Full wwPDB X-ray Structure Validation Report (i)

Dec 13, 2023 – 09:22 pm GMT

PDB ID	:	4CPZ
Title	:	Structure of the Neuraminidase from the B/Lyon/CHU/15.216/2011 virus in complex with Zanamivir
Authors	:	Vachieri, S.G.; Collins, P.J.; Escuret, V.; Casalegno, J.S.; Cattle, N.; Ferraris, O.; Sabatier, M.; Frobert, E.; Caro, V.; Skehel, J.J.; Gamblin, S.J.; Valla, F.; Valette, M.; Ottmann, M.; McCauley, J.W.; Daniels, R.S.; Lina, B.
Deposited on	:	2014-02-09
Resolution	:	2.20 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 (i) 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 ①) were used in the production of this report:

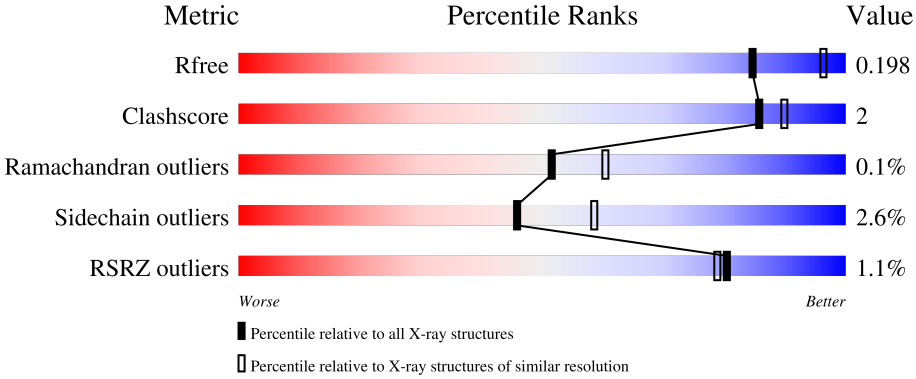
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (2.20-2.20)

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	466	79% • 16%
1	B	466	80% • 16%
1	C	466	80% • 16%
1	D	466	78% 5% 16%
1	E	466	2% 74% 9% • 16%

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Mol	Chain	Length	Quality of chain
1	F	466	2% 77% 6% 16%
1	G	466	% 74% 10% 16%
1	H	466	2% 76% 7% 16%
2	I	3	67% 33%
2	J	3	33% 67%
2	L	3	100%
2	M	3	33% 67%
2	N	3	33% 67%
2	O	3	67% 33%
3	K	2	100%
3	P	2	50% 50%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	NAG	H	1469	-	-	-	X

2 Entry composition (i)

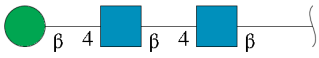
There are 8 unique types of molecules in this entry. The entry contains 25984 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 NEURAMINIDASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	390	3017	1891	520	577	29	0	0	0
1	B	390	3017	1891	520	577	29	0	0	0
1	C	390	3017	1891	520	577	29	0	0	0
1	D	390	3017	1891	520	577	29	0	0	0
1	E	390	3013	1890	520	574	29	0	0	0
1	F	390	3014	1890	520	575	29	0	0	0
1	G	390	3014	1890	520	575	29	0	0	0
1	H	390	3017	1891	520	577	29	0	0	0

- Molecule 2 is an oligosaccharide called 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
			Total	C	N	O			
2	I	3	39	22	2	15	0	0	0
2	J	3	39	22	2	15	0	0	0
2	L	3	39	22	2	15	0	0	0
2	M	3	39	22	2	15	0	0	0

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
2	N	3	39	22	2	15	0	0	0
			Total	C	N	O			
2	O	3	39	22	2	15	0	0	0

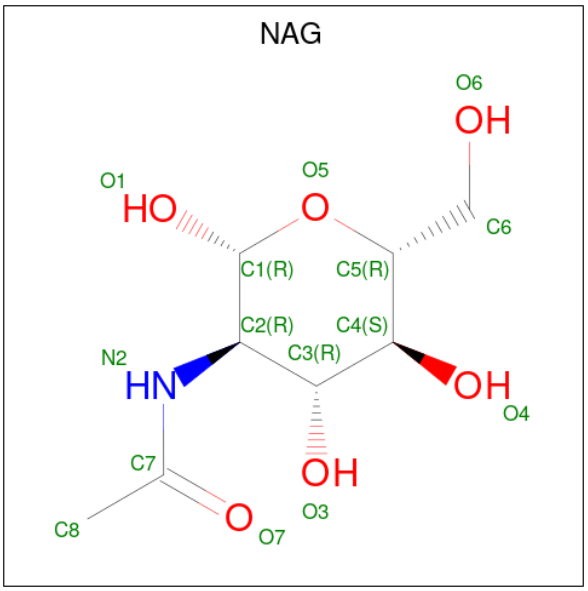
- Molecule 3 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
3	K	2	28	16	2	10	0	0	0
			Total	C	N	O			
3	P	2	28	16	2	10	0	0	0

- Molecule 4 is CALCIUM ION (three-letter code: CA) (formula: Ca).

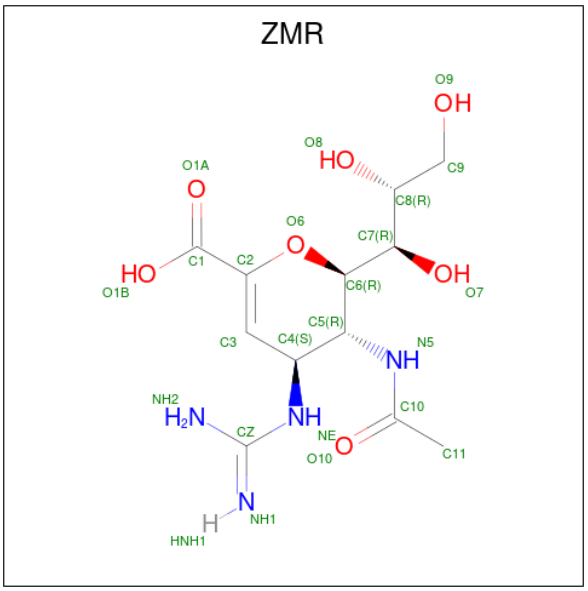
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Ca		
4	A	1	1	1	0	0
			Total	Ca		
4	B	1	1	1	0	0
			Total	Ca		
4	C	1	1	1	0	0
			Total	Ca		
4	D	1	1	1	0	0
			Total	Ca		
4	E	1	1	1	0	0
			Total	Ca		
4	F	1	1	1	0	0
			Total	Ca		
4	G	1	1	1	0	0
			Total	Ca		
4	H	1	1	1	0	0

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



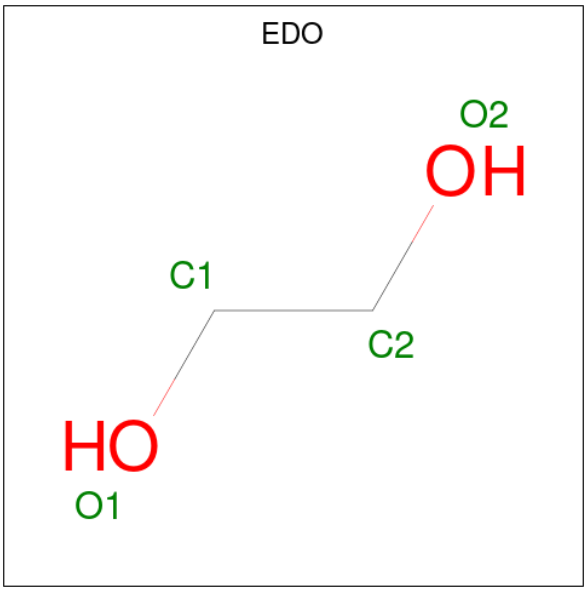
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
5	A	1	14	8	1	5	0	0
5	B	1	14	8	1	5	0	0
5	C	1	14	8	1	5	0	0
5	D	1	14	8	1	5	0	0
5	E	1	14	8	1	5	0	0
5	G	1	14	8	1	5	0	0
5	H	1	14	8	1	5	0	0

- Molecule 6 is ZANAMIVIR (three-letter code: ZMR) (formula: $C_{12}H_{20}N_4O_7$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
6	A	1	23	12	4	7	0	0
			Total	C	N	O		
6	B	1	23	12	4	7	0	0
			Total	C	N	O		
6	C	1	23	12	4	7	0	0
			Total	C	N	O		
6	D	1	23	12	4	7	0	0
			Total	C	N	O		
6	E	1	23	12	4	7	0	0
			Total	C	N	O		
6	F	1	23	12	4	7	0	0
			Total	C	N	O		
6	G	1	23	12	4	7	0	0
			Total	C	N	O		
6	H	1	23	12	4	7	0	0

- Molecule 7 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
7	D	1	4	2	2	0	0

- Molecule 8 is water.

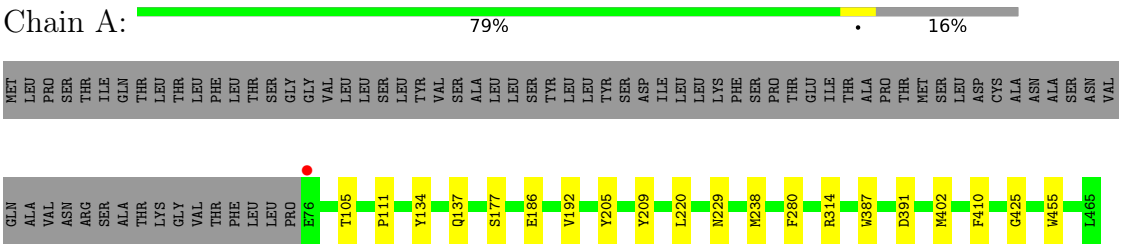
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
8	A	314	314	314	0	0
8	B	251	251	251	0	0
8	C	255	255	255	0	0
8	D	188	188	188	0	0
8	E	102	102	102	0	0
8	F	50	50	50	0	0
8	G	58	58	58	0	0
8	H	56	56	56	0	0

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.

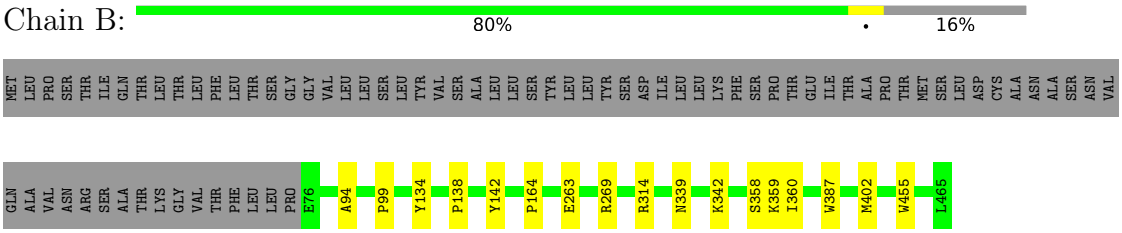
- Molecule 1: NEURAMINIDASE

Chain A:



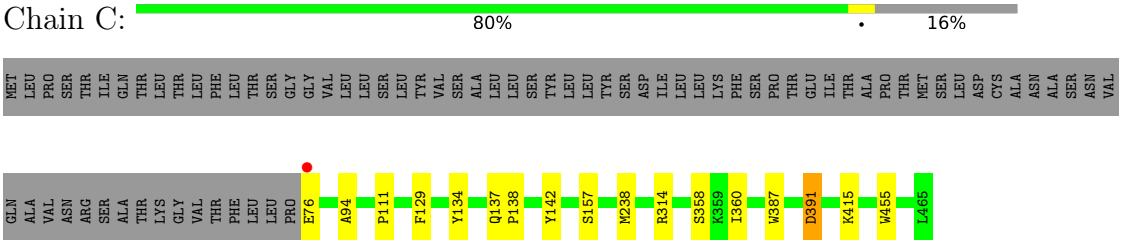
- Molecule 1: NEURAMINIDASE

Chain B:



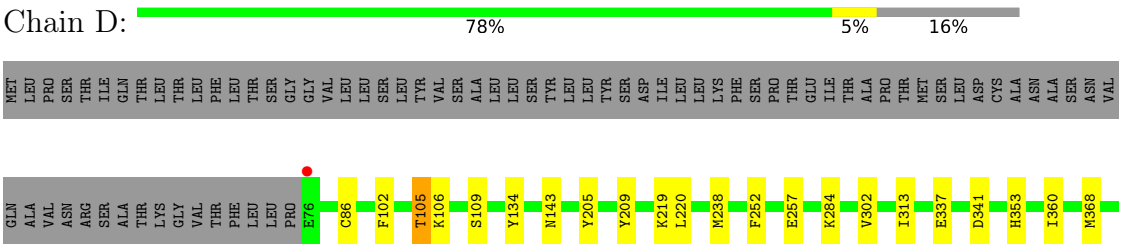
- Molecule 1: NEURAMINIDASE

Chain C:



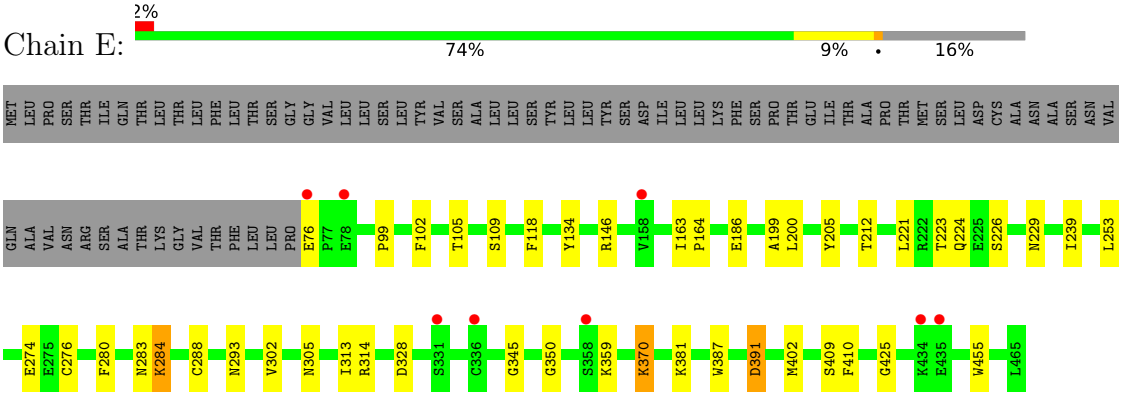
- Molecule 1: NEURAMINIDASE

Chain D:



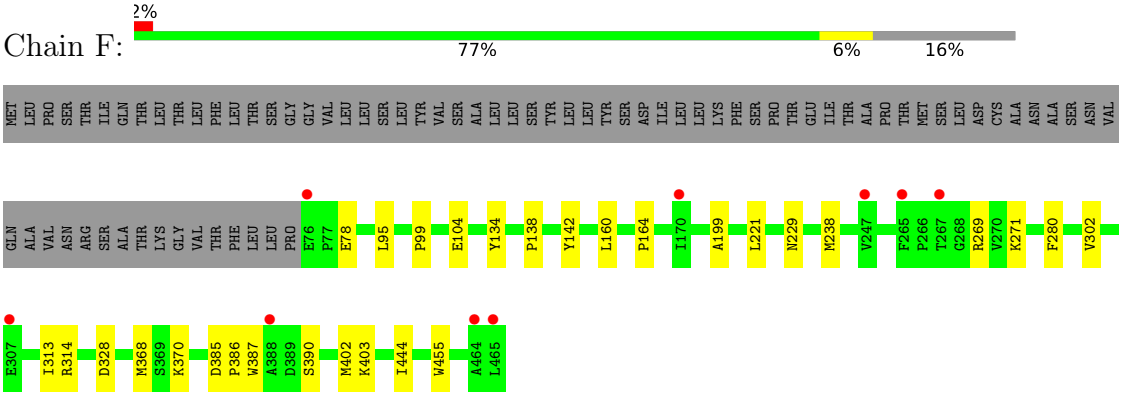
• Molecule 1: NEURAMINIDASE

Chain E:



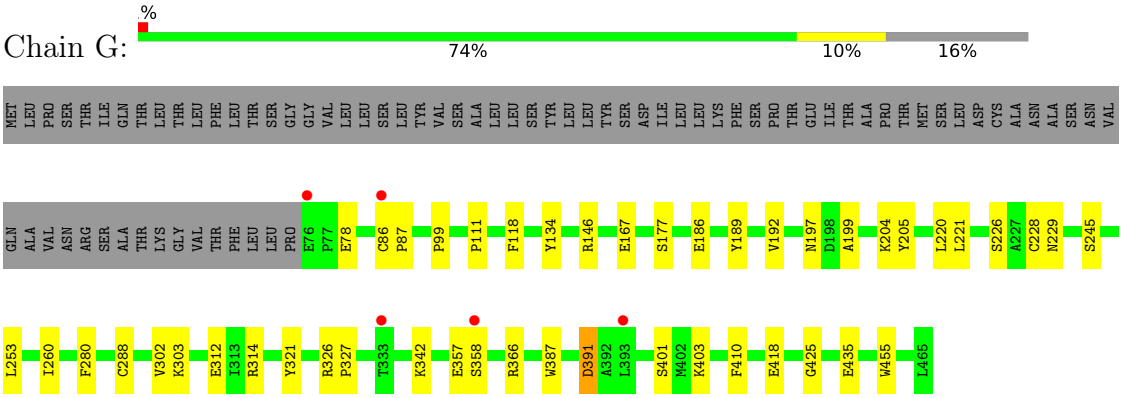
• Molecule 1: NEURAMINIDASE

Chain F:



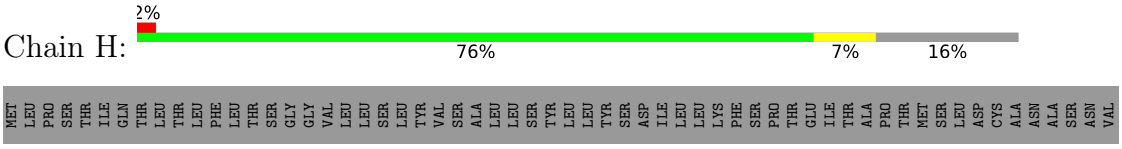
• Molecule 1: NEURAMINIDASE

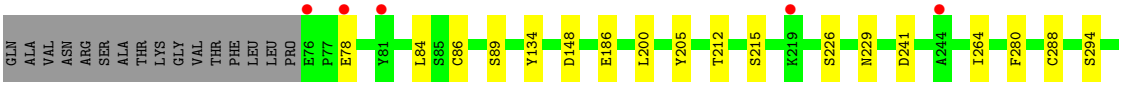
Chain G:

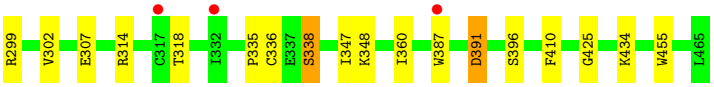


• Molecule 1: NEURAMINIDASE

Chain H:





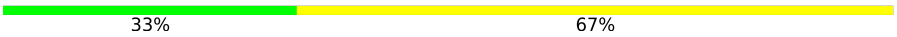


• Molecule 2: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain I:

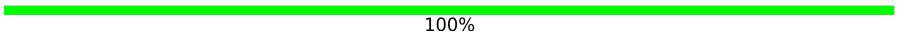
• Molecule 2: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain J:



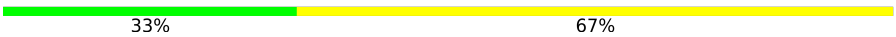
• Molecule 2: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain L:



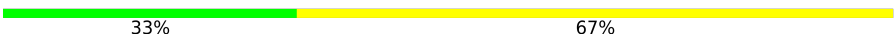
• Molecule 2: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain M:



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

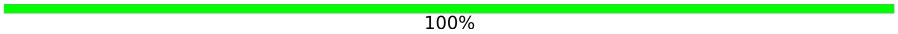
Chain N:



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

Chain O:

• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain K: 

• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain P:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	89.34Å 163.25Å 123.45Å 90.00° 108.31° 90.00°	Depositor
Resolution (Å)	48.50 – 2.20 48.50 – 2.20	Depositor EDS
% Data completeness (in resolution range)	96.8 (48.50-2.20) 96.4 (48.50-2.20)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.31 (at 2.20Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.153 , 0.200 0.151 , 0.198	Depositor DCC
R_{free} test set	8173 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å^2)	34.4	Xtriage
Anisotropy	0.711	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 45.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	0.029 for h,-k,-h-l	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	25984	wwPDB-VP
Average B, all atoms (Å^2)	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.45% 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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: CA, ZMR, BMA, NAG, EDO

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	0.47	0/3091	0.61	0/4176
1	B	0.41	0/3091	0.57	0/4176
1	C	0.45	0/3091	0.60	0/4176
1	D	0.42	0/3091	0.57	0/4176
1	E	0.31	0/3087	0.50	0/4172
1	F	0.31	0/3088	0.50	0/4172
1	G	0.32	0/3088	0.52	0/4172
1	H	0.30	0/3091	0.51	0/4176
All	All	0.38	0/24718	0.55	0/33396

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	3017	0	2891	8	0
1	B	3017	0	2891	9	0
1	C	3017	0	2891	6	0
1	D	3017	0	2891	15	0
1	E	3013	0	2889	23	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	F	3014	0	2890	12	0
1	G	3014	0	2889	20	0
1	H	3017	0	2891	14	0
2	I	39	0	34	1	0
2	J	39	0	34	1	0
2	L	39	0	34	0	0
2	M	39	0	34	1	0
2	N	39	0	34	0	0
2	O	39	0	34	0	0
3	K	28	0	25	0	0
3	P	28	0	25	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
4	E	1	0	0	0	0
4	F	1	0	0	0	0
4	G	1	0	0	0	0
4	H	1	0	0	0	0
5	A	14	0	13	0	0
5	B	14	0	13	0	0
5	C	14	0	13	0	0
5	D	14	0	13	0	0
5	E	14	0	13	0	0
5	G	14	0	13	0	0
5	H	14	0	13	0	0
6	A	23	0	19	0	0
6	B	23	0	19	0	0
6	C	23	0	19	0	0
6	D	23	0	18	0	0
6	E	23	0	19	0	0
6	F	23	0	19	0	0
6	G	23	0	19	0	0
6	H	23	0	19	1	0
7	D	4	0	6	2	0
8	A	314	0	0	2	1
8	B	251	0	0	3	0
8	C	255	0	0	0	1
8	D	188	0	0	4	0
8	E	102	0	0	1	0
8	F	50	0	0	0	0
8	G	58	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	H	56	0	0	0	0
All	All	25984	0	23625	105	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 2.

All (105) 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:D:86:CYS:HB2	8:D:2009:HOH:O	1.90	0.71
1:G:312:GLU:OE2	1:G:314:ARG:NH2	2.28	0.66
1:B:358:SER:O	8:B:2209:HOH:O	2.14	0.66
1:E:359:LYS:NZ	8:E:2084:HOH:O	2.21	0.63
1:H:200:LEU:HD11	1:H:212:THR:HB	1.82	0.61
1:B:314:ARG:HB2	1:B:387:TRP:CD1	2.37	0.60
1:F:302:VAL:HG22	1:F:313:ILE:HG12	1.85	0.58
1:H:314:ARG:HB2	1:H:387:TRP:CD1	2.38	0.57
1:E:350:GLY:N	1:E:409:SER:OG	2.37	0.57
1:E:391:ASP:OD1	1:E:391:ASP:N	2.38	0.57
1:G:401:SER:HB2	1:G:403:LYS:HE3	1.88	0.56
1:E:314:ARG:HB2	1:E:387:TRP:CD1	2.41	0.55
1:F:95:LEU:HD23	1:F:444:ILE:HD12	1.87	0.55
1:H:391:ASP:N	1:H:391:ASP:OD1	2.40	0.55
1:E:284:LYS:HD2	1:E:305:ASN:HD21	1.73	0.54
1:D:368:MET:HB2	1:D:402:MET:HG3	1.89	0.53
1:F:368:MET:HB2	1:F:402:MET:HG3	1.91	0.53
1:D:205:TYR:CE1	7:D:1472:EDO:H11	2.44	0.52
1:G:99:PRO:HB2	1:G:111:PRO:HB3	1.92	0.52
1:D:302:VAL:HG22	1:D:313:ILE:HG12	1.92	0.52
1:C:391:ASP:OD1	1:C:391:ASP:N	2.34	0.51
1:E:200:LEU:HD11	1:E:212:THR:HB	1.93	0.51
1:C:314:ARG:HB2	1:C:387:TRP:CD1	2.46	0.51
1:H:229:ASN:HB3	1:H:280:PHE:CE2	2.46	0.51
1:F:199:ALA:HB3	1:F:221:LEU:HB3	1.93	0.51
1:F:328:ASP:OD1	1:F:370:LYS:HE2	2.11	0.50
1:E:223:THR:OG1	1:E:224:GLN:N	2.43	0.49
1:G:391:ASP:N	1:G:391:ASP:OD1	2.44	0.49
1:E:276:CYS:HB3	1:E:288:CYS:HB3	1.95	0.48
1:H:299:ARG:HH22	1:H:347:ILE:HG23	1.77	0.48
1:F:99:PRO:HG3	1:F:164:PRO:HD2	1.94	0.48
1:A:314:ARG:HB2	1:A:387:TRP:CD1	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:335:PRO:O	1:H:338:SER:OG	2.32	0.48
1:F:269:ARG:NH2	1:F:271:LYS:HE2	2.30	0.47
1:H:288:CYS:HB2	1:H:302:VAL:HB	1.96	0.47
1:A:111:PRO:HD2	1:A:137:GLN:O	2.15	0.46
1:A:391:ASP:OD1	8:A:2275:HOH:O	2.20	0.46
1:D:341:ASP:N	8:D:2137:HOH:O	2.48	0.46
1:E:99:PRO:HG3	1:E:164:PRO:HD2	1.97	0.46
1:F:314:ARG:HB2	1:F:387:TRP:CD1	2.50	0.46
1:G:118:PHE:CG	1:G:226:SER:HA	2.51	0.46
1:C:111:PRO:HD2	1:C:137:GLN:O	2.16	0.46
1:E:328:ASP:OD1	1:E:370:LYS:HE2	2.16	0.46
1:F:138:PRO:HA	1:F:142:TYR:OH	2.15	0.46
1:D:105:THR:HG22	8:D:2020:HOH:O	2.14	0.45
1:E:229:ASN:HB3	1:E:280:PHE:CE1	2.51	0.45
1:G:253:LEU:HD13	1:G:260:ILE:HD13	1.97	0.45
1:B:138:PRO:HA	1:B:142:TYR:OH	2.16	0.45
1:D:106:LYS:HB2	8:D:2021:HOH:O	2.15	0.45
1:E:199:ALA:HB3	1:E:221:LEU:HB3	1.98	0.45
1:G:229:ASN:HB3	1:G:280:PHE:CE2	2.52	0.45
1:H:148:ASP:OD1	6:H:1470:ZMR:NE	2.49	0.45
1:G:189:TYR:HB2	1:G:204:LYS:HB3	1.99	0.45
1:B:94:ALA:HB1	1:D:209:TYR:CZ	2.52	0.45
1:C:138:PRO:HA	1:C:142:TYR:OH	2.17	0.44
1:A:177:SER:HB3	1:A:192:VAL:HB	1.98	0.44
1:A:410:PHE:CZ	1:A:425:GLY:HA3	2.53	0.44
1:G:177:SER:HB3	1:G:192:VAL:HB	2.00	0.44
1:E:163:ILE:HA	1:E:164:PRO:HD3	1.81	0.44
1:B:269:ARG:HH21	1:B:339:ASN:HD21	1.65	0.44
1:B:402:MET:SD	1:G:435:GLU:HG2	2.57	0.44
1:D:353:HIS:HD2	1:D:360:ILE:HD11	1.82	0.44
1:H:186:GLU:HB3	1:H:205:TYR:CZ	2.52	0.44
1:G:86:CYS:HB3	1:G:87:PRO:HD2	2.00	0.44
1:G:199:ALA:HB3	1:G:221:LEU:HB3	1.99	0.44
1:D:257:GLU:N	7:D:1472:EDO:H22	2.31	0.43
1:G:327:PRO:HD3	1:G:342:LYS:HB2	2.00	0.43
1:H:226:SER:HB3	1:H:348:LYS:HE3	1.99	0.43
1:B:359:LYS:HB3	8:B:2209:HOH:O	2.17	0.43
1:E:302:VAL:HG22	1:E:313:ILE:HG12	2.01	0.43
1:G:167:GLU:OE2	8:G:2029:HOH:O	2.21	0.43
1:E:381:LYS:HE2	1:E:391:ASP:HB2	2.01	0.43
1:D:102:PHE:O	1:D:109:SER:HB2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:209:TYR:CZ	1:C:94:ALA:HB1	2.54	0.42
8:A:2207:HOH:O	2:I:1:NAG:H83	2.18	0.42
1:B:269:ARG:HH21	1:B:339:ASN:ND2	2.17	0.42
1:F:385:ASP:HA	1:F:386:PRO:HD2	1.93	0.42
1:E:186:GLU:HB3	1:E:205:TYR:CZ	2.54	0.42
1:F:160:LEU:HD11	1:F:444:ILE:HD11	2.02	0.42
1:G:288:CYS:HB2	1:G:302:VAL:HB	2.01	0.42
1:D:341:ASP:OD1	1:H:434:LYS:HG2	2.19	0.42
1:H:215:SER:OG	1:H:241:ASP:OD2	2.23	0.42
1:E:239:ILE:HD13	1:E:253:LEU:HD11	2.02	0.42
1:G:321:TYR:O	1:G:366:ARG:NH1	2.49	0.42
1:E:274:GLU:OE2	1:E:293:ASN:HB2	2.20	0.41
1:C:129:PHE:CD1	1:C:157:SER:HB3	2.56	0.41
1:E:118:PHE:CG	1:E:226:SER:HA	2.55	0.41
1:E:283:ASN:HD22	2:M:1:NAG:H83	1.85	0.41
8:B:2162:HOH:O	2:J:1:NAG:H83	2.20	0.41
1:E:102:PHE:O	1:E:109:SER:HB2	2.21	0.41
1:D:410:PHE:CZ	1:D:425:GLY:HA3	2.56	0.41
1:E:293:ASN:HA	1:E:345:GLY:O	2.21	0.41
1:G:326:ARG:CZ	1:G:366:ARG:HD2	2.50	0.41
1:A:229:ASN:HB3	1:A:280:PHE:CE2	2.56	0.41
1:H:84:LEU:HA	1:H:84:LEU:HD23	1.85	0.41
1:G:410:PHE:CZ	1:G:425:GLY:HA3	2.56	0.41
1:H:410:PHE:CZ	1:H:425:GLY:HA3	2.56	0.41
1:A:186:GLU:HB3	1:A:205:TYR:CZ	2.57	0.40
1:D:353:HIS:CD2	1:D:360:ILE:HD11	2.56	0.40
1:F:229:ASN:HB3	1:F:280:PHE:CE2	2.57	0.40
1:G:303:LYS:HG3	1:G:387:TRP:CZ2	2.57	0.40
1:E:410:PHE:CZ	1:E:425:GLY:HA3	2.57	0.40
1:G:186:GLU:HB3	1:G:205:TYR:CZ	2.56	0.40
1:D:238:MET:HB2	1:D:252:PHE:CE2	2.56	0.40
1:B:99:PRO:HG3	1:B:164:PRO:HD2	2.03	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)
8:A:2305:HOH:O	8:C:2147:HOH:O[1_455]	2.19	0.01

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	388/466 (83%)	375 (97%)	12 (3%)	1 (0%)	41	46
1	B	388/466 (83%)	376 (97%)	12 (3%)	0	100	100
1	C	388/466 (83%)	376 (97%)	12 (3%)	0	100	100
1	D	388/466 (83%)	373 (96%)	14 (4%)	1 (0%)	41	46
1	E	388/466 (83%)	375 (97%)	13 (3%)	0	100	100
1	F	388/466 (83%)	375 (97%)	13 (3%)	0	100	100
1	G	388/466 (83%)	372 (96%)	15 (4%)	1 (0%)	41	46
1	H	388/466 (83%)	374 (96%)	14 (4%)	0	100	100
All	All	3104/3728 (83%)	2996 (96%)	105 (3%)	3 (0%)	51	60

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	G	220	LEU
1	A	220	LEU
1	D	220	LEU

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	323/390 (83%)	318 (98%)	5 (2%)	65	78
1	B	323/390 (83%)	318 (98%)	5 (2%)	65	78

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	323/390 (83%)	315 (98%)	8 (2%)	47	60
1	D	323/390 (83%)	316 (98%)	7 (2%)	52	65
1	E	322/390 (83%)	313 (97%)	9 (3%)	43	56
1	F	322/390 (83%)	315 (98%)	7 (2%)	52	65
1	G	322/390 (83%)	311 (97%)	11 (3%)	37	47
1	H	323/390 (83%)	309 (96%)	14 (4%)	29	36
All	All	2581/3120 (83%)	2515 (97%)	66 (3%)	46	58

All (66) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	105	THR
1	A	134	TYR
1	A	238	MET
1	A	402	MET
1	A	455	TRP
1	B	134	TYR
1	B	263	GLU
1	B	342	LYS
1	B	360	ILE
1	B	455	TRP
1	C	76	GLU
1	C	134	TYR
1	C	238	MET
1	C	358	SER
1	C	360	ILE
1	C	391	ASP
1	C	415	LYS
1	C	455	TRP
1	D	105	THR
1	D	134	TYR
1	D	143	ASN
1	D	219	LYS
1	D	284	LYS
1	D	337	GLU
1	D	455	TRP
1	E	76	GLU
1	E	105	THR
1	E	134	TYR
1	E	146	ARG

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Mol	Chain	Res	Type
1	E	284	LYS
1	E	370	LYS
1	E	391	ASP
1	E	402	MET
1	E	455	TRP
1	F	78	GLU
1	F	104	GLU
1	F	134	TYR
1	F	238	MET
1	F	390	SER
1	F	403	LYS
1	F	455	TRP
1	G	78	GLU
1	G	134	TYR
1	G	146	ARG
1	G	197	ASN
1	G	228	CYS
1	G	245	SER
1	G	357	GLU
1	G	358	SER
1	G	391	ASP
1	G	418	GLU
1	G	455	TRP
1	H	78	GLU
1	H	86	CYS
1	H	89	SER
1	H	134	TYR
1	H	264	ILE
1	H	294	SER
1	H	307	GLU
1	H	318	THR
1	H	336	CYS
1	H	338	SER
1	H	360	ILE
1	H	391	ASP
1	H	396	SER
1	H	455	TRP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	339	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)

22 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	I	1	1,2	14,14,15	0.38	0	17,19,21	0.41	0
2	NAG	I	2	2	14,14,15	0.42	0	17,19,21	0.43	0
2	BMA	I	3	2	11,11,12	1.00	0	15,15,17	0.81	0
2	NAG	J	1	1,2	14,14,15	0.56	0	17,19,21	0.53	0
2	NAG	J	2	2	14,14,15	0.26	0	17,19,21	0.50	0
2	BMA	J	3	2	11,11,12	1.53	2 (18%)	15,15,17	1.91	4 (26%)
3	NAG	K	1	1,3	14,14,15	0.41	0	17,19,21	0.34	0
3	NAG	K	2	3	14,14,15	0.18	0	17,19,21	0.46	0
2	NAG	L	1	1,2	14,14,15	0.45	0	17,19,21	0.47	0
2	NAG	L	2	2	14,14,15	0.32	0	17,19,21	0.56	0
2	BMA	L	3	2	11,11,12	0.81	0	15,15,17	0.85	0
2	NAG	M	1	1,2	14,14,15	0.40	0	17,19,21	0.35	0
2	NAG	M	2	2	14,14,15	0.28	0	17,19,21	0.42	0
2	BMA	M	3	2	11,11,12	0.55	0	15,15,17	0.96	1 (6%)
2	NAG	N	1	1,2	14,14,15	0.41	0	17,19,21	0.63	0
2	NAG	N	2	2	14,14,15	0.78	1 (7%)	17,19,21	1.10	1 (5%)
2	BMA	N	3	2	11,11,12	1.10	1 (9%)	15,15,17	0.90	0
2	NAG	O	1	1,2	14,14,15	0.27	0	17,19,21	0.41	0
2	NAG	O	2	2	14,14,15	0.30	0	17,19,21	0.42	0
2	BMA	O	3	2	11,11,12	1.09	1 (9%)	15,15,17	0.82	0
3	NAG	P	1	1,3	14,14,15	0.43	0	17,19,21	1.69	4 (23%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	NAG	P	2	3	14,14,15	0.40	0	17,19,21	0.49	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	I	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	I	2	2	-	0/6/23/26	0/1/1/1
2	BMA	I	3	2	-	0/2/19/22	0/1/1/1
2	NAG	J	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	J	2	2	-	2/6/23/26	0/1/1/1
2	BMA	J	3	2	-	2/2/19/22	0/1/1/1
3	NAG	K	1	1,3	-	4/6/23/26	0/1/1/1
3	NAG	K	2	3	-	2/6/23/26	0/1/1/1
2	NAG	L	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	L	2	2	-	0/6/23/26	0/1/1/1
2	BMA	L	3	2	-	2/2/19/22	0/1/1/1
2	NAG	M	1	1,2	-	4/6/23/26	0/1/1/1
2	NAG	M	2	2	-	2/6/23/26	0/1/1/1
2	BMA	M	3	2	-	0/2/19/22	0/1/1/1
2	NAG	N	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	N	2	2	-	2/6/23/26	0/1/1/1
2	BMA	N	3	2	-	0/2/19/22	0/1/1/1
2	NAG	O	1	1,2	-	4/6/23/26	0/1/1/1
2	NAG	O	2	2	-	1/6/23/26	0/1/1/1
2	BMA	O	3	2	-	2/2/19/22	0/1/1/1
3	NAG	P	1	1,3	-	3/6/23/26	0/1/1/1
3	NAG	P	2	3	-	0/6/23/26	0/1/1/1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	J	3	BMA	C2-C3	3.67	1.57	1.52
2	J	3	BMA	C1-C2	3.02	1.59	1.52
2	N	2	NAG	O5-C1	2.51	1.47	1.43
2	N	3	BMA	C4-C3	2.30	1.58	1.52
2	O	3	BMA	C1-C2	2.13	1.57	1.52

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	J	3	BMA	C1-C2-C3	5.12	115.96	109.67
3	P	1	NAG	C2-N2-C7	4.79	129.73	122.90
2	N	2	NAG	C1-O5-C5	4.34	118.08	112.19
2	J	3	BMA	O5-C1-C2	3.08	115.53	110.77
3	P	1	NAG	C1-C2-N2	3.03	115.67	110.49
2	J	3	BMA	C2-C3-C4	2.67	115.51	110.89
3	P	1	NAG	C4-C3-C2	-2.36	107.56	111.02
2	M	3	BMA	O2-C2-C3	-2.26	105.61	110.14
3	P	1	NAG	C1-O5-C5	2.12	115.06	112.19
2	J	3	BMA	O2-C2-C3	-2.04	106.06	110.14

There are no chirality outliers.

All (38) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	N	2	NAG	O5-C5-C6-O6
3	K	2	NAG	C4-C5-C6-O6
2	L	3	BMA	O5-C5-C6-O6
2	J	3	BMA	O5-C5-C6-O6
2	O	1	NAG	O5-C5-C6-O6
3	K	2	NAG	O5-C5-C6-O6
2	M	2	NAG	O5-C5-C6-O6
2	J	3	BMA	C4-C5-C6-O6
2	O	3	BMA	O5-C5-C6-O6
2	L	3	BMA	C4-C5-C6-O6
2	O	1	NAG	C4-C5-C6-O6
2	I	1	NAG	C8-C7-N2-C2
2	I	1	NAG	O7-C7-N2-C2
2	J	1	NAG	C8-C7-N2-C2
2	J	1	NAG	O7-C7-N2-C2
2	L	1	NAG	C8-C7-N2-C2
2	L	1	NAG	O7-C7-N2-C2
2	M	1	NAG	C8-C7-N2-C2
2	M	1	NAG	O7-C7-N2-C2
2	N	1	NAG	C8-C7-N2-C2
2	N	1	NAG	O7-C7-N2-C2
2	O	1	NAG	C8-C7-N2-C2
2	O	1	NAG	O7-C7-N2-C2
3	K	1	NAG	C8-C7-N2-C2
3	K	1	NAG	O7-C7-N2-C2
3	P	1	NAG	C8-C7-N2-C2

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Mol	Chain	Res	Type	Atoms
3	P	1	NAG	O7-C7-N2-C2
2	M	2	NAG	C4-C5-C6-O6
3	K	1	NAG	O5-C5-C6-O6
2	N	2	NAG	C4-C5-C6-O6
3	K	1	NAG	C4-C5-C6-O6
2	O	2	NAG	O5-C5-C6-O6
2	M	1	NAG	C4-C5-C6-O6
2	O	3	BMA	C4-C5-C6-O6
2	M	1	NAG	O5-C5-C6-O6
2	J	2	NAG	C4-C5-C6-O6
3	P	1	NAG	C1-C2-N2-C7
2	J	2	NAG	O5-C5-C6-O6

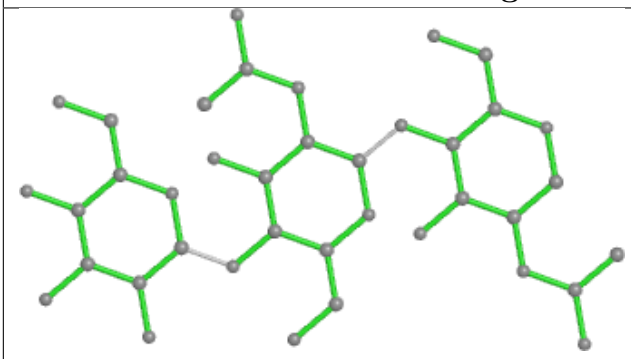
There are no ring outliers.

3 monomers are involved in 3 short contacts:

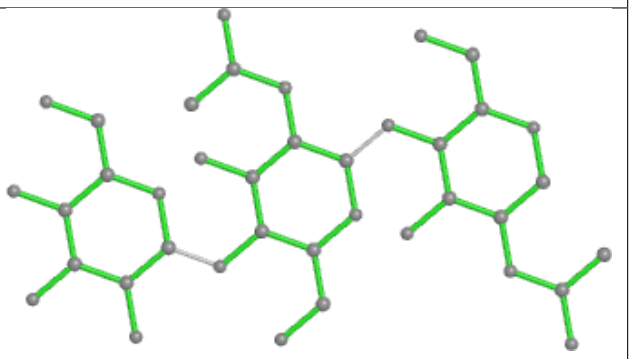
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	J	1	NAG	1	0
2	I	1	NAG	1	0
2	M	1	NAG	1	0

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

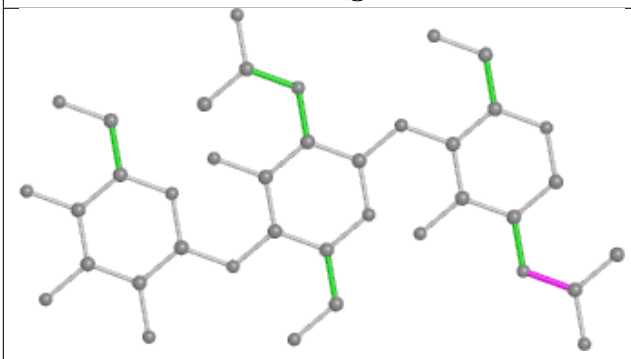
Oligosaccharide Chain I



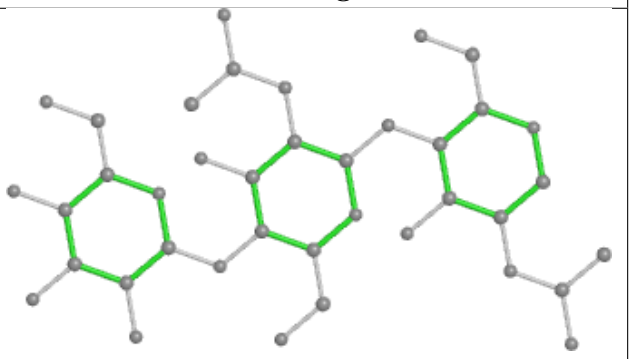
Bond lengths



Bond angles

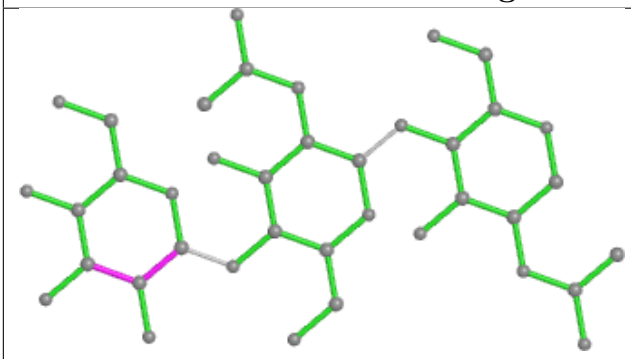


Torsions

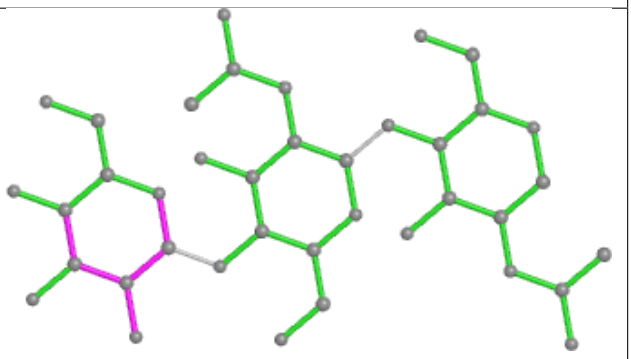


Rings

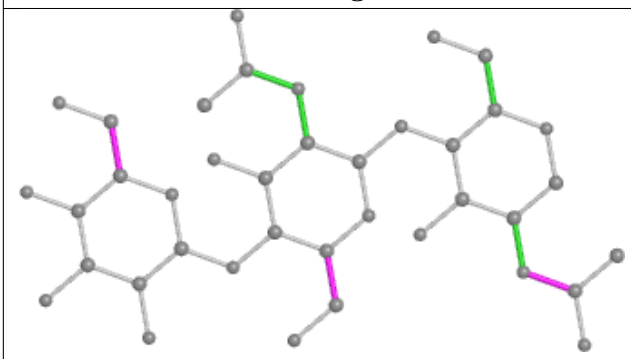
Oligosaccharide Chain J



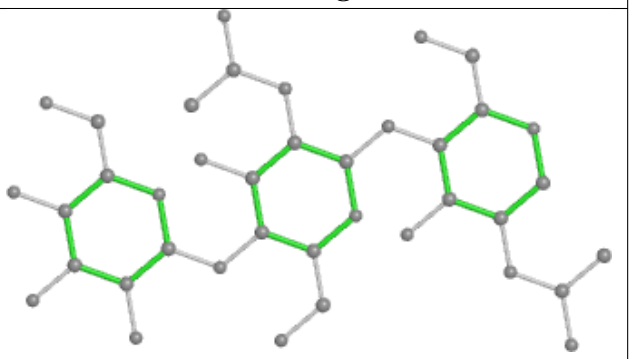
Bond lengths



Bond angles

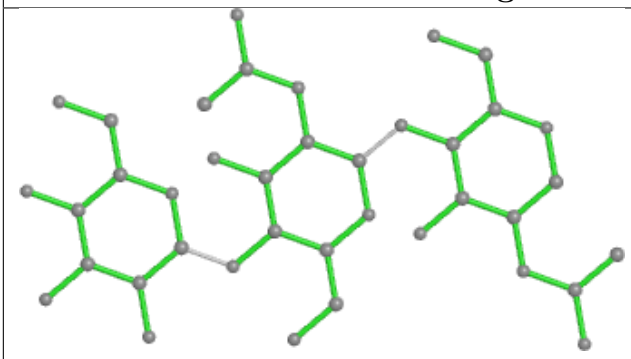


Torsions

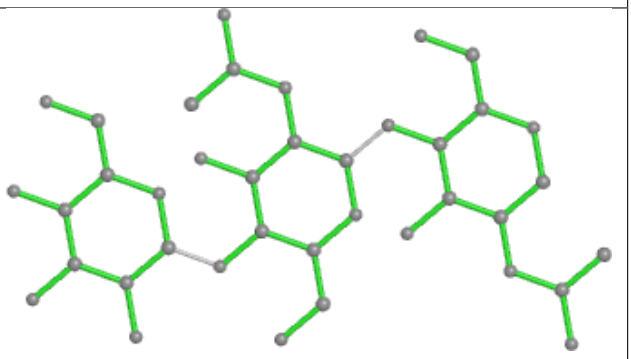


Rings

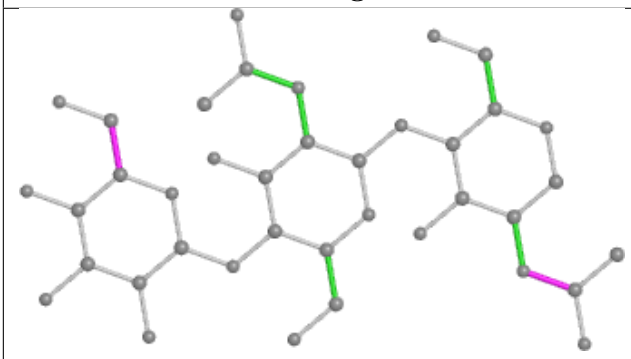
Oligosaccharide Chain L



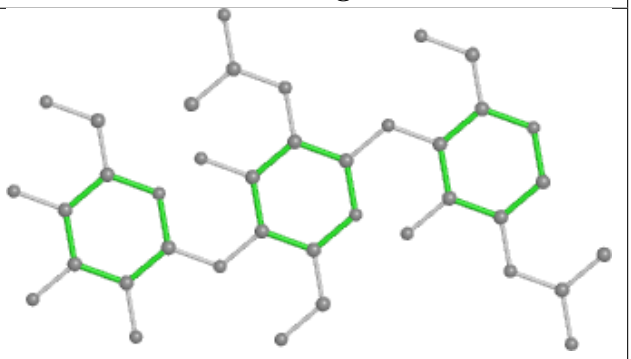
Bond lengths



Bond angles

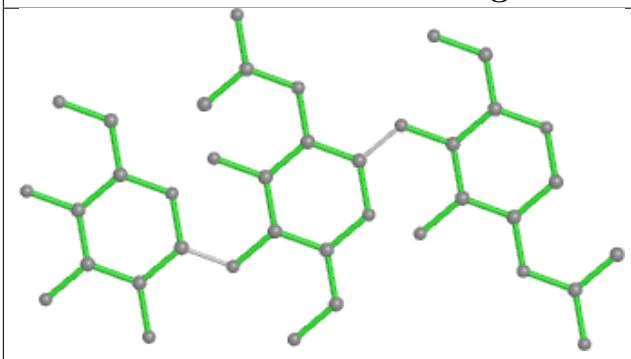


Torsions

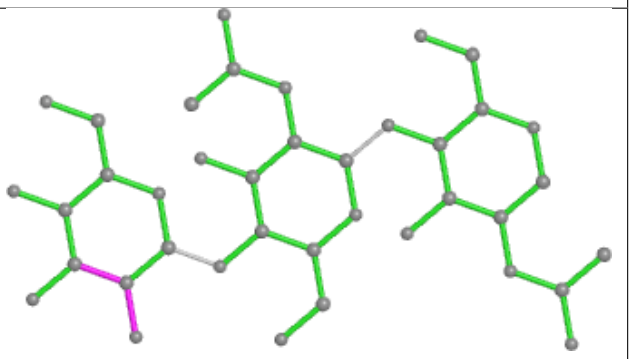


Rings

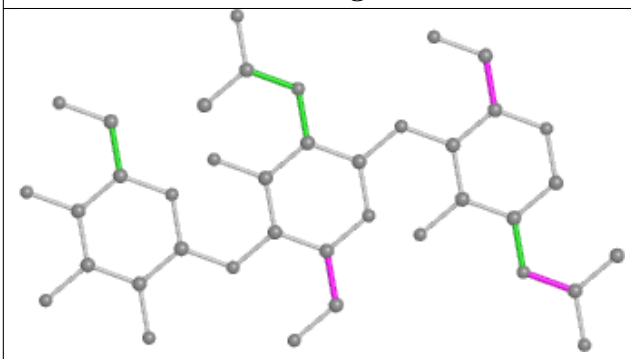
Oligosaccharide Chain M



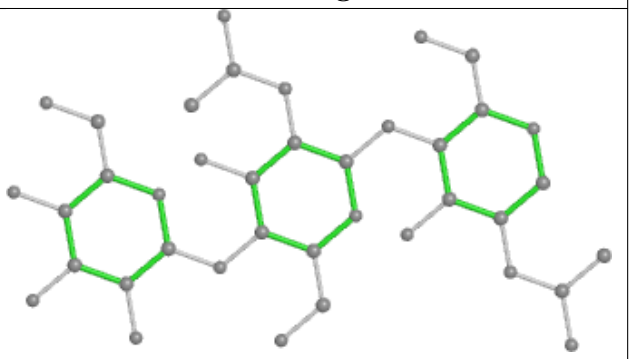
Bond lengths



Bond angles

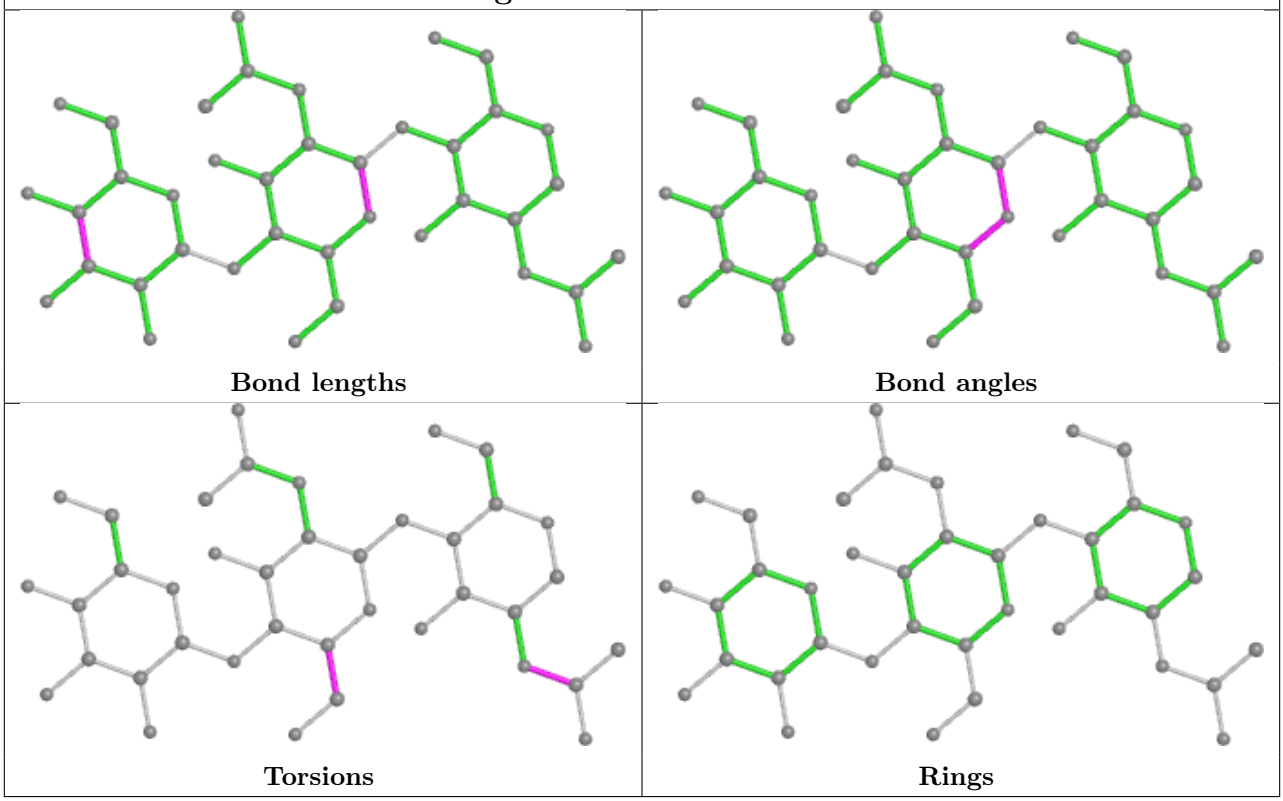


Torsions

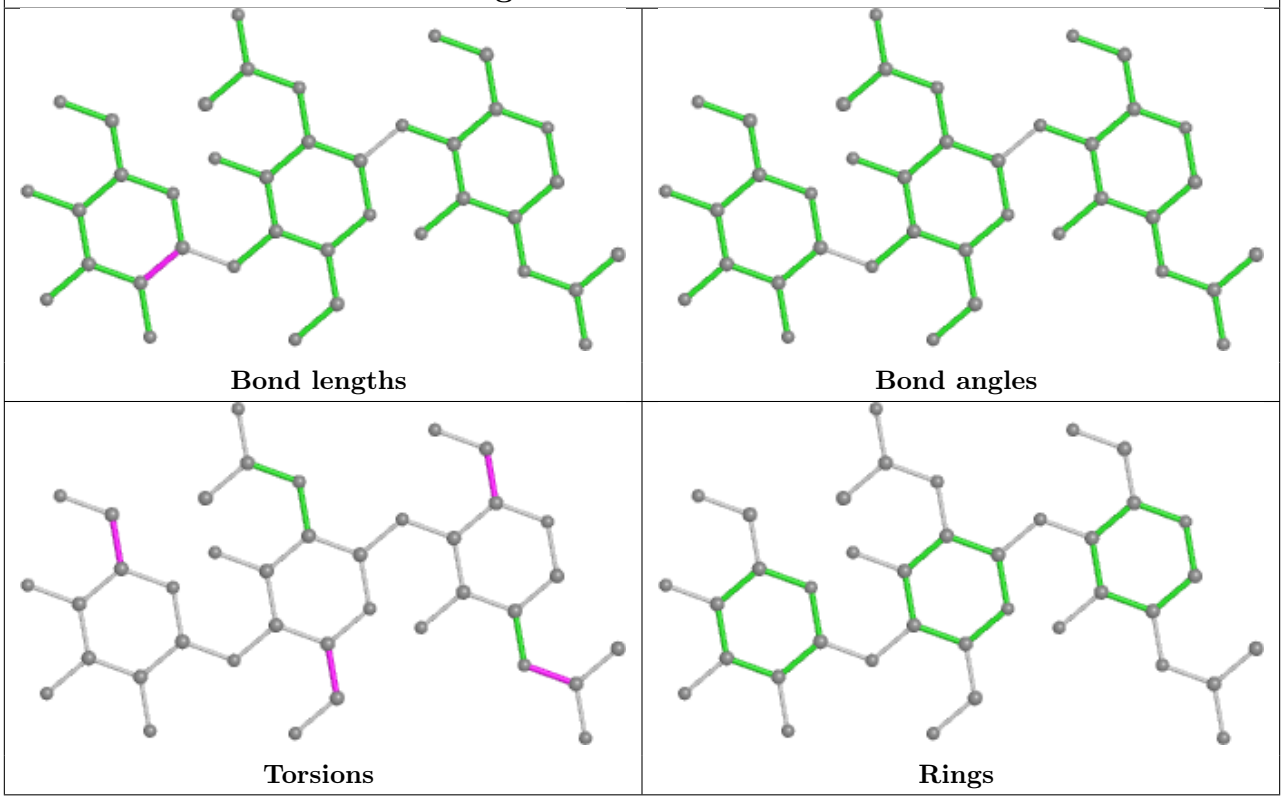


Rings

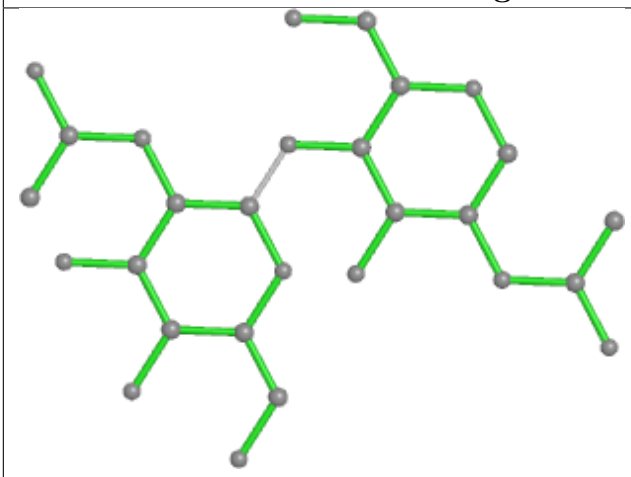
Oligosaccharide Chain N



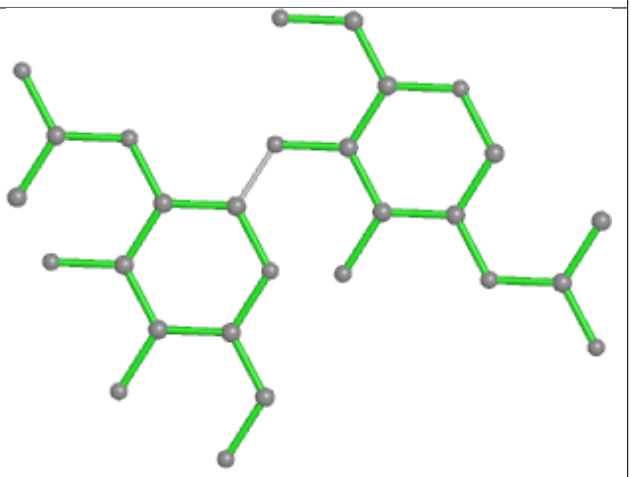
Oligosaccharide Chain O



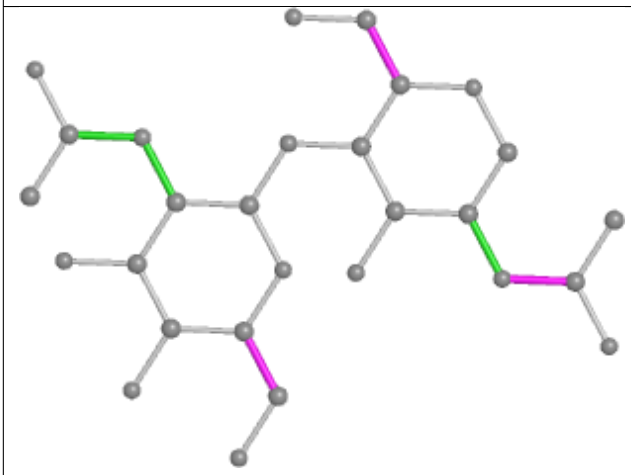
Oligosaccharide Chain K



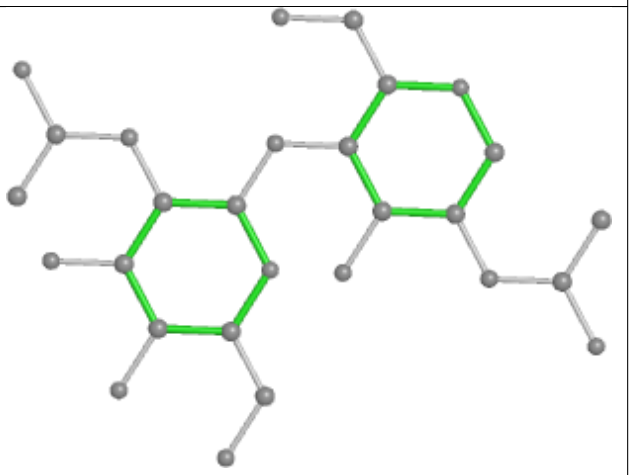
Bond lengths



Bond angles

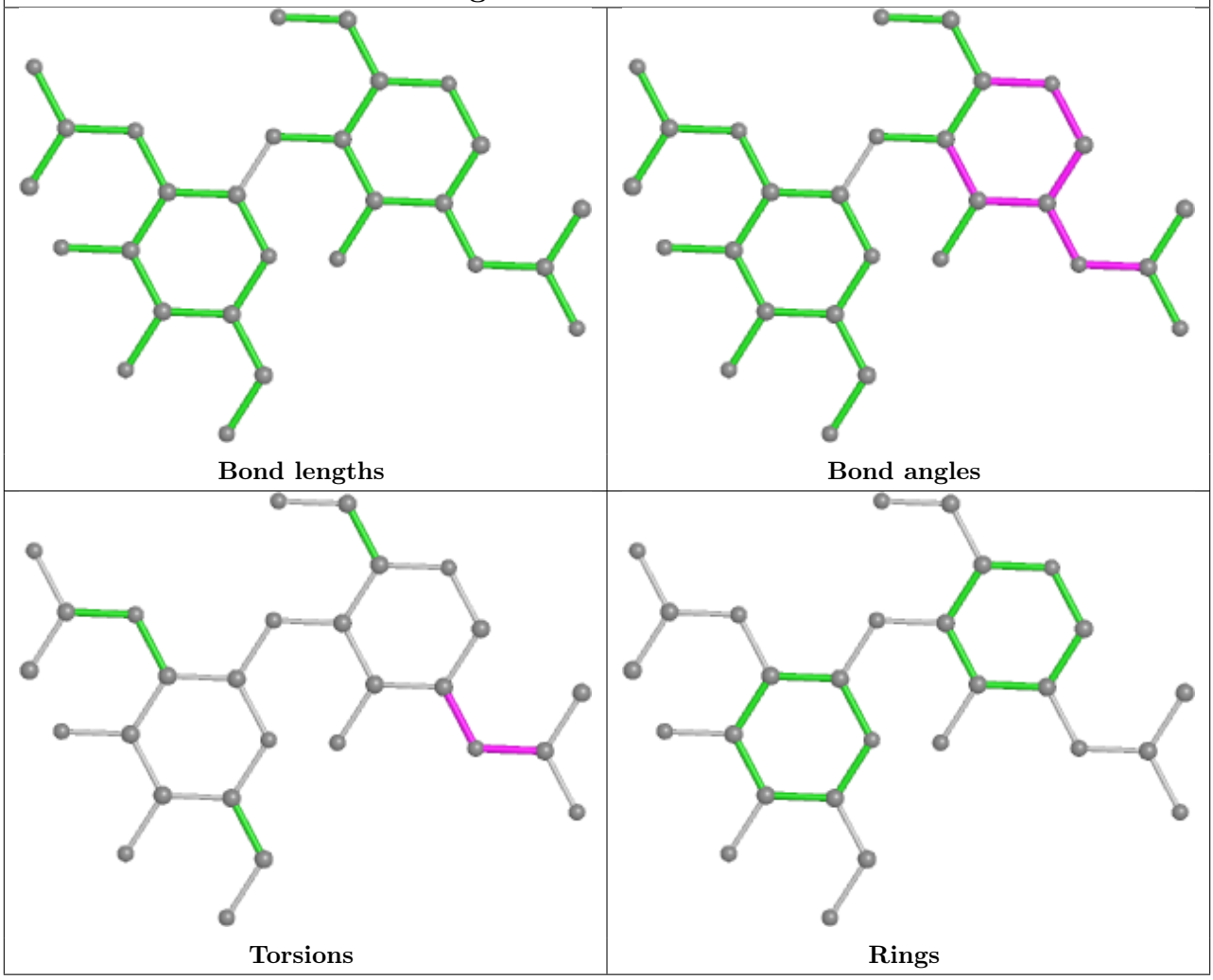


Torsions



Rings

Oligosaccharide Chain P



5.6 Ligand geometry (i)

Of 24 ligands modelled in this entry, 8 are monoatomic - leaving 16 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
5	NAG	C	1469	1	14,14,15	0.27	0	17,19,21	0.44	0
6	ZMR	D	1471	-	22,23,23	4.40	10 (45%)	24,32,32	3.32	6 (25%)
6	ZMR	F	1470	-	22,23,23	4.35	11 (50%)	24,32,32	3.70	4 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
6	ZMR	A	1471	-	22,23,23	4.49	10 (45%)	24,32,32	3.58	7 (29%)
5	NAG	G	1470	1	14,14,15	0.40	0	17,19,21	0.67	1 (5%)
5	NAG	A	1470	1	14,14,15	0.37	0	17,19,21	0.47	0
5	NAG	B	1470	1	14,14,15	0.65	0	17,19,21	0.53	0
5	NAG	H	1469	1	14,14,15	0.50	0	17,19,21	0.49	0
6	ZMR	C	1470	-	22,23,23	4.30	10 (45%)	24,32,32	3.38	4 (16%)
5	NAG	E	1470	1	14,14,15	0.44	0	17,19,21	0.43	0
7	EDO	D	1472	-	3,3,3	0.46	0	2,2,2	0.13	0
5	NAG	D	1470	1	14,14,15	0.47	0	17,19,21	0.50	0
6	ZMR	G	1471	-	22,23,23	4.43	11 (50%)	24,32,32	3.33	4 (16%)
6	ZMR	B	1471	-	22,23,23	4.49	10 (45%)	24,32,32	3.13	4 (16%)
6	ZMR	E	1471	-	22,23,23	4.39	11 (50%)	24,32,32	3.35	6 (25%)
6	ZMR	H	1470	-	22,23,23	4.42	11 (50%)	24,32,32	3.62	5 (20%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	C	1469	1	-	2/6/23/26	0/1/1/1
6	ZMR	D	1471	-	-	1/22/38/38	0/1/1/1
6	ZMR	F	1470	-	-	3/22/38/38	0/1/1/1
6	ZMR	A	1471	-	-	1/22/38/38	0/1/1/1
5	NAG	G	1470	1	-	2/6/23/26	0/1/1/1
5	NAG	A	1470	1	-	0/6/23/26	0/1/1/1
5	NAG	B	1470	1	-	2/6/23/26	0/1/1/1
5	NAG	H	1469	1	-	0/6/23/26	0/1/1/1
6	ZMR	C	1470	-	-	1/22/38/38	0/1/1/1
5	NAG	E	1470	1	-	2/6/23/26	0/1/1/1
7	EDO	D	1472	-	-	1/1/1/1	-
5	NAG	D	1470	1	-	0/6/23/26	0/1/1/1
6	ZMR	G	1471	-	-	2/22/38/38	0/1/1/1
6	ZMR	B	1471	-	-	1/22/38/38	0/1/1/1
6	ZMR	E	1471	-	-	2/22/38/38	0/1/1/1
6	ZMR	H	1470	-	-	3/22/38/38	0/1/1/1

All (84) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	1471	ZMR	C3-C2	15.23	1.57	1.33
6	B	1471	ZMR	C3-C2	14.91	1.56	1.33
6	G	1471	ZMR	C3-C2	14.17	1.55	1.33
6	D	1471	ZMR	C3-C2	14.12	1.55	1.33
6	E	1471	ZMR	C3-C2	13.98	1.55	1.33
6	C	1470	ZMR	C3-C2	13.98	1.55	1.33
6	F	1470	ZMR	C3-C2	13.76	1.54	1.33
6	H	1470	ZMR	C3-C2	13.58	1.54	1.33
6	H	1470	ZMR	C4-NE	7.46	1.56	1.46
6	D	1471	ZMR	CZ-NE	7.27	1.45	1.33
6	B	1471	ZMR	C4-NE	7.22	1.56	1.46
6	E	1471	ZMR	C5-N5	7.07	1.57	1.45
6	G	1471	ZMR	C4-NE	7.07	1.56	1.46
6	F	1470	ZMR	C4-NE	7.04	1.56	1.46
6	H	1470	ZMR	CZ-NE	6.99	1.45	1.33
6	A	1471	ZMR	C4-NE	6.96	1.56	1.46
6	D	1471	ZMR	C4-NE	6.92	1.56	1.46
6	C	1470	ZMR	C4-NE	6.90	1.56	1.46
6	G	1471	ZMR	C5-N5	6.90	1.56	1.45
6	G	1471	ZMR	CZ-NE	6.88	1.45	1.33
6	A	1471	ZMR	CZ-NE	6.85	1.45	1.33
6	E	1471	ZMR	C4-NE	6.85	1.55	1.46
6	H	1470	ZMR	C5-N5	6.81	1.56	1.45
6	C	1470	ZMR	CZ-NE	6.73	1.45	1.33
6	E	1471	ZMR	CZ-NE	6.72	1.45	1.33
6	B	1471	ZMR	C5-N5	6.69	1.56	1.45
6	F	1470	ZMR	C5-N5	6.61	1.56	1.45
6	D	1471	ZMR	C5-N5	6.61	1.56	1.45
6	F	1470	ZMR	CZ-NE	6.58	1.44	1.33
6	B	1471	ZMR	CZ-NE	6.55	1.44	1.33
6	C	1470	ZMR	C5-N5	6.04	1.55	1.45
6	A	1471	ZMR	C5-N5	5.97	1.55	1.45
6	H	1470	ZMR	C2-C1	-5.79	1.34	1.48
6	F	1470	ZMR	C2-C1	-5.35	1.35	1.48
6	E	1471	ZMR	C2-C1	-5.29	1.35	1.48
6	C	1470	ZMR	C2-C1	-5.11	1.36	1.48
6	G	1471	ZMR	C2-C1	-5.09	1.36	1.48
6	D	1471	ZMR	C2-C1	-4.94	1.36	1.48
6	A	1471	ZMR	C6-C5	-4.85	1.45	1.53
6	B	1471	ZMR	C6-C5	-4.59	1.45	1.53
6	F	1470	ZMR	C6-C5	-4.59	1.45	1.53
6	B	1471	ZMR	C2-C1	-4.59	1.37	1.48
6	H	1470	ZMR	C6-C5	-4.51	1.45	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	D	1471	ZMR	C6-C5	-4.49	1.45	1.53
6	C	1470	ZMR	C6-C5	-4.40	1.45	1.53
6	A	1471	ZMR	C2-C1	-4.33	1.38	1.48
6	E	1471	ZMR	C6-C5	-4.20	1.46	1.53
6	G	1471	ZMR	C6-C5	-4.20	1.46	1.53
6	B	1471	ZMR	O6-C2	3.30	1.50	1.37
6	G	1471	ZMR	O6-C2	3.23	1.50	1.37
6	F	1470	ZMR	O6-C2	3.21	1.50	1.37
6	E	1471	ZMR	O6-C2	3.16	1.50	1.37
6	A	1471	ZMR	O6-C2	3.10	1.49	1.37
6	E	1471	ZMR	C10-N5	3.02	1.44	1.34
6	H	1470	ZMR	C10-N5	2.87	1.44	1.34
6	D	1471	ZMR	O6-C2	2.85	1.48	1.37
6	G	1471	ZMR	C10-N5	2.83	1.44	1.34
6	H	1470	ZMR	O6-C2	2.83	1.48	1.37
6	F	1470	ZMR	C10-N5	2.78	1.43	1.34
6	C	1470	ZMR	O6-C2	2.77	1.48	1.37
6	D	1471	ZMR	C10-N5	2.74	1.43	1.34
6	B	1471	ZMR	C10-N5	2.72	1.43	1.34
6	D	1471	ZMR	O7-C7	-2.66	1.36	1.43
6	G	1471	ZMR	O7-C7	-2.60	1.36	1.43
6	A	1471	ZMR	C10-N5	2.57	1.43	1.34
6	F	1470	ZMR	O8-C8	-2.56	1.37	1.43
6	H	1470	ZMR	O8-C8	-2.52	1.38	1.43
6	A	1471	ZMR	O7-C7	-2.51	1.37	1.43
6	G	1471	ZMR	O8-C8	-2.50	1.38	1.43
6	B	1471	ZMR	O7-C7	-2.49	1.37	1.43
6	C	1470	ZMR	O7-C7	-2.46	1.37	1.43
6	D	1471	ZMR	O8-C8	-2.45	1.38	1.43
6	C	1470	ZMR	C10-N5	2.41	1.42	1.34
6	H	1470	ZMR	O7-C7	-2.39	1.37	1.43
6	E	1471	ZMR	O7-C7	-2.37	1.37	1.43
6	C	1470	ZMR	O8-C8	-2.37	1.38	1.43
6	E	1471	ZMR	O8-C8	-2.36	1.38	1.43
6	G	1471	ZMR	C4-C3	-2.35	1.47	1.50
6	F	1470	ZMR	O7-C7	-2.35	1.37	1.43
6	A	1471	ZMR	O8-C8	-2.26	1.38	1.43
6	B	1471	ZMR	O8-C8	-2.23	1.38	1.43
6	H	1470	ZMR	C4-C3	-2.23	1.47	1.50
6	F	1470	ZMR	C4-C3	-2.19	1.47	1.50
6	E	1471	ZMR	C4-C3	-2.11	1.47	1.50

All (41) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	H	1470	ZMR	O6-C2-C3	-16.09	105.85	124.61
6	A	1471	ZMR	O6-C2-C3	-15.82	106.17	124.61
6	F	1470	ZMR	O6-C2-C3	-15.62	106.39	124.61
6	C	1470	ZMR	O6-C2-C3	-15.50	106.54	124.61
6	D	1471	ZMR	O6-C2-C3	-14.84	107.31	124.61
6	E	1471	ZMR	O6-C2-C3	-14.62	107.56	124.61
6	G	1471	ZMR	O6-C2-C3	-13.64	108.71	124.61
6	B	1471	ZMR	O6-C2-C3	-13.24	109.17	124.61
6	G	1471	ZMR	C3-C2-C1	-6.93	108.70	123.65
6	F	1470	ZMR	C3-C2-C1	-6.25	110.15	123.65
6	H	1470	ZMR	C3-C2-C1	-4.83	113.22	123.65
6	B	1471	ZMR	C3-C2-C1	-4.65	113.62	123.65
6	E	1471	ZMR	C3-C2-C1	-4.16	114.68	123.65
6	F	1470	ZMR	O9-C9-C8	3.78	119.31	111.07
6	H	1470	ZMR	O9-C9-C8	3.52	118.74	111.07
6	A	1471	ZMR	C3-C2-C1	-3.43	116.25	123.65
6	B	1471	ZMR	O1B-C1-C2	3.34	122.53	114.20
6	A	1471	ZMR	O6-C2-C1	-3.16	105.74	112.06
6	D	1471	ZMR	C3-C2-C1	-3.10	116.97	123.65
6	A	1471	ZMR	O1B-C1-C2	2.94	121.55	114.20
6	D	1471	ZMR	O9-C9-C8	2.92	117.43	111.07
6	G	1471	ZMR	O9-C9-C8	2.91	117.42	111.07
6	B	1471	ZMR	O6-C2-C1	-2.91	106.24	112.06
6	C	1470	ZMR	O9-C9-C8	2.90	117.38	111.07
6	F	1470	ZMR	O1B-C1-C2	2.83	121.25	114.20
6	C	1470	ZMR	O1B-C1-C2	2.82	121.24	114.20
6	E	1471	ZMR	O9-C9-C8	2.79	117.16	111.07
6	E	1471	ZMR	O1B-C1-C2	2.60	120.68	114.20
6	A	1471	ZMR	O1B-C1-O1A	-2.58	117.70	123.61
6	C	1470	ZMR	C3-C2-C1	-2.50	118.25	123.65
6	A	1471	ZMR	C6-C5-N5	-2.38	106.96	110.91
6	E	1471	ZMR	C11-C10-N5	2.35	120.07	116.10
6	D	1471	ZMR	O1B-C1-C2	2.21	119.72	114.20
6	D	1471	ZMR	C11-C10-N5	2.20	119.82	116.10
6	G	1471	ZMR	O1B-C1-C2	2.14	119.53	114.20
5	G	1470	NAG	C1-O5-C5	2.12	115.06	112.19
6	D	1471	ZMR	C5-N5-C10	-2.07	118.15	123.18
6	A	1471	ZMR	C8-C7-C6	-2.06	109.12	113.03
6	E	1471	ZMR	C8-C7-C6	-2.05	109.14	113.03
6	H	1470	ZMR	C5-N5-C10	-2.02	118.26	123.18
6	H	1470	ZMR	C11-C10-N5	2.00	119.49	116.10

There are no chirality outliers.

All (23) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	H	1470	ZMR	O1A-C1-C2-O6
5	G	1470	NAG	C4-C5-C6-O6
5	C	1469	NAG	C4-C5-C6-O6
5	B	1470	NAG	O5-C5-C6-O6
5	G	1470	NAG	O5-C5-C6-O6
5	B	1470	NAG	C4-C5-C6-O6
5	C	1469	NAG	O5-C5-C6-O6
6	A	1471	ZMR	O1A-C1-C2-O6
6	E	1471	ZMR	O1A-C1-C2-O6
6	G	1471	ZMR	O1A-C1-C2-O6
7	D	1472	EDO	O1-C1-C2-O2
6	D	1471	ZMR	O1A-C1-C2-O6
6	F	1470	ZMR	O1A-C1-C2-O6
6	E	1471	ZMR	O1B-C1-C2-O6
6	G	1471	ZMR	O1B-C1-C2-O6
6	H	1470	ZMR	O1B-C1-C2-O6
6	B	1471	ZMR	O1A-C1-C2-O6
6	C	1470	ZMR	O1A-C1-C2-O6
6	F	1470	ZMR	C6-C7-C8-O8
5	E	1470	NAG	C4-C5-C6-O6
5	E	1470	NAG	O5-C5-C6-O6
6	H	1470	ZMR	O1A-C1-C2-C3
6	F	1470	ZMR	O7-C7-C8-O8

There are no ring outliers.

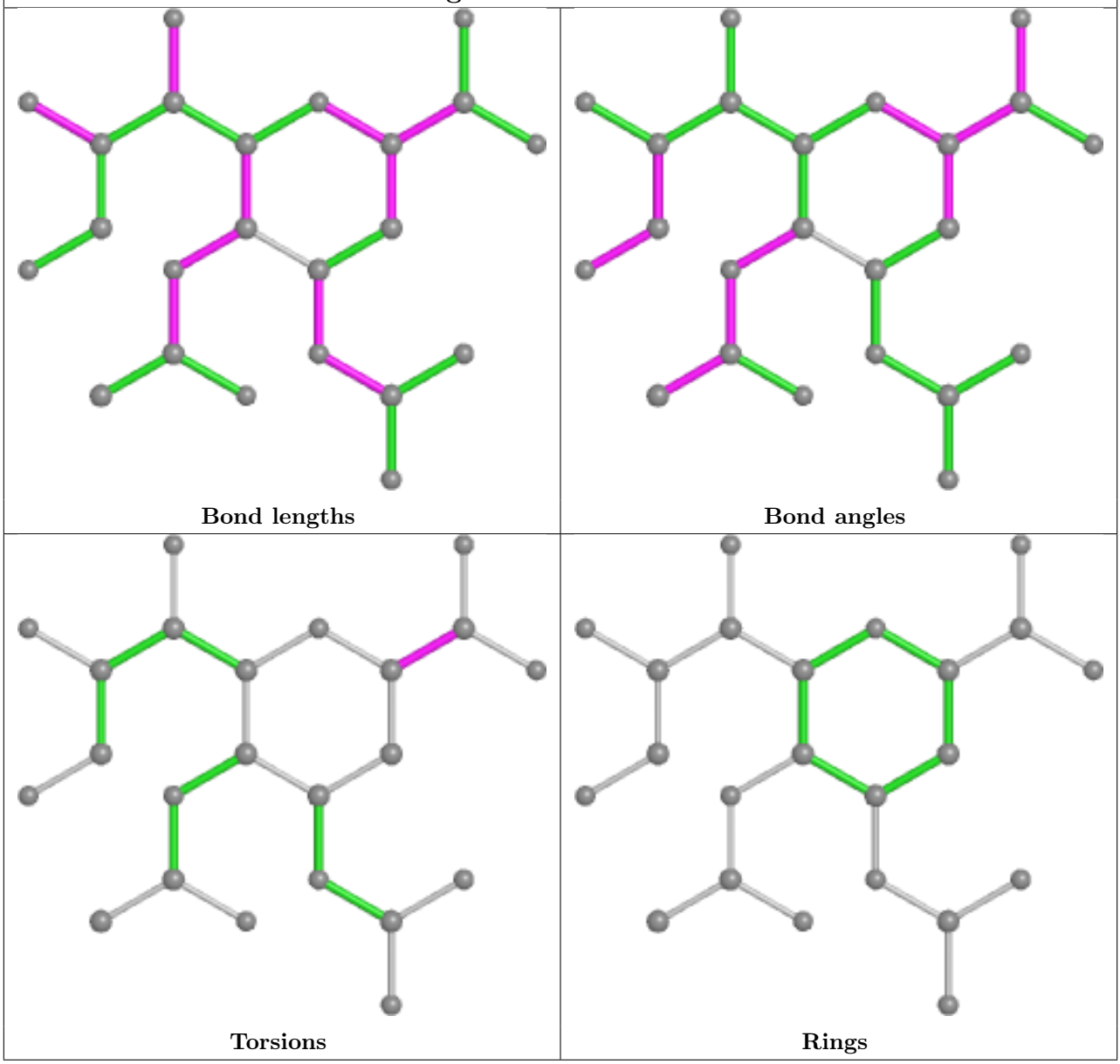
2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	D	1472	EDO	2	0
6	H	1470	ZMR	1	0

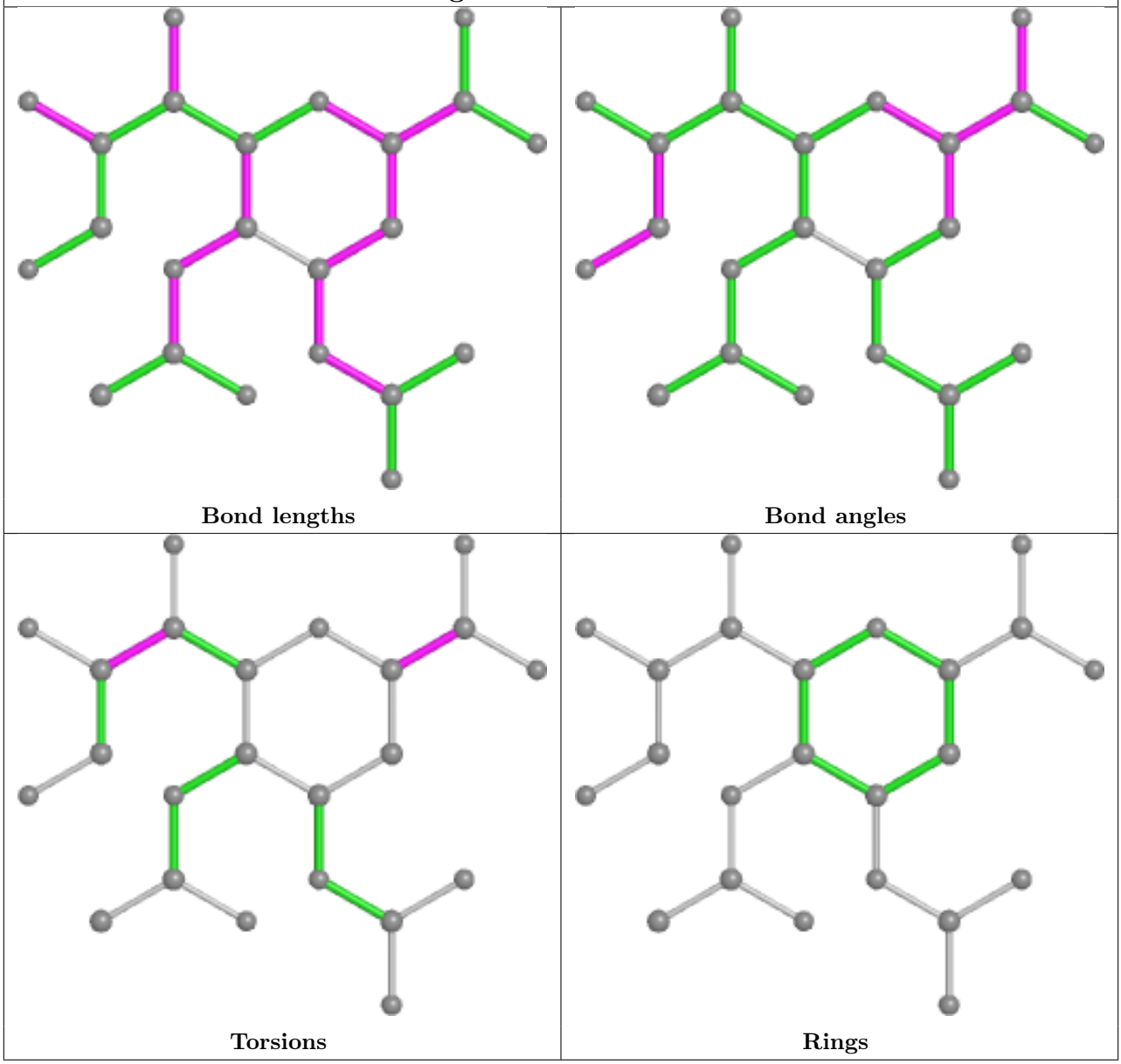
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

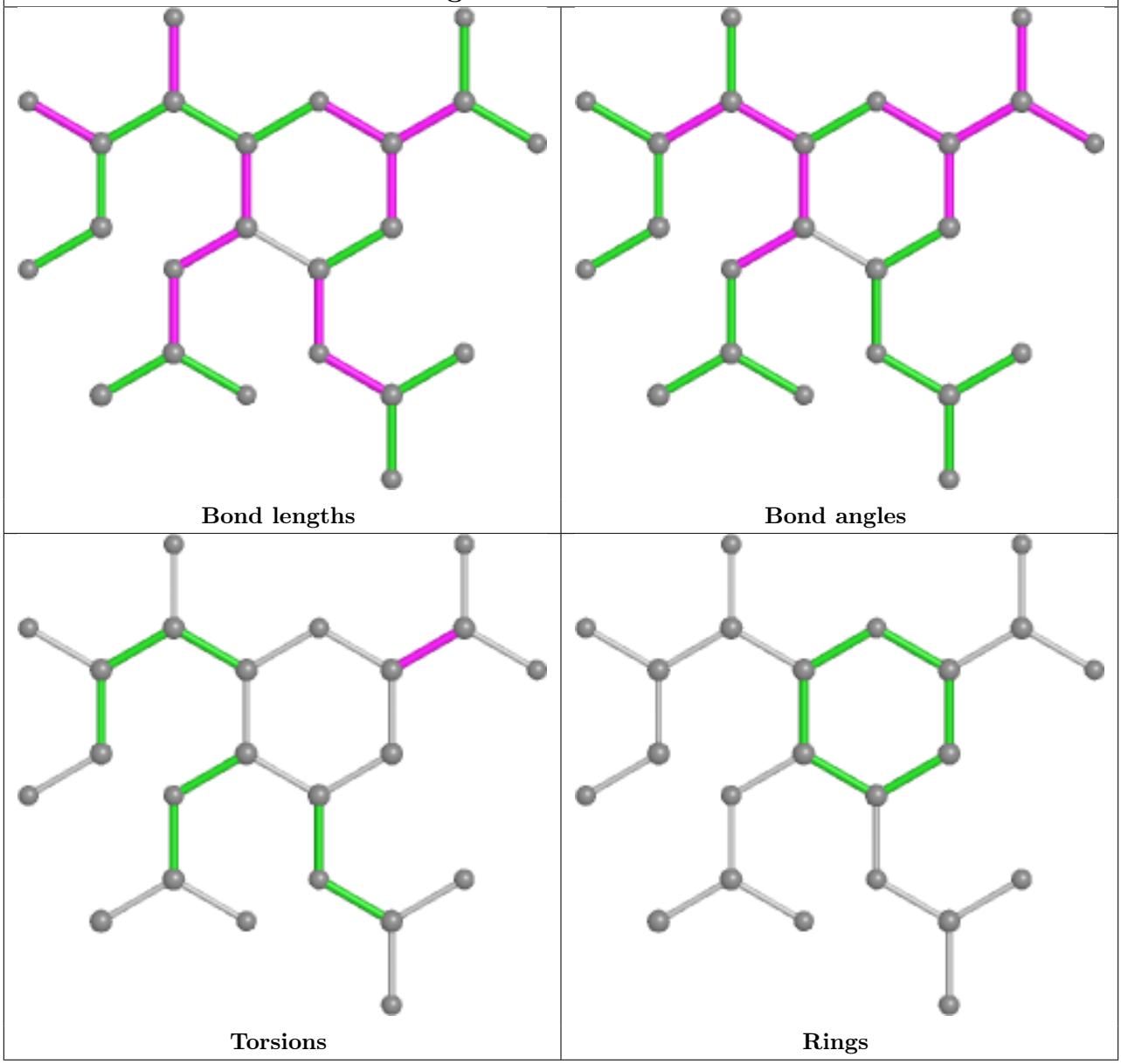
Ligand ZMR D 1471



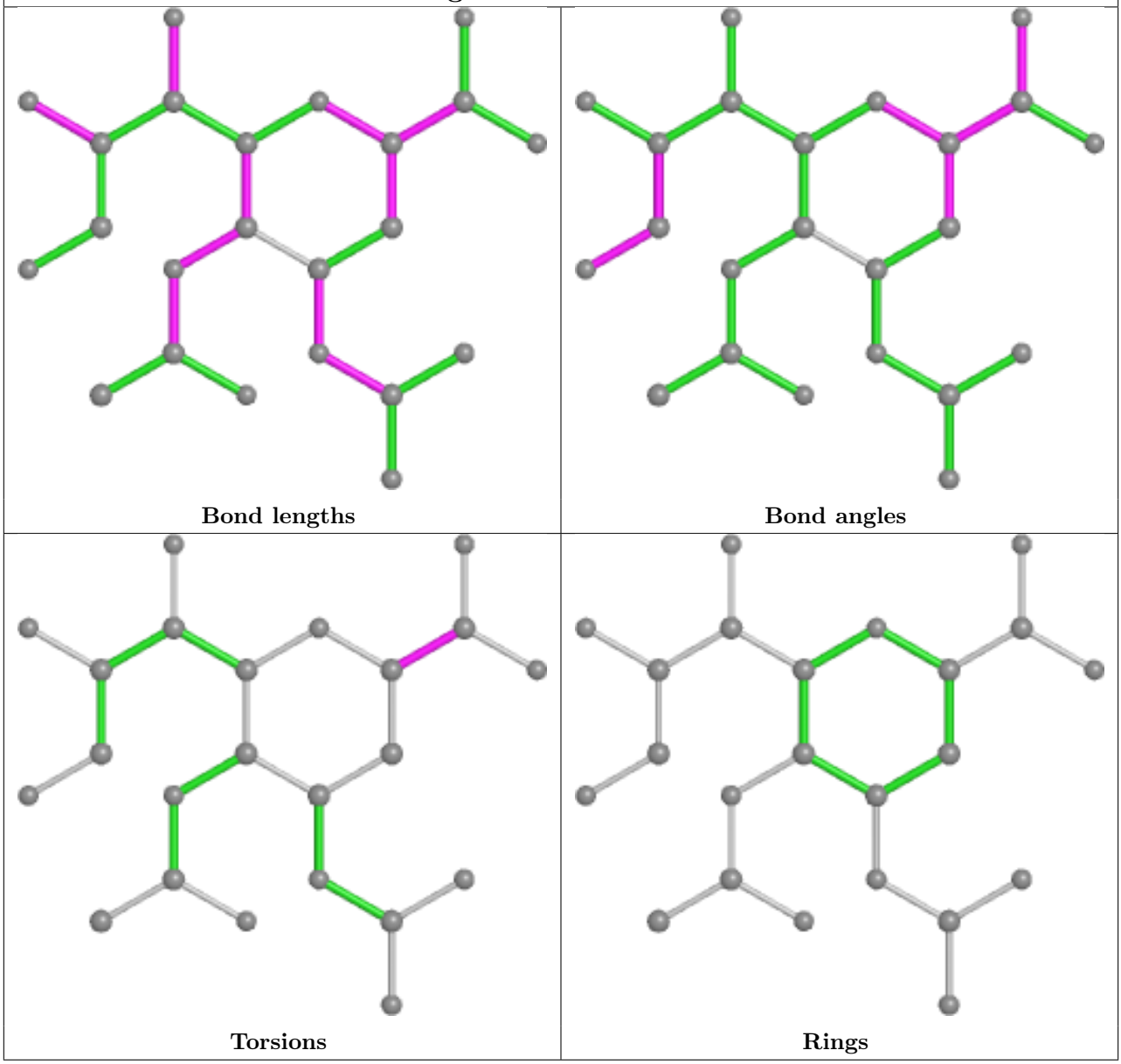
Ligand ZMR F 1470



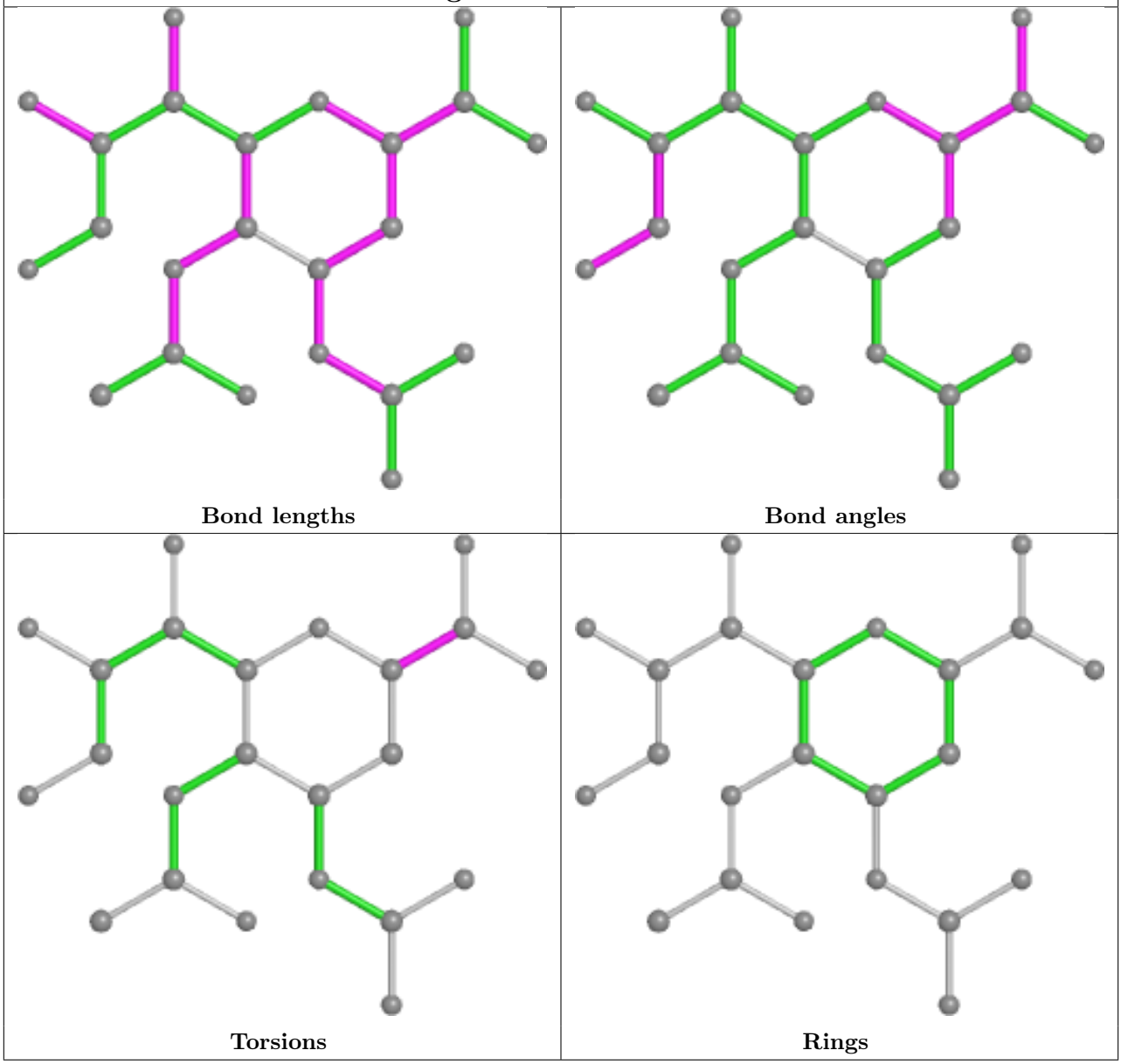
Ligand ZMR A 1471



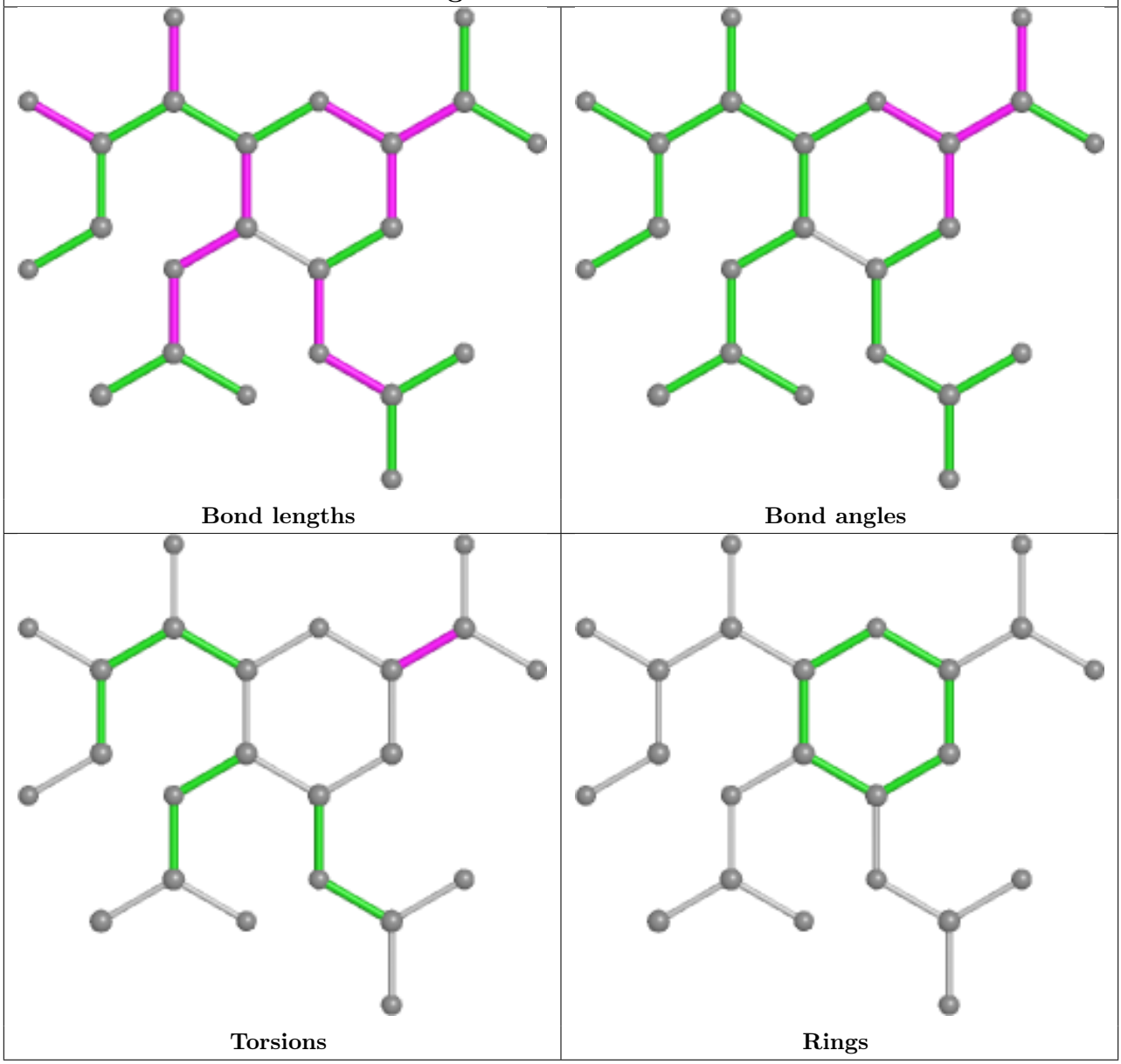
Ligand ZMR C 1470



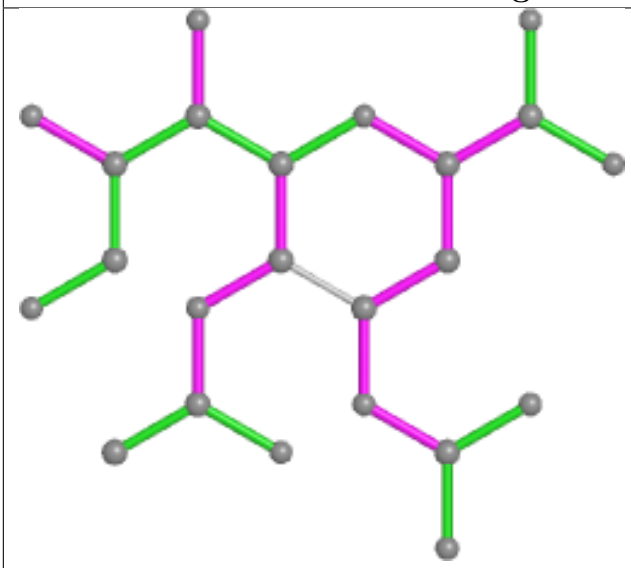
Ligand ZMR G 1471



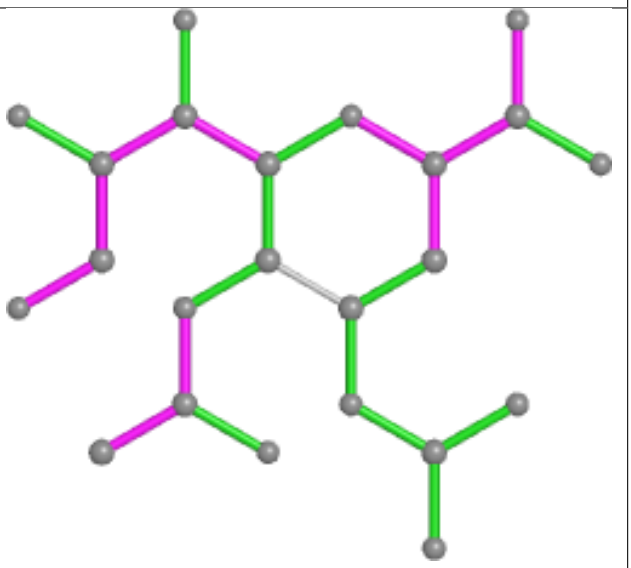
Ligand ZMR B 1471



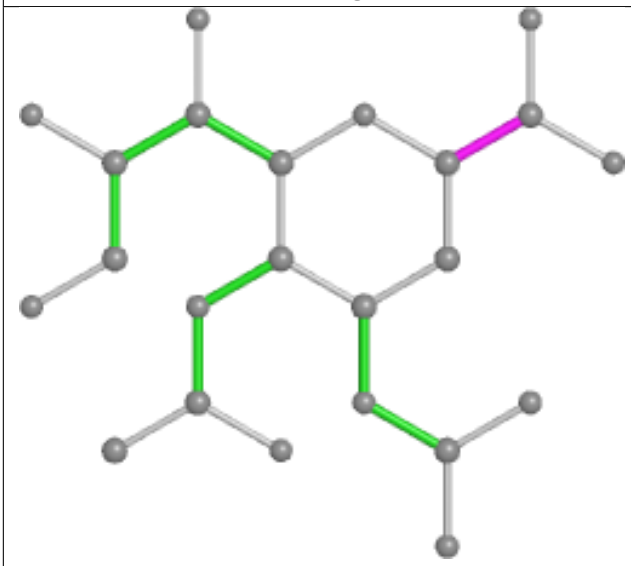
Ligand ZMR E 1471



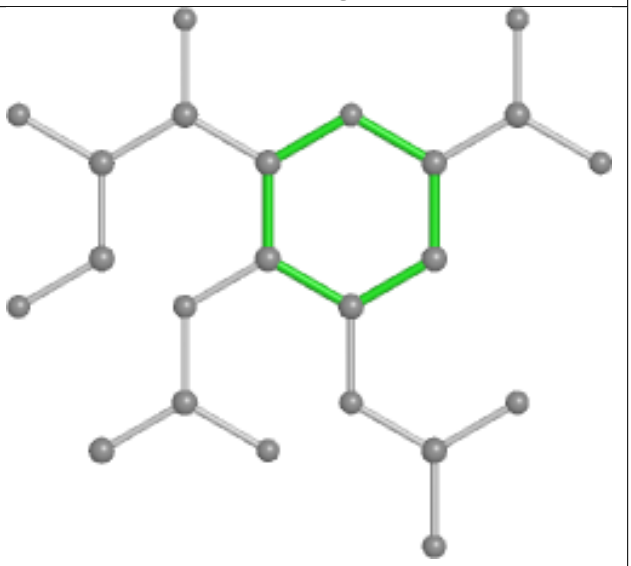
Bond lengths



Bond angles

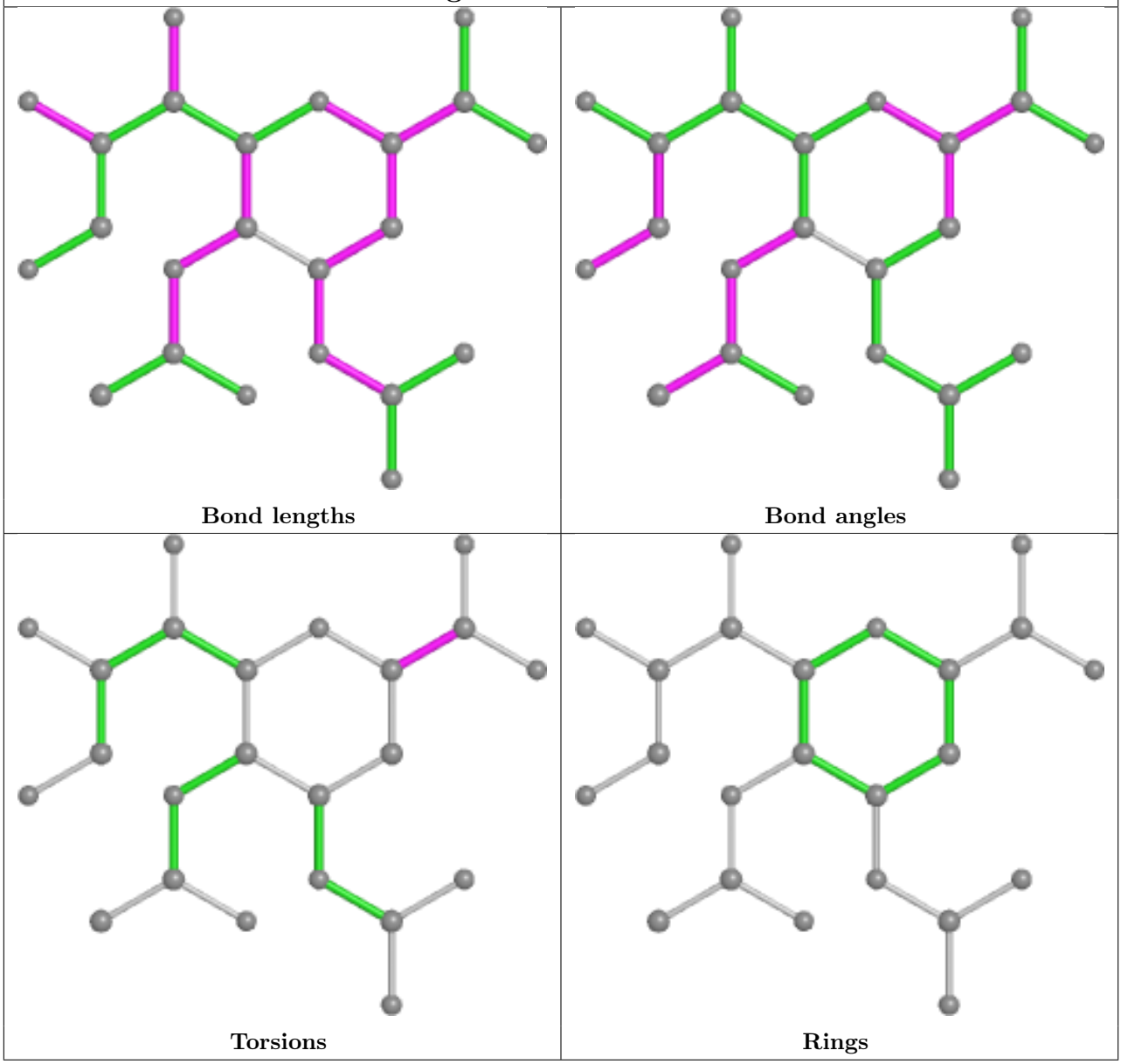


Torsions



Rings

Ligand ZMR H 1470



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	390/466 (83%)	-0.56	1 (0%)	94	93	15, 24, 41, 78	0
1	B	390/466 (83%)	-0.63	0	100	100	17, 27, 44, 100	0
1	C	390/466 (83%)	-0.45	1 (0%)	94	93	18, 29, 44, 94	0
1	D	390/466 (83%)	-0.49	1 (0%)	94	93	20, 34, 54, 100	0
1	E	390/466 (83%)	-0.11	8 (2%)	63	61	32, 49, 73, 106	0
1	F	390/466 (83%)	-0.11	9 (2%)	60	58	30, 48, 67, 106	0
1	G	390/466 (83%)	-0.15	5 (1%)	77	75	32, 52, 81, 109	0
1	H	390/466 (83%)	-0.05	8 (2%)	63	61	35, 55, 80, 102	0
All	All	3120/3728 (83%)	-0.32	33 (1%)	80	79	15, 40, 71, 109	0

All (33) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	76	GLU	5.3
1	F	76	GLU	3.9
1	D	76	GLU	3.8
1	H	76	GLU	3.6
1	H	317	CYS	3.5
1	E	358	SER	3.3
1	H	332	ILE	3.3
1	E	336	CYS	3.3
1	H	244	ALA	3.3
1	E	78	GLU	3.3
1	H	81	TYR	3.1
1	E	434	LYS	2.9
1	F	464	ALA	2.8
1	G	393	LEU	2.7
1	G	358	SER	2.7
1	A	76	GLU	2.6

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Mol	Chain	Res	Type	RSRZ
1	H	219	LYS	2.6
1	E	435	GLU	2.6
1	C	76	GLU	2.5
1	G	76	GLU	2.4
1	F	465	LEU	2.4
1	F	247	VAL	2.4
1	F	265	PHE	2.4
1	E	158	VAL	2.3
1	G	86	CYS	2.2
1	G	333	THR	2.2
1	H	387	TRP	2.2
1	F	170	ILE	2.2
1	F	307	GLU	2.1
1	H	78	GLU	2.1
1	E	331	SER	2.1
1	F	267	THR	2.1
1	F	388	ALA	2.1

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

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

6.3 Carbohydrates (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	BMA	O	3	11/12	0.50	0.36	80,92,112,113	0
2	BMA	J	3	11/12	0.68	0.36	92,96,116,117	0
2	BMA	I	3	11/12	0.72	0.35	96,101,113,114	0
2	BMA	N	3	11/12	0.79	0.35	80,107,110,110	0
2	BMA	L	3	11/12	0.81	0.40	83,93,103,106	0
2	BMA	M	3	11/12	0.83	0.27	81,84,87,90	0
3	NAG	P	1	14/15	0.83	0.25	74,79,85,90	0
2	NAG	O	2	14/15	0.84	0.27	80,88,96,107	0
2	NAG	I	2	14/15	0.88	0.21	50,68,81,91	0
2	NAG	L	2	14/15	0.90	0.33	65,74,83,92	0
3	NAG	K	2	14/15	0.90	0.24	70,83,93,99	0

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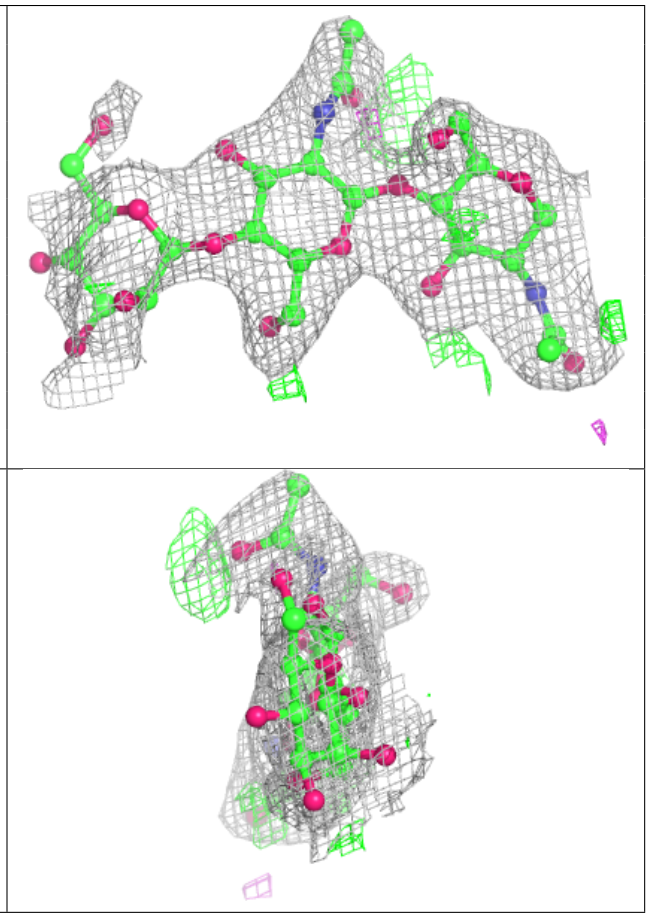
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	NAG	N	2	14/15	0.90	0.29	64,83,92,101	0
2	NAG	M	2	14/15	0.91	0.24	63,75,79,86	0
2	NAG	J	2	14/15	0.91	0.27	51,67,78,88	0
3	NAG	P	2	14/15	0.91	0.33	92,99,102,103	0
2	NAG	O	1	14/15	0.92	0.17	64,72,85,87	0
2	NAG	I	1	14/15	0.93	0.15	37,50,55,60	0
2	NAG	J	1	14/15	0.93	0.14	34,43,54,62	0
2	NAG	M	1	14/15	0.94	0.17	53,60,69,75	0
2	NAG	N	1	14/15	0.95	0.17	58,64,69,72	0
3	NAG	K	1	14/15	0.96	0.18	40,53,65,77	0
2	NAG	L	1	14/15	0.97	0.20	29,47,56,58	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.

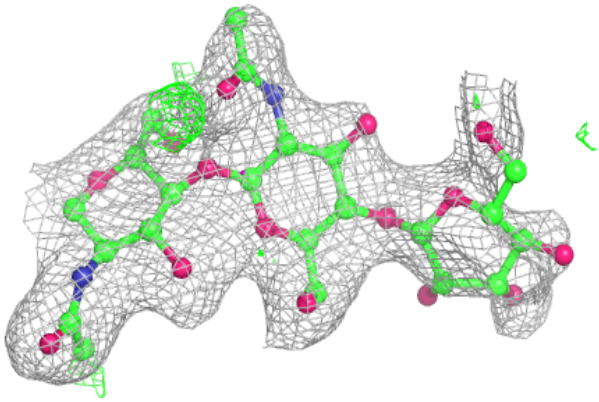
Electron density around Chain I:

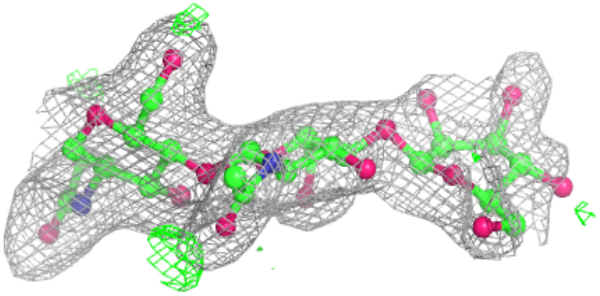
2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative) and green (positive)

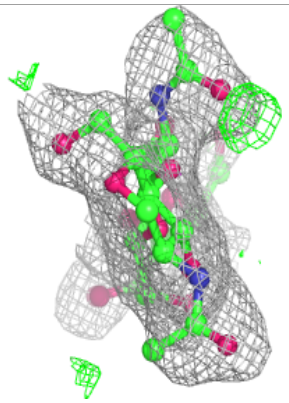


Electron density around Chain J:

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

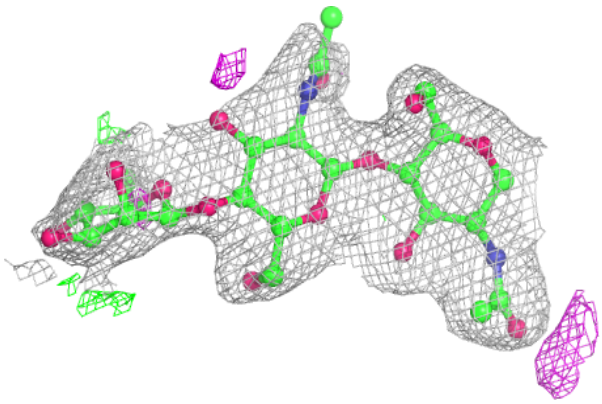


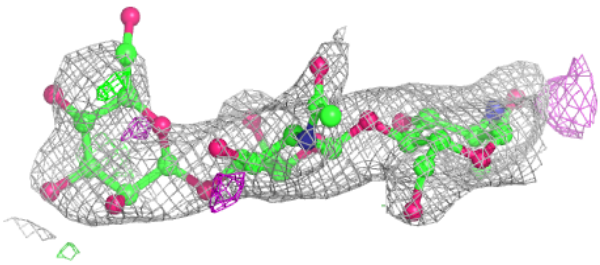


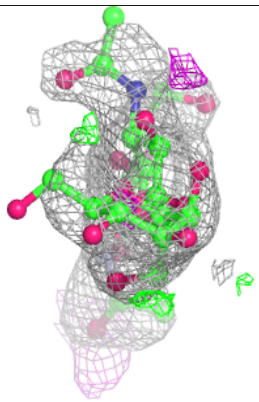


Electron density around Chain L:

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

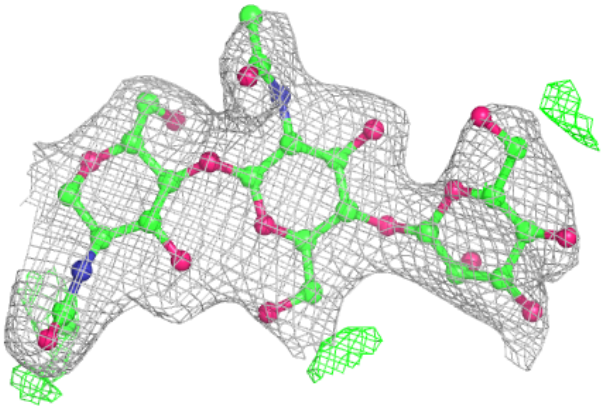


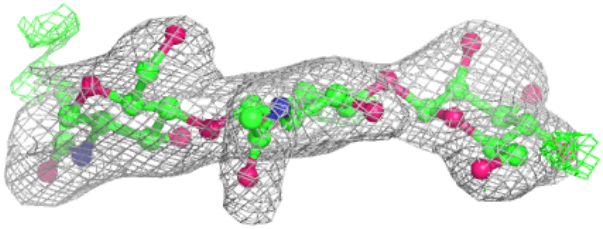


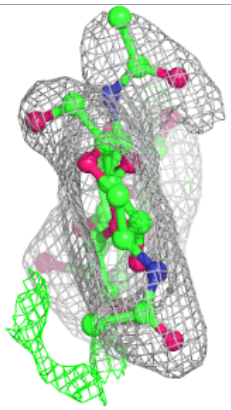


Electron density around Chain M:

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

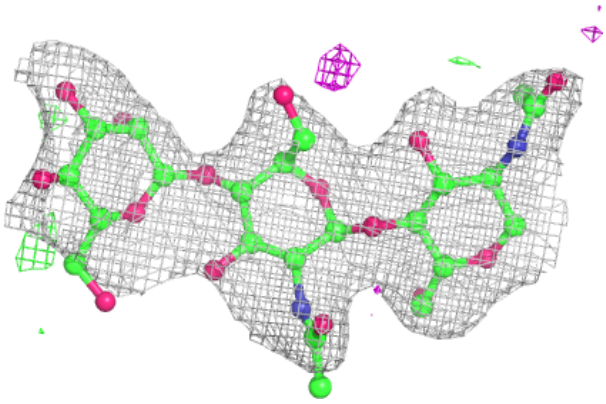


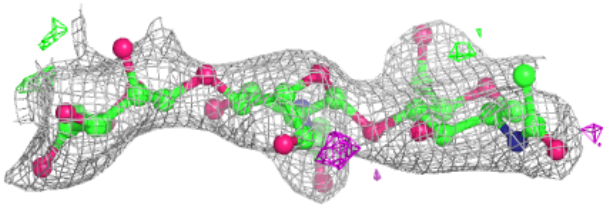


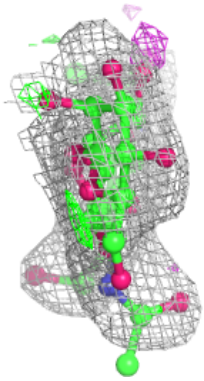


Electron density around Chain N:

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

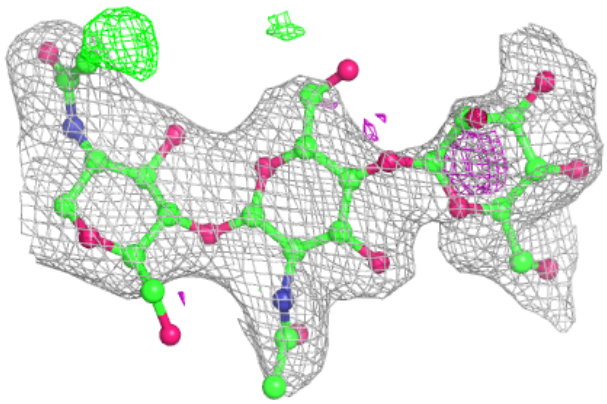


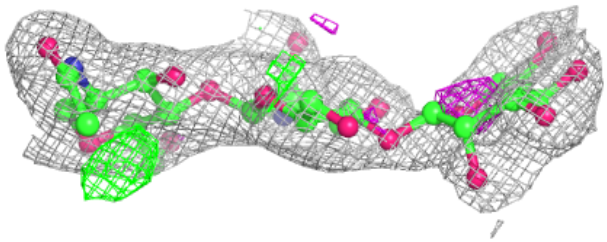


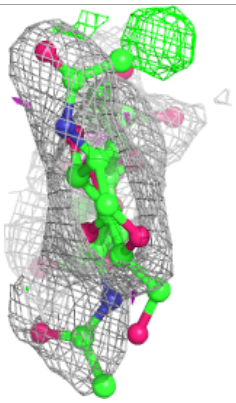


Electron density around Chain O:

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

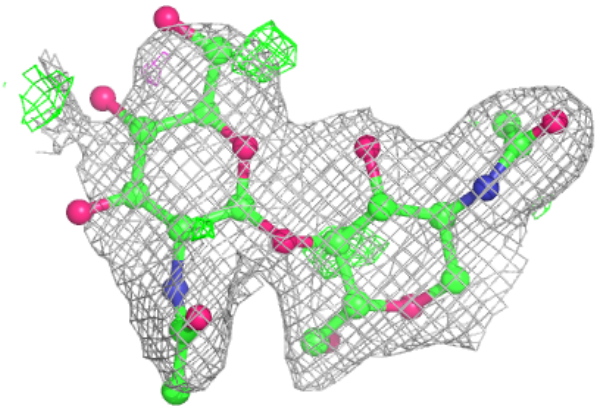


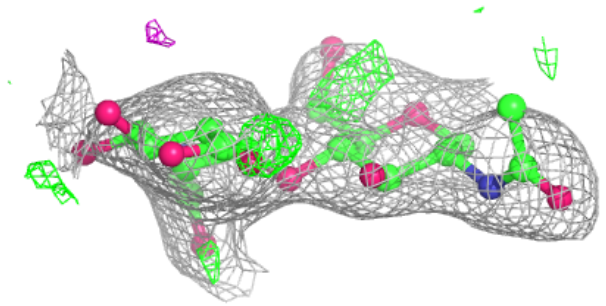


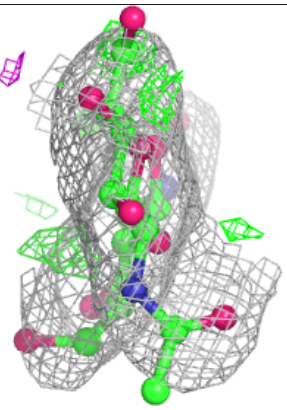


Electron density around Chain K:

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

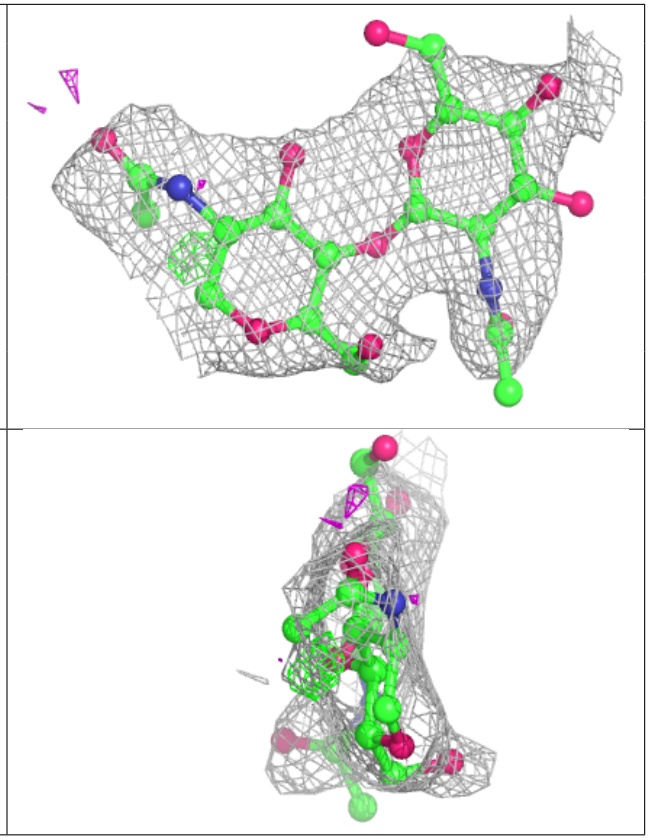






Electron density around Chain P:

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



6.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	NAG	H	1469	14/15	0.74	0.43	86,98,103,103	0
5	NAG	B	1470	14/15	0.81	0.28	79,86,99,99	0
5	NAG	E	1470	14/15	0.86	0.33	78,89,99,99	0
5	NAG	C	1469	14/15	0.86	0.21	64,70,78,85	0
5	NAG	G	1470	14/15	0.87	0.16	69,79,91,92	0
4	CA	G	1466	1/1	0.90	0.05	70,70,70,70	0
5	NAG	D	1470	14/15	0.91	0.12	73,80,85,86	0
5	NAG	A	1470	14/15	0.92	0.18	48,54,72,74	0
4	CA	H	1466	1/1	0.94	0.04	74,74,74,74	0
6	ZMR	G	1471	23/23	0.94	0.11	36,47,56,65	0
6	ZMR	H	1470	23/23	0.94	0.10	45,57,61,65	0
6	ZMR	D	1471	23/23	0.96	0.10	26,34,40,44	0
6	ZMR	F	1470	23/23	0.96	0.10	38,46,55,56	0
7	EDO	D	1472	4/4	0.96	0.21	26,31,32,37	0

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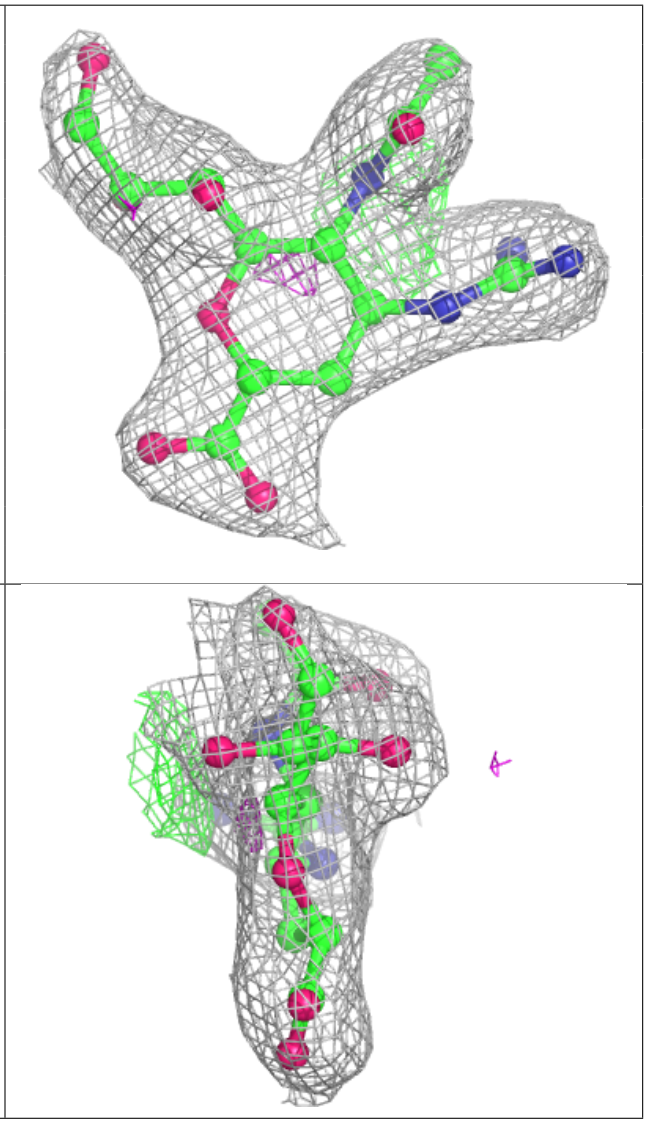
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
6	ZMR	E	1471	23/23	0.97	0.10	48,51,60,61	0
4	CA	D	1466	1/1	0.98	0.04	42,42,42,42	0
4	CA	E	1466	1/1	0.98	0.09	66,66,66,66	0
4	CA	F	1466	1/1	0.98	0.07	59,59,59,59	0
6	ZMR	A	1471	23/23	0.98	0.09	15,22,27,30	0
6	ZMR	B	1471	23/23	0.98	0.08	19,27,33,35	0
6	ZMR	C	1470	23/23	0.98	0.08	21,27,32,33	0
4	CA	B	1466	1/1	0.99	0.03	35,35,35,35	0
4	CA	A	1466	1/1	0.99	0.05	28,28,28,28	0
4	CA	C	1466	1/1	1.00	0.08	34,34,34,34	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.

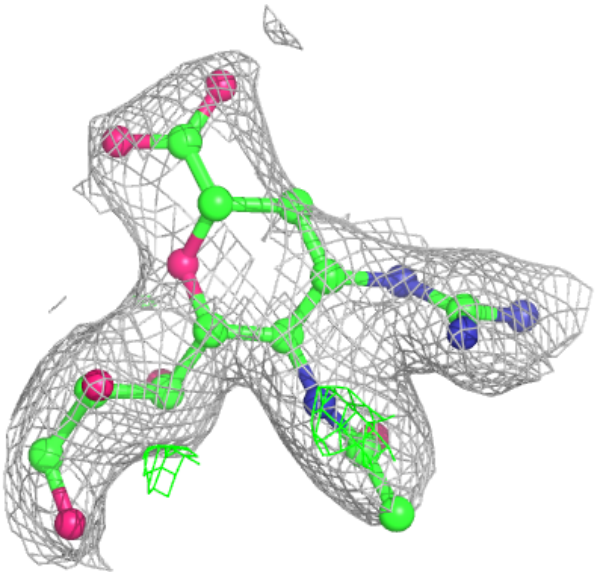
Electron density around ZMR G 1471:

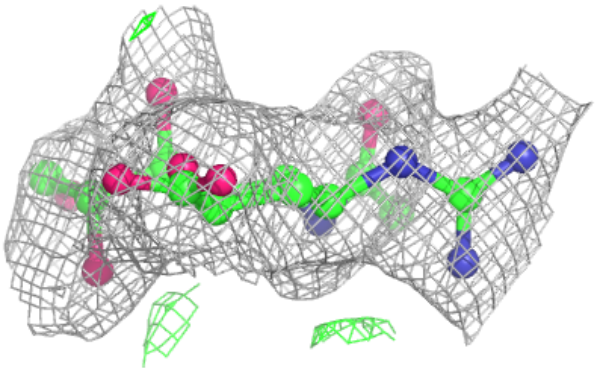
2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

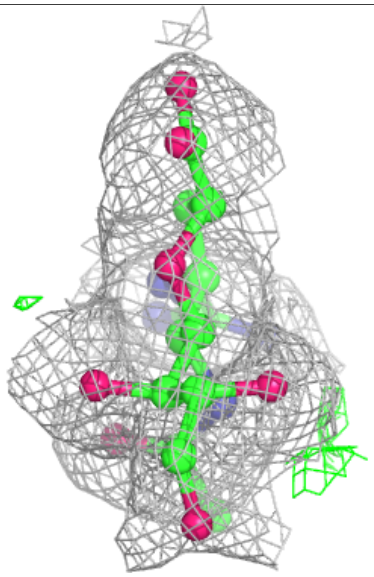


Electron density around ZMR H 1470:

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

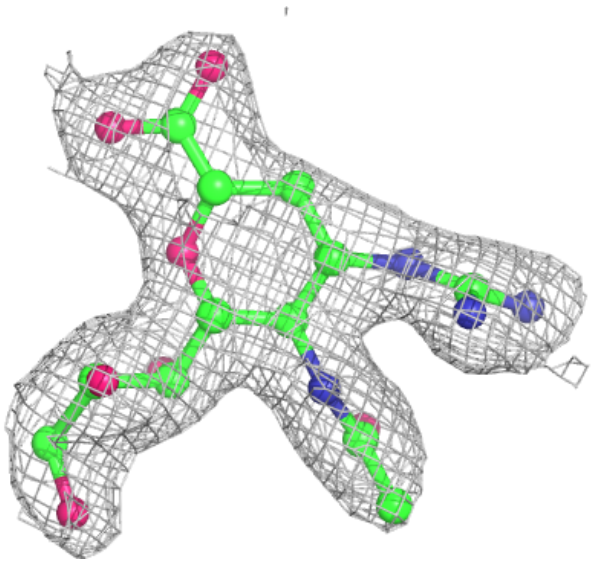


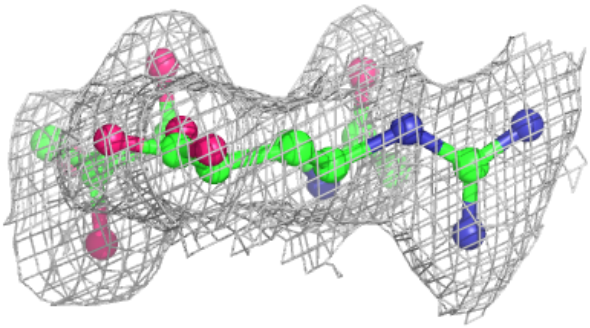


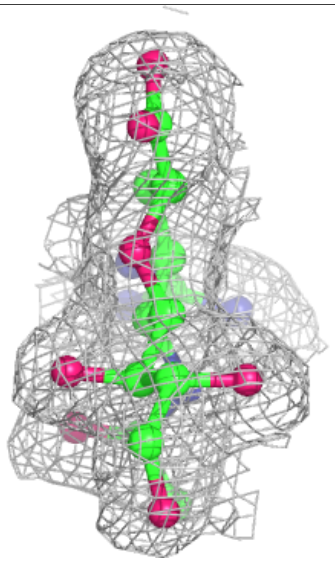


Electron density around ZMR D 1471:

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

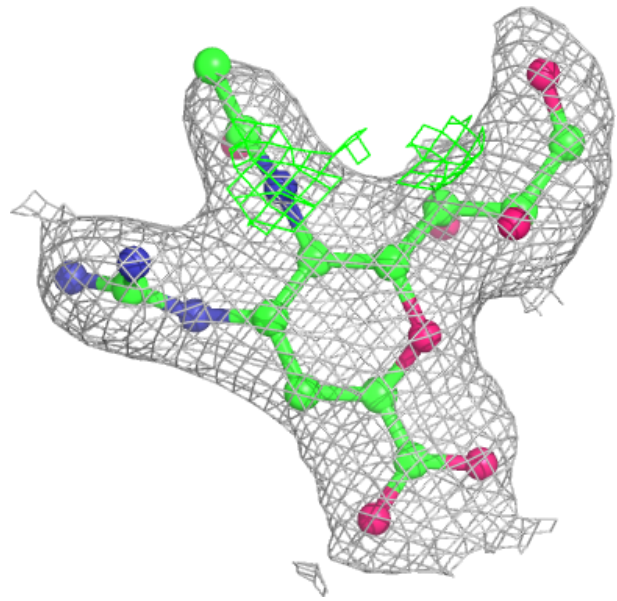


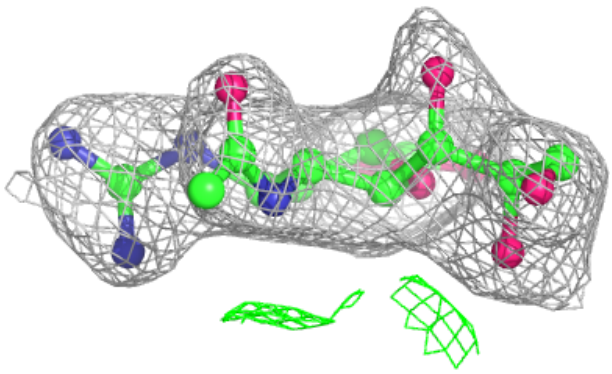


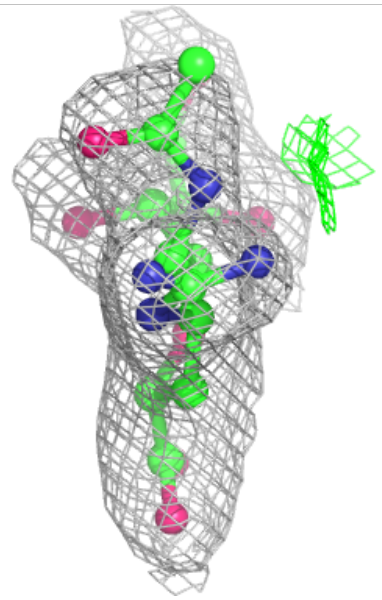


Electron density around ZMR F 1470:

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

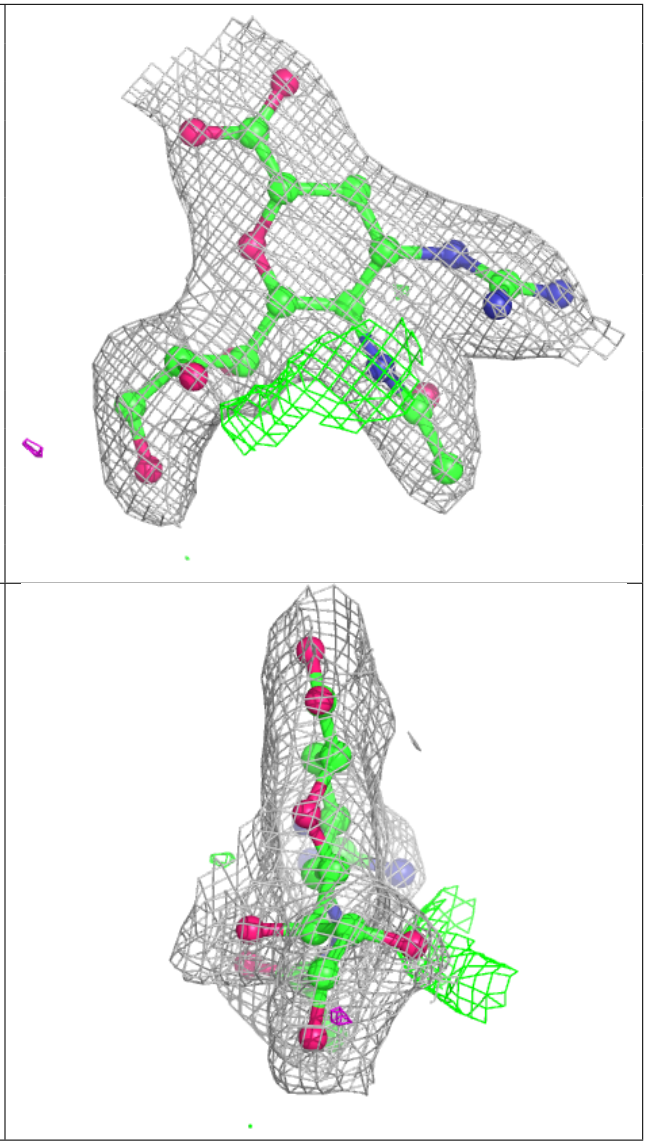






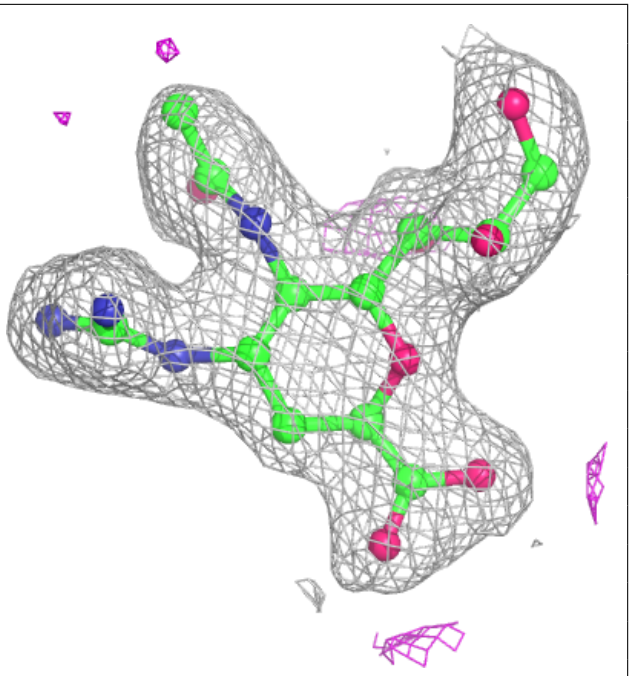
Electron density around ZMR E 1471:

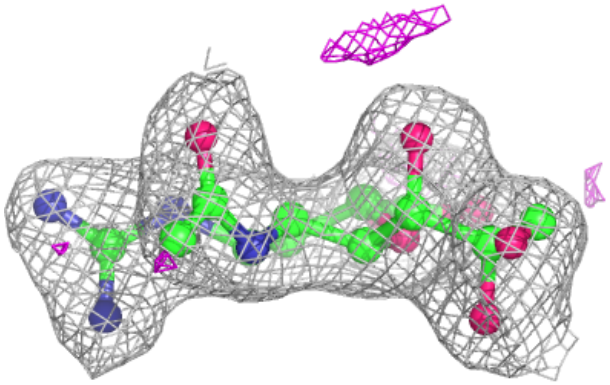
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

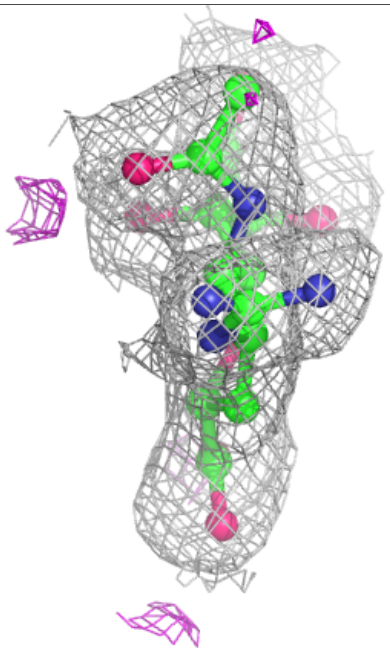


Electron density around ZMR A 1471:

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

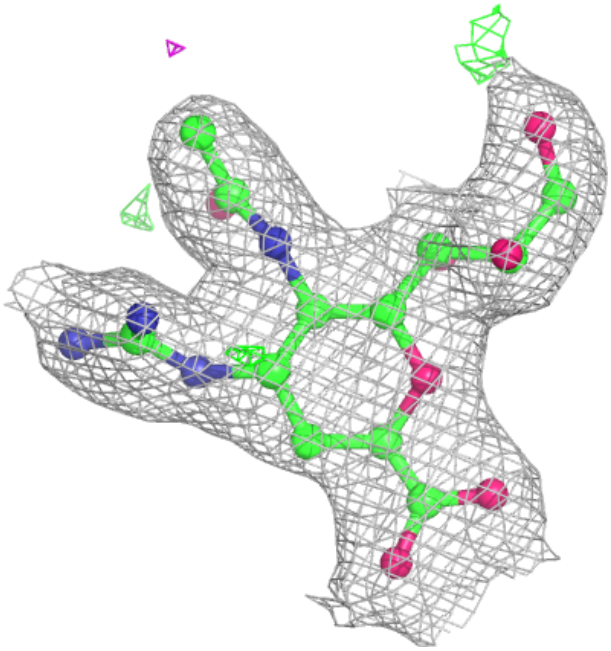


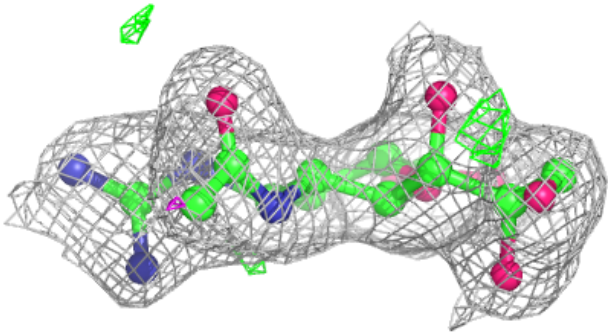


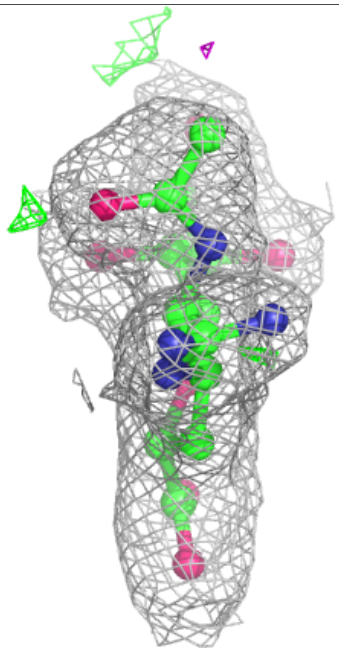


Electron density around ZMR B 1471:

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

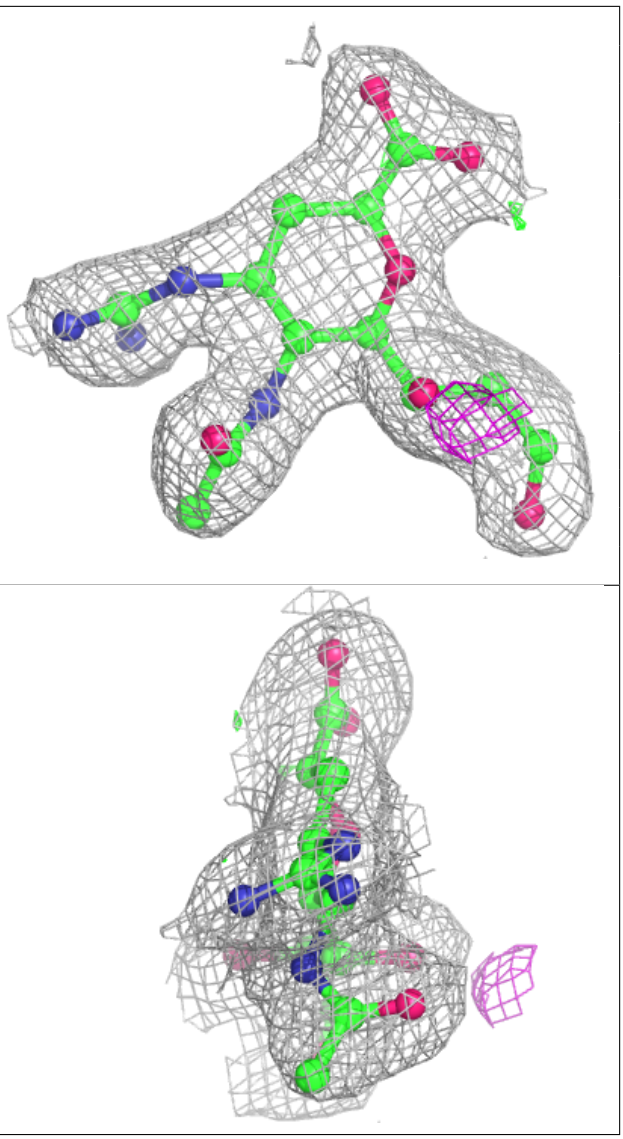






Electron density around ZMR C 1470:

$2mF_o$-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.