Full wwPDB X-ray Structure Validation Report ⓘ

Aug 8, 2020 – 03:04 PM BST

PDB ID	:	6SKA
Title	:	Teneurin 2 in complex with Latrophilin 1 Lec-Olf domains
Authors	:	Chu, A.; Carrasquero, M.A.; Lowe, E.; Seiradake, E.
Deposited on	:	2019-08-15
Resolution	:	3.86 Å(reported)

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

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

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

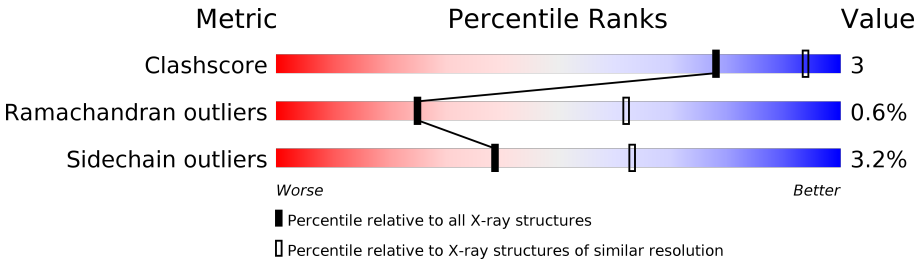
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.13.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.13.1

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 3.86 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))
Clashscore	141614	1015 (4.08-3.64)
Ramachandran outliers	138981	1069 (4.10-3.62)
Sidechain outliers	138945	1062 (4.10-3.62)

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 on 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%

Mol	Chain	Length	Quality of chain
1	A	1836	91% 8%
2	D	347	80% 17%
3	B	8	25% 75%
4	C	2	100%
4	E	2	100%
4	F	2	50% 50%
4	G	2	100%
4	H	2	50% 50%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 17628 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 Teneurin-2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	1836	14513	9168	2508	2774	63	0	1	0

There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	LYS	deletion	UNP Q9DER5
A	?	-	THR	deletion	UNP Q9DER5
A	?	-	GLU	deletion	UNP Q9DER5
A	?	-	GLU	deletion	UNP Q9DER5
A	?	-	ASN	deletion	UNP Q9DER5
A	?	-	SER	deletion	UNP Q9DER5
A	?	-	ILE	deletion	UNP Q9DER5

- Molecule 2 is a protein called Adhesion G protein-coupled receptor L1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	D	347	2810	1775	479	539	17	0	0	0

There are 11 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	132	VAL	ILE	conflict	UNP Q80TR1
D	?	-	VAL	deletion	UNP Q80TR1
D	?	-	TYR	deletion	UNP Q80TR1
D	?	-	VAL	deletion	UNP Q80TR1
D	?	-	ASP	deletion	UNP Q80TR1
D	?	-	ASP	deletion	UNP Q80TR1
D	?	-	ASP	deletion	UNP Q80TR1
D	?	-	SER	deletion	UNP Q80TR1
D	?	-	GLU	deletion	UNP Q80TR1

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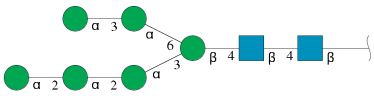
Chain	Residue	Modelled	Actual	Comment	Reference
D	?	-	ALA	deletion	UNP Q80TR1
D	?	-	ALA	deletion	UNP Q80TR1

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

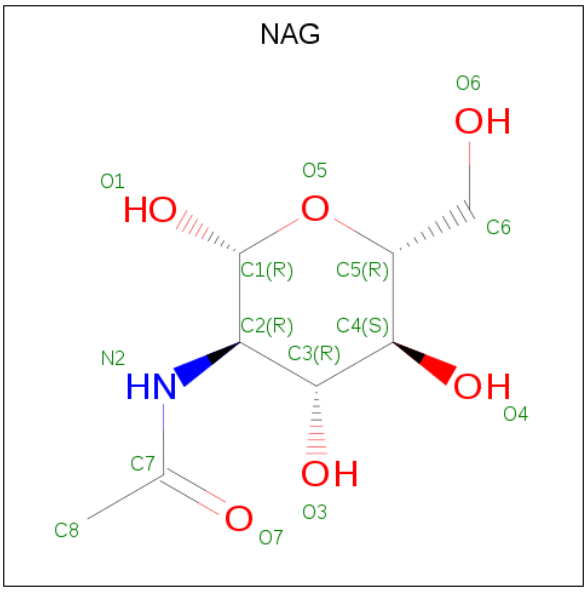


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
3	B	8	Total C N O 94 52 2 40	0	0	0

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
4	C	2	Total C N O 28 16 2 10	0	0	0
4	E	2	Total C N O 28 16 2 10	0	0	0
4	F	2	Total C N O 28 16 2 10	0	0	0
4	G	2	Total C N O 28 16 2 10	0	0	0
4	H	2	Total C N O 28 16 2 10	0	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
5	A	1	Total C N O 14 8 1 5	0	0
5	A	1	Total C N O 14 8 1 5	0	0
5	A	1	Total C N O 14 8 1 5	0	0
5	A	1	Total C N O 14 8 1 5	0	0
5	A	1	Total C N O 14 8 1 5	0	0

- Molecule 6 is CALCIUM ION (three-letter code: CA) (formula: Ca).

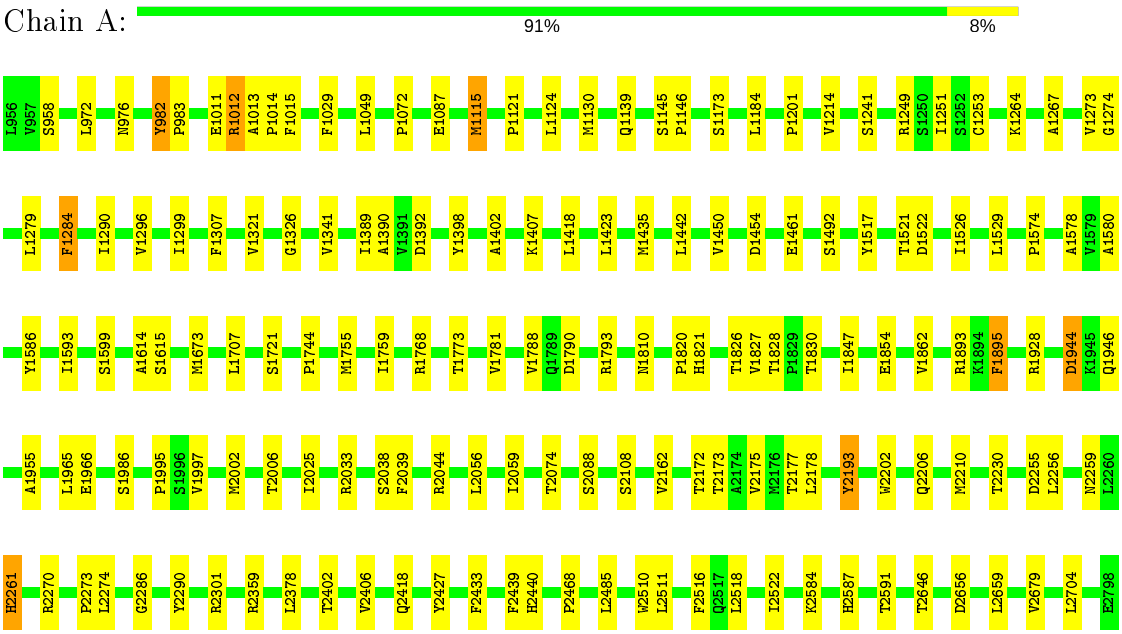
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	D	1	Total Ca 1 1	0	0

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. 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. 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.

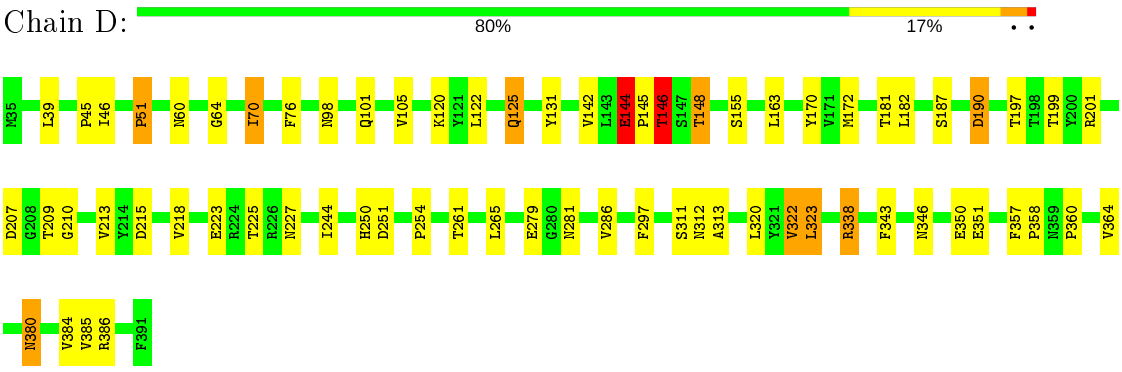
- Molecule 1: Teneurin-2

Chain A:



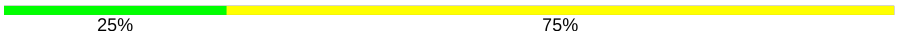
- Molecule 2: Adhesion G protein-coupled receptor L1

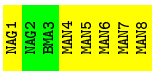
Chain D:



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

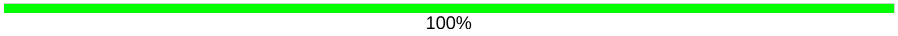
Chain B:





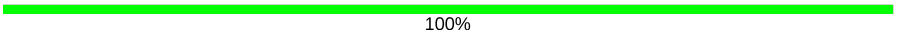
• Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain C:



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

Chain E:



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

Chain F:

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

Chain G:

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

Chain H:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 43 2 2	Depositor
Cell constants a, b, c, α, β, γ	96.26Å 96.26Å 809.22Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	52.09 – 3.86 202.31 – 3.86	Depositor EDS
% Data completeness (in resolution range)	91.0 (52.09-3.86) 91.0 (202.31-3.86)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.71 (at 3.89Å)	Xtriage
Refinement program	BUSTER	Depositor
R, R_{free}	(Not available) , (Not available) 0.277 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å^2)	104.8	Xtriage
Anisotropy	0.063	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 109.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.41$, $< L^2 > = 0.23$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.78	EDS
Total number of atoms	17628	wwPDB-VP
Average B, all atoms (Å^2)	134.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.67% 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: CA, BMA, NAG, MAN

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	0.36	0/14825	0.60	0/20101
2	D	0.37	0/2886	0.57	0/3935
All	All	0.36	0/17711	0.59	0/24036

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	A	14513	0	14252	73	0
2	D	2810	0	2639	28	0
3	B	94	0	79	0	0
4	C	28	0	25	0	0
4	E	28	0	25	0	0
4	F	28	0	25	0	0
4	G	28	0	25	0	0
4	H	28	0	25	0	0
5	A	70	0	65	0	0
6	D	1	0	0	0	0
All	All	17628	0	17160	99	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 3.

All (99) 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:D:364:VAL:HA	2:D:380:ASN:HB2	1.58	0.85
1:A:1821:HIS:HD2	1:A:1830:THR:HG21	1.44	0.81
1:A:982:TYR:HB3	1:A:983:PRO:HD3	1.63	0.78
1:A:982:TYR:HB3	1:A:983:PRO:CD	2.17	0.74
1:A:2468:PRO:HB3	1:A:2485:LEU:HB3	1.76	0.67
1:A:1821:HIS:CD2	1:A:1830:THR:HG21	2.28	0.66
1:A:2172:THR:HG21	2:D:51:PRO:HA	1.79	0.65
1:A:1201:PRO:HB3	1:A:1214:VAL:HB	1.81	0.63
1:A:1130:MET:HB2	1:A:1173:SER:HB2	1.81	0.62
1:A:1521:THR:HB	1:A:1574:PRO:HD2	1.83	0.59
2:D:148:THR:HB	2:D:384:VAL:HG23	1.84	0.59
2:D:251:ASP:HA	2:D:254:PRO:HG3	1.85	0.58
1:A:972:LEU:HD22	1:A:1012:ARG:HE	1.69	0.57
1:A:1895:PHE:HE1	1:A:2511:LEU:HA	1.68	0.57
1:A:1744:PRO:HB2	1:A:2006:THR:HG21	1.86	0.57
2:D:338:ARG:HA	2:D:357:PHE:HB3	1.86	0.56
1:A:1130:MET:HG2	1:A:1139:GLN:HG2	1.88	0.55
1:A:1773:THR:HG23	1:A:1788:VAL:HB	1.88	0.55
1:A:2406:VAL:HG11	1:A:2433:PHE:HE2	1.71	0.55
1:A:2418:GLN:HB2	1:A:2427:TYR:HB3	1.89	0.55
1:A:2173:THR:HG22	1:A:2175:VAL:H	1.72	0.54
2:D:170:TYR:HB3	2:D:182:LEU:HD11	1.90	0.54
2:D:311:SER:HB2	2:D:323:LEU:HB3	1.89	0.54
2:D:163:LEU:HD13	2:D:215:ASP:H	1.73	0.54
1:A:2511:LEU:HD13	1:A:2518:LEU:HD11	1.91	0.53
1:A:1274:GLY:HA2	1:A:1321:VAL:HG11	1.91	0.53
1:A:1390:ALA:HB1	1:A:1450:VAL:HG23	1.89	0.52
1:A:1279:LEU:HD23	1:A:1290:ILE:HD12	1.92	0.52
1:A:1995:PRO:HB2	1:A:2256:LEU:HB3	1.92	0.52
2:D:144:GLU:H	2:D:145:PRO:HD3	1.75	0.51
2:D:187:SER:H	2:D:190:ASP:HB2	1.76	0.51
1:A:2056:LEU:HD21	1:A:2059:ILE:HD11	1.93	0.51
1:A:1955:ALA:HB3	1:A:2210:MET:HE3	1.94	0.50
1:A:1273:VAL:HG23	1:A:1578:ALA:HB1	1.92	0.50
1:A:2290:TYR:CZ	1:A:2301:ARG:HG3	2.47	0.50
1:A:1290:ILE:HG12	1:A:1296:VAL:HG22	1.94	0.50
2:D:45:PRO:HB3	2:D:105:VAL:HG22	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1827:VAL:HG13	1:A:1828:THR:HG23	1.93	0.49
1:A:1013:ALA:HB3	1:A:1014:PRO:HD3	1.95	0.49
1:A:1299:ILE:HD12	1:A:1341:VAL:HG11	1.94	0.49
2:D:207:ASP:HB2	2:D:223:GLU:HA	1.95	0.49
2:D:343:PHE:HD1	2:D:350:GLU:HB3	1.76	0.49
2:D:60:ASN:HB3	2:D:125:GLN:HB2	1.95	0.49
1:A:1820:PRO:HB3	1:A:1826:THR:HA	1.95	0.48
1:A:2261:HIS:HA	1:A:2274:LEU:HB2	1.95	0.48
2:D:142:VAL:HB	2:D:358:PRO:HD3	1.95	0.48
1:A:2039:PHE:HB2	1:A:2044:ARG:HB2	1.93	0.48
1:A:1854:GLU:HB2	1:A:1862:VAL:HB	1.94	0.48
1:A:2584:LYS:HB3	1:A:2587:HIS:HB2	1.95	0.48
1:A:1895:PHE:HZ	1:A:2510:TRP:HB3	1.78	0.47
2:D:313:ALA:HB2	2:D:322:VAL:HG13	1.97	0.47
1:A:2402:THR:HG23	1:A:2439:PHE:HA	1.96	0.47
2:D:244:ILE:HD12	2:D:297:PHE:HZ	1.80	0.47
1:A:1522:ASP:HB2	1:A:1526:ILE:HB	1.96	0.46
1:A:1755:MET:HG3	1:A:1759:ILE:HG12	1.97	0.46
1:A:1580:ALA:HB2	1:A:1586:TYR:CE2	2.51	0.46
1:A:1517:TYR:HB3	1:A:1529:LEU:HD11	1.98	0.46
2:D:213:VAL:HG22	2:D:218:VAL:HG22	1.97	0.46
1:A:982:TYR:CB	1:A:983:PRO:CD	2.91	0.46
1:A:1893:ARG:HB2	2:D:70:ILE:HD12	1.97	0.46
1:A:2178:LEU:HD13	1:A:2193:TYR:CD2	2.51	0.46
2:D:281:ASN:HD22	2:D:286:VAL:HG22	1.81	0.46
2:D:181:THR:HG22	2:D:201:ARG:HA	1.99	0.45
1:A:1788:VAL:HG22	1:A:1793:ARG:HG2	1.97	0.45
1:A:1121:PRO:HG2	1:A:1124:LEU:HB2	1.98	0.45
2:D:146:THR:HB	2:D:386:ARG:HB2	1.98	0.45
1:A:1249:ARG:HB3	1:A:1264:LYS:HB3	2.00	0.44
1:A:2646:THR:HG22	1:A:2704:LEU:HD22	1.98	0.44
1:A:1012:ARG:HD2	1:A:1015:PHE:HD2	1.82	0.44
2:D:209:THR:H	2:D:261:THR:HG22	1.83	0.44
1:A:1267:ALA:HB3	1:A:1284:PHE:HB2	2.00	0.44
1:A:1442:LEU:HG	1:A:1461:GLU:HG3	2.00	0.43
1:A:2659:LEU:HD21	1:A:2679:VAL:HG11	1.99	0.43
1:A:1072:PRO:HB2	1:A:1087:GLU:HG2	2.00	0.43
1:A:1251:ILE:HB	1:A:1307:PHE:HD2	1.83	0.43
1:A:2088:SER:HB3	1:A:2108:SER:HB3	2.00	0.42
2:D:244:ILE:HD12	2:D:297:PHE:CZ	2.54	0.42
1:A:1115:MET:HG2	1:A:1115:MET:H	1.73	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1707:LEU:HB3	1:A:1721:SER:HB2	2.00	0.42
1:A:2025:ILE:HB	1:A:2038:SER:HB2	2.01	0.42
1:A:2518:LEU:HB3	1:A:2522:ILE:HD12	2.01	0.42
1:A:976:ASN:HB3	1:A:1011:GLU:HB2	2.01	0.42
1:A:2406:VAL:HG11	1:A:2433:PHE:CE2	2.54	0.42
2:D:46:ILE:HG21	2:D:122:LEU:HD23	2.02	0.42
2:D:64:GLY:HA2	2:D:120:LYS:HG2	2.01	0.42
1:A:1614:ALA:HB3	1:A:1828:THR:HG21	2.02	0.42
1:A:2511:LEU:O	1:A:2516:PHE:HB2	2.20	0.42
1:A:1145:SER:C	1:A:1146:PRO:N	2.74	0.41
1:A:1944:ASP:HB3	1:A:1946:GLN:H	1.85	0.41
1:A:1398:TYR:CE1	1:A:1407:LYS:HG2	2.56	0.41
2:D:313:ALA:HB1	2:D:320:LEU:HD11	2.03	0.41
1:A:1049:LEU:HD12	1:A:1184:LEU:HD23	2.03	0.41
1:A:2255:ASP:HB3	1:A:2259:ASN:H	1.86	0.41
2:D:144:GLU:N	2:D:145:PRO:CD	2.84	0.41
1:A:2162:VAL:HG11	1:A:2378:LEU:HD11	2.03	0.40
1:A:1768:ARG:HH22	1:A:2033:ARG:HD2	1.85	0.40
1:A:1810:ASN:HA	1:A:2074:THR:HB	2.03	0.40
1:A:2172:THR:HG22	1:A:2177:THR:HG22	2.02	0.40
1:A:2273:PRO:HD2	1:A:2286:GLY:HA2	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	1829/1836 (100%)	1758 (96%)	63 (3%)	8 (0%)	34 70
2	D	343/347 (99%)	310 (90%)	27 (8%)	6 (2%)	9 42
All	All	2172/2183 (100%)	2068 (95%)	90 (4%)	14 (1%)	25 62

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	982	TYR
2	D	360	PRO
1	A	1284	PHE
2	D	210	GLY
1	A	1966	GLU
1	A	1402	ALA
2	D	250	HIS
1	A	1492	SER
1	A	1790	ASP
1	A	1997	VAL
2	D	146	THR
2	D	144	GLU
1	A	1326	GLY
2	D	51	PRO

5.3.2 Protein sidechains

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	1601/1600 (100%)	1567 (98%)	34 (2%)	53 73
2	D	306/306 (100%)	279 (91%)	27 (9%)	10 37
All	All	1907/1906 (100%)	1846 (97%)	61 (3%)	39 63

All (61) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	958	SER
1	A	1012	ARG
1	A	1029	PHE
1	A	1115	MET
1	A	1241	SER
1	A	1253	CYS
1	A	1389	ILE
1	A	1392	ASP
1	A	1418	LEU

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Mol	Chain	Res	Type
1	A	1423	LEU
1	A	1435	MET
1	A	1454	ASP
1	A	1593	ILE
1	A	1599	SER
1	A	1615	SER
1	A	1673	MET
1	A	1781	VAL
1	A	1847	ILE
1	A	1895	PHE
1	A	1928	ARG
1	A	1944	ASP
1	A	1965	LEU
1	A	1986	SER
1	A	2002	MET
1	A	2193	TYR
1	A	2202	TRP
1	A	2206	GLN
1	A	2230	THR
1	A	2261	HIS
1	A	2270	ARG
1	A	2359	ARG
1	A	2440	HIS
1	A	2591	THR
1	A	2656	ASP
2	D	39	LEU
2	D	70	ILE
2	D	76	PHE
2	D	98	ASN
2	D	101	GLN
2	D	125	GLN
2	D	131	TYR
2	D	144	GLU
2	D	146	THR
2	D	148	THR
2	D	155	SER
2	D	172	MET
2	D	190	ASP
2	D	197	THR
2	D	199	THR
2	D	225	THR
2	D	227	ASN

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Mol	Chain	Res	Type
2	D	265	LEU
2	D	279	GLU
2	D	312	ASN
2	D	322	VAL
2	D	323	LEU
2	D	338	ARG
2	D	346	ASN
2	D	351	GLU
2	D	380	ASN
2	D	385	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1285	ASN
2	D	281	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

18 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	B	1	1,3	14,14,15	0.41	0	17,19,21	0.67	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	NAG	B	2	3	14,14,15	0.42	0	17,19,21	0.53	0
3	BMA	B	3	3	11,11,12	0.50	0	15,15,17	0.52	0
3	MAN	B	4	3	11,11,12	0.52	0	15,15,17	1.05	2 (13%)
3	MAN	B	5	3	11,11,12	0.57	0	15,15,17	0.90	1 (6%)
3	MAN	B	6	3	11,11,12	0.56	0	15,15,17	0.92	2 (13%)
3	MAN	B	7	3	11,11,12	0.56	0	15,15,17	0.93	2 (13%)
3	MAN	B	8	3	11,11,12	0.56	0	15,15,17	1.01	2 (13%)
4	NAG	C	1	1,4	14,14,15	0.44	0	17,19,21	0.68	0
4	NAG	C	2	4	14,14,15	0.44	0	17,19,21	0.58	0
4	NAG	E	1	1,4	14,14,15	0.42	0	17,19,21	0.64	0
4	NAG	E	2	4	14,14,15	0.43	0	17,19,21	0.57	0
4	NAG	F	1	1,4	14,14,15	0.42	0	17,19,21	0.66	1 (5%)
4	NAG	F	2	4	14,14,15	0.44	0	17,19,21	0.58	0
4	NAG	G	1	1,4	14,14,15	0.43	0	17,19,21	0.60	0
4	NAG	G	2	4	14,14,15	0.43	0	17,19,21	0.52	0
4	NAG	H	1	1,4	14,14,15	0.43	0	17,19,21	0.69	1 (5%)
4	NAG	H	2	4	14,14,15	0.42	0	17,19,21	0.51	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	B	1	1,3	-	4/6/23/26	0/1/1/1
3	NAG	B	2	3	-	2/6/23/26	0/1/1/1
3	BMA	B	3	3	-	0/2/19/22	0/1/1/1
3	MAN	B	4	3	-	2/2/19/22	0/1/1/1
3	MAN	B	5	3	-	1/2/19/22	0/1/1/1
3	MAN	B	6	3	-	0/2/19/22	0/1/1/1
3	MAN	B	7	3	-	0/2/19/22	0/1/1/1
3	MAN	B	8	3	-	0/2/19/22	0/1/1/1
4	NAG	C	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	C	2	4	-	3/6/23/26	0/1/1/1
4	NAG	E	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	E	2	4	-	2/6/23/26	0/1/1/1
4	NAG	F	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	F	2	4	-	2/6/23/26	0/1/1/1
4	NAG	G	1	1,4	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	G	2	4	-	2/6/23/26	0/1/1/1
4	NAG	H	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	H	2	4	-	4/6/23/26	0/1/1/1

There are no bond length outliers.

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	5	MAN	C1-O5-C5	2.70	115.85	112.19
3	B	4	MAN	C1-C2-C3	2.68	112.96	109.67
3	B	8	MAN	C1-O5-C5	2.57	115.68	112.19
3	B	7	MAN	C1-O5-C5	2.36	115.39	112.19
3	B	8	MAN	C1-C2-C3	2.35	112.56	109.67
3	B	6	MAN	C1-C2-C3	2.34	112.54	109.67
3	B	6	MAN	C1-O5-C5	2.21	115.19	112.19
3	B	4	MAN	C1-O5-C5	2.16	115.11	112.19
3	B	7	MAN	C1-C2-C3	2.16	112.31	109.67
3	B	1	NAG	C1-O5-C5	2.10	115.04	112.19
4	F	1	NAG	C1-O5-C5	2.09	115.02	112.19
4	H	1	NAG	C1-O5-C5	2.03	114.95	112.19

There are no chirality outliers.

All (32) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	G	1	NAG	C8-C7-N2-C2
4	G	1	NAG	O7-C7-N2-C2
4	F	1	NAG	O7-C7-N2-C2
4	H	1	NAG	C8-C7-N2-C2
4	H	1	NAG	O7-C7-N2-C2
4	G	2	NAG	C8-C7-N2-C2
4	G	2	NAG	O7-C7-N2-C2
4	C	2	NAG	C8-C7-N2-C2
4	C	2	NAG	O7-C7-N2-C2
4	E	1	NAG	C8-C7-N2-C2
4	E	1	NAG	O7-C7-N2-C2
4	E	2	NAG	C8-C7-N2-C2
4	E	2	NAG	O7-C7-N2-C2
4	F	2	NAG	C8-C7-N2-C2
4	F	2	NAG	O7-C7-N2-C2

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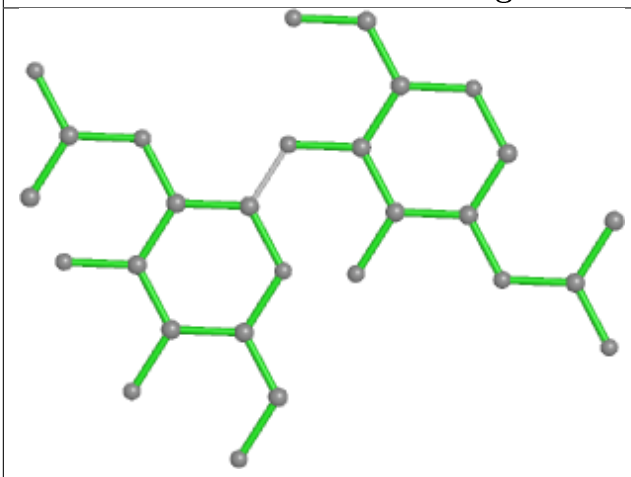
Mol	Chain	Res	Type	Atoms
4	H	2	NAG	C8-C7-N2-C2
4	H	2	NAG	O7-C7-N2-C2
3	B	2	NAG	C8-C7-N2-C2
3	B	2	NAG	O7-C7-N2-C2
3	B	1	NAG	C8-C7-N2-C2
3	B	1	NAG	O7-C7-N2-C2
4	F	1	NAG	C8-C7-N2-C2
3	B	1	NAG	O5-C5-C6-O6
3	B	1	NAG	C4-C5-C6-O6
4	C	2	NAG	O5-C5-C6-O6
3	B	4	MAN	C4-C5-C6-O6
4	C	1	NAG	C4-C5-C6-O6
4	H	2	NAG	C4-C5-C6-O6
3	B	4	MAN	O5-C5-C6-O6
3	B	5	MAN	C4-C5-C6-O6
4	C	1	NAG	O5-C5-C6-O6
4	H	2	NAG	O5-C5-C6-O6

There are no ring outliers.

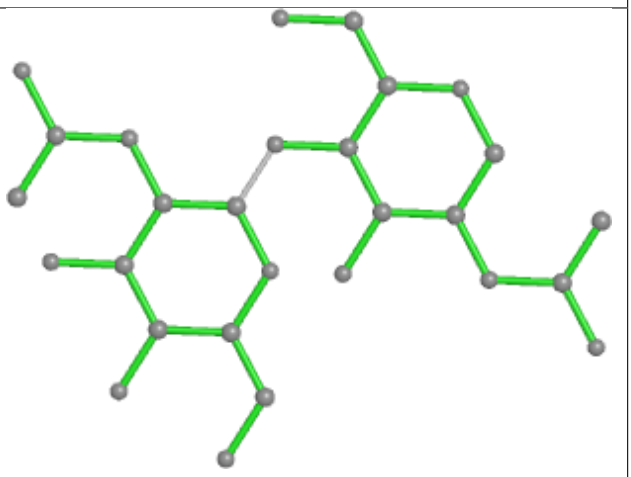
No monomer is involved in short contacts.

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

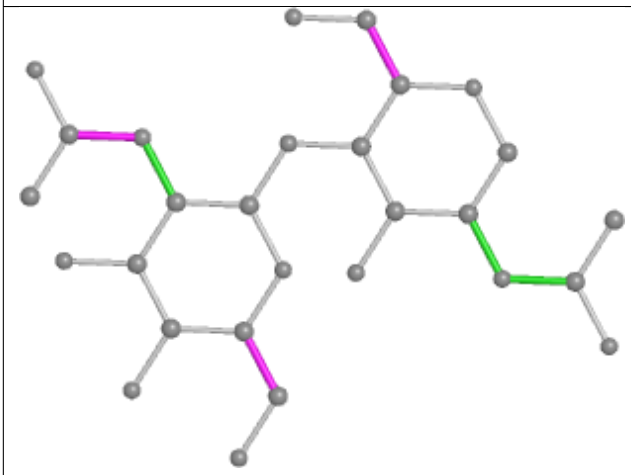
Oligosaccharide Chain C



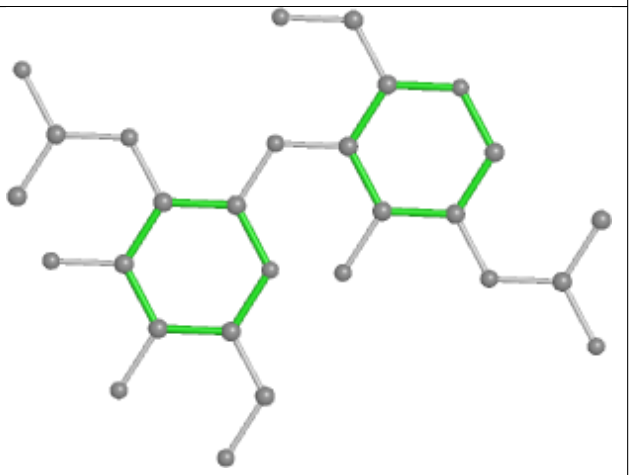
Bond lengths



Bond angles

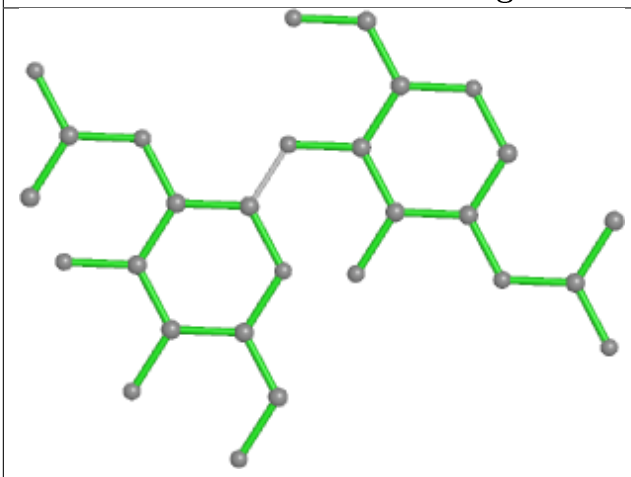


Torsions

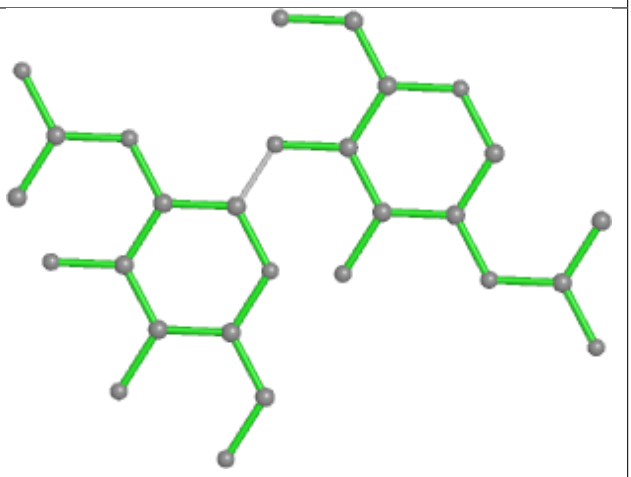


Rings

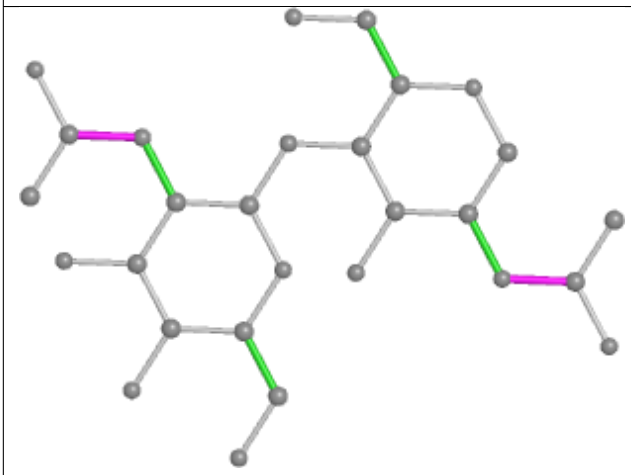
Oligosaccharide Chain E



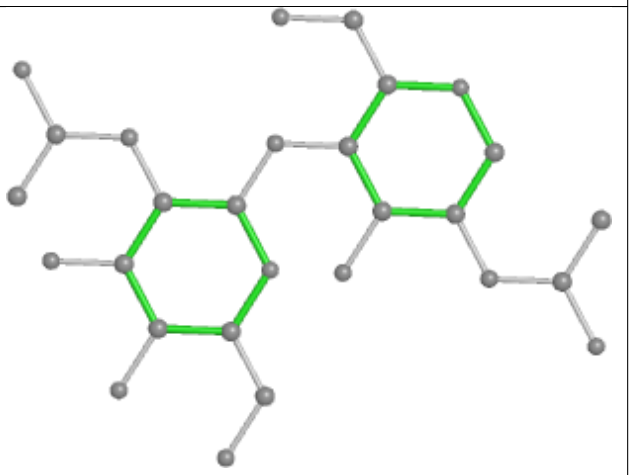
Bond lengths



Bond angles

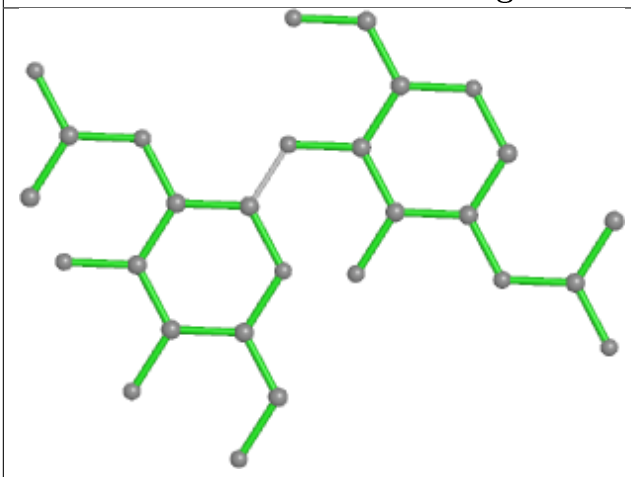


Torsions

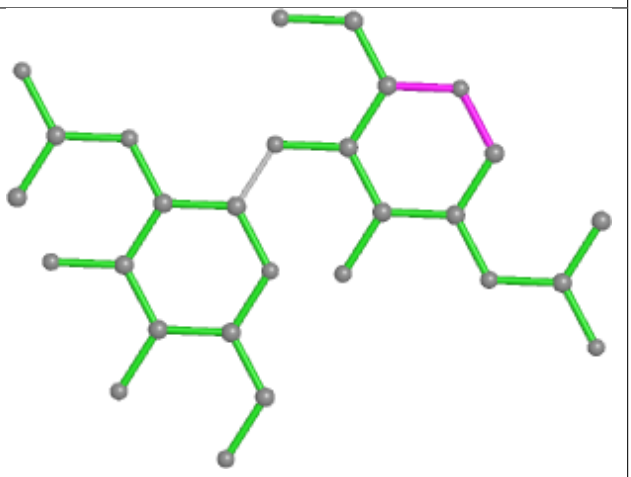


Rings

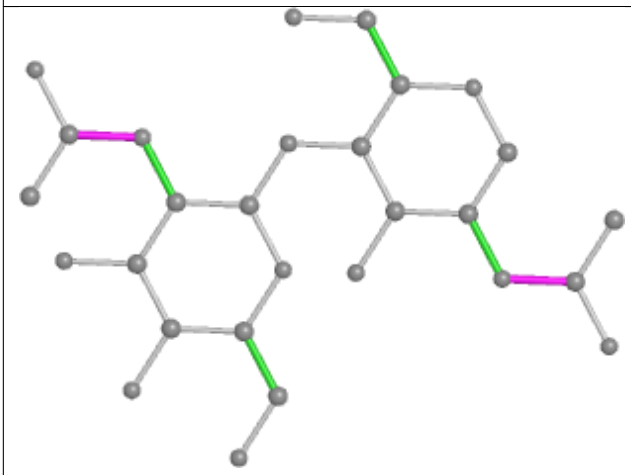
Oligosaccharide Chain F



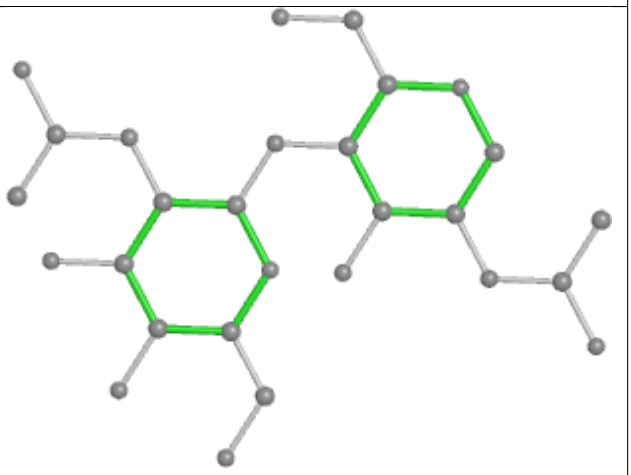
Bond lengths



Bond angles

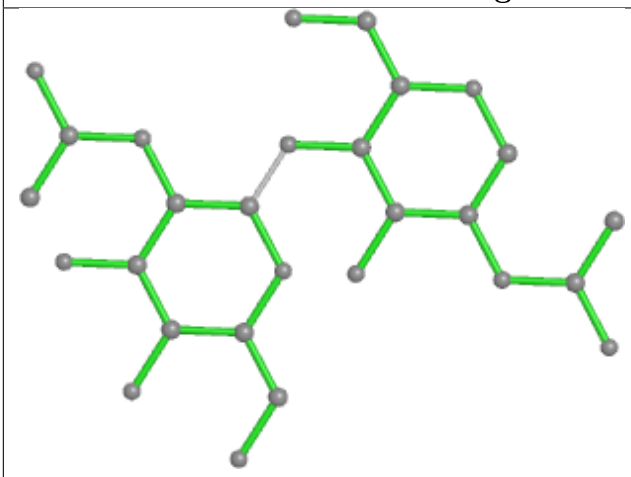


Torsions

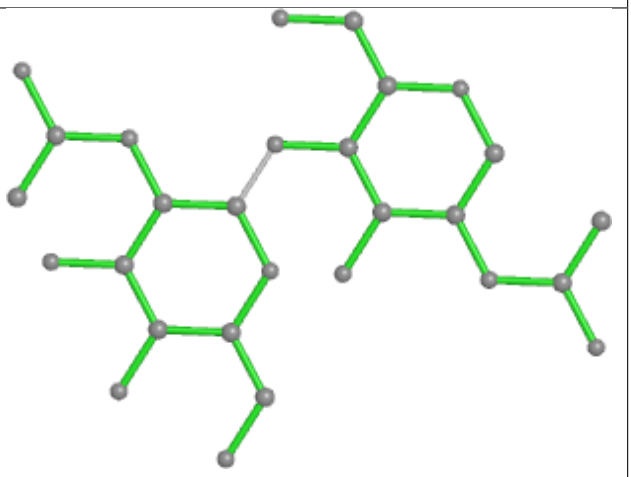


Rings

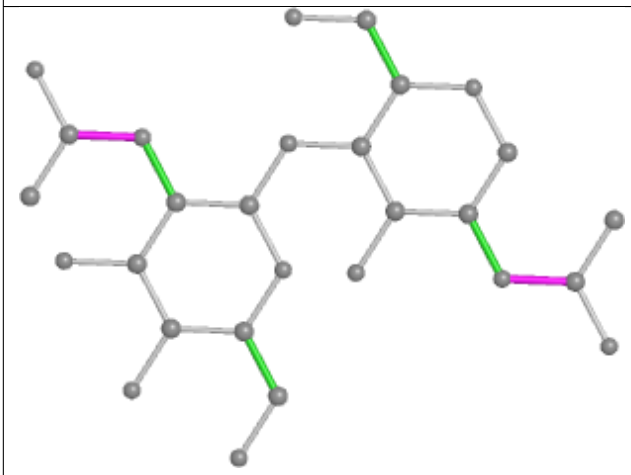
Oligosaccharide Chain G



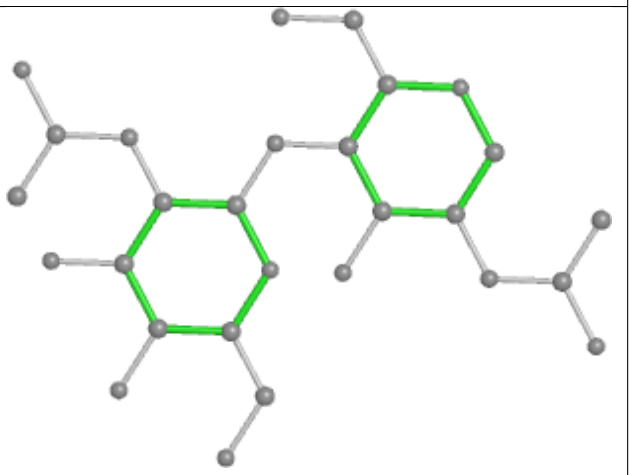
Bond lengths



Bond angles

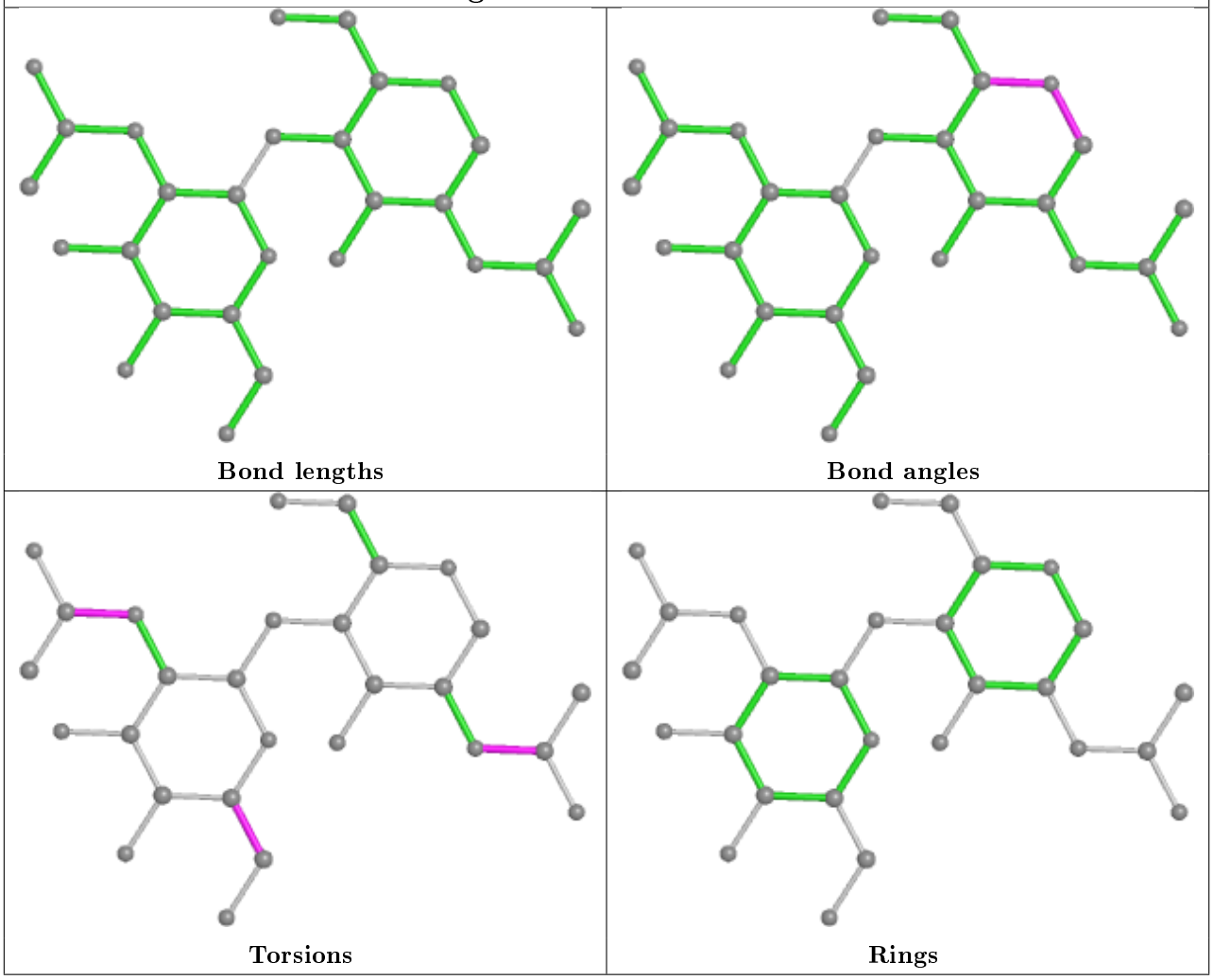


Torsions



Rings

Oligosaccharide Chain H



5.6 Ligand geometry

Of 6 ligands modelled in this entry, 1 is monoatomic - leaving 5 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	A	3014	1	14,14,15	0.43	0	17,19,21	1.10	2 (11%)
5	NAG	A	3022	1	14,14,15	0.43	0	17,19,21	0.67	0
5	NAG	A	3019	1	14,14,15	0.44	0	17,19,21	0.62	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
5	NAG	A	3000	1	14,14,15	0.43	0	17,19,21	0.50	0
5	NAG	A	3011	1	14,14,15	0.43	0	17,19,21	0.62	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
5	NAG	A	3014	1	-	4/6/23/26	0/1/1/1
5	NAG	A	3022	1	-	4/6/23/26	0/1/1/1
5	NAG	A	3019	1	-	2/6/23/26	0/1/1/1
5	NAG	A	3000	1	-	2/6/23/26	0/1/1/1
5	NAG	A	3011	1	-	4/6/23/26	0/1/1/1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	A	3014	NAG	C2-N2-C7	3.06	127.27	122.90
5	A	3014	NAG	C1-C2-N2	2.98	115.59	110.49

There are no chirality outliers.

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	3019	NAG	C8-C7-N2-C2
5	A	3019	NAG	O7-C7-N2-C2
5	A	3014	NAG	C8-C7-N2-C2
5	A	3014	NAG	O7-C7-N2-C2
5	A	3000	NAG	C8-C7-N2-C2
5	A	3000	NAG	O7-C7-N2-C2
5	A	3011	NAG	C8-C7-N2-C2
5	A	3011	NAG	O7-C7-N2-C2
5	A	3022	NAG	C8-C7-N2-C2
5	A	3011	NAG	O5-C5-C6-O6
5	A	3022	NAG	O7-C7-N2-C2
5	A	3014	NAG	C1-C2-N2-C7
5	A	3022	NAG	O5-C5-C6-O6
5	A	3014	NAG	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
5	A	3011	NAG	C4-C5-C6-O6
5	A	3022	NAG	C4-C5-C6-O6

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	3
2	D	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	1037:MET	C	1045:PRO	N	15.82
1	D	325:SER	C	336:GLY	N	7.27
1	A	1891:ASP	C	1892:HIS	N	3.08
1	A	1145:SER	C	1146:PRO	N	2.74

6 Fit of model and data

6.1 Protein, DNA and RNA chains

Unable to reproduce the depositors R factor - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains

Unable to reproduce the depositors R factor - this section is therefore empty.

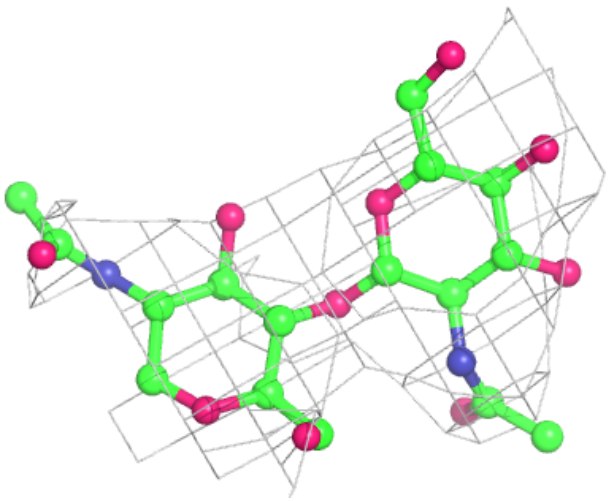
6.3 Carbohydrates

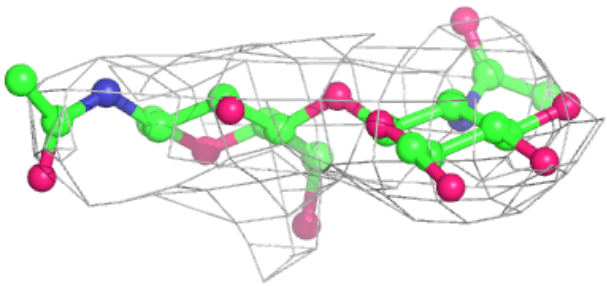
Unable to reproduce the depositors R factor - this section is therefore empty.

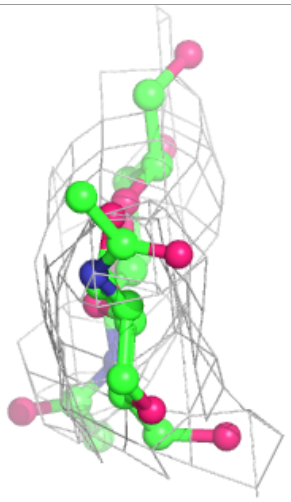
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around Chain C:

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

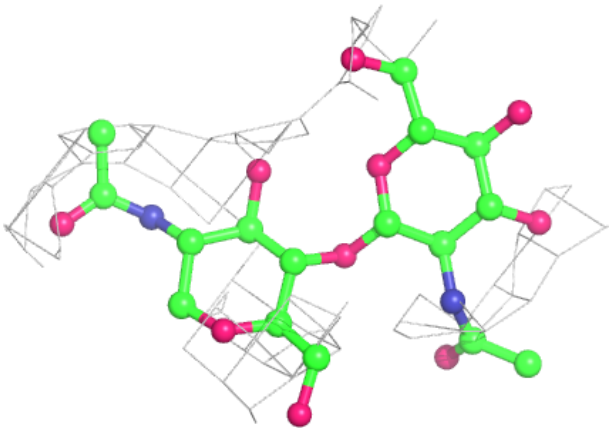


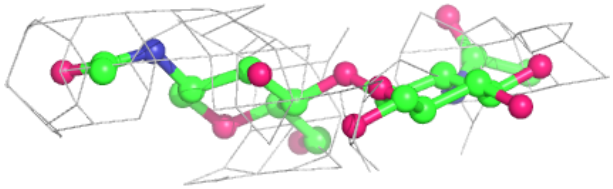


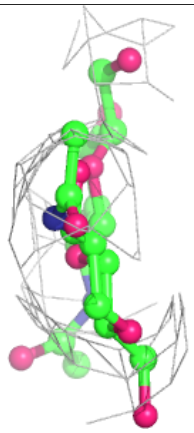


Electron density around Chain E:

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

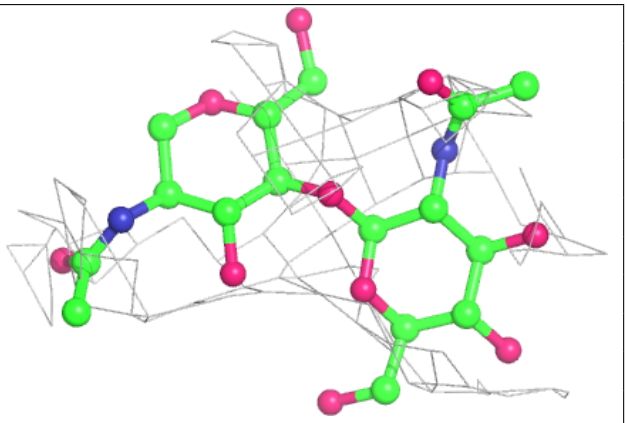


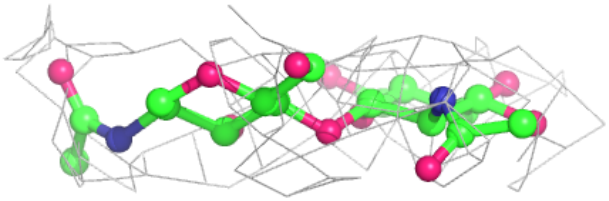


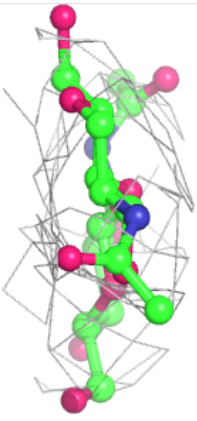


Electron density around Chain F:

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

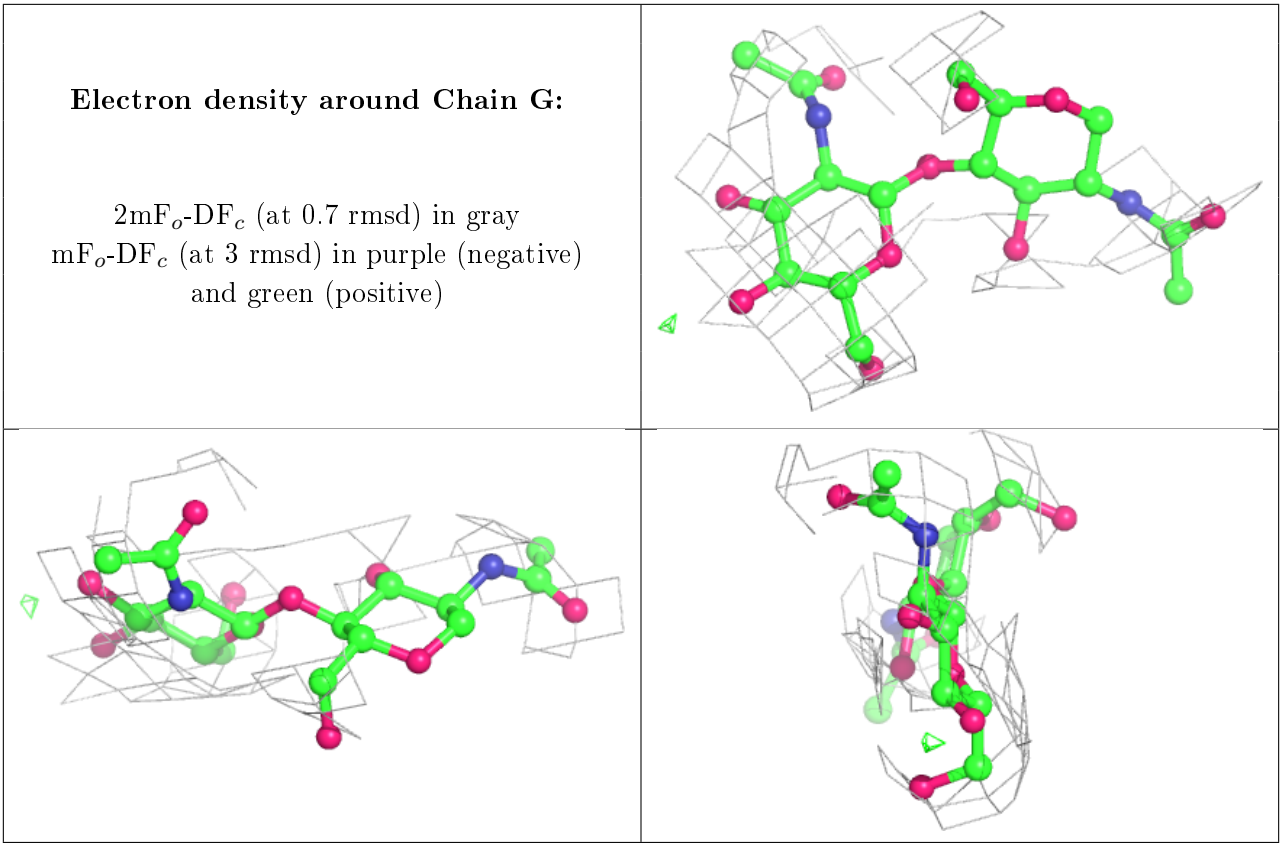






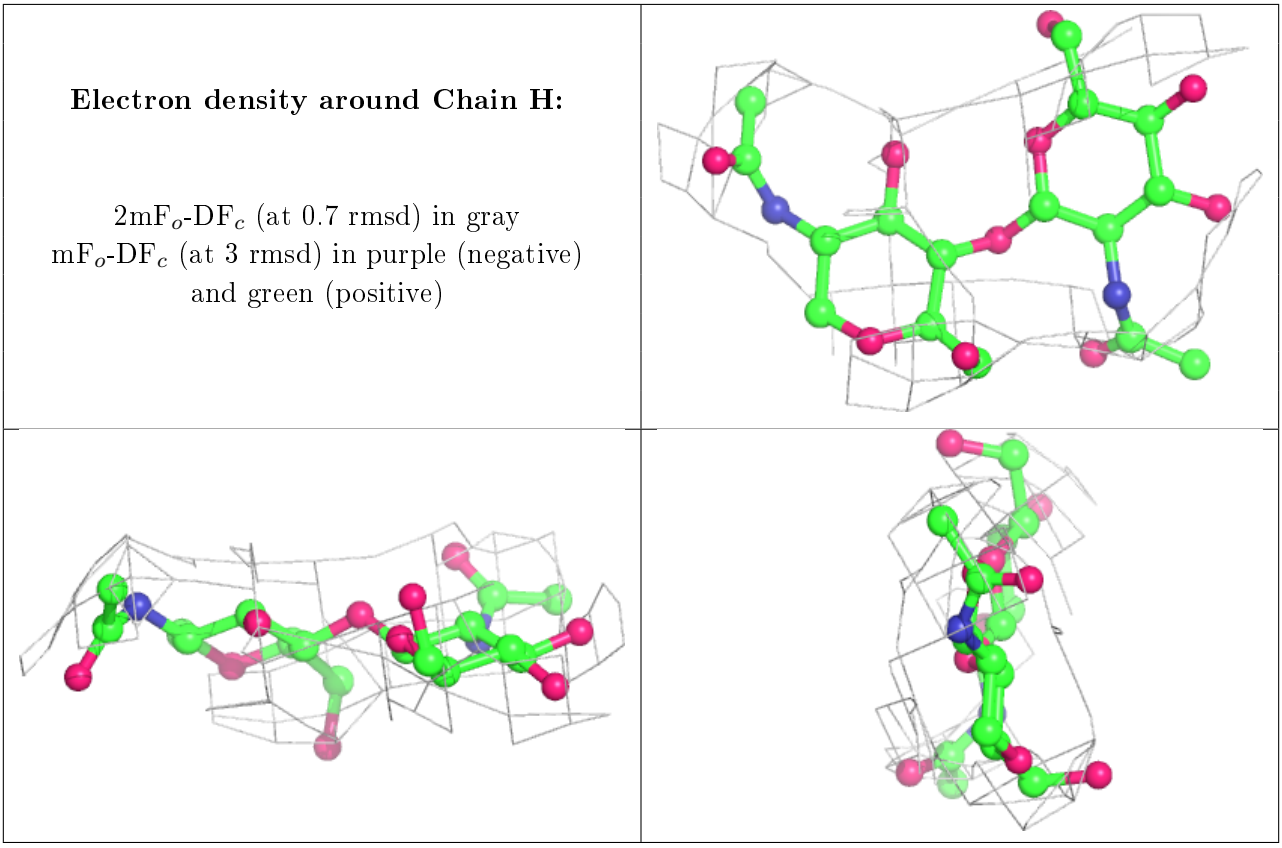
Electron density around Chain G:

$2mF_o$-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)



6.4 Ligands

Unable to reproduce the depositors R factor - this section is therefore empty.

6.5 Other polymers

Unable to reproduce the depositors R factor - this section is therefore empty.