



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 4, 2026 – 05:50 PM UTC

PDB ID : 6KZK / pdb_00006kzk
Title : Structure of alginate lyase Aly36B mutant K143A/M171A in complex with alginate trisaccharide
Authors : Zhang, Y.Z.; Dong, F.; Chen, X.L.
Deposited on : 2019-09-24
Resolution : 2.79 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

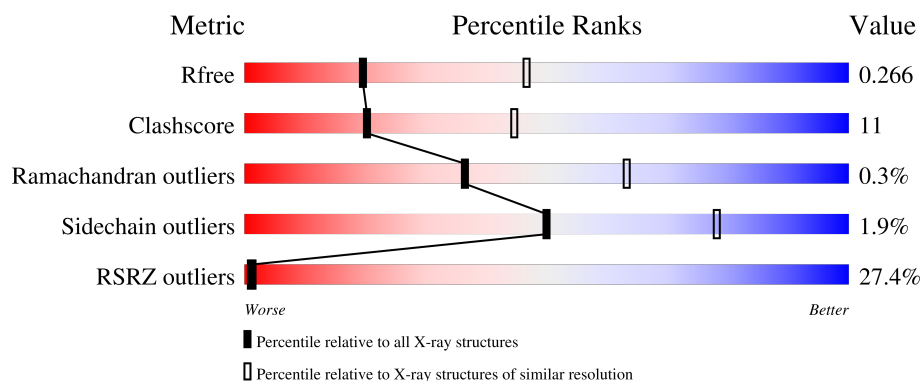
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.79 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.



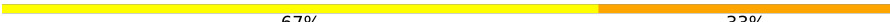
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	5248 (2.80-2.76)
Clashscore	190562	5693 (2.80-2.76)
Ramachandran outliers	187476	5590 (2.80-2.76)
Sidechain outliers	187428	5592 (2.80-2.76)
RSRZ outliers	180081	5251 (2.80-2.76)

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	241	32% 76% 24%
1	B	241	17% 78% 22%
1	C	241	34% 74% 24%
2	D	3	67% 33%
2	E	3	67% 33%

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Mol	Chain	Length	Quality of chain
2	F	3	 67%33%

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
2	BEM	F	1	-	-	X	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 5933 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.

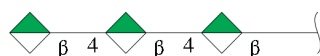
- Molecule 1 is a protein called Alginate lyase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	241	Total	C	N	O	S	0	0	0
			1875	1176	330	367	2			
1	B	241	Total	C	N	O	S	0	0	0
			1875	1176	330	367	2			
1	C	241	Total	C	N	O	S	0	0	0
			1875	1176	330	367	2			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	109	ALA	LYS	engineered mutation	UNP A0A249T061
A	137	ALA	MET	engineered mutation	UNP A0A249T061
B	109	ALA	LYS	engineered mutation	UNP A0A249T061
B	137	ALA	MET	engineered mutation	UNP A0A249T061
C	109	ALA	LYS	engineered mutation	UNP A0A249T061
C	137	ALA	MET	engineered mutation	UNP A0A249T061

- Molecule 2 is an oligosaccharide called beta-D-mannopyranuronic acid-(1-4)-beta-D-mannopyranuronic acid-(1-4)-beta-D-mannopyranuronic acid.



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
2	D	3	Total	C	O	0	0	0
			37	18	19			
2	E	3	Total	C	O	0	0	0
			37	18	19			
2	F	3	Total	C	O	0	0	0
			37	18	19			

- Molecule 3 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total 1	Ca 1	0	0
3	B	1	Total 1	Ca 1	0	0
3	C	1	Total 1	Ca 1	0	0

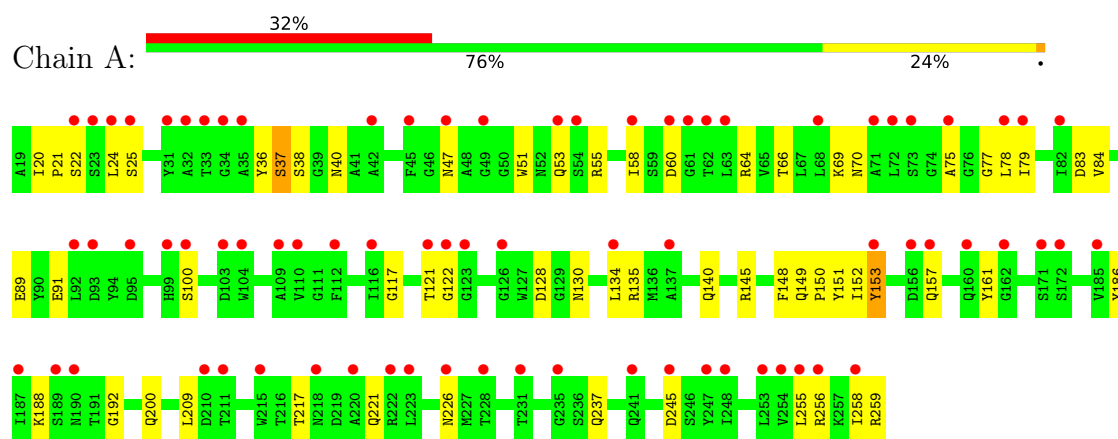
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	62	Total 62	O 62	0	0
4	B	62	Total 62	O 62	0	0
4	C	70	Total 70	O 70	0	0

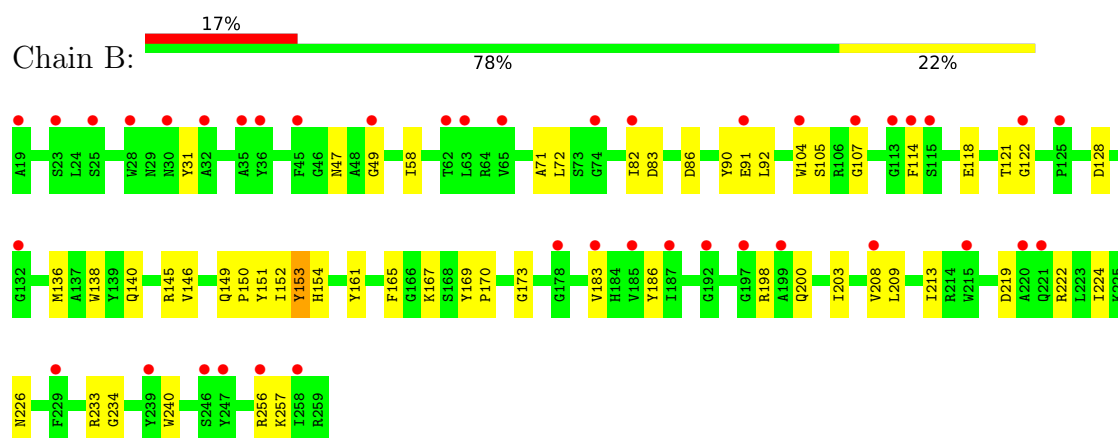
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

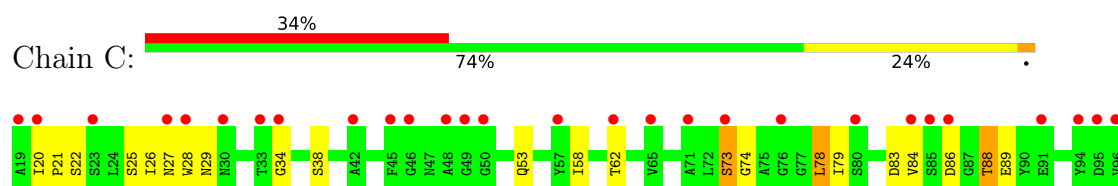
• Molecule 1: Alginate lyase

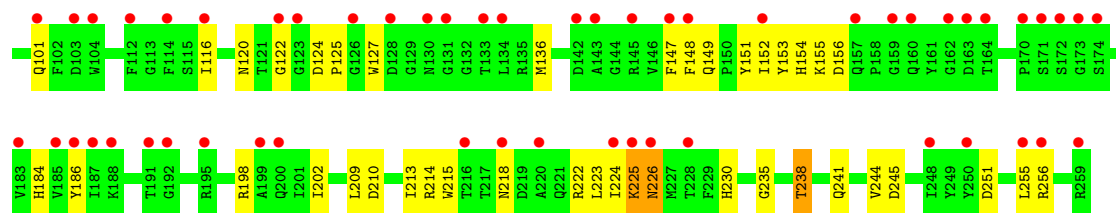


• Molecule 1: Alginate lyase

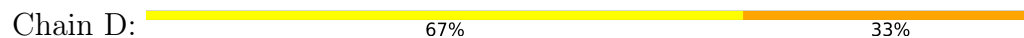


• Molecule 1: Alginate lyase





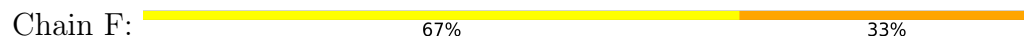
- Molecule 2: beta-D-mannopyranuronic acid-(1-4)-beta-D-mannopyranuronic acid-(1-4)-beta-D-mannopyranuronic acid



- Molecule 2: beta-D-mannopyranuronic acid-(1-4)-beta-D-mannopyranuronic acid-(1-4)-beta-D-mannopyranuronic acid



- Molecule 2: beta-D-mannopyranuronic acid-(1-4)-beta-D-mannopyranuronic acid-(1-4)-beta-D-mannopyranuronic acid



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	105.77Å 188.32Å 91.11Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.84 – 2.79 40.84 – 2.79	Depositor EDS
% Data completeness (in resolution range)	94.3 (40.84-2.79) 94.3 (40.84-2.79)	Depositor EDS
R_{merge}	0.18	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.43 (at 2.81Å)	Xtriage
Refinement program	PHENIX 1.10.1_2155	Depositor
R, R_{free}	0.195 , 0.273 0.199 , 0.266	Depositor DCC
R_{free} test set	1018 reflections (4.41%)	wwPDB-VP
Wilson B-factor (Å ²)	26.6	Xtriage
Anisotropy	0.725	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 33.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.003 for 1/2*h-1/2*k,-3/2*h-1/2*k,-l 0.012 for 1/2*h+1/2*k,3/2*h-1/2*k,-l	Xtriage
F_o, F_c correlation	0.73	EDS
Total number of atoms	5933	wwPDB-VP
Average B, all atoms (Å ²)	22.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.16% 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: BEM, CA

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	0.63	6/1925 (0.3%)	0.74	4/2614 (0.2%)
1	B	0.64	4/1925 (0.2%)	0.80	4/2614 (0.2%)
1	C	0.92	6/1925 (0.3%)	0.84	11/2614 (0.4%)
All	All	0.74	16/5775 (0.3%)	0.80	19/7842 (0.2%)

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	78	LEU	C-O	-7.64	1.14	1.24
1	C	26	ILE	C-O	-6.26	1.17	1.24
1	A	149	GLN	C-O	-5.85	1.18	1.24
1	B	150	PRO	C-O	-5.79	1.16	1.23
1	A	150	PRO	C-O	-5.75	1.17	1.23
1	C	218	ASN	C-O	-5.67	1.17	1.24
1	A	20	ILE	C-O	-5.67	1.17	1.24
1	A	148	PHE	C-O	-5.66	1.17	1.23
1	B	153	TYR	C-O	-5.58	1.17	1.24
1	C	154	HIS	C-O	-5.56	1.16	1.24
1	B	151	TYR	C-O	-5.21	1.18	1.23
1	A	153	TYR	C-O	-5.16	1.18	1.24
1	B	47	ASN	C-O	-5.04	1.17	1.23
1	C	22	SER	C-O	-5.01	1.16	1.23
1	A	20	ILE	CA-C	-5.00	1.47	1.52
1	C	226	ASN	CA-C	-5.00	1.46	1.52

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	49	GLY	N-CA-C	17.97	136.94	114.66
1	A	20	ILE	N-CA-C	-9.96	87.36	108.88

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	152	ILE	N-CA-C	9.34	122.07	108.53
1	A	152	ILE	N-CA-C	8.74	122.52	108.97
1	B	152	ILE	N-CA-C	8.59	121.26	108.46
1	C	20	ILE	N-CA-C	-7.94	91.74	108.88
1	C	147	PHE	N-CA-C	7.41	119.31	108.86
1	C	222	ARG	N-CA-C	7.10	121.70	112.89
1	C	21	PRO	N-CA-C	6.23	120.41	111.13
1	C	226	ASN	N-CA-C	5.96	117.54	108.07
1	C	222	ARG	N-CA-CB	-5.40	101.60	110.40
1	B	152	ILE	CB-CA-C	-5.34	102.27	110.50
1	C	149	GLN	CA-C-N	-5.26	114.82	120.03
1	C	149	GLN	C-N-CA	-5.26	114.82	120.03
1	C	20	ILE	CA-C-N	-5.22	115.35	120.52
1	C	20	ILE	C-N-CA	-5.22	115.35	120.52
1	B	149	GLN	N-CA-C	5.17	116.60	108.23
1	A	20	ILE	CA-C-N	-5.12	115.32	120.85
1	A	20	ILE	C-N-CA	-5.12	115.32	120.85

There are no chirality outliers.

There are no planarity outliers.

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	1875	0	1746	44	0
1	B	1875	0	1747	34	0
1	C	1875	0	1747	45	0
2	D	37	0	21	1	0
2	E	37	0	21	3	0
2	F	37	0	21	8	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	1	0
4	A	62	0	0	4	0
4	B	62	0	0	5	0
4	C	70	0	0	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	5933	0	5303	125	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 11.

All (125) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:122:GLY:O	1:C:153:TYR:OH	1.87	0.92
1:C:151:TYR:OH	2:F:1:BEM:O6B	1.91	0.88
1:A:38:SER:H	1:A:53:GLN:NE2	1.73	0.86
1:A:38:SER:H	1:A:53:GLN:HE21	1.22	0.84
1:C:235:GLY:N	2:F:1:BEM:H3	1.92	0.84
1:C:251:ASP:OD1	4:C:401:HOH:O	1.95	0.84
1:B:122:GLY:O	1:B:153:TYR:OH	1.96	0.84
1:A:38:SER:N	1:A:53:GLN:HG2	1.93	0.83
1:C:73:SER:OG	2:F:1:BEM:O1	2.02	0.77
1:A:47:ASN:HD21	1:A:83:ASP:H	1.29	0.77
1:C:116:ILE:HD11	1:C:224:ILE:HG12	1.69	0.74
1:C:73:SER:HG	2:F:1:BEM:HO1	1.35	0.74
1:A:38:SER:N	1:A:53:GLN:HE21	1.86	0.73
1:B:118:GLU:OE1	4:B:401:HOH:O	2.06	0.73
1:C:116:ILE:CD1	1:C:224:ILE:HG12	2.20	0.72
1:B:91:GLU:CD	1:B:256:ARG:HH21	1.98	0.71
2:E:1:BEM:O6B	2:E:1:BEM:O1	2.07	0.71
1:A:135:ARG:NH1	4:A:404:HOH:O	2.24	0.70
1:C:58:ILE:O	4:C:402:HOH:O	2.11	0.69
1:C:235:GLY:H	2:F:1:BEM:H3	1.57	0.69
1:C:27:ASN:HA	4:C:401:HOH:O	1.93	0.68
1:C:255:LEU:HG	1:C:256:ARG:N	2.08	0.68
1:C:34:GLY:O	4:C:402:HOH:O	2.14	0.66
1:C:84:VAL:O	4:C:403:HOH:O	2.14	0.66
1:A:38:SER:H	1:A:53:GLN:HG2	1.61	0.64
1:B:91:GLU:OE2	1:B:256:ARG:NH2	2.28	0.64
1:C:79:ILE:HG23	1:C:230:HIS:CD2	2.34	0.64
1:C:29:ASN:OD1	3:C:304:CA:CA	1.76	0.63
1:A:38:SER:H	1:A:53:GLN:CG	2.11	0.62
1:A:55:ARG:HA	1:A:66:THR:HG22	1.85	0.59
1:B:203:ILE:HD12	1:B:208:VAL:HG21	1.84	0.59
1:A:55:ARG:NH2	1:A:75:ALA:O	2.35	0.59
1:C:225:LYS:O	1:C:226:ASN:HB3	2.01	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:64:ARG:O	4:A:402:HOH:O	2.16	0.58
1:A:151:TYR:OH	2:D:2:BEM:H2	2.04	0.57
1:A:245:ASP:OD2	4:A:403:HOH:O	2.17	0.57
1:A:55:ARG:NH1	1:A:77:GLY:O	2.34	0.57
1:B:136:MET:HE1	1:B:183:VAL:HG21	1.88	0.56
1:B:145:ARG:NH1	1:B:173:GLY:O	2.36	0.56
1:C:151:TYR:CZ	2:F:1:BEM:O6B	2.58	0.55
1:A:122:GLY:O	1:A:153:TYR:OH	2.20	0.55
1:C:151:TYR:CE2	2:F:1:BEM:O6B	2.59	0.55
1:A:38:SER:H	1:A:53:GLN:CD	2.14	0.55
1:A:51:TRP:HA	1:A:78:LEU:HD11	1.89	0.54
1:C:255:LEU:HG	1:C:256:ARG:H	1.72	0.54
1:B:90:TYR:HB3	1:B:114:PHE:CZ	2.42	0.54
1:C:34:GLY:N	4:C:402:HOH:O	2.20	0.53
1:C:213:ILE:HG21	1:C:215:TRP:CE2	2.43	0.52
1:A:84:VAL:HG22	1:A:226:ASN:HA	1.91	0.52
1:A:256:ARG:NH1	1:A:258:ILE:HG12	2.25	0.52
1:A:24:LEU:HD12	1:A:255:LEU:HD23	1.92	0.52
1:A:89:GLU:HG2	1:A:188:LYS:HG3	1.91	0.52
1:B:92:LEU:HD23	1:B:114:PHE:CE2	2.45	0.52
1:B:104:TRP:CD2	1:B:146:VAL:HG11	2.45	0.52
1:B:161:TYR:HB2	4:B:432:HOH:O	2.09	0.51
1:C:244:VAL:HG12	1:C:245:ASP:O	2.11	0.51
1:B:169:TYR:HA	1:B:170:PRO:C	2.37	0.50
1:A:157:GLN:NE2	1:A:161:TYR:O	2.45	0.49
1:A:186:TYR:HB3	1:A:200:GLN:HB3	1.94	0.48
1:C:83:ASP:OD2	1:C:225:LYS:HE2	2.12	0.48
1:A:38:SER:N	1:A:53:GLN:CG	2.66	0.48
1:A:200:GLN:HA	1:A:209:LEU:O	2.12	0.48
1:B:121:THR:OG1	4:B:402:HOH:O	2.13	0.48
1:B:200:GLN:HA	1:B:209:LEU:O	2.13	0.48
1:C:238:THR:O	1:C:241:GLN:HG3	2.14	0.47
1:B:186:TYR:HE2	1:B:198:ARG:HG2	1.77	0.47
1:A:128:ASP:OD1	1:A:130:ASN:HB2	2.14	0.47
1:A:192:GLY:O	1:A:217:THR:HA	2.14	0.47
1:C:27:ASN:C	1:C:29:ASN:H	2.23	0.47
1:B:105:SER:HB3	1:B:233:ARG:NH1	2.30	0.47
1:C:38:SER:H	1:C:53:GLN:HG2	1.79	0.46
1:C:74:GLY:HA2	1:C:79:ILE:HD13	1.97	0.46
1:C:86:ASP:HB3	1:C:223:LEU:HD13	1.97	0.46
1:B:83:ASP:HA	1:B:226:ASN:HB3	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:120:ASN:HB3	1:C:124:ASP:O	2.16	0.46
2:F:1:BEM:HO3	2:F:2:BEM:C1	2.25	0.46
1:B:256:ARG:HG2	1:B:257:LYS:O	2.16	0.46
1:B:107:GLY:HA2	1:B:138:TRP:NE1	2.31	0.46
1:C:116:ILE:HD13	1:C:224:ILE:HG12	1.96	0.46
1:A:37:SER:O	1:A:40:ASN:HB2	2.16	0.46
1:B:31:TYR:HB2	1:B:58:ILE:HG21	1.97	0.45
1:B:71:ALA:O	1:B:72:LEU:HD23	2.15	0.45
1:B:122:GLY:N	2:E:1:BEM:O6B	2.44	0.45
1:B:122:GLY:HA2	2:E:1:BEM:O2	2.16	0.45
1:A:140:GLN:HA	1:A:145:ARG:O	2.17	0.45
1:C:155:LYS:HB3	1:C:214:ARG:O	2.17	0.45
1:B:154:HIS:CG	1:B:213:ILE:HD11	2.52	0.45
1:C:184:HIS:HD2	1:C:202:ILE:HD12	1.81	0.44
1:C:84:VAL:HG22	1:C:226:ASN:HA	2.00	0.44
1:C:186:TYR:HE2	1:C:198:ARG:HG2	1.83	0.44
1:B:86:ASP:OD1	4:B:403:HOH:O	2.21	0.44
1:B:128:ASP:OD2	4:B:401:HOH:O	2.21	0.44
1:A:47:ASN:HD21	1:A:83:ASP:N	2.04	0.43
1:A:78:LEU:HD12	1:A:79:ILE:H	1.83	0.43
1:B:234:GLY:HA2	1:B:240:TRP:CD2	2.53	0.43
1:B:140:GLN:HA	1:B:145:ARG:O	2.18	0.43
1:C:101:GLN:HA	1:C:101:GLN:OE1	2.19	0.43
1:A:55:ARG:CA	1:A:66:THR:HG22	2.47	0.43
1:C:136:MET:HE3	1:C:148:PHE:CD1	2.54	0.43
1:A:83:ASP:HA	1:A:226:ASN:HB3	2.01	0.43
1:B:92:LEU:CD2	1:B:114:PHE:CE2	3.01	0.43
1:B:82:ILE:HD12	1:B:82:ILE:N	2.34	0.43
1:A:78:LEU:HD12	1:A:79:ILE:N	2.34	0.42
1:A:259:ARG:NH2	4:A:409:HOH:O	2.43	0.42
1:B:219:ASP:HA	1:B:222:ARG:HB2	2.01	0.42
1:C:256:ARG:O	1:C:256:ARG:HG3	2.18	0.42
1:A:36:TYR:CD1	1:A:58:ILE:HD11	2.54	0.42
1:B:86:ASP:HA	1:B:224:ILE:O	2.19	0.42
1:A:21:PRO:HG3	1:A:24:LEU:HD11	2.01	0.42
1:A:117:GLY:HA3	1:A:221:GLN:HB3	2.02	0.42
1:C:156:ASP:CG	1:C:214:ARG:HH21	2.27	0.41
1:B:165:PHE:O	1:B:167:LYS:HG2	2.21	0.41
1:C:88:THR:HG22	1:C:89:GLU:HG3	2.02	0.41
1:A:55:ARG:HA	1:A:66:THR:CG2	2.49	0.41
1:C:58:ILE:HA	1:C:62:THR:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:91:GLU:OE2	1:A:256:ARG:NH1	2.49	0.41
1:A:121:THR:HG22	1:A:135:ARG:NH1	2.35	0.41
1:A:237:GLN:H	1:A:237:GLN:CD	2.28	0.41
1:C:38:SER:N	1:C:53:GLN:HG2	2.36	0.40
1:A:91:GLU:CG	1:A:258:ILE:HD11	2.51	0.40
1:B:82:ILE:O	1:B:226:ASN:HB2	2.21	0.40
1:C:125:PRO:C	1:C:127:TRP:H	2.29	0.40
1:C:209:LEU:HG	1:C:210:ASP:N	2.35	0.40
1:C:73:SER:HB3	1:C:74:GLY:H	1.65	0.40
1:A:69:LYS:HG3	1:A:70:ASN:ND2	2.36	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	239/241 (99%)	220 (92%)	18 (8%)	1 (0%)	30	57
1	B	239/241 (99%)	225 (94%)	14 (6%)	0	100	100
1	C	239/241 (99%)	224 (94%)	14 (6%)	1 (0%)	30	57
All	All	717/723 (99%)	669 (93%)	46 (6%)	2 (0%)	36	63

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	60	ASP
1	C	28	TRP

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	194/194 (100%)	189 (97%)	5 (3%)	40	72
1	B	194/194 (100%)	194 (100%)	0	100	100
1	C	194/194 (100%)	188 (97%)	6 (3%)	35	68
All	All	582/582 (100%)	571 (98%)	11 (2%)	50	78

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

Mol	Chain	Res	Type
1	A	22	SER
1	A	25	SER
1	A	37	SER
1	A	100	SER
1	A	134	LEU
1	C	25	SER
1	C	73	SER
1	C	78	LEU
1	C	88	THR
1	C	225	LYS
1	C	238	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	47	ASN
1	A	53	GLN
1	A	70	ASN
1	A	160	GLN
1	A	194	ASN
1	A	200	GLN
1	A	241	GLN
1	B	81	ASN
1	B	154	HIS
1	B	221	GLN

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Mol	Chain	Res	Type
1	B	226	ASN
1	B	252	ASN
1	C	157	GLN
1	C	194	ASN
1	C	221	GLN
1	C	226	ASN
1	C	252	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 ⓘ

9 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	BEM	D	1	2	13,13,13	1.59	4 (30%)	18,19,19	3.33	9 (50%)
2	BEM	D	2	2	12,12,13	1.94	5 (41%)	14,17,19	2.64	6 (42%)
2	BEM	D	3	2	12,12,13	1.32	1 (8%)	14,17,19	2.03	5 (35%)
2	BEM	E	1	2	13,13,13	0.79	0	18,19,19	1.03	1 (5%)
2	BEM	E	2	2	12,12,13	0.71	0	14,17,19	0.64	0
2	BEM	E	3	2	12,12,13	0.72	0	14,17,19	0.64	0
2	BEM	F	1	2	13,13,13	0.76	0	18,19,19	0.56	0
2	BEM	F	2	2	12,12,13	1.86	4 (33%)	14,17,19	2.47	6 (42%)
2	BEM	F	3	2	12,12,13	1.42	2 (16%)	14,17,19	0.92	1 (7%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	BEM	D	1	2	-	2/4/24/24	0/1/1/1
2	BEM	D	2	2	-	1/4/21/24	0/1/1/1
2	BEM	D	3	2	-	0/4/21/24	0/1/1/1
2	BEM	E	1	2	-	1/4/24/24	0/1/1/1
2	BEM	E	2	2	-	0/4/21/24	0/1/1/1
2	BEM	E	3	2	-	0/4/21/24	0/1/1/1
2	BEM	F	1	2	-	0/4/24/24	0/1/1/1
2	BEM	F	2	2	-	0/4/21/24	0/1/1/1
2	BEM	F	3	2	-	0/4/21/24	0/1/1/1

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	2	BEM	C5-C6	-3.28	1.46	1.53
2	F	2	BEM	C5-C6	-3.23	1.46	1.53
2	D	2	BEM	O6B-C6	-3.18	1.20	1.30
2	D	1	BEM	O6B-C6	-3.04	1.21	1.30
2	D	3	BEM	O6B-C6	-2.83	1.21	1.30
2	F	3	BEM	O6B-C6	-2.71	1.22	1.30
2	F	2	BEM	O5-C1	-2.68	1.39	1.43
2	F	2	BEM	O6B-C6	-2.59	1.22	1.30
2	F	2	BEM	O2-C2	-2.58	1.37	1.43
2	D	2	BEM	C2-C3	-2.55	1.48	1.52
2	D	2	BEM	O2-C2	-2.54	1.38	1.43
2	D	1	BEM	C1-C2	-2.28	1.47	1.52
2	F	3	BEM	O5-C1	-2.25	1.39	1.43
2	D	1	BEM	O5-C1	-2.08	1.37	1.42
2	D	1	BEM	O3-C3	-2.07	1.37	1.43
2	D	2	BEM	O5-C1	-2.07	1.40	1.43

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	1	BEM	O3-C3-C2	-9.02	89.11	110.38
2	D	2	BEM	O3-C3-C2	-5.67	98.48	110.05
2	D	1	BEM	O6B-C6-O6A	-5.54	111.51	124.08
2	F	2	BEM	O3-C3-C2	-5.35	99.13	110.05
2	D	2	BEM	O2-C2-C3	-4.84	100.13	110.15

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	2	BEM	C2-C3-C4	4.66	119.06	110.86
2	D	1	BEM	C1-O5-C5	4.42	118.72	112.22
2	D	1	BEM	O5-C1-C2	-4.23	102.86	110.30
2	D	3	BEM	O4-C4-C5	4.18	119.30	109.76
2	D	2	BEM	C1-C2-C3	4.14	115.68	109.64
2	D	3	BEM	C3-C4-C5	-3.61	103.09	109.30
2	F	2	BEM	C1-C2-C3	3.27	114.41	109.64
2	D	1	BEM	O1-C1-O5	-3.20	100.91	110.41
2	D	3	BEM	O6B-C6-O6A	-3.08	117.09	124.08
2	F	2	BEM	O4-C4-C5	2.76	116.06	109.76
2	D	1	BEM	O2-C2-C1	-2.69	103.04	109.25
2	D	3	BEM	C2-C3-C4	-2.68	106.15	110.86
2	F	2	BEM	O4-C4-C3	-2.66	104.09	110.38
2	D	2	BEM	O5-C1-C2	2.63	117.07	110.79
2	E	1	BEM	C3-C4-C5	2.55	113.68	109.30
2	D	1	BEM	O1-C1-C2	-2.49	101.77	108.98
2	D	2	BEM	O2-C2-C1	2.45	114.84	109.22
2	D	1	BEM	O2-C2-C3	-2.33	104.89	110.38
2	D	3	BEM	O6B-C6-C5	2.24	121.72	113.64
2	D	1	BEM	C3-C4-C5	2.14	112.99	109.30
2	D	2	BEM	O6B-C6-O6A	-2.12	119.26	124.08
2	F	3	BEM	O6B-C6-O6A	-2.08	119.36	124.08
2	F	2	BEM	O6A-C6-C5	-2.07	113.34	120.81

There are no chirality outliers.

All (4) torsion outliers are listed below:

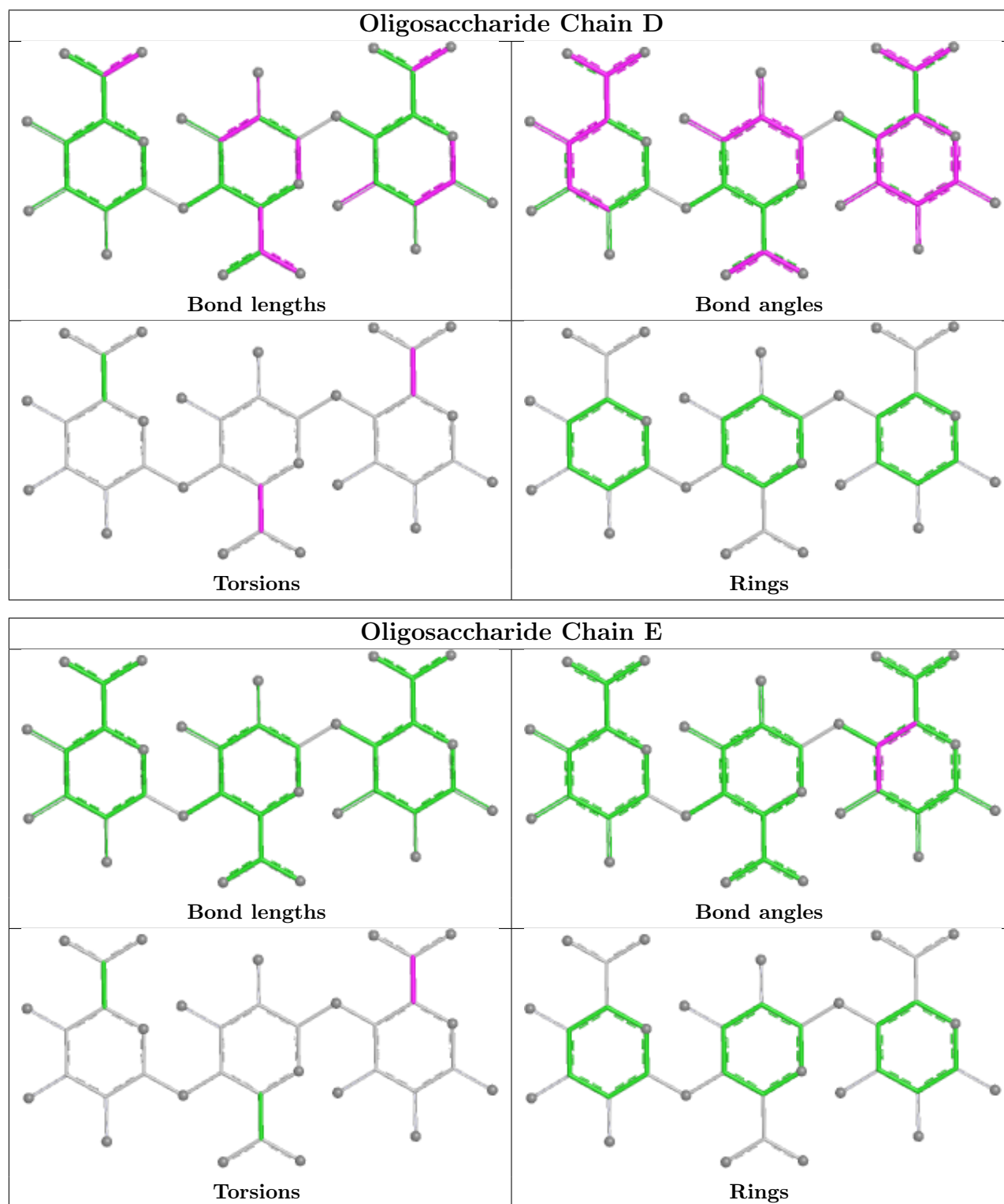
Mol	Chain	Res	Type	Atoms
2	D	1	BEM	C4-C5-C6-O6A
2	D	2	BEM	O5-C5-C6-O6B
2	E	1	BEM	O5-C5-C6-O6B
2	D	1	BEM	C4-C5-C6-O6B

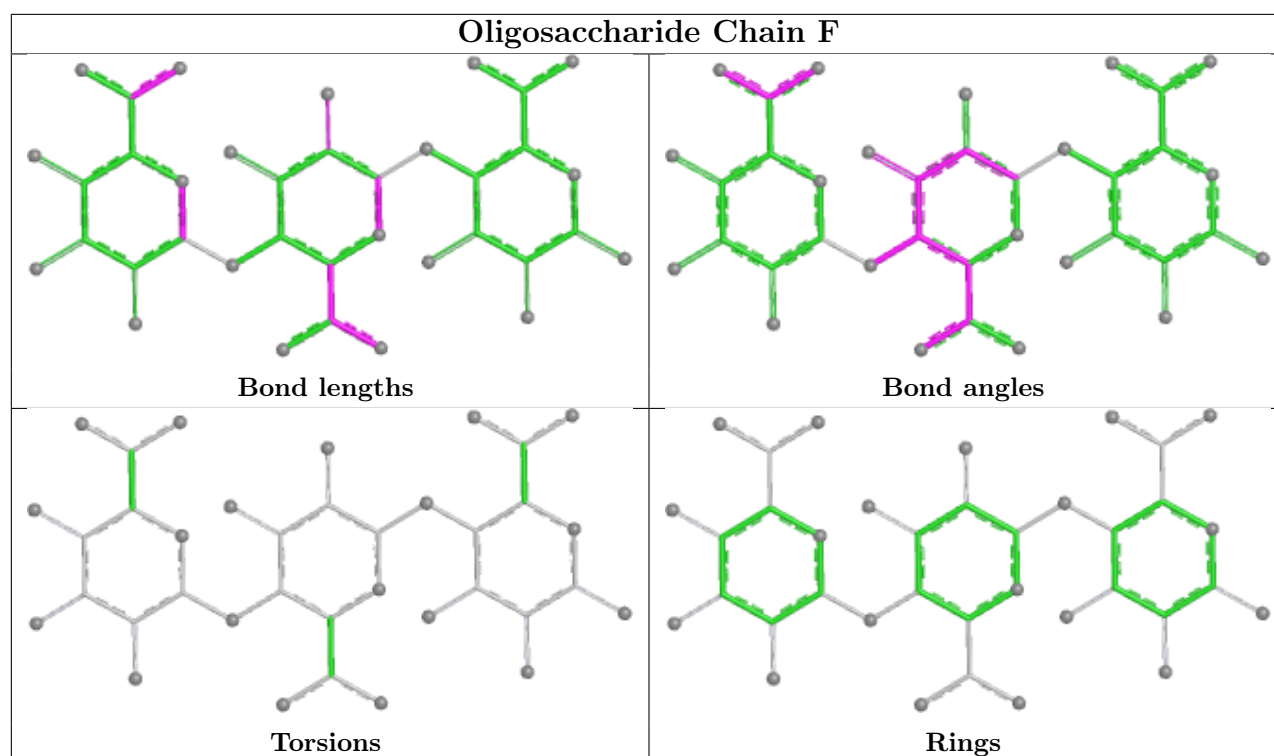
There are no ring outliers.

4 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	1	BEM	3	0
2	F	2	BEM	1	0
2	F	1	BEM	8	0
2	D	2	BEM	1	0

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





5.6 Ligand geometry [i](#)

Of 3 ligands modelled in this entry, 3 are monoatomic - leaving 0 for Mogul analysis.

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	241/241 (100%)	1.65	76 (31%) 1 1	14, 23, 33, 43	0
1	B	241/241 (100%)	1.43	41 (17%) 4 3	11, 20, 28, 42	0
1	C	241/241 (100%)	1.74	81 (33%) 1 1	10, 24, 32, 44	0
All	All	723/723 (100%)	1.61	198 (27%) 1 1	10, 22, 32, 44	0

All (198) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	49	GLY	5.7
1	A	49	GLY	5.5
1	C	171	SER	5.3
1	A	189	SER	4.3
1	B	49	GLY	4.0
1	C	225	LYS	3.9
1	C	19	ALA	3.8
1	A	228	THR	3.7
1	A	73	SER	3.7
1	C	185	VAL	3.5
1	C	172	SER	3.5
1	A	172	SER	3.4
1	A	220	ALA	3.4
1	B	107	GLY	3.4
1	C	199	ALA	3.4
1	A	218	ASN	3.4
1	B	82	ILE	3.3
1	B	113	GLY	3.3
1	A	24	LEU	3.3
1	C	23	SER	3.3
1	C	122	GLY	3.2
1	B	65	VAL	3.2
1	A	255	LEU	3.2

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Mol	Chain	Res	Type	RSRZ
1	C	33	THR	3.2
1	C	256	ARG	3.1
1	C	73	SER	3.1
1	A	82	ILE	3.1
1	B	19	ALA	3.1
1	B	183	VAL	3.1
1	B	74	GLY	3.1
1	A	35	ALA	3.1
1	C	20	ILE	3.1
1	B	197	GLY	3.0
1	B	220	ALA	3.0
1	C	103	ASP	3.0
1	C	200	GLN	3.0
1	B	246	SER	2.9
1	A	78	LEU	2.9
1	B	30	ASN	2.9
1	A	45	PHE	2.9
1	A	68	LEU	2.9
1	C	45	PHE	2.9
1	C	91	GLU	2.9
1	A	79	ILE	2.9
1	C	57	TYR	2.9
1	A	103	ASP	2.9
1	A	31	TYR	2.9
1	A	95	ASP	2.8
1	A	122	GLY	2.8
1	C	48	ALA	2.8
1	B	256	ARG	2.8
1	C	30	ASN	2.8
1	A	162	GLY	2.8
1	C	248	ILE	2.8
1	C	95	ASP	2.8
1	C	142	ASP	2.8
1	A	116	ILE	2.8
1	C	173	GLY	2.8
1	C	152	ILE	2.7
1	B	185	VAL	2.7
1	B	229	PHE	2.7
1	B	258	ILE	2.7
1	C	126	GLY	2.7
1	C	160	GLN	2.7
1	A	104	TRP	2.7

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Mol	Chain	Res	Type	RSRZ
1	C	34	GLY	2.7
1	C	159	GLY	2.7
1	C	42	ALA	2.7
1	C	255	LEU	2.6
1	C	183	VAL	2.6
1	A	215	TRP	2.6
1	A	156	ASP	2.6
1	A	58	ILE	2.6
1	B	247	TYR	2.6
1	A	99	HIS	2.6
1	B	114	PHE	2.6
1	B	45	PHE	2.6
1	C	148	PHE	2.6
1	A	54	SER	2.5
1	A	253	LEU	2.5
1	A	226	ASN	2.5
1	A	171	SER	2.5
1	A	247	TYR	2.5
1	B	122	GLY	2.5
1	C	96	VAL	2.5
1	C	27	ASN	2.5
1	A	248	ILE	2.5
1	C	94	TYR	2.5
1	C	50	GLY	2.5
1	A	109	ALA	2.5
1	C	130	ASN	2.5
1	C	195	ARG	2.5
1	C	192	GLY	2.5
1	C	114	PHE	2.5
1	C	218	ASN	2.4
1	C	259	ARG	2.4
1	C	116	ILE	2.4
1	B	208	VAL	2.4
1	A	75	ALA	2.4
1	A	23	SER	2.4
1	A	71	ALA	2.4
1	A	137	ALA	2.4
1	A	256	ARG	2.4
1	B	32	ALA	2.4
1	C	112	PHE	2.4
1	A	190	ASN	2.4
1	C	80	SER	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	160	GLN	2.4
1	C	71	ALA	2.4
1	B	187	ILE	2.3
1	B	221	GLN	2.3
1	A	72	LEU	2.3
1	A	92	LEU	2.3
1	A	210	ASP	2.3
1	C	104	TRP	2.3
1	B	239	TYR	2.3
1	C	188	LYS	2.3
1	B	115	SER	2.3
1	C	28	TRP	2.3
1	C	145	ARG	2.3
1	A	61	GLY	2.3
1	A	235	GLY	2.3
1	A	258	ILE	2.3
1	A	47	ASN	2.3
1	C	85	SER	2.3
1	C	162	GLY	2.3
1	C	147	PHE	2.3
1	C	187	ILE	2.2
1	A	25	SER	2.2
1	C	163	ASP	2.2
1	A	134	LEU	2.2
1	B	28	TRP	2.2
1	B	63	LEU	2.2
1	A	187	ILE	2.2
1	C	143	ALA	2.2
1	C	216	THR	2.2
1	A	222	ARG	2.2
1	C	174	SER	2.2
1	A	110	VAL	2.2
1	C	84	VAL	2.2
1	B	35	ALA	2.2
1	C	220	ALA	2.2
1	C	62	THR	2.2
1	C	228	THR	2.2
1	A	153	TYR	2.2
1	A	241	GLN	2.2
1	A	34	GLY	2.2
1	A	126	GLY	2.2
1	A	22	SER	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	91	GLU	2.2
1	A	211	THR	2.2
1	C	164	THR	2.2
1	B	132	GLY	2.2
1	C	76	GLY	2.2
1	A	60	ASP	2.2
1	A	62	THR	2.1
1	B	125	PRO	2.1
1	B	36	TYR	2.1
1	C	134	LEU	2.1
1	C	46	GLY	2.1
1	C	131	GLY	2.1
1	A	93	ASP	2.1
1	B	25	SER	2.1
1	C	65	VAL	2.1
1	A	33	THR	2.1
1	C	191	THR	2.1
1	A	53	GLN	2.1
1	C	101	GLN	2.1
1	A	123	GLY	2.1
1	B	192	GLY	2.1
1	C	86	ASP	2.1
1	C	224	ILE	2.1
1	B	23	SER	2.1
1	A	231	THR	2.1
1	C	170	PRO	2.1
1	C	157	GLN	2.1
1	B	178	GLY	2.1
1	A	254	VAL	2.1
1	A	112	PHE	2.1
1	A	42	ALA	2.1
1	B	215	TRP	2.1
1	C	133	THR	2.1
1	A	157	GLN	2.1
1	A	63	LEU	2.1
1	A	223	LEU	2.1
1	C	123	GLY	2.1
1	C	186	TYR	2.1
1	C	128	ASP	2.0
1	A	32	ALA	2.0
1	B	199	ALA	2.0
1	A	185	VAL	2.0

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Mol	Chain	Res	Type	RSRZ
1	C	250	TYR	2.0
1	A	245	ASP	2.0
1	A	100	SER	2.0
1	A	121	THR	2.0
1	B	62	THR	2.0
1	B	104	TRP	2.0
1	C	226	ASN	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](#)

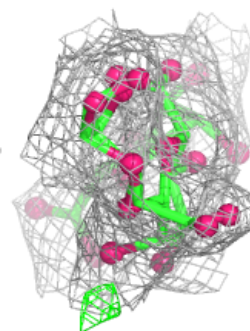
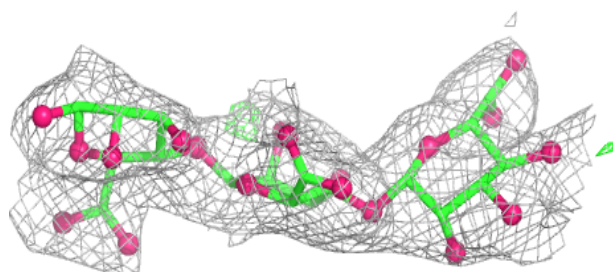
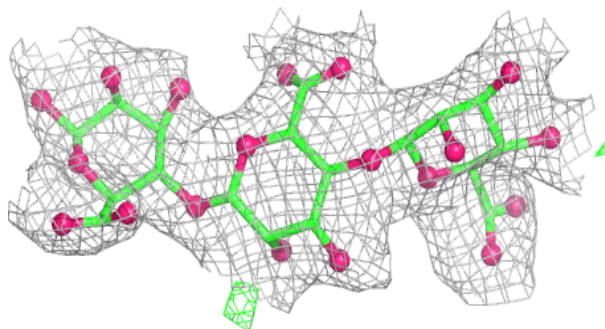
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	BEM	F	3	12/13	0.69	0.19	16,30,34,49	0
2	BEM	E	3	12/13	0.72	0.18	21,24,31,32	0
2	BEM	F	1	13/13	0.72	0.22	19,26,34,43	0
2	BEM	E	1	13/13	0.72	0.25	24,31,43,49	0
2	BEM	D	1	13/13	0.76	0.17	24,29,36,38	0
2	BEM	D	3	12/13	0.78	0.15	19,27,31,33	0
2	BEM	D	2	12/13	0.81	0.16	17,25,33,34	0
2	BEM	E	2	12/13	0.85	0.19	19,26,33,33	0
2	BEM	F	2	12/13	0.86	0.14	18,23,27,31	0

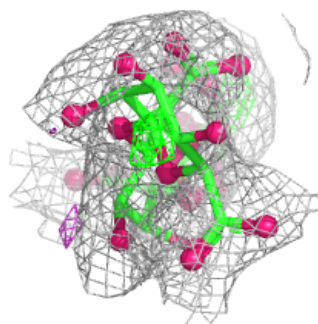
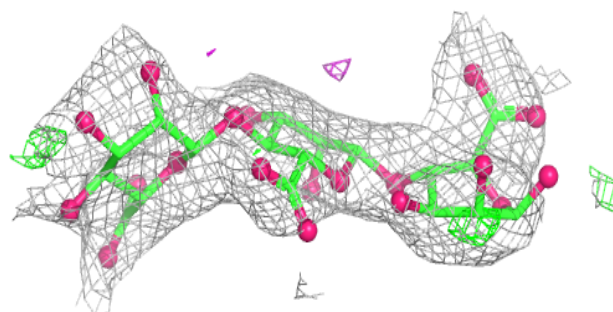
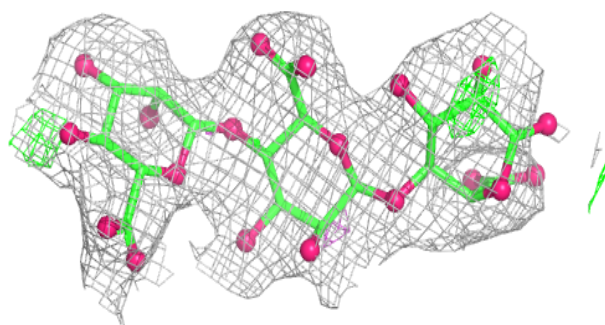
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

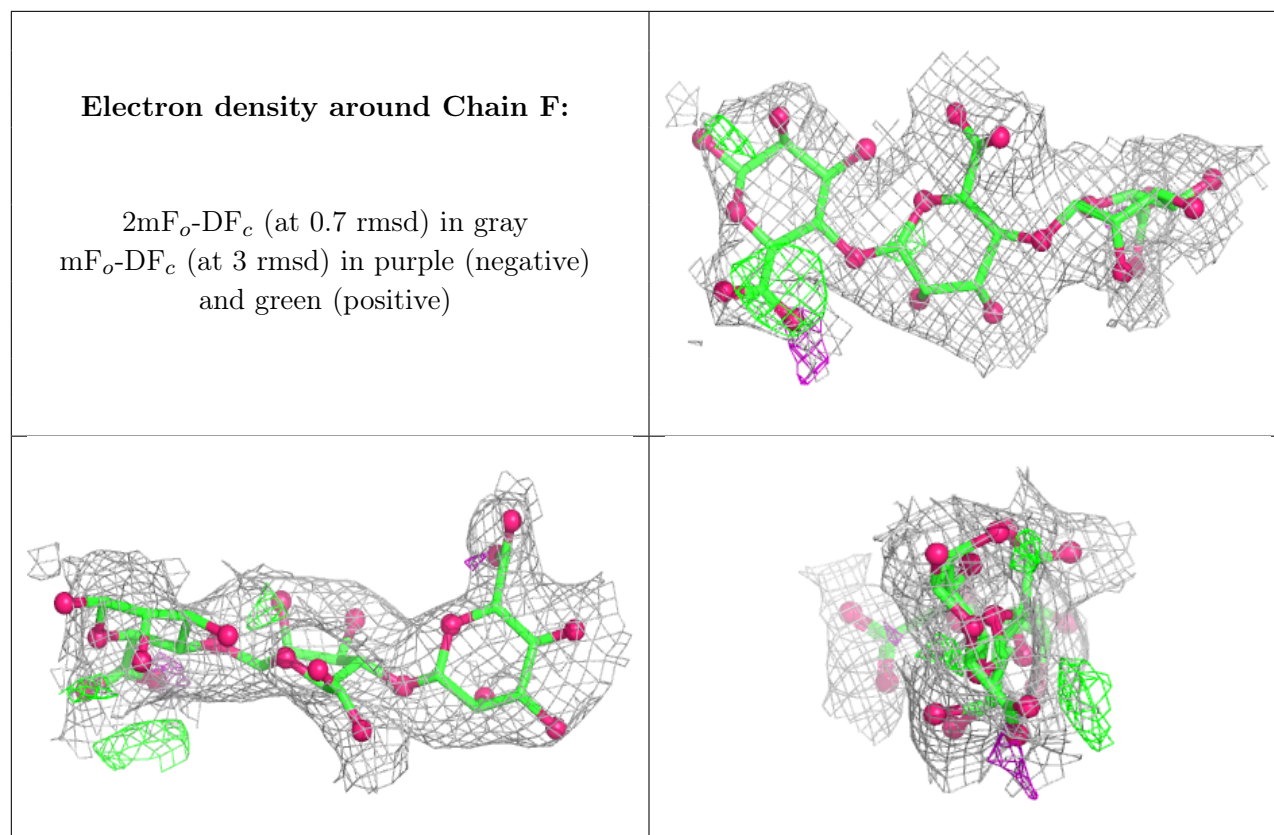
Electron density around Chain D:

$2mF_o-DF_c$ (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)





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($\text{\AA}^2$)	Q<0.9
3	CA	C	304	1/1	0.86	0.07	31,31,31,31	0
3	CA	B	304	1/1	0.91	0.08	31,31,31,31	0
3	CA	A	304	1/1	0.92	0.08	35,35,35,35	0

6.5 Other polymers [i](#)

There are no such residues in this entry.