



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 06:15 AM UTC

PDB ID : 5DK3 / pdb_00005dk3
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 : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

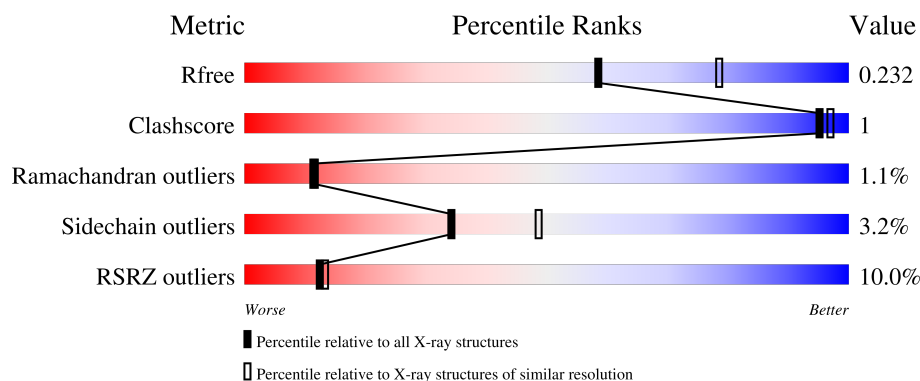
1 Overall quality at a glance

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}	180053	9078 (2.30-2.26)
Clashscore	190562	9802 (2.30-2.26)
Ramachandran outliers	187476	9690 (2.30-2.26)
Sidechain outliers	187428	9691 (2.30-2.26)
RSRZ outliers	180081	9085 (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	96% .
1	F	218	11% 94% 6%
2	B	444	13% 92% 5% ..
2	G	444	11% 92% 7% .
3	C	7	29% 57% 14%

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Mol	Chain	Length	Quality of chain
4	D	7	 43% 57%
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.

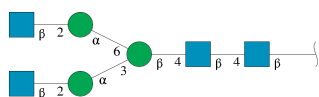
- Molecule 1 is a protein called Light Chain.

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.

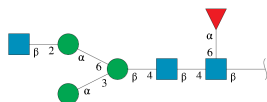
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	441	Total	C	N	O	S	0	0	0
			3344	2115	549	663	17			
2	G	438	Total	C	N	O	S	0	0	0
			3350	2120	548	664	18			

- 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.



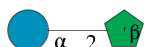
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	C	7	Total	C	N	O	0	0	0
			89	50	4	35			

- 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.



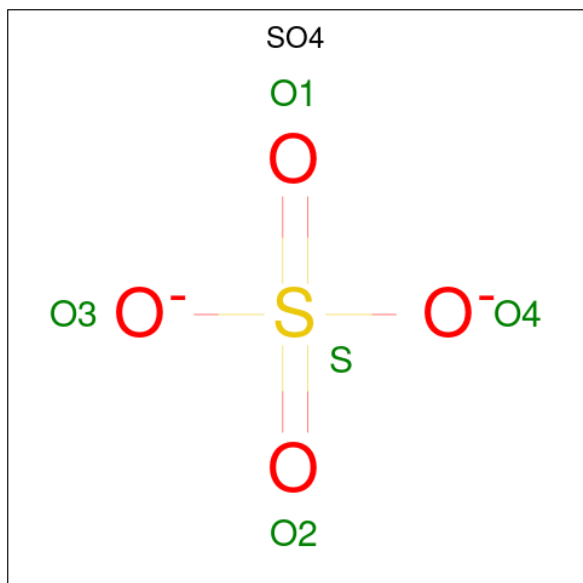
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	D	7	Total	C	N	O	0	0	0
			85	48	3	34			

- 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 (CCD ID: 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		

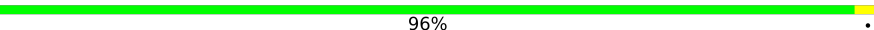
- Molecule 7 is water.

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](#)

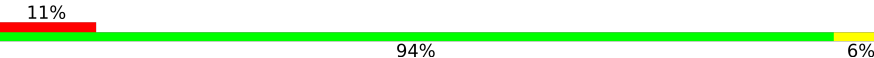
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

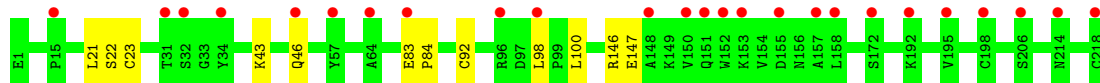
- Molecule 1: Light Chain

Chain A:  96%

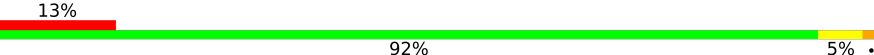


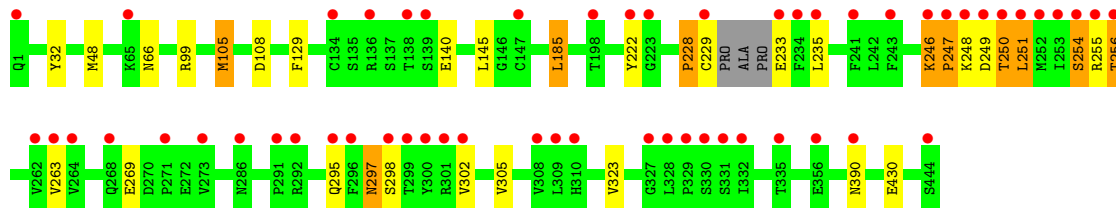
- Molecule 1: Light Chain

Chain F:  11% 94% 6%

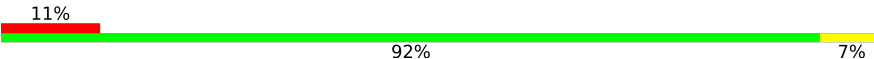


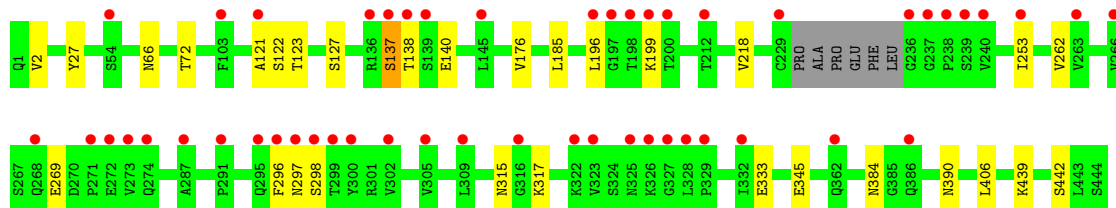
- Molecule 2: Heavy Chain

Chain B:  13% 92% 5% ..



- Molecule 2: Heavy Chain

Chain G:  11% 92% 7%



- 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-mannopyra

nose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain C:  29% 57% 14%



- 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

Chain D:  43% 57%



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

Chain E:  50% 50%



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

Chain H:  50% 50%



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

Chain I:  50% 50%



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 33.38 – 2.28	Depositor EDS
% Data completeness (in resolution range)	100.0 (33.38-2.28) 99.9 (33.38-2.28)	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 , 69.2	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

5.1 Standard geometry

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

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	0.95	0/1706	1.07	1/2318 (0.0%)
1	F	0.78	0/1676	1.02	0/2286
2	B	0.94	5/3434 (0.1%)	1.10	14/4697 (0.3%)
2	G	0.82	0/3440	1.06	10/4698 (0.2%)
All	All	0.88	5/10256 (0.0%)	1.07	25/13999 (0.2%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	105	MET	SD-CE	-8.47	1.58	1.79
2	B	48	MET	SD-CE	7.13	1.97	1.79
2	B	222	TYR	CA-C	6.12	1.61	1.52
2	B	32	TYR	CA-C	-5.12	1.46	1.52
2	B	129	PHE	CA-C	-5.10	1.47	1.52

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	222	TYR	N-CA-C	9.46	124.90	113.16
2	G	121	ALA	CA-C-N	8.69	137.34	121.70
2	G	121	ALA	C-N-CA	8.69	137.34	121.70
2	B	250	THR	N-CA-C	8.38	120.30	108.74
2	B	390	ASN	CA-CB-CG	8.20	120.80	112.60
2	G	297	ASN	OD1-CG-ND2	-6.77	115.83	122.60
2	G	297	ASN	CB-CG-ND2	6.15	125.62	116.40
2	B	108	ASP	CA-CB-CG	6.14	118.74	112.60
2	G	298	SER	N-CA-C	-6.04	104.51	112.72
2	G	127	SER	N-CA-C	-6.01	99.44	109.24
2	B	251	LEU	CA-C-N	5.96	132.42	121.70
2	B	251	LEU	C-N-CA	5.96	132.42	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	315	ASN	CA-CB-CG	5.89	118.49	112.60
2	B	222	TYR	CA-C-N	5.71	131.99	121.70
2	B	222	TYR	C-N-CA	5.71	131.99	121.70
2	G	297	ASN	N-CA-C	-5.68	101.50	109.69
2	B	250	THR	CA-C-N	5.52	130.47	121.74
2	B	250	THR	C-N-CA	5.52	130.47	121.74
2	G	345	GLU	N-CA-C	5.25	116.26	109.65
2	B	254	SER	CA-C-N	5.17	131.00	121.70
2	B	254	SER	C-N-CA	5.17	131.00	121.70
2	G	137	SER	N-CA-C	-5.06	100.02	110.80
1	A	141	ASN	N-CA-C	5.03	117.43	109.24
2	B	228	PRO	CA-C-N	5.00	130.71	121.70
2	B	228	PRO	C-N-CA	5.00	130.71	121.70

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
2	B	3344	0	3142	10	0
2	G	3350	0	3182	4	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	1	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	21	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 (21) 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
7:A:537:HOH:O	2:B:105:MET:HE2	2.14	0.47
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:406:LEU:C	2:G:406:LEU:HD12	2.43	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:G:185:LEU:C	2:G:185:LEU:HD12	2.46	0.41
2:B:297:ASN:HD22	3:C:1:NAG:C1	2.28	0.41
2:B:185:LEU:HD12	2:B:185:LEU:C	2.47	0.40
2:B:228:PRO:O	2:B:229:CYS:HB2	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	216/218 (99%)	209 (97%)	7 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	F	216/218 (99%)	207 (96%)	9 (4%)	0	100	100
2	B	437/444 (98%)	409 (94%)	20 (5%)	8 (2%)	6	5
2	G	434/444 (98%)	411 (95%)	17 (4%)	6 (1%)	9	8
All	All	1303/1324 (98%)	1236 (95%)	53 (4%)	14 (1%)	11	11

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%)	183 (97%)	5 (3%)	39	55
1	F	181/189 (96%)	177 (98%)	4 (2%)	45	62
2	B	374/398 (94%)	361 (96%)	13 (4%)	32	45
2	G	380/398 (96%)	366 (96%)	14 (4%)	30	43
All	All	1123/1174 (96%)	1087 (97%)	36 (3%)	34	49

All (36) 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
1	A	195	VAL
2	B	99	ARG
2	B	140	GLU
2	B	145	LEU
2	B	185	LEU
2	B	235	LEU
2	B	248	LYS
2	B	250	THR
2	B	251	LEU
2	B	256	THR
2	B	269	GLU
2	B	302	VAL
2	B	305	VAL
2	B	430	GLU
1	F	21	LEU
1	F	22	SER
1	F	146	ARG
1	F	147	GLU
2	G	72	THR
2	G	123	THR
2	G	140	GLU
2	G	176	VAL
2	G	196	LEU
2	G	199	LYS
2	G	218	VAL
2	G	253	ILE
2	G	262	VAL
2	G	269	GLU
2	G	333	GLU
2	G	390	ASN
2	G	439	LYS
2	G	442	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	46	GLN

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Mol	Chain	Res	Type
1	A	164	GLN
2	B	276	ASN
2	B	297	ASN
1	F	142	ASN
1	F	164	GLN
2	G	59	ASN
2	G	66	ASN
2	G	276	ASN
2	G	418	GLN
2	G	434	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	1.14	1 (5%)
3	NAG	C	2	3	14,14,15	0.29	0	17,19,21	0.81	1 (5%)
3	BMA	C	3	3	11,11,12	0.28	0	15,15,17	0.85	1 (6%)
3	MAN	C	4	3	11,11,12	0.33	0	15,15,17	0.61	0
3	NAG	C	5	3	14,14,15	0.28	0	17,19,21	0.82	1 (5%)
3	MAN	C	6	3	11,11,12	0.34	0	15,15,17	0.64	0
3	NAG	C	7	3	14,14,15	0.27	0	17,19,21	0.74	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
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	0.29	0	17,19,21	0.96	1 (5%)
4	BMA	D	3	4	11,11,12	0.19	0	15,15,17	0.74	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	0.58	0
4	MAN	D	6	4	11,11,12	0.27	0	15,15,17	0.57	0
4	FUC	D	7	4	10,10,11	0.49	0	14,14,16	0.73	0
5	GLC	E	1	5	11,11,12	0.33	0	15,15,17	0.75	1 (6%)
5	FRU	E	2	5	11,12,12	0.65	0	10,18,18	0.38	0
5	GLC	H	1	5	11,11,12	0.26	0	15,15,17	0.76	1 (6%)
5	FRU	H	2	5	11,12,12	0.47	0	10,18,18	0.46	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	0.61	0	10,18,18	0.56	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	-	1/6/23/26	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	4.64	118.41	112.19
4	D	1	NAG	C1-O5-C5	4.11	117.70	112.19
3	C	1	NAG	O5-C1-C2	-4.01	105.08	111.29
4	D	2	NAG	O5-C1-C2	-3.14	106.43	111.29
3	C	3	BMA	C1-O5-C5	2.98	116.18	112.19
4	D	4	MAN	C1-O5-C5	2.81	115.95	112.19
5	H	1	GLC	C1-O5-C5	2.74	115.85	112.19
3	C	2	NAG	O5-C1-C2	-2.67	107.16	111.29
4	D	3	BMA	C1-O5-C5	2.62	115.70	112.19
3	C	5	NAG	O5-C1-C2	-2.33	107.68	111.29
5	E	1	GLC	C1-O5-C5	2.33	115.31	112.19
3	C	7	NAG	O5-C1-C2	-2.02	108.17	111.29

There are no chirality outliers.

All (8) torsion outliers are listed below:

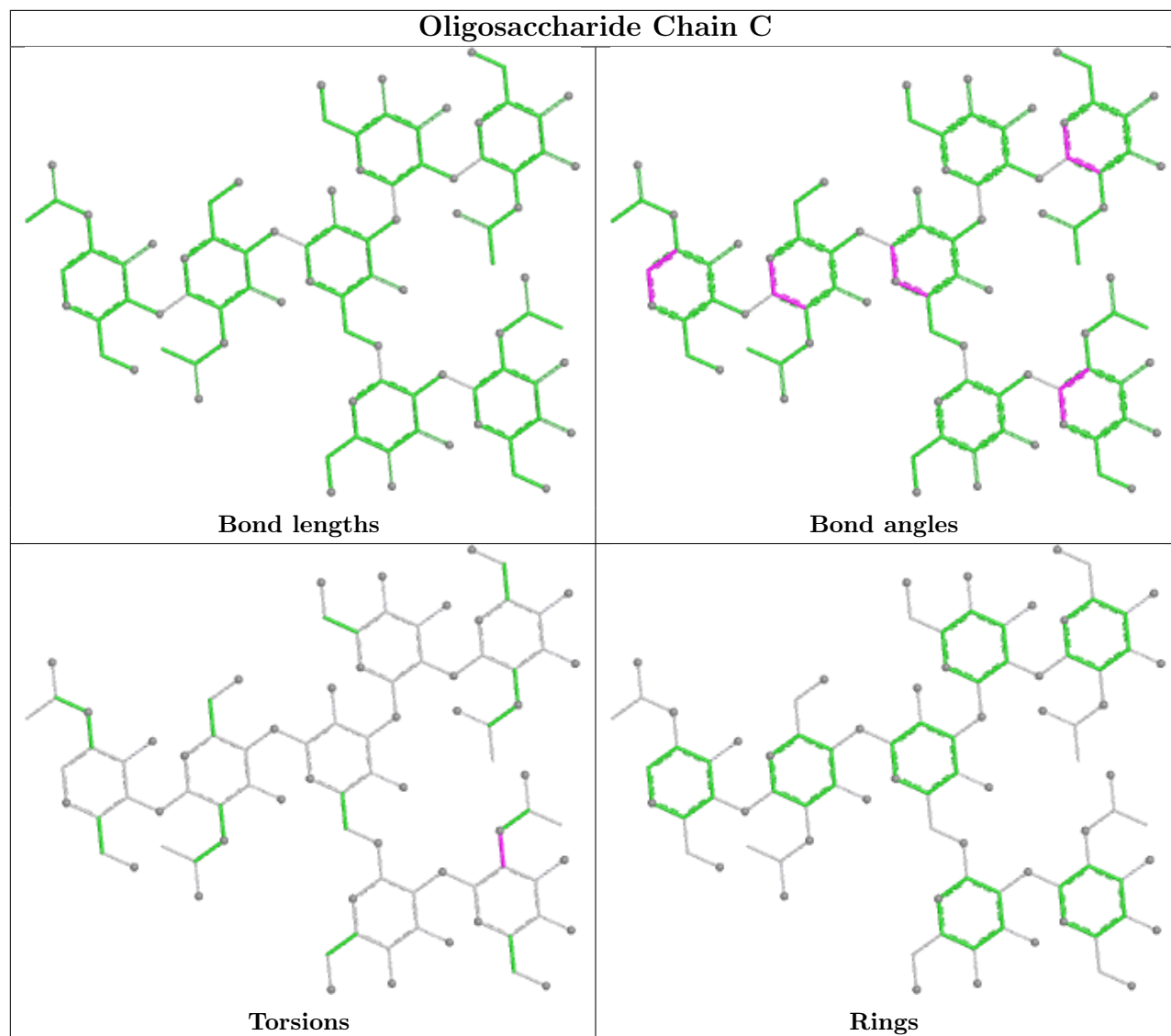
Mol	Chain	Res	Type	Atoms
5	E	2	FRU	O1-C1-C2-C3
5	E	2	FRU	O1-C1-C2-O2
5	E	2	FRU	O1-C1-C2-O5
4	D	2	NAG	C4-C5-C6-O6
4	D	2	NAG	O5-C5-C6-O6
5	I	1	GLC	O5-C5-C6-O6
3	C	7	NAG	C1-C2-N2-C7
5	I	2	FRU	O1-C1-C2-C3

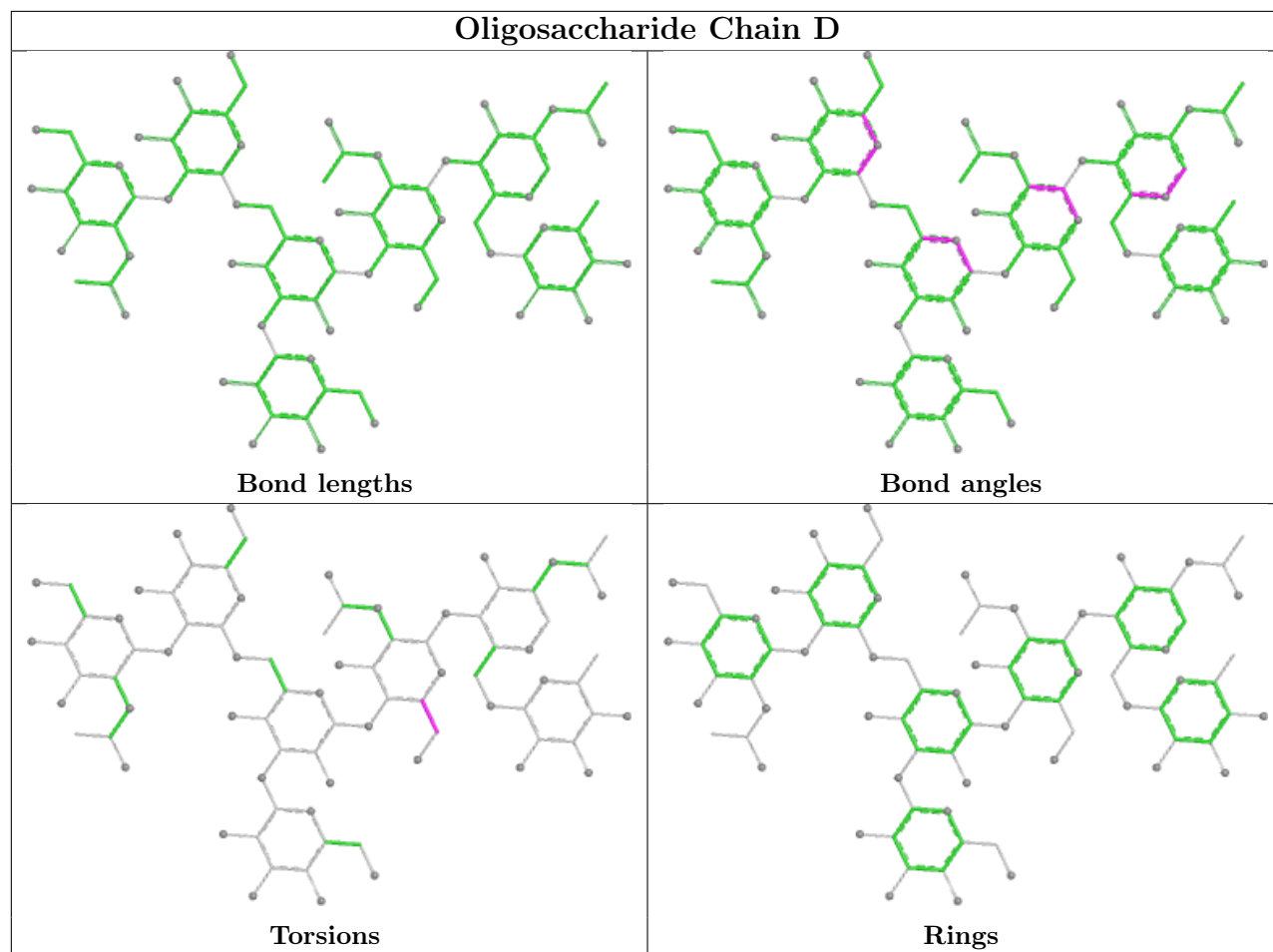
There are no ring outliers.

1 monomer is involved in 3 short contacts:

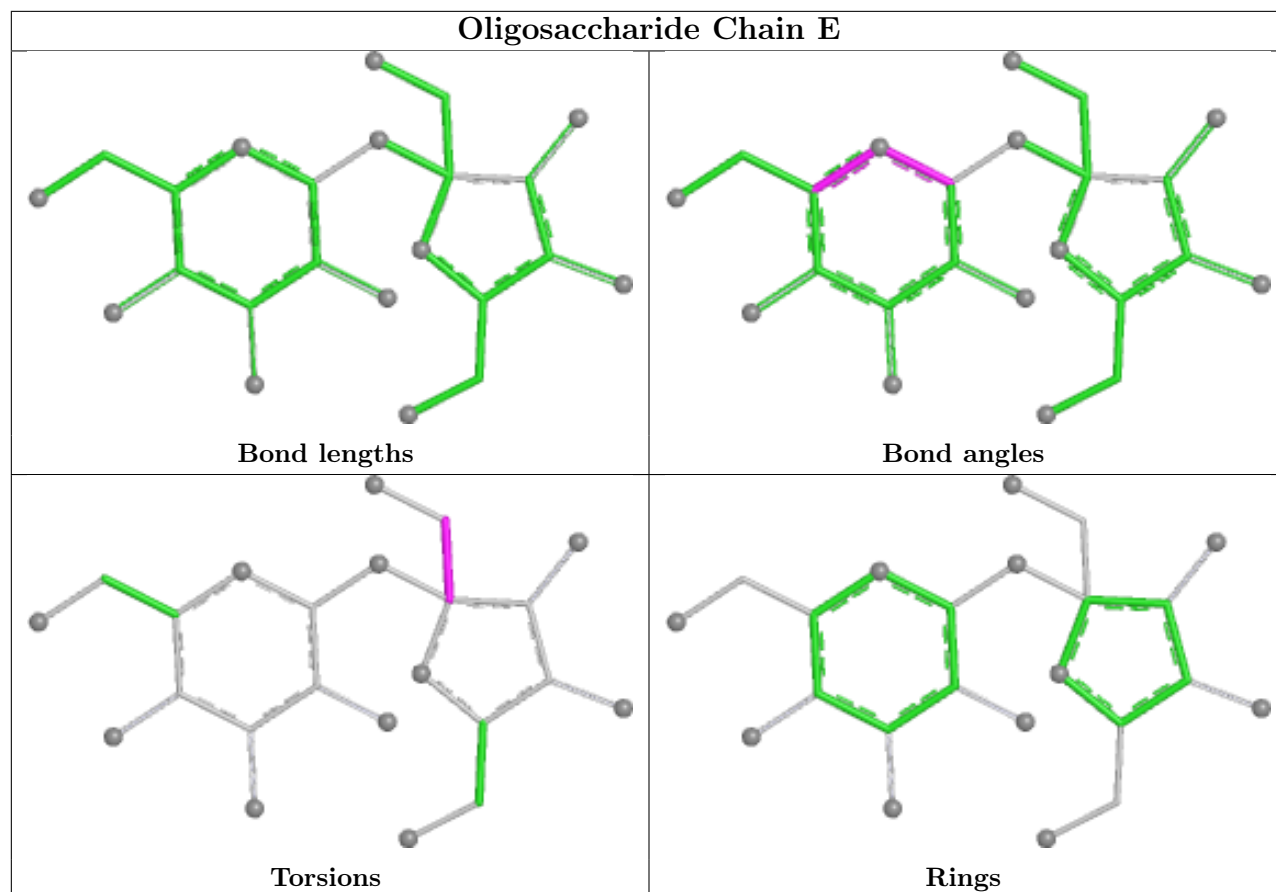
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	1	NAG	3	0

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

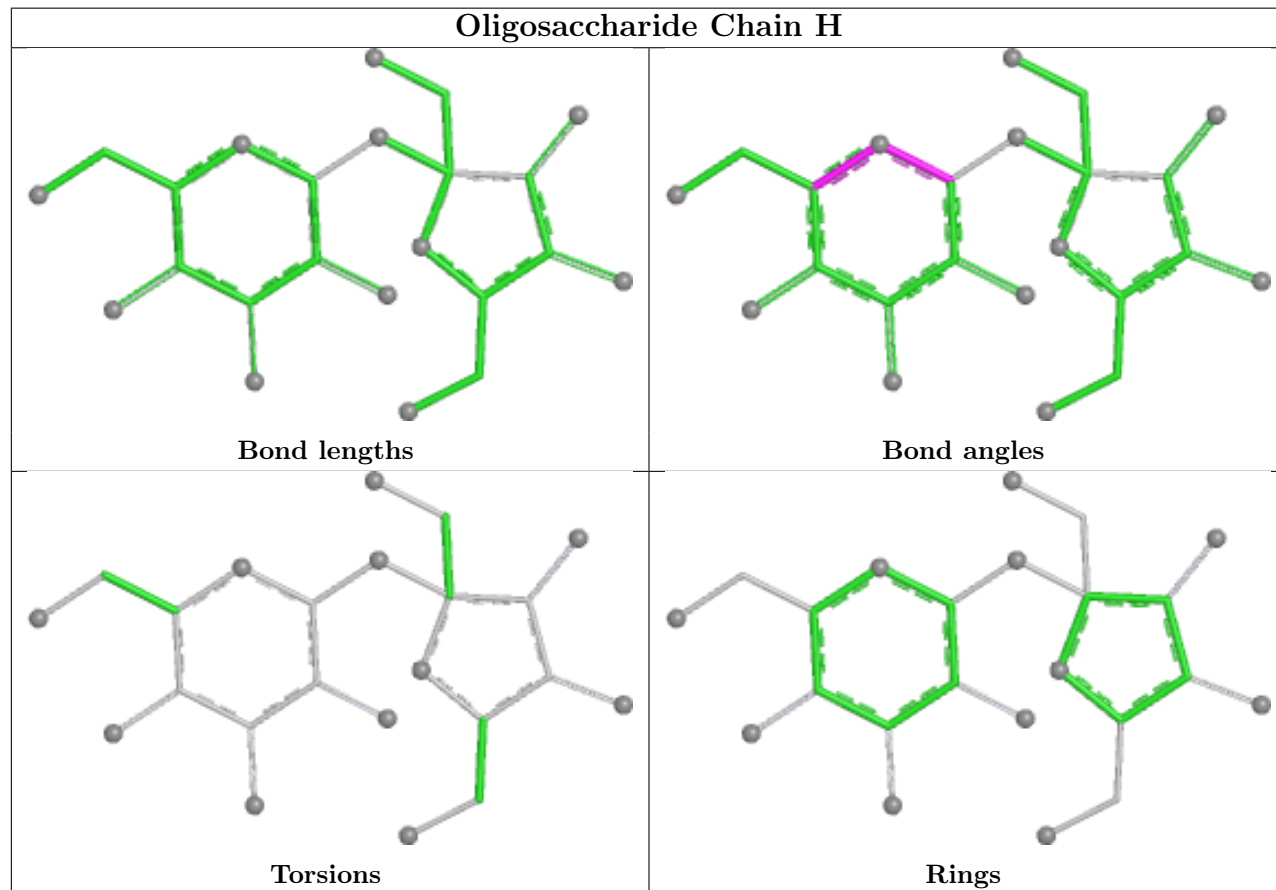


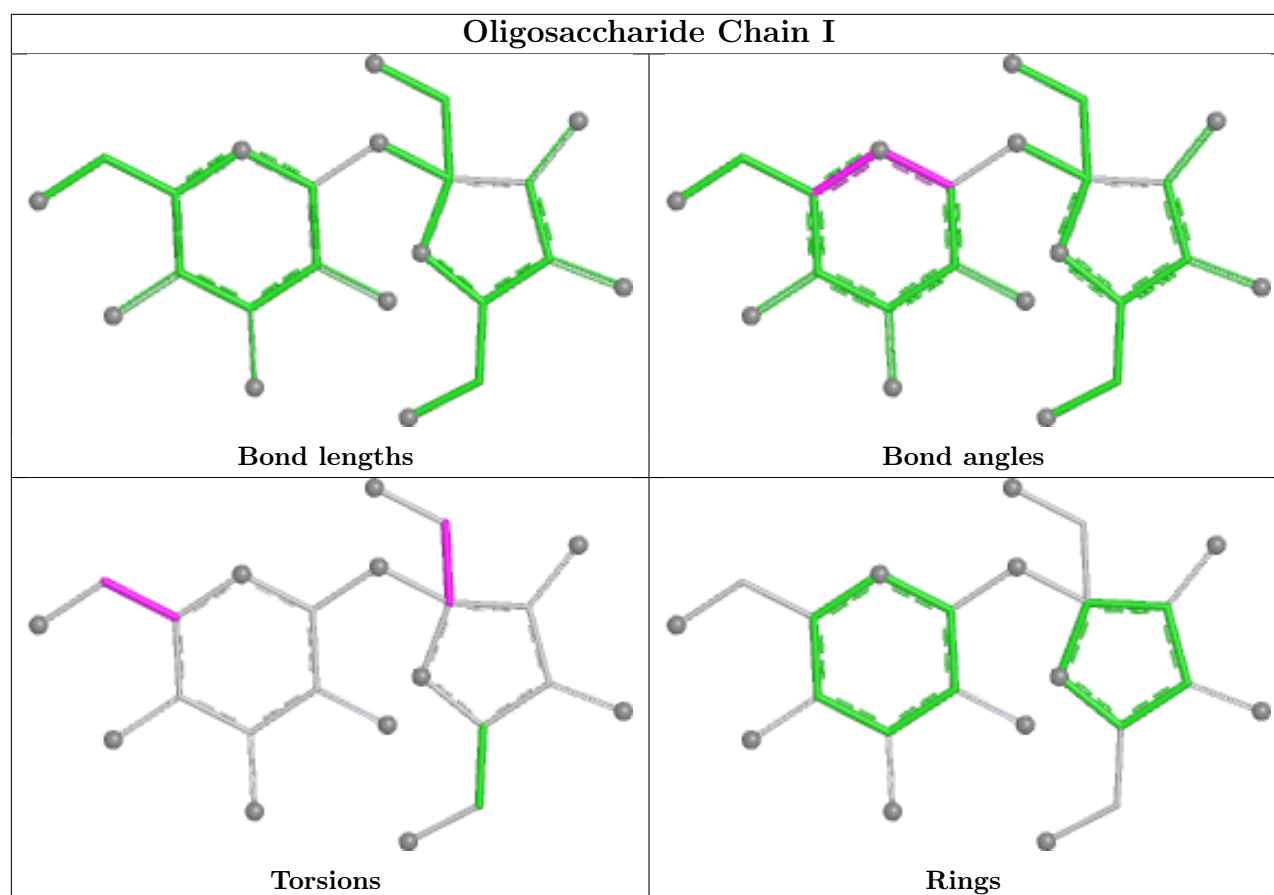


Oligosaccharide Chain E



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	504	-	4,4,4	0.33	0	6,6,6	0.19	0
6	SO4	B	501	-	4,4,4	0.38	0	6,6,6	0.25	0
6	SO4	B	503	-	4,4,4	0.38	0	6,6,6	0.26	0
6	SO4	A	301	-	4,4,4	0.61	0	6,6,6	0.39	0
6	SO4	B	502	-	4,4,4	0.18	0	6,6,6	0.21	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

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	A	218/218 (100%)	-0.29	1 (0%) 87 88	29, 41, 64, 98	0
1	F	218/218 (100%)	1.07	25 (11%) 9 10	35, 87, 121, 139	0
2	B	441/444 (99%)	0.41	56 (12%) 8 8	30, 49, 109, 133	0
2	G	438/444 (98%)	0.71	50 (11%) 10 10	37, 65, 107, 125	0
All	All	1315/1324 (99%)	0.50	132 (10%) 12 13	29, 59, 111, 139	0

All (132) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	57	TYR	7.5
2	B	252	MET	6.8
2	G	273	VAL	6.6
2	B	251	LEU	6.5
2	B	254	SER	6.1
2	G	103	PHE	5.9
2	B	247	PRO	5.7
2	B	302	VAL	5.2
2	B	331	SER	5.2
1	F	98	LEU	5.2
2	B	229	CYS	4.8
2	G	196	LEU	4.7
2	G	229	CYS	4.7
2	G	298	SER	4.5
2	B	296	PHE	4.3
2	G	329	PRO	4.3
2	G	199	LYS	4.2
2	G	238	PRO	4.1
2	B	253	ILE	4.1
1	F	83	GLU	4.0
2	G	138	THR	4.0

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Mol	Chain	Res	Type	RSRZ
2	B	138	THR	3.9
2	B	235	LEU	3.9
1	F	64	ALA	3.9
1	F	218	CYS	3.9
2	G	266	VAL	3.9
2	G	237	GLY	3.9
2	G	309	LEU	3.8
2	B	271	PRO	3.8
2	B	250	THR	3.7
2	B	249	ASP	3.7
2	G	299	THR	3.7
2	G	274	GLN	3.6
2	G	386	GLN	3.5
2	B	248	LYS	3.5
2	G	328	LEU	3.4
2	G	296	PHE	3.4
2	B	256	THR	3.4
2	G	136	ARG	3.4
2	B	330	SER	3.3
1	F	192	LYS	3.3
2	B	300	TYR	3.3
2	G	332	ILE	3.3
2	G	236	GLY	3.2
2	B	329	PRO	3.2
2	B	241	PHE	3.2
2	B	263	VAL	3.2
2	B	444	SER	3.2
2	G	300	TYR	3.2
2	G	198	THR	3.1
1	F	198	CYS	3.1
1	F	32	SER	3.1
2	G	268	GLN	3.1
2	B	310	HIS	3.0
2	G	295	GLN	3.0
1	A	218	CYS	3.0
2	G	271	PRO	3.0
2	B	222	TYR	3.0
2	B	291	PRO	3.0
2	B	308	VAL	2.9
2	B	328	LEU	2.9
2	B	268	GLN	2.8
2	G	200	THR	2.8

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Mol	Chain	Res	Type	RSRZ
2	B	262	VAL	2.8
2	B	198	THR	2.8
2	B	299	THR	2.8
1	F	34	TYR	2.8
2	B	301	ARG	2.8
2	G	263	VAL	2.7
1	F	151	GLN	2.6
1	F	96	ARG	2.6
1	F	46	GLN	2.6
2	G	287	ALA	2.6
2	G	121	ALA	2.6
2	G	302	VAL	2.6
1	F	15	PRO	2.6
2	B	332	ILE	2.6
2	B	295	GLN	2.5
2	G	326	LYS	2.5
2	G	139	SER	2.5
1	F	31	THR	2.5
1	F	157	ALA	2.5
2	B	243	PHE	2.4
2	B	139	SER	2.4
2	B	147	CYS	2.4
2	B	390	ASN	2.4
2	B	264	VAL	2.4
2	B	273	VAL	2.4
2	B	136	ARG	2.4
2	G	316	GLY	2.4
2	G	272	GLU	2.4
2	B	246	LYS	2.3
2	G	212	THR	2.3
2	G	253	ILE	2.3
2	G	362	GLN	2.3
2	B	65	LYS	2.3
2	G	322	LYS	2.3
2	G	54	SER	2.3
1	F	195	VAL	2.3
2	B	327	GLY	2.3
1	F	172	SER	2.3
2	G	137	SER	2.3
2	G	305	VAL	2.3
1	F	214	ASN	2.2
2	G	297	ASN	2.2

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Mol	Chain	Res	Type	RSRZ
1	F	153	LYS	2.2
2	G	325	ASN	2.2
2	G	291	PRO	2.2
2	B	233	GLU	2.2
1	F	148	ALA	2.2
2	B	234	PHE	2.2
1	F	155	ASP	2.2
2	B	223	GLY	2.2
2	B	1	GLN	2.2
2	G	323	VAL	2.2
2	B	356	GLU	2.2
2	B	255	ARG	2.1
1	F	158	LEU	2.1
2	G	145	LEU	2.1
2	G	197	GLY	2.1
2	B	335	THR	2.1
2	B	292	ARG	2.1
2	B	298	SER	2.1
2	B	309	LEU	2.1
2	G	240	VAL	2.1
2	B	286	ASN	2.1
1	F	150	VAL	2.1
2	B	134	CYS	2.0
2	G	327	GLY	2.0
1	F	152	TRP	2.0
1	F	206	SER	2.0
2	G	239	SER	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($\text{\AA}^2$)	Q<0.9
3	NAG	C	1	14/15	-	-	99,104,109,111	0

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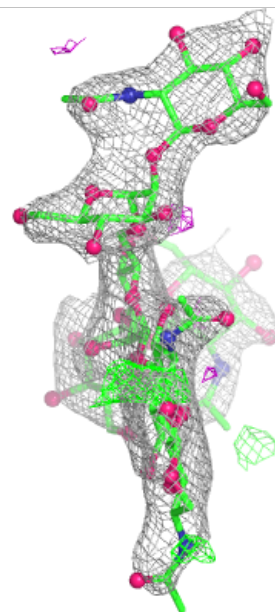
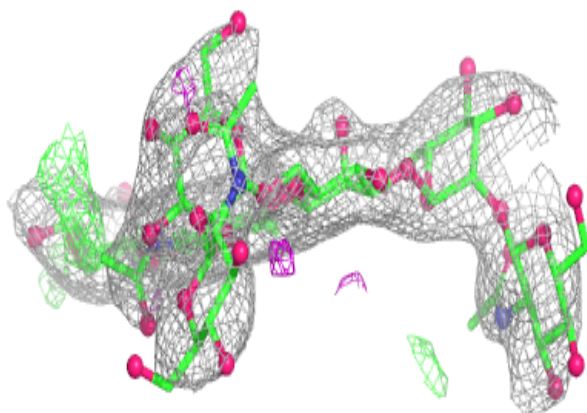
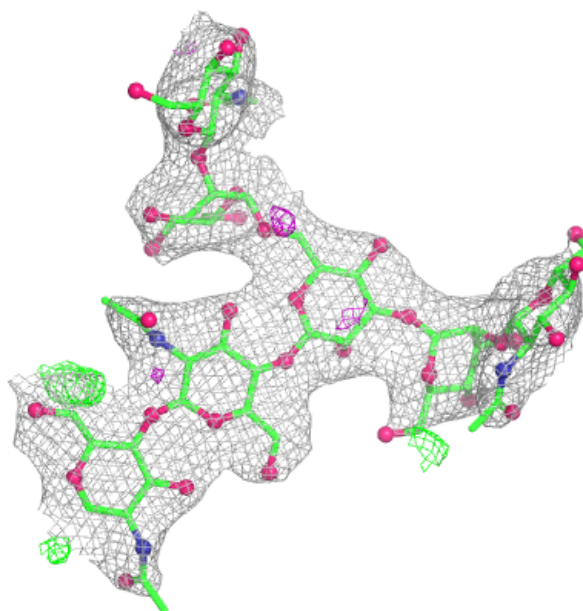
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	NAG	C	2	14/15	-	-	89,92,95,95	0
3	BMA	C	3	11/12	-	-	88,91,94,95	0
3	MAN	C	4	11/12	-	-	98,103,105,107	0
3	NAG	C	5	14/15	-	-	105,110,113,115	0
3	MAN	C	6	11/12	-	-	94,97,98,101	0
3	NAG	C	7	14/15	-	-	105,108,112,113	0
4	NAG	D	1	14/15	-	-	82,90,95,96	0
4	NAG	D	2	14/15	-	-	73,80,87,87	0
4	BMA	D	3	11/12	-	-	80,89,94,98	0
4	MAN	D	4	11/12	-	-	79,82,87,88	0
4	NAG	D	5	14/15	-	-	79,82,90,92	0
4	MAN	D	6	11/12	-	-	104,108,111,112	0
4	FUC	D	7	10/11	-	-	79,80,81,83	0
5	GLC	E	1	11/12	-	-	43,54,57,58	0
5	FRU	E	2	12/12	-	-	45,63,67,69	0
5	FRU	I	2	12/12	0.77	0.16	84,88,91,92	0
5	GLC	I	1	11/12	0.82	0.13	66,82,86,88	0
5	FRU	H	2	12/12	0.84	0.12	63,70,71,74	0
5	GLC	H	1	11/12	0.94	0.09	68,73,76,77	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.

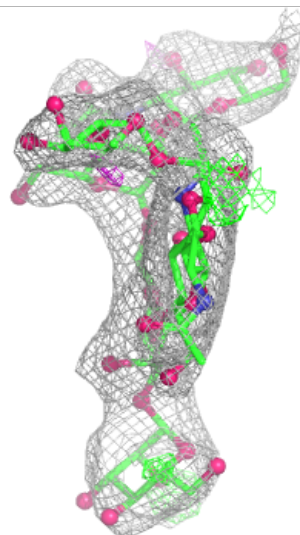
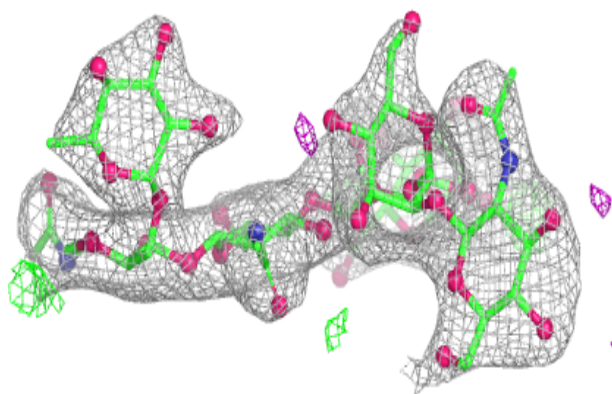
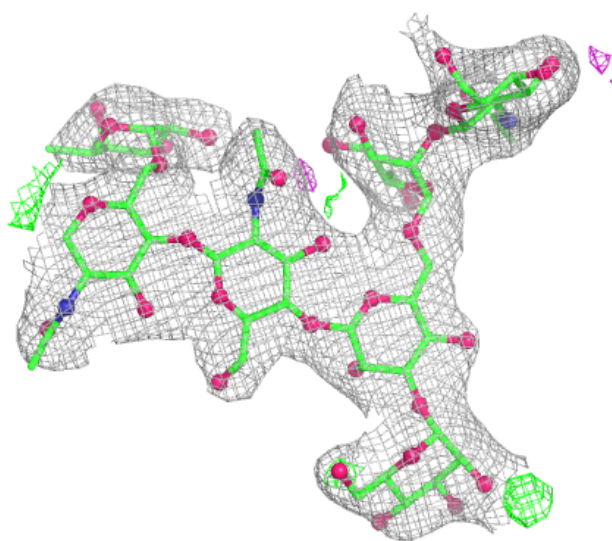
Electron density around Chain C:

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



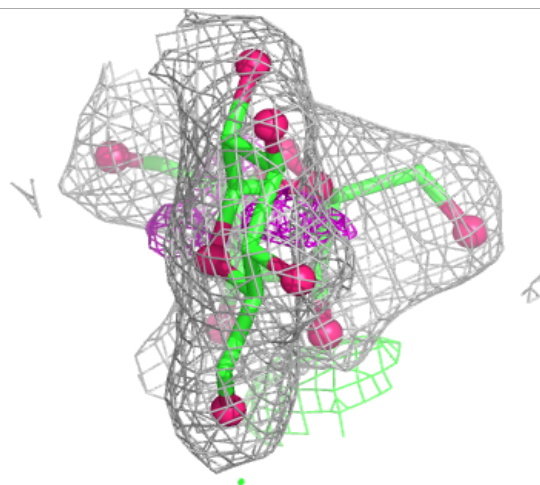
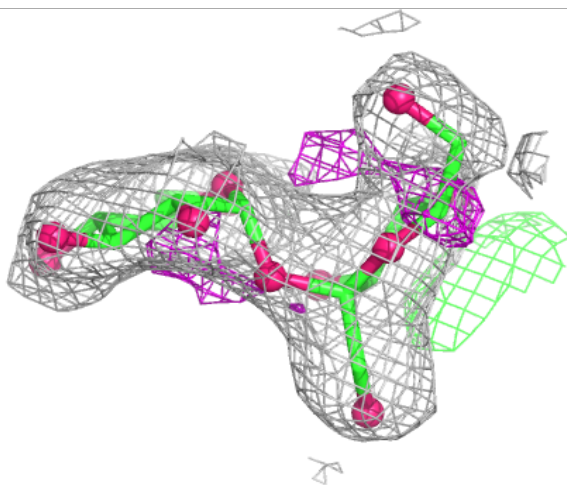
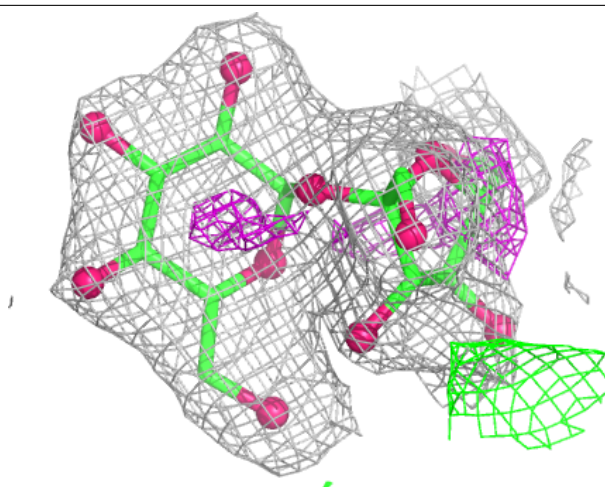
Electron density around Chain D:

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



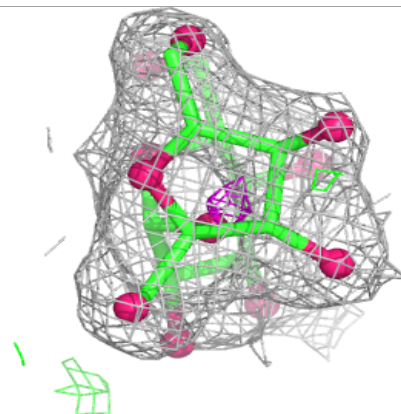
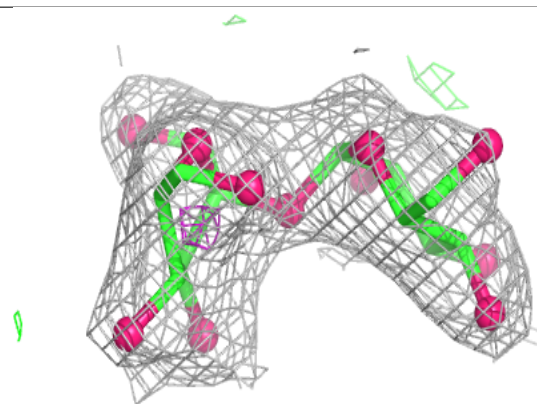
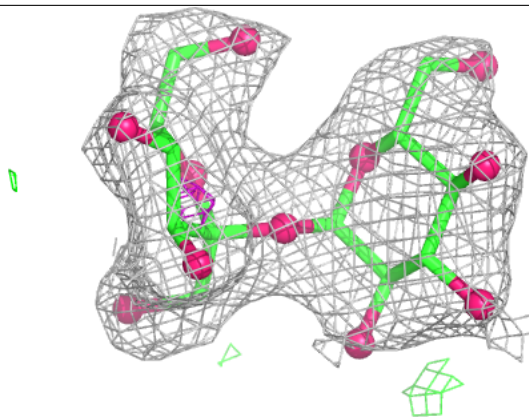
Electron density around Chain E:

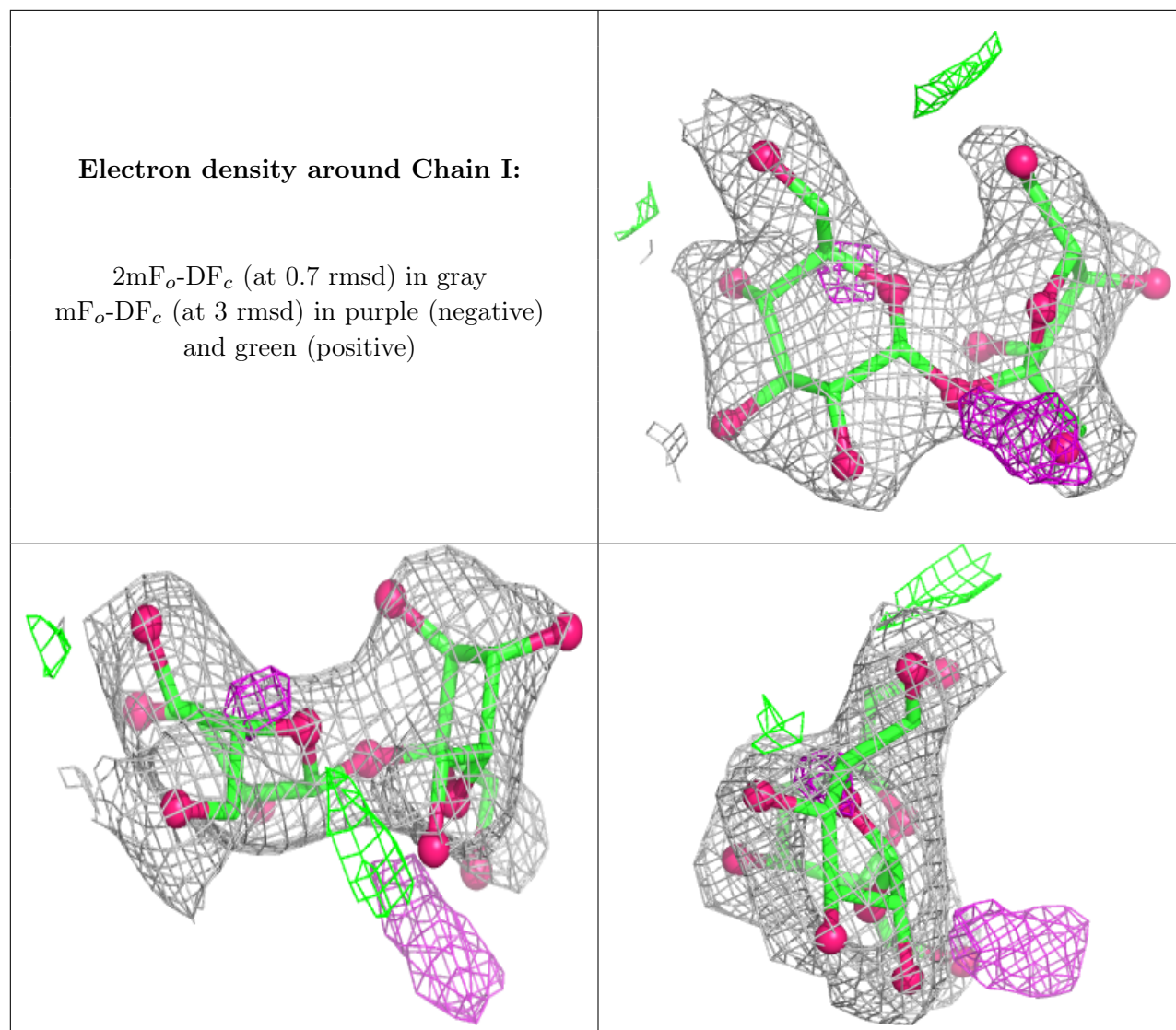
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



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 [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
6	SO4	B	504	5/5	0.57	0.16	113,113,114,115	0
6	SO4	A	301	5/5	0.91	0.14	59,70,72,75	0
6	SO4	B	502	5/5	0.92	0.09	82,84,84,89	0
6	SO4	B	501	5/5	0.92	0.08	99,99,99,100	0
6	SO4	B	503	5/5	0.93	0.09	69,77,78,79	0

6.5 Other polymers [i](#)

There are no such residues in this entry.