Full wwPDB X-ray Structure Validation Report ⓘ

Nov 25, 2024 – 03:02 PM EST

PDB ID	:	1GQG
Title	:	Quercetin 2,3-dioxygenase in complex with the inhibitor diethyldithiocarbamate
Authors	:	Steiner, R.A.; Dijkstra, B.W.
Deposited on	:	2001-11-23
Resolution	:	1.70 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 ⓘ symbol.

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

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

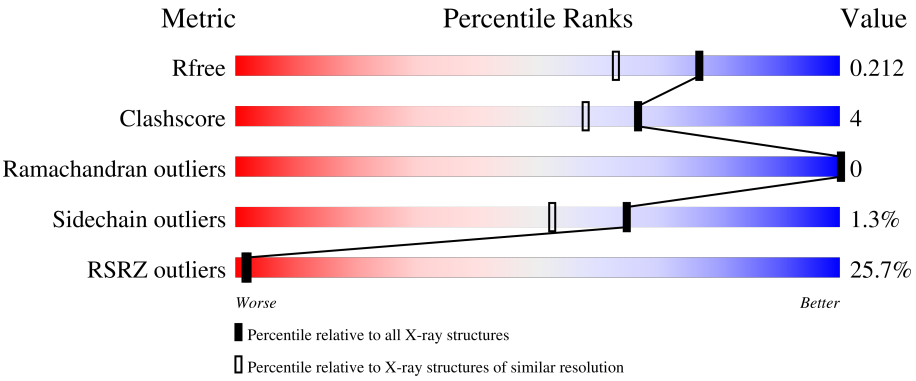
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.21
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.004 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.40

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 1.70 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	5161 (1.70-1.70)
Clashscore	180529	5671 (1.70-1.70)
Ramachandran outliers	177936	5594 (1.70-1.70)
Sidechain outliers	177891	5594 (1.70-1.70)
RSRZ outliers	164620	5159 (1.70-1.70)

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%

Mol	Chain	Length	Quality of chain
1	A	350	85% 10% 5%
1	B	350	91% • • 5%
1	C	350	91% 5% • •
1	D	350	94% 89% 6% 5%
2	E	3	33% 33% 33%
2	F	3	67% 33%

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Mol	Chain	Length	Quality of chain
3	G	2	

2 Entry composition (i)

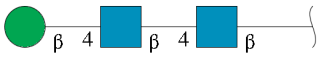
There are 7 unique types of molecules in this entry. The entry contains 12136 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 QUERCETIN 2,3-DIOXYGENASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	333	Total	C	N	O	S	0	8	0
			2595	1654	420	515	6			
1	B	334	Total	C	N	O	S	0	4	0
			2590	1648	421	516	5			
1	C	337	Total	C	N	O	S	0	3	0
			2605	1655	424	521	5			
1	D	333	Total	C	N	O	S	0	3	0
			2578	1642	419	512	5			

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

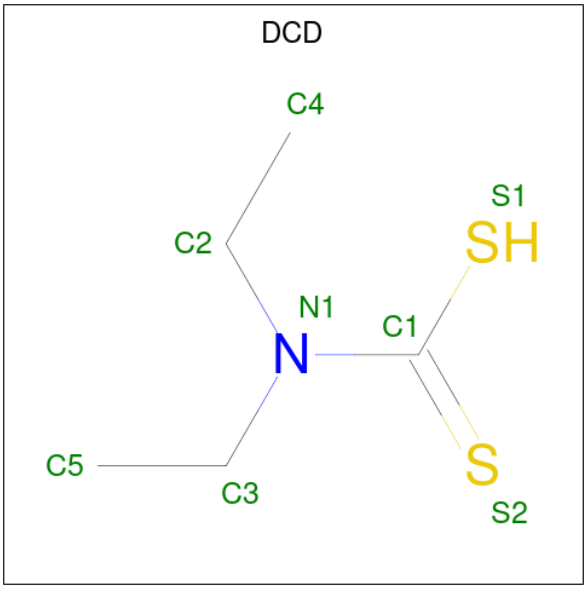


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	E	3	Total	C	N	O	0	0	0
			39	22	2	15			
2	F	3	Total	C	N	O	0	0	0
			39	22	2	15			

- 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	G	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 4 is DIETHYLCARBAMODITHIOIC ACID (three-letter code: DCD) (formula: $C_5H_{11}NS_2$).

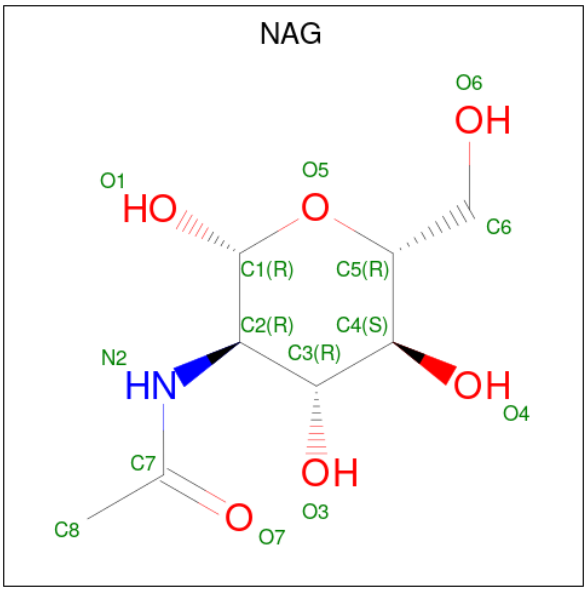


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C N S 8 5 1 2	0	0
4	B	1	Total C N S 8 5 1 2	0	0
4	C	1	Total C N S 8 5 1 2	0	0
4	D	1	Total C N S 8 5 1 2	0	0

- Molecule 5 is COPPER (II) ION (three-letter code: CU) (formula: Cu).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total Cu 1 1	0	0
5	B	1	Total Cu 1 1	0	0
5	C	1	Total Cu 1 1	0	0
5	D	1	Total Cu 1 1	0	0

- Molecule 6 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



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

- Molecule 7 is water.

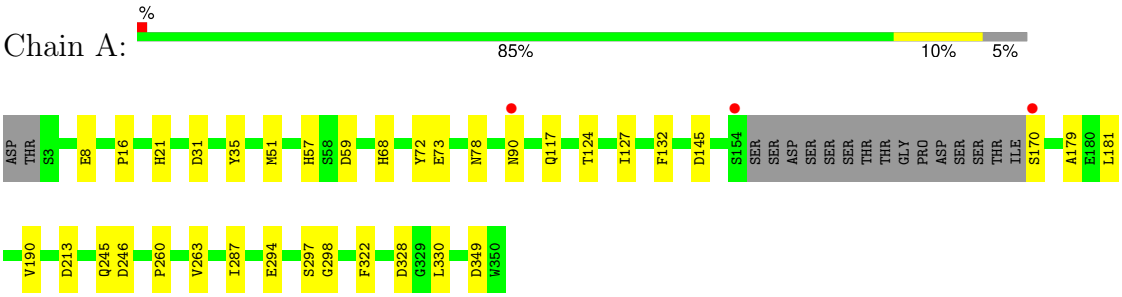
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	411	Total O 411 411	0	0
7	B	346	Total O 346 346	0	0
7	C	345	Total O 345 345	0	0
7	D	342	Total O 342 342	0	0

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.

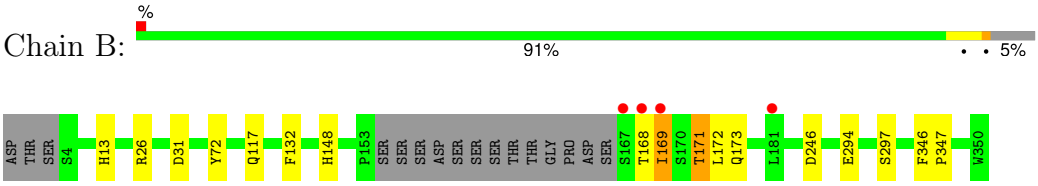
• Molecule 1: QUERCETIN 2,3-DIOXYGENASE

Chain A:



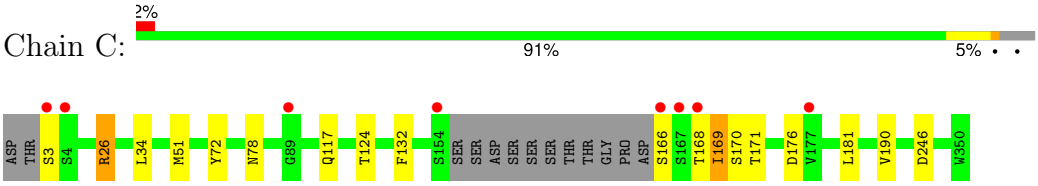
• Molecule 1: QUERCETIN 2,3-DIOXYGENASE

Chain B:



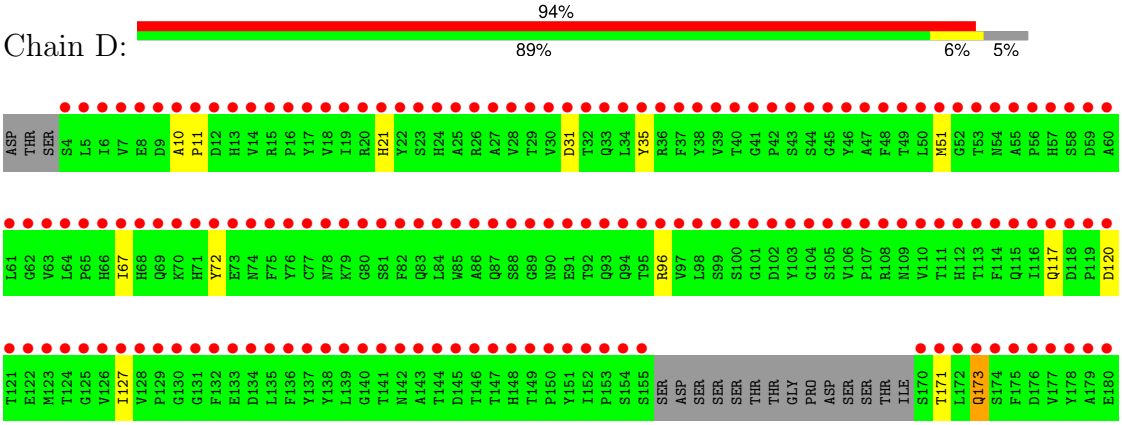
• Molecule 1: QUERCETIN 2,3-DIOXYGENASE

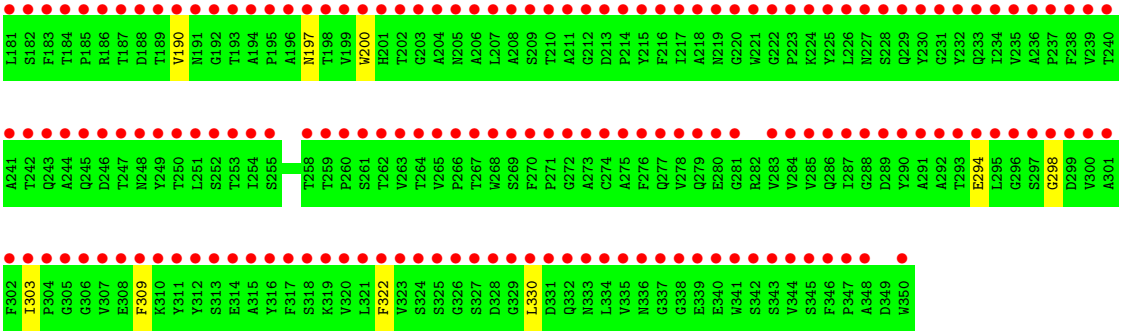
Chain C:



• Molecule 1: QUERCETIN 2,3-DIOXYGENASE

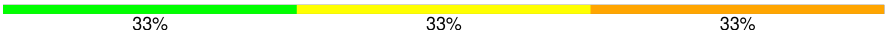
Chain D:





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

Chain E:



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

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	108.94Å 55.65Å 123.86Å 90.00° 98.26° 90.00°	Depositor
Resolution (Å)	19.92 – 1.70 19.92 – 1.70	Depositor EDS
% Data completeness (in resolution range)	91.3 (19.92-1.70) 91.2 (19.92-1.70)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	4.64 (at 1.70Å)	Xtriage
Refinement program	REFMAC 5.0	Depositor
R, R_{free}	0.161 , 0.183 0.198 , 0.212	Depositor DCC
R_{free} test set	7426 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å^2)	21.9	Xtriage
Anisotropy	0.617	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 42.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	12136	wwPDB-VP
Average B, all atoms (Å^2)	18.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.12% 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: DCD, NAG, CU, BMA

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	0.49	0/2710	0.78	6/3713 (0.2%)
1	B	0.43	0/2687	0.77	2/3684 (0.1%)
1	C	0.41	0/2698	0.73	2/3698 (0.1%)
1	D	0.43	0/2670	0.75	2/3660 (0.1%)
All	All	0.44	0/10765	0.76	12/14755 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2

There are no bond length outliers.

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	176	ASP	CB-CG-OD2	6.08	123.77	118.30
1	A	31	ASP	CB-CG-OD2	5.86	123.58	118.30
1	D	31	ASP	CB-CG-OD2	5.79	123.51	118.30
1	B	31	ASP	CB-CG-OD2	5.73	123.46	118.30
1	D	120	ASP	CB-CG-OD2	5.62	123.36	118.30
1	B	246	ASP	CB-CG-OD2	5.42	123.18	118.30
1	A	145	ASP	CB-CG-OD2	5.37	123.13	118.30
1	A	328	ASP	CB-CG-OD2	5.34	123.11	118.30
1	A	246	ASP	CB-CG-OD2	5.33	123.10	118.30
1	A	213	ASP	CB-CG-OD2	5.15	122.94	118.30
1	A	349	ASP	CB-CG-OD2	5.10	122.89	118.30
1	C	246	ASP	CB-CG-OD2	5.07	122.87	118.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	8[A]	GLU	Sidechain
1	A	8[B]	GLU	Sidechain

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2595	0	2405	28	0
1	B	2590	0	2399	13	0
1	C	2605	0	2411	20	0
1	D	2578	0	2385	15	0
2	E	39	0	34	1	0
2	F	39	0	34	1	0
3	G	28	0	25	1	0
4	A	8	0	10	1	0
4	B	8	0	11	0	0
4	C	8	0	10	3	0
4	D	8	0	11	0	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
5	C	1	0	0	0	0
5	D	1	0	0	0	0
6	A	42	0	39	0	0
6	B	56	0	52	0	0
6	C	42	0	39	0	0
6	D	42	0	39	0	0
7	A	411	0	0	8	0
7	B	346	0	0	4	0
7	C	345	0	0	5	0
7	D	342	0	0	4	0
All	All	12136	0	9904	75	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 (75) close contacts within the same asymmetric unit are listed below, sorted by their clash

magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:78[A]:ASN:OD1	7:C:2112:HOH:O	1.74	1.04
1:D:171:THR:HA	1:D:173:GLN:OE1	1.68	0.93
1:A:73:GLU:HG3	1:A:127[A]:ILE:HD12	1.55	0.86
1:A:181[B]:LEU:HD23	7:A:2103:HOH:O	1.79	0.82
1:A:78[B]:ASN:ND2	1:A:124:THR:OG1	2.12	0.82
1:B:297:SER:HB3	7:B:2270:HOH:O	1.86	0.76
1:A:78[A]:ASN:OD1	7:A:2125:HOH:O	2.05	0.73
1:A:260[B]:PRO:HG2	1:A:263:VAL:CG2	2.19	0.71
1:A:245:GLN:HG3	7:A:2285:HOH:O	1.91	0.71
1:A:57:HIS:HE1	1:A:59:ASP:OD1	1.75	0.68
1:C:190:VAL:HG11	2:F:1:NAG:H82	1.79	0.65
1:C:117:GLN:HB2	7:C:2155:HOH:O	1.97	0.65
1:D:173:GLN:H	1:D:173:GLN:CD	2.03	0.62
1:A:170:SER:HB3	1:A:179:ALA:HB2	1.84	0.60
1:A:78[B]:ASN:HD21	1:A:124:THR:CB	2.15	0.60
1:C:169:ILE:CG2	1:C:170:SER:N	2.64	0.59
1:B:148:HIS:HE1	7:B:2004:HOH:O	1.86	0.59
1:C:181:LEU:HD12	1:C:181:LEU:H	1.69	0.58
1:B:169:ILE:O	1:B:173:GLN:HG3	2.04	0.57
1:B:117:GLN:HG3	7:D:2212:HOH:O	2.03	0.56
1:C:181:LEU:HD12	1:C:181:LEU:N	2.22	0.54
1:A:73:GLU:CG	1:A:127[A]:ILE:HD12	2.35	0.54
1:D:190:VAL:HG11	3:G:1:NAG:H82	1.89	0.54
1:A:179:ALA:HB1	1:A:181[A]:LEU:CD1	2.37	0.54
1:C:51:MET:CE	4:C:1351:DCD:H3C2	2.39	0.53
1:A:68:HIS:CE1	1:A:132:PHE:HZ	2.27	0.53
1:A:127[A]:ILE:HD11	4:A:1351:DCD:H5C1	1.92	0.52
1:A:190:VAL:HG11	2:E:1:NAG:H82	1.92	0.51
1:C:132:PHE:HB3	7:C:2081:HOH:O	2.10	0.51
1:A:35:TYR:HD2	1:A:51[B]:MET:CE	2.25	0.50
1:A:179:ALA:HB1	1:A:181[A]:LEU:HD12	1.94	0.50
1:A:260[B]:PRO:HG2	1:A:263:VAL:HG23	1.93	0.50
1:C:78[B]:ASN:ND2	1:C:124:THR:OG1	2.37	0.50
1:B:132:PHE:HB3	7:B:2066:HOH:O	2.11	0.49
1:C:166:SER:O	1:C:169:ILE:HG22	2.13	0.49
1:A:16:PRO:HB3	1:A:287:ILE:HG21	1.96	0.48
1:C:132:PHE:CB	7:C:2081:HOH:O	2.62	0.47
1:A:294:GLU:HG2	7:A:2339:HOH:O	2.14	0.47
1:D:67:ILE:HD11	7:D:2145:HOH:O	2.14	0.46
1:B:13:HIS:HB2	1:C:171:THR:HG23	1.97	0.46
1:B:168:THR:O	1:B:171:THR:N	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:294:GLU:HG2	7:B:2284:HOH:O	2.17	0.45
1:A:322:PHE:CZ	1:A:330:LEU:HB3	2.52	0.45
1:D:294:GLU:HG2	7:D:2288:HOH:O	2.17	0.45
1:C:169:ILE:HD12	1:C:169:ILE:HA	1.70	0.45
1:A:132:PHE:CB	7:A:2179:HOH:O	2.65	0.44
1:B:171:THR:HG22	7:C:2026:HOH:O	2.16	0.44
1:A:57:HIS:CE1	1:A:59:ASP:OD1	2.63	0.44
1:B:168:THR:O	1:B:169:ILE:C	2.55	0.44
1:D:171:THR:CA	1:D:173:GLN:OE1	2.54	0.43
1:C:169:ILE:HG22	1:C:170:SER:H	1.84	0.43
1:A:132:PHE:HB2	7:A:2179:HOH:O	2.18	0.43
1:A:170:SER:CB	1:A:179:ALA:HB2	2.49	0.42
1:D:21:HIS:CG	1:D:298:GLY:HA3	2.53	0.42
1:B:346:PHE:HB2	1:B:347:PRO:HD2	2.00	0.42
1:C:169:ILE:HG22	1:C:170:SER:N	2.33	0.42
1:D:35:TYR:HD2	1:D:51:MET:CE	2.32	0.42
1:C:51:MET:HE1	4:C:1351:DCD:H3C2	2.01	0.42
1:D:322:PHE:CZ	1:D:330:LEU:HB3	2.55	0.41
1:A:181[A]:LEU:CD1	7:A:2221:HOH:O	2.67	0.41
1:D:10:ALA:HA	1:D:11:PRO:HD3	1.90	0.41
1:C:169:ILE:HG23	1:C:170:SER:N	2.36	0.41
1:D:96:ARG:HD2	1:D:200:TRP:CD2	2.56	0.41
1:B:346:PHE:HB2	1:B:347:PRO:CD	2.50	0.41
1:C:34:LEU:C	1:C:34:LEU:HD23	2.40	0.41
1:A:57:HIS:HD2	1:A:117:GLN:O	2.02	0.41
1:D:197:ASN:CG	1:D:197:ASN:O	2.59	0.41
1:A:21:HIS:CG	1:A:298:GLY:HA3	2.56	0.41
1:A:117:GLN:HB2	7:A:2166:HOH:O	2.20	0.41
1:C:51:MET:HE2	4:C:1351:DCD:H3C2	2.02	0.41
1:B:172:LEU:HD23	1:B:172:LEU:HA	1.94	0.40
1:D:117:GLN:NE2	7:D:2149:HOH:O	2.54	0.40
1:C:26:ARG:HH11	1:C:26:ARG:HG2	1.86	0.40
1:D:303:ILE:HG21	1:D:309:PHE:CD1	2.56	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	337/350 (96%)	329 (98%)	8 (2%)	0	100	100
1	B	334/350 (95%)	325 (97%)	9 (3%)	0	100	100
1	C	336/350 (96%)	324 (96%)	12 (4%)	0	100	100
1	D	332/350 (95%)	323 (97%)	9 (3%)	0	100	100
All	All	1339/1400 (96%)	1301 (97%)	38 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	284/294 (97%)	280 (99%)	4 (1%)	62	49
1	B	282/294 (96%)	278 (99%)	4 (1%)	62	49
1	C	284/294 (97%)	279 (98%)	5 (2%)	54	39
1	D	279/294 (95%)	277 (99%)	2 (1%)	81	75
All	All	1129/1176 (96%)	1114 (99%)	15 (1%)	65	52

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	72	TYR
1	A	90	ASN

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Mol	Chain	Res	Type
1	A	297[A]	SER
1	A	297[B]	SER
1	B	26	ARG
1	B	72	TYR
1	B	169	ILE
1	B	171	THR
1	C	3	SER
1	C	26	ARG
1	C	72	TYR
1	C	168	THR
1	C	169	ILE
1	D	72	TYR
1	D	173	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	57	HIS
1	A	332	GLN
1	A	336	ASN
1	B	83	GLN
1	B	117	GLN
1	B	148	HIS
1	B	173	GLN
1	B	332	GLN
1	B	336	ASN
1	C	83	GLN
1	C	332	GLN
1	C	336	ASN
1	D	332	GLN
1	D	336	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)

8 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	NAG	E	1	1,2	14,14,15	0.45	0	17,19,21	1.16	2 (11%)
2	NAG	E	2	2	14,14,15	0.48	0	17,19,21	1.02	1 (5%)
2	BMA	E	3	2	11,11,12	0.59	0	15,15,17	0.53	0
2	NAG	F	1	1,2	14,14,15	0.50	0	17,19,21	0.99	0
2	NAG	F	2	2	14,14,15	0.50	0	17,19,21	1.07	0
2	BMA	F	3	2	11,11,12	0.63	0	15,15,17	0.52	0
3	NAG	G	1	1,3	14,14,15	0.54	0	17,19,21	1.37	2 (11%)
3	NAG	G	2	3	14,14,15	0.58	0	17,19,21	0.85	0

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

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

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	G	1	NAG	C2-N2-C7	-3.35	118.41	122.90
3	G	1	NAG	O5-C1-C2	-3.12	106.46	111.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	E	1	NAG	O5-C1-C2	-3.06	106.56	111.29
2	E	2	NAG	O4-C4-C3	-2.03	105.60	110.38
2	E	1	NAG	C2-N2-C7	-2.00	120.22	122.90

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	E	2	NAG	C4-C5-C6-O6
3	G	1	NAG	C4-C5-C6-O6
2	E	2	NAG	O5-C5-C6-O6
3	G	1	NAG	O5-C5-C6-O6

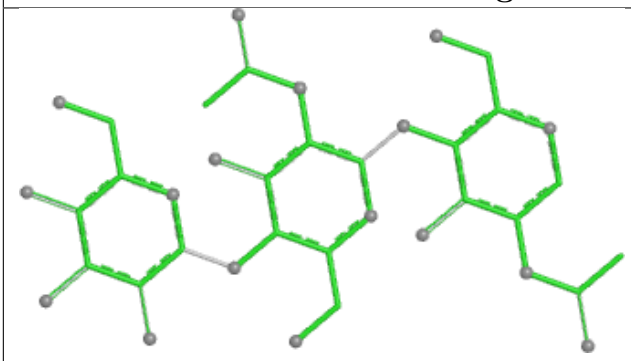
There are no ring outliers.

3 monomers are involved in 3 short contacts:

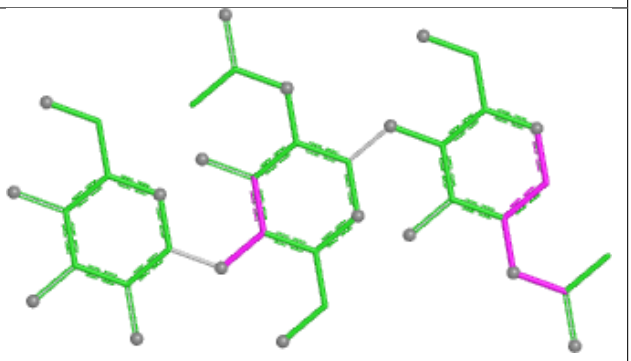
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	F	1	NAG	1	0
2	E	1	NAG	1	0
3	G	1	NAG	1	0

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

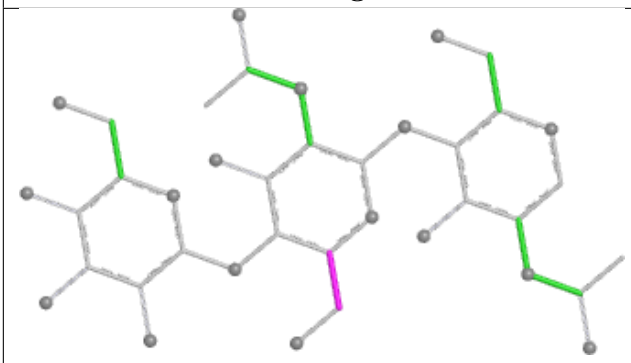
Oligosaccharide Chain E



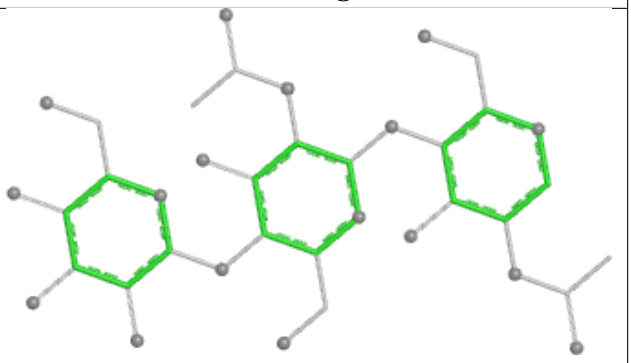
Bond lengths



Bond angles

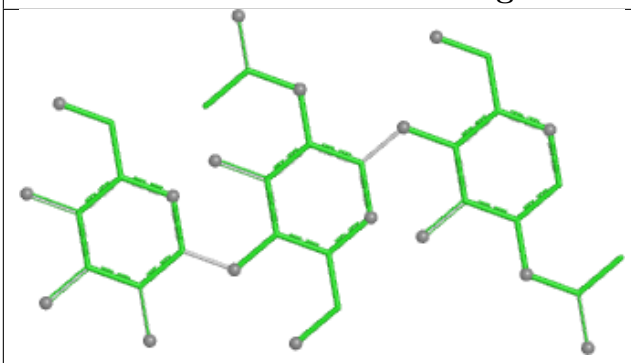


Torsions

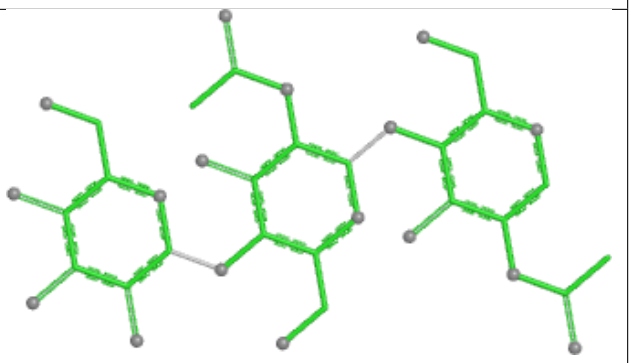


Rings

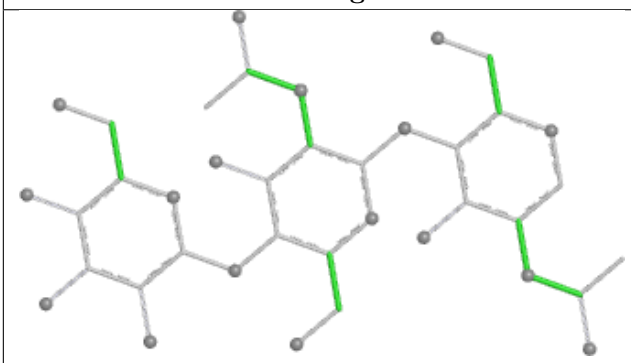
Oligosaccharide Chain F



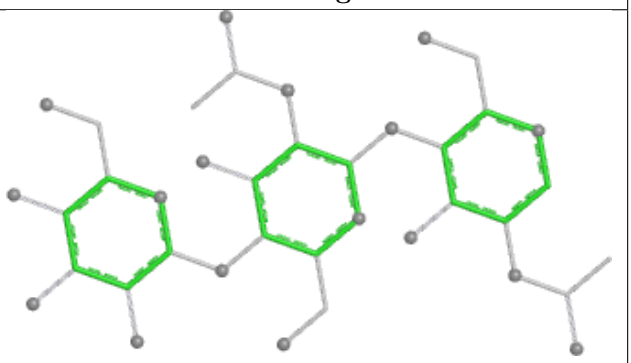
Bond lengths



Bond angles

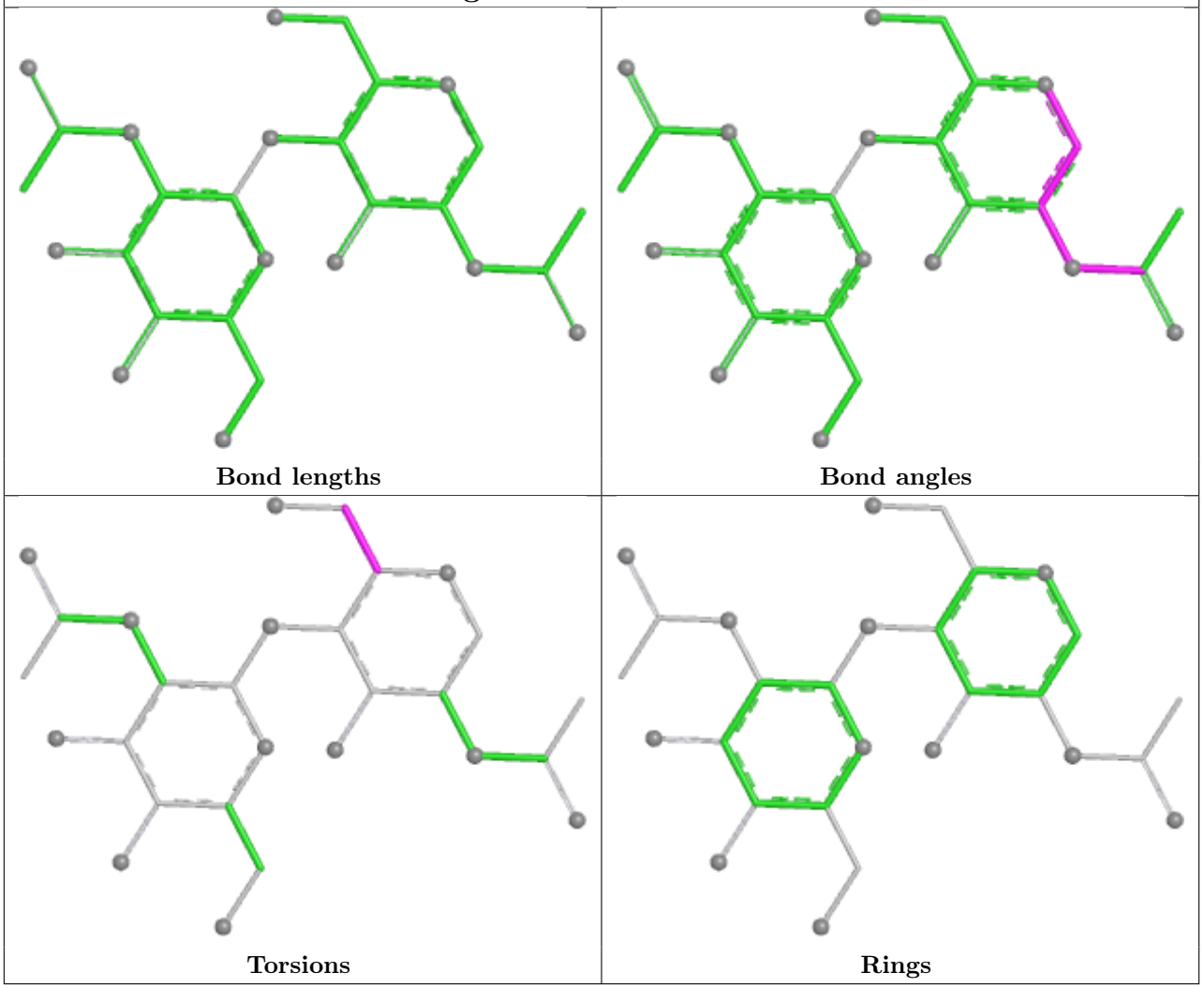


Torsions



Rings

Oligosaccharide Chain G



5.6 Ligand geometry (i)

Of 21 ligands modelled in this entry, 4 are monoatomic - leaving 17 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	$\#\|Z\| > 2$
4	DCD	A	1351	5	6,7,7	0.97	0	6,8,8	0.93	0
6	NAG	C	1356	1	14,14,15	0.60	0	17,19,21	1.03	1 (5%)
6	NAG	B	1354	1	14,14,15	0.55	0	17,19,21	1.26	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
4	DCD	D	1351	5	6,7,7	1.61	1 (16%)	6,8,8	1.46	1 (16%)
6	NAG	A	1357	1	14,14,15	0.63	0	17,19,21	0.85	0
6	NAG	A	1356	1	14,14,15	0.60	0	17,19,21	0.91	1 (5%)
6	NAG	B	1356	1	14,14,15	0.59	0	17,19,21	0.77	0
6	NAG	B	1353	1	14,14,15	0.60	0	17,19,21	0.89	1 (5%)
6	NAG	C	1357	1	14,14,15	0.64	0	17,19,21	1.26	2 (11%)
6	NAG	A	1353	1	14,14,15	0.46	0	17,19,21	0.85	0
6	NAG	C	1353	1	14,14,15	0.48	0	17,19,21	0.60	0
6	NAG	D	1353	1	14,14,15	0.51	0	17,19,21	1.24	2 (11%)
6	NAG	D	1356	1	14,14,15	0.51	0	17,19,21	0.91	0
4	DCD	B	1351	5	6,7,7	1.33	1 (16%)	6,8,8	0.91	0
4	DCD	C	1351	5	6,7,7	1.09	1 (16%)	6,8,8	0.58	0
6	NAG	D	1357	1	14,14,15	0.64	0	17,19,21	1.11	1 (5%)
6	NAG	B	1355	1	14,14,15	0.66	0	17,19,21	1.49	2 (11%)

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	DCD	A	1351	5	-	0/8/8/8	-
6	NAG	C	1356	1	-	0/6/23/26	0/1/1/1
6	NAG	B	1354	1	-	0/6/23/26	0/1/1/1
4	DCD	D	1351	5	-	0/8/8/8	-
6	NAG	A	1357	1	-	0/6/23/26	0/1/1/1
6	NAG	A	1356	1	-	0/6/23/26	0/1/1/1
6	NAG	B	1356	1	-	0/6/23/26	0/1/1/1
6	NAG	B	1353	1	-	0/6/23/26	0/1/1/1
6	NAG	C	1357	1	-	0/6/23/26	0/1/1/1
6	NAG	A	1353	1	-	0/6/23/26	0/1/1/1
6	NAG	C	1353	1	-	0/6/23/26	0/1/1/1
6	NAG	D	1353	1	-	0/6/23/26	0/1/1/1
6	NAG	D	1356	1	-	0/6/23/26	0/1/1/1
4	DCD	B	1351	5	-	0/8/8/8	-
4	DCD	C	1351	5	-	0/8/8/8	-
6	NAG	D	1357	1	-	0/6/23/26	0/1/1/1
6	NAG	B	1355	1	-	0/6/23/26	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	1351	DCD	C1-S2	-3.54	1.59	1.66
4	B	1351	DCD	C1-S2	-3.05	1.60	1.66
4	C	1351	DCD	C1-S2	-2.35	1.61	1.66

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	B	1355	NAG	O5-C1-C2	-4.42	104.46	111.29
6	B	1354	NAG	C2-N2-C7	-4.10	117.40	122.90
6	C	1357	NAG	O5-C1-C2	-3.33	106.14	111.29
4	D	1351	DCD	S2-C1-N1	-3.14	117.98	123.70
6	B	1355	NAG	C2-N2-C7	-2.93	118.97	122.90
6	D	1353	NAG	C6-C5-C4	-2.87	105.98	113.02
6	D	1357	NAG	O5-C1-C2	-2.56	107.33	111.29
6	C	1356	NAG	O5-C1-C2	-2.50	107.42	111.29
6	B	1353	NAG	C2-N2-C7	-2.13	120.05	122.90
6	C	1357	NAG	C2-N2-C7	-2.12	120.05	122.90
6	D	1353	NAG	C4-C3-C2	-2.07	107.99	111.02
6	A	1356	NAG	C2-N2-C7	-2.04	120.17	122.90

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1351	DCD	1	0
4	C	1351	DCD	3	0

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

Warning: The R factor obtained from EDS is 0.2703, which does not match the depositor's R factor of 0.161. Please interpret the results in this section carefully.

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	333/350 (95%)	-0.11	3 (0%)	81	83	10, 15, 20, 27	8 (2%)
1	B	334/350 (95%)	-0.03	4 (1%)	76	79	11, 15, 19, 28	4 (1%)
1	C	337/350 (96%)	0.21	8 (2%)	59	62	10, 15, 20, 34	3 (0%)
1	D	333/350 (95%)	4.87	329 (98%)	0	0	9, 15, 20, 34	3 (0%)
All	All	1337/1400 (95%)	1.23	344 (25%)	2	2	9, 15, 20, 34	18 (1%)

All (344) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	155	SER	12.6
1	D	154	SER	11.9
1	D	138	TYR	11.2
1	D	170	SER	10.3
1	D	262	THR	10.0
1	D	181	LEU	9.4
1	D	137	TYR	9.4
1	D	171	THR	9.2
1	D	263	VAL	9.2
1	D	117	GLN	9.2
1	D	289	ASP	9.2
1	D	342	SER	9.0
1	D	190	VAL	9.0
1	D	183	PHE	8.9
1	D	132	PHE	8.7
1	D	261	SER	8.4
1	D	27	ALA	8.4
1	D	116	ILE	8.2
1	D	80	GLY	8.2

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Mol	Chain	Res	Type	RSRZ
1	D	63	VAL	8.0
1	D	58	SER	7.9
1	D	28	VAL	7.9
1	D	143	ALA	7.9
1	D	328	ASP	7.9
1	D	146	THR	7.8
1	D	34	LEU	7.8
1	D	153	PRO	7.7
1	D	37	PHE	7.5
1	D	189	THR	7.5
1	D	55	ALA	7.4
1	D	75	PHE	7.4
1	D	82	PHE	7.3
1	D	152	ILE	7.2
1	D	175	PHE	7.2
1	D	177	VAL	7.2
1	D	89	GLY	7.2
1	D	173	GLN	7.1
1	D	67	ILE	7.0
1	D	29	THR	7.0
1	D	182	SER	7.0
1	D	150	PRO	7.0
1	D	139	LEU	6.9
1	D	151	TYR	6.9
1	D	216	PHE	6.8
1	D	350	TRP	6.8
1	D	115	GLN	6.8
1	D	178	TYR	6.8
1	D	225	TYR	6.8
1	D	98	LEU	6.8
1	D	14	VAL	6.7
1	D	97	VAL	6.7
1	D	77	CYS	6.6
1	D	110	VAL	6.6
1	D	90	ASN	6.6
1	D	22	TYR	6.6
1	D	172	LEU	6.6
1	D	290	TYR	6.6
1	D	120	ASP	6.6
1	D	54	ASN	6.6
1	D	57	HIS	6.6
1	D	35	TYR	6.4

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Mol	Chain	Res	Type	RSRZ
1	D	6	ILE	6.4
1	D	81	SER	6.4
1	D	214	PRO	6.4
1	D	144	THR	6.3
1	D	341	TRP	6.3
1	D	78	ASN	6.3
1	D	61	LEU	6.3
1	D	127[A]	ILE	6.3
1	D	149	THR	6.3
1	D	141	THR	6.2
1	D	228[A]	SER	6.2
1	D	46	TYR	6.2
1	D	84	LEU	6.2
1	D	230	TYR	6.1
1	D	135	LEU	6.1
1	D	106	VAL	6.1
1	D	207	LEU	6.0
1	D	30	VAL	6.0
1	D	85	TRP	6.0
1	D	229	GLN	6.0
1	D	51	MET	6.0
1	D	327	SER	6.0
1	D	121	THR	6.0
1	D	226	LEU	5.9
1	D	136	PHE	5.8
1	D	208	ALA	5.8
1	D	4	SER	5.8
1	D	31	ASP	5.8
1	D	107	PRO	5.8
1	D	217	ILE	5.7
1	D	99	SER	5.7
1	D	211	ALA	5.7
1	D	111	THR	5.7
1	D	303	ILE	5.6
1	D	64	LEU	5.6
1	D	72	TYR	5.6
1	D	5	LEU	5.6
1	D	259	THR	5.6
1	D	7	VAL	5.5
1	D	340	GLU	5.5
1	D	238	PHE	5.4
1	D	23	SER	5.4

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Mol	Chain	Res	Type	RSRZ
1	D	101	GLY	5.4
1	D	60	ALA	5.4
1	D	113	THR	5.4
1	D	147	THR	5.4
1	D	184	THR	5.4
1	D	335	VAL	5.4
1	D	19	ILE	5.3
1	D	33	GLN	5.3
1	D	69	GLN	5.3
1	D	32	THR	5.3
1	D	193	THR	5.3
1	D	200	TRP	5.3
1	D	56	PRO	5.3
1	D	131	GLY	5.3
1	D	24	HIS	5.3
1	D	123	MET	5.3
1	D	128	VAL	5.3
1	D	215	TYR	5.3
1	D	100[A]	SER	5.2
1	D	50	LEU	5.2
1	D	48	PHE	5.2
1	D	264	THR	5.2
1	D	59	ASP	5.1
1	D	76	TYR	5.1
1	D	47	ALA	5.1
1	D	71	HIS	5.1
1	D	92	THR	5.0
1	D	17	TYR	5.0
1	D	52	GLY	5.0
1	D	260	PRO	5.0
1	D	134	ASP	5.0
1	D	249	TYR	5.0
1	D	114	PHE	5.0
1	D	191	ASN	4.9
1	D	247	THR	4.9
1	D	38	TYR	4.9
1	D	70	LYS	4.9
1	D	142	ASN	4.8
1	D	10	ALA	4.8
1	D	86	ALA	4.8
1	D	298	GLY	4.8
1	D	62	GLY	4.8

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Mol	Chain	Res	Type	RSRZ
1	D	66	HIS	4.7
1	D	9	ASP	4.7
1	D	293	THR	4.7
1	D	39	VAL	4.7
1	D	213	ASP	4.7
1	C	167	SER	4.7
1	D	180	GLU	4.7
1	D	8	GLU	4.7
1	D	187	THR	4.6
1	D	130	GLY	4.6
1	D	79	LYS	4.6
1	D	42	PRO	4.6
1	D	221	TRP	4.6
1	D	336	ASN	4.6
1	D	252	SER	4.6
1	D	297	SER	4.6
1	D	306	GLY	4.6
1	D	129	PRO	4.6
1	D	145	ASP	4.5
1	D	53	THR	4.5
1	D	104	GLY	4.5
1	D	192	GLY	4.5
1	D	308	GLU	4.5
1	D	103	TYR	4.5
1	D	309	PHE	4.5
1	D	312	TYR	4.5
1	D	339	GLU	4.4
1	D	235	VAL	4.4
1	D	73	GLU	4.4
1	D	194	ALA	4.4
1	D	108	ARG	4.4
1	D	202	THR	4.4
1	D	251	LEU	4.4
1	D	188	ASP	4.4
1	D	246	ASP	4.4
1	D	21	HIS	4.4
1	D	18	VAL	4.4
1	D	271	PRO	4.4
1	D	13	HIS	4.3
1	D	11	PRO	4.3
1	D	242	THR	4.3
1	D	87	GLN	4.3

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Mol	Chain	Res	Type	RSRZ
1	D	65	PRO	4.3
1	D	124	THR	4.3
1	D	43	SER	4.3
1	D	174	SER	4.3
1	D	333	ASN	4.2
1	D	40	THR	4.2
1	D	49	THR	4.2
1	D	337	GLY	4.2
1	D	95	THR	4.2
1	D	185	PRO	4.2
1	D	218	ALA	4.2
1	D	273	ALA	4.2
1	D	140	GLY	4.2
1	D	323	VAL	4.1
1	D	205	ASN	4.1
1	D	223	PRO	4.1
1	D	270	PHE	4.1
1	D	302	PHE	4.1
1	D	288	GLY	4.1
1	D	199	VAL	4.1
1	D	239	VAL	4.1
1	D	278	VAL	4.1
1	D	326	GLY	4.1
1	D	300	VAL	4.1
1	D	102	ASP	4.0
1	D	206	ALA	4.0
1	D	91	GLU	4.0
1	D	310	LYS	4.0
1	D	198	THR	4.0
1	D	176	ASP	4.0
1	D	201	HIS	4.0
1	D	119	PRO	4.0
1	D	83	GLN	4.0
1	D	179	ALA	4.0
1	D	236	ALA	4.0
1	D	244	ALA	4.0
1	D	275	ALA	4.0
1	D	276	PHE	3.9
1	D	126	VAL	3.9
1	D	274	CYS	3.9
1	D	25	ALA	3.9
1	D	269	SER	3.8

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Mol	Chain	Res	Type	RSRZ
1	D	315	ALA	3.8
1	D	250	THR	3.7
1	D	209	SER	3.7
1	D	118	ASP	3.7
1	D	272	GLY	3.7
1	C	168	THR	3.7
1	D	44	SER	3.7
1	D	266	PRO	3.7
1	D	292	ALA	3.7
1	D	291	ALA	3.7
1	D	321	LEU	3.7
1	D	26	ARG	3.7
1	D	232	TYR	3.6
1	D	268	TRP	3.6
1	D	122	GLU	3.6
1	D	212	GLY	3.6
1	D	301	ALA	3.6
1	D	237	PRO	3.6
1	D	133	GLU	3.6
1	D	41	GLY	3.5
1	D	68	HIS	3.5
1	D	96	ARG	3.5
1	D	286	GLN	3.5
1	C	4	SER	3.5
1	D	325	SER	3.5
1	D	304	PRO	3.5
1	D	36	ARG	3.5
1	D	204	ALA	3.5
1	D	317	PHE	3.5
1	D	219	ASN	3.5
1	D	258	THR	3.5
1	D	241	ALA	3.4
1	D	344	VAL	3.4
1	D	234	ILE	3.4
1	D	319	LYS	3.4
1	D	195	PRO	3.4
1	D	320	VAL	3.4
1	D	93	GLN	3.4
1	D	88	SER	3.4
1	D	296	GLY	3.4
1	D	243	GLN	3.4
1	D	330	LEU	3.3

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Mol	Chain	Res	Type	RSRZ
1	D	196	ALA	3.3
1	C	166	SER	3.3
1	D	203	GLY	3.2
1	D	338	GLY	3.2
1	D	94	GLN	3.2
1	D	245	GLN	3.2
1	D	287	ILE	3.2
1	D	316	TYR	3.2
1	D	267	THR	3.2
1	D	283	VAL	3.2
1	D	332	GLN	3.2
1	D	224	LYS	3.1
1	D	322	PHE	3.1
1	D	231	GLY	3.1
1	D	329	GLY	3.1
1	D	210	THR	3.1
1	D	285	VAL	3.1
1	D	125	GLY	3.1
1	D	12	ASP	3.0
1	D	284	VAL	3.0
1	D	307	VAL	3.0
1	D	331	ASP	3.0
1	D	74	ASN	3.0
1	D	109	ASN	3.0
1	D	248	ASN	3.0
1	D	299	ASP	3.0
1	D	294	GLU	3.0
1	D	254	ILE	2.9
1	D	305	GLY	2.9
1	D	240	THR	2.9
1	B	169	ILE	2.9
1	D	105	SER	2.9
1	B	167	SER	2.9
1	D	334	LEU	2.9
1	D	15	ARG	2.9
1	D	45	GLY	2.9
1	D	220	GLY	2.9
1	D	112	HIS	2.8
1	D	265	VAL	2.8
1	D	314	GLU	2.8
1	D	197	ASN	2.8
1	D	253	THR	2.8

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Mol	Chain	Res	Type	RSRZ
1	D	148	HIS	2.8
1	D	16	PRO	2.8
1	D	324	SER	2.7
1	D	295	LEU	2.7
1	D	279	GLN	2.7
1	C	89	GLY	2.7
1	D	222	GLY	2.7
1	D	255	SER	2.7
1	D	345	SER	2.7
1	B	168	THR	2.6
1	A	90	ASN	2.6
1	B	181	LEU	2.6
1	A	154	SER	2.6
1	D	280	GLU	2.5
1	D	20	ARG	2.5
1	D	281	GLY	2.5
1	C	3	SER	2.5
1	D	311	TYR	2.5
1	D	347	PRO	2.4
1	D	318	SER	2.4
1	D	186	ARG	2.4
1	C	154	SER	2.4
1	D	346	PHE	2.3
1	D	277	GLN	2.3
1	D	343	SER	2.3
1	D	227	ASN	2.2
1	D	348	ALA	2.1
1	D	313	SER	2.1
1	D	233	GLN	2.1
1	A	170	SER	2.1
1	C	177	VAL	2.1

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

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

6.3 Carbohydrates (i)

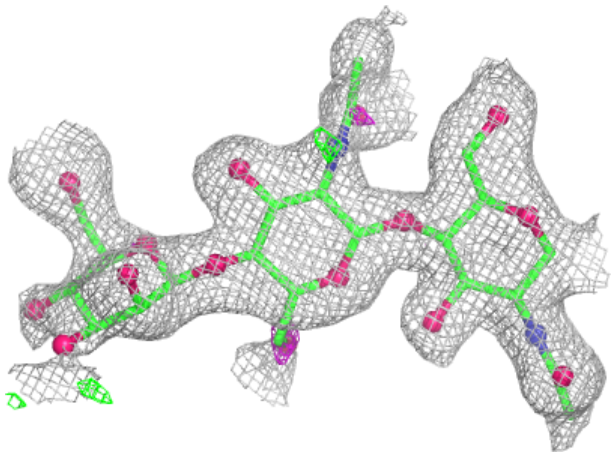
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

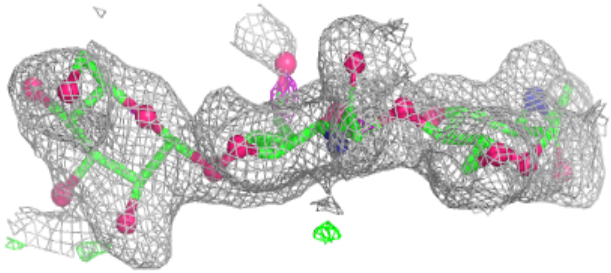
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	BMA	E	3	11/12	0.67	0.13	48,49,50,50	0
2	BMA	F	3	11/12	0.68	0.11	52,55,56,56	0
3	NAG	G	1	14/15	0.74	0.13	31,36,39,40	0
2	NAG	E	2	14/15	0.75	0.12	36,41,44,46	0
2	NAG	F	1	14/15	0.76	0.12	31,36,42,45	0
2	NAG	F	2	14/15	0.78	0.12	35,40,43,48	0
2	NAG	E	1	14/15	0.82	0.10	31,36,39,40	0
3	NAG	G	2	14/15	0.82	0.10	36,39,43,45	0

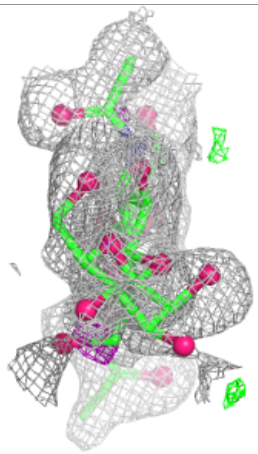
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

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)

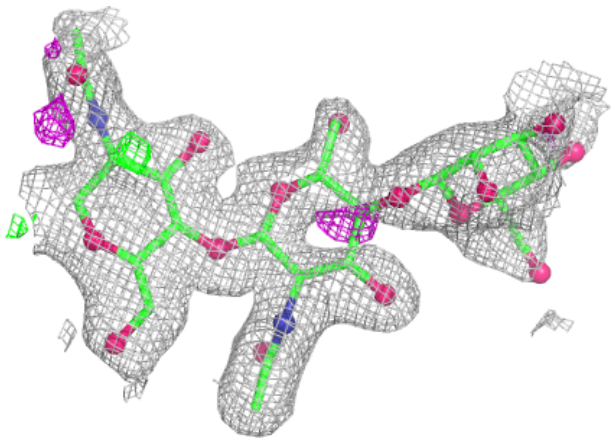


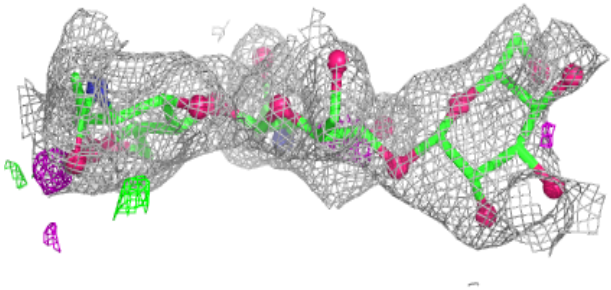


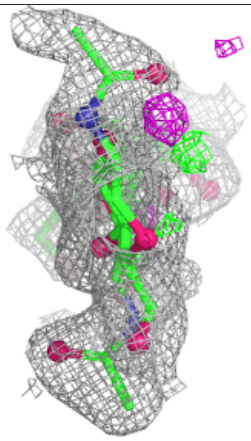


Electron density around Chain F:

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

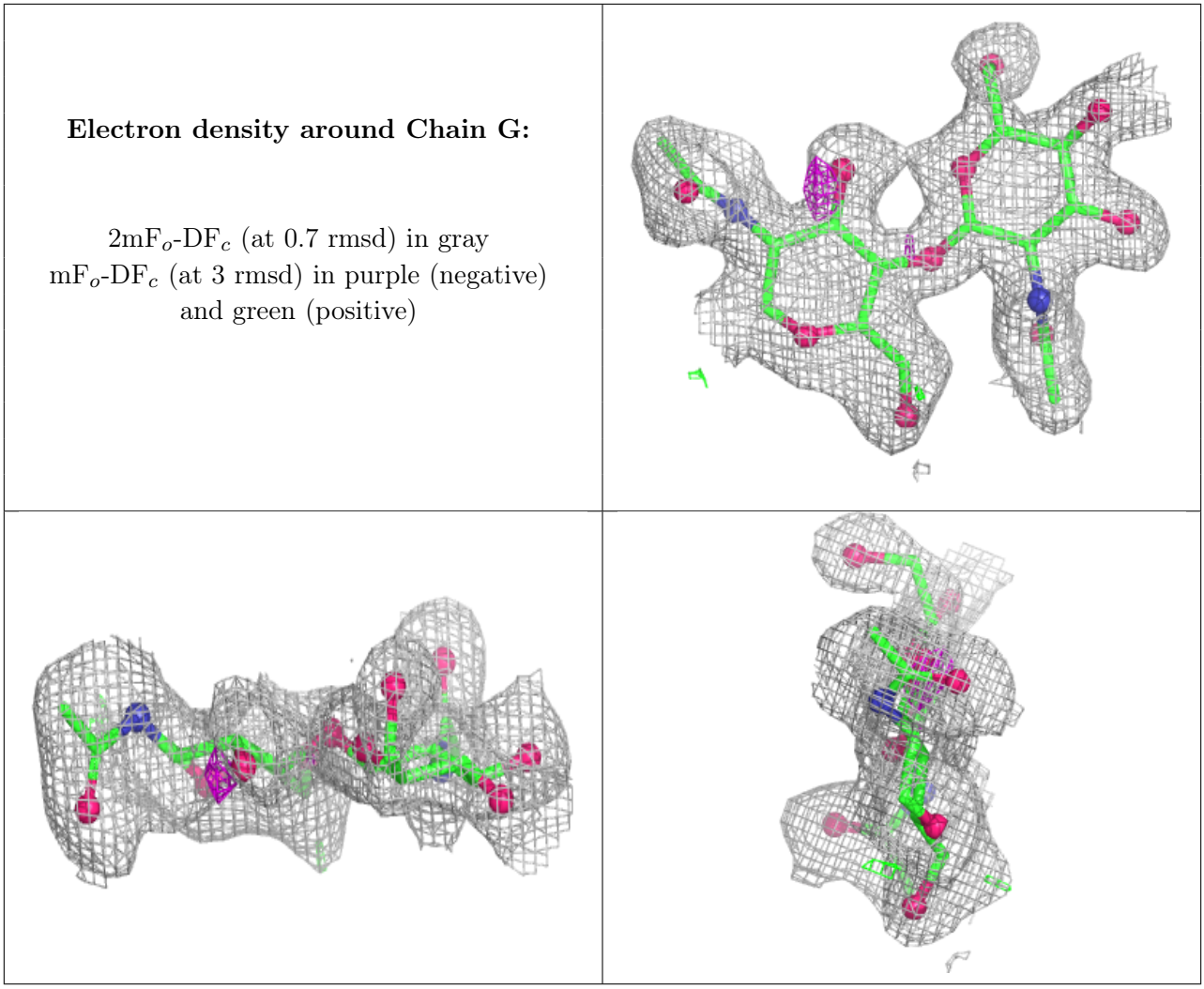






Electron density around Chain G:

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



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
5	CU	D	1352	1/1	0.43	0.48	17,17,17,17	0
6	NAG	A	1357	14/15	0.68	0.13	32,36,42,44	0
6	NAG	D	1356	14/15	0.72	0.12	29,33,37,38	0
6	NAG	B	1354	14/15	0.74	0.12	40,45,47,48	0
6	NAG	D	1353	14/15	0.76	0.12	33,39,42,43	0
6	NAG	B	1355	14/15	0.78	0.11	28,34,45,46	0
6	NAG	C	1353	14/15	0.78	0.12	34,39,44,46	0
6	NAG	B	1356	14/15	0.80	0.11	35,42,45,45	0
6	NAG	D	1357	14/15	0.81	0.11	32,38,44,45	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	DCD	D	1351	8/8	0.82	0.34	19,20,23,23	0
6	NAG	C	1357	14/15	0.83	0.11	32,39,42,43	0
6	NAG	C	1356	14/15	0.84	0.10	34,39,46,46	0
6	NAG	A	1356	14/15	0.86	0.10	27,32,41,43	0
6	NAG	B	1353	14/15	0.89	0.07	29,34,38,38	0
6	NAG	A	1353	14/15	0.89	0.08	26,32,35,36	0
4	DCD	C	1351	8/8	0.91	0.11	20,21,22,23	0
4	DCD	B	1351	8/8	0.96	0.09	22,23,24,24	0
4	DCD	A	1351	8/8	0.97	0.07	17,18,20,20	0
5	CU	B	1352	1/1	0.98	0.03	17,17,17,17	0
5	CU	C	1352	1/1	0.98	0.04	17,17,17,17	0
5	CU	A	1352	1/1	0.99	0.03	17,17,17,17	0

6.5 Other polymers (i)

There are no such residues in this entry.