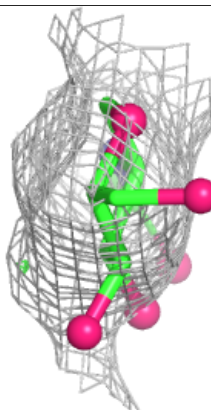
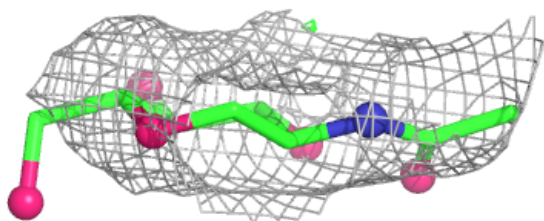
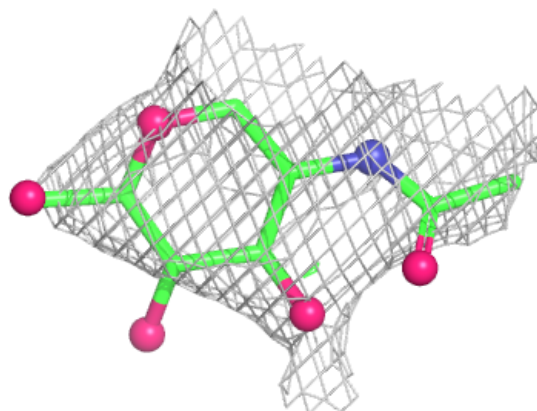
**Electron density around NAG G 501:**

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

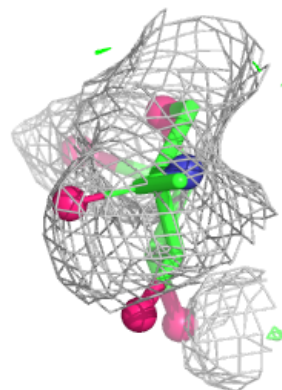
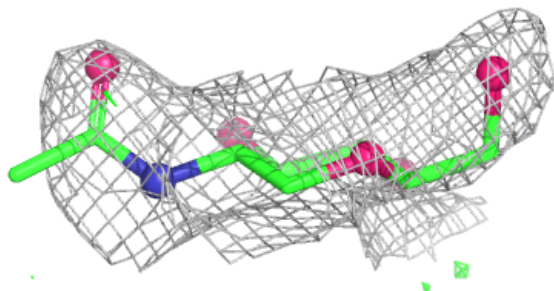
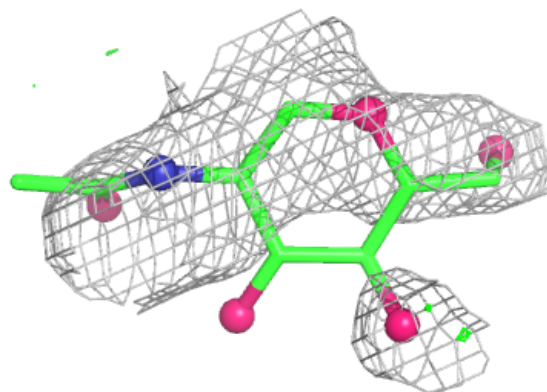


Electron density around NAG C 1611:

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

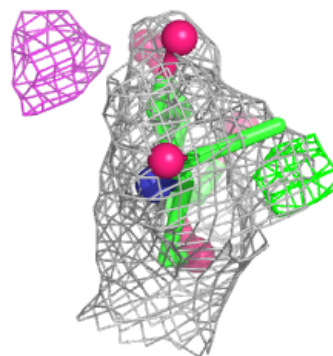
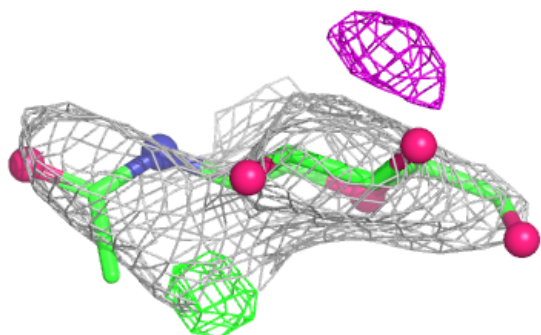
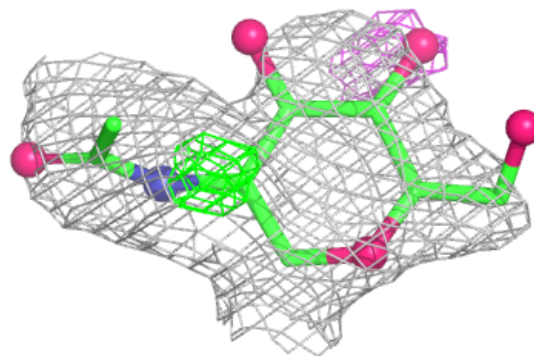
**Electron density around NAG G 507:**

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

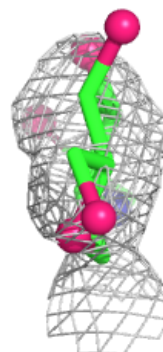
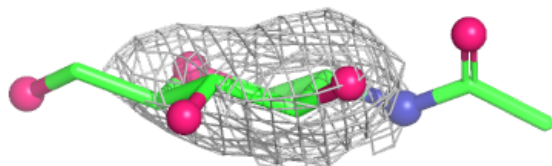
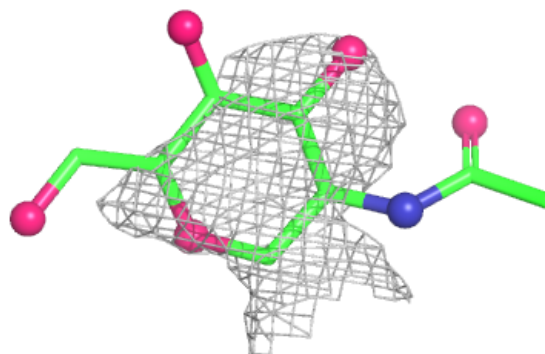


Electron density around NAG G 506:

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

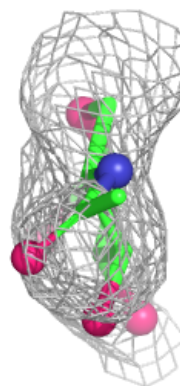
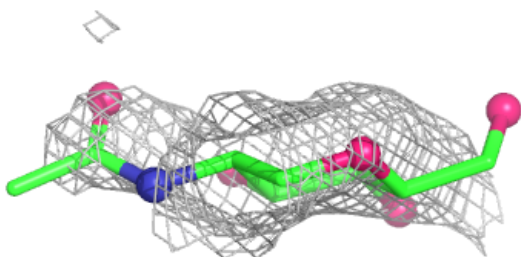
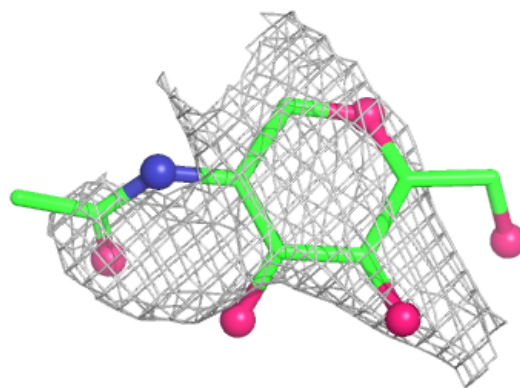
**Electron density around NAG G 508:**

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

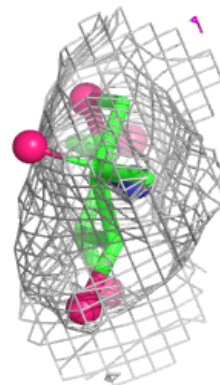
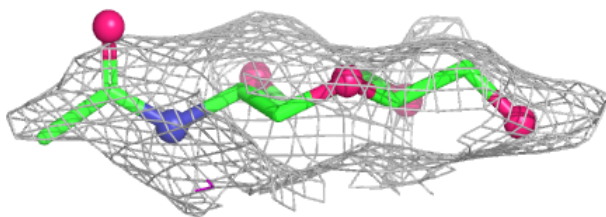
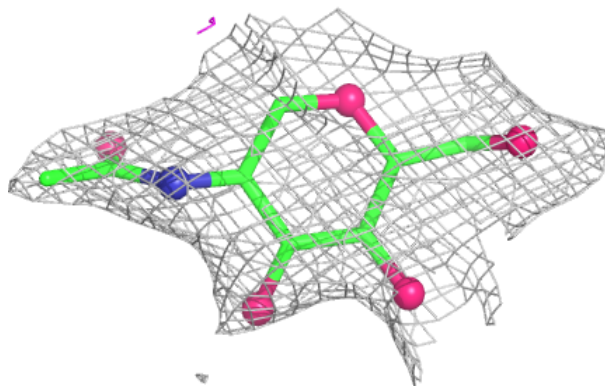


Electron density around NAG C 1601:

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

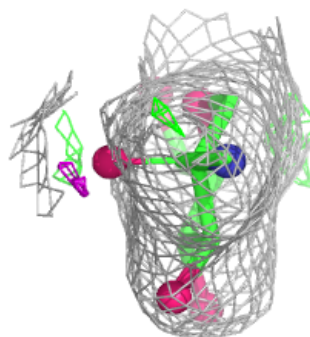
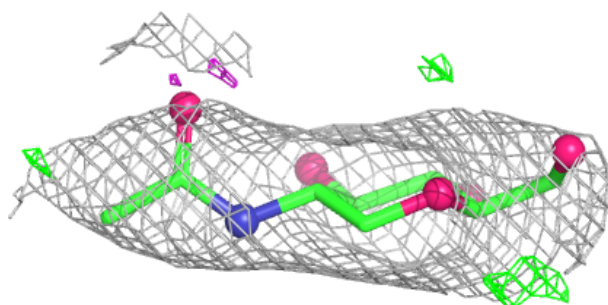
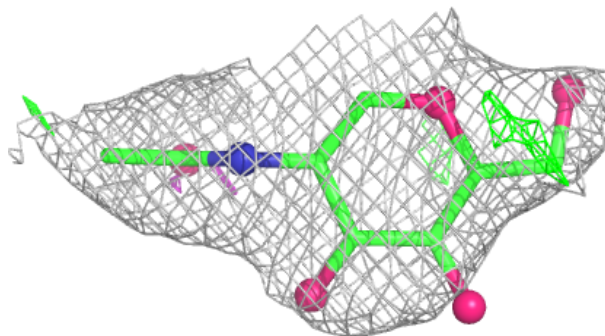
**Electron density around NAG C 1602:**

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

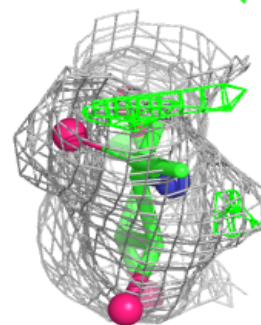
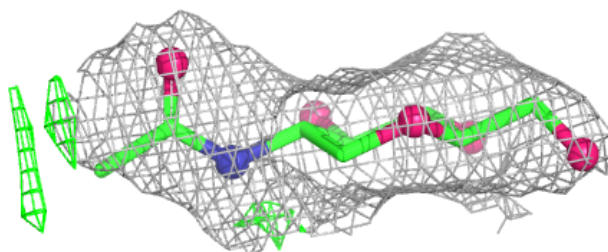
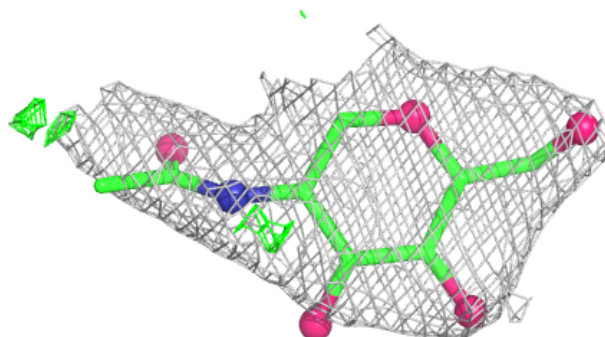


Electron density around NAG G 505:

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

**Electron density around NAG G 504:**

$2mF_o-DF_c$ (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.