Full wwPDB X-ray Structure Validation Report (i)

May 6, 2025 – 06:11 PM JST

PDB ID	:	8ZE6 / pdb_00008ze6
Title	:	Crystal structure of MjHKU4r-CoV-1 RBD bound to MjDPP4
Authors	:	Yang, M.; Li, Z.; Xu, Y.; Zhang, S.
Deposited on	:	2024-05-04
Resolution	:	2.70 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 (i)) were used in the production of this report:

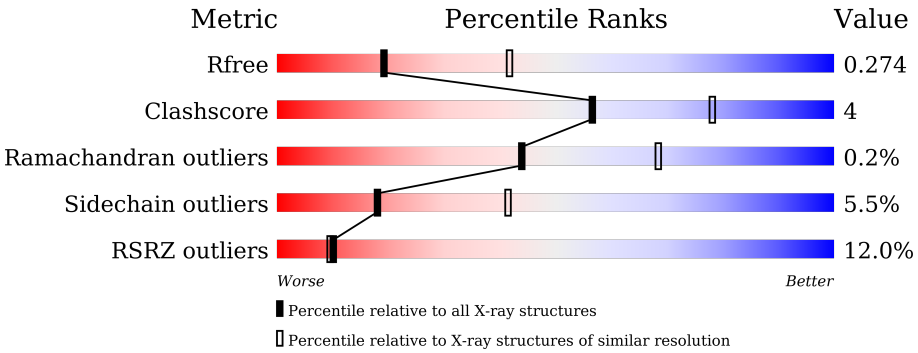
MolProbity	:	4-5-2 with Phenix2.0rc1
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	2.0rc1
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.006 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.43.1

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 2.70 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}	164625	3333 (2.70-2.70)
Clashscore	180529	3684 (2.70-2.70)
Ramachandran outliers	177936	3633 (2.70-2.70)
Sidechain outliers	177891	3633 (2.70-2.70)
RSRZ outliers	164620	3333 (2.70-2.70)

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	B	728	7% 86% 13%
1	D	728	8% 87% 13%
2	A	203	32% 69% 26%
2	C	203	23% 75% 23%
3	E	2	50% 50%
3	F	2	100%

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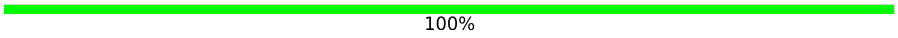
Mol	Chain	Length	Quality of chain
3	G	2	
3	H	2	
3	I	2	
3	J	2	

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 15431 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 Dipeptidyl peptidase 4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	726	Total	C	N	O	S	0	0	0
			5944	3814	989	1119	22			
1	D	728	Total	C	N	O	S	0	0	0
			5960	3823	994	1121	22			

- Molecule 2 is a protein called Spike glycoprotein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	201	Total	C	N	O	S	0	0	0
			1564	1000	253	299	12			
2	A	201	Total	C	N	O	S	0	0	0
			1562	998	253	299	12			

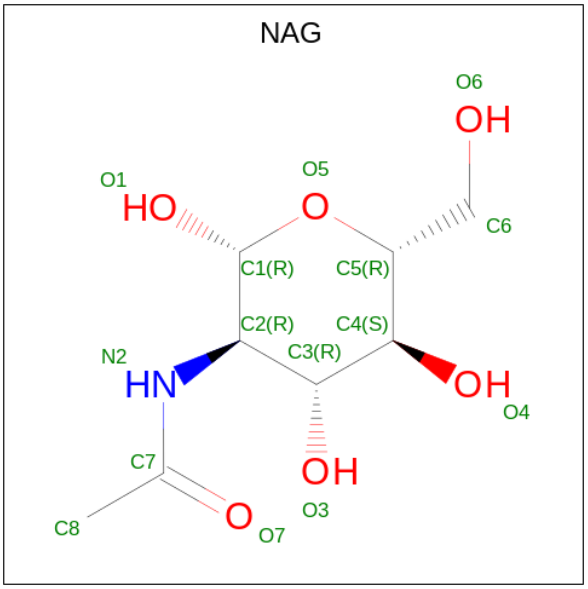
There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	388	ASP	SER	conflict	UNP A0AAE8ZFM2
C	482	ALA	SER	conflict	UNP A0AAE8ZFM2
C	544	GLU	VAL	conflict	UNP A0AAE8ZFM2
A	388	ASP	SER	conflict	UNP A0AAE8ZFM2
A	482	ALA	SER	conflict	UNP A0AAE8ZFM2
A	544	GLU	VAL	conflict	UNP A0AAE8ZFM2

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

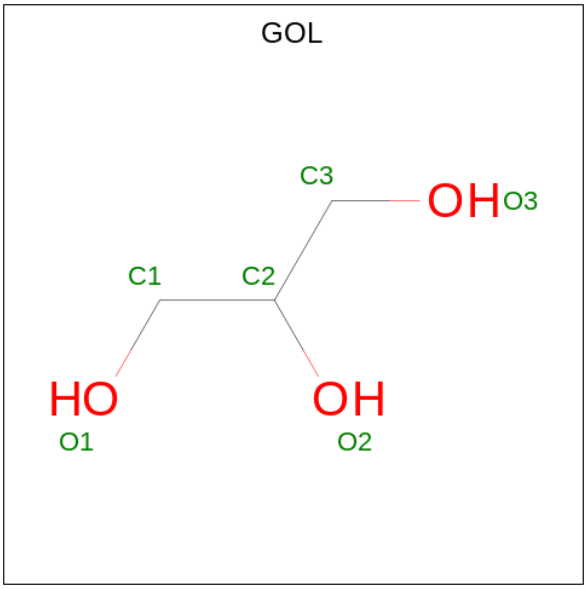
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
3	E	2	Total C N O 28 16 2 10	0	0	0
3	F	2	Total C N O 28 16 2 10	0	0	0
3	G	2	Total C N O 28 16 2 10	0	0	0
3	H	2	Total C N O 28 16 2 10	0	0	0
3	I	2	Total C N O 28 16 2 10	0	0	0
3	J	2	Total C N O 28 16 2 10	0	0	0

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	1	Total C N O 14 8 1 5	0	0
4	B	1	Total C N O 14 8 1 5	0	0
4	D	1	Total C N O 14 8 1 5	0	0
4	D	1	Total C N O 14 8 1 5	0	0
4	D	1	Total C N O 14 8 1 5	0	0

- Molecule 5 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	1	Total C O 6 3 3	0	0

- Molecule 6 is water.

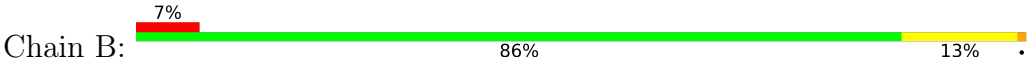
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	B	65	Total O 65 65	0	0
6	C	14	Total O 14 14	0	0
6	D	70	Total O 70 70	0	0
6	A	8	Total O 8 8	0	0

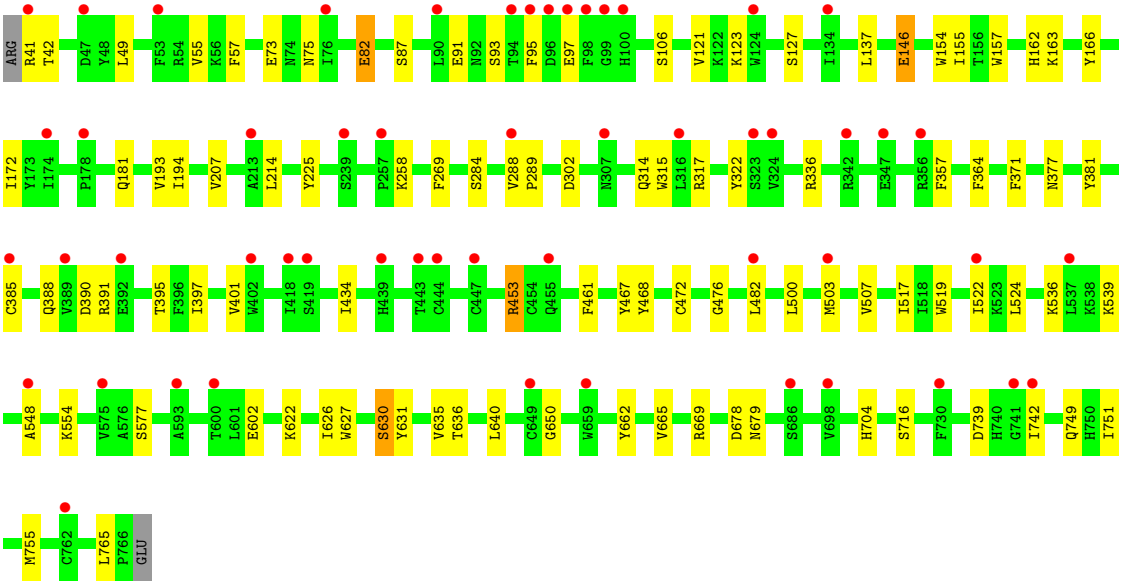
3 Residue-property plots (i)

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: Dipeptidyl peptidase 4

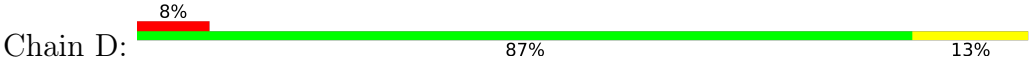
Chain B:

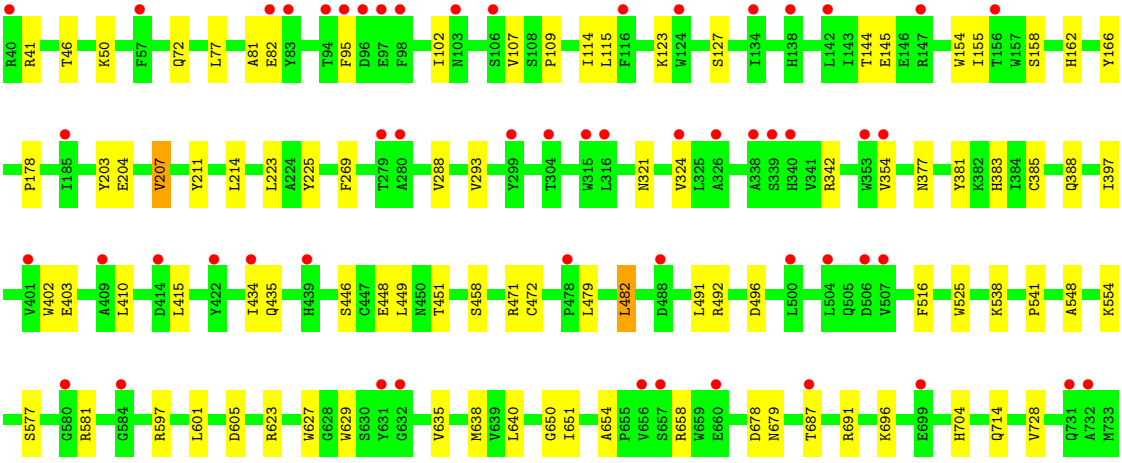




• Molecule 1: Dipeptidyl peptidase 4

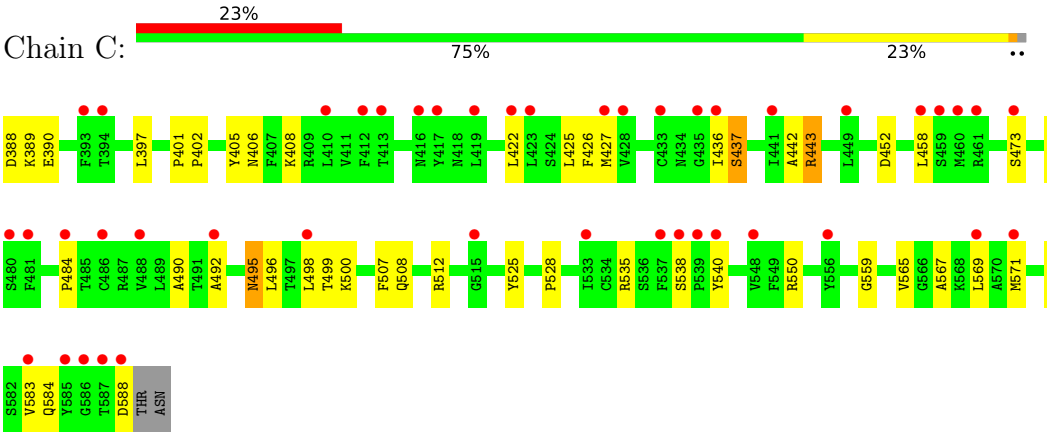
Chain D:





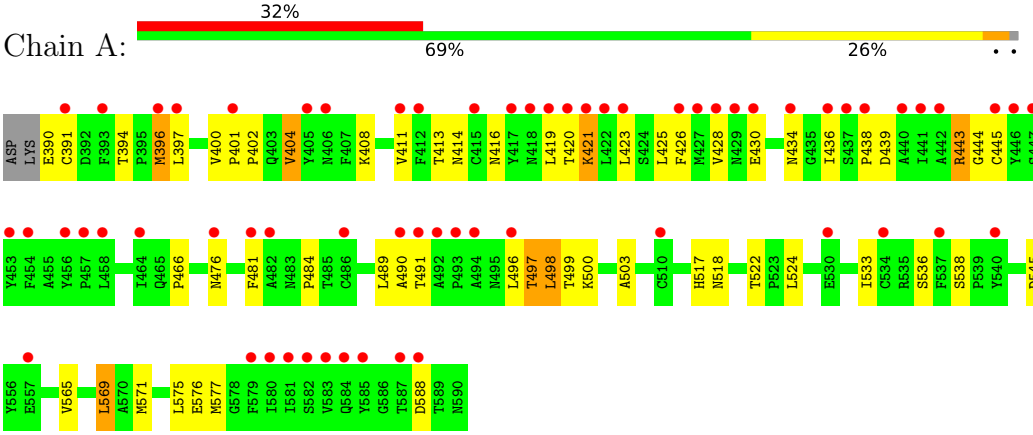
• Molecule 2: Spike glycoprotein

Chain C:



• Molecule 2: Spike glycoprotein

Chain A:

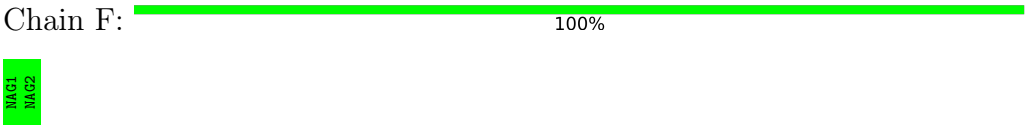


• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain E:

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

Chain F:



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

Chain G:

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

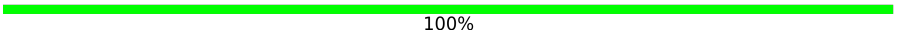
Chain H:

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

Chain I:

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

Chain J:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	96.53Å 121.44Å 110.62Å 90.00° 105.13° 90.00°	Depositor
Resolution (Å)	47.49 – 2.70 47.49 – 2.70	Depositor EDS
% Data completeness (in resolution range)	98.8 (47.49-2.70) 98.8 (47.49-2.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.12 (at 2.69Å)	Xtriage
Refinement program	PHENIX (1.20.1_4487: ???)	Depositor
R, R_{free}	0.242 , 0.274 0.242 , 0.274	Depositor DCC
R_{free} test set	3345 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å^2)	57.8	Xtriage
Anisotropy	0.516	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 51.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	15431	wwPDB-VP
Average B, all atoms (Å^2)	66.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.38% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	B	0.09	0/6118	0.26	0/8322
1	D	0.08	0/6134	0.26	0/8343
2	A	0.10	0/1601	0.33	0/2174
2	C	0.10	0/1603	0.28	0/2175
All	All	0.09	0/15456	0.27	0/21014

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

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	5944	0	5667	43	0
1	D	5960	0	5679	46	0
2	A	1562	0	1507	24	0
2	C	1564	0	1511	25	0
3	E	28	0	25	2	0
3	F	28	0	25	0	0
3	G	28	0	25	1	0
3	H	28	0	25	0	0
3	I	28	0	25	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	J	28	0	25	0	0
4	B	28	0	26	0	0
4	D	42	0	39	0	0
5	B	6	0	8	1	0
6	A	8	0	0	0	0
6	B	65	0	0	0	0
6	C	14	0	0	0	0
6	D	70	0	0	1	0
All	All	15431	0	14587	134	0

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

All (134) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:405:TYR:HB3	2:C:476:ASN:HD22	1.45	0.81
1:B:146:GLU:HG2	1:B:181:GLN:HA	1.66	0.77
1:B:302:ASP:HB3	1:B:314:GLN:HB2	1.73	0.71
1:D:410:LEU:HD13	1:D:415:LEU:HD12	1.74	0.69
2:C:492:ALA:HB1	2:C:498:LEU:HD21	1.76	0.68
1:D:123:LYS:O	1:D:127:SER:OG	2.09	0.68
2:C:436:ILE:HG12	2:C:437:SER:H	1.58	0.68
2:A:436:ILE:HB	2:A:484:PRO:HG3	1.76	0.66
1:D:696:LYS:HG3	1:D:728:VAL:HG22	1.77	0.66
1:D:203:TYR:HA	1:D:207:VAL:HG13	1.76	0.66
1:D:581:ARG:HD3	1:D:605:ASP:OD2	1.96	0.66
2:A:491:THR:HG22	2:A:576:GLU:HG2	1.80	0.63
2:C:401:PRO:HG3	2:C:575:LEU:HD21	1.81	0.62
1:B:123:LYS:O	1:B:127:SER:OG	2.13	0.62
1:B:317:ARG:NH2	2:A:518:ASN:O	2.30	0.62
1:B:87:SER:HB2	3:E:1:NAG:H81	1.82	0.61
1:D:742:ILE:HG13	1:D:751:ILE:HD12	1.83	0.61
1:D:640:LEU:HD11	1:D:650:GLY:HA3	1.81	0.61
1:D:81:ALA:O	1:D:492:ARG:NH2	2.34	0.60
2:C:525:TYR:OH	1:D:342:ARG:NH2	2.35	0.60
1:B:336:ARG:NH2	2:A:545:ASP:OD1	2.34	0.60
2:A:404:VAL:HB	2:A:476:ASN:HD22	1.68	0.59
1:B:49:LEU:HB3	1:B:749:GLN:HG2	1.85	0.58
1:B:388:GLN:HB2	1:B:391:ARG:HB2	1.84	0.58
2:A:419:LEU:H	2:A:419:LEU:HD23	1.68	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:640:LEU:HD11	1:B:650:GLY:HA3	1.86	0.58
2:C:397:LEU:HD21	2:C:425:LEU:HD13	1.86	0.58
1:D:154:TRP:HD1	1:D:214:LEU:HD12	1.69	0.57
2:C:452:ASP:HB2	2:C:580:ILE:HB	1.85	0.57
2:C:508:GLN:HG3	2:C:567:ALA:HB2	1.86	0.57
1:B:377:ASN:HD21	1:B:381:TYR:HB2	1.69	0.56
2:C:495:ASN:OD1	2:C:495:ASN:N	2.38	0.56
1:D:554:LYS:HB3	1:D:577:SER:HB3	1.87	0.56
1:B:453:ARG:HG2	1:B:476:GLY:HA3	1.86	0.56
1:B:751:ILE:HG12	1:B:755:MET:HE2	1.88	0.55
2:A:402:PRO:HG3	2:A:408:LYS:HG3	1.89	0.55
1:B:626:ILE:HG23	1:B:636:THR:HG23	1.89	0.54
1:D:581:ARG:HG2	1:D:601:LEU:HD23	1.90	0.54
2:C:427:MET:SD	2:C:427:MET:N	2.81	0.53
1:D:107:VAL:HG22	1:D:114:ILE:HG12	1.90	0.53
2:C:565:VAL:HG11	1:D:288:VAL:HG11	1.89	0.53
1:D:479:LEU:HD12	1:D:496:ASP:HA	1.92	0.52
1:D:46:THR:HG23	1:D:50:LYS:HD2	1.91	0.51
1:B:289:PRO:HB3	1:B:315:TRP:CE2	2.46	0.51
2:C:436:ILE:HB	2:C:484:PRO:HB3	1.93	0.51
2:A:420:THR:HA	2:A:423:LEU:HB2	1.93	0.49
1:D:109:PRO:HG2	1:D:158:SER:O	2.11	0.49
1:B:662:TYR:CZ	5:B:803:GOL:H32	2.47	0.49
1:B:317:ARG:HD2	1:B:322:TYR:HB3	1.95	0.49
1:B:41:ARG:NH1	1:B:42:THR:O	2.46	0.48
2:C:512:ARG:NH1	2:C:559:GLY:O	2.47	0.48
2:C:402:PRO:HD3	2:C:408:LYS:NZ	2.28	0.48
2:A:419:LEU:O	2:A:421:LYS:N	2.41	0.48
1:B:214:LEU:HD23	1:B:225:TYR:HB3	1.95	0.48
2:C:500:LYS:HB3	2:C:571:MET:HE2	1.94	0.48
3:I:1:NAG:H62	3:I:2:NAG:N2	2.28	0.48
1:B:288:VAL:HG11	2:A:565:VAL:HG11	1.96	0.47
2:C:406:ASN:OD1	2:C:535:ARG:NE	2.35	0.47
2:C:402:PRO:HG3	2:C:408:LYS:HG3	1.96	0.47
1:D:448:GLU:HA	1:D:451:THR:HG23	1.96	0.47
2:A:401:PRO:HB3	2:A:577:MET:HE1	1.96	0.47
1:B:742:ILE:HD12	1:B:751:ILE:HD12	1.95	0.47
2:C:426:PHE:HB3	2:C:490:ALA:HB1	1.97	0.47
1:B:82:GLU:HG2	1:B:467:TYR:OH	2.15	0.47
1:B:548:ALA:HB3	1:B:635:VAL:HG21	1.97	0.46
2:A:524:LEU:HD13	2:A:533:ILE:HD12	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:519:TRP:O	1:B:522:ILE:HG12	2.14	0.46
1:D:458:SER:HG	1:D:471:ARG:HB2	1.81	0.46
1:B:461:PHE:CD2	1:B:468:TYR:HB3	2.51	0.46
1:D:115:LEU:HD21	1:D:155:ILE:HD13	1.98	0.46
1:B:704:HIS:ND1	1:B:716:SER:OG	2.33	0.46
1:D:742:ILE:HG22	1:D:747:ALA:HB1	1.98	0.46
1:B:357:PHE:O	1:B:669:ARG:NH1	2.49	0.46
1:D:225:TYR:CZ	1:D:269:PHE:HB2	2.51	0.46
2:A:430:GLU:HB3	2:A:489:LEU:HB2	1.98	0.45
1:D:638:MET:O	1:D:691:ARG:NH1	2.50	0.45
1:B:554:LYS:HB3	1:B:577:SER:HB3	1.98	0.45
2:C:476:ASN:HD21	2:C:507:PHE:H	1.64	0.45
1:B:154:TRP:HD1	1:B:214:LEU:HD12	1.80	0.45
1:B:172:ILE:HD13	1:B:214:LEU:HD21	1.98	0.45
2:A:443:ARG:HB3	2:A:444:GLY:H	1.55	0.45
1:B:73:GLU:O	1:B:75:ASN:ND2	2.50	0.45
1:D:548:ALA:HB3	1:D:635:VAL:HG21	1.99	0.45
2:C:422:LEU:HA	2:C:425:LEU:HD12	1.98	0.44
1:D:403:GLU:OE2	6:D:901:HOH:O	2.21	0.44
2:C:500:LYS:HG2	2:C:575:LEU:HB2	2.00	0.44
1:B:87:SER:HB2	3:E:1:NAG:C8	2.47	0.43
1:D:127:SER:N	1:D:204:GLU:OE2	2.47	0.43
2:A:466:PRO:HB3	2:A:481:PHE:CZ	2.53	0.43
1:B:397:ILE:HD12	1:B:434:ILE:HD13	2.01	0.43
1:D:516:PHE:HB3	1:D:525:TRP:CD2	2.53	0.43
1:B:269:PHE:HB3	1:B:284:SER:HB3	2.00	0.43
1:B:500:LEU:HA	1:B:503:MET:HE3	2.01	0.43
1:B:536:LYS:HB2	1:B:536:LYS:HE2	1.75	0.43
1:D:127:SER:HB3	1:D:211:TYR:CD1	2.53	0.43
1:D:321:ASN:HA	1:D:354:VAL:HG23	2.00	0.43
1:B:630:SER:HB3	1:B:631:TYR:H	1.68	0.43
2:A:500:LYS:H	2:A:500:LYS:HG3	1.72	0.43
2:A:503:ALA:HB1	2:A:569:LEU:O	2.19	0.43
1:D:482:LEU:HD12	1:D:491:LEU:HD12	2.00	0.43
2:C:442:ALA:HB3	2:C:443:ARG:HH21	1.83	0.43
1:D:541:PRO:HG3	1:D:623:ARG:CZ	2.48	0.43
1:D:377:ASN:OD1	1:D:381:TYR:N	2.47	0.43
1:D:658:ARG:HG3	1:D:687:THR:HG22	2.01	0.43
1:B:93:SER:O	1:B:97:GLU:HG3	2.19	0.42
1:B:193:VAL:HG12	1:B:194:ILE:HG12	2.00	0.42
1:D:162:HIS:HD2	1:D:178:PRO:HD3	1.83	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:419:LEU:H	2:A:419:LEU:CD2	2.33	0.42
2:C:496:LEU:HB3	2:C:498:LEU:HD22	2.01	0.42
1:D:446:SER:HA	1:D:449:LEU:HD13	2.02	0.42
1:D:155:ILE:HG13	1:D:166:TYR:HB3	2.02	0.42
1:D:397:ILE:HD12	1:D:434:ILE:HD13	2.02	0.42
1:D:458:SER:OG	1:D:471:ARG:HB2	2.20	0.42
1:D:102:ILE:HD13	1:D:102:ILE:HA	1.90	0.41
2:A:426:PHE:HB3	2:A:490:ALA:HB1	2.01	0.41
1:D:214:LEU:HD22	1:D:223:LEU:HD11	2.02	0.41
1:D:629:TRP:CZ2	1:D:742:ILE:HG12	2.55	0.41
2:A:517:HIS:CG	3:G:1:NAG:H83	2.55	0.41
2:C:498:LEU:HG	2:C:575:LEU:HD23	2.02	0.41
1:D:383:HIS:NE2	1:D:402:TRP:O	2.54	0.41
2:A:498:LEU:HD13	2:A:498:LEU:HA	1.93	0.41
1:D:538:LYS:HA	1:D:538:LYS:HD3	1.87	0.41
1:D:654:ALA:HA	1:D:704:HIS:ND1	2.34	0.41
2:A:555:GLN:CD	2:A:555:GLN:H	2.29	0.41
1:B:678:ASP:HB3	1:B:679:ASN:H	1.68	0.41
1:B:207:VAL:HG22	1:B:665:VAL:HG11	2.03	0.40
1:B:364:PHE:CD2	1:B:371:PHE:HB3	2.57	0.40
1:D:627:TRP:HB2	1:D:651:ILE:HB	2.03	0.40
1:B:106:SER:HG	1:B:157:TRP:CD1	2.40	0.40
2:A:397:LEU:O	2:A:497:THR:HG23	2.21	0.40
2:C:478:LYS:HD3	2:C:528:PRO:HG3	2.03	0.40
1:B:155:ILE:HG13	1:B:166:TYR:HB3	2.04	0.40
1:D:678:ASP:HB3	1:D:679:ASN:H	1.72	0.40
2:A:396:MET:HE3	2:A:396:MET:HB3	1.89	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	B	724/728 (100%)	689 (95%)	34 (5%)	1 (0%)	48 73
1	D	726/728 (100%)	696 (96%)	30 (4%)	0	100 100
2	A	199/203 (98%)	176 (88%)	21 (11%)	2 (1%)	13 33
2	C	199/203 (98%)	188 (94%)	11 (6%)	0	100 100
All	All	1848/1862 (99%)	1749 (95%)	96 (5%)	3 (0%)	44 68

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	A	438	PRO
2	A	497	THR
1	B	401	VAL

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	B	648/650 (100%)	621 (96%)	27 (4%)	25 53
1	D	649/650 (100%)	630 (97%)	19 (3%)	37 67
2	A	173/175 (99%)	144 (83%)	29 (17%)	1 4
2	C	173/175 (99%)	157 (91%)	16 (9%)	7 18
All	All	1643/1650 (100%)	1552 (94%)	91 (6%)	18 41

All (91) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	55	VAL
1	B	57	PHE
1	B	82	GLU
1	B	91	GLU
1	B	95	PHE
1	B	121	VAL
1	B	137	LEU
1	B	146	GLU

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Mol	Chain	Res	Type
1	B	162	HIS
1	B	163	LYS
1	B	258	LYS
1	B	385	CYS
1	B	390	ASP
1	B	395	THR
1	B	453	ARG
1	B	472	CYS
1	B	482	LEU
1	B	507	VAL
1	B	517	ILE
1	B	524	LEU
1	B	539	LYS
1	B	602	GLU
1	B	622	LYS
1	B	627	TRP
1	B	630	SER
1	B	739	ASP
1	B	765	LEU
2	C	388	ASP
2	C	389	LYS
2	C	390	GLU
2	C	437	SER
2	C	443	ARG
2	C	458	LEU
2	C	473	SER
2	C	495	ASN
2	C	499	THR
2	C	538	SER
2	C	540	TYR
2	C	550	ARG
2	C	569	LEU
2	C	583	VAL
2	C	584	GLN
2	C	588	ASP
1	D	41	ARG
1	D	72	GLN
1	D	77	LEU
1	D	82	GLU
1	D	95	PHE
1	D	144	THR
1	D	145	GLU

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Mol	Chain	Res	Type
1	D	207	VAL
1	D	293	VAL
1	D	324	VAL
1	D	385	CYS
1	D	388	GLN
1	D	435	GLN
1	D	472	CYS
1	D	482	LEU
1	D	597	ARG
1	D	714	GLN
1	D	740	HIS
1	D	742	ILE
2	A	390	GLU
2	A	391	CYS
2	A	394	THR
2	A	396	MET
2	A	400	VAL
2	A	404	VAL
2	A	411	VAL
2	A	413	THR
2	A	414	ASN
2	A	416	ASN
2	A	421	LYS
2	A	425	LEU
2	A	428	VAL
2	A	434	ASN
2	A	439	ASP
2	A	443	ARG
2	A	445	CYS
2	A	449	LEU
2	A	496	LEU
2	A	498	LEU
2	A	499	THR
2	A	522	THR
2	A	536	SER
2	A	538	SER
2	A	552	GLN
2	A	569	LEU
2	A	571	MET
2	A	575	LEU
2	A	588	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18)

such sidechains are listed below:

Mol	Chain	Res	Type
1	B	80	ASN
1	B	344	GLN
1	B	345	HIS
1	B	455	GLN
2	C	414	ASN
2	C	429	ASN
2	C	476	ASN
2	C	552	GLN
1	D	74	ASN
1	D	103	ASN
1	D	179	ASN
1	D	344	GLN
1	D	388	GLN
1	D	553	GLN
1	D	595	ASN
1	D	754	HIS
2	A	429	ASN
2	A	495	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)

12 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	NAG	E	1	1,3	14,14,15	0.81	1 (7%)	17,19,21	1.16	2 (11%)
3	NAG	E	2	3	14,14,15	0.47	0	17,19,21	0.52	0
3	NAG	F	1	1,3	14,14,15	0.33	0	17,19,21	0.45	0
3	NAG	F	2	3	14,14,15	0.27	0	17,19,21	0.46	0
3	NAG	G	1	1,3	14,14,15	1.90	1 (7%)	17,19,21	1.41	2 (11%)
3	NAG	G	2	3	14,14,15	0.32	0	17,19,21	0.52	0
3	NAG	H	1	1,3	14,14,15	1.11	1 (7%)	17,19,21	1.14	2 (11%)
3	NAG	H	2	3	14,14,15	0.49	0	17,19,21	0.51	0
3	NAG	I	1	1,3	14,14,15	0.69	1 (7%)	17,19,21	1.05	1 (5%)
3	NAG	I	2	3	14,14,15	0.23	0	17,19,21	0.55	0
3	NAG	J	1	1,3	14,14,15	0.18	0	17,19,21	0.46	0
3	NAG	J	2	3	14,14,15	0.26	0	17,19,21	0.46	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
3	NAG	E	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	E	2	3	-	0/6/23/26	0/1/1/1
3	NAG	F	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	F	2	3	-	2/6/23/26	0/1/1/1
3	NAG	G	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	G	2	3	-	2/6/23/26	0/1/1/1
3	NAG	H	1	1,3	-	3/6/23/26	0/1/1/1
3	NAG	H	2	3	-	2/6/23/26	0/1/1/1
3	NAG	I	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	I	2	3	-	0/6/23/26	0/1/1/1
3	NAG	J	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	J	2	3	-	2/6/23/26	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	G	1	NAG	O5-C1	-6.72	1.33	1.43
3	H	1	NAG	O5-C1	-4.01	1.37	1.43
3	E	1	NAG	O5-C1	2.87	1.48	1.43
3	I	1	NAG	O5-C1	-2.31	1.40	1.43

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	G	1	NAG	C3-C4-C5	4.24	117.81	110.24
3	I	1	NAG	C1-O5-C5	3.29	116.65	112.19
3	E	1	NAG	C1-O5-C5	3.17	116.49	112.19
3	H	1	NAG	C3-C4-C5	2.83	115.29	110.24
3	H	1	NAG	O4-C4-C5	-2.72	102.55	109.30
3	E	1	NAG	C4-C3-C2	-2.09	107.96	111.02
3	G	1	NAG	C4-C3-C2	2.02	113.97	111.02

There are no chirality outliers.

All (15) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	G	2	NAG	O5-C5-C6-O6
3	G	2	NAG	C4-C5-C6-O6
3	J	1	NAG	C4-C5-C6-O6
3	H	1	NAG	O5-C5-C6-O6
3	E	1	NAG	C8-C7-N2-C2
3	E	1	NAG	O7-C7-N2-C2
3	J	2	NAG	C4-C5-C6-O6
3	F	2	NAG	O5-C5-C6-O6
3	J	1	NAG	O5-C5-C6-O6
3	F	2	NAG	C4-C5-C6-O6
3	J	2	NAG	O5-C5-C6-O6
3	H	1	NAG	C4-C5-C6-O6
3	H	2	NAG	C1-C2-N2-C7
3	H	1	NAG	C1-C2-N2-C7
3	H	2	NAG	C3-C2-N2-C7

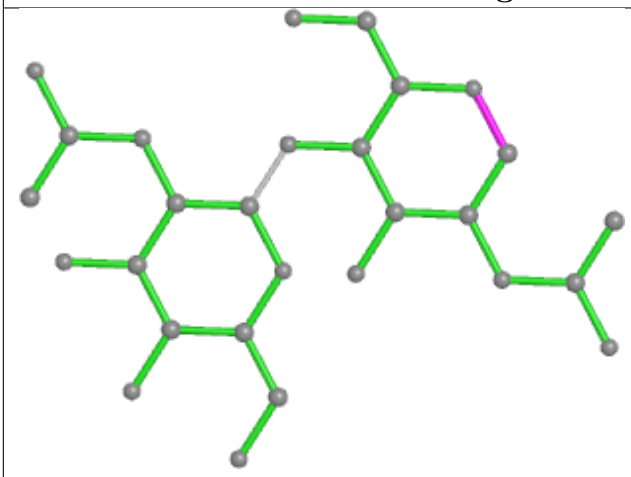
There are no ring outliers.

4 monomers are involved in 4 short contacts:

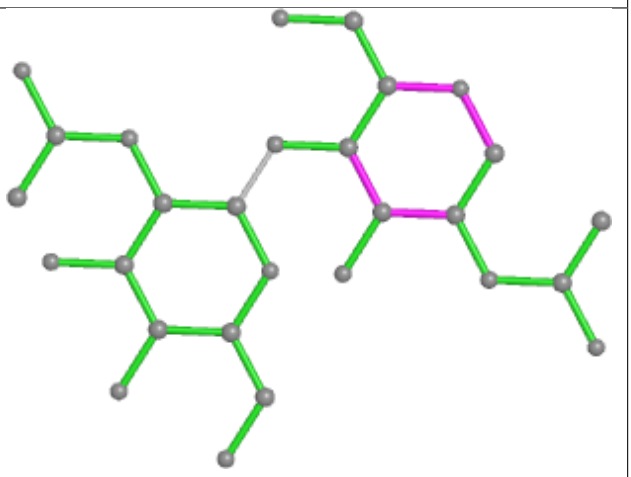
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	I	2	NAG	1	0
3	E	1	NAG	2	0
3	G	1	NAG	1	0
3	I	1	NAG	1	0

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

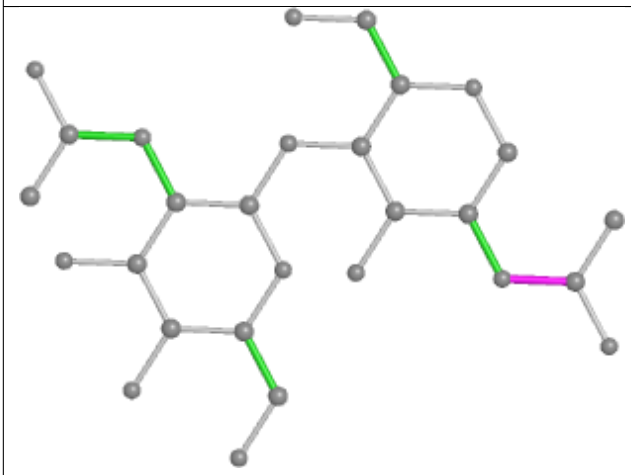
Oligosaccharide Chain E



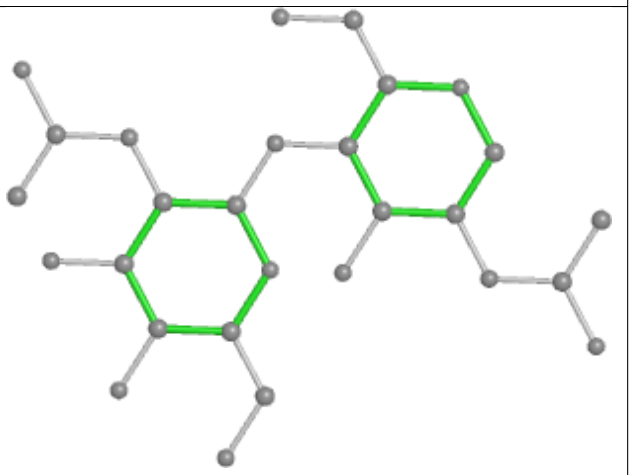
Bond lengths



Bond angles

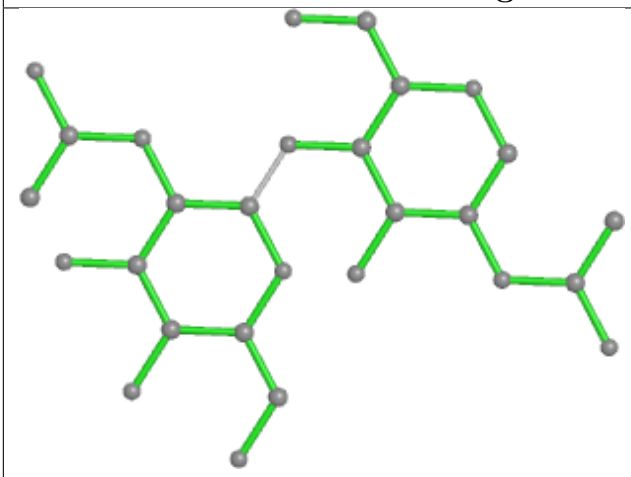


Torsions

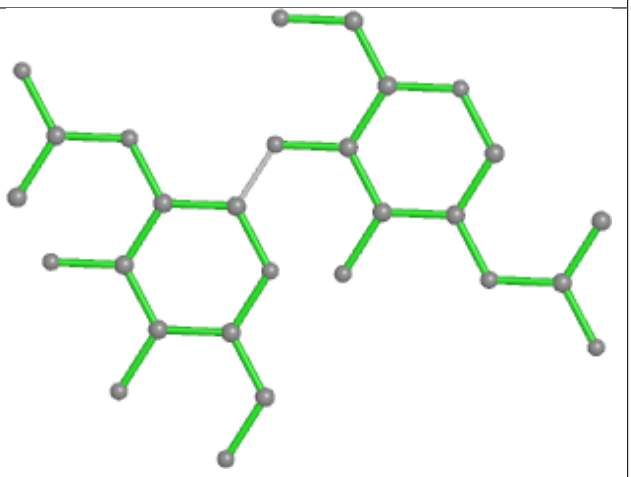


Rings

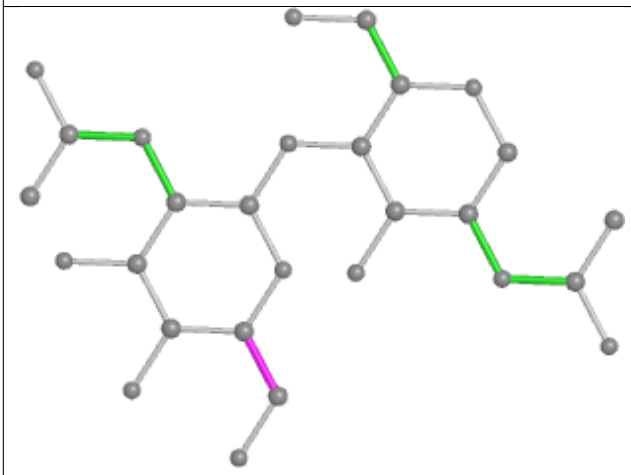
Oligosaccharide Chain F



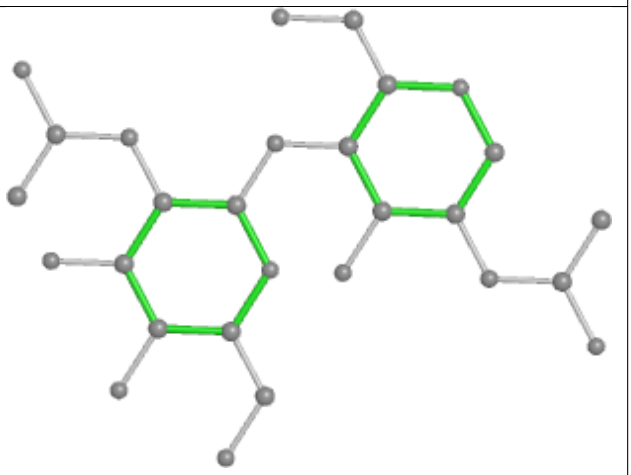
Bond lengths



Bond angles

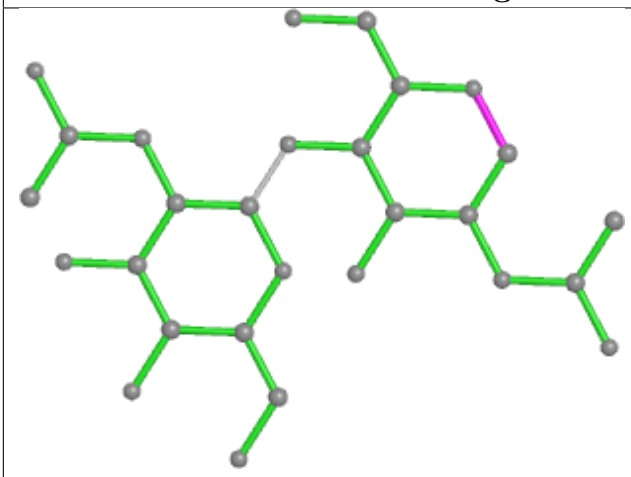


Torsions

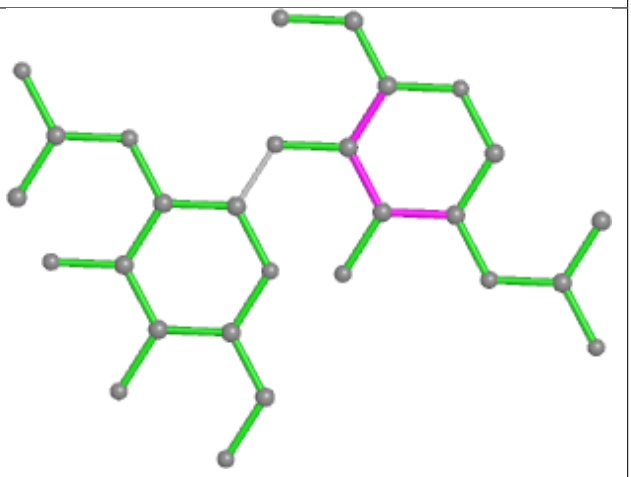


Rings

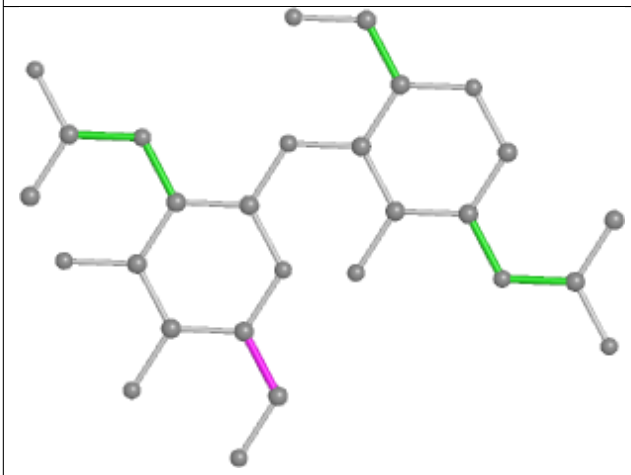
Oligosaccharide Chain G



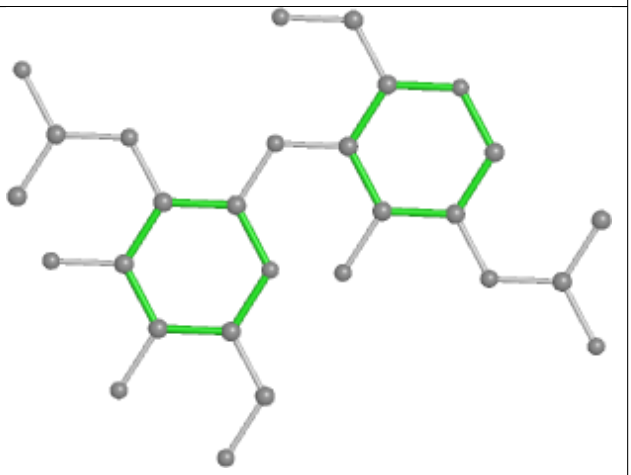
Bond lengths



Bond angles

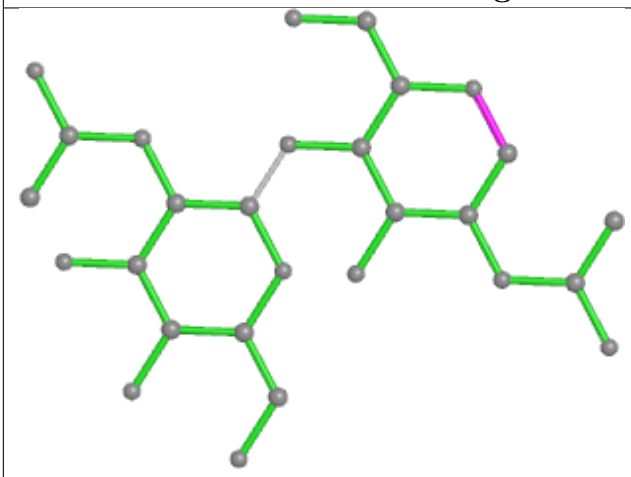


Torsions

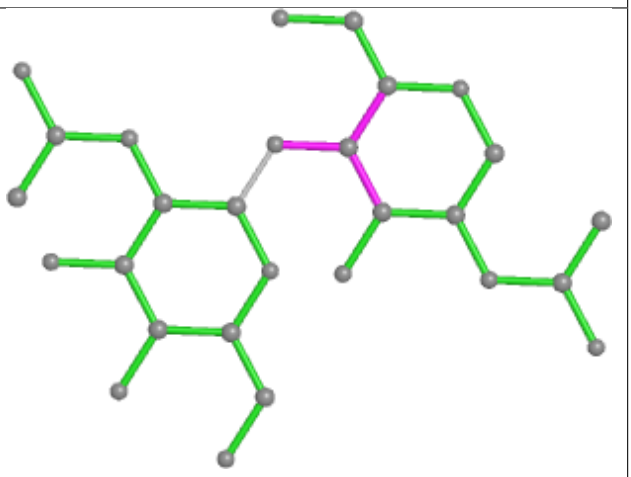


Rings

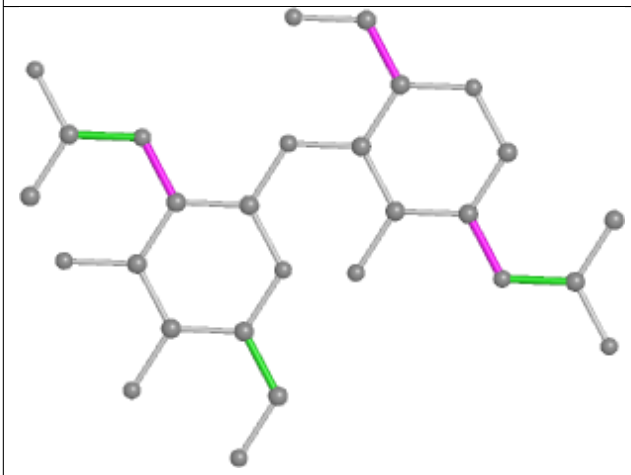
Oligosaccharide Chain H



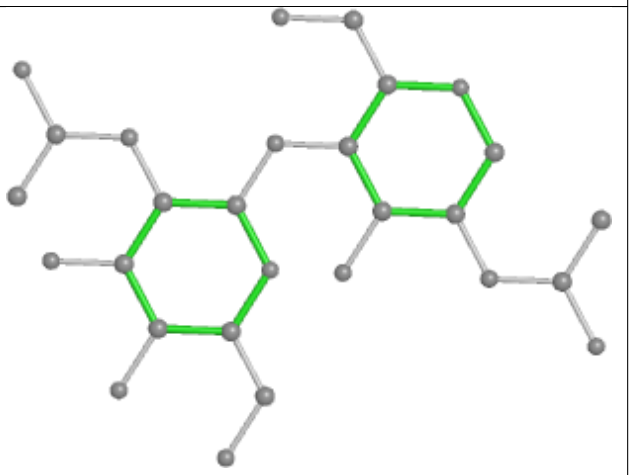
Bond lengths



Bond angles

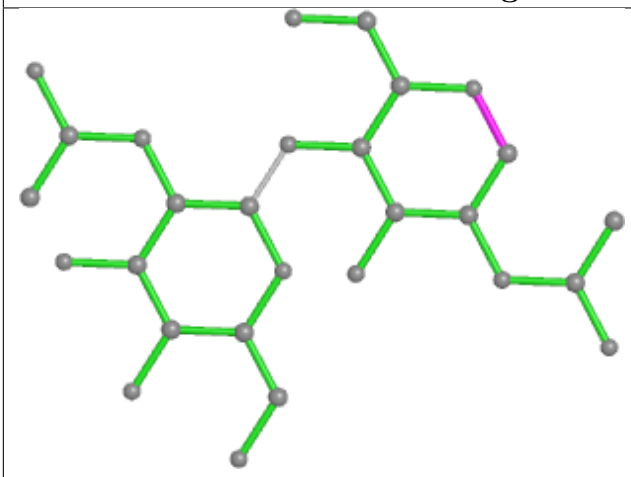


Torsions

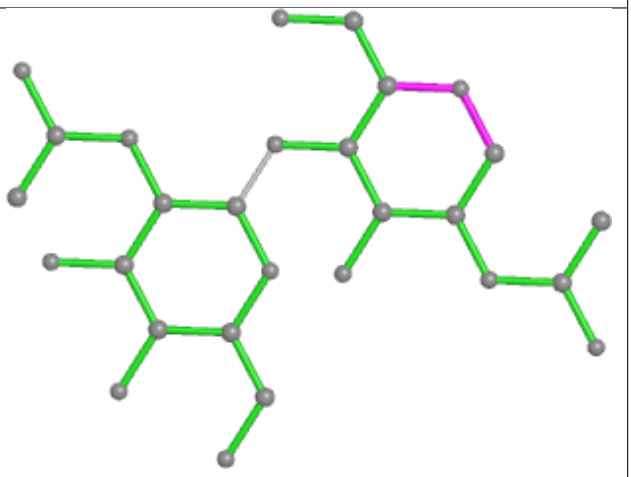


Rings

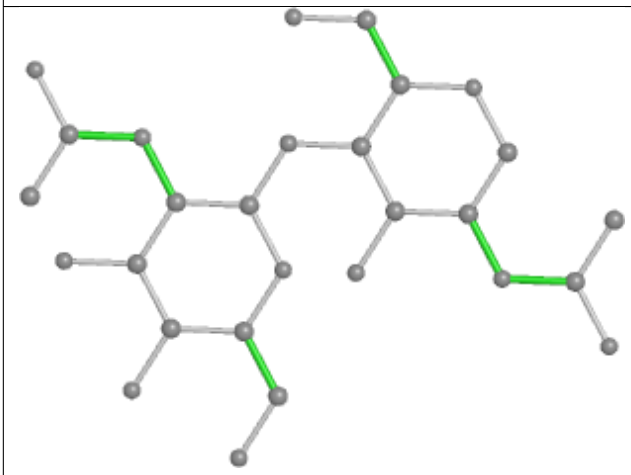
Oligosaccharide Chain I



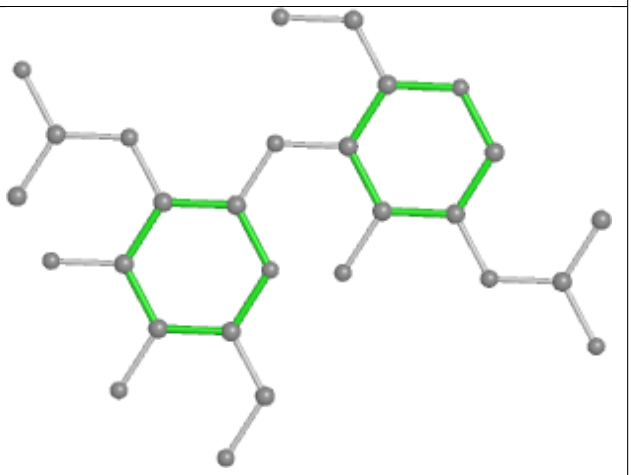
Bond lengths



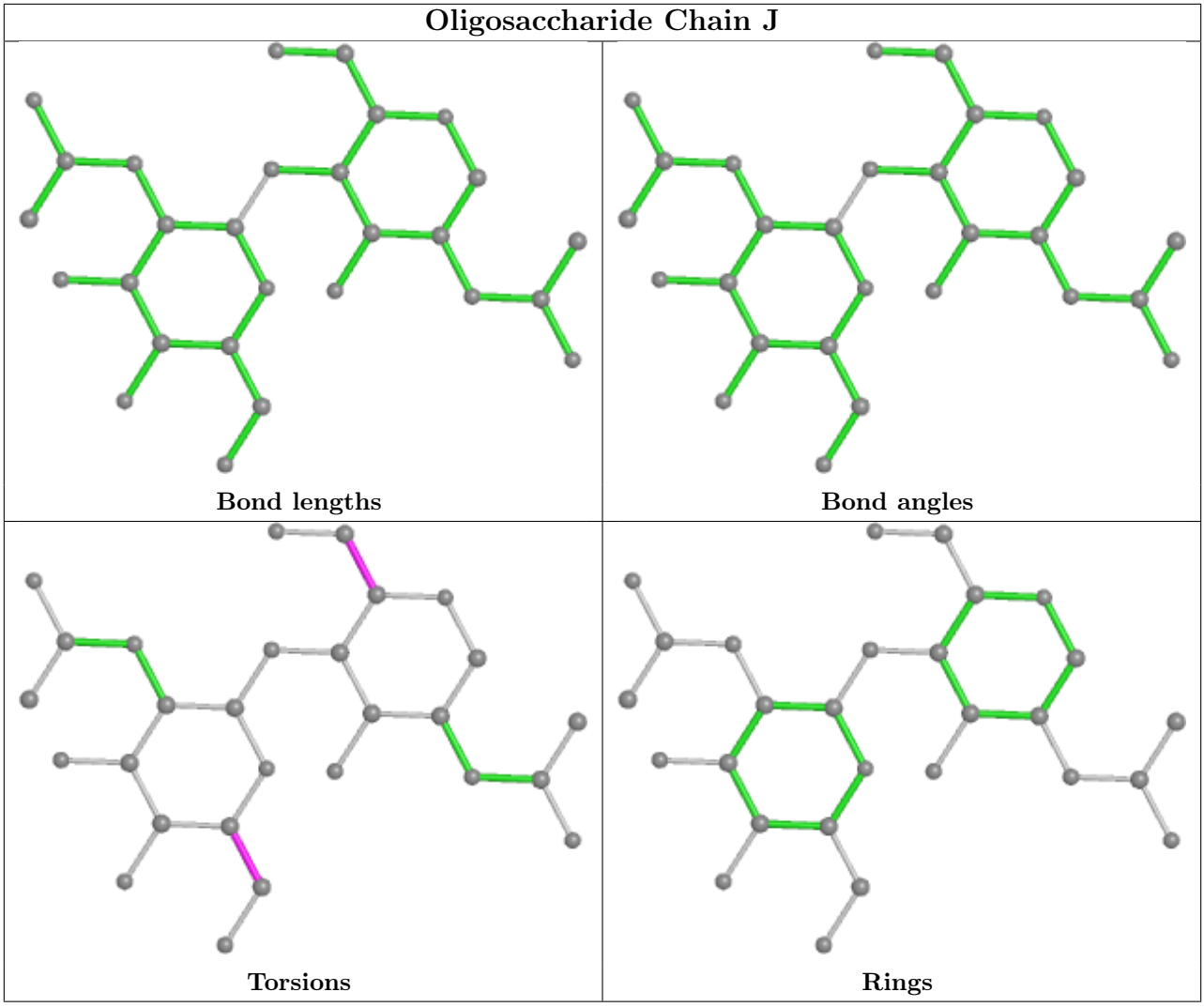
Bond angles



Torsions



Rings



5.6 Ligand geometry (i)

6 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	NAG	D	801	1	14,14,15	0.28	0	17,19,21	0.48	0
4	NAG	B	802	1	14,14,15	0.71	0	17,19,21	0.94	1 (5%)
5	GOL	B	803	-	5,5,5	0.84	0	5,5,5	1.09	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
4	NAG	D	802	1	14,14,15	0.24	0	17,19,21	0.50	0
4	NAG	D	803	1	14,14,15	0.31	0	17,19,21	0.47	0
4	NAG	B	801	1	14,14,15	0.21	0	17,19,21	0.48	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	D	801	1	-	2/6/23/26	0/1/1/1
4	NAG	B	802	1	-	1/6/23/26	0/1/1/1
5	GOL	B	803	-	-	2/4/4/4	-
4	NAG	D	802	1	-	2/6/23/26	0/1/1/1
4	NAG	D	803	1	-	2/6/23/26	0/1/1/1
4	NAG	B	801	1	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	B	802	NAG	C1-O5-C5	3.32	116.69	112.19

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	B	803	GOL	O1-C1-C2-C3
4	D	801	NAG	C4-C5-C6-O6
4	B	801	NAG	O5-C5-C6-O6
4	B	801	NAG	C4-C5-C6-O6
4	D	802	NAG	O5-C5-C6-O6
4	D	803	NAG	C4-C5-C6-O6
4	D	802	NAG	C4-C5-C6-O6
4	D	801	NAG	O5-C5-C6-O6
4	D	803	NAG	O5-C5-C6-O6
5	B	803	GOL	O1-C1-C2-O2
4	B	802	NAG	O5-C5-C6-O6

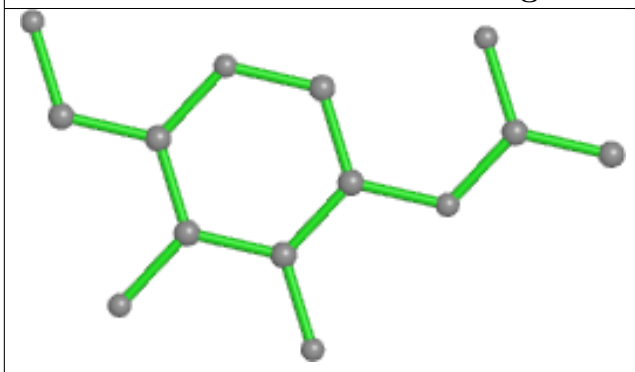
There are no ring outliers.

1 monomer is involved in 1 short contact:

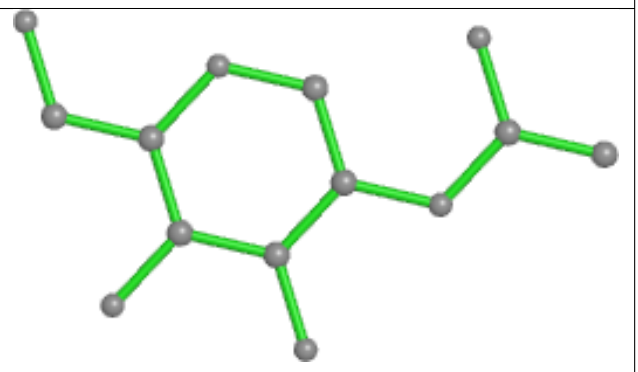
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	803	GOL	1	0

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.

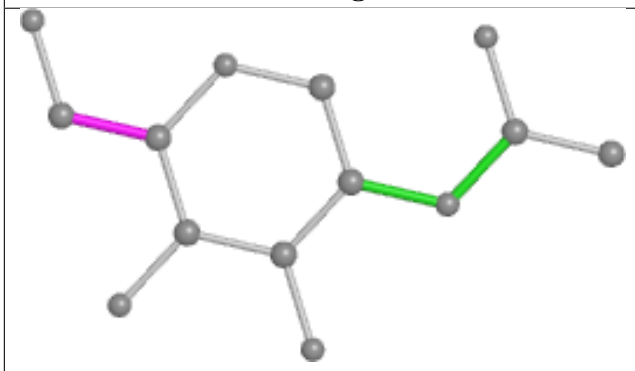
Ligand NAG D 801



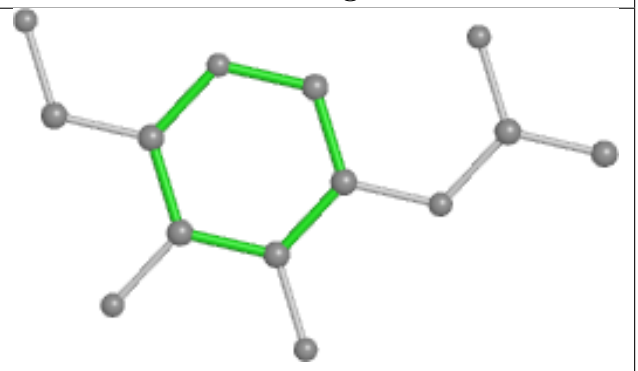
Bond lengths



Bond angles

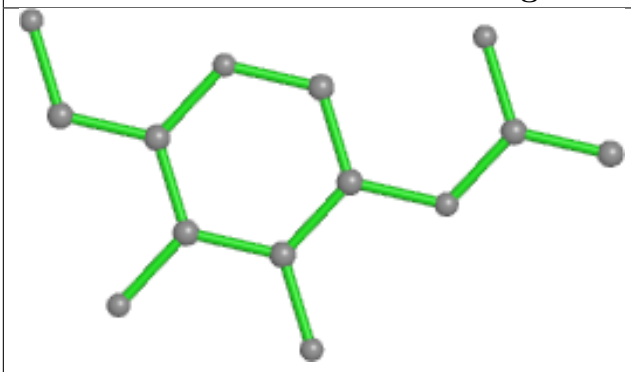


Torsions

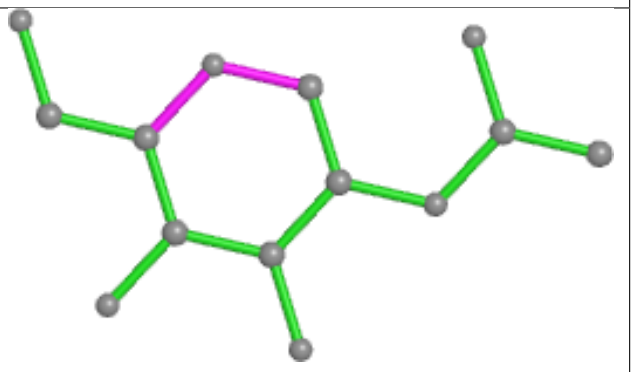


Rings

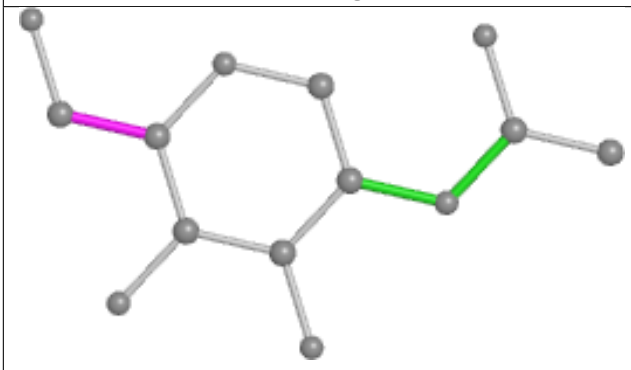
Ligand NAG B 802



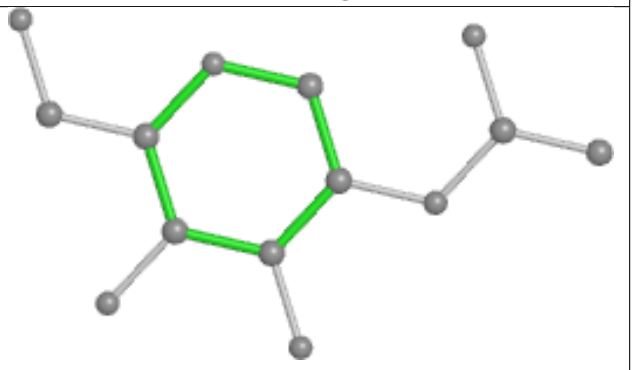
Bond lengths



Bond angles

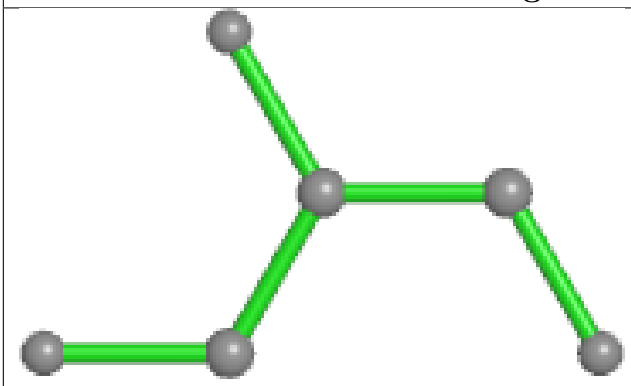


Torsions

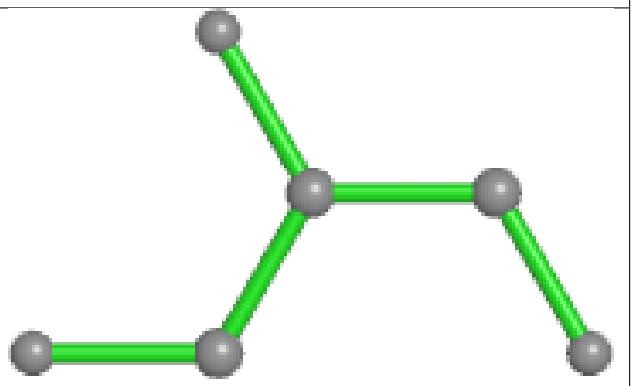


Rings

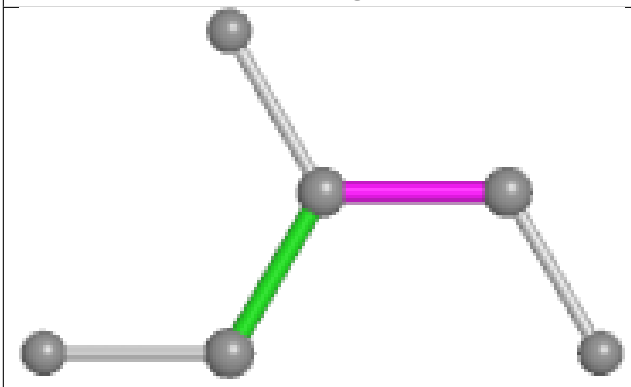
Ligand GOL B 803



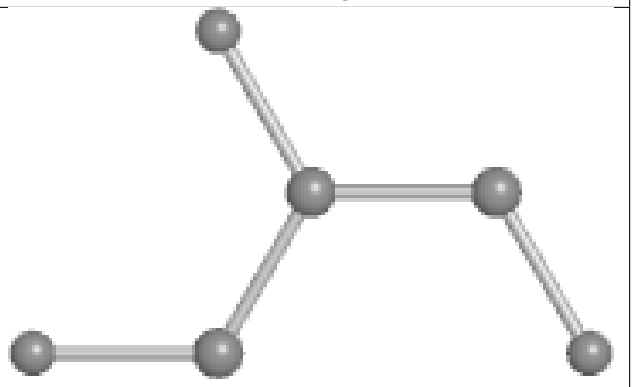
Bond lengths



Bond angles

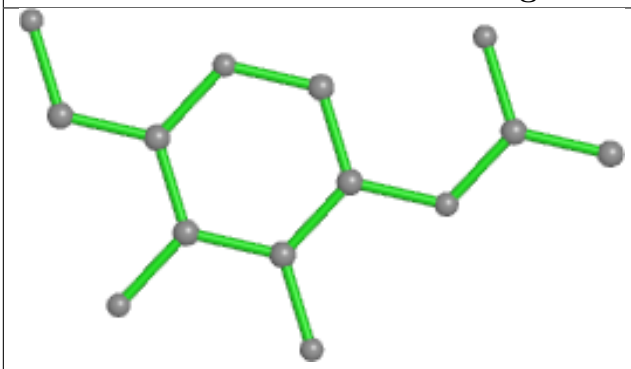


Torsions

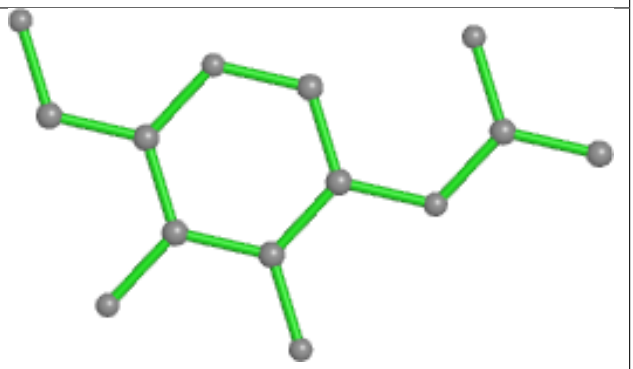


Rings

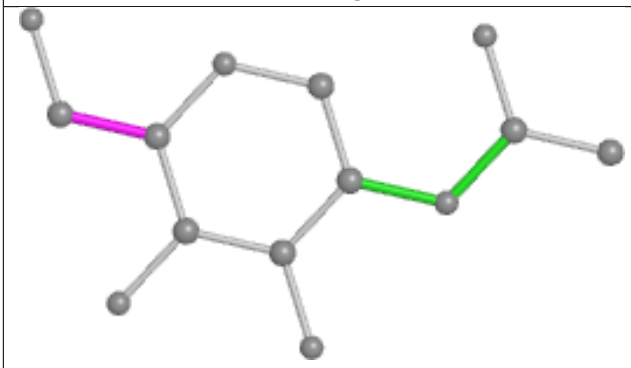
Ligand NAG D 802



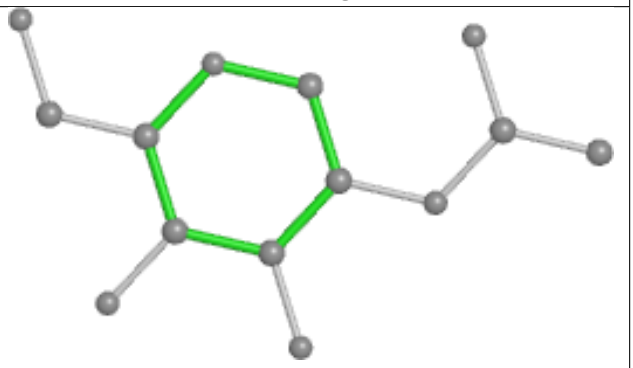
Bond lengths



Bond angles

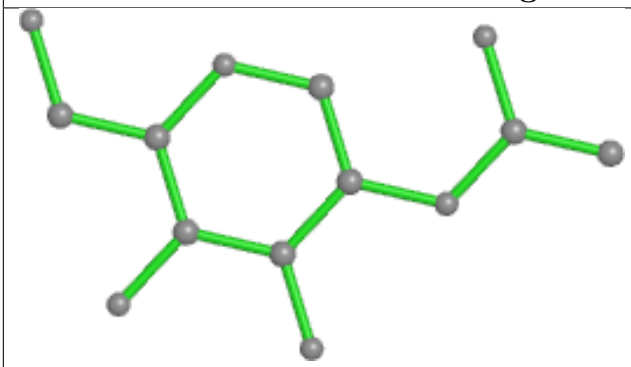


Torsions

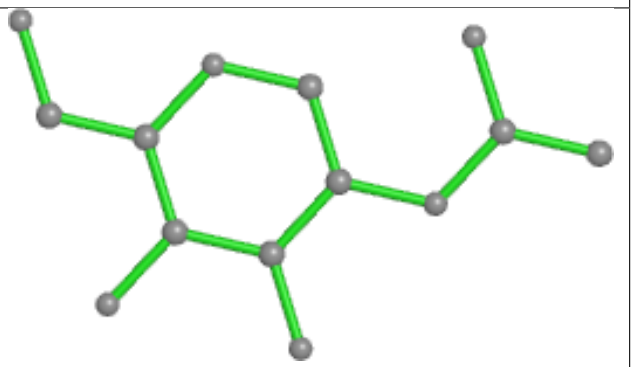


Rings

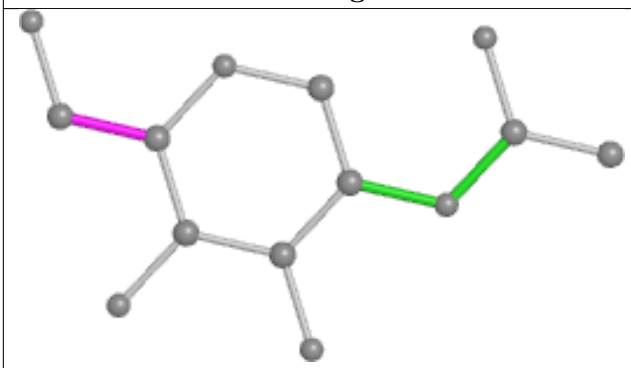
Ligand NAG D 803



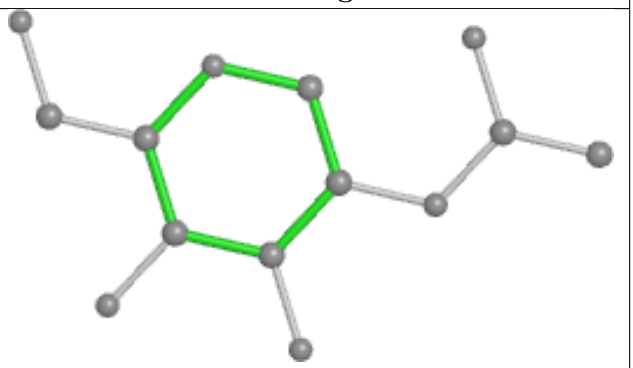
Bond lengths



Bond angles

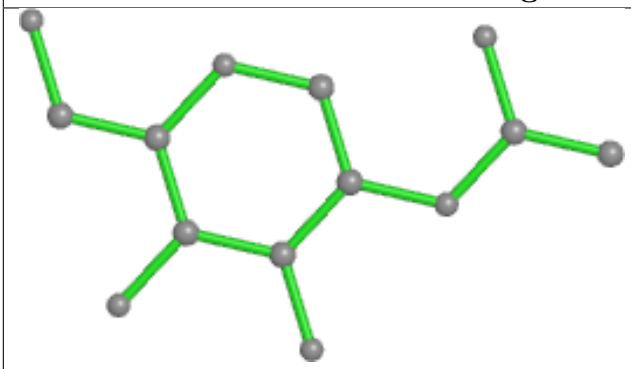


Torsions

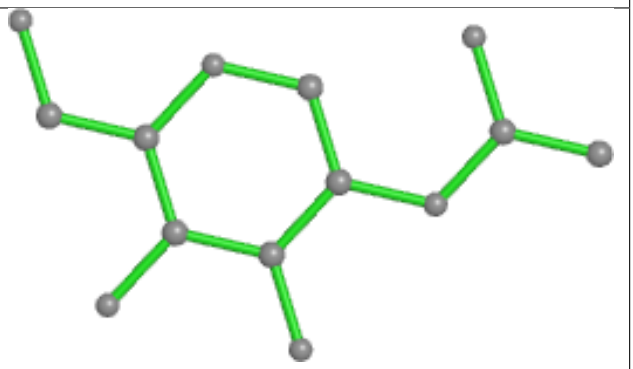


Rings

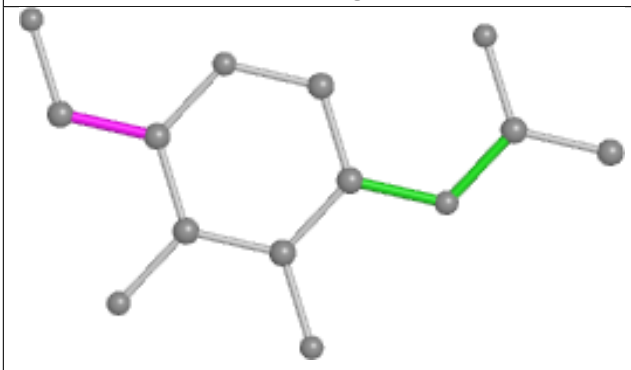
Ligand NAG B 801



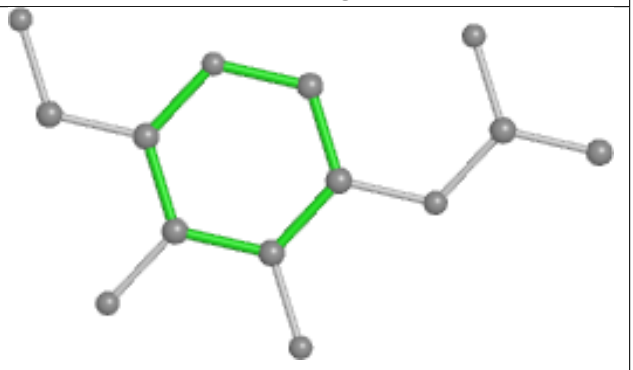
Bond lengths



Bond angles



Torsions



Rings

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, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	B	726/728 (99%)	0.86	54 (7%)	22	20	35, 55, 85, 150	0
1	D	728/728 (100%)	0.86	58 (7%)	20	18	37, 56, 86, 119	0
2	A	201/203 (99%)	1.73	65 (32%)	1	1	45, 96, 149, 171	0
2	C	201/203 (99%)	1.47	46 (22%)	2	3	50, 85, 148, 164	0
All	All	1856/1862 (99%)	1.02	223 (12%)	10	9	35, 59, 123, 171	0

All (223) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	A	441	ILE	8.0
2	A	585	TYR	7.1
2	A	426	PHE	5.6
2	A	422	LEU	5.4
2	C	422	LEU	4.6
2	A	423	LEU	4.6
2	C	488	VAL	4.5
2	C	441	ILE	4.5
2	A	393	PHE	4.4
2	A	534	CYS	4.4
1	D	507	VAL	4.3
1	D	40	ARG	4.1
1	B	95	PHE	4.1
2	A	417	TYR	4.1
1	B	257	PRO	4.0
2	A	436	ILE	4.0
2	A	582	SER	4.0
1	D	97	GLU	4.0
1	D	732	ALA	3.8
2	C	540	TYR	3.8
2	A	440	ALA	3.8

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Mol	Chain	Res	Type	RSRZ
2	A	437	SER	3.8
2	A	411	VAL	3.7
2	C	492	ALA	3.7
1	D	95	PHE	3.7
2	A	494	ALA	3.7
2	A	427	MET	3.6
1	B	649	CYS	3.6
2	A	490	ALA	3.6
2	A	415	CYS	3.5
1	B	96	ASP	3.5
2	C	484	PRO	3.4
2	C	480	SER	3.4
1	B	98	PHE	3.4
1	B	402	TRP	3.3
1	D	338	ALA	3.3
2	A	456	TYR	3.3
1	B	124	TRP	3.3
2	C	533	ILE	3.3
2	A	496	LEU	3.3
1	D	657	SER	3.2
1	D	506	ASP	3.2
2	C	587	THR	3.2
1	D	353	TRP	3.1
2	A	587	THR	3.1
1	B	239	SER	3.1
2	C	428	VAL	3.1
2	A	493	PRO	3.1
2	A	492	ALA	3.1
2	C	585	TYR	3.1
2	A	540	TYR	3.1
2	A	530	GLU	3.0
1	D	504	LEU	3.0
1	D	156	THR	3.0
2	C	556	TYR	3.0
2	A	442	ALA	3.0
2	A	438	PRO	3.0
1	B	342	ARG	3.0
1	B	447	CYS	2.9
2	C	393	PHE	2.9
2	A	405	TYR	2.9
1	B	537	LEU	2.9
2	A	421	LYS	2.8

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Mol	Chain	Res	Type	RSRZ
2	A	449	LEU	2.8
2	A	447	SER	2.8
2	A	428	VAL	2.8
1	D	116	PHE	2.8
1	B	90	LEU	2.8
2	C	433	CYS	2.8
2	C	486	CYS	2.8
1	D	478	PRO	2.8
2	A	537	PHE	2.8
2	C	586	GLY	2.8
1	B	347	GLU	2.7
2	A	579	PHE	2.7
2	A	397	LEU	2.7
1	B	392	GLU	2.7
1	D	94	THR	2.7
1	D	106	SER	2.7
2	A	406	ASN	2.7
1	B	444	CYS	2.7
2	C	515	GLY	2.7
2	C	571	MET	2.7
2	C	419	LEU	2.7
2	A	486	CYS	2.7
2	C	538	SER	2.7
2	A	446	TYR	2.6
2	A	430	GLU	2.6
2	C	458	LEU	2.6
1	D	584	GLY	2.6
2	C	436	ILE	2.6
2	A	464	ILE	2.6
2	C	423	LEU	2.6
2	C	548	VAL	2.6
1	D	57	PHE	2.6
1	D	580	GLY	2.6
1	D	82	GLU	2.6
1	D	414	ASP	2.6
2	A	418	ASN	2.6
1	D	401	VAL	2.6
1	B	443	THR	2.6
1	D	734	TRP	2.6
1	D	500	LEU	2.6
1	D	324	VAL	2.5
2	A	583	VAL	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	53	PHE	2.5
2	A	412	PHE	2.5
1	B	503	MET	2.5
1	B	522	ILE	2.5
1	B	41	ARG	2.5
2	C	477	TYR	2.5
2	C	481	PHE	2.5
1	B	307	ASN	2.5
2	A	581	ILE	2.5
2	C	410	LEU	2.4
2	A	401	PRO	2.4
2	A	457	PRO	2.4
1	D	354	VAL	2.4
2	C	537	PHE	2.4
2	A	453	TYR	2.4
2	A	476	ASN	2.4
2	A	450	THR	2.4
2	C	569	LEU	2.4
1	B	323	SER	2.4
1	D	98	PHE	2.4
1	D	340	HIS	2.4
2	A	481	PHE	2.4
1	B	97	GLU	2.4
1	D	316	LEU	2.4
1	B	659	TRP	2.4
2	C	460	MET	2.4
1	B	455	GLN	2.4
1	D	138	HIS	2.4
2	A	510	CYS	2.4
1	D	304	THR	2.4
1	B	482	LEU	2.4
1	B	100	HIS	2.4
1	D	439	HIS	2.4
1	D	656	VAL	2.4
1	D	185	ILE	2.4
1	D	409	ALA	2.4
1	D	660	GLU	2.3
1	B	174	ILE	2.3
2	C	459	SER	2.3
2	A	391	CYS	2.3
2	C	498	LEU	2.3
2	A	419	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	178	PRO	2.3
1	D	339	SER	2.3
1	D	83	TYR	2.3
1	D	142	LEU	2.3
1	D	422	TYR	2.3
1	B	686	SER	2.3
2	A	420	THR	2.3
1	B	385	CYS	2.3
1	B	439	HIS	2.3
1	B	389	VAL	2.3
1	D	134	ILE	2.3
1	B	213	ALA	2.3
1	D	124	TRP	2.3
1	D	326	ALA	2.3
2	A	396	MET	2.2
2	A	491	THR	2.2
2	A	588	ASP	2.2
2	C	581	ILE	2.2
1	D	280	ALA	2.2
1	D	632	GLY	2.2
1	D	147	ARG	2.2
1	D	699	GLU	2.2
2	C	416	ASN	2.2
2	C	427	MET	2.2
1	D	315	TRP	2.2
1	D	631	TYR	2.2
1	D	488	ASP	2.2
1	B	593	ALA	2.2
1	B	419	SER	2.2
2	C	473	SER	2.2
2	C	539	PRO	2.2
1	D	96	ASP	2.2
1	D	731	GLN	2.2
1	B	99	GLY	2.2
1	D	687	THR	2.1
1	D	103	ASN	2.1
1	B	134	ILE	2.1
1	B	742	ILE	2.1
1	B	741	GLY	2.1
2	C	435	GLY	2.1
1	D	766	PRO	2.1
2	C	394	THR	2.1

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Mol	Chain	Res	Type	RSRZ
2	C	413	THR	2.1
1	B	324	VAL	2.1
2	A	454	PHE	2.1
1	B	316	LEU	2.1
1	B	356	ARG	2.1
1	B	94	THR	2.1
1	B	600	THR	2.1
1	B	76	ILE	2.1
1	B	418	ILE	2.1
1	B	730	PHE	2.1
2	C	583	VAL	2.1
1	D	767	GLU	2.1
1	D	434	ILE	2.1
2	A	580	ILE	2.1
2	A	584	GLN	2.1
1	B	47	ASP	2.1
1	D	299	TYR	2.1
2	C	461	ARG	2.1
2	C	588	ASP	2.1
1	B	762	CYS	2.0
1	D	279	THR	2.0
1	B	288	VAL	2.0
1	B	698	VAL	2.0
2	C	412	PHE	2.0
2	A	458	LEU	2.0
2	A	434	ASN	2.0
2	C	417	TYR	2.0
2	A	557	GLU	2.0
2	A	445	CYS	2.0
1	B	575	VAL	2.0
2	C	449	LEU	2.0
2	A	429	ASN	2.0
1	B	548	ALA	2.0
2	A	482	ALA	2.0

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

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

6.3 Carbohydrates (i)

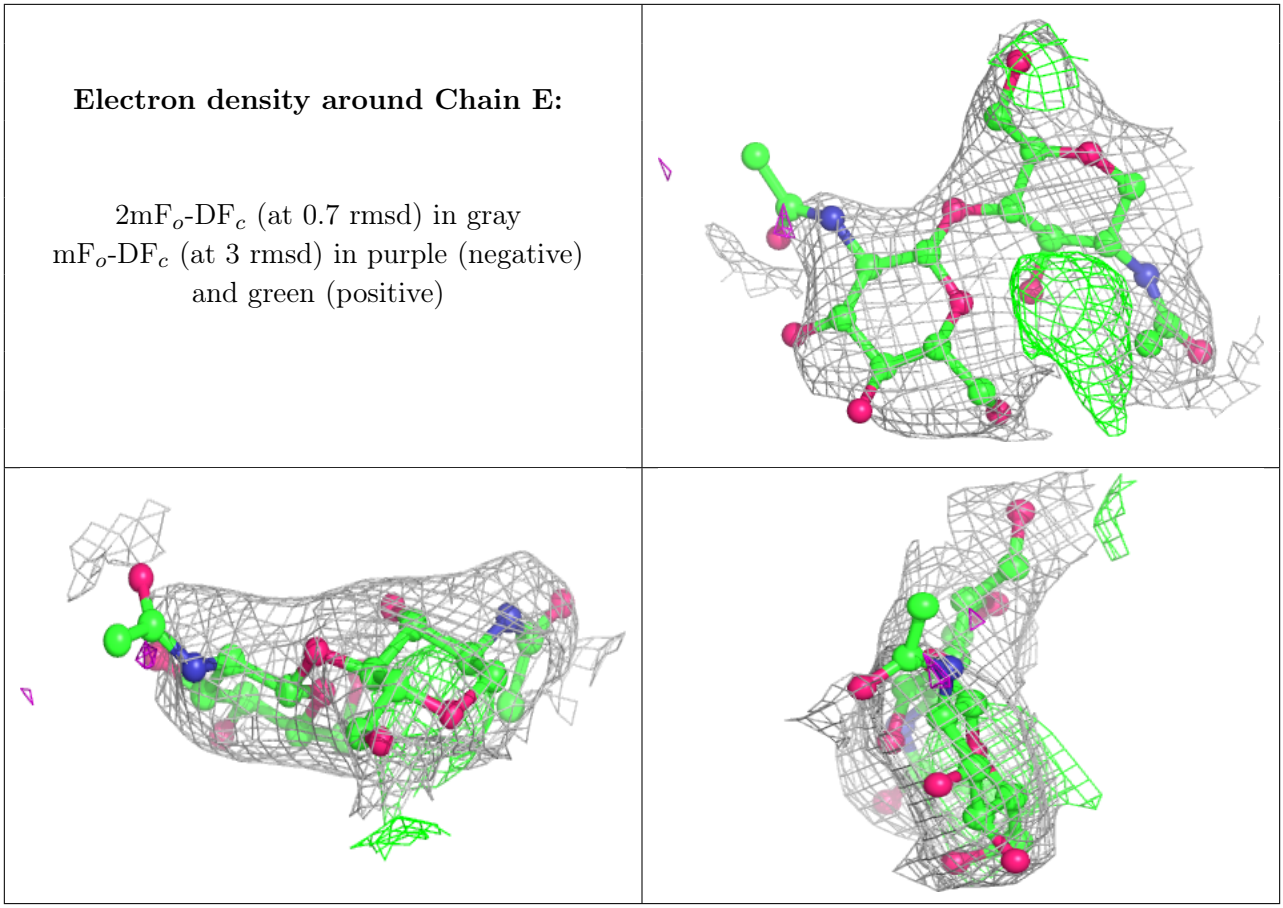
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	NAG	G	2	14/15	0.55	0.15	65,96,106,106	0
3	NAG	H	1	14/15	0.65	0.18	54,67,75,78	0
3	NAG	H	2	14/15	0.67	0.23	73,85,98,98	0
3	NAG	F	2	14/15	0.72	0.14	68,78,85,87	0
3	NAG	E	1	14/15	0.72	0.14	59,62,78,83	0
3	NAG	I	2	14/15	0.75	0.12	68,75,84,95	0
3	NAG	I	1	14/15	0.76	0.16	51,62,69,73	0
3	NAG	G	1	14/15	0.76	0.17	77,84,94,97	0
3	NAG	E	2	14/15	0.77	0.21	79,85,89,99	0
3	NAG	J	2	14/15	0.79	0.14	73,85,97,103	0
3	NAG	J	1	14/15	0.80	0.14	64,72,80,81	0
3	NAG	F	1	14/15	0.91	0.09	45,57,63,64	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.

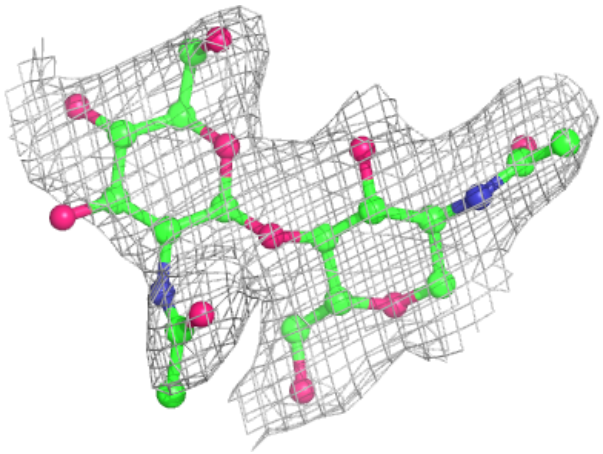
Electron density around Chain E:

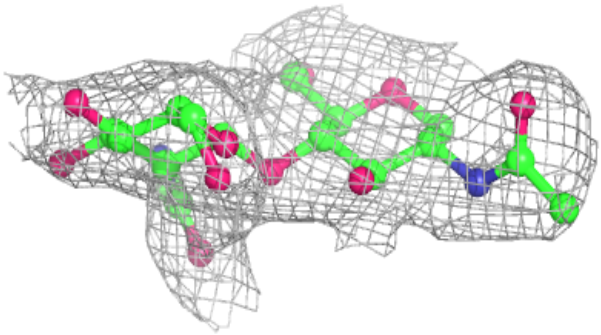
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

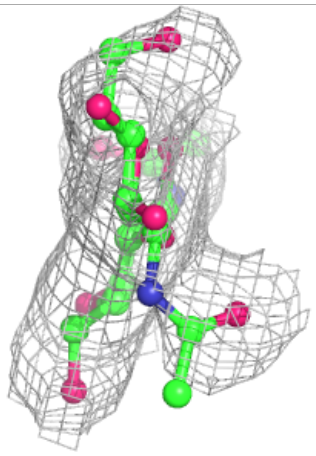


Electron density around Chain F:

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

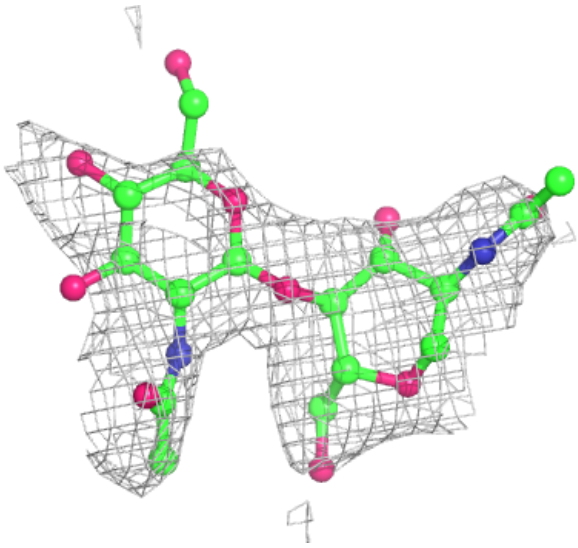


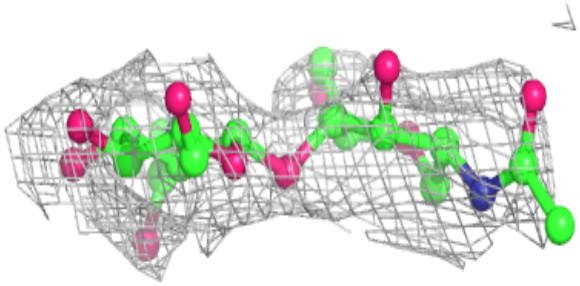


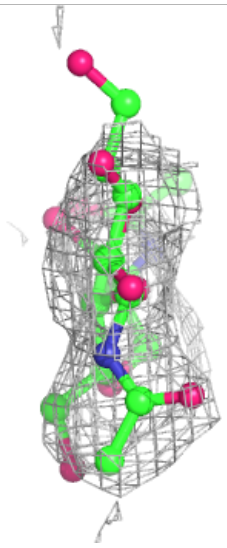


Electron density around Chain G:

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

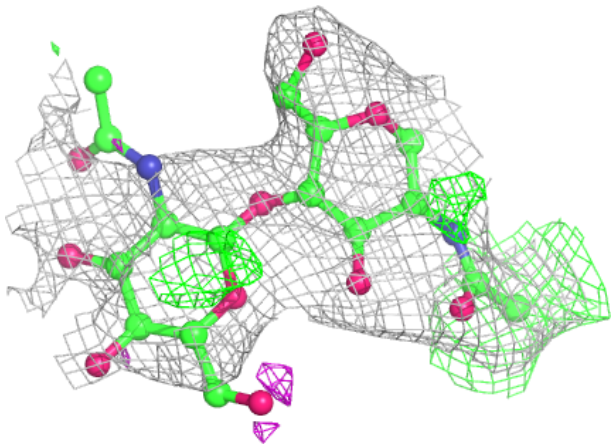


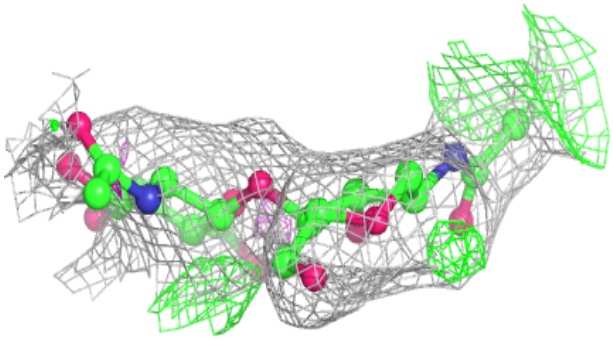


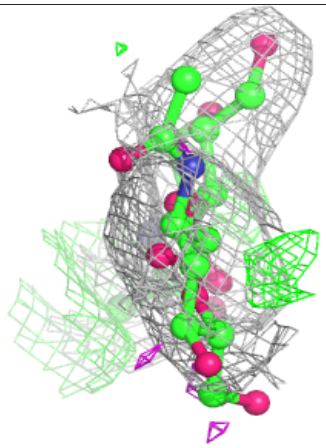


Electron density around Chain H:

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

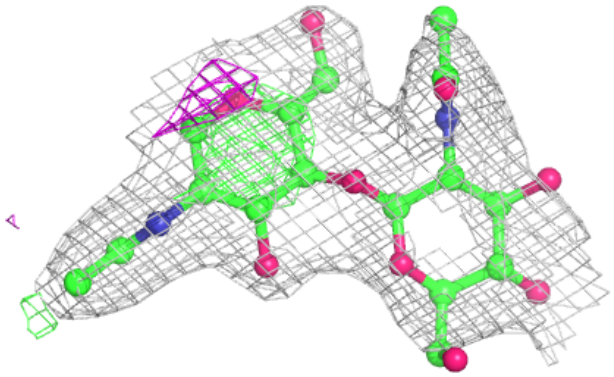


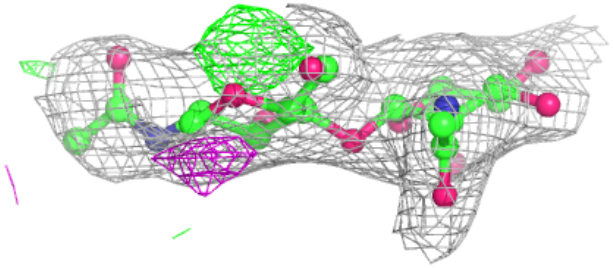


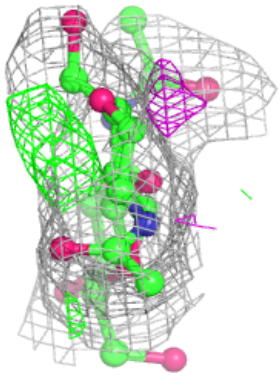


Electron density around Chain I:

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

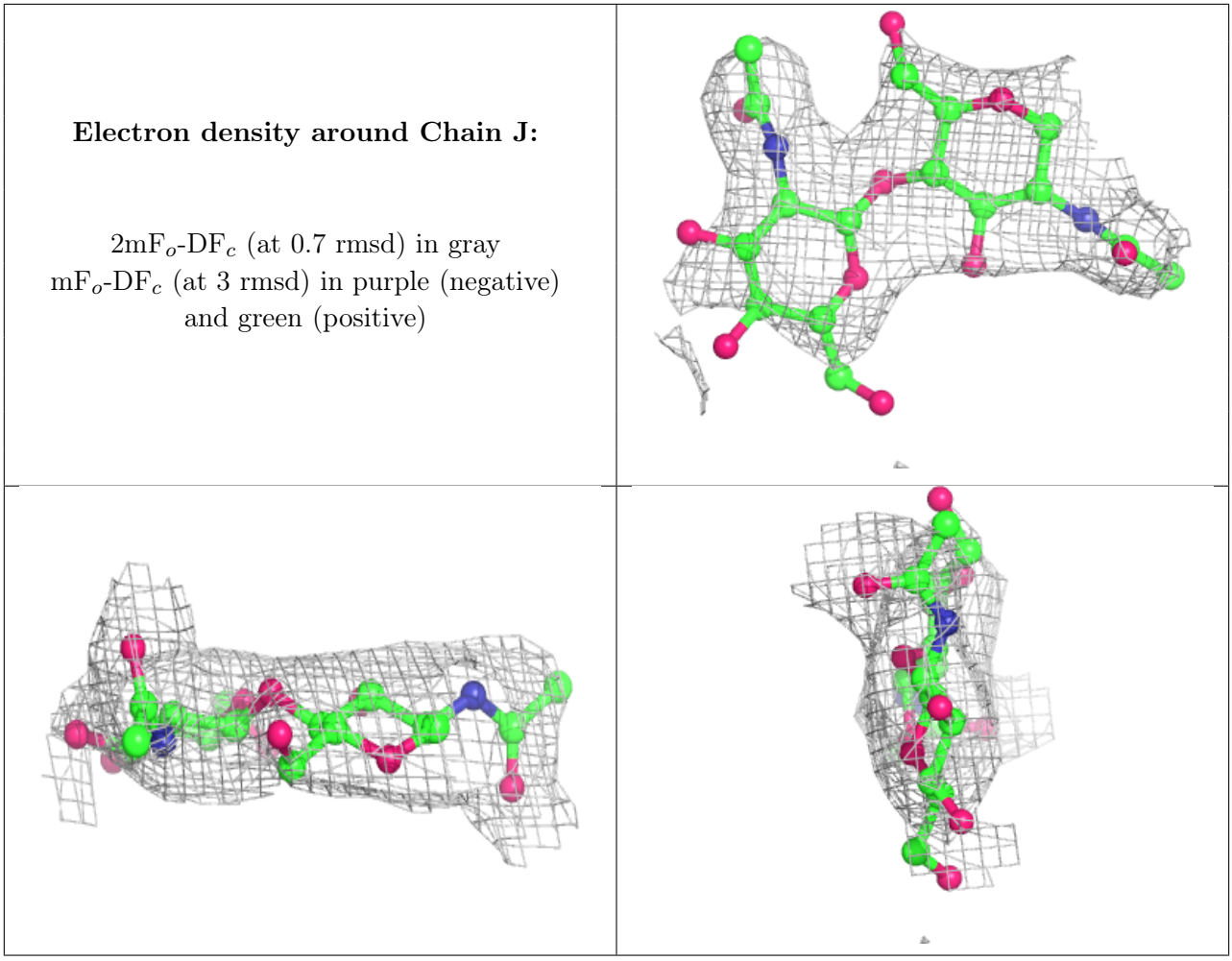






Electron density around Chain J:

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



6.4 Ligands

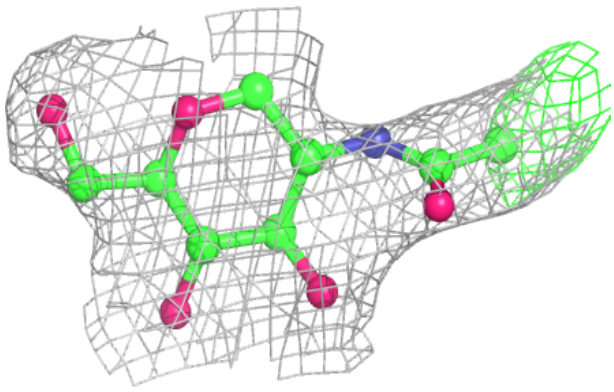
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

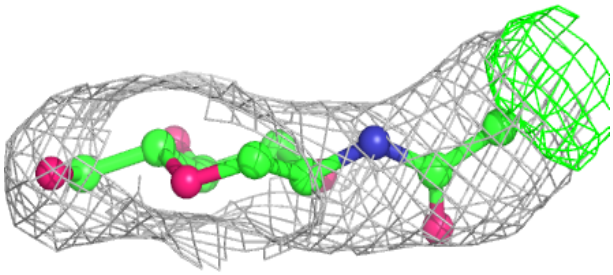
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	NAG	B	802	14/15	0.61	0.15	54,76,81,81	0
4	NAG	D	802	14/15	0.67	0.17	74,89,96,98	0
4	NAG	D	801	14/15	0.74	0.14	69,83,88,89	0
4	NAG	B	801	14/15	0.74	0.16	72,76,79,80	0
4	NAG	D	803	14/15	0.81	0.10	70,72,75,75	0
5	GOL	B	803	6/6	0.85	0.19	50,52,55,58	0

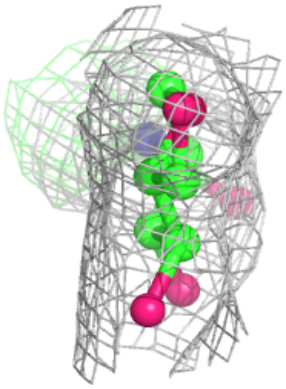
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around NAG B 802:

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

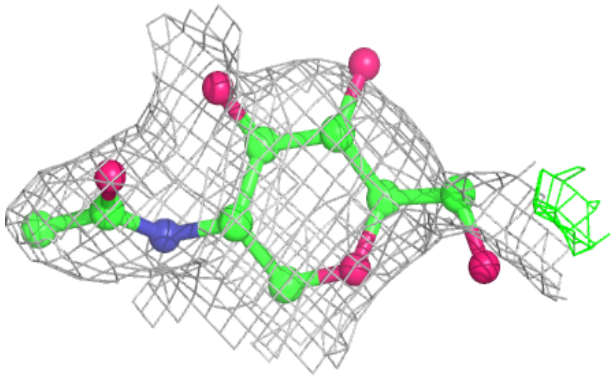


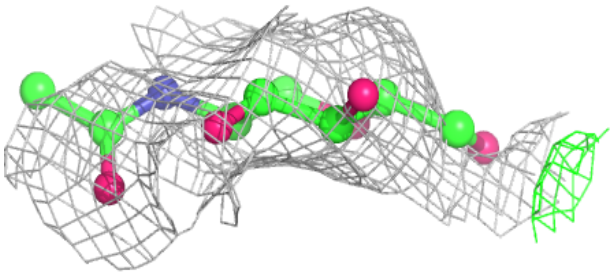


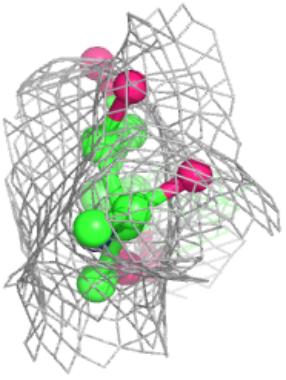


Electron density around NAG D 802:

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

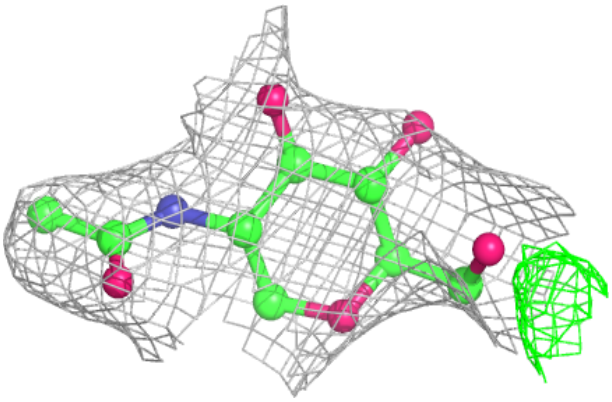


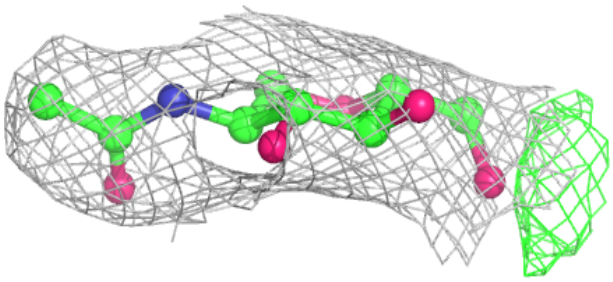


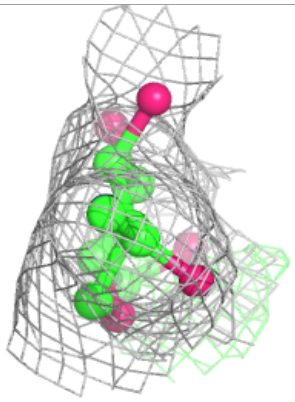


Electron density around NAG D 801:

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

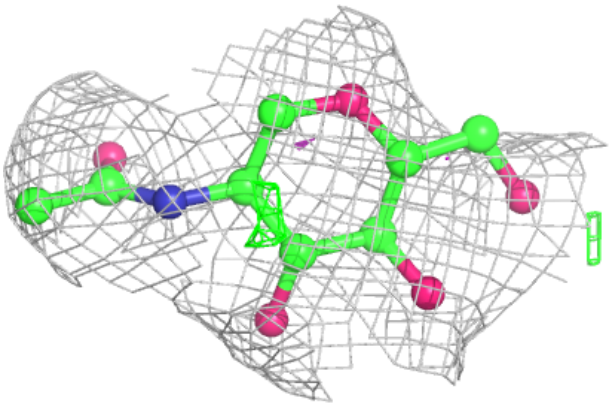


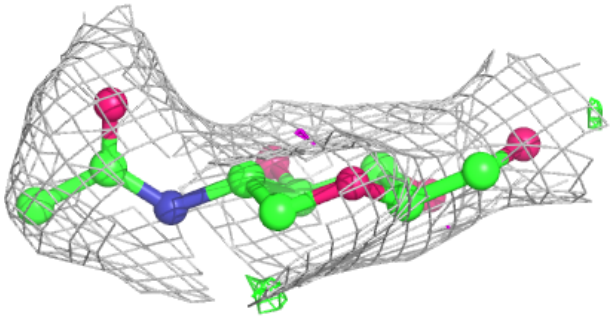


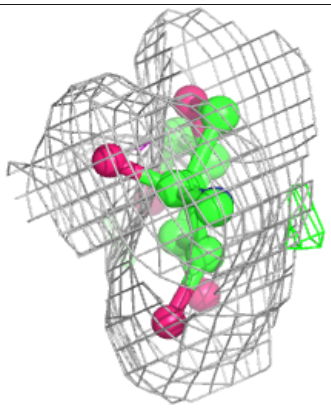


Electron density around NAG B 801:

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

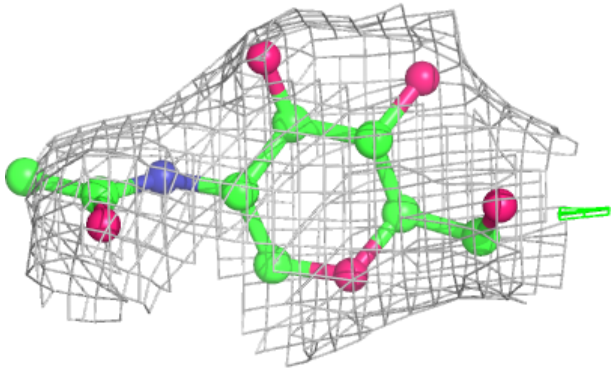


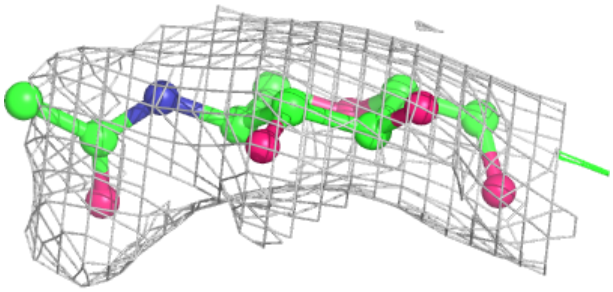


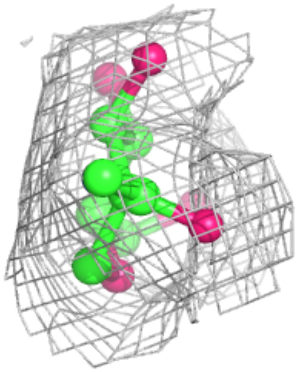


Electron density around NAG D 803:

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

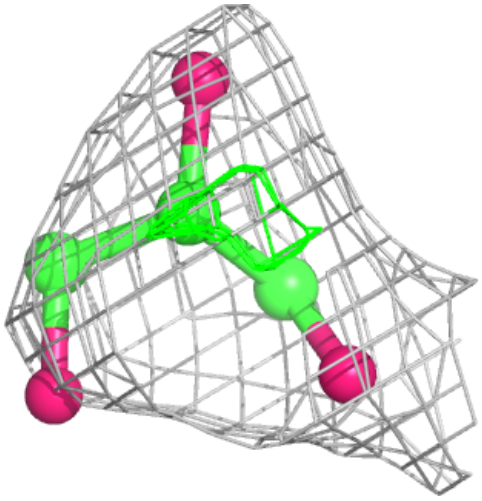


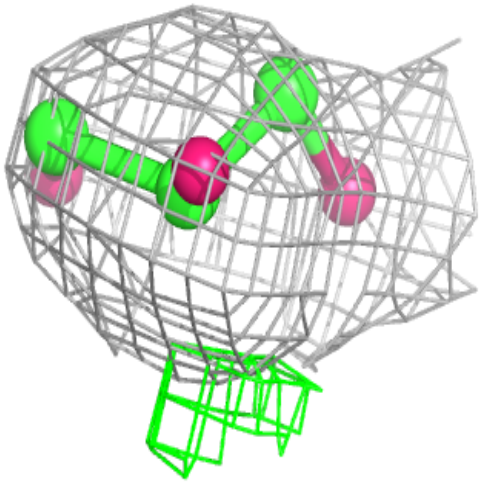


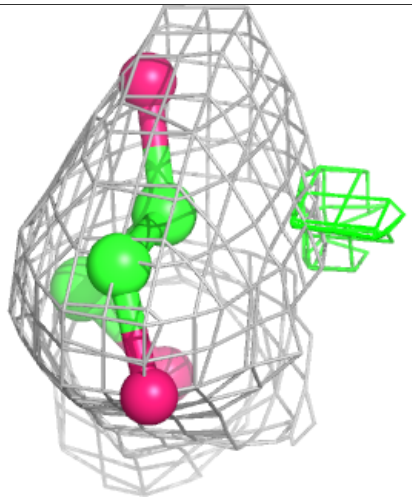


Electron density around GOL B 803:

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







6.5 Other polymers

There are no such residues in this entry.