



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 22, 2024 – 09:20 PM EDT

PDB ID : 5DK3
Title : Crystal Structure of Pembrolizumab, a full length IgG4 antibody
Authors : Scapin, G.; Prosise, W.; Reichert, P.
Deposited on : 2015-09-02
Resolution : 2.28 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	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

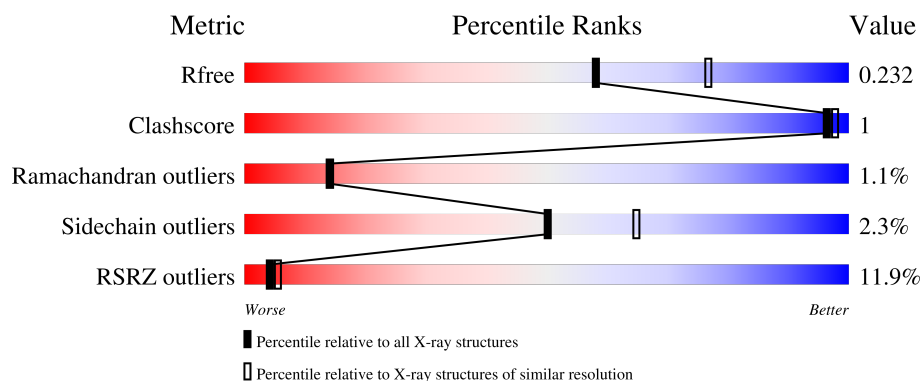
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.28 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}	130704	6980 (2.30-2.26)
Clashscore	141614	7711 (2.30-2.26)
Ramachandran outliers	138981	7597 (2.30-2.26)
Sidechain outliers	138945	7598 (2.30-2.26)
RSRZ outliers	127900	6849 (2.30-2.26)

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	A	218	<div> <div>4%</div> <div>97%</div> <div>..</div> </div>
1	F	218	<div> <div>21%</div> <div>95%</div> <div>5%</div> </div>
2	B	444	<div> <div>11%</div> <div>94%</div> <div>5% ..</div> </div>
2	G	444	<div> <div>12%</div> <div>94%</div> <div>5% .</div> </div>
3	C	7	<div> <div>43%</div> <div>43%</div> <div>14%</div> </div>

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Mol	Chain	Length	Quality of chain
4	D	7	 29% 71%
5	E	2	 50% 50%
5	H	2	 50% 50%
5	I	2	 50% 50%

2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 10749 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.

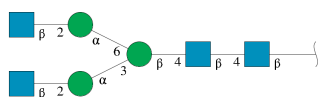
- Molecule 1 is a protein called Light Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	218	Total	C	N	O	S	0	0	0
			1668	1049	280	334	5			
1	F	218	Total	C	N	O	S	0	0	0
			1638	1029	272	332	5			

- Molecule 2 is a protein called Heavy Chain.

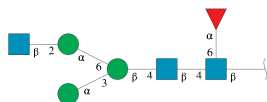
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	441	Total	C	N	O	S	0	0	0
			3344	2115	549	663	17			
2	G	438	Total	C	N	O	S	0	0	0
			3350	2120	548	664	18			

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



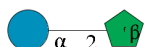
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	C	7	Total	C	N	O	0	0	0
			89	50	4	35			

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



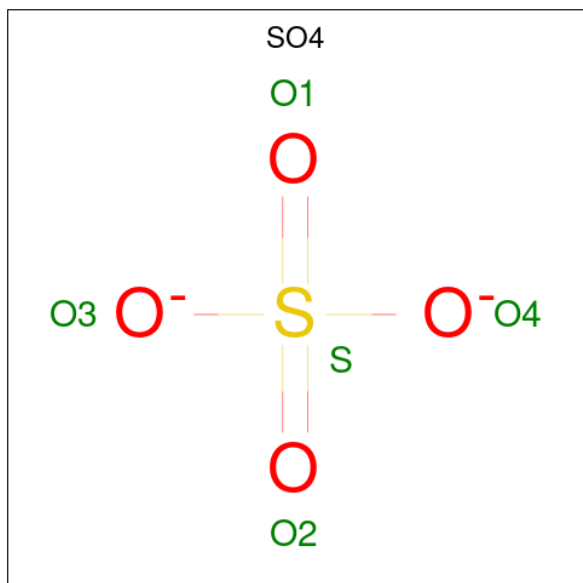
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	D	7	Total	C	N	O	0	0	0
			85	48	3	34			

- Molecule 5 is an oligosaccharide called beta-D-fructofuranose-(2-1)-alpha-D-glucopyranose.



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
5	E	2	Total	C	O	0	0	0
			23	12	11			
5	H	2	Total	C	O	0	0	0
			23	12	11			
5	I	2	Total	C	O	0	0	0
			23	12	11			

- Molecule 6 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	O	S	0	0
			5	4	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	B	1	Total	O	S	0	0
			5	4	1		
6	B	1	Total	O	S	0	0
			5	4	1		
6	B	1	Total	O	S	0	0
			5	4	1		
6	B	1	Total	O	S	0	0
			5	4	1		

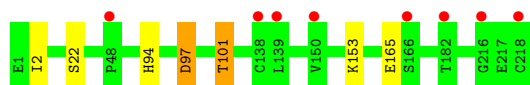
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	152	Total	O	0	0
			152	152		
7	B	209	Total	O	0	0
			209	209		
7	F	16	Total	O	0	0
			16	16		
7	G	104	Total	O	0	0
			104	104		

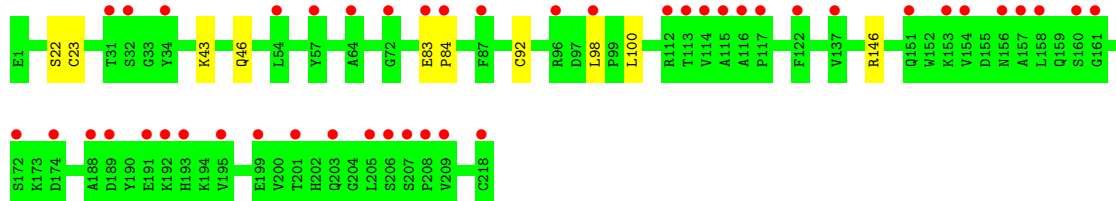
3 Residue-property plots [i](#)

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.

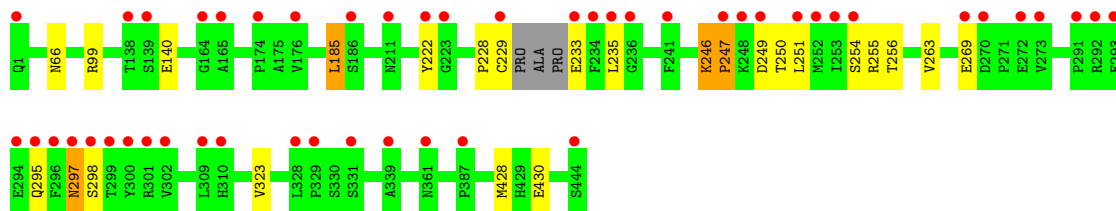
• Molecule 1: Light Chain



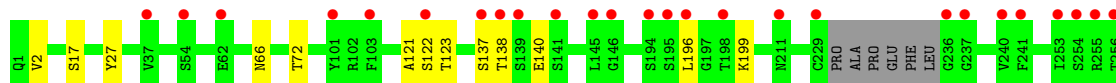
• Molecule 1: Light Chain

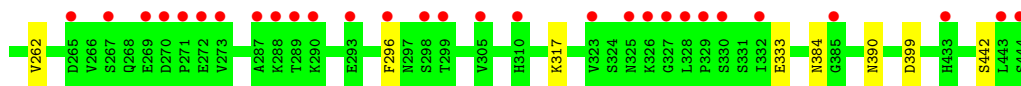


• Molecule 2: Heavy Chain



• Molecule 2: Heavy Chain

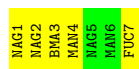
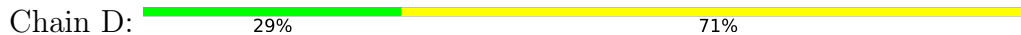




- Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



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



- Molecule 5: beta-D-fructofuranose-(2-1)-alpha-D-glucopyranose



- Molecule 5: beta-D-fructofuranose-(2-1)-alpha-D-glucopyranose



- Molecule 5: beta-D-fructofuranose-(2-1)-alpha-D-glucopyranose



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	63.83Å 110.83Å 264.96Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	33.38 – 2.28 33.12 – 2.28	Depositor EDS
% Data completeness (in resolution range)	100.0 (33.38-2.28) 100.0 (33.12-2.28)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.36 (at 2.29Å)	Xtriage
Refinement program	BUSTER 2.11.5	Depositor
R, R_{free}	0.184 , 0.224 0.199 , 0.232	Depositor DCC
R_{free} test set	4386 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å ²)	46.5	Xtriage
Anisotropy	0.335	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 67.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	10749	wwPDB-VP
Average B, all atoms (Å ²)	63.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.87% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: MAN, FUC, BMA, FRU, SO4, GLC, NAG

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	0.60	0/1706	0.75	2/2318 (0.1%)
1	F	0.44	0/1676	0.66	0/2286
2	B	0.57	0/3434	0.75	2/4697 (0.0%)
2	G	0.48	0/3440	0.68	1/4698 (0.0%)
All	All	0.53	0/10256	0.71	5/13999 (0.0%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	121	ALA	C-N-CA	6.26	137.34	121.70
2	B	185	LEU	CA-CB-CG	5.37	127.65	115.30
1	A	97	ASP	CB-CA-C	-5.15	100.10	110.40
2	B	222	TYR	N-CA-C	5.15	124.90	111.00
1	A	165	GLU	CB-CA-C	-5.04	100.33	110.40

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	1668	0	1626	2	0
1	F	1638	0	1556	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	3344	0	3142	8	0
2	G	3350	0	3182	2	0
3	C	89	0	76	3	0
4	D	85	0	73	0	0
5	E	23	0	21	0	0
5	H	23	0	21	0	0
5	I	23	0	21	0	0
6	A	5	0	0	0	0
6	B	20	0	0	0	0
7	A	152	0	0	0	0
7	B	209	0	0	0	0
7	F	16	0	0	0	0
7	G	104	0	0	0	0
All	All	10749	0	9718	17	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 1.

All (17) 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:B:297:ASN:ND2	3:C:1:NAG:O5	1.91	1.02
1:F:83:GLU:HG3	1:F:84:PRO:CD	1.90	1.02
1:F:83:GLU:HG3	1:F:84:PRO:HD2	1.62	0.81
2:B:297:ASN:ND2	3:C:1:NAG:C1	2.49	0.76
1:A:2:ILE:O	1:A:101:THR:HG21	1.95	0.67
1:F:83:GLU:HG3	1:F:84:PRO:HD3	1.75	0.66
2:B:233:GLU:N	2:G:137:SER:HG	1.99	0.60
1:A:94:HIS:CD2	1:A:101:THR:HG22	2.43	0.53
2:B:263:VAL:HG21	2:B:323:VAL:HG11	1.95	0.48
2:B:254:SER:N	2:B:255:ARG:CB	2.76	0.48
1:F:43:LYS:HB2	1:F:46:GLN:OE1	2.13	0.48
1:F:98:LEU:HD23	1:F:100:LEU:CD2	2.46	0.45
2:B:246:LYS:CB	2:B:247:PRO:HA	2.48	0.43
2:G:2:VAL:HG13	2:G:27:TYR:CD1	2.54	0.41
1:F:23:CYS:HG	1:F:92:CYS:CB	2.28	0.41
2:B:297:ASN:HD22	3:C:1:NAG:C1	2.28	0.41
2:B:228:PRO:O	2:B:229:CYS:HB2	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	216/218 (99%)	209 (97%)	7 (3%)	0	100	100
1	F	216/218 (99%)	207 (96%)	9 (4%)	0	100	100
2	B	437/444 (98%)	409 (94%)	20 (5%)	8 (2%)	8	7
2	G	434/444 (98%)	411 (95%)	17 (4%)	6 (1%)	11	10
All	All	1303/1324 (98%)	1236 (95%)	53 (4%)	14 (1%)	14	14

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	246	LYS
2	B	247	PRO
2	B	298	SER
2	G	138	THR
2	G	122	SER
2	G	296	PHE
2	B	295	GLN
2	B	297	ASN
2	G	66	ASN
2	G	317	LYS
2	G	384	ASN
2	B	66	ASN
2	B	249	ASP
2	B	256	THR

5.3.2 Protein sidechains

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	188/189 (100%)	184 (98%)	4 (2%)	53	68
1	F	181/189 (96%)	179 (99%)	2 (1%)	73	84
2	B	374/398 (94%)	365 (98%)	9 (2%)	49	63
2	G	380/398 (96%)	369 (97%)	11 (3%)	42	56
All	All	1123/1174 (96%)	1097 (98%)	26 (2%)	50	65

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	22	SER
1	A	97	ASP
1	A	101	THR
1	A	153	LYS
2	B	99	ARG
2	B	140	GLU
2	B	185	LEU
2	B	235	LEU
2	B	250	THR
2	B	251	LEU
2	B	269	GLU
2	B	428	MET
2	B	430	GLU
1	F	22	SER
1	F	146	ARG
2	G	17	SER
2	G	72	THR
2	G	123	THR
2	G	140	GLU
2	G	196	LEU
2	G	199	LYS
2	G	262	VAL
2	G	333	GLU
2	G	390	ASN
2	G	399	ASP
2	G	442	SER

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

Mol	Chain	Res	Type
2	B	297	ASN
2	G	59	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 ⓘ

20 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	NAG	C	1	3	14,14,15	0.24	0	17,19,21	1.11	1 (5%)
3	NAG	C	2	3	14,14,15	0.28	0	17,19,21	0.79	1 (5%)
3	BMA	C	3	3	11,11,12	0.29	0	15,15,17	0.84	1 (6%)
3	MAN	C	4	3	11,11,12	0.34	0	15,15,17	0.63	0
3	NAG	C	5	3	14,14,15	0.27	0	17,19,21	0.79	1 (5%)
3	MAN	C	6	3	11,11,12	0.35	0	15,15,17	0.66	0
3	NAG	C	7	3	14,14,15	0.26	0	17,19,21	0.71	0
4	NAG	D	1	2,4	14,14,15	0.47	0	17,19,21	1.21	1 (5%)
4	NAG	D	2	4	14,14,15	0.28	0	17,19,21	0.94	1 (5%)
4	BMA	D	3	4	11,11,12	0.19	0	15,15,17	0.73	1 (6%)
4	MAN	D	4	4	11,11,12	0.26	0	15,15,17	0.79	1 (6%)
4	NAG	D	5	4	14,14,15	0.28	0	17,19,21	0.56	0
4	MAN	D	6	4	11,11,12	0.27	0	15,15,17	0.58	0
4	FUC	D	7	4	10,10,11	0.51	0	14,14,16	0.82	1 (7%)
5	GLC	E	1	5	11,11,12	0.34	0	15,15,17	0.77	1 (6%)
5	FRU	E	2	5	11,12,12	0.64	0	10,18,18	0.37	0
5	GLC	H	1	5	11,11,12	0.27	0	15,15,17	0.75	1 (6%)
5	FRU	H	2	5	11,12,12	0.46	0	10,18,18	0.44	0
5	GLC	I	1	5	11,11,12	0.33	0	15,15,17	1.25	1 (6%)
5	FRU	I	2	5	11,12,12	0.60	0	10,18,18	0.55	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	C	1	3	-	0/6/23/26	0/1/1/1
3	NAG	C	2	3	-	0/6/23/26	0/1/1/1
3	BMA	C	3	3	-	0/2/19/22	0/1/1/1
3	MAN	C	4	3	-	0/2/19/22	0/1/1/1
3	NAG	C	5	3	-	0/6/23/26	0/1/1/1
3	MAN	C	6	3	-	0/2/19/22	0/1/1/1
3	NAG	C	7	3	-	0/6/23/26	0/1/1/1
4	NAG	D	1	2,4	-	0/6/23/26	0/1/1/1
4	NAG	D	2	4	-	2/6/23/26	0/1/1/1
4	BMA	D	3	4	-	0/2/19/22	0/1/1/1
4	MAN	D	4	4	-	0/2/19/22	0/1/1/1
4	NAG	D	5	4	-	0/6/23/26	0/1/1/1
4	MAN	D	6	4	-	0/2/19/22	0/1/1/1
4	FUC	D	7	4	-	-	0/1/1/1
5	GLC	E	1	5	-	0/2/19/22	0/1/1/1
5	FRU	E	2	5	-	3/5/24/24	0/1/1/1
5	GLC	H	1	5	-	0/2/19/22	0/1/1/1
5	FRU	H	2	5	-	0/5/24/24	0/1/1/1
5	GLC	I	1	5	-	1/2/19/22	0/1/1/1
5	FRU	I	2	5	-	1/5/24/24	0/1/1/1

There are no bond length outliers.

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	I	1	GLC	C1-O5-C5	4.59	118.41	112.19
4	D	1	NAG	C1-O5-C5	4.06	117.70	112.19
3	C	1	NAG	O5-C1-C2	-3.93	105.08	111.29
4	D	2	NAG	O5-C1-C2	-3.08	106.43	111.29
3	C	3	BMA	C1-O5-C5	2.95	116.18	112.19
4	D	4	MAN	C1-O5-C5	2.77	115.95	112.19
5	H	1	GLC	C1-O5-C5	2.70	115.85	112.19
3	C	2	NAG	O5-C1-C2	-2.61	107.16	111.29
4	D	3	BMA	C1-O5-C5	2.59	115.70	112.19
5	E	1	GLC	C1-O5-C5	2.30	115.31	112.19
3	C	5	NAG	O5-C1-C2	-2.28	107.68	111.29
4	D	7	FUC	C1-C2-C3	2.14	112.30	109.67

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	E	2	FRU	O1-C1-C2-C3
5	E	2	FRU	O1-C1-C2-O2
5	E	2	FRU	O1-C1-C2-O5
4	D	2	NAG	C4-C5-C6-O6
4	D	2	NAG	O5-C5-C6-O6
5	I	1	GLC	O5-C5-C6-O6
5	I	2	FRU	O1-C1-C2-C3

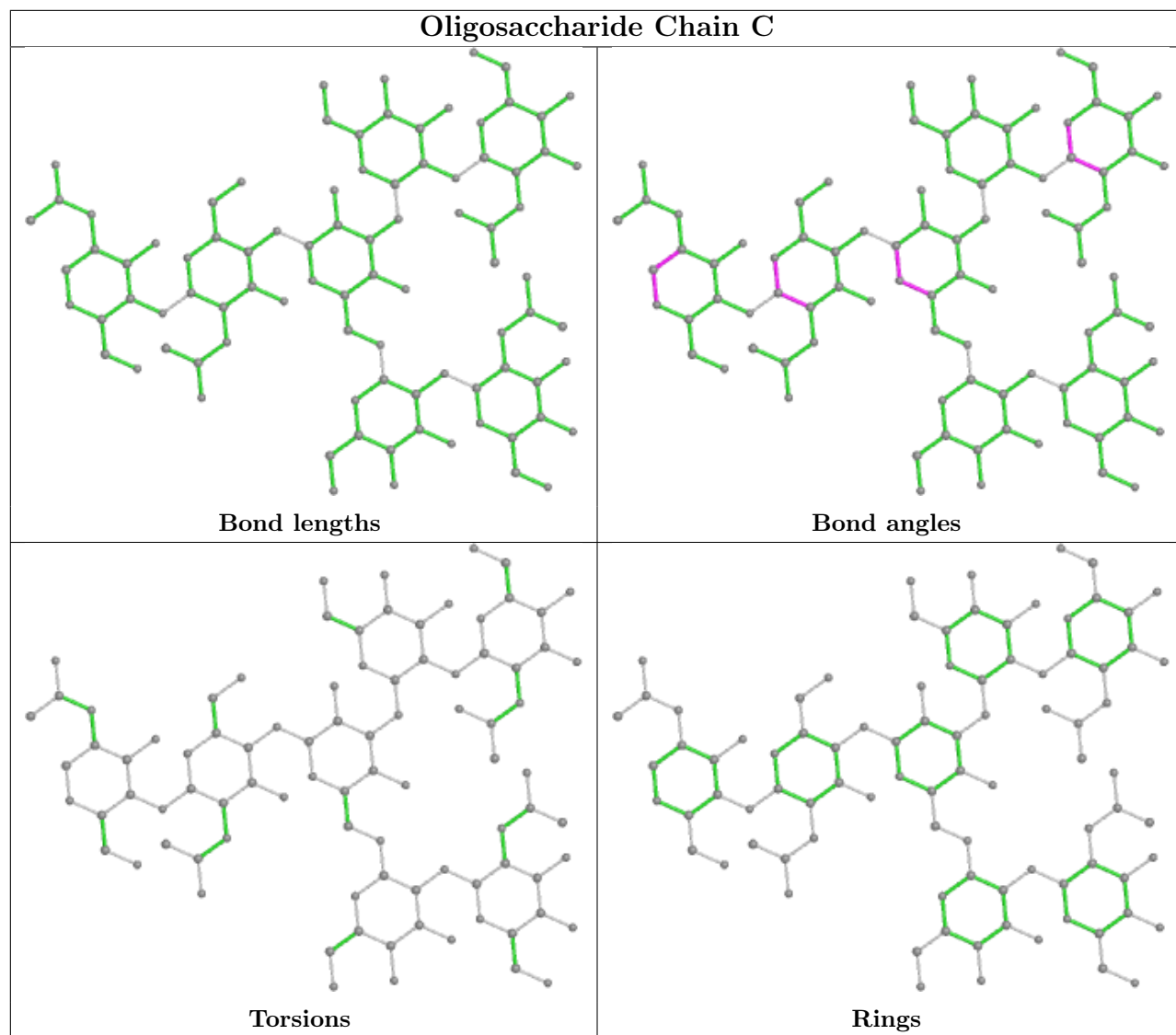
There are no ring outliers.

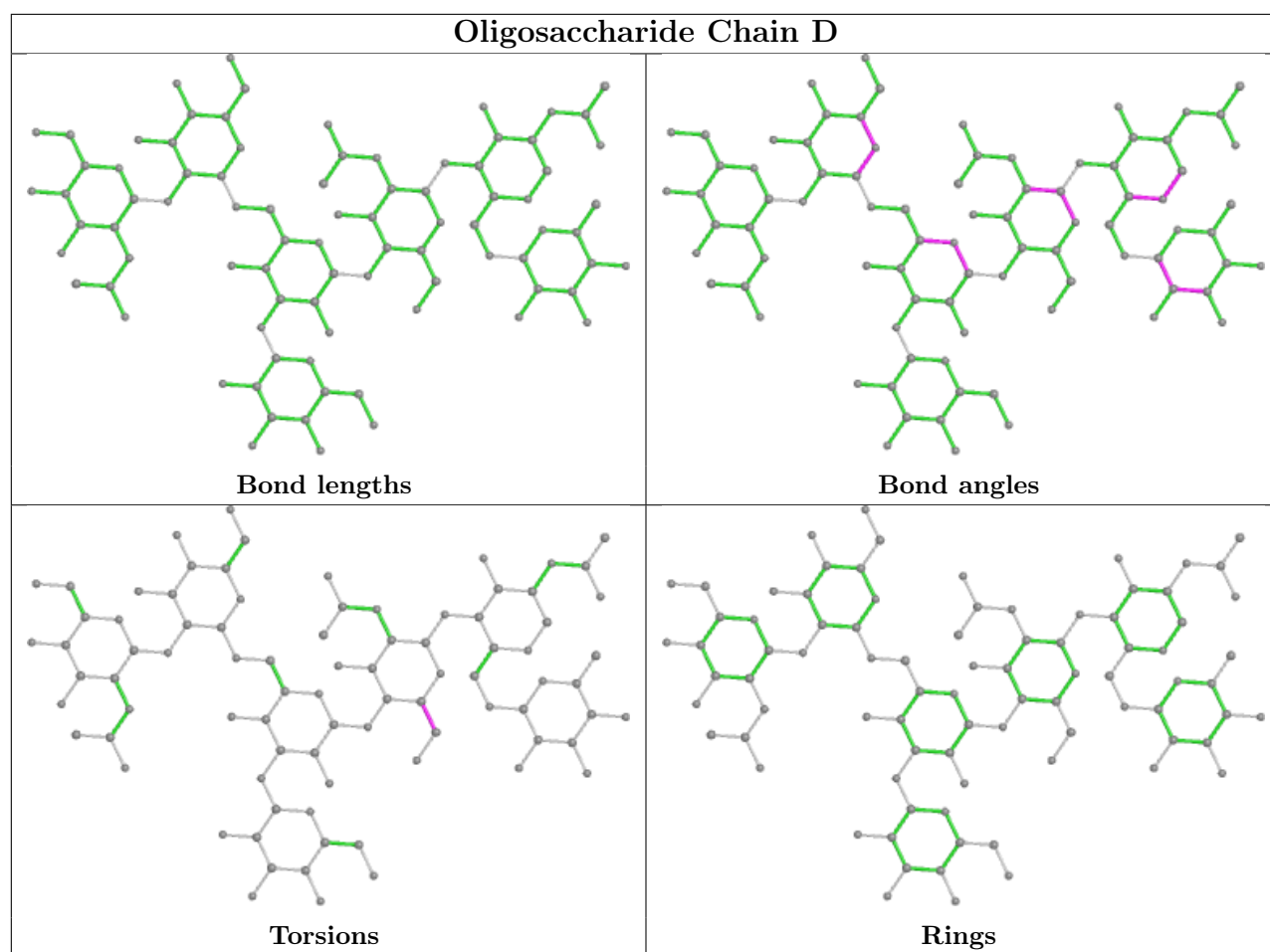
1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	1	NAG	3	0

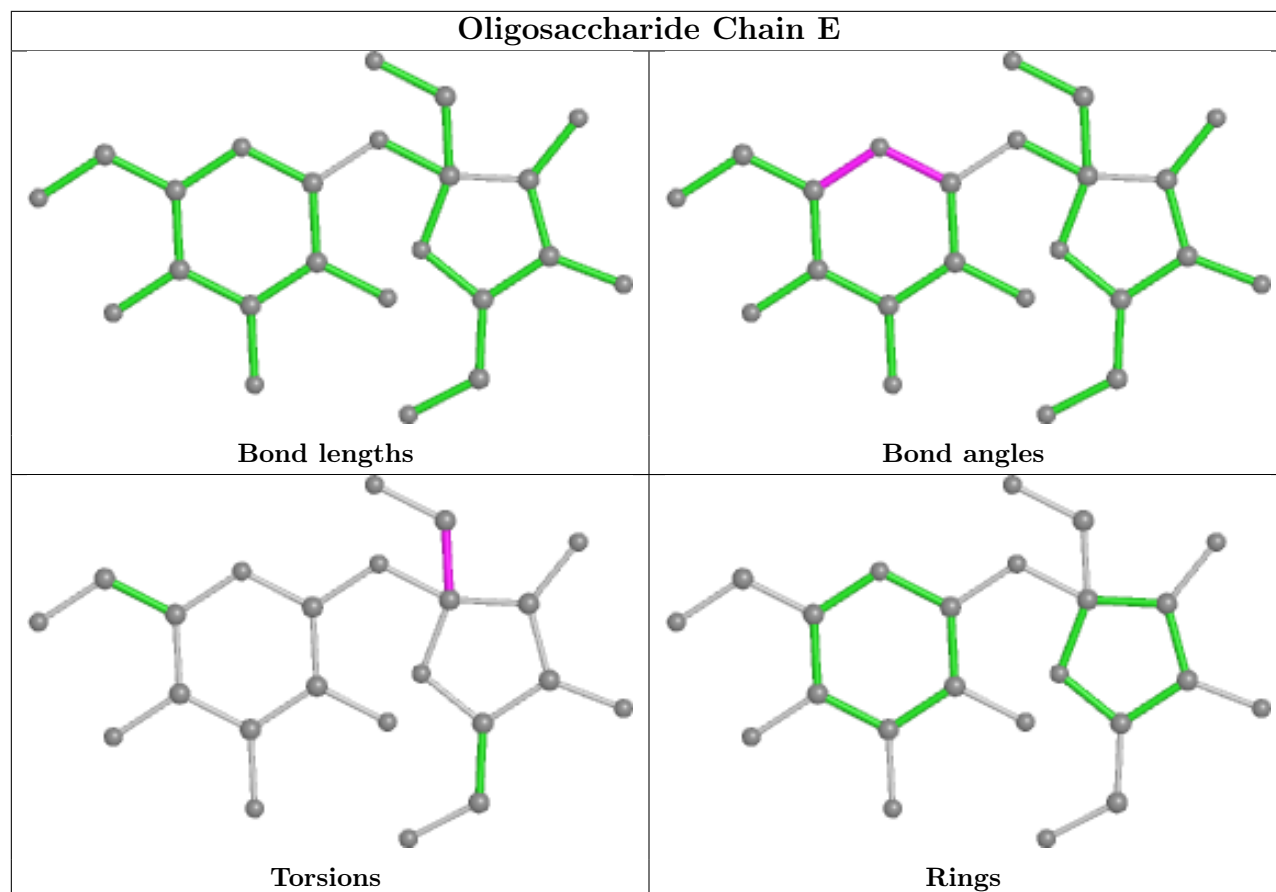
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

Oligosaccharide Chain C

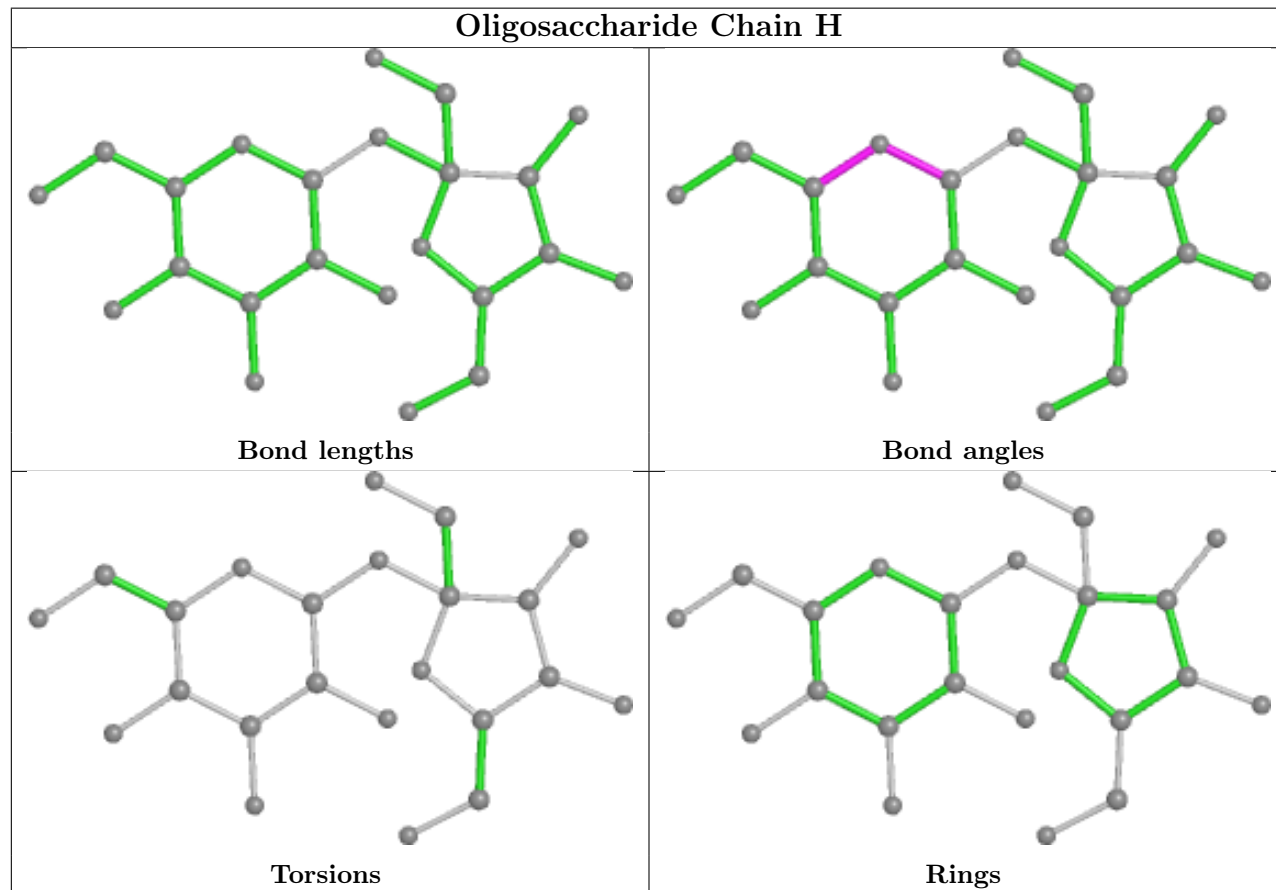


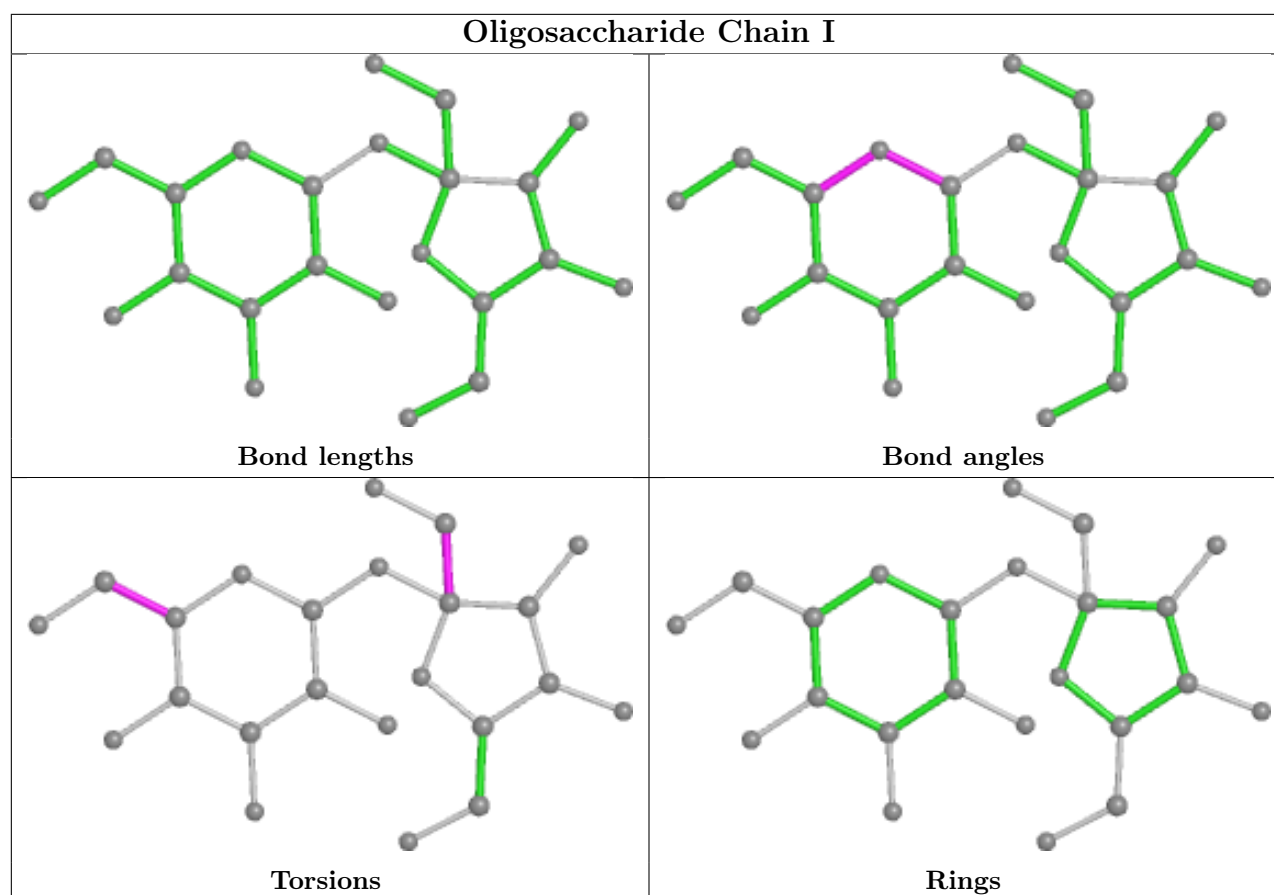


Oligosaccharide Chain E



Oligosaccharide Chain H





5.6 Ligand geometry [i](#)

5 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	$\# Z > 2$
6	SO4	B	501	-	4,4,4	0.30	0	6,6,6	0.32	0
6	SO4	B	504	-	4,4,4	0.22	0	6,6,6	0.17	0
6	SO4	A	301	-	4,4,4	0.52	0	6,6,6	0.35	0
6	SO4	B	502	-	4,4,4	0.08	0	6,6,6	0.20	0
6	SO4	B	503	-	4,4,4	0.27	0	6,6,6	0.28	0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	A	218/218 (100%)	0.29	8 (3%) 41 47	31, 41, 64, 98	0
1	F	218/218 (100%)	1.08	45 (20%) 1 1	35, 87, 121, 139	0
2	B	441/444 (99%)	0.51	49 (11%) 5 7	30, 49, 109, 133	0
2	G	438/444 (98%)	0.70	55 (12%) 3 4	37, 65, 107, 125	0
All	All	1315/1324 (99%)	0.63	157 (11%) 4 5	30, 59, 111, 139	0

All (157) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	247	PRO	9.9
1	F	64	ALA	9.9
2	G	298	SER	9.3
2	G	103	PHE	9.2
2	G	236	GLY	9.1
2	B	254	SER	8.5
2	G	273	VAL	8.0
2	G	329	PRO	7.8
2	G	328	LEU	7.1
2	B	296	PHE	7.1
1	F	57	TYR	6.9
2	G	332	ILE	6.7
1	F	192	LYS	6.7
2	B	300	TYR	6.5
1	F	206	SER	6.5
2	B	329	PRO	6.0
2	B	249	ASP	5.8
2	B	295	GLN	5.8
1	F	98	LEU	5.6
2	G	237	GLY	5.5
2	G	269	GLU	5.4

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Mol	Chain	Res	Type	RSRZ
2	G	326	LYS	5.3
1	F	158	LEU	5.3
1	F	218	CYS	5.3
2	G	240	VAL	5.2
1	F	113	THR	5.1
1	F	207	SER	5.0
2	B	444	SER	4.7
1	F	188	ALA	4.7
2	G	287	ALA	4.6
2	G	139	SER	4.6
1	F	153	LYS	4.5
2	B	234	PHE	4.5
2	B	302	VAL	4.4
2	G	327	GLY	4.3
1	F	156	ASN	4.1
2	G	198	THR	4.1
2	B	252	MET	4.0
1	F	205	LEU	4.0
1	F	34	TYR	4.0
1	F	172	SER	4.0
1	F	151	GLN	4.0
2	G	138	THR	4.0
2	G	254	SER	3.9
2	G	288	LYS	3.9
2	G	330	SER	3.9
2	B	299	THR	3.9
2	G	272	GLU	3.9
1	F	157	ALA	3.7
2	B	331	SER	3.7
2	B	235	LEU	3.7
2	B	301	ARG	3.7
2	B	270	ASP	3.5
2	B	294	GLU	3.5
2	G	270	ASP	3.5
2	B	138	THR	3.5
2	G	325	ASN	3.4
1	F	208	PRO	3.4
2	G	299	THR	3.4
1	F	83	GLU	3.4
1	F	189	ASP	3.3
2	B	292	ARG	3.3
2	B	297	ASN	3.3

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Mol	Chain	Res	Type	RSRZ
2	G	256	THR	3.3
2	B	293	GLU	3.2
1	F	54	LEU	3.2
1	F	116	ALA	3.2
2	G	444	SER	3.2
2	B	253	ILE	3.2
1	F	174	ASP	3.2
1	F	31	THR	3.1
2	G	196	LEU	3.1
2	G	253	ILE	3.1
2	B	139	SER	3.0
1	F	203	GLN	3.0
1	F	87	PHE	3.0
2	B	248	LYS	3.0
1	F	72	GLY	3.0
2	G	290	LYS	3.0
1	F	209	VAL	2.9
2	G	271	PRO	2.9
2	G	54	SER	2.9
1	F	115	ALA	2.9
2	B	241	PHE	2.9
2	B	298	SER	2.9
2	B	236	GLY	2.9
2	G	145	LEU	2.9
2	G	443	LEU	2.9
2	B	291	PRO	2.8
2	G	267	SER	2.8
2	G	146	GLY	2.8
2	G	211	ASN	2.8
1	A	166	SER	2.7
2	G	289	THR	2.7
1	F	161	GLY	2.7
2	B	165	ALA	2.7
1	F	195	VAL	2.7
2	G	101	TYR	2.7
1	F	154	VAL	2.7
1	F	114	VAL	2.7
2	B	222	TYR	2.6
2	B	176	VAL	2.6
2	G	122	SER	2.6
1	A	138	CYS	2.6
1	A	218	CYS	2.6

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Mol	Chain	Res	Type	RSRZ
2	B	229	CYS	2.6
2	G	229	CYS	2.6
2	B	1	GLN	2.6
2	G	241	PHE	2.6
1	F	199	GLU	2.6
1	F	193	HIS	2.6
2	G	385	GLY	2.6
1	F	84	PRO	2.5
1	A	139	LEU	2.5
2	G	433	HIS	2.5
2	B	273	VAL	2.5
2	G	137	SER	2.5
2	B	387	PRO	2.5
1	F	32	SER	2.4
2	G	37	VAL	2.4
2	B	269	GLU	2.4
2	B	328	LEU	2.4
2	B	310	HIS	2.4
2	G	255	ARG	2.4
2	B	339	ALA	2.4
2	B	186	SER	2.4
1	A	150	VAL	2.3
2	G	305	VAL	2.3
2	B	309	LEU	2.3
1	F	191	GLU	2.3
2	B	164	GLY	2.2
2	G	310	HIS	2.2
2	G	323	VAL	2.2
2	G	62	GLU	2.2
2	B	211	ASN	2.2
1	F	112	ARG	2.2
1	F	160	SER	2.2
2	G	195	SER	2.2
2	B	233	GLU	2.2
1	A	182	THR	2.1
2	B	174	PRO	2.1
2	B	361	ASN	2.1
2	G	265	ASP	2.1
1	F	96	ARG	2.1
1	F	117	PRO	2.1
2	B	272	GLU	2.1
2	G	141	SER	2.1

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Mol	Chain	Res	Type	RSRZ
1	F	122	PHE	2.1
2	G	194	SER	2.1
1	A	216	GLY	2.1
2	G	296	PHE	2.1
1	F	201	THR	2.0
1	F	137	VAL	2.0
2	B	251	LEU	2.0
2	G	293	GLU	2.0
2	B	223	GLY	2.0
1	A	48	PRO	2.0

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, 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
5	GLC	I	1	11/12	0.83	0.26	66,82,86,88	0
3	NAG	C	7	14/15	0.87	0.22	105,108,112,113	0
3	NAG	C	5	14/15	0.87	0.34	105,110,113,115	0
4	MAN	D	6	11/12	0.88	0.21	104,108,111,112	0
4	MAN	D	4	11/12	0.88	0.18	79,82,87,88	0
5	FRU	I	2	12/12	0.88	0.31	84,88,91,92	0
4	NAG	D	5	14/15	0.89	0.18	79,82,90,92	0
5	FRU	E	2	12/12	0.89	0.16	45,63,67,69	0
5	GLC	E	1	11/12	0.91	0.16	43,54,57,58	0
3	NAG	C	1	14/15	0.91	0.21	99,104,109,111	0
5	FRU	H	2	12/12	0.92	0.18	63,70,71,74	0
3	MAN	C	4	11/12	0.92	0.17	98,103,105,107	0
3	NAG	C	2	14/15	0.92	0.18	89,92,95,95	0
4	BMA	D	3	11/12	0.93	0.15	80,89,94,98	0
3	MAN	C	6	11/12	0.93	0.17	94,97,98,101	0
3	BMA	C	3	11/12	0.93	0.14	88,91,94,95	0
4	NAG	D	1	14/15	0.93	0.16	82,90,95,96	0
4	FUC	D	7	10/11	0.93	0.31	79,80,81,83	0

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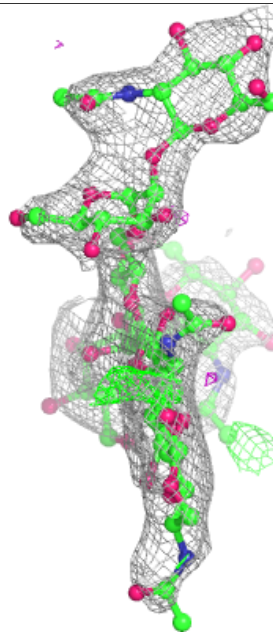
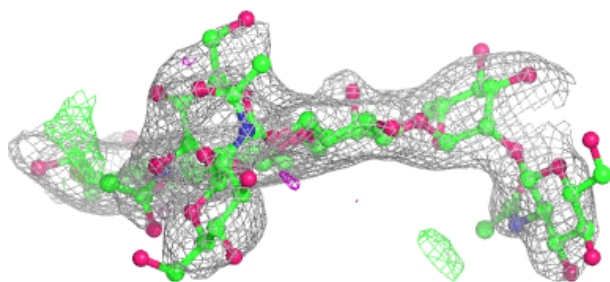
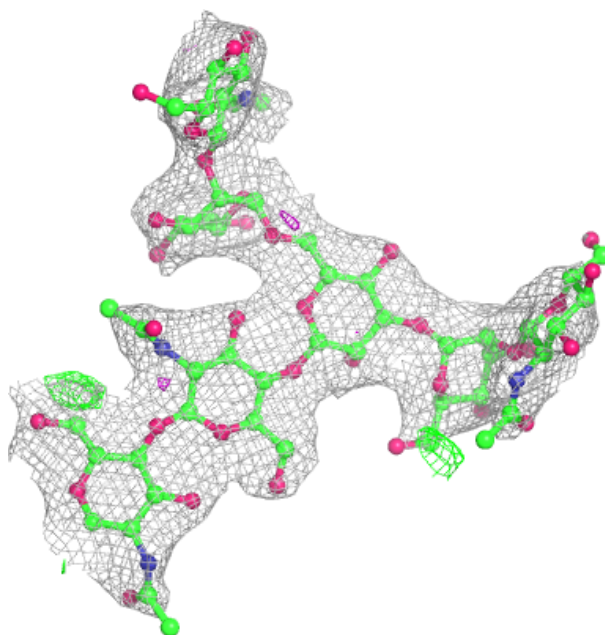
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
5	GLC	H	1	11/12	0.94	0.17	68,73,76,77	0
4	NAG	D	2	14/15	0.96	0.12	73,80,87,87	0

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.

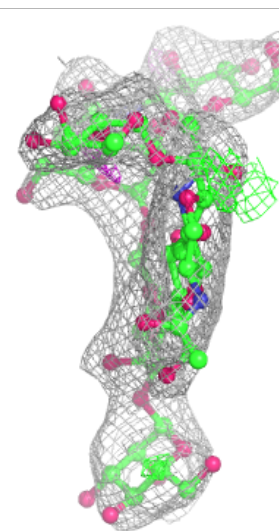
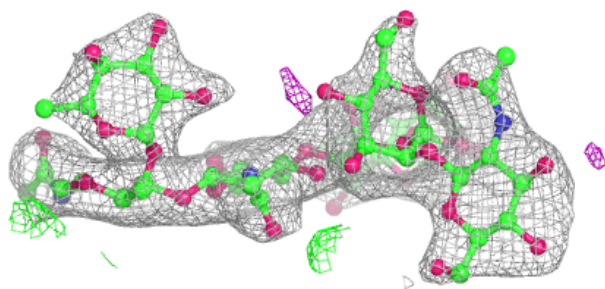
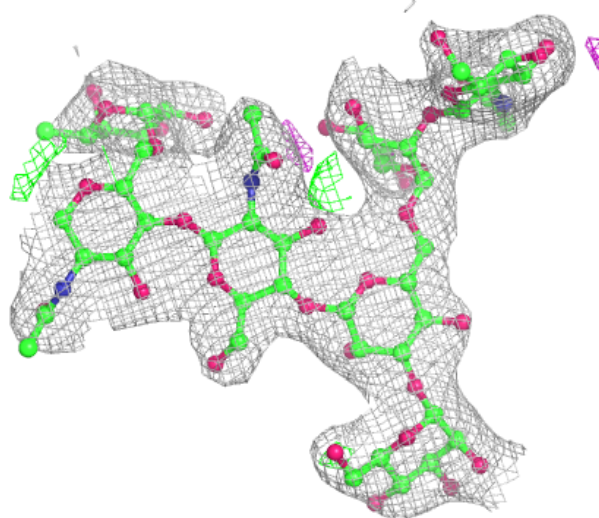
Electron density around Chain C:

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



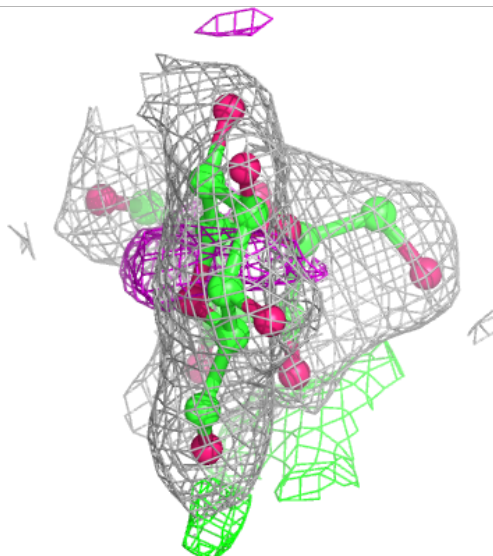
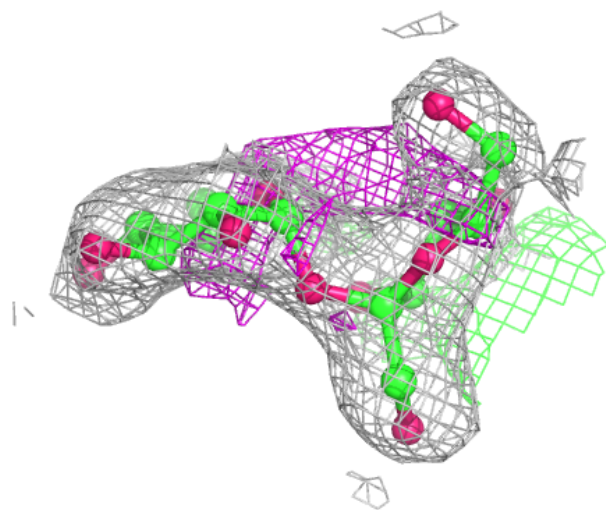
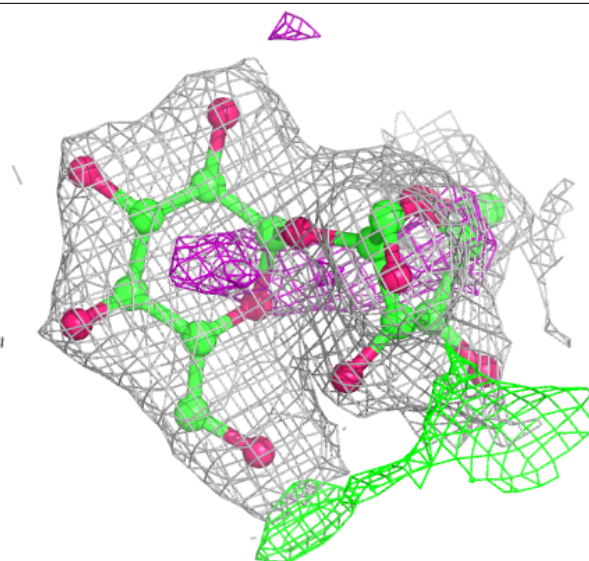
Electron density around Chain D:

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



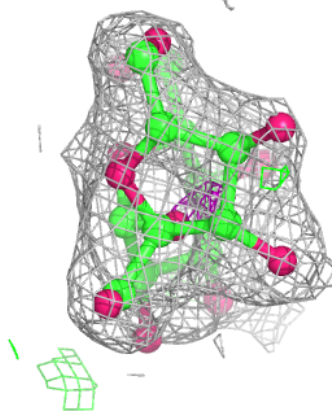
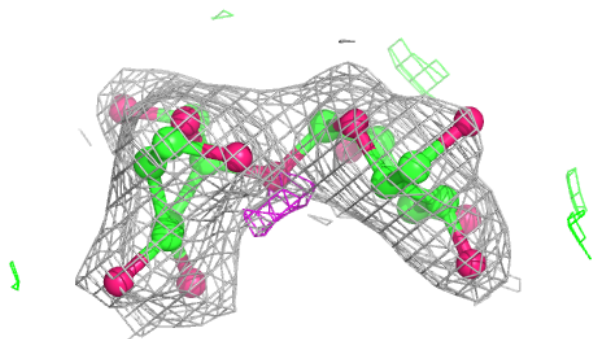
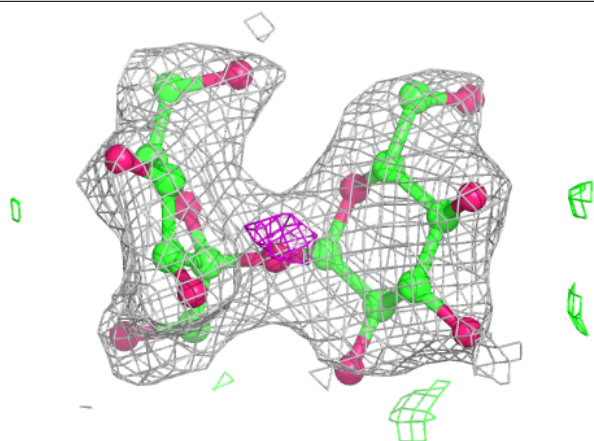
Electron density around Chain E:

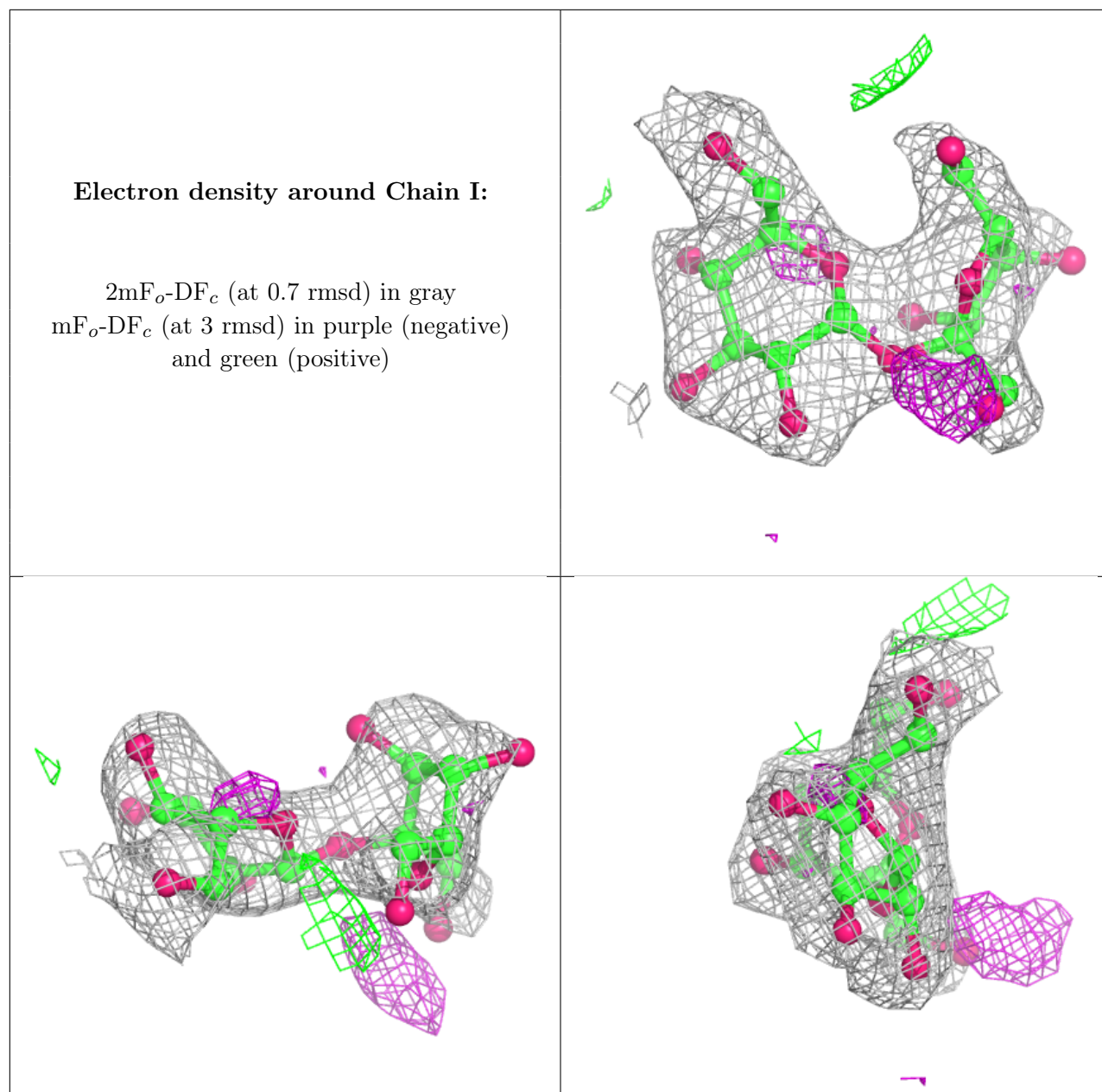
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around Chain 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, 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
6	SO4	B	504	5/5	0.86	0.25	113,113,114,115	0
6	SO4	B	501	5/5	0.94	0.15	99,99,99,100	0
6	SO4	A	301	5/5	0.95	0.14	59,70,72,75	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
6	SO4	B	503	5/5	0.96	0.11	69,77,78,79	0
6	SO4	B	502	5/5	0.98	0.18	82,84,84,89	0

6.5 Other polymers [i](#)

There are no such residues in this entry.