wwPDB X-ray Structure Validation Summary Report (i)

Aug 3, 2023 – 12:21 AM EDT

PDB ID	:	1G82
Title	:	STRUCTURE OF FIBROBLAST GROWTH FACTOR 9
Authors	:	Hecht, H.J.; Adar, R.; Hofmann, B.; Bogin, O.; Weich, H.; Yayon, A.
Deposited on	:	2000-11-16
Resolution	:	2.60 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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:

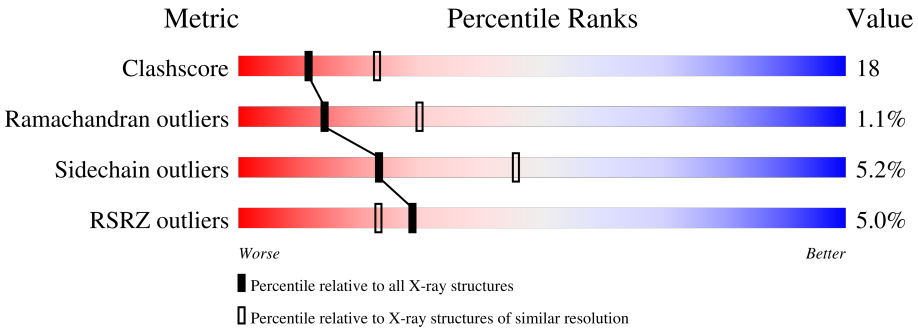
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.34
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.34

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 2.60 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	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)

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

Mol	Chain	Length	Quality of chain
1	A	160	2% 63% 25% 9%
1	B	160	16% 41% 51% 5%
1	C	160	67% 24% 5%
1	D	160	% 59% 32%
2	E	3	100%
2	F	3	33% 67%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	G	3	33% 67%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	NAG	E	2	X	-	-	-
2	NAG	G	2	X	-	-	-
2	FUC	G	3	X	-	-	-

2 Entry composition (i)

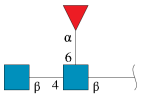
There are 5 unique types of molecules in this entry. The entry contains 5480 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 FIBROBLAST GROWTH FACTOR 9.

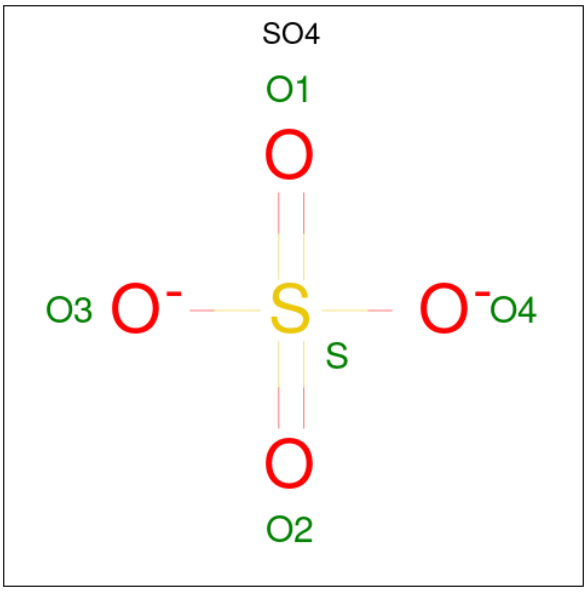
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	157	Total	C	N	O	S	0	0	0
			1295	819	234	239	3			
1	B	157	Total	C	N	O	S	0	0	0
			1295	821	234	237	3			
1	C	155	Total	C	N	O	S	0	0	0
			1279	811	231	234	3			
1	D	155	Total	C	N	O	S	0	0	0
			1276	809	231	233	3			

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



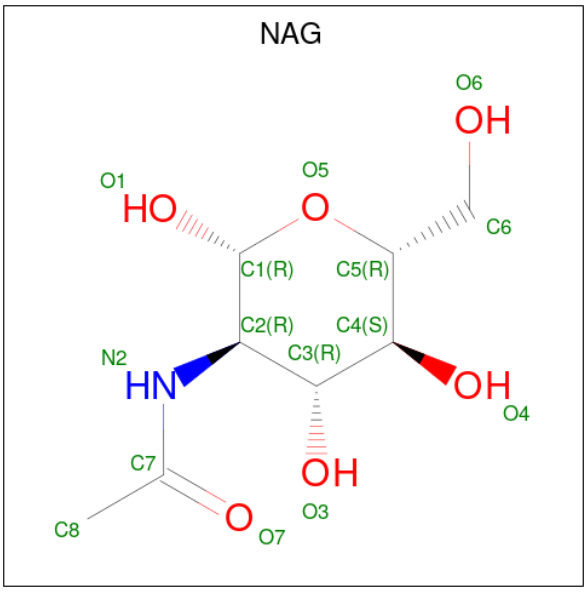
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	E	3	Total	C	N	O	0	0	0
			38	22	2	14			
2	F	3	Total	C	N	O	0	0	0
			38	22	2	14			
2	G	3	Total	C	N	O	0	0	0
			38	22	2	14			

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total O S 5 4 1	0	0
3	A	1	Total O S 5 4 1	0	0
3	A	1	Total O S 5 4 1	0	0
3	B	1	Total O S 5 4 1	0	0
3	B	1	Total O S 5 4 1	0	0
3	C	1	Total O S 5 4 1	0	0
3	C	1	Total O S 5 4 1	0	0
3	C	1	Total O S 5 4 1	0	0
3	C	1	Total O S 5 4 1	0	0
3	D	1	Total O S 5 4 1	0	0
3	D	1	Total O S 5 4 1	0	0
3	D	1	Total O S 5 4 1	0	0

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



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

- Molecule 5 is water.

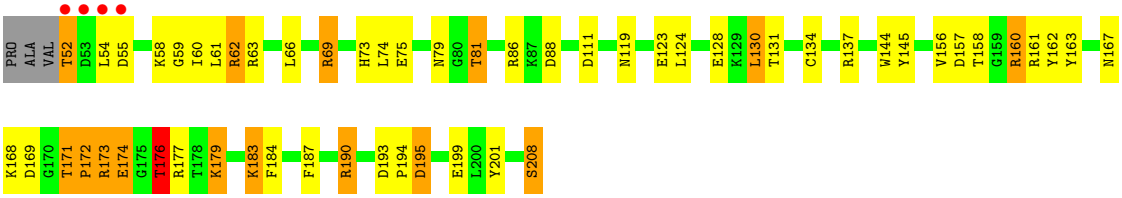
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	59	Total O 59 59	0	0
5	B	4	Total O 4 4	0	0
5	C	35	Total O 35 35	0	0
5	D	49	Total O 49 49	0	0

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.

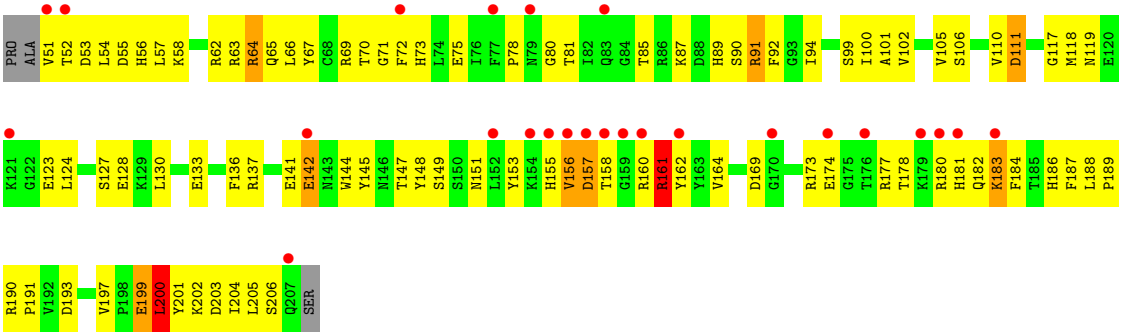
• Molecule 1: FIBROBLAST GROWTH FACTOR 9

Chain A:



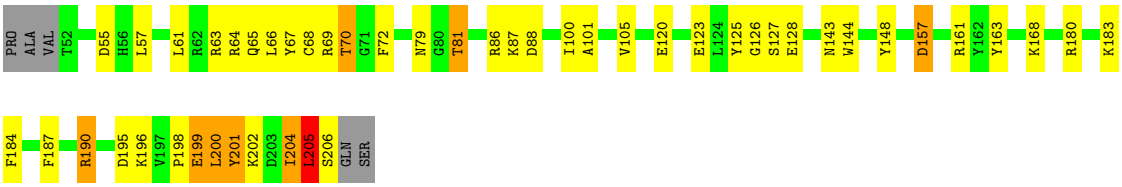
• Molecule 1: FIBROBLAST GROWTH FACTOR 9

Chain B:



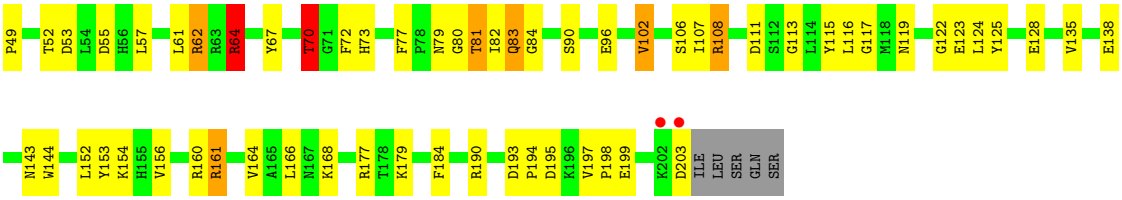
• Molecule 1: FIBROBLAST GROWTH FACTOR 9

Chain C:



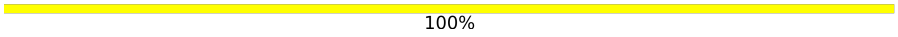
• Molecule 1: FIBROBLAST GROWTH FACTOR 9

Chain D:



• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain E:



• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain F:

• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain G:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	I 41	Depositor
Cell constants a, b, c, α, β, γ	151.95Å 151.95Å 117.23Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.60 39.66 – 2.60	Depositor EDS
% Data completeness (in resolution range)	99.9 (50.00-2.60) 100.0 (39.66-2.60)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	0.05	Depositor
$< I/\sigma(I) >$ [1]	5.52 (at 2.61Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.208 , 0.248 0.211 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å^2)	52.4	Xtriage
Anisotropy	0.220	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 58.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.018 for -k,-h,-l	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	5480	wwPDB-VP
Average B, all atoms (Å^2)	55.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.72% 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: SO4, NAG, FUC

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	1.80	22/1325 (1.7%)	1.54	18/1783 (1.0%)
1	B	1.25	3/1325 (0.2%)	1.21	12/1785 (0.7%)
1	C	1.66	9/1309 (0.7%)	1.36	14/1763 (0.8%)
1	D	1.86	28/1307 (2.1%)	1.48	15/1761 (0.9%)
All	All	1.66	62/5266 (1.2%)	1.40	59/7092 (0.8%)

The worst 5 of 62 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	120	GLU	CD-OE2	8.82	1.35	1.25
1	A	195	ASP	CB-CG	8.26	1.69	1.51
1	A	179	LYS	CE-NZ	8.12	1.69	1.49
1	A	162	TYR	CD2-CE2	-8.07	1.27	1.39
1	D	123	GLU	CD-OE1	7.68	1.34	1.25

The worst 5 of 59 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	64	ARG	NE-CZ-NH2	-12.57	114.01	120.30
1	A	62	ARG	NE-CZ-NH2	-12.02	114.29	120.30
1	A	190	ARG	NE-CZ-NH2	-11.65	114.48	120.30
1	A	62	ARG	NE-CZ-NH1	11.48	126.04	120.30
1	A	195	ASP	CB-CG-OD2	10.39	127.65	118.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1295	0	1272	31	0
1	B	1295	0	1275	96	0
1	C	1279	0	1259	29	0
1	D	1276	0	1254	32	0
2	E	38	0	34	0	0
2	F	38	0	34	4	0
2	G	38	0	34	1	0
3	A	15	0	0	1	0
3	B	10	0	0	1	0
3	C	20	0	0	0	0
3	D	15	0	0	1	0
4	B	14	0	13	0	0
5	A	59	0	0	2	0
5	B	4	0	0	0	0
5	C	35	0	0	0	0
5	D	49	0	0	3	0
All	All	5480	0	5175	185	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 18.

The worst 5 of 185 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:179:LYS:CE	1:A:179:LYS:NZ	1.69	1.49
1:B:158:THR:CG2	1:B:160:ARG:HG2	1.61	1.30
1:B:64:ARG:HH11	1:B:64:ARG:CG	1.43	1.27
1:B:155:HIS:HD2	1:B:162:TYR:CE1	1.62	1.16
1:B:158:THR:HG21	1:B:160:ARG:HG2	1.19	1.09

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	155/160 (97%)	149 (96%)	6 (4%)	0	100 100
1	B	155/160 (97%)	136 (88%)	16 (10%)	3 (2%)	8 15
1	C	153/160 (96%)	142 (93%)	7 (5%)	4 (3%)	5 9
1	D	153/160 (96%)	147 (96%)	6 (4%)	0	100 100
All	All	616/640 (96%)	574 (93%)	35 (6%)	7 (1%)	14 30

5 of 7 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	53	ASP
1	B	156	VAL
1	C	200	LEU
1	B	183	LYS
1	C	202	LYS

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	141/143 (99%)	133 (94%)	8 (6%)	20 41
1	B	141/143 (99%)	131 (93%)	10 (7%)	14 29
1	C	139/143 (97%)	136 (98%)	3 (2%)	52 76
1	D	138/143 (96%)	130 (94%)	8 (6%)	20 40
All	All	559/572 (98%)	530 (95%)	29 (5%)	23 46

5 of 29 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	161	ARG
1	D	160	ARG
1	B	206	SER
1	D	81	THR
1	B	200	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 8 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	186	HIS
1	B	207	GLN
1	B	155	HIS
1	B	151	ASN
1	B	181	HIS

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)

9 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	2,1	14,14,15	2.65	5 (35%)	17,19,21	4.50	11 (64%)
2	NAG	E	2	2	14,14,15	0.97	0	17,19,21	2.60	6 (35%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	FUC	E	3	2	10,10,11	1.41	2 (20%)	14,14,16	1.82	3 (21%)
2	NAG	F	1	2,1	14,14,15	1.24	1 (7%)	17,19,21	2.76	9 (52%)
2	NAG	F	2	2	14,14,15	1.34	2 (14%)	17,19,21	4.24	10 (58%)
2	FUC	F	3	2	10,10,11	1.45	1 (10%)	14,14,16	3.08	6 (42%)
2	NAG	G	1	2,1	14,14,15	1.78	2 (14%)	17,19,21	3.37	6 (35%)
2	NAG	G	2	2	14,14,15	1.19	1 (7%)	17,19,21	2.25	5 (29%)
2	FUC	G	3	2	10,10,11	0.96	1 (10%)	14,14,16	2.23	7 (50%)

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	2,1	-	4/6/23/26	0/1/1/1
2	NAG	E	2	2	1/1/5/7	2/6/23/26	0/1/1/1
2	FUC	E	3	2	-	-	0/1/1/1
2	NAG	F	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	F	2	2	-	5/6/23/26	0/1/1/1
2	FUC	F	3	2	-	-	0/1/1/1
2	NAG	G	1	2,1	-	5/6/23/26	0/1/1/1
2	NAG	G	2	2	1/1/5/7	2/6/23/26	0/1/1/1
2	FUC	G	3	2	1/1/4/5	-	0/1/1/1

The worst 5 of 15 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	1	NAG	C2-N2	-7.28	1.33	1.46
2	G	1	NAG	O7-C7	5.00	1.34	1.23
2	E	1	NAG	C4-C5	-4.18	1.44	1.53
2	F	2	NAG	C1-C2	3.64	1.57	1.52
2	E	1	NAG	C4-C3	-3.49	1.43	1.52

The worst 5 of 63 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	F	2	NAG	O5-C1-C2	10.40	127.70	111.29
2	E	1	NAG	C8-C7-N2	10.17	133.31	116.10
2	F	2	NAG	O5-C5-C6	8.87	121.10	107.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	F	3	FUC	C2-C3-C4	-8.02	97.02	110.89
2	E	1	NAG	C3-C4-C5	-7.55	96.78	110.24

All (3) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	E	2	NAG	C1
2	G	2	NAG	C1
2	G	3	FUC	C1

5 of 20 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	E	1	NAG	C8-C7-N2-C2
2	E	1	NAG	O7-C7-N2-C2
2	F	1	NAG	C8-C7-N2-C2
2	F	1	NAG	O7-C7-N2-C2
2	F	2	NAG	C3-C2-N2-C7

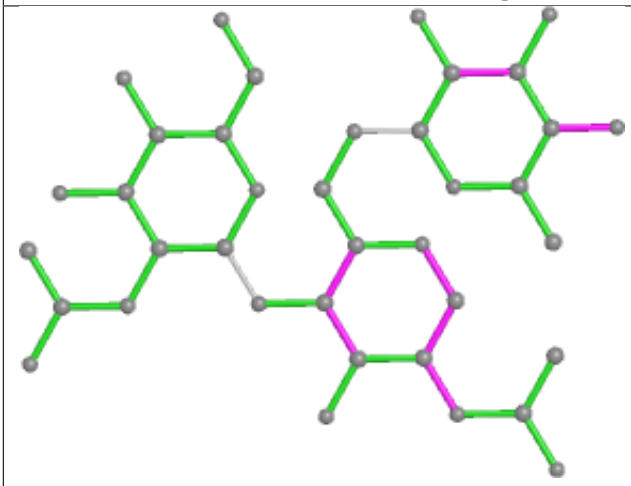
There are no ring outliers.

4 monomers are involved in 5 short contacts:

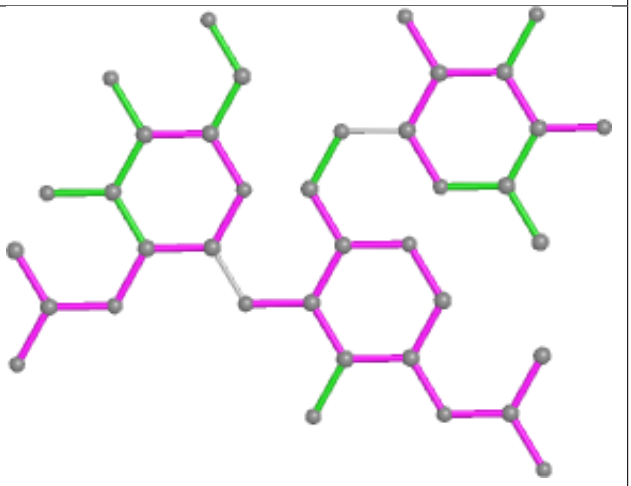
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	G	2	NAG	1	0
2	F	1	NAG	2	0
2	F	2	NAG	2	0
2	G	1	NAG	1	0

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

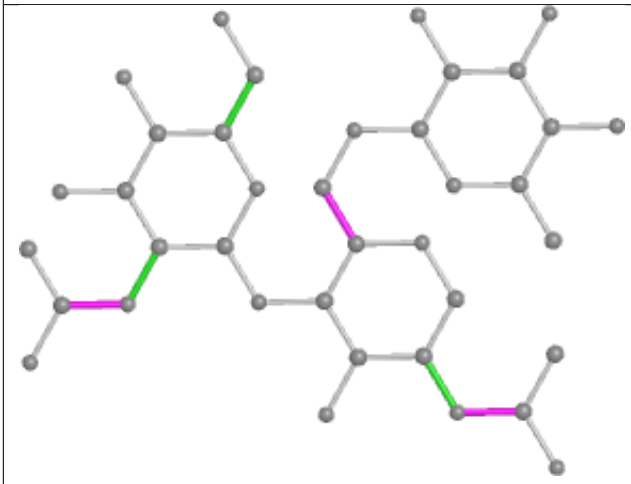
Oligosaccharide Chain E



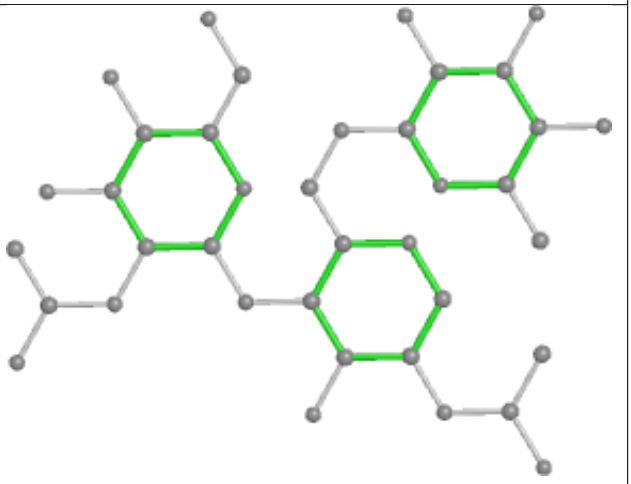
Bond lengths



Bond angles

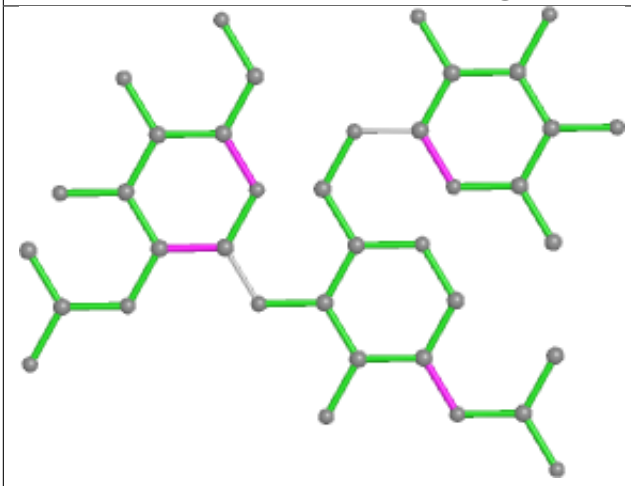


Torsions

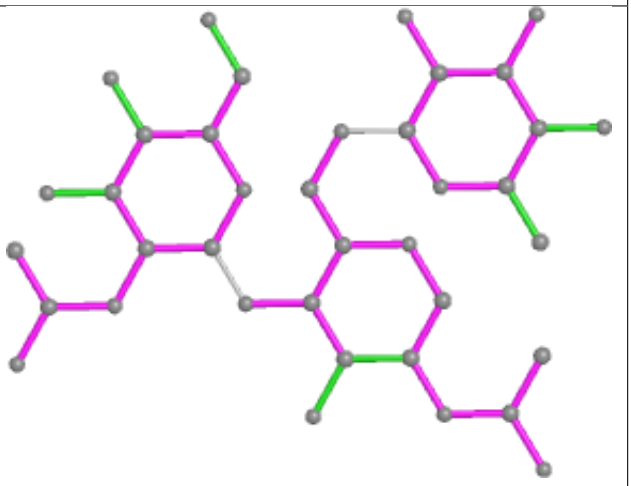


Rings

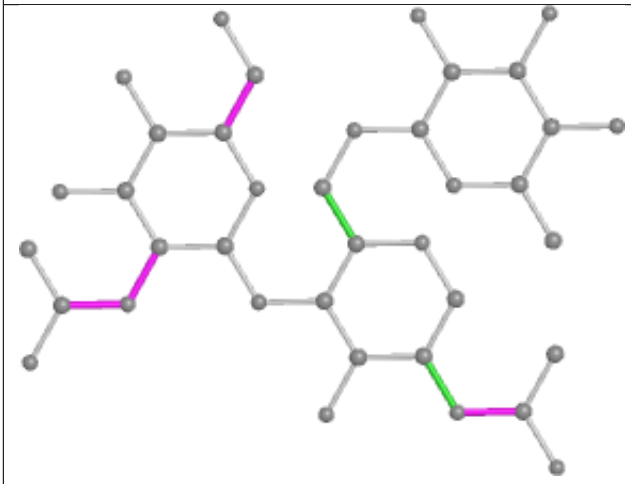
Oligosaccharide Chain F



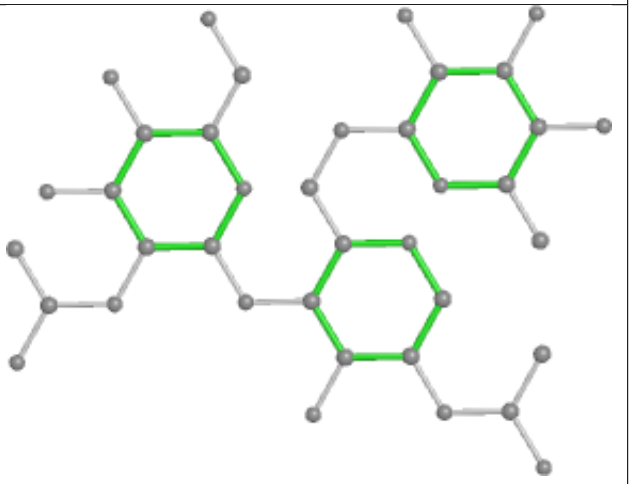
Bond lengths



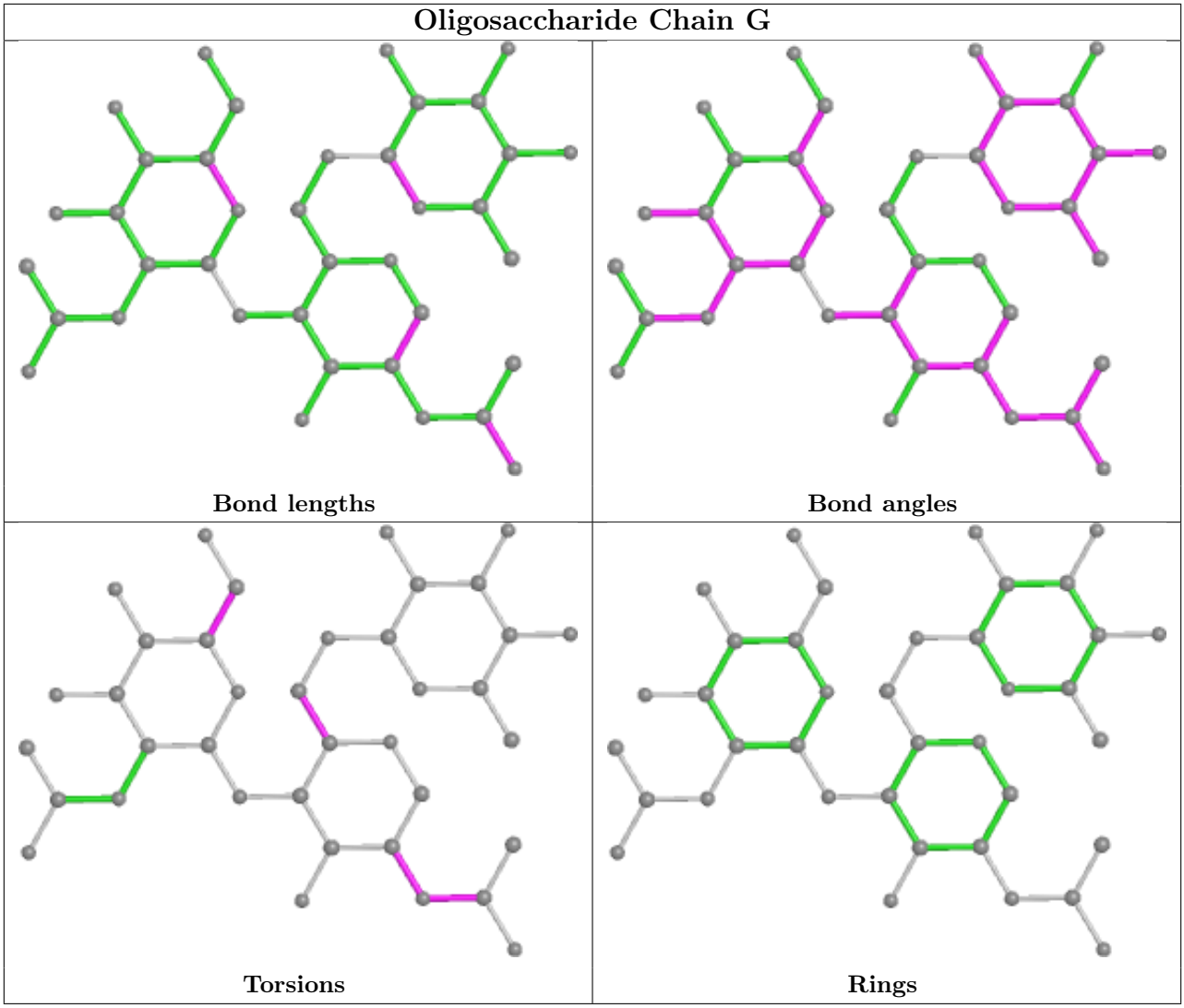
Bond angles



Torsions



Rings



5.6 Ligand geometry (i)

13 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	B	651	1	14,14,15	1.07	1 (7%)	17,19,21	2.01	3 (17%)
3	SO4	A	290	-	4,4,4	0.74	0	6,6,6	0.85	0
3	SO4	D	300	-	4,4,4	0.18	0	6,6,6	0.50	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	SO4	C	301	-	4,4,4	0.12	0	6,6,6	0.25	0
3	SO4	C	296	-	4,4,4	0.24	0	6,6,6	0.60	0
3	SO4	B	295	-	4,4,4	0.56	0	6,6,6	1.06	0
3	SO4	D	293	-	4,4,4	0.65	0	6,6,6	1.52	1 (16%)
3	SO4	D	297	-	4,4,4	0.21	0	6,6,6	1.08	1 (16%)
3	SO4	A	299	-	4,4,4	0.37	0	6,6,6	0.60	0
3	SO4	A	294	-	4,4,4	0.36	0	6,6,6	1.17	0
3	SO4	C	292	-	4,4,4	0.83	0	6,6,6	0.66	0
3	SO4	B	291	-	4,4,4	0.28	0	6,6,6	1.00	0
3	SO4	C	298	-	4,4,4	0.37	0	6,6,6	0.77	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	B	651	1	-	6/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	651	NAG	C1-C2	3.49	1.57	1.52

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	B	651	NAG	O5-C1-C2	5.04	119.24	111.29
4	B	651	NAG	C1-O5-C5	4.63	118.47	112.19
3	D	293	SO4	O4-S-O1	-3.13	92.95	109.31
4	B	651	NAG	O5-C5-C6	3.03	111.95	107.20
3	D	297	SO4	O3-S-O2	-2.08	98.45	109.31

There are no chirality outliers.

5 of 6 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	651	NAG	C8-C7-N2-C2
4	B	651	NAG	O7-C7-N2-C2
4	B	651	NAG	O5-C5-C6-O6
4	B	651	NAG	C4-C5-C6-O6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
4	B	651	NAG	C1-C2-N2-C7

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	300	SO4	1	0
3	B	295	SO4	1	0
3	A	294	SO4	1	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

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	157/160 (98%)	-0.11	4 (2%) 57 51	29, 41, 60, 87	0
1	B	157/160 (98%)	0.91	25 (15%) 1 1	51, 79, 103, 110	0
1	C	155/160 (96%)	-0.22	0 100 100	34, 47, 77, 108	0
1	D	155/160 (96%)	-0.06	2 (1%) 77 73	30, 42, 66, 100	0
All	All	624/640 (97%)	0.13	31 (4%) 28 23	29, 47, 96, 110	0

The worst 5 of 31 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	83	GLN	6.1
1	B	155	HIS	6.0
1	B	157	ASP	5.2
1	B	160	ARG	5.2
1	B	51	VAL	4.9

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

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

6.3 Carbohydrates

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	NAG	F	2	14/15	0.76	0.28	82,90,99,103	0
2	NAG	G	2	14/15	0.81	0.32	69,87,92,93	0

Continued on next page...

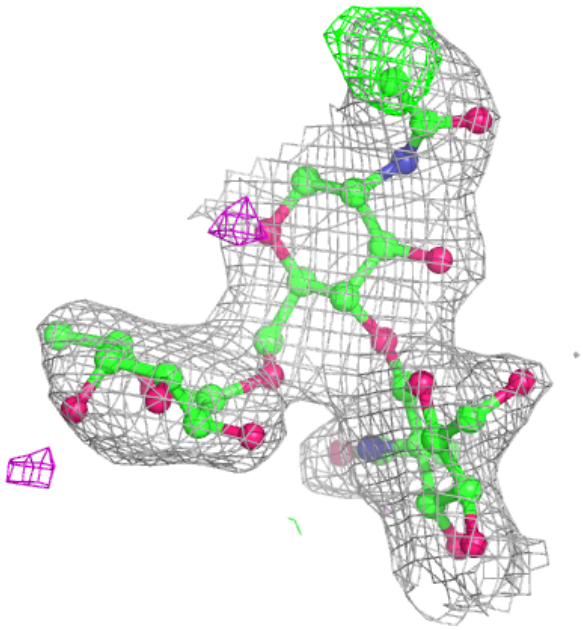
Continued from previous page...

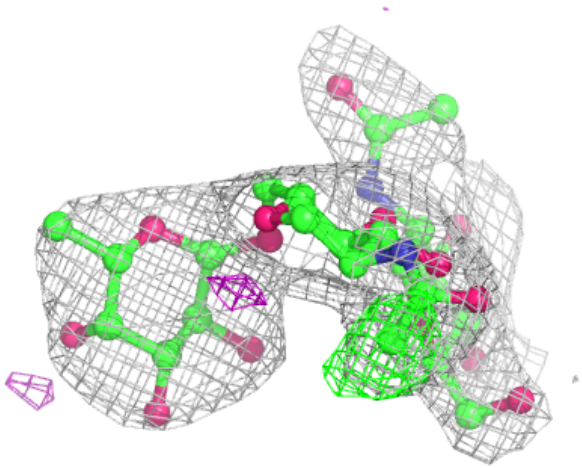
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	NAG	E	2	14/15	0.82	0.24	67,76,85,88	0
2	NAG	G	1	14/15	0.86	0.21	60,69,74,80	0
2	NAG	E	1	14/15	0.86	0.17	56,60,71,73	0
2	NAG	F	1	14/15	0.90	0.17	57,67,75,81	0
2	FUC	F	3	10/11	0.94	0.20	59,66,69,69	0
2	FUC	E	3	10/11	0.95	0.22	60,68,71,74	0
2	FUC	G	3	10/11	0.95	0.20	63,69,72,72	0

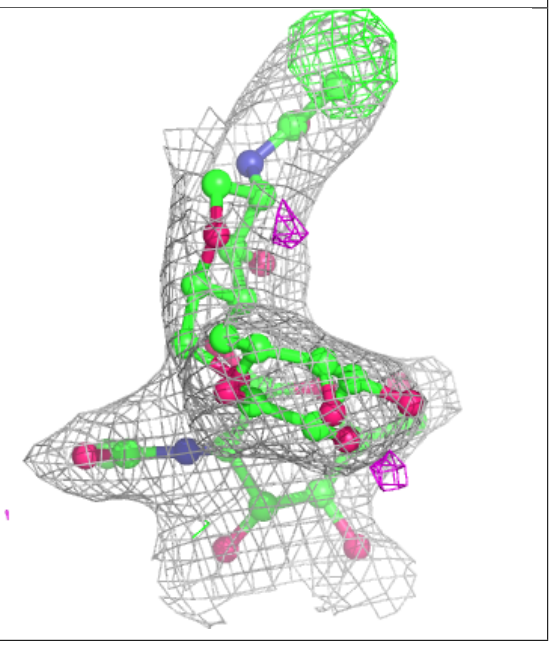
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

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)

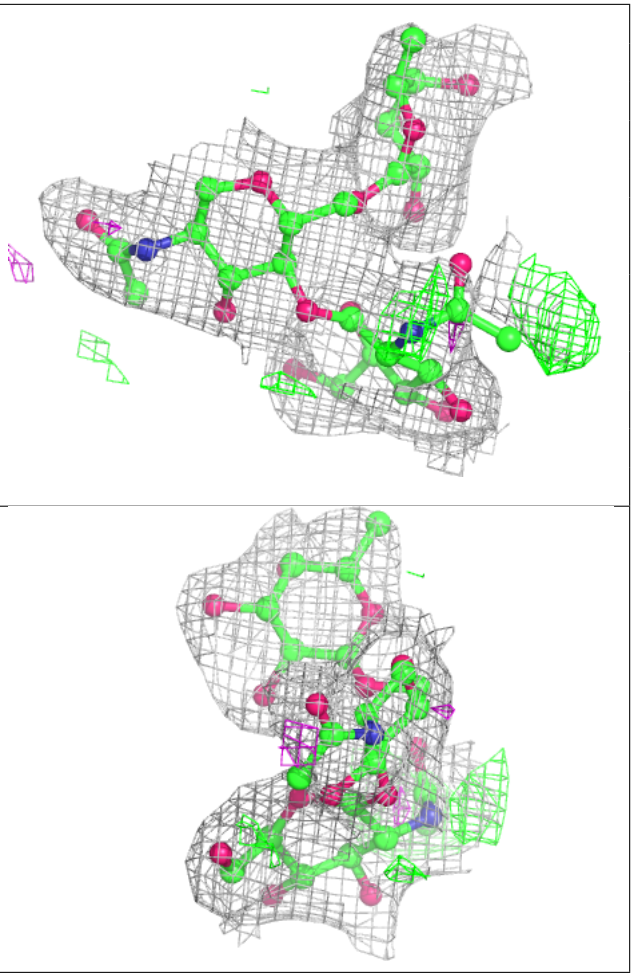






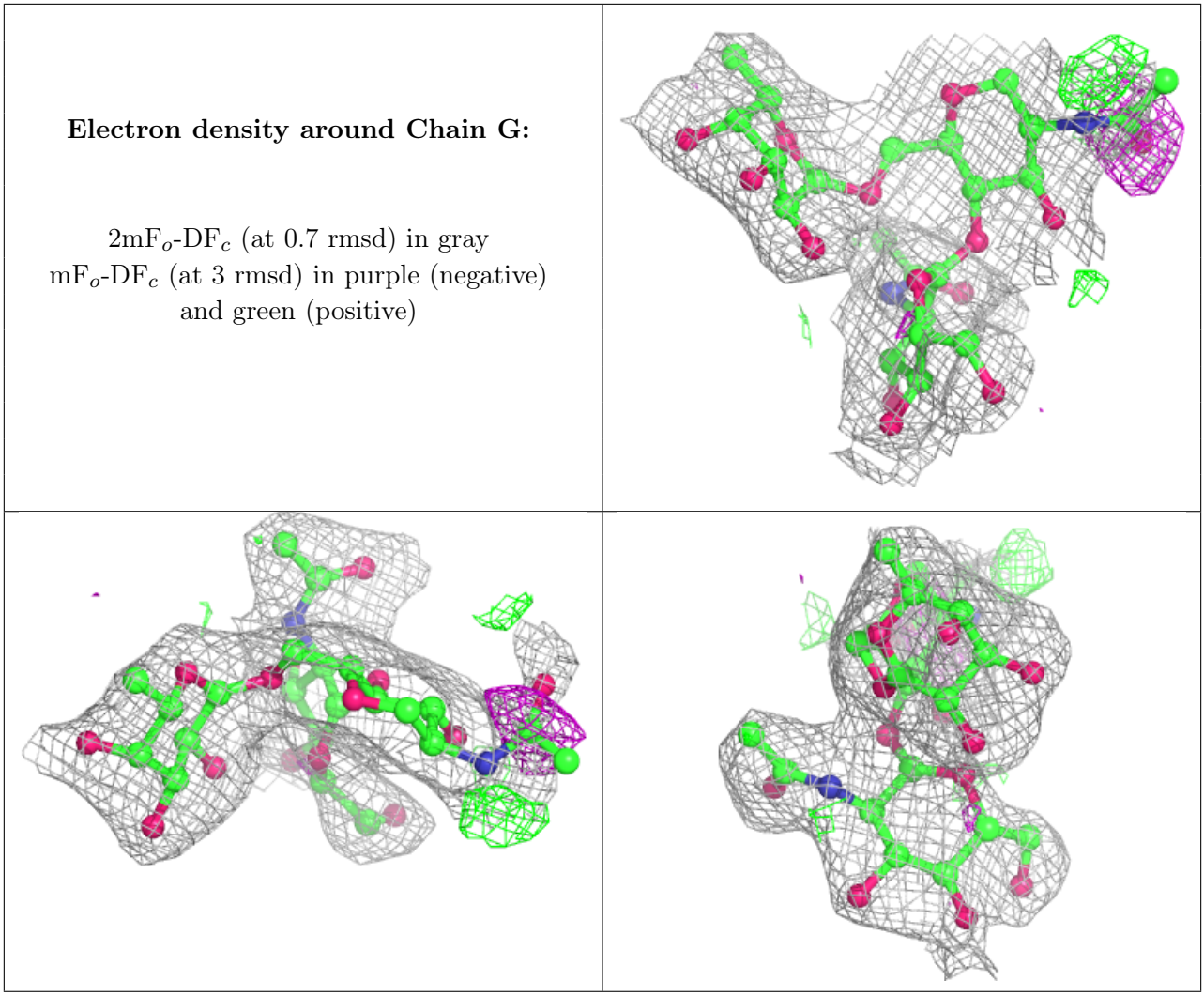
Electron density around Chain F:

$2mF_o$-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
4	NAG	B	651	14/15	0.32	0.26	120,124,126,126	0
3	SO4	C	301	5/5	0.78	0.19	118,120,120,123	0
3	SO4	A	294	5/5	0.78	0.22	66,68,78,81	0
3	SO4	D	300	5/5	0.80	0.22	125,126,127,129	0
3	SO4	B	295	5/5	0.80	0.37	97,97,102,102	0
3	SO4	C	298	5/5	0.88	0.38	89,90,91,95	0
3	SO4	C	296	5/5	0.89	0.25	82,88,89,90	0
3	SO4	A	299	5/5	0.90	0.17	80,86,88,93	0
3	SO4	B	291	5/5	0.91	0.22	83,83,86,86	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	SO4	D	297	5/5	0.95	0.16	64,68,71,74	0
3	SO4	A	290	5/5	0.96	0.12	48,49,51,56	0
3	SO4	D	293	5/5	0.98	0.12	41,45,51,53	0
3	SO4	C	292	5/5	0.98	0.14	52,54,58,59	0

6.5 Other polymers (i)

There are no such residues in this entry.