



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 18, 2025 – 07:29 PM EDT

PDB ID : 1LK9
Title : The Three-dimensional Structure of Alliinase from Garlic
Authors : Kuettner, E.B.; Hilgenfeld, R.; Weiss, M.S.
Deposited on : 2002-04-24
Resolution : 1.53 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 : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 1.21
EDS : 3.0
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4 : 9.0.004 (Gargrove)
Density-Fitness : 1.0.11
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.41.4

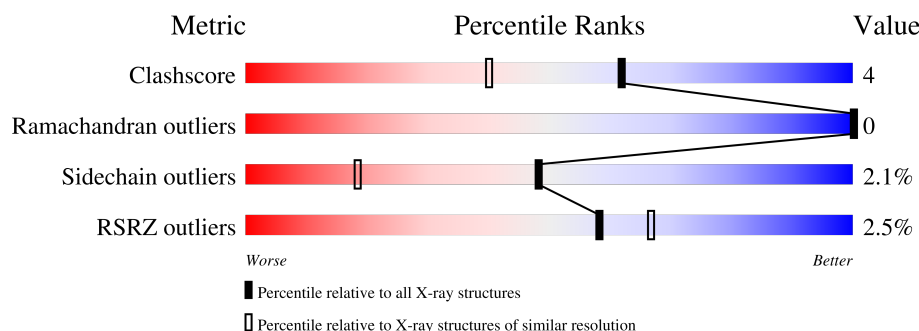
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.53 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	180529	3784 (1.56-1.52)
Ramachandran outliers	177936	3720 (1.56-1.52)
Sidechain outliers	177891	3717 (1.56-1.52)
RSRZ outliers	164620	3510 (1.56-1.52)

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	448	<div> <div>3%</div> <div> <div></div> <div>84%</div> <div>10%</div> <div>5%</div> </div> </div>
1	B	448	<div> <div>2%</div> <div> <div></div> <div>84%</div> <div>10%</div> <div>5%</div> </div> </div>
2	C	4	<div> <div>25%</div> <div>75%</div> </div>
3	D	2	<div> <div>50%</div> <div>50%</div> </div>
3	F	2	<div> <div>100%</div> </div>
4	E	2	<div> <div>50%</div> <div>50%</div> </div>

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
9	DHA	B	850[A]	-	X	X	-

2 Entry composition [i](#)

There are 10 unique types of molecules in this entry. The entry contains 7996 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.

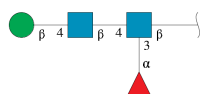
- Molecule 1 is a protein called ALLIIN LYASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	425	Total	C	N	O	S	0	11	0
			3453	2200	579	650	24			
1	B	427	Total	C	N	O	S	0	6	0
			3461	2208	580	649	24			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	176	ASP	ASN	SEE REMARK 999	UNP Q01594
B	176	ASP	ASN	SEE REMARK 999	UNP Q01594

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	C	4	Total	C	N	O	0	0	0
			49	28	2	19			

- Molecule 3 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



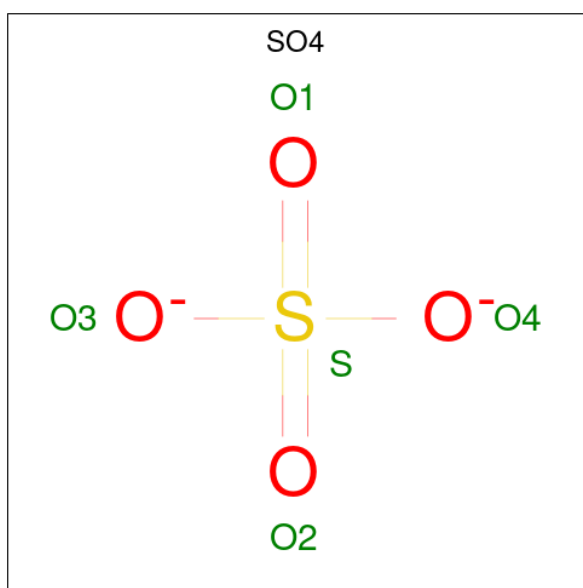
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	D	2	Total	C	N	O	0	0	0
			28	16	2	10			
3	F	2	Total	C	N	O	0	0	0
			28	16	2	10			

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	E	2	Total	C	N	O	0	0	0
			24	14	1	9			

- Molecule 5 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



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

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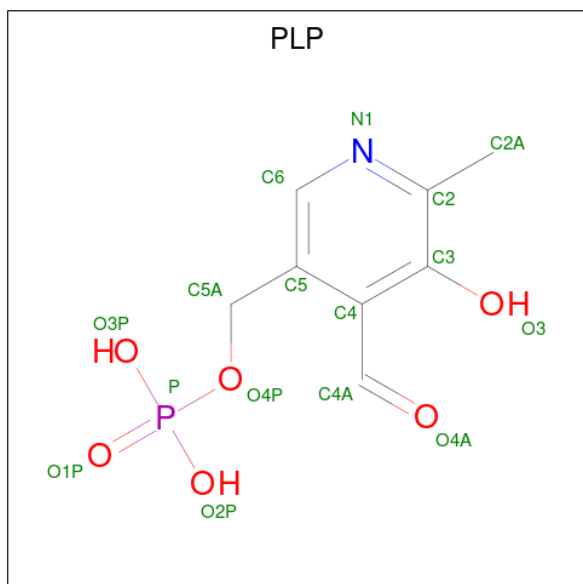
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	O	S	0	0
			5	4	1		
5	A	1	Total	O	S	0	0
			5	4	1		
5	B	1	Total	O	S	0	0
			5	4	1		
5	B	1	Total	O	S	0	0
			5	4	1		
5	B	1	Total	O	S	0	0
			5	4	1		
5	B	1	Total	O	S	0	0
			5	4	1		

- Molecule 6 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

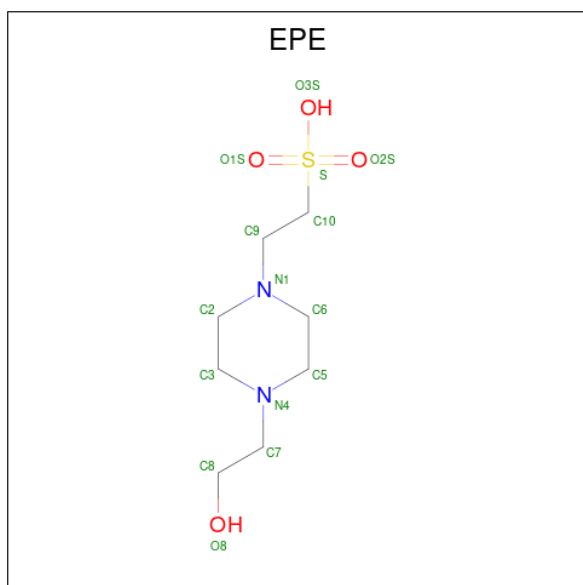
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	1	Total	Cl	0	0
			1	1		
6	B	1	Total	Cl	0	0
			1	1		

- Molecule 7 is PYRIDOXAL-5'-PHOSPHATE (three-letter code: PLP) (formula: C₈H₁₀NO₆P).



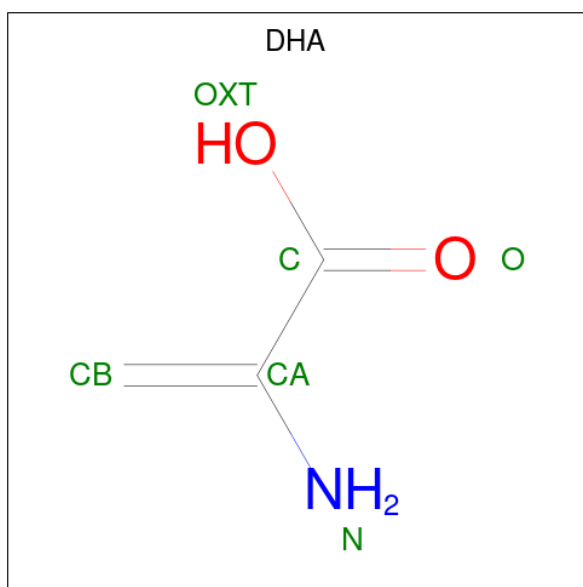
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
7	A	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
7	B	1	Total	C	N	O	P	0	0
			15	8	1	5	1		

- Molecule 8 is 4-(2-HYDROXYETHYL)-1-PIPERAZINE ETHANESULFONIC ACID (three-letter code: EPE) (formula: $C_8H_{18}N_2O_4S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
8	A	1	Total	C	N	O	S	0	1
			15	8	2	4	1		
8	A	1	Total	C	N	O	S	0	1
			15	8	2	4	1		

- Molecule 9 is 2-AMINO-ACRYLIC ACID (three-letter code: DHA) (formula: $C_3H_5NO_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
9	B	1	Total	C	N	O	0	1
			6	3	1	2		

- Molecule 10 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	394	Total	O	0	0
			394	394		
10	B	436	Total	O	0	0
			436	436		

- Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain F:  100%

MAG1
MAG2

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

Chain E:  50% 50%

MAG1
FUC2

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	68.45Å 101.07Å 155.69Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	12.00 – 1.53 12.00 – 1.53	Depositor EDS
% Data completeness (in resolution range)	98.7 (12.00-1.53) 98.6 (12.00-1.53)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.71 (at 1.53Å)	Xtriage
Refinement program	REFMAC 4.0.6	Depositor
R, R_{free}	0.193 , 0.221 0.184 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	20.4	Xtriage
Anisotropy	0.147	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.41 , 46.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	7996	wwPDB-VP
Average B, all atoms (Å ²)	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.45% 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: PLP, DHA, SO4, EPE, FUC, BMA, CL, 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	0.55	0/3601	1.21	22/4874 (0.5%)
1	B	0.58	0/3579	1.22	20/4846 (0.4%)
All	All	0.57	0/7180	1.22	42/9720 (0.4%)

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	1
1	B	0	1
All	All	0	2

There are no bond length outliers.

All (42) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	213	ARG	NE-CZ-NH2	-12.96	113.82	120.30
1	A	25	ARG	NE-CZ-NH1	11.00	125.80	120.30
1	A	89	ARG	NE-CZ-NH1	9.31	124.95	120.30
1	B	128	PHE	CB-CG-CD2	-8.95	114.53	120.80
1	A	25	ARG	NE-CZ-NH2	-8.74	115.93	120.30
1	B	89	ARG	NE-CZ-NH2	-8.13	116.24	120.30
1	A	323	ARG	NE-CZ-NH1	7.48	124.04	120.30
1	B	312	ARG	CD-NE-CZ	7.47	134.06	123.60
1	A	128	PHE	CB-CG-CD2	-7.24	115.73	120.80
1	B	128	PHE	CB-CG-CD1	7.07	125.75	120.80
1	A	128	PHE	CB-CG-CD1	6.99	125.69	120.80
1	A	287	ARG	NE-CZ-NH2	-6.98	116.81	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	325	ARG	NE-CZ-NH2	-6.86	116.87	120.30
1	B	287	ARG	NE-CZ-NH2	6.81	123.70	120.30
1	A	357	ARG	NE-CZ-NH2	-6.69	116.95	120.30
1	A	208	PRO	N-CA-C	6.54	129.09	112.10
1	B	312	ARG	NE-CZ-NH2	6.45	123.52	120.30
1	B	213	ARG	NH1-CZ-NH2	6.41	126.45	119.40
1	A	123[A]	ASP	N-CA-CB	-6.37	99.14	110.60
1	A	123[B]	ASP	N-CA-CB	-6.37	99.14	110.60
1	A	259	ARG	NE-CZ-NH1	6.35	123.47	120.30
1	B	401	ARG	NE-CZ-NH1	6.30	123.45	120.30
1	B	323	ARG	NE-CZ-NH2	-6.07	117.27	120.30
1	B	259	ARG	NE-CZ-NH2	6.04	123.32	120.30
1	B	337	ASP	CB-CG-OD1	6.04	123.74	118.30
1	B	352	TYR	CB-CG-CD1	-5.92	117.45	121.00
1	B	89	ARG	NE-CZ-NH1	5.91	123.25	120.30
1	A	100	PHE	CB-CG-CD1	5.87	124.91	120.80
1	A	100	PHE	CB-CG-CD2	-5.78	116.75	120.80
1	B	338	ARG	NE-CZ-NH1	-5.74	117.43	120.30
1	A	357	ARG	NE-CZ-NH1	-5.58	117.51	120.30
1	A	357	ARG	NH1-CZ-NH2	5.58	125.53	119.40
1	B	68	PHE	CB-CG-CD1	5.54	124.68	120.80
1	A	412	ASP	CB-CG-OD1	5.52	123.27	118.30
1	A	400	VAL	CG1-CB-CG2	5.51	119.72	110.90
1	A	29	ASP	CB-CG-OD1	5.41	123.17	118.30
1	A	213	ARG	NE-CZ-NH2	-5.34	117.63	120.30
1	B	259	ARG	NE-CZ-NH1	-5.26	117.67	120.30
1	A	241	ASP	CB-CG-OD2	-5.21	113.61	118.30
1	B	29	ASP	CB-CG-OD2	-5.08	113.72	118.30
1	A	384	ARG	NE-CZ-NH2	-5.03	117.79	120.30
1	B	124	ARG	NE-CZ-NH1	5.01	122.81	120.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	146	ASN	Sidechain
1	B	146	ASN	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	A	3453	0	3329	28	0
1	B	3461	0	3351	28	0
2	C	49	0	43	0	0
3	D	28	0	25	0	0
3	F	28	0	25	0	0
4	E	24	0	22	4	0
5	A	30	0	0	0	0
5	B	25	0	0	0	0
6	A	1	0	0	0	0
6	B	1	0	0	0	0
7	A	15	0	7	0	0
7	B	15	0	7	1	0
8	A	30	0	36	3	0
9	B	6	0	3	4	0
10	A	394	0	0	1	0
10	B	436	0	0	3	0
All	All	7996	0	6848	56	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 4.

All (56) 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)
4:E:2:FUC:H63	4:E:2:FUC:H2	1.47	0.97
1:B:425:LYS:HD2	1:B:426:ARG:H	1.30	0.94
1:A:106:GLU:HG3	1:A:126:ILE:HD12	1.74	0.69
1:B:251:LYS:CE	9:B:850[A]:DHA:HB1	2.22	0.69
1:B:251:LYS:HE2	9:B:850[A]:DHA:HB1	1.74	0.68
1:A:286:PRO:HG2	1:B:286:PRO:HG2	1.76	0.68
1:A:177:LYS:HA	1:B:177:LYS:HG2	1.78	0.64
4:E:2:FUC:H63	4:E:2:FUC:C2	2.23	0.64
1:A:177:LYS:HB2	1:B:177:LYS:HE2	1.81	0.63
1:B:141:ILE:HD12	1:B:277[B]:TYR:CE1	2.35	0.60
1:B:144[B]:SER:HB3	1:B:145:PRO:HD2	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:425:LYS:HD2	1:B:426:ARG:N	2.10	0.58
1:B:115[A]:VAL:HG13	1:B:304:VAL:HG11	1.84	0.58
1:B:420:ASP:HA	1:B:423:LYS:HE2	1.86	0.57
1:A:177:LYS:HB2	1:B:177:LYS:CE	2.35	0.57
1:B:267[A]:ASP:OD2	1:B:269:SER:OG	2.15	0.56
1:A:311:MET:CE	1:A:316:THR:HG22	2.37	0.55
1:A:336:SER:HB3	1:A:422:VAL:HG13	1.88	0.55
1:A:279:THR:CG2	8:A:851[B]:EPE:H72	2.37	0.54
1:A:141:ILE:HD12	1:A:277[B]:TYR:CE1	2.42	0.54
1:A:311:MET:HA	1:A:311:MET:HE2	1.90	0.54
1:A:311:MET:CE	1:A:320:LYS:HD2	2.38	0.53
1:B:144[A]:SER:HB2	1:B:145:PRO:HD2	1.91	0.51
1:A:7:LYS:HD3	1:A:10:GLU:OE1	2.10	0.51
1:B:251:LYS:HE2	9:B:850[A]:DHA:CB	2.42	0.50
4:E:2:FUC:C2	4:E:2:FUC:C6	2.84	0.49
1:B:320:LYS:O	1:B:324:GLU:HG3	2.13	0.48
1:A:144[A]:SER:HB3	1:A:145:PRO:HD2	1.96	0.48
1:B:326:TRP:HB2	10:B:1112:HOH:O	2.13	0.48
1:B:311:MET:SD	1:B:320:LYS:HD3	2.53	0.48
1:A:144[B]:SER:HB2	1:A:145:PRO:HD2	1.96	0.47
1:B:125:TYR:HB3	1:B:271:TYR:CD1	2.49	0.47
1:A:110:LYS:HE3	1:A:126:ILE:HD11	1.97	0.47
1:A:283:GLU:OE2	8:A:851[B]:EPE:N4	2.47	0.47
1:A:207:ASN:HA	1:A:208:PRO:HA	1.69	0.46
1:A:311:MET:HE3	1:A:320:LYS:HD2	1.97	0.46
1:A:232:HIS:ND1	1:A:318:GLY:HA3	2.31	0.46
1:A:125:TYR:HB3	1:A:271:TYR:CD1	2.52	0.45
7:B:600:PLP:O3	9:B:850[A]:DHA:N	2.50	0.44
1:B:427:LYS:HG2	10:B:1232:HOH:O	2.18	0.44
1:A:176:ASP:HB3	1:B:178:LYS:CE	2.48	0.43
1:B:148:THR:HG23	1:B:178:LYS:HZ1	1.82	0.43
1:A:110:LYS:HE3	1:A:126:ILE:CD1	2.48	0.43
1:A:7:LYS:HD2	10:A:1160:HOH:O	2.18	0.43
1:B:101:ILE:HG23	1:B:128:PHE:CE2	2.54	0.43
1:A:419:LYS:O	1:A:423:LYS:HG2	2.18	0.43
1:B:148:THR:HG23	1:B:178:LYS:NZ	2.35	0.42
4:E:2:FUC:H2	4:E:2:FUC:C6	2.28	0.42
1:B:137:HIS:CE1	1:B:141:ILE:HD11	2.54	0.42
1:B:157:LYS:HE3	1:B:197:GLN:HB3	2.02	0.42
1:A:56:GLY:O	1:A:384:ARG:NH2	2.53	0.42
1:A:177:LYS:HG3	1:B:176:ASP:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:311:MET:HE1	1:A:316:THR:HG22	2.01	0.41
8:A:852[B]:EPE:H61	8:A:852[B]:EPE:H102	1.65	0.41
1:A:370:TRP:CH2	1:A:425:LYS:HG2	2.55	0.41
1:B:15[A]:VAL:HG23	10:B:1139:HOH: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	A	434/448 (97%)	417 (96%)	17 (4%)	0	100	100
1	B	431/448 (96%)	419 (97%)	12 (3%)	0	100	100
All	All	865/896 (96%)	836 (97%)	29 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	383/395 (97%)	375 (98%)	8 (2%)	48	18
1	B	380/395 (96%)	371 (98%)	9 (2%)	44	14
All	All	763/790 (97%)	746 (98%)	17 (2%)	48	17

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	25	ARG
1	A	55	GLN
1	A	157	LYS
1	A	281	ASN
1	A	336	SER
1	A	337	ASP
1	A	384	ARG
1	A	400	VAL
1	B	6	MET
1	B	25	ARG
1	B	115[A]	VAL
1	B	115[B]	VAL
1	B	157	LYS
1	B	232	HIS
1	B	281	ASN
1	B	425	LYS
1	B	427	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	381	GLN
1	A	386	ASN
1	B	408	GLN

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 ⓘ

10 monosaccharides are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NAG	C	1	2,1	14,14,15	1.08	1 (7%)	17,19,21	1.25	2 (11%)
2	NAG	C	2	2	14,14,15	1.05	1 (7%)	17,19,21	1.34	3 (17%)
2	BMA	C	3	2	11,11,12	0.97	0	15,15,17	0.53	0
2	FUC	C	4	2	10,10,11	1.05	1 (10%)	14,14,16	0.77	0
3	NAG	D	1	1,3	14,14,15	1.08	1 (7%)	17,19,21	1.11	1 (5%)
3	NAG	D	2	3	14,14,15	0.85	0	17,19,21	0.80	0
4	NAG	E	1	4,1	14,14,15	1.05	1 (7%)	17,19,21	1.62	4 (23%)
4	FUC	E	2	4	10,10,11	1.13	1 (10%)	14,14,16	0.92	1 (7%)
3	NAG	F	1	1,3	14,14,15	1.03	0	17,19,21	1.25	3 (17%)
3	NAG	F	2	3	14,14,15	1.03	1 (7%)	17,19,21	1.52	2 (11%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	C	1	2,1	-	1/6/23/26	0/1/1/1
2	NAG	C	2	2	-	1/6/23/26	0/1/1/1
2	BMA	C	3	2	-	2/2/19/22	0/1/1/1
2	FUC	C	4	2	-	-	0/1/1/1
3	NAG	D	1	1,3	-	1/6/23/26	0/1/1/1
3	NAG	D	2	3	-	2/6/23/26	0/1/1/1
4	NAG	E	1	4,1	-	2/6/23/26	0/1/1/1
4	FUC	E	2	4	-	-	0/1/1/1
3	NAG	F	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	F	2	3	-	2/6/23/26	0/1/1/1

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	E	1	NAG	C1-C2	2.43	1.55	1.52
3	D	1	NAG	C1-C2	2.39	1.55	1.52
2	C	1	NAG	C1-C2	2.36	1.55	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	2	NAG	C1-C2	2.36	1.55	1.52
3	F	2	NAG	C1-C2	2.07	1.55	1.52
2	C	4	FUC	C2-C3	2.04	1.55	1.52
4	E	2	FUC	C2-C3	2.01	1.55	1.52

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	2	NAG	C2-N2-C7	4.54	128.98	122.90
4	E	1	NAG	C4-C3-C2	-3.77	105.50	111.02
3	F	1	NAG	C4-C3-C2	-3.34	106.12	111.02
2	C	1	NAG	O7-C7-C8	-3.30	116.18	122.05
4	E	1	NAG	C2-N2-C7	-3.27	118.52	122.90
3	D	1	NAG	O7-C7-C8	-3.20	116.36	122.05
2	C	1	NAG	C1-C2-N2	-2.73	106.14	110.43
2	C	2	NAG	O5-C1-C2	-2.70	107.11	111.29
4	E	1	NAG	C1-O5-C5	2.65	115.73	112.19
2	C	2	NAG	C1-O5-C5	-2.35	109.04	112.19
3	F	2	NAG	O7-C7-C8	-2.28	118.00	122.05
2	C	2	NAG	C4-C3-C2	-2.21	107.78	111.02
4	E	1	NAG	O7-C7-C8	-2.21	118.12	122.05
4	E	2	FUC	O5-C5-C6	2.15	112.07	107.40
3	F	1	NAG	O7-C7-C8	-2.07	118.37	122.05
3	F	1	NAG	O7-C7-N2	2.03	125.57	121.98

There are no chirality outliers.

All (11) torsion outliers are listed below:

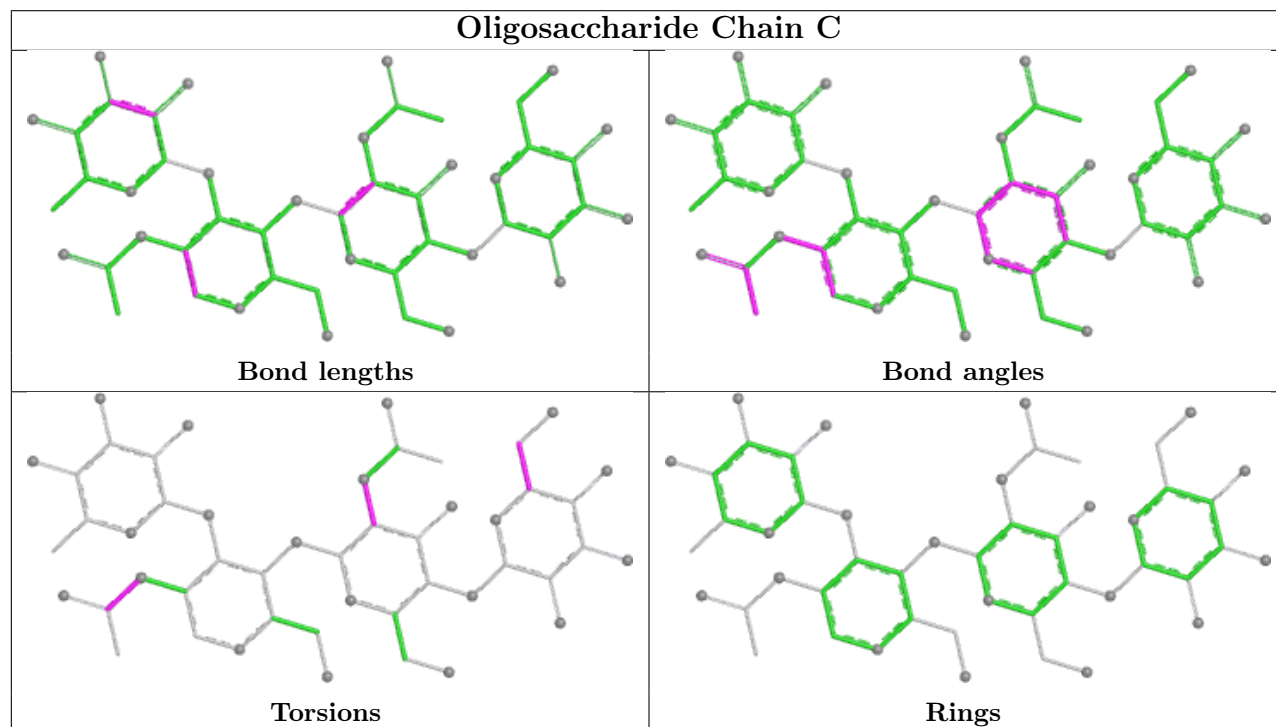
Mol	Chain	Res	Type	Atoms
2	C	2	NAG	C3-C2-N2-C7
3	D	2	NAG	O5-C5-C6-O6
3	F	2	NAG	O5-C5-C6-O6
2	C	3	BMA	C4-C5-C6-O6
3	F	2	NAG	C4-C5-C6-O6
3	D	2	NAG	C4-C5-C6-O6
2	C	3	BMA	O5-C5-C6-O6
4	E	1	NAG	O7-C7-N2-C2
2	C	1	NAG	O7-C7-N2-C2
3	D	1	NAG	O7-C7-N2-C2
4	E	1	NAG	C4-C5-C6-O6

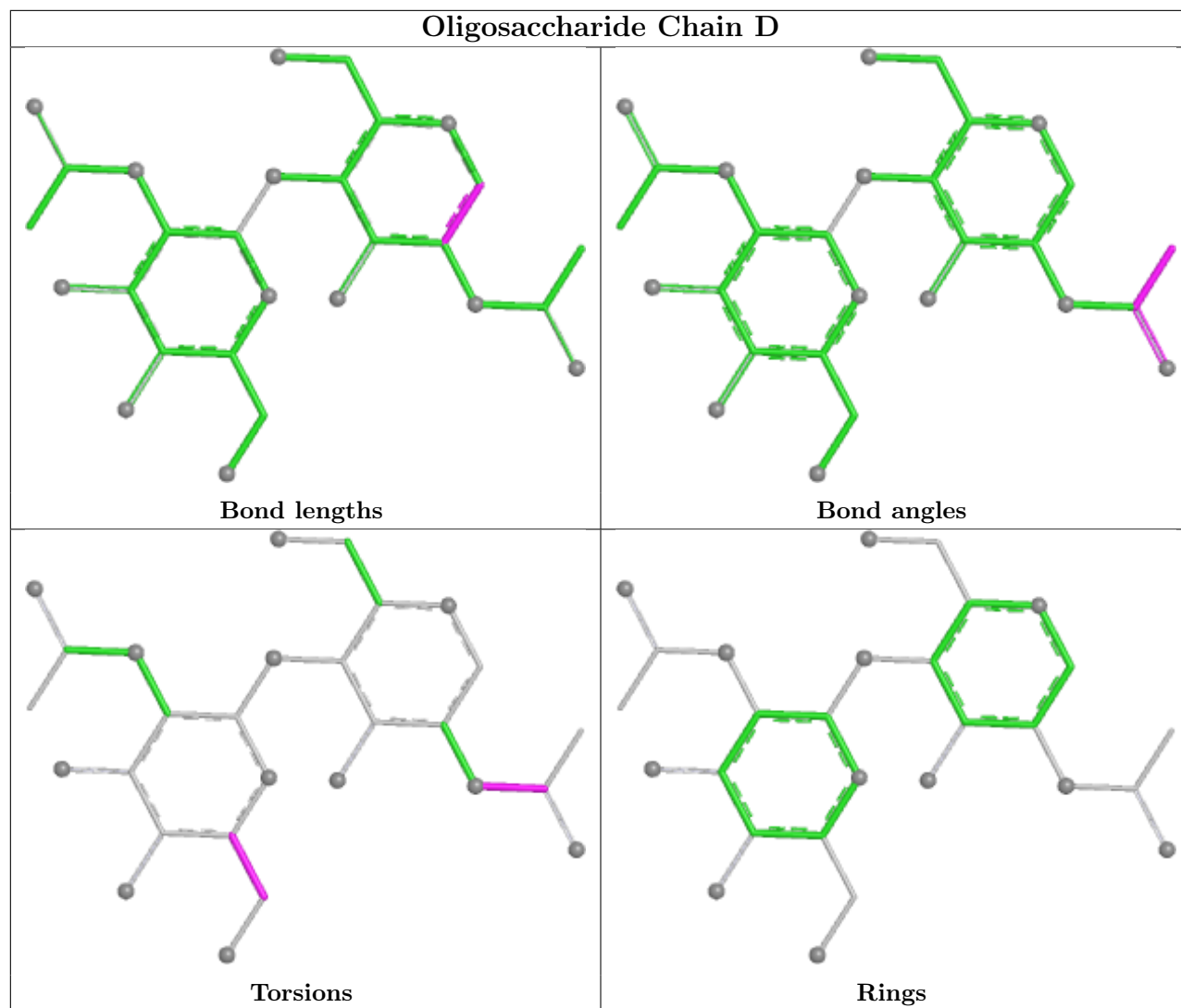
There are no ring outliers.

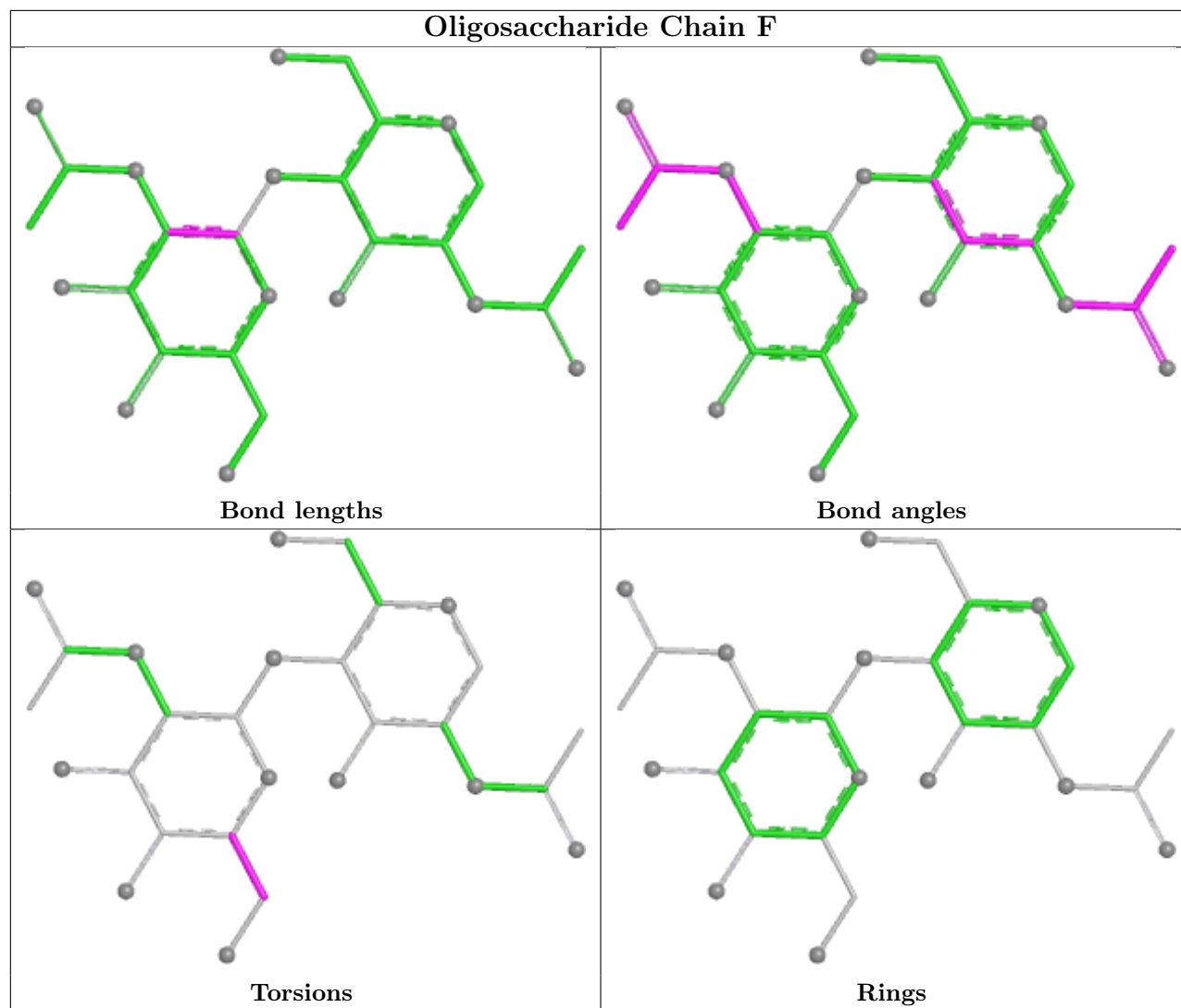
1 monomer is involved in 4 short contacts:

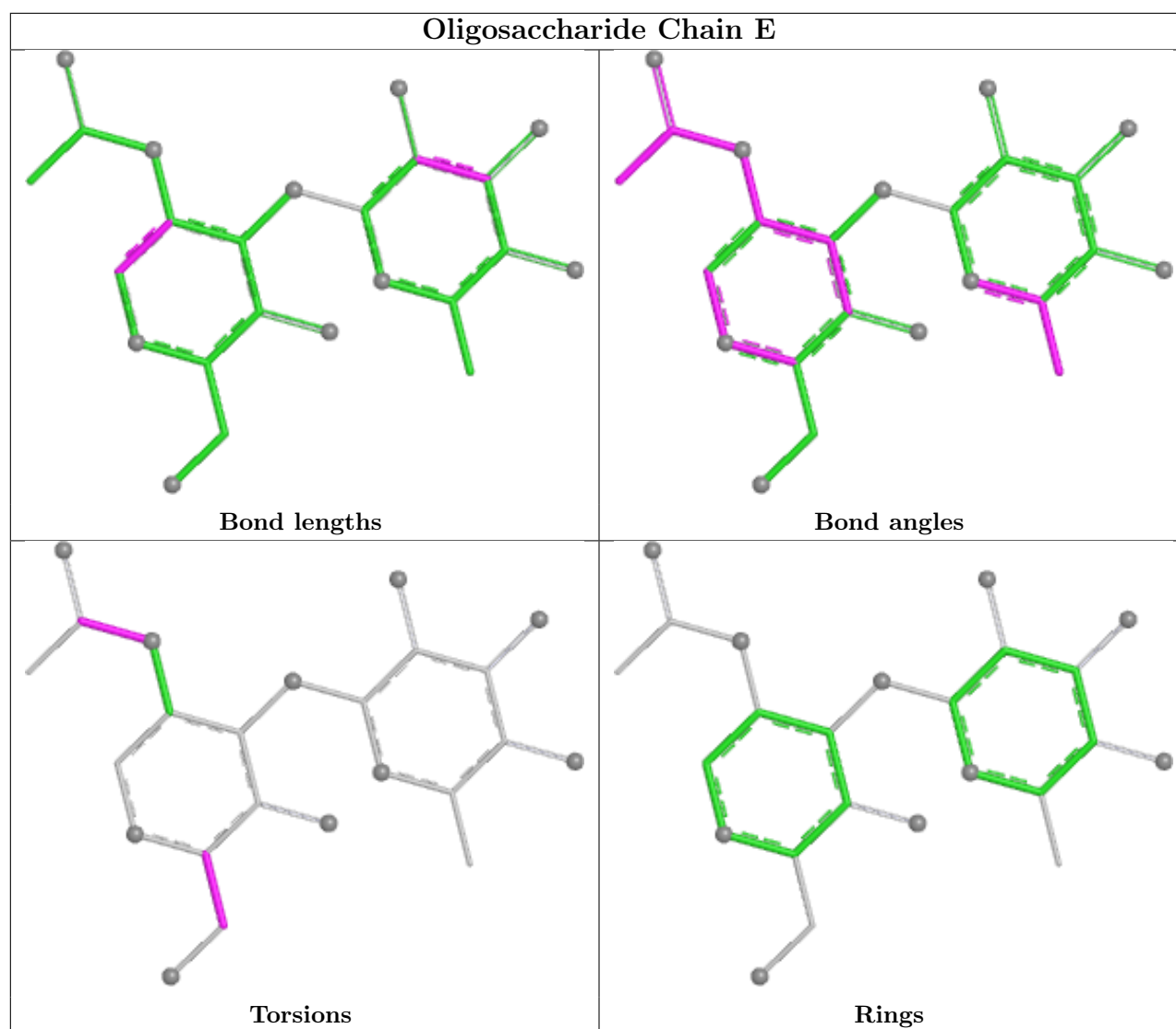
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	E	2	FUC	4	0

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









5.6 Ligand geometry [i](#)

Of 18 ligands modelled in this entry, 2 are monoatomic - leaving 16 for Mogul analysis.

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	SO4	B	902	-	4,4,4	0.66	0	6,6,6	0.48	0
5	SO4	B	909	-	4,4,4	0.68	0	6,6,6	0.21	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	PLP	B	600	9,1	15,15,16	1.47	4 (26%)	21,22,23	1.78	5 (23%)
9	DHA	B	850[A]	7	4,5,5	2.98	2 (50%)	5,6,6	2.54	5 (100%)
7	PLP	A	600	1	15,15,16	1.38	1 (6%)	21,22,23	1.66	3 (14%)
5	SO4	B	908	-	4,4,4	0.62	0	6,6,6	0.21	0
5	SO4	B	901	-	4,4,4	0.87	0	6,6,6	0.42	0
5	SO4	A	906	-	4,4,4	0.66	0	6,6,6	0.26	0
5	SO4	A	907	-	4,4,4	0.66	0	6,6,6	0.19	0
5	SO4	A	905	-	4,4,4	0.73	0	6,6,6	0.15	0
8	EPE	A	851[B]	-	15,15,15	1.77	2 (13%)	19,20,20	1.94	7 (36%)
8	EPE	A	852[B]	-	15,15,15	1.69	2 (13%)	19,20,20	1.71	5 (26%)
5	SO4	A	911	-	4,4,4	0.67	0	6,6,6	0.12	0
5	SO4	B	903	-	4,4,4	0.69	0	6,6,6	0.47	0
5	SO4	A	910	-	4,4,4	0.75	0	6,6,6	0.47	0
5	SO4	A	904	-	4,4,4	0.68	0	6,6,6	0.07	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
7	PLP	B	600	9,1	-	1/6/6/8	0/1/1/1
9	DHA	B	850[A]	7	-	2/2/4/4	-
7	PLP	A	600	1	-	0/6/6/8	0/1/1/1
8	EPE	A	851[B]	-	-	3/9/19/19	0/1/1/1
8	EPE	A	852[B]	-	-	4/9/19/19	0/1/1/1

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	B	850[A]	DHA	O-C	5.39	1.35	1.22
8	A	851[B]	EPE	O3S-S	4.77	1.65	1.47
8	A	852[B]	EPE	O3S-S	4.76	1.65	1.47
8	A	851[B]	EPE	C10-S	3.54	1.82	1.77
8	A	852[B]	EPE	C10-S	3.29	1.82	1.77
7	B	600	PLP	C2A-C2	3.03	1.55	1.50
9	B	850[A]	DHA	OXT-C	-2.51	1.23	1.30
7	B	600	PLP	P-O1P	2.49	1.58	1.50
7	A	600	PLP	C2A-C2	2.45	1.54	1.50
7	B	600	PLP	C4A-C4	2.44	1.56	1.51
7	B	600	PLP	C5A-C5	2.03	1.56	1.50

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	600	PLP	C4A-C4-C5	4.82	125.91	120.94
8	A	851[B]	EPE	O2S-S-C10	4.34	113.28	106.73
7	B	600	PLP	C4A-C4-C5	3.98	125.04	120.94
9	B	850[A]	DHA	O-C-CA	-3.94	115.56	123.60
8	A	852[B]	EPE	O2S-S-C10	3.90	112.62	106.73
7	B	600	PLP	C5A-C5-C6	-3.62	113.46	119.36
8	A	852[B]	EPE	O3S-S-O1S	-3.26	103.25	111.40
7	A	600	PLP	C3-C4-C5	-3.20	114.75	118.59
8	A	851[B]	EPE	O1S-S-C10	-2.98	102.23	106.73
8	A	851[B]	EPE	C7-N4-C3	2.63	118.26	111.24
7	B	600	PLP	C4A-C4-C3	-2.58	116.22	120.52
7	A	600	PLP	C5A-C5-C6	-2.46	115.34	119.36
7	B	600	PLP	O4P-C5A-C5	-2.45	104.76	109.36
8	A	851[B]	EPE	C6-C5-N4	-2.39	105.84	110.65
8	A	851[B]	EPE	C6-N1-C2	2.36	113.92	108.84
8	A	852[B]	EPE	O2S-S-O1S	2.34	121.42	113.82
7	B	600	PLP	C5A-C5-C4	2.27	127.12	122.64
8	A	851[B]	EPE	O3S-S-O1S	-2.24	105.78	111.40
8	A	851[B]	EPE	C3-C2-N1	2.23	115.15	110.65
8	A	852[B]	EPE	O1S-S-C10	-2.17	103.45	106.73
9	B	850[A]	DHA	OXT-C-O	2.12	128.96	123.90
8	A	852[B]	EPE	C2-C3-N4	2.09	114.87	110.65
9	B	850[A]	DHA	OXT-C-CA	2.02	115.38	112.44
9	B	850[A]	DHA	CB-CA-C	-2.02	116.18	121.06
9	B	850[A]	DHA	CB-CA-N	-2.01	120.92	125.76

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	A	851[B]	EPE	C9-C10-S-O1S
8	A	852[B]	EPE	C9-C10-S-O2S
9	B	850[A]	DHA	OXT-C-CA-CB
8	A	851[B]	EPE	N4-C7-C8-O8
8	A	852[B]	EPE	N4-C7-C8-O8
9	B	850[A]	DHA	O-C-CA-CB
7	B	600	PLP	C6-C5-C5A-O4P
8	A	852[B]	EPE	C9-C10-S-O1S
8	A	852[B]	EPE	C9-C10-S-O3S
8	A	851[B]	EPE	C9-C10-S-O2S

There are no ring outliers.

4 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	B	600	PLP	1	0
9	B	850[A]	DHA	4	0
8	A	851[B]	EPE	2	0
8	A	852[B]	EPE	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	A	425/448 (94%)	0.13	12 (2%) 55 63	11, 24, 38, 53	11 (2%)
1	B	427/448 (95%)	-0.19	9 (2%) 63 72	12, 20, 37, 55	6 (1%)
All	All	852/896 (95%)	-0.03	21 (2%) 58 67	11, 22, 38, 55	17 (1%)

All (21) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1	LYS	3.8
1	B	149	ALA	3.0
1	A	424	ALA	2.8
1	B	178	LYS	2.7
1	B	177	LYS	2.6
1	A	327	VAL	2.6
1	B	148	THR	2.6
1	A	123[A]	ASP	2.6
1	A	337	ASP	2.6
1	B	427	LYS	2.5
1	B	191	ASN	2.4
1	A	370	TRP	2.4
1	B	176	ASP	2.4
1	A	55	GLN	2.3
1	A	176	ASP	2.3
1	A	416	TYR	2.2
1	B	114	GLU	2.1
1	A	151	PRO	2.1
1	A	425	LYS	2.1
1	B	192	VAL	2.1
1	A	149	ALA	2.1

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 ⓘ

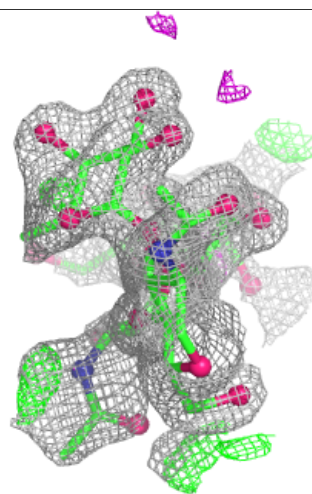
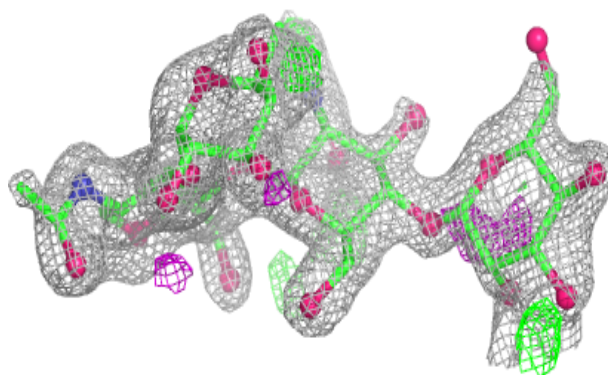
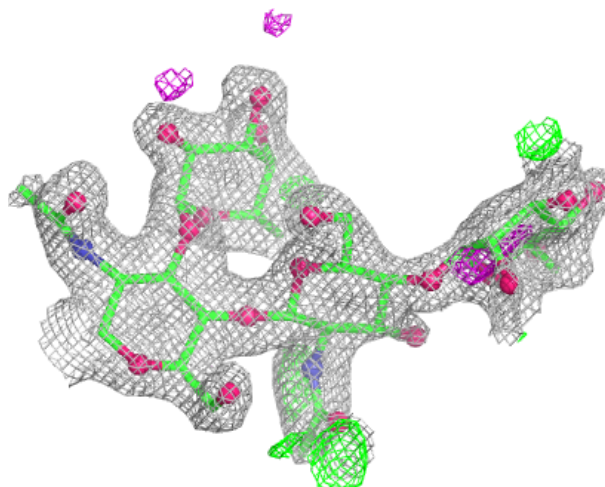
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	NAG	E	1	14/15	0.48	0.17	49,56,60,61	0
4	FUC	E	2	10/11	0.56	0.16	41,48,50,50	0
3	NAG	D	2	14/15	0.57	0.17	56,62,66,70	0
2	BMA	C	3	11/12	0.66	0.13	55,57,59,61	0
3	NAG	F	2	14/15	0.71	0.14	45,55,59,62	0
2	NAG	C	2	14/15	0.79	0.13	38,44,50,56	0
3	NAG	D	1	14/15	0.84	0.09	31,34,42,49	0
2	FUC	C	4	10/11	0.85	0.10	39,41,44,48	0
3	NAG	F	1	14/15	0.89	0.09	25,28,40,43	0
2	NAG	C	1	14/15	0.91	0.09	28,31,38,39	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.

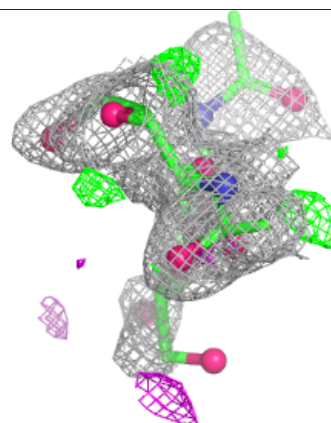
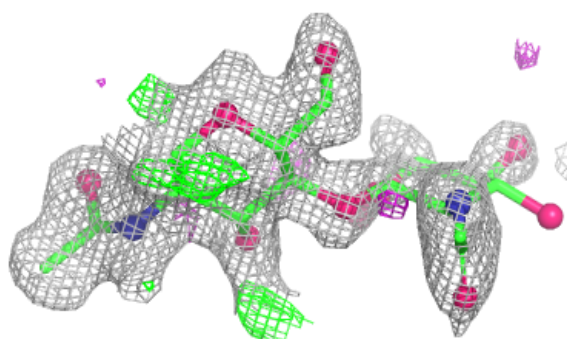
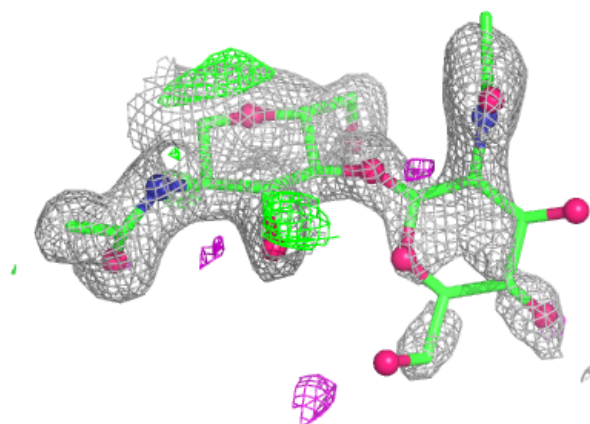
Electron density around Chain C:

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

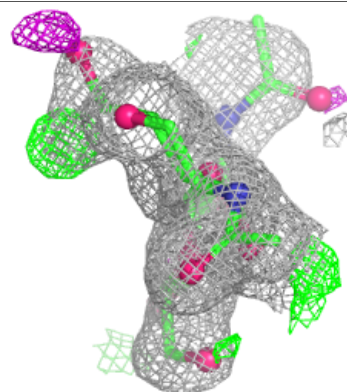
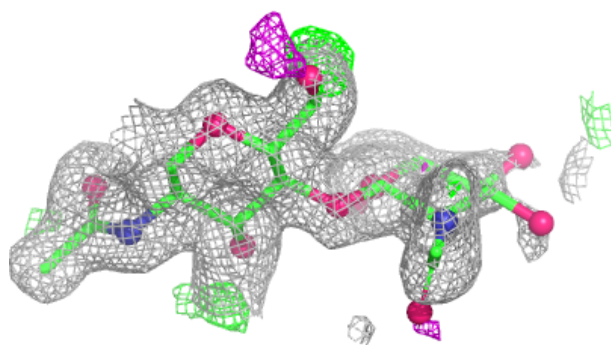
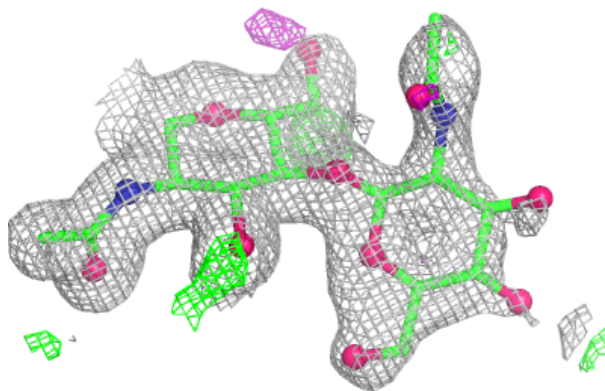


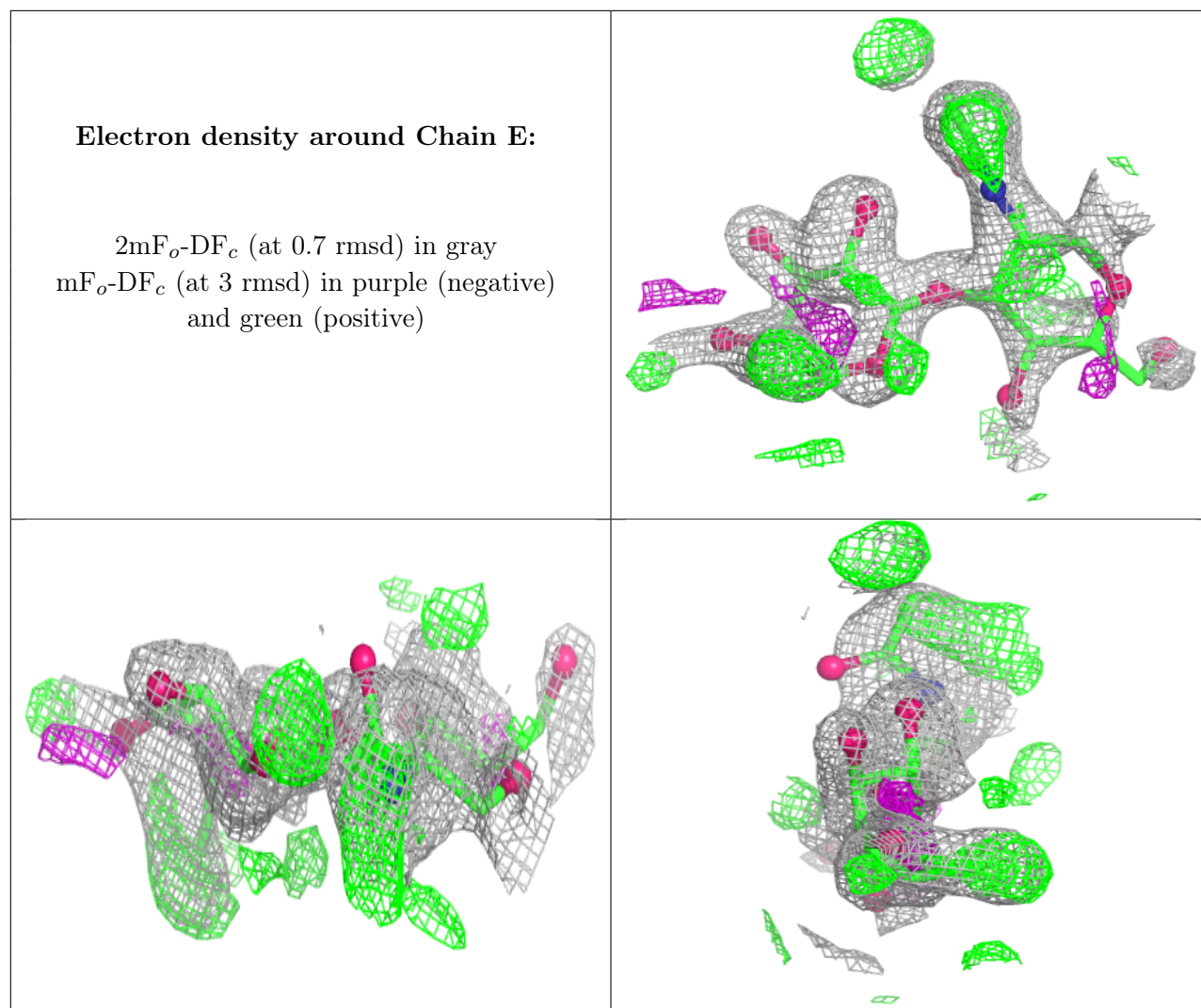
Electron density around Chain D:

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

**Electron density around Chain F:**

$2mF_o-DF_c$ (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
5	SO4	A	906	5/5	0.82	0.16	31,32,32,32	5
5	SO4	B	908	5/5	0.84	0.17	36,36,36,37	5
8	EPE	A	852[B]	15/15	0.84	0.15	22,24,28,30	15
5	SO4	A	910	5/5	0.85	0.13	26,27,28,28	5
9	DHA	B	850[A]	6/6	0.86	0.12	20,22,25,26	6
5	SO4	B	909	5/5	0.87	0.14	29,30,31,31	5
8	EPE	A	851[B]	15/15	0.87	0.13	24,26,30,31	15
5	SO4	A	911	5/5	0.90	0.09	58,58,58,58	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
5	SO4	A	904	5/5	0.92	0.09	60,60,60,60	0
5	SO4	B	903	5/5	0.93	0.15	35,35,36,36	0
5	SO4	A	905	5/5	0.93	0.08	48,48,48,48	0
5	SO4	A	907	5/5	0.93	0.08	50,50,50,50	0
5	SO4	B	902	5/5	0.95	0.08	40,40,41,41	0
7	PLP	A	600	15/16	0.97	0.06	19,23,29,37	0
6	CL	B	1002	1/1	0.98	0.05	19,19,19,19	0
5	SO4	B	901	5/5	0.98	0.10	25,26,29,29	0
7	PLP	B	600	15/16	0.98	0.05	16,18,25,28	0
6	CL	A	1001	1/1	0.99	0.04	18,18,18,18	0

6.5 Other polymers [i](#)

There are no such residues in this entry.