wwPDB X-ray Structure Validation Summary Report (i)

Oct 6, 2024 – 09:31 AM EDT

PDB ID	:	2A74
Title	:	Human Complement Component C3c
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Deposited on	:	2005-07-04
Resolution	:	2.40 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:

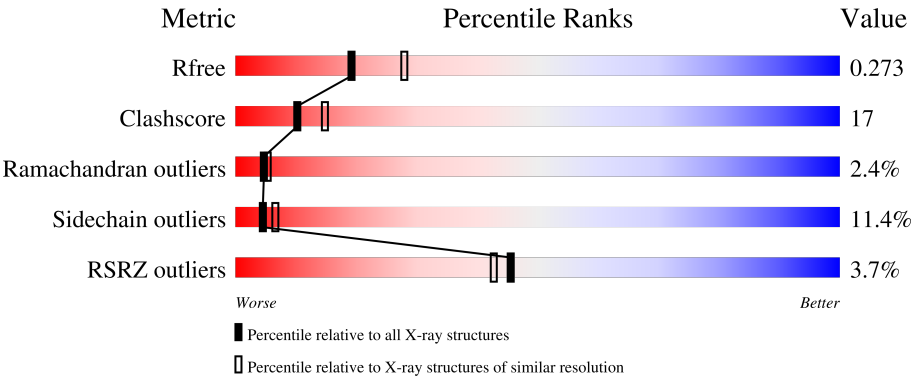
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

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 2.40 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	4642 (2.40-2.40)
Clashscore	180529	5218 (2.40-2.40)
Ramachandran outliers	177936	5158 (2.40-2.40)
Sidechain outliers	177891	5159 (2.40-2.40)
RSRZ outliers	164620	4642 (2.40-2.40)

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	643	3% 65% 26% 6%
1	D	643	5% 66% 24% 7%
2	B	188	2% 78% 14% 5%
2	E	188	6% 69% 21% 6%
3	C	343	3% 51% 26% 7% 14%

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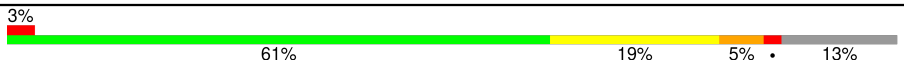
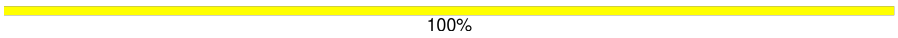
Mol	Chain	Length	Quality of chain
3	F	343	
4	G	2	
4	H	2	

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
4	NDG	G	2	X	-	-	-
4	NDG	H	2	X	-	-	-
5	GOL	A	712	-	-	X	-
5	GOL	D	711	-	-	X	-

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 18389 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 Complement Component C3c.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	630	Total	C	N	O	S	0	0	0
			4907	3127	828	937	15			
1	D	633	Total	C	N	O	S	0	0	0
			4933	3144	833	941	15			

- Molecule 2 is a protein called Complement Component C3c.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	183	Total	C	N	O	S	0	0	0
			1480	950	249	276	5			
2	E	184	Total	C	N	O	S	0	0	0
			1484	954	250	275	5			

- Molecule 3 is a protein called Complement Component C3c.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	296	Total	C	N	O	S	0	0	0
			2407	1517	395	475	20			
3	F	298	Total	C	N	O	S	0	0	0
			2421	1524	397	480	20			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	G	2	Total	C	N	O	0	0	0
			28	16	2	10			

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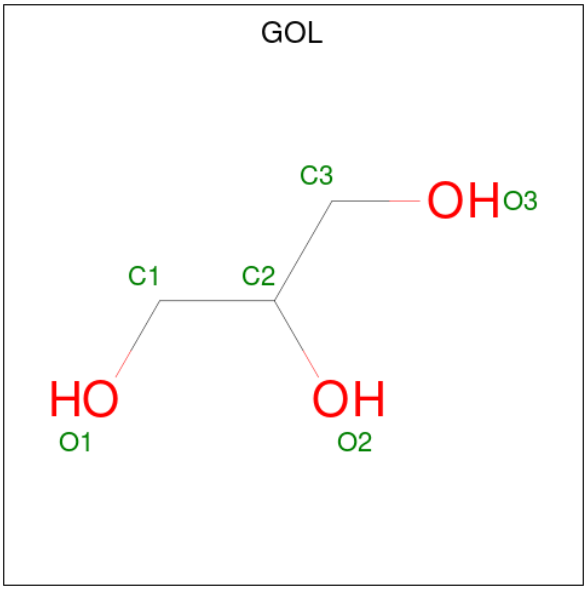
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
4	H	2	Total C N O 28 16 2 10	0	0	0

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

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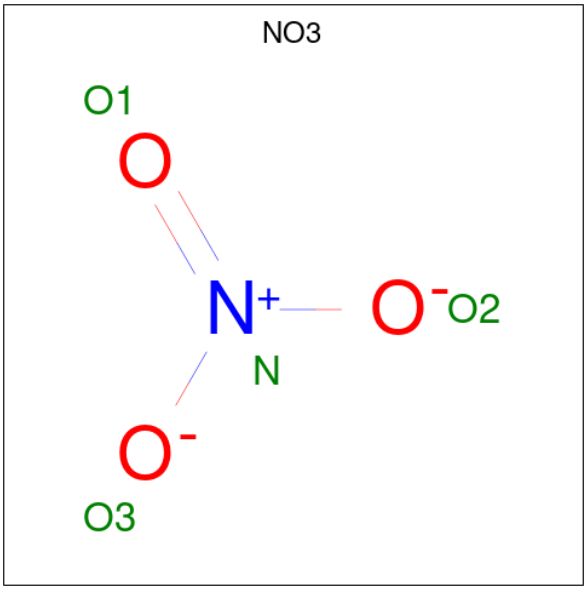
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	E	1	Total C O 6 3 3	0	0
5	F	1	Total C O 6 3 3	0	0
5	F	1	Total C O 6 3 3	0	0

- Molecule 6 is NITRATE ION (three-letter code: NO3) (formula: NO_3).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	C	1	Total N O 4 1 3	0	0
6	F	1	Total N O 4 1 3	0	0
6	F	1	Total N O 4 1 3	0	0

- Molecule 7 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	188	Total O 188 188	0	0
7	B	58	Total O 58 58	0	0
7	C	71	Total O 71 71	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	D	148	Total O 148 148	0	0
7	E	53	Total O 53 53	0	0
7	F	93	Total O 93 93	0	0

3 Residue-property plots (i)

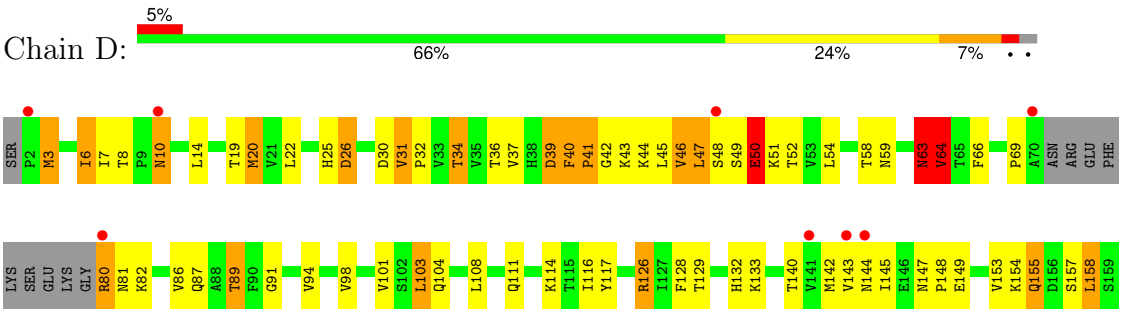
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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.

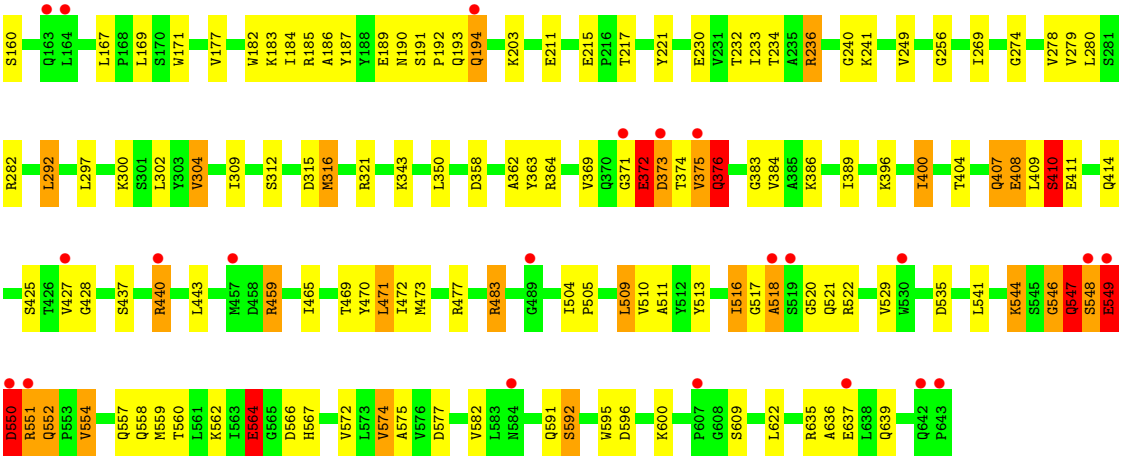
• Molecule 1: Complement Component C3c

Chain A:

• Molecule 1: Complement Component C3c

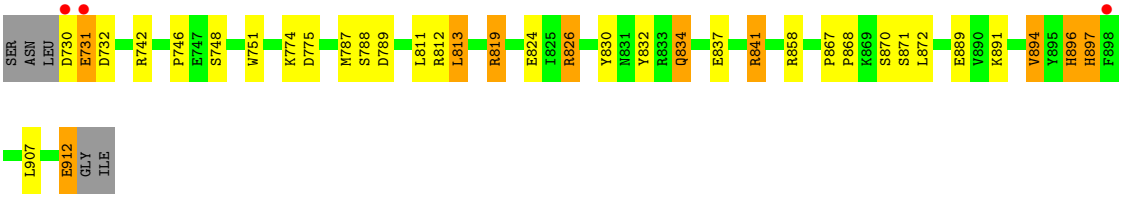
Chain D:





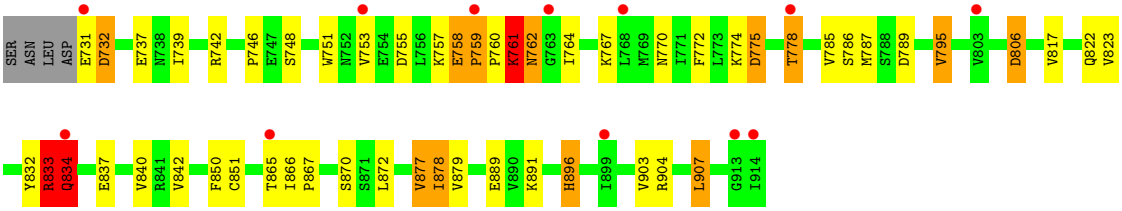
• Molecule 2: Complement Component C3c

Chain B:



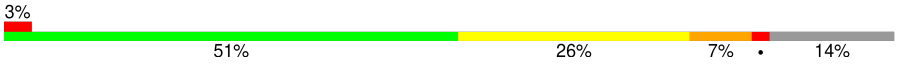
• Molecule 2: Complement Component C3c

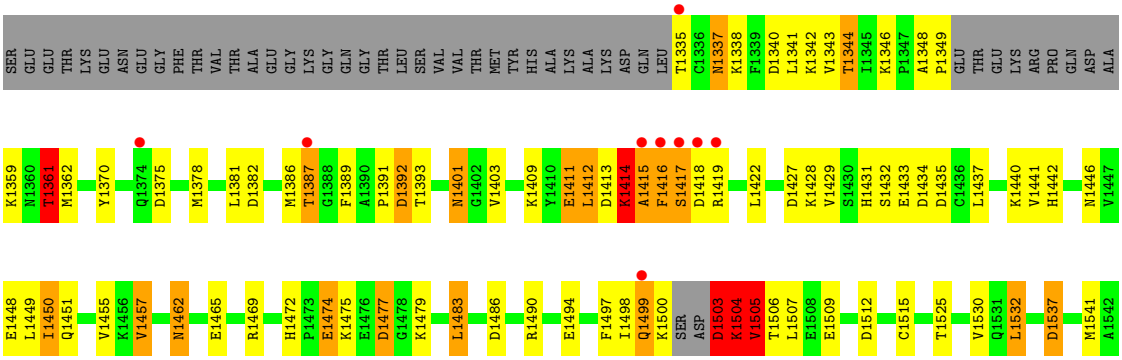
Chain E:

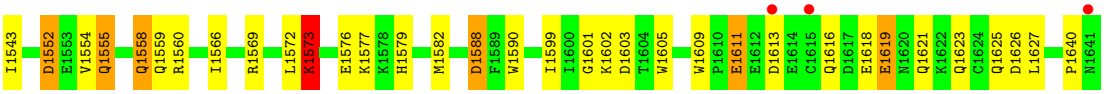


• Molecule 3: Complement Component C3c

Chain C:

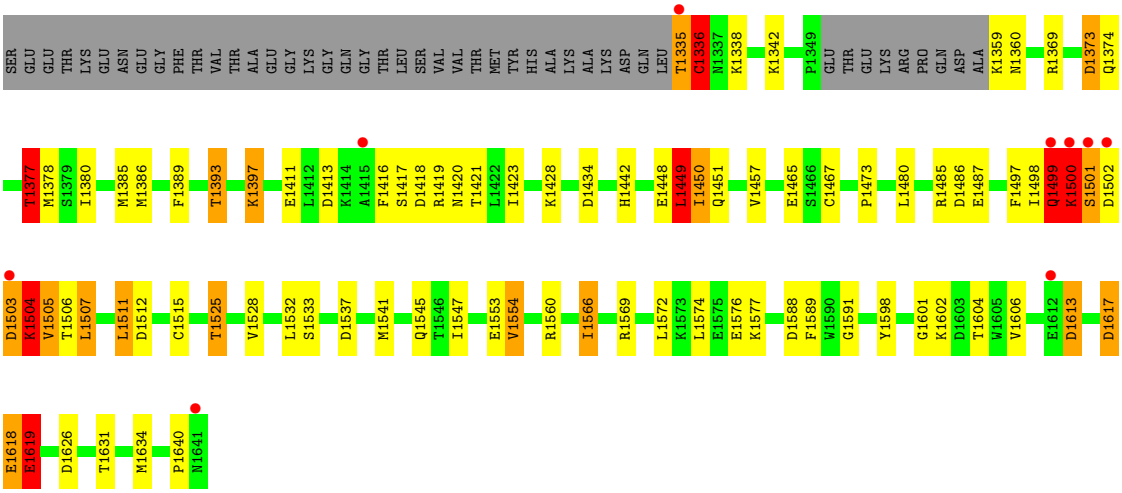






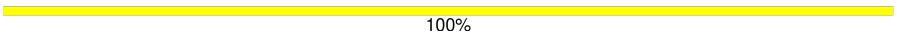
• Molecule 3: Complement Component C3c

Chain F:



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

Chain G:



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

Chain H:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α, β, γ	126.87Å 246.86Å 87.38Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.00 – 2.40 40.00 – 2.40	Depositor EDS
% Data completeness (in resolution range)	97.4 (40.00-2.40) 97.3 (40.00-2.40)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.71 (at 2.31Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.215 , 0.275 0.213 , 0.273	Depositor DCC
R_{free} test set	3124 reflections (2.97%)	wwPDB-VP
Wilson B-factor (Å^2)	47.0	Xtriage
Anisotropy	0.511	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 51.4	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	0.93	EDS
Total number of atoms	18389	wwPDB-VP
Average B, all atoms (Å^2)	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 56.48 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 2.7203e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[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: NDG, GOL, NO3

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	0.45	2/5004 (0.0%)	0.72	11/6799 (0.2%)
1	D	0.65	10/5032 (0.2%)	0.71	10/6839 (0.1%)
2	B	0.49	1/1512 (0.1%)	0.70	1/2055 (0.0%)
2	E	1.21	16/1516 (1.1%)	0.76	6/2060 (0.3%)
3	C	0.40	1/2453 (0.0%)	0.76	16/3305 (0.5%)
3	F	0.59	7/2468 (0.3%)	0.78	11/3327 (0.3%)
All	All	0.62	37/17985 (0.2%)	0.73	55/24385 (0.2%)

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	5
1	D	0	8
3	C	0	1
3	F	0	3
All	All	0	17

The worst 5 of 37 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	564	GLU	CG-CD	19.98	1.81	1.51
2	E	837	GLU	CD-OE1	16.09	1.43	1.25
2	E	761	LYS	CE-NZ	13.09	1.81	1.49
2	E	758	GLU	CD-OE2	12.47	1.39	1.25
3	F	1397	LYS	CE-NZ	12.42	1.80	1.49

The worst 5 of 55 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	564	GLU	OE1-CD-OE2	7.91	132.80	123.30
2	E	761	LYS	CD-CE-NZ	-7.19	95.16	111.70
3	C	1413	ASP	CB-CG-OD2	6.27	123.94	118.30
3	F	1397	LYS	CD-CE-NZ	-6.14	97.58	111.70
1	A	30	ASP	CB-CG-OD2	5.94	123.65	118.30

There are no chirality outliers.

5 of 17 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	255	ASP	Peptide
1	A	403	ARG	Peptide
1	A	549	GLU	Peptide
1	A	63	ASN	Peptide
1	A	69	PRO	Peptide

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	4907	0	4970	204	0
1	D	4933	0	4996	195	0
2	B	1480	0	1501	30	0
2	E	1484	0	1511	46	0
3	C	2407	0	2316	97	0
3	F	2421	0	2326	62	0
4	G	28	0	23	2	0
4	H	28	0	19	1	0
5	A	18	0	24	6	0
5	B	12	0	16	2	0
5	C	12	0	16	0	0
5	D	6	0	8	5	0
5	E	18	0	24	2	0
5	F	12	0	16	4	0
6	C	4	0	0	0	0
6	F	8	0	0	0	0
7	A	188	0	0	11	0
7	B	58	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	C	71	0	0	6	0
7	D	148	0	0	3	0
7	E	53	0	0	2	0
7	F	93	0	0	2	0
All	All	18389	0	17766	601	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 17.

The worst 5 of 601 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:564:GLU:CG	1:D:564:GLU:CD	1.81	1.49
3:F:1397:LYS:CE	3:F:1397:LYS:NZ	1.80	1.44
1:D:544:LYS:CE	1:D:544:LYS:NZ	1.79	1.43
2:E:761:LYS:CE	2:E:761:LYS:NZ	1.81	1.42
1:A:6:ILE:HD11	1:A:20:MET:CG	1.53	1.39

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	624/643 (97%)	582 (93%)	27 (4%)	15 (2%)	5 5
1	D	629/643 (98%)	593 (94%)	21 (3%)	15 (2%)	5 5
2	B	181/188 (96%)	172 (95%)	8 (4%)	1 (1%)	22 33
2	E	182/188 (97%)	167 (92%)	13 (7%)	2 (1%)	12 18
3	C	290/343 (84%)	270 (93%)	9 (3%)	11 (4%)	2 2
3	F	294/343 (86%)	274 (93%)	11 (4%)	9 (3%)	3 3

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	2200/2348 (94%)	2058 (94%)	89 (4%)	53 (2%)	5 5

5 of 53 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	410	SER
1	A	550	ASP
3	C	1361	THR
1	D	41	PRO
1	D	372	GLU

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	555/567 (98%)	498 (90%)	57 (10%)	6 9
1	D	558/567 (98%)	487 (87%)	71 (13%)	3 4
2	B	171/175 (98%)	156 (91%)	15 (9%)	8 13
2	E	171/175 (98%)	155 (91%)	16 (9%)	7 11
3	C	270/309 (87%)	232 (86%)	38 (14%)	3 3
3	F	272/309 (88%)	242 (89%)	30 (11%)	5 7
All	All	1997/2102 (95%)	1770 (89%)	227 (11%)	4 6

5 of 227 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	34	THR
3	F	1553	GLU
1	D	297	LEU
3	F	1528	VAL
3	F	1342	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 49 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	38	HIS
1	D	318	GLN
1	D	81	ASN
1	D	155	GLN
1	D	376	GLN

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)

4 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	$\#\|Z\| > 2$
4	NDG	G	1	4	14,14,15	0.60	0	17,19,21	0.66	0
4	NDG	G	2	4	14,14,15	0.54	0	17,19,21	0.76	0
4	NDG	H	1	4	14,14,15	0.55	0	17,19,21	1.07	1 (5%)
4	NDG	H	2	4	14,14,15	0.92	1 (7%)	17,19,21	0.72	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	NDG	G	1	4	-	0/6/23/26	0/1/1/1
4	NDG	G	2	4	1/1/5/7	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NDG	H	1	4	-	2/6/23/26	0/1/1/1
4	NDG	H	2	4	1/1/5/7	4/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	H	2	NDG	C1-C2	-2.91	1.48	1.52

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	H	1	NDG	O4-C4-C5	2.71	116.00	109.32

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	G	2	NDG	C1
4	H	2	NDG	C1

5 of 8 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	H	2	NDG	C8-C7-N2-C2
4	H	2	NDG	O7-C7-N2-C2
4	G	2	NDG	O5-C5-C6-O6
4	H	1	NDG	O5-C5-C6-O6
4	H	2	NDG	O5-C5-C6-O6

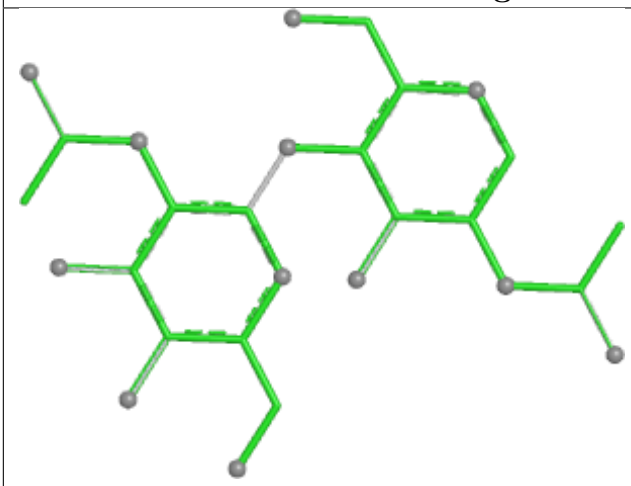
There are no ring outliers.

3 monomers are involved in 3 short contacts:

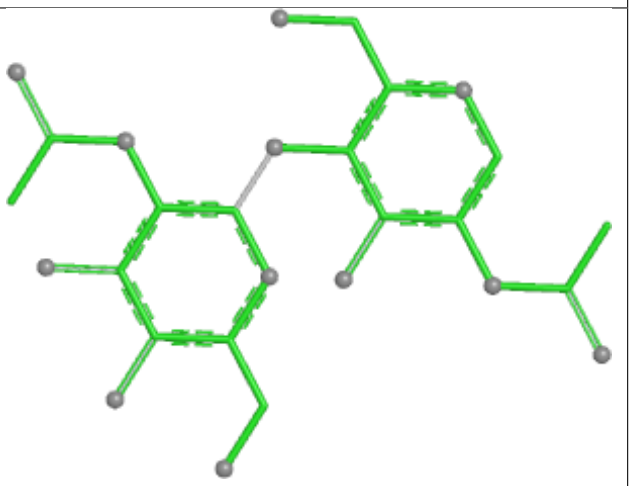
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	G	1	NDG	2	0
4	H	1	NDG	1	0
4	G	2	NDG	1	0

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

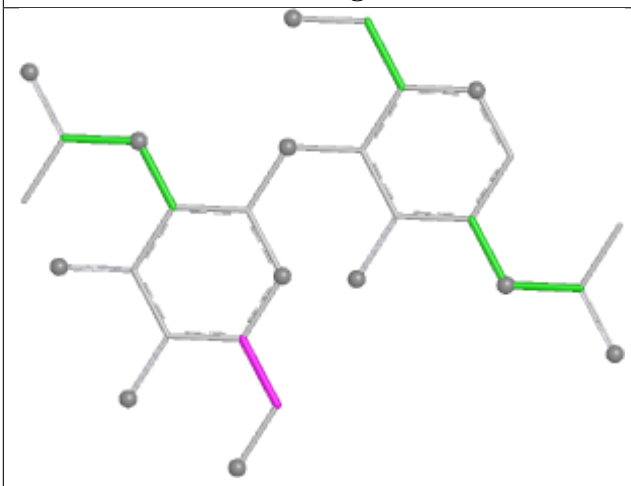
Oligosaccharide Chain G



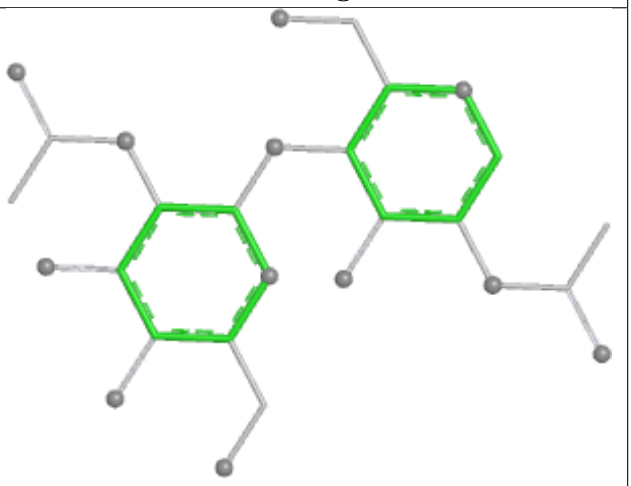
Bond lengths



Bond angles

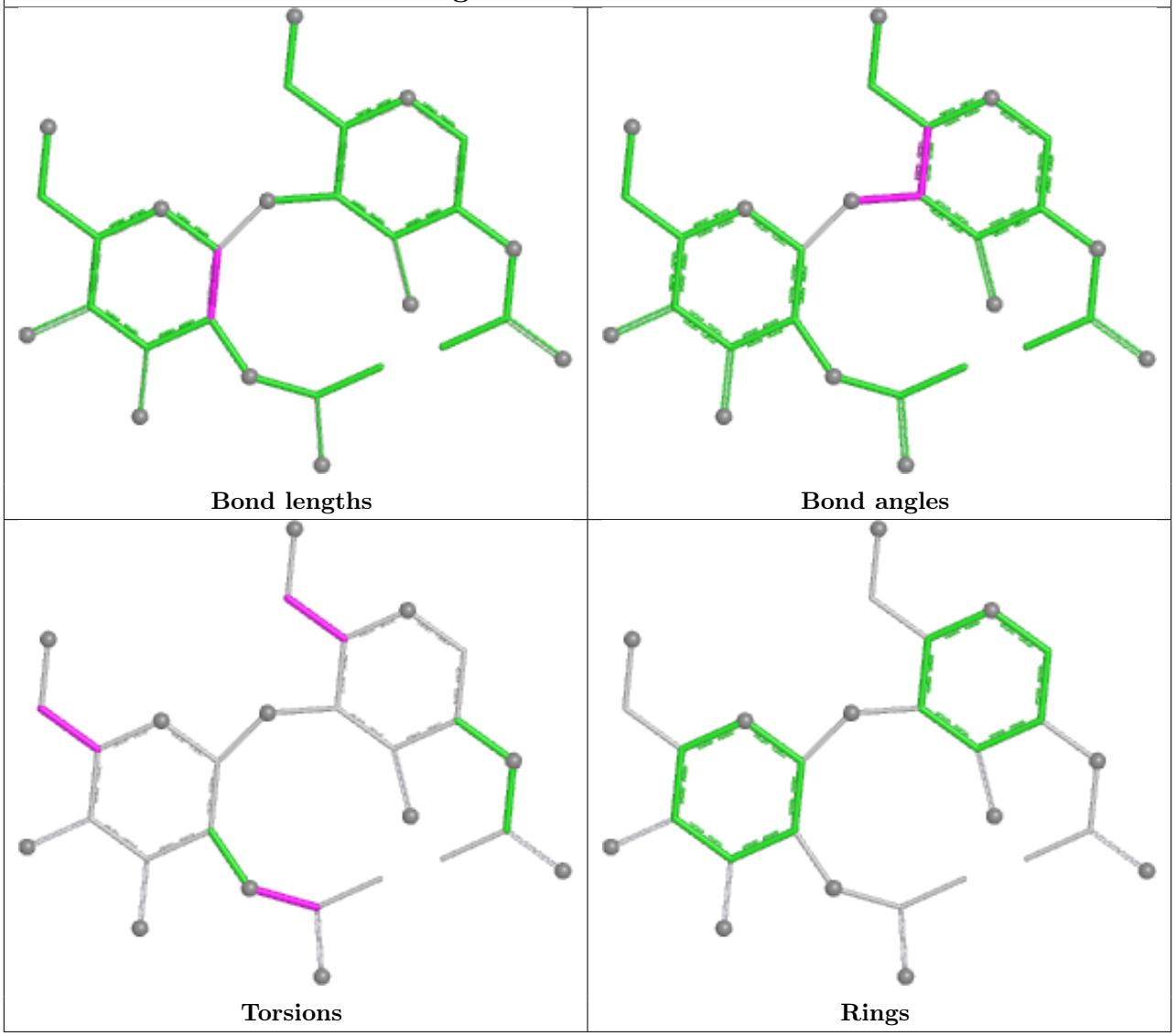


Torsions



Rings

Oligosaccharide Chain H



5.6 Ligand geometry (i)

16 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	$\#\|Z\| > 2$
5	GOL	F	707	-	5,5,5	0.38	0	5,5,5	0.29	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
5	GOL	A	712	-	5,5,5	0.33	0	5,5,5	0.43	0
5	GOL	E	706	-	5,5,5	0.38	0	5,5,5	0.50	0
6	NO3	C	801	-	1,3,3	3.33	1 (100%)	0,3,3	-	-
5	GOL	C	708	-	5,5,5	0.31	0	5,5,5	0.44	0
5	GOL	B	701	-	5,5,5	0.40	0	5,5,5	0.54	0
5	GOL	F	710	-	5,5,5	0.36	0	5,5,5	0.25	0
5	GOL	B	702	-	5,5,5	0.41	0	5,5,5	0.24	0
6	NO3	F	802	-	1,3,3	3.33	1 (100%)	0,3,3	-	-
6	NO3	F	803	-	1,3,3	3.26	1 (100%)	0,3,3	-	-
5	GOL	C	709	-	5,5,5	0.32	0	5,5,5	0.45	0
5	GOL	A	713	-	5,5,5	0.44	0	5,5,5	0.40	0
5	GOL	E	705	-	5,5,5	0.38	0	5,5,5	0.37	0
5	GOL	D	711	-	5,5,5	0.39	0	5,5,5	0.39	0
5	GOL	E	704	-	5,5,5	0.43	0	5,5,5	0.50	0
5	GOL	A	703	-	5,5,5	0.35	0	5,5,5	0.23	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	GOL	F	707	-	-	3/4/4/4	-
5	GOL	A	712	-	-	0/4/4/4	-
5	GOL	E	706	-	-	2/4/4/4	-
5	GOL	C	708	-	-	2/4/4/4	-
5	GOL	B	701	-	-	4/4/4/4	-
5	GOL	F	710	-	-	3/4/4/4	-
5	GOL	B	702	-	-	3/4/4/4	-
5	GOL	C	709	-	-	0/4/4/4	-
5	GOL	A	713	-	-	1/4/4/4	-
5	GOL	E	705	-	-	2/4/4/4	-
5	GOL	D	711	-	-	0/4/4/4	-
5	GOL	E	704	-	-	1/4/4/4	-
5	GOL	A	703	-	-	2/4/4/4	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	C	801	NO3	O1-N	3.33	1.40	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	F	802	NO3	O1-N	3.33	1.40	1.24
6	F	803	NO3	O1-N	3.26	1.40	1.24

There are no bond angle outliers.

There are no chirality outliers.

5 of 23 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	703	GOL	C1-C2-C3-O3
5	B	701	GOL	O1-C1-C2-C3
5	B	701	GOL	C1-C2-C3-O3
5	B	701	GOL	O2-C2-C3-O3
5	B	702	GOL	O1-C1-C2-C3

There are no ring outliers.

7 monomers are involved in 19 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	F	707	GOL	3	0
5	A	712	GOL	4	0
5	B	701	GOL	2	0
5	F	710	GOL	1	0
5	E	705	GOL	2	0
5	D	711	GOL	5	0
5	A	703	GOL	2	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	630/643 (97%)	0.40	17 (2%)	56	53	30, 44, 55, 73	0
1	D	633/643 (98%)	0.58	30 (4%)	37	34	33, 44, 56, 78	0
2	B	183/188 (97%)	0.21	3 (1%)	70	67	32, 44, 52, 59	0
2	E	184/188 (97%)	0.70	12 (6%)	26	24	37, 44, 51, 71	0
3	C	296/343 (86%)	0.33	12 (4%)	42	39	33, 45, 56, 65	0
3	F	298/343 (86%)	0.45	9 (3%)	52	49	30, 45, 57, 68	0
All	All	2224/2348 (94%)	0.46	83 (3%)	45	43	30, 44, 55, 78	0

The worst 5 of 83 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	F	1502	ASP	4.8
3	F	1501	SER	4.7
3	C	1416	PHE	4.6
3	F	1335	THR	3.9
3	C	1417	SER	3.6

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

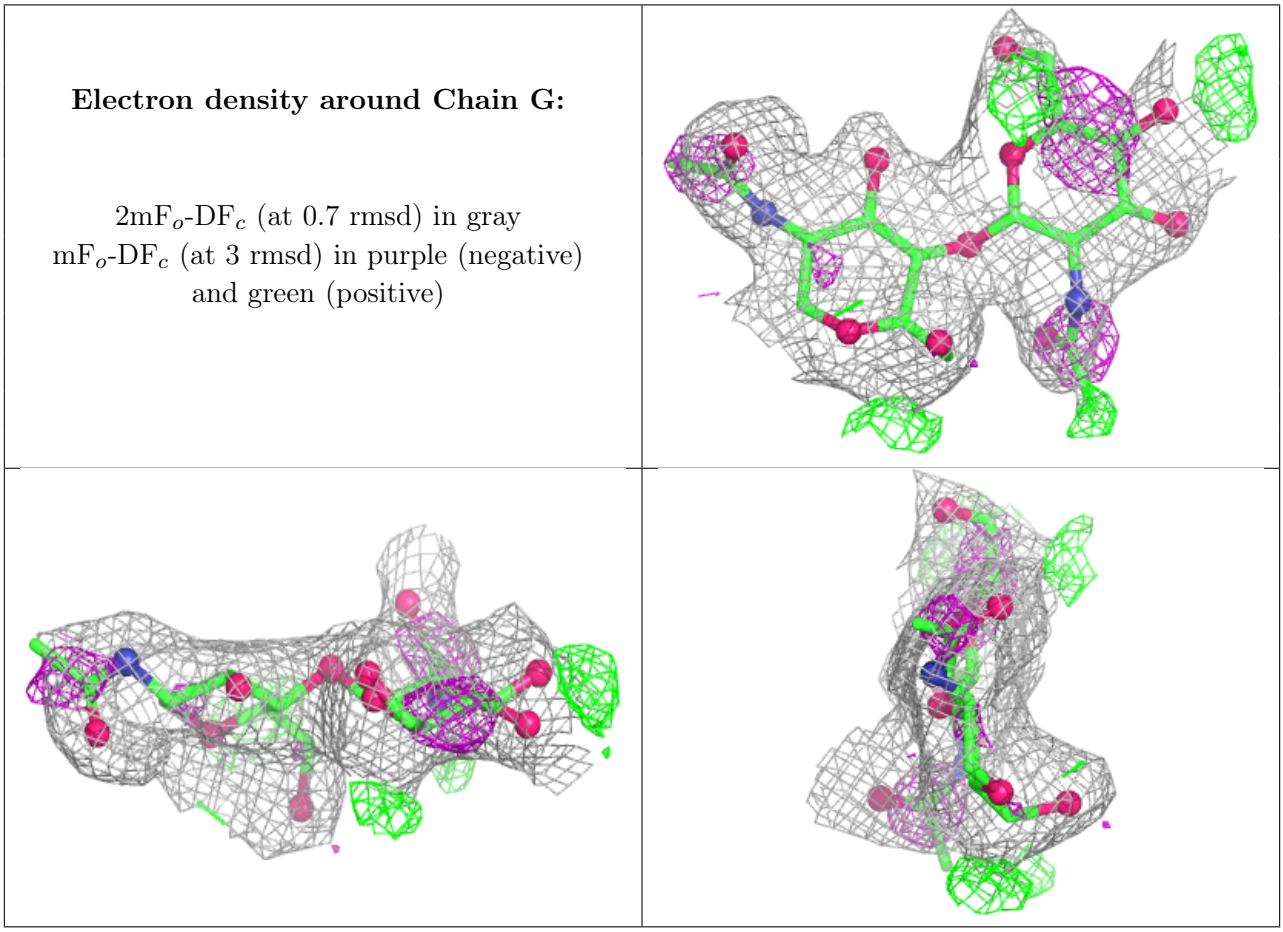
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' 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
4	NDG	H	2	14/15	0.24	0.19	75,76,78,79	0
4	NDG	G	2	14/15	0.54	0.17	64,66,69,69	0
4	NDG	H	1	14/15	0.70	0.14	61,66,70,73	0
4	NDG	G	1	14/15	0.79	0.12	54,57,59,62	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.

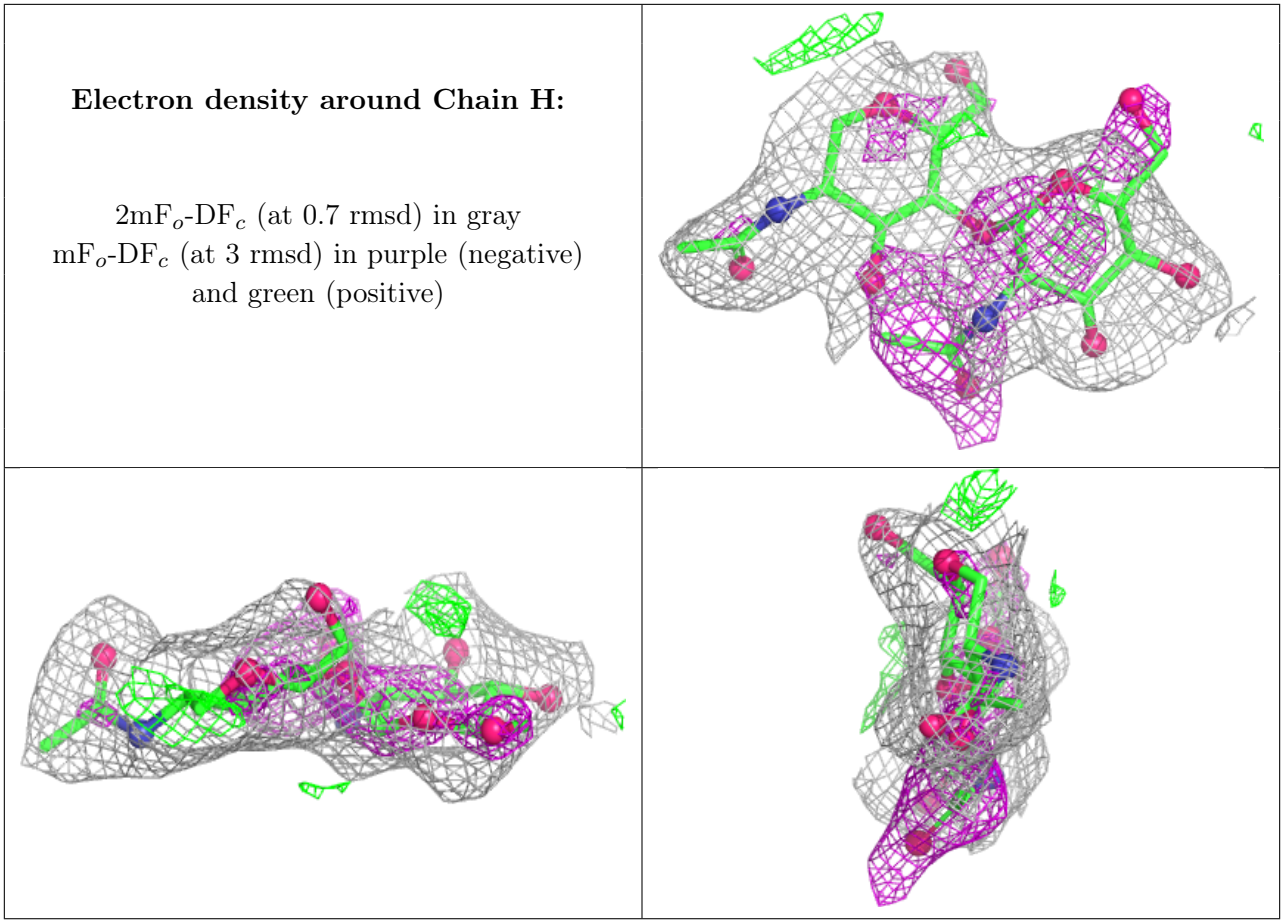
Electron density around Chain G:

$2mF_o$-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

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	GOL	F	707	6/6	0.62	0.16	86,88,88,89	0
5	GOL	A	712	6/6	0.65	0.18	78,81,82,85	0
5	GOL	C	708	6/6	0.70	0.23	66,72,73,75	0
5	GOL	E	706	6/6	0.72	0.27	57,60,63,64	0
5	GOL	A	703	6/6	0.73	0.23	60,62,63,65	0
5	GOL	B	702	6/6	0.75	0.15	87,88,88,89	0
5	GOL	C	709	6/6	0.75	0.17	90,90,91,91	0
5	GOL	F	710	6/6	0.75	0.20	72,73,73,74	0
5	GOL	D	711	6/6	0.76	0.15	81,83,84,88	0
5	GOL	A	713	6/6	0.77	0.20	61,65,66,68	0
6	NO3	F	802	4/4	0.79	0.22	89,89,89,90	0
6	NO3	F	803	4/4	0.79	0.18	73,73,73,73	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
6	NO3	C	801	4/4	0.82	0.17	77,77,77,77	0
5	GOL	E	705	6/6	0.84	0.26	62,66,66,67	0
5	GOL	E	704	6/6	0.86	0.19	45,49,51,52	0
5	GOL	B	701	6/6	0.87	0.15	45,46,48,48	0

6.5 Other polymers (i)

There are no such residues in this entry.