



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 7, 2025 – 06:20 am BST

PDB ID : 9Q8L / pdb_00009q8l
Title : Crystal Structure of 21A08Ap1-Fab in Complex with Human PD-1 at 1.85 angstrom Resolution
Authors : Murer, P.; Petersen, L.; Egli, N.; Salazar, U.; Neubert, P.; Zurbach, A.; Rau, A.; Stocker, C.; Katopodis, A.; Huber, C.; Carr, K.; Arduin, A.
Deposited on : 2025-02-25
Resolution : 1.85 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 : 4-5-2 with Phenix2.0rc1
Mogul : 1.8.4, CSD as541be (2020)
Xtriage (Phenix) : 2.0rc1
EDS : 3.0
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4 : 9.0.006 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.45.1

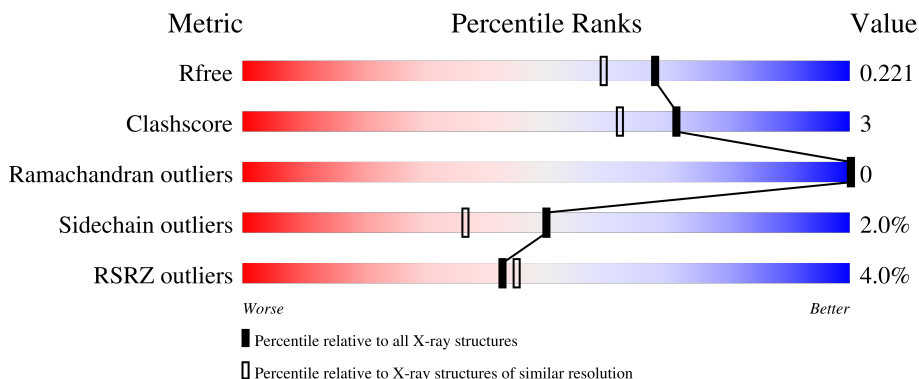
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.85 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	3097 (1.86-1.86)
Clashscore	180529	3359 (1.86-1.86)
Ramachandran outliers	177936	3335 (1.86-1.86)
Sidechain outliers	177891	3335 (1.86-1.86)
RSRZ outliers	164620	3097 (1.86-1.86)

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 $\leq 5\%$. 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	H	218	<div> <div>2%</div> <div> <div></div> <div>93%</div> <div>7%</div> </div> </div>
2	L	216	<div> <div>3%</div> <div> <div></div> <div>86%</div> <div>12%</div> </div> </div>
3	A	147	<div> <div>7%</div> <div> <div></div> <div>67%</div> <div>9%</div> <div>24%</div> </div> </div>
4	B	3	<div> <div></div> <div> <div>67%</div> <div>33%</div> </div> </div>
4	C	3	<div> <div></div> <div>100%</div> </div>

2 Entry composition [i](#)

There are 9 unique types of molecules in this entry. The entry contains 4593 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 Heavy chain of huIgG1-Fab.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	H	218	Total	C	N	O	S	0	4	0
			1625	1023	268	324	10			

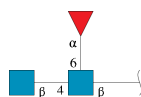
- Molecule 2 is a protein called Light chain of huIgG1-Fab.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	L	215	Total	C	N	O	S	0	7	0
			1621	1011	271	334	5			

- Molecule 3 is a protein called Programmed cell death protein 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	A	112	Total	C	N	O	S	0	2	0
			889	557	163	164	5			

- Molecule 4 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.



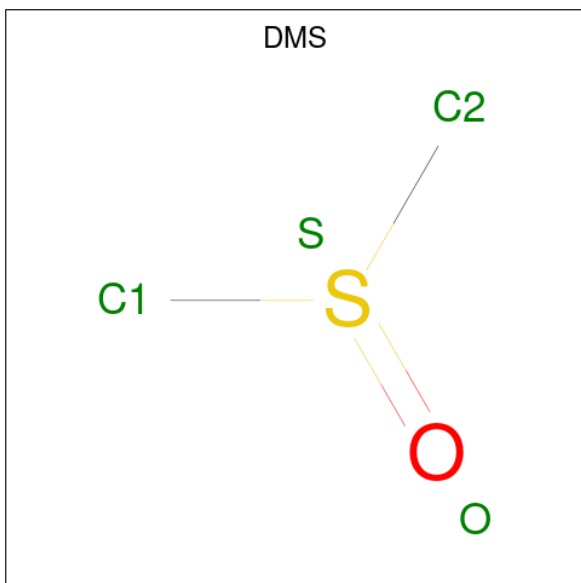
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	B	3	Total	C	N	O		0	0	0
			38	22	2	14				
4	C	3	Total	C	N	O		0	0	0
			38	22	2	14				

- Molecule 5 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



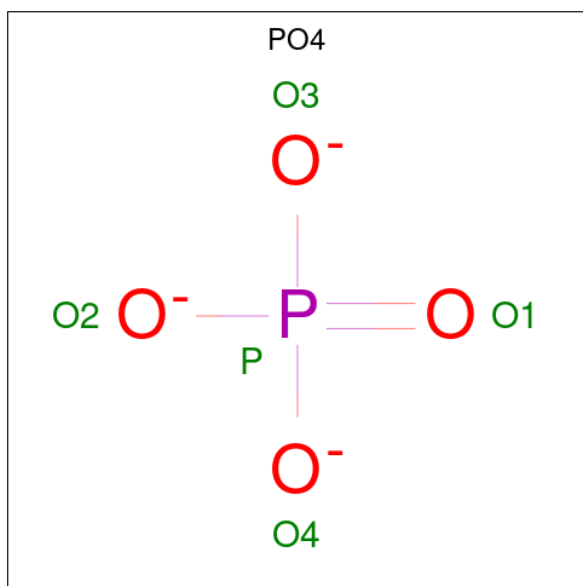
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	H	1	Total	C	O	0	0
			4	2	2		
5	H	1	Total	C	O	0	0
			4	2	2		
5	H	1	Total	C	O	0	0
			4	2	2		
5	L	1	Total	C	O	0	0
			4	2	2		

- Molecule 6 is DIMETHYL SULFOXIDE (CCD ID: DMS) (formula: C_2H_6OS).



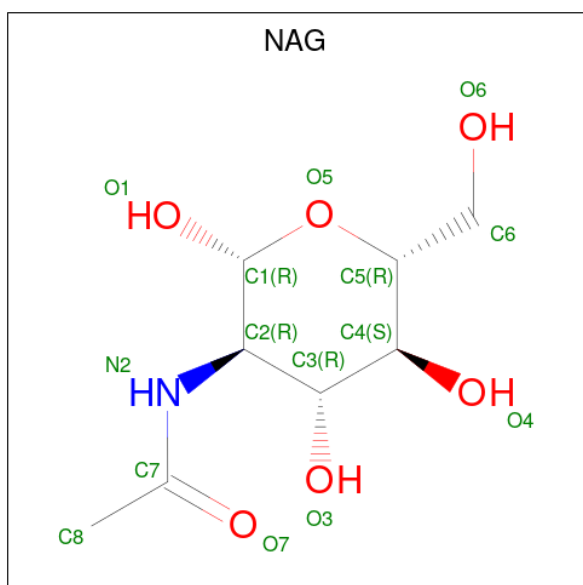
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	H	1	Total	C	O	S	0	0
			4	2	1	1		

- Molecule 7 is PHOSPHATE ION (CCD ID: PO4) (formula: O_4P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	L	1	Total	O	P	0	0
			5	4	1		

- Molecule 8 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



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

- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	H	142	Total	O	0	0
			142	142		
9	L	135	Total	O	0	0
			135	135		
9	A	66	Total	O	0	0
			66	66		

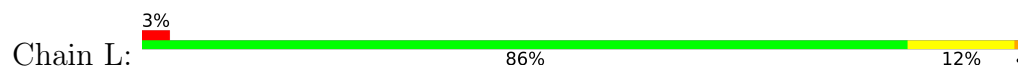
3 Residue-property plots [i](#)

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.

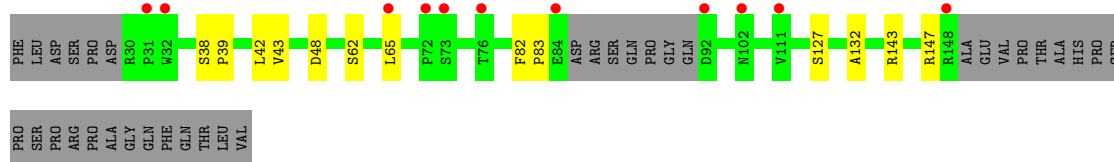
- Molecule 1: Heavy chain of huIgG1-Fab



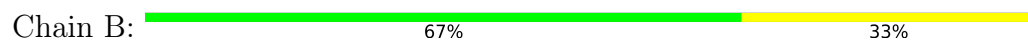
- Molecule 2: Light chain of huIgG1-Fab



- Molecule 3: Programmed cell death protein 1



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



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



MAG1
MAG2
FUC3

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	61.84Å 70.24Å 163.68Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	81.84 – 1.85 81.84 – 1.85	Depositor EDS
% Data completeness (in resolution range)	100.0 (81.84-1.85) 100.0 (81.84-1.85)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.20 (at 1.84Å)	Xtriage
Refinement program	REFMAC 5.8.0430	Depositor
R, R_{free}	0.178 , 0.216 0.188 , 0.221	Depositor DCC
R_{free} test set	3096 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	29.7	Xtriage
Anisotropy	0.016	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 38.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	4593	wwPDB-VP
Average B, all atoms (Å ²)	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.90% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ 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: PO4, EDO, NAG, FUC, DMS

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	H	0.67	0/1668	1.04	0/2271
2	L	0.68	0/1673	1.13	7/2287 (0.3%)
3	A	0.69	0/912	1.12	1/1239 (0.1%)
All	All	0.68	0/4253	1.09	8/5797 (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
2	L	0	3
3	A	0	2
All	All	0	5

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L	62	ARG	CD-NE-CZ	6.91	134.07	124.40
2	L	62	ARG	NE-CZ-NH2	-6.44	113.40	119.20
2	L	5	THR	CA-CB-OG1	-6.32	100.12	109.60
2	L	160	LYS	CB-CA-C	6.11	120.02	109.15
3	A	48	ASP	CA-CB-CG	5.92	118.53	112.60
2	L	3	VAL	N-CA-CB	-5.55	98.99	111.87
2	L	94	ASP	CA-CB-CG	5.22	117.82	112.60
2	L	170	LYS	CB-CA-C	5.11	118.16	109.53

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	A	143	ARG	Sidechain
3	A	147	ARG	Sidechain
2	L	17	ARG	Sidechain
2	L	62	ARG	Sidechain
2	L	80	ARG	Sidechain

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	H	1625	0	1580	9	0
2	L	1621	0	1560	15	0
3	A	889	0	862	4	0
4	B	38	0	34	0	0
4	C	38	0	34	0	0
5	H	12	0	18	0	0
5	L	4	0	6	1	0
6	H	4	0	6	0	0
7	L	5	0	0	0	0
8	A	14	0	13	0	0
9	A	66	0	0	0	0
9	H	142	0	0	0	0
9	L	135	0	0	4	0
All	All	4593	0	4113	27	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 3.

All (27) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:209[A]:THR:HG23	9:L:443:HOH:O	1.82	0.80
2:L:171:GLN:HE21	2:L:177:ALA:HB2	1.47	0.80
2:L:108:THR:HG23	9:L:476:HOH:O	1.84	0.76
2:L:124:PRO:HD3	2:L:136:LEU:CD2	2.20	0.71
3:A:39:PRO:HG3	3:A:42:LEU:HD13	1.84	0.59
2:L:142:ASP:H	2:L:171:GLN:HE22	1.52	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:48:VAL:HG13	1:H:64:LEU:HD11	1.89	0.55
2:L:142:ASP:H	2:L:171:GLN:NE2	2.09	0.51
1:H:166:HIS:HD2	9:L:480:HOH:O	1.94	0.50
1:H:212:ARG:HD3	1:H:214:GLU:OE1	2.12	0.49
3:A:127:SER:O	3:A:132:ALA:HA	2.13	0.48
1:H:180:LEU:C	1:H:180:LEU:HD12	2.38	0.48
1:H:125:PRO:HD3	1:H:211:LYS:HE2	1.96	0.47
2:L:6:GLN:HE21	2:L:102:GLY:HA3	1.78	0.46
2:L:6:GLN:HE22	2:L:88:TYR:HA	1.79	0.46
2:L:92:TRP:CH2	3:A:43:VAL:HG11	2.51	0.46
2:L:170:LYS:HE3	2:L:174:ASN:HA	1.98	0.46
1:H:83:MET:HE1	1:H:94:TYR:CZ	2.51	0.45
2:L:79:LEU:HD11	2:L:107:LEU:HD21	1.99	0.45
1:H:203:LYS:N	1:H:204:PRO:CD	2.80	0.44
1:H:198[A]:CYS:SG	1:H:211:LYS:HB3	2.59	0.43
3:A:82:PHE:HA	3:A:83:PRO:C	2.45	0.41
1:H:166:HIS:HE1	9:L:403:HOH:O	2.03	0.41
2:L:124:PRO:HD3	2:L:136:LEU:HD23	2.01	0.41
2:L:40:LEU:HD23	2:L:85:ALA:HB2	2.03	0.41
2:L:120:THR:OG1	5:L:302:EDO:H12	2.21	0.41
2:L:55[A]:ARG:HD3	2:L:63:PHE:O	2.21	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	H	220/218 (101%)	217 (99%)	3 (1%)	0	100	100
2	L	220/216 (102%)	212 (96%)	8 (4%)	0	100	100
3	A	110/147 (75%)	107 (97%)	3 (3%)	0	100	100
All	All	550/581 (95%)	536 (98%)	14 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	H	183/182 (100%)	180 (98%)	3 (2%)	58	46
2	L	184/181 (102%)	180 (98%)	4 (2%)	47	32
3	A	98/129 (76%)	94 (96%)	4 (4%)	26	11
All	All	465/492 (94%)	454 (98%)	11 (2%)	50	29

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	H	32	ASN
1	H	140	LEU
1	H	152	VAL
2	L	3	VAL
2	L	71	SER
2	L	204[A]	SER
2	L	204[B]	SER
3	A	38[A]	SER
3	A	38[B]	SER
3	A	62	SER
3	A	65	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	H	84	ASN
1	H	166	HIS
2	L	6	GLN
2	L	112	GLN
2	L	130	GLN
2	L	171	GLN
2	L	192	HIS

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Mol	Chain	Res	Type
3	A	33	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

6 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	NAG	B	1	4,3	14,14,15	0.41	0	17,19,21	0.45	0
4	NAG	B	2	4	14,14,15	0.42	0	17,19,21	0.61	0
4	FUC	B	3	4	10,10,11	0.30	0	14,14,16	0.60	1 (7%)
4	NAG	C	1	4,3	14,14,15	0.54	0	17,19,21	1.00	1 (5%)
4	NAG	C	2	4	14,14,15	1.00	2 (14%)	17,19,21	1.61	3 (17%)
4	FUC	C	3	4	10,10,11	0.53	0	14,14,16	0.95	1 (7%)

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	1	4,3	-	2/6/23/26	0/1/1/1
4	NAG	B	2	4	-	0/6/23/26	0/1/1/1
4	FUC	B	3	4	-	-	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	C	1	4,3	-	0/6/23/26	0/1/1/1
4	NAG	C	2	4	-	0/6/23/26	0/1/1/1
4	FUC	C	3	4	-	-	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	2	NAG	O5-C1	2.59	1.47	1.43
4	C	2	NAG	C1-C2	2.28	1.55	1.52

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	2	NAG	O5-C1-C2	5.17	119.45	111.29
4	C	2	NAG	O3-C3-C2	-2.86	103.55	109.47
4	C	3	FUC	O5-C1-C2	2.22	114.19	110.77
4	C	1	NAG	O4-C4-C5	-2.15	103.95	109.30
4	B	3	FUC	C1-C2-C3	2.10	112.25	109.67
4	C	2	NAG	C1-O5-C5	2.10	115.03	112.19

There are no chirality outliers.

All (2) torsion outliers are listed below:

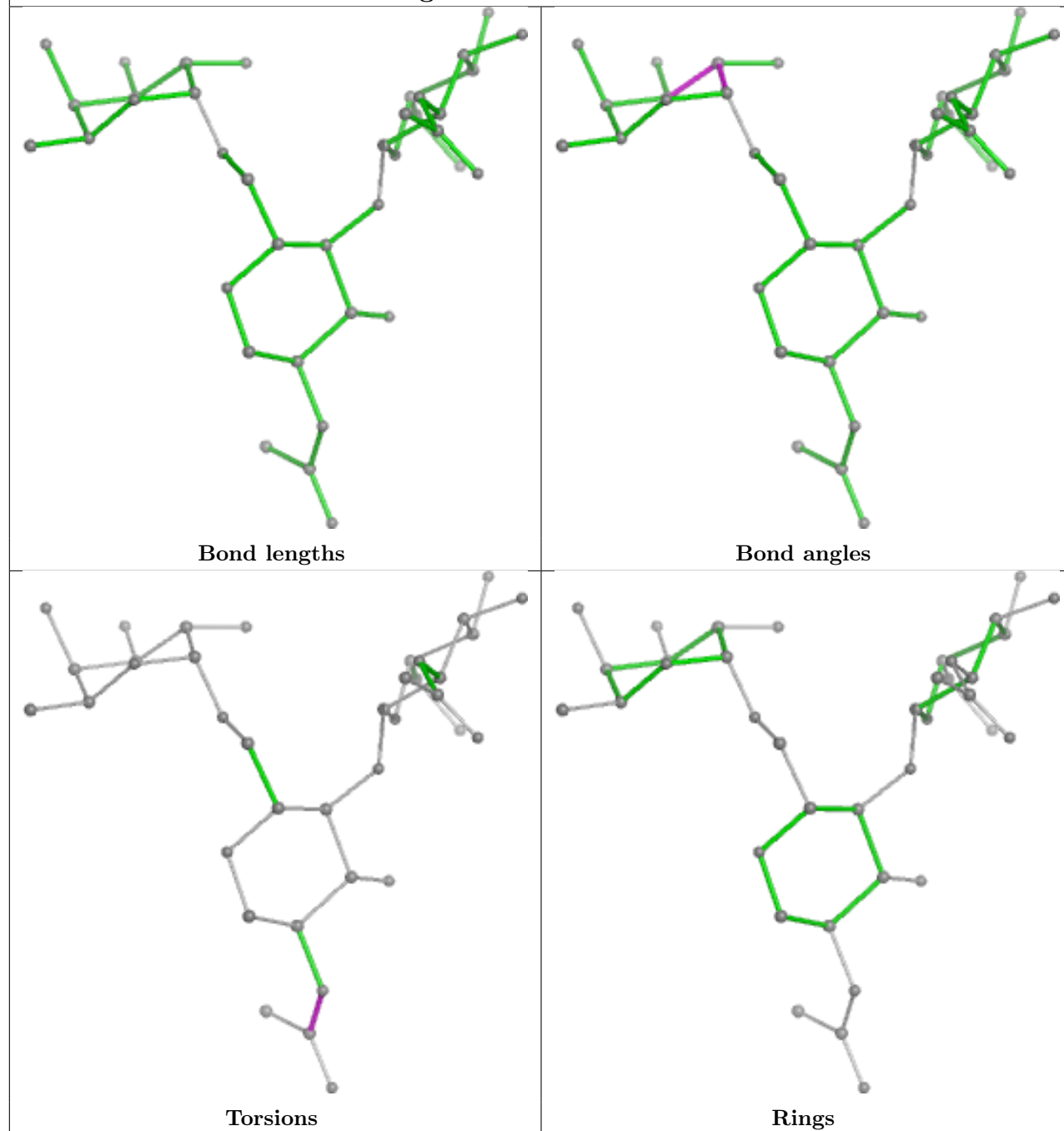
Mol	Chain	Res	Type	Atoms
4	B	1	NAG	C8-C7-N2-C2
4	B	1	NAG	O7-C7-N2-C2

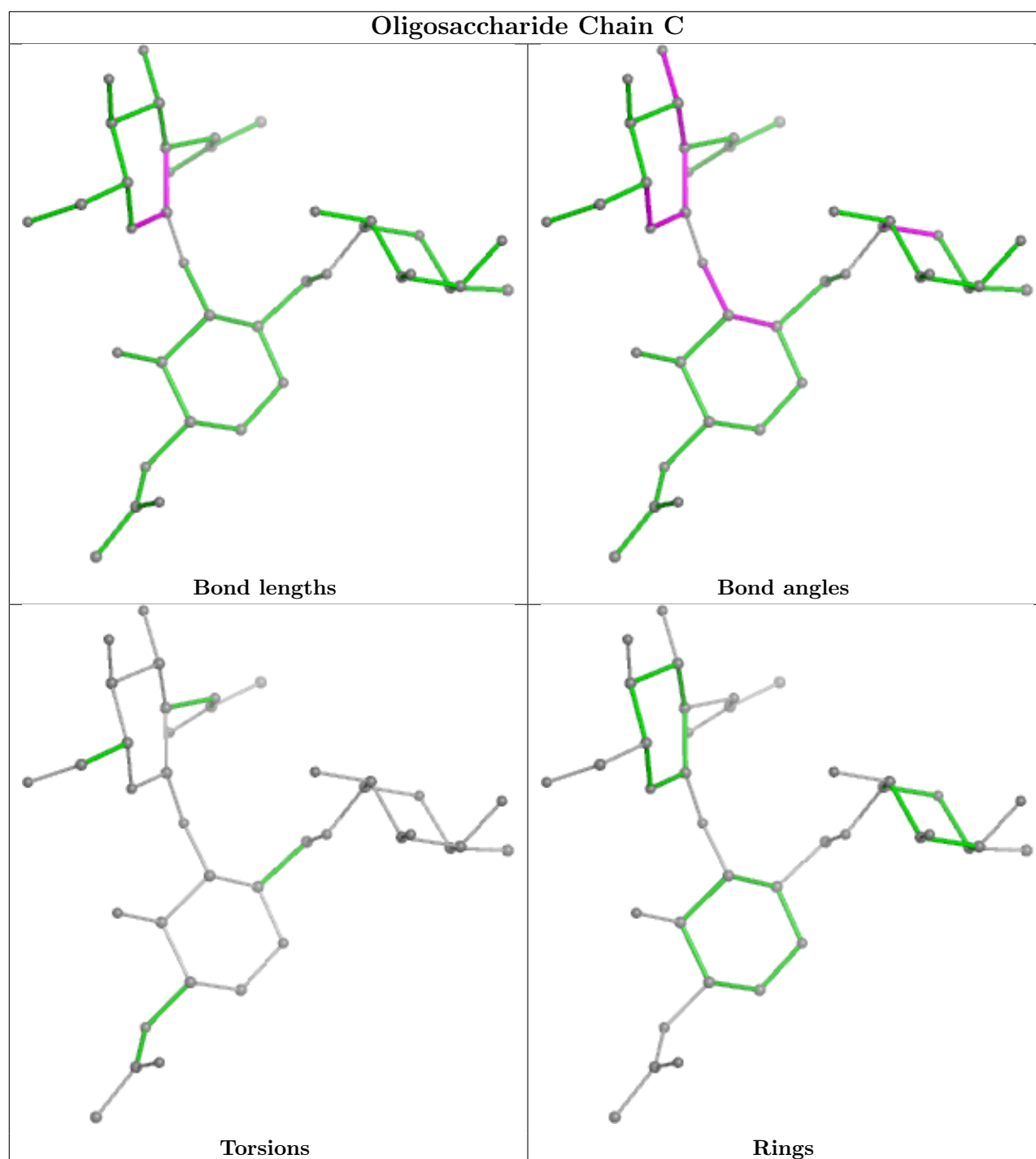
There are no ring outliers.

No monomer is involved in short contacts.

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

Oligosaccharide Chain B





5.6 Ligand geometry [i](#)

7 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	$\# Z > 2$
8	NAG	A	201	3	14,14,15	0.39	0	17,19,21	0.58	0
5	EDO	H	302	-	3,3,3	0.11	0	2,2,2	0.25	0
6	DMS	H	304	-	3,3,3	0.46	0	3,3,3	0.18	0
5	EDO	L	302	-	3,3,3	0.51	0	2,2,2	0.62	0
5	EDO	H	301	-	3,3,3	0.25	0	2,2,2	0.43	0
7	PO4	L	301	-	4,4,4	1.22	1 (25%)	6,6,6	0.42	0
5	EDO	H	303	-	3,3,3	0.46	0	2,2,2	0.49	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
8	NAG	A	201	3	-	3/6/23/26	0/1/1/1
5	EDO	H	302	-	-	1/1/1/1	-
5	EDO	L	302	-	-	1/1/1/1	-
5	EDO	H	301	-	-	0/1/1/1	-
5	EDO	H	303	-	-	1/1/1/1	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	L	301	PO4	P-O1	2.20	1.56	1.50

There are no bond angle outliers.

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	A	201	NAG	C8-C7-N2-C2
8	A	201	NAG	O7-C7-N2-C2
5	H	302	EDO	O1-C1-C2-O2
5	H	303	EDO	O1-C1-C2-O2
5	L	302	EDO	O1-C1-C2-O2
8	A	201	NAG	C1-C2-N2-C7

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	L	302	EDO	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, 95th 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	H	218/218 (100%)	-0.01	5 (2%) 61 63	11, 29, 48, 62	4 (1%)
2	L	215/216 (99%)	0.13	6 (2%) 55 58	15, 30, 51, 68	7 (3%)
3	A	112/147 (76%)	0.75	11 (9%) 14 14	17, 39, 67, 84	2 (1%)
All	All	545/581 (93%)	0.20	22 (4%) 43 45	11, 31, 54, 84	13 (2%)

All (22) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	L	216	SER	4.3
3	A	92	ASP	4.1
1	H	56	PHE	4.0
1	H	64	LEU	3.5
2	L	215	CYS	3.4
3	A	31	PRO	3.2
1	H	5	LEU	2.8
2	L	2	SER	2.8
3	A	111	VAL	2.8
3	A	32	TRP	2.8
3	A	148	ARG	2.7
3	A	76	THR	2.7
3	A	72	PRO	2.7
3	A	73	SER	2.5
2	L	191	SER	2.5
3	A	84	GLU	2.5
1	H	65	LYS	2.4
2	L	108	THR	2.4
3	A	102	ASN	2.3
1	H	9	GLY	2.2
2	L	3	VAL	2.0
3	A	65	LEU	2.0

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 ⓘ

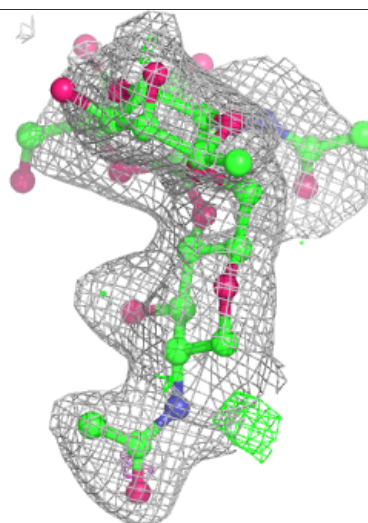
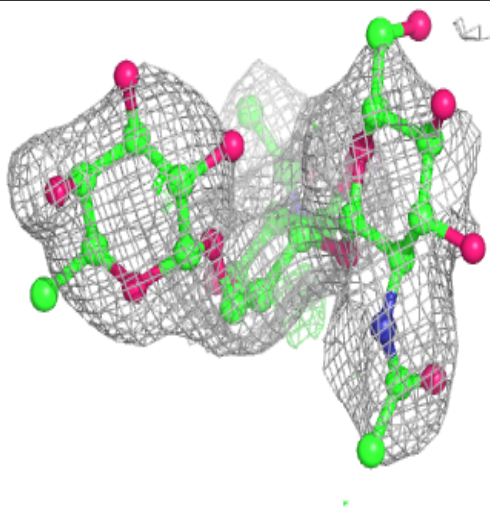
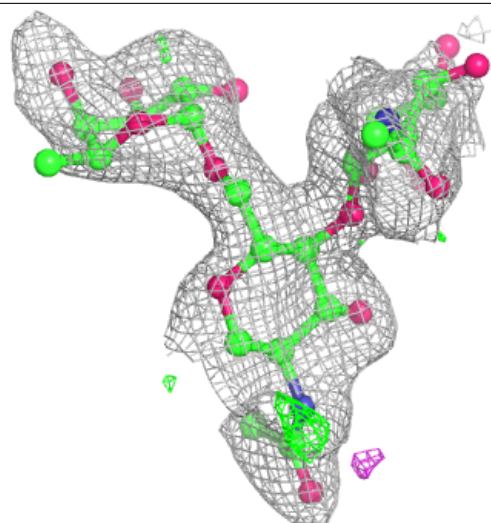
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

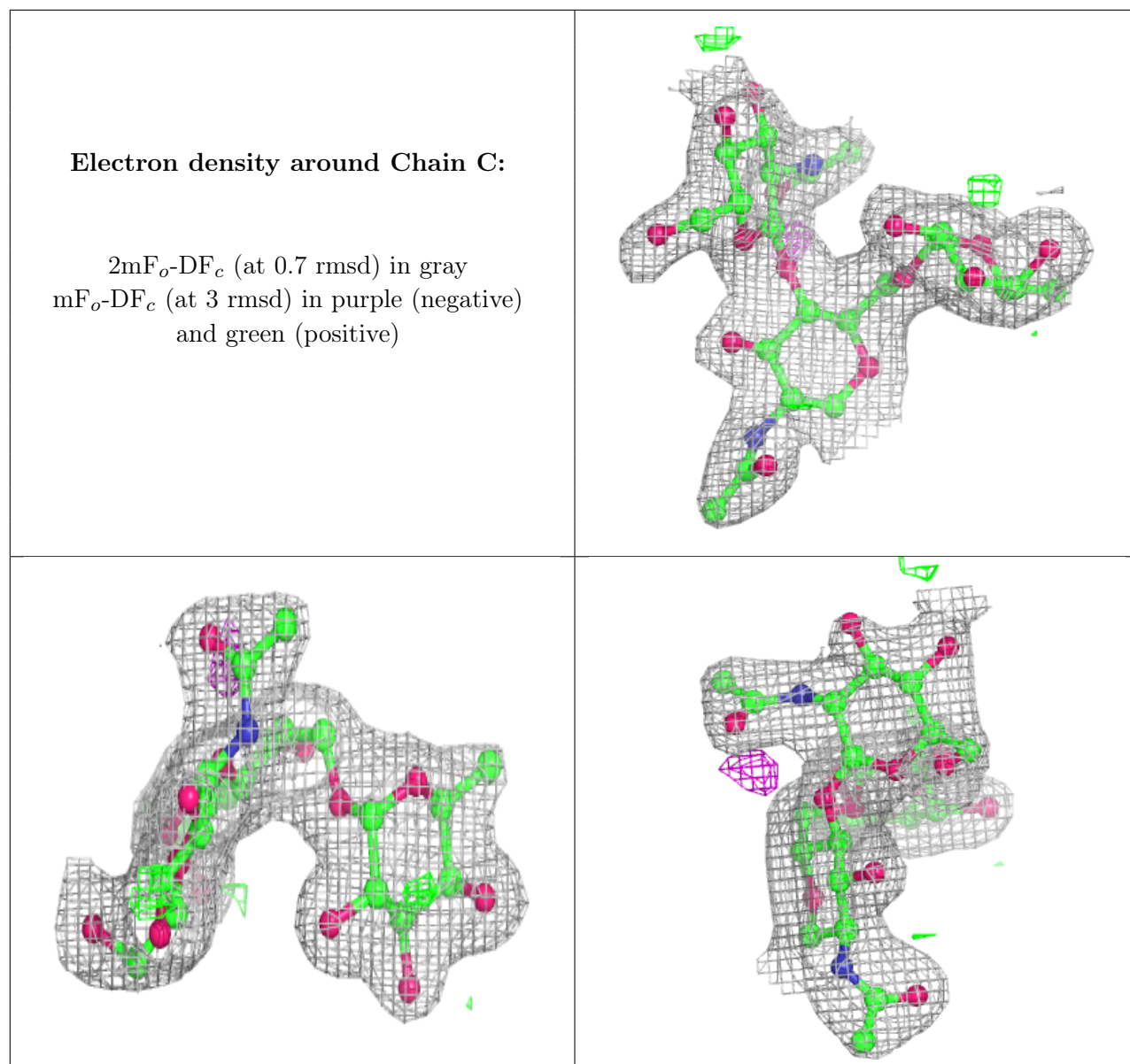
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	NAG	B	1	14/15	-	-	49,53,65,75	0
4	NAG	B	2	14/15	-	-	74,86,97,102	0
4	FUC	B	3	10/11	-	-	70,75,77,79	0
4	NAG	C	1	14/15	-	-	38,41,45,54	0
4	NAG	C	2	14/15	-	-	44,64,70,75	0
4	FUC	C	3	10/11	-	-	38,43,46,50	0

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 B:

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





6.4 Ligands [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, 95th 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
8	NAG	A	201	14/15	0.51	0.20	87,103,110,114	0
5	EDO	L	302	4/4	0.76	0.29	40,46,50,55	0
7	PO4	L	301	5/5	0.85	0.11	56,62,66,77	0
5	EDO	H	303	4/4	0.88	0.13	45,48,49,56	0
5	EDO	H	302	4/4	0.90	0.16	49,50,52,55	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
5	EDO	H	301	4/4	0.92	0.11	36,36,37,37	0
6	DMS	H	304	4/4	0.92	0.15	44,48,58,61	0

6.5 Other polymers [i](#)

There are no such residues in this entry.