



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 02:36 PM UTC

PDB ID : 4KGL / pdb_00004kgl
Title : Crystal structure of human alpha-L-iduronidase complex with [2R,3R,4R,5S]-2-carboxy-3,4,5-trihydroxy-piperidine
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Deposited on : 2013-04-29
Resolution : 2.70 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

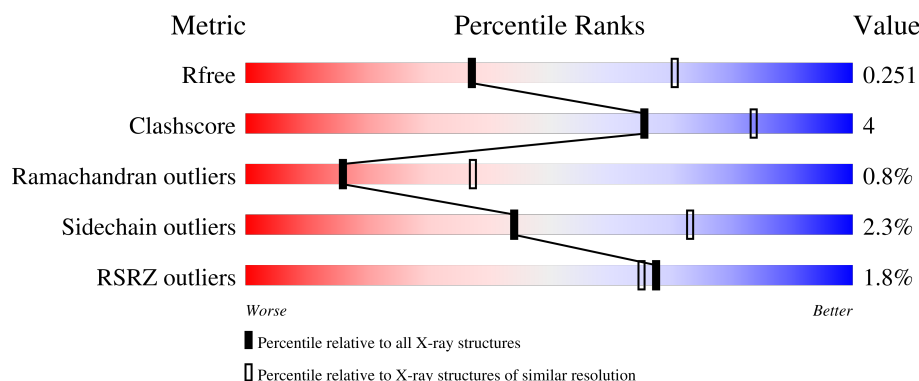
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

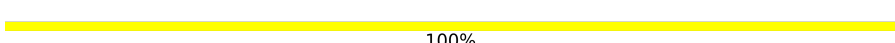
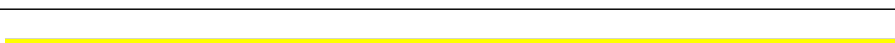
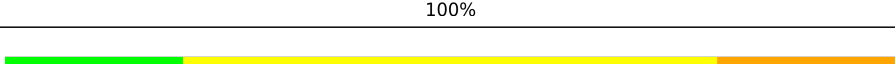
The reported resolution of this entry is 2.70 Å.

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.



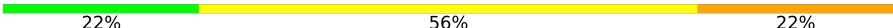
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	3538 (2.70-2.70)
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (2.70-2.70)

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	627	
1	B	627	
2	C	2	
2	E	2	
3	D	5	

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Mol	Chain	Length	Quality of chain
4	F	9	 A horizontal bar chart showing the quality of chain F. The bar is divided into three segments: a green segment on the left labeled '22%', a yellow segment in the middle labeled '56%', and an orange segment on the right labeled '22%'. The segments are separated by thin black lines.

2 Entry composition [i](#)

There are 9 unique types of molecules in this entry. The entry contains 9990 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 Alpha-L-iduronidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	595	Total	C	N	O	S	0	0	0
			4734	3030	852	840	12			
1	B	612	Total	C	N	O	S	0	4	0
			4888	3121	886	867	14			

There are 6 discrepancies between the modelled and reference sequences:

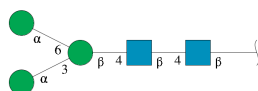
Chain	Residue	Modelled	Actual	Comment	Reference
A	33	GLN	HIS	SEE REMARK 999	UNP P35475
A	63	PRO	GLN	SEE REMARK 999	UNP P35475
A	105	GLN	ARG	SEE REMARK 999	UNP P35475
B	33	GLN	HIS	SEE REMARK 999	UNP P35475
B	63	PRO	GLN	SEE REMARK 999	UNP P35475
B	105	GLN	ARG	SEE REMARK 999	UNP P35475

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



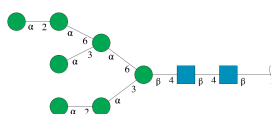
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	C	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	E	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 3 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-[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.



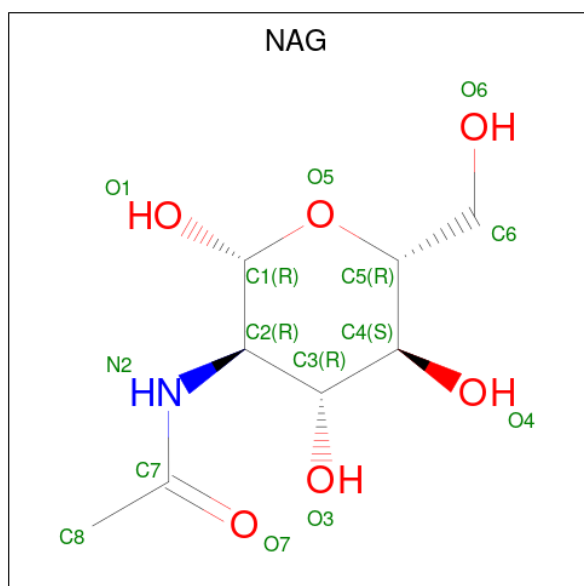
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	D	5	Total	C	N	O	0	0	0
			61	34	2	25			

- Molecule 4 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)]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
4	F	9	Total	C	N	O	0	0	0
			105	58	2	45			

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).



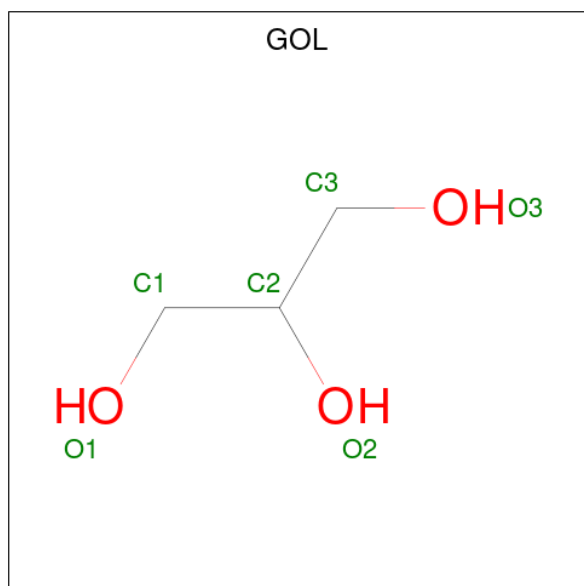
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O	0	0
			14	8	1	5		

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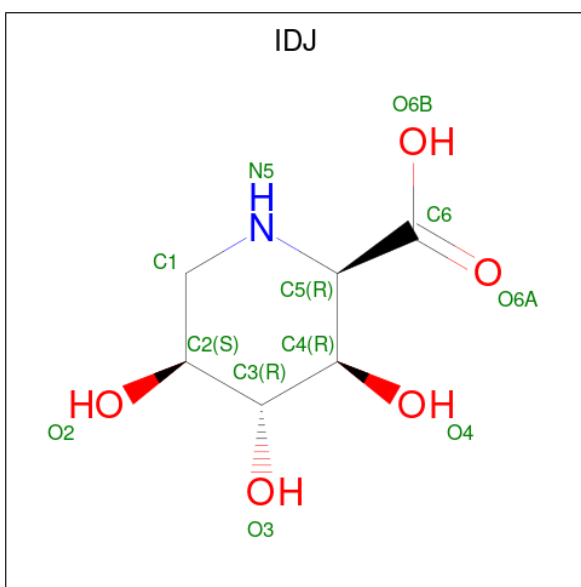
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	B	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 6 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



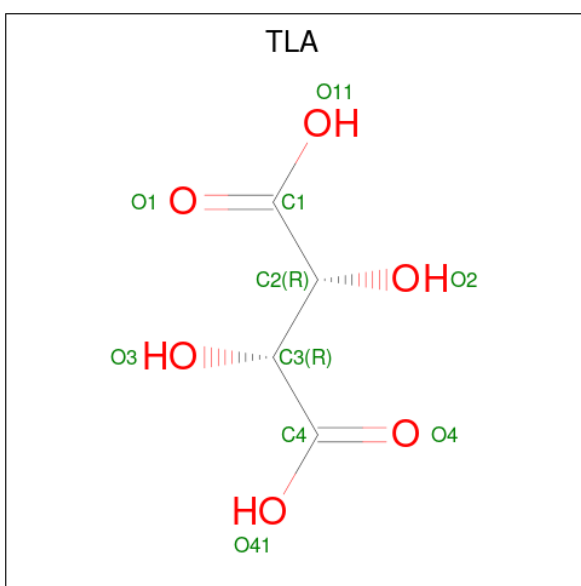
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			6	3	3		
6	B	1	Total	C	O	0	0
			6	3	3		
6	B	1	Total	C	O	0	0
			6	3	3		
6	B	1	Total	C	O	0	0
			6	3	3		
6	B	1	Total	C	O	0	0
			6	3	3		

- Molecule 7 is (2R,3R,4R,5S)-3,4,5-trihydroxypiperidine-2-carboxylic acid (CCD ID: IDJ) (formula: $C_6H_{11}NO_5$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	A	1	Total	C	N	O	0	0
			12	6	1	5		
7	B	1	Total	C	N	O	0	0
			12	6	1	5		

- Molecule 8 is L(+)-TARTARIC ACID (CCD ID: TLA) (formula: $C_4H_6O_6$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	B	1	Total	C	O	0	0
			10	4	6		

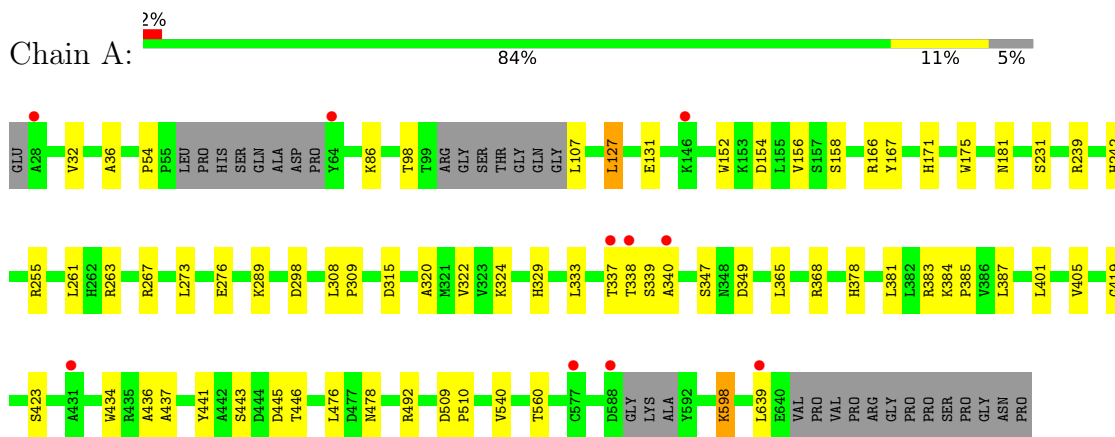
- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	20	Total 20	O 20	0	0
9	B	34	Total 34	O 34	0	0

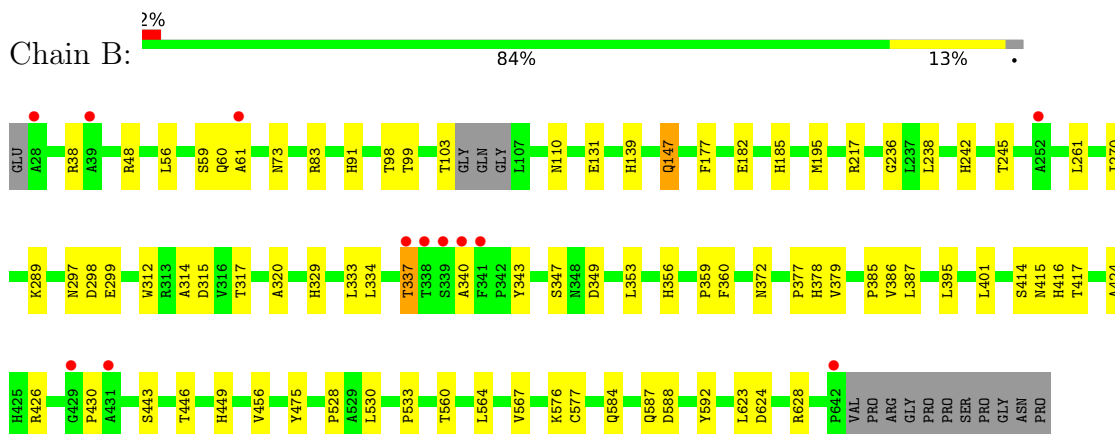
3 Residue-property plots [i](#)

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.

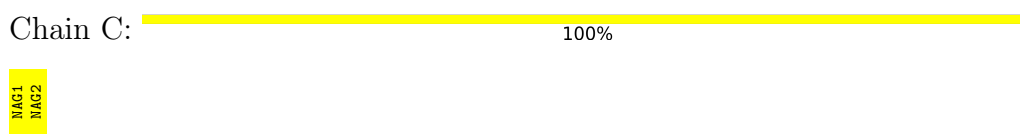
- Molecule 1: Alpha-L-iduronidase



- Molecule 1: Alpha-L-iduronidase



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



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

Chain E:  100%

NAG1
NAG2

- Molecule 3: alpha-D-mannopyranose-(1-3)-[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

Chain D:  20% 60% 20%

NAG1
NAG2
BMA3
MAN4
MAN5

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

Chain F:  22% 56% 22%

NAG1
NAG2
BMA3
MAN4
MAN5
MAN6
MAN7
MAN8
MAN9

4 Data and refinement statistics

Property	Value	Source
Space group	H 3	Depositor
Cell constants a, b, c, α , β , γ	259.36Å 259.36Å 71.57Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	49.06 – 2.70 49.06 – 2.70	Depositor EDS
% Data completeness (in resolution range)	99.4 (49.06-2.70) 99.4 (49.06-2.70)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.25 (at 2.69Å)	Xtriage
Refinement program	REFMAC 5.7.0032	Depositor
R, R_{free}	0.204 , 0.254 0.202 , 0.251	Depositor DCC
R_{free} test set	2481 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	48.2	Xtriage
Anisotropy	0.797	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 40.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.007 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	9990	wwPDB-VP
Average B, all atoms (Å ²)	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.89% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: IDJ, GOL, BMA, MAN, NAG, TLA

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	0.46	1/4879 (0.0%)	0.79	1/6666 (0.0%)
1	B	0.46	0/5039	0.80	2/6886 (0.0%)
All	All	0.46	1/9918 (0.0%)	0.80	3/13552 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	54	PRO	CA-C	5.03	1.54	1.51

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	449	HIS	CA-C-N	5.65	125.32	119.56
1	B	449	HIS	C-N-CA	5.65	125.32	119.56
1	A	445	ASP	CB-CA-C	-5.00	110.42	117.23

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	4734	0	4632	34	0
1	B	4888	0	4786	39	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	28	0	25	0	0
2	E	28	0	25	1	0
3	D	61	0	52	2	0
4	F	105	0	88	2	0
5	A	14	0	13	0	0
5	B	14	0	13	0	0
6	A	6	0	8	2	0
6	B	24	0	32	2	0
7	A	12	0	10	0	0
7	B	12	0	10	0	0
8	B	10	0	4	0	0
9	A	20	0	0	0	0
9	B	34	0	0	1	0
All	All	9990	0	9698	75	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 (75) 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:B:577[A]:CYS:O	1:B:577[A]:CYS:SG	2.33	0.86
1:A:315:ASP:HB2	1:A:478:ASN:OD1	1.77	0.83
1:A:324:LYS:HZ3	6:A:909:GOL:H11	1.54	0.71
3:D:3:BMA:H61	3:D:5:MAN:H5	1.74	0.69
1:B:195:MET:HE1	1:B:236:GLY:HA3	1.77	0.66
1:B:270:ILE:HD11	2:E:1:NAG:H82	1.80	0.63
1:B:334:LEU:HD21	1:B:343:TYR:HB3	1.80	0.63
1:B:320:ALA:HB1	1:B:443:SER:HB2	1.81	0.61
1:A:152:TRP:O	1:A:156:VAL:HG23	2.01	0.61
1:A:131:GLU:OE2	1:A:181:ASN:HB2	2.01	0.60
1:B:356:HIS:HB2	6:B:914:GOL:H31	1.82	0.60
1:A:273:LEU:HD11	1:A:333:LEU:HD13	1.84	0.59
1:A:298:ASP:HA	1:A:347:SER:HB3	1.84	0.59
1:B:414:SER:C	1:B:416:HIS:H	2.11	0.58
1:B:359:PRO:HG3	6:B:914:GOL:H12	1.85	0.58
1:A:378:HIS:CD2	1:A:560:THR:HB	2.38	0.58
1:A:36:ALA:HA	1:A:401:LEU:HD13	1.86	0.57
3:D:3:BMA:H61	3:D:5:MAN:C5	2.35	0.57
1:A:324:LYS:NZ	6:A:909:GOL:H11	2.18	0.55
1:A:166:ARG:HG3	1:A:166:ARG:HH11	1.75	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:476:LEU:HG	1:A:510:PRO:HB3	1.91	0.52
1:B:242:HIS:CD2	1:B:289:LYS:HB2	2.45	0.51
1:B:56:LEU:HD13	4:F:5:MAN:H3	1.91	0.51
1:A:242:HIS:CD2	1:A:289:LYS:HB2	2.46	0.51
1:A:261:LEU:HD13	1:A:263:ARG:HG2	1.92	0.50
1:B:315:ASP:HA	1:B:385:PRO:HG2	1.93	0.50
1:A:492:ARG:NH2	4:F:3:BMA:O2	2.46	0.49
1:A:368:ARG:HA	1:A:381:LEU:HD23	1.95	0.48
1:A:434:TRP:CH2	1:A:436:ALA:HB2	2.48	0.48
1:A:383:ARG:HG2	1:A:387:LEU:HD23	1.95	0.48
1:B:584:GLN:HB3	1:B:592:TYR:HB3	1.96	0.48
1:A:267:ARG:HG2	1:A:446:THR:HG21	1.95	0.48
1:B:98:THR:OG1	1:B:110:ASN:HB3	2.13	0.48
1:A:276:GLU:OE1	1:A:329:HIS:NE2	2.44	0.47
1:B:564:LEU:HD12	1:B:564:LEU:C	2.39	0.47
1:A:32:VAL:HG22	1:A:405:VAL:HG22	1.96	0.46
1:A:315:ASP:HA	1:A:385:PRO:HG2	1.97	0.46
1:B:242:HIS:NE2	1:B:289:LYS:HB2	2.31	0.46
1:B:401:LEU:HD21	1:B:424:ALA:HB2	1.97	0.46
1:A:365:LEU:O	1:A:384:LYS:HB2	2.16	0.45
1:B:386:VAL:HG13	1:B:387:LEU:N	2.31	0.45
1:B:73:ASN:HB2	1:B:353:LEU:HD21	1.97	0.45
1:B:314:ALA:HB1	1:B:360:PHE:HB3	1.98	0.45
1:A:419:GLY:HA3	1:A:441:TYR:CE1	2.52	0.45
1:A:171:HIS:CD2	1:A:175:TRP:HE1	2.35	0.45
1:A:509:ASP:HB2	1:A:598:LYS:HE3	2.00	0.44
1:A:86:LYS:HE2	1:A:127:LEU:HD11	2.00	0.44
1:A:154:ASP:O	1:A:158:SER:HB2	2.18	0.44
1:A:242:HIS:NE2	1:A:289:LYS:HB2	2.33	0.44
1:B:298:ASP:HA	1:B:347:SER:HB3	1.99	0.43
1:A:166:ARG:HD3	1:A:167:TYR:CZ	2.54	0.43
1:B:99:THR:HG21	1:B:139:HIS:HB2	2.01	0.43
1:B:475:TYR:HE1	1:B:530:LEU:HD22	1.84	0.43
1:B:91:HIS:ND1	1:B:131:GLU:OE1	2.52	0.43
1:B:378:HIS:CD2	1:B:560:THR:HB	2.54	0.43
1:B:456:VAL:O	1:B:528:PRO:HD2	2.18	0.43
1:B:182:GLU:HB3	1:B:185:HIS:HB2	2.01	0.42
1:B:48:ARG:HD2	1:B:83:ARG:O	2.18	0.42
1:B:395:LEU:HD22	1:B:576:LYS:HB3	2.01	0.42
1:A:320:ALA:HB1	1:A:443:SER:HB2	2.01	0.42
1:A:255:ARG:HD2	1:A:255:ARG:C	2.44	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:317:THR:HA	1:B:533:PRO:HG3	2.02	0.42
1:B:624:ASP:OD2	1:B:628:ARG:HB2	2.20	0.42
1:A:263:ARG:HD3	1:A:263:ARG:HA	1.87	0.42
1:B:414:SER:C	1:B:416:HIS:N	2.77	0.42
1:B:372:ASN:HA	1:B:377:PRO:HB3	2.02	0.41
1:B:337:THR:HG21	9:B:1022:HOH:O	2.19	0.41
1:B:329:HIS:O	1:B:333:LEU:HB3	2.21	0.41
1:B:298:ASP:O	1:B:299:GLU:HG3	2.19	0.41
1:B:312:TRP:CD2	1:B:446:THR:HG22	2.56	0.41
1:A:423:SER:OG	1:A:437:ALA:HB3	2.21	0.41
1:B:103:THR:HG21	1:B:147:GLN:HE21	1.85	0.41
1:A:308:LEU:HA	1:A:309:PRO:HD3	1.91	0.40
1:B:177:PHE:HB2	1:B:217:ARG:O	2.21	0.40
1:B:261:LEU:O	1:B:297:ASN:HA	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	587/627 (94%)	543 (92%)	41 (7%)	3 (0%)	24	48
1	B	612/627 (98%)	569 (93%)	36 (6%)	7 (1%)	11	29
All	All	1199/1254 (96%)	1112 (93%)	77 (6%)	10 (1%)	16	37

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	338	THR
1	A	339	SER
1	A	340	ALA
1	B	340	ALA

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Mol	Chain	Res	Type
1	B	60	GLN
1	B	415	ASN
1	B	61	ALA
1	B	587	GLN
1	B	588	ASP
1	B	430	PRO

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	503/527 (95%)	492 (98%)	11 (2%)	45	74
1	B	520/527 (99%)	508 (98%)	12 (2%)	44	73
All	All	1023/1054 (97%)	1000 (98%)	23 (2%)	44	74

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	98	THR
1	A	107	LEU
1	A	127	LEU
1	A	231	SER
1	A	239	ARG
1	A	322	VAL
1	A	337	THR
1	A	349	ASP
1	A	540	VAL
1	A	598	LYS
1	A	639	LEU
1	B	38	ARG
1	B	59	SER
1	B	147	GLN
1	B	238	LEU
1	B	245	THR
1	B	337	THR

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Mol	Chain	Res	Type
1	B	349	ASP
1	B	379	VAL
1	B	417	THR
1	B	426	ARG
1	B	567	VAL
1	B	623	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	87	GLN
1	A	113	HIS
1	A	186	HIS
1	A	281	GLN
1	A	330	GLN
1	A	336	ASN
1	A	358	HIS
1	A	587	GLN
1	B	70	GLN
1	B	73	ASN
1	B	139	HIS
1	B	147	GLN
1	B	185	HIS
1	B	196	GLN
1	B	200	ASN
1	B	563	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

18 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	0.53	0	17,19,21	1.41	2 (11%)
2	NAG	C	2	2	14,14,15	0.59	0	17,19,21	0.93	1 (5%)
3	NAG	D	1	3,1	14,14,15	0.56	0	17,19,21	1.07	1 (5%)
3	NAG	D	2	3	14,14,15	0.53	0	17,19,21	1.47	1 (5%)
3	BMA	D	3	3	11,11,12	0.40	0	15,15,17	0.83	0
3	MAN	D	4	3	11,11,12	0.56	0	15,15,17	0.63	0
3	MAN	D	5	3	11,11,12	0.56	0	15,15,17	1.83	2 (13%)
2	NAG	E	1	2,1	14,14,15	0.55	0	17,19,21	0.89	0
2	NAG	E	2	2	14,14,15	0.53	0	17,19,21	1.36	2 (11%)
4	NAG	F	1	4,1	14,14,15	0.48	0	17,19,21	1.23	2 (11%)
4	NAG	F	2	4	14,14,15	0.55	0	17,19,21	1.12	1 (5%)
4	BMA	F	3	4	11,11,12	0.62	0	15,15,17	1.34	1 (6%)
4	MAN	F	4	4	11,11,12	0.65	0	15,15,17	0.88	0
4	MAN	F	5	4	11,11,12	0.49	0	15,15,17	1.31	1 (6%)
4	MAN	F	6	4	11,11,12	0.55	0	15,15,17	0.69	1 (6%)
4	MAN	F	7	4	11,11,12	0.56	0	15,15,17	1.02	1 (6%)
4	MAN	F	8	4	11,11,12	0.54	0	15,15,17	0.71	0
4	MAN	F	9	4	11,11,12	0.72	0	15,15,17	1.39	3 (20%)

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	-	2/6/23/26	0/1/1/1
2	NAG	C	2	2	-	2/6/23/26	0/1/1/1
3	NAG	D	1	3,1	-	1/6/23/26	0/1/1/1
3	NAG	D	2	3	-	2/6/23/26	0/1/1/1
3	BMA	D	3	3	-	2/2/19/22	0/1/1/1
3	MAN	D	4	3	-	0/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	MAN	D	5	3	-	2/2/19/22	0/1/1/1
2	NAG	E	1	2,1	-	3/6/23/26	0/1/1/1
2	NAG	E	2	2	-	0/6/23/26	0/1/1/1
4	NAG	F	1	4,1	-	0/6/23/26	0/1/1/1
4	NAG	F	2	4	-	0/6/23/26	0/1/1/1
4	BMA	F	3	4	-	0/2/19/22	0/1/1/1
4	MAN	F	4	4	-	0/2/19/22	0/1/1/1
4	MAN	F	5	4	-	2/2/19/22	0/1/1/1
4	MAN	F	6	4	-	0/2/19/22	0/1/1/1
4	MAN	F	7	4	-	2/2/19/22	0/1/1/1
4	MAN	F	8	4	-	2/2/19/22	0/1/1/1
4	MAN	F	9	4	-	2/2/19/22	0/1/1/1

There are no bond length outliers.

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	5	MAN	C1-O5-C5	5.63	119.74	112.19
4	F	5	MAN	C1-O5-C5	4.48	118.19	112.19
2	C	1	NAG	C1-O5-C5	4.46	118.17	112.19
3	D	2	NAG	C1-O5-C5	4.21	117.83	112.19
4	F	3	BMA	C1-C2-C3	3.56	114.82	109.64
4	F	9	MAN	C2-C3-C4	3.38	116.80	110.86
3	D	5	MAN	C1-C2-C3	3.33	114.49	109.64
2	E	2	NAG	C1-O5-C5	3.18	116.45	112.19
4	F	1	NAG	O5-C1-C2	-3.02	106.62	111.29
4	F	2	NAG	C1-O5-C5	2.98	116.18	112.19
2	E	2	NAG	C2-N2-C7	2.97	126.89	122.90
4	F	7	MAN	C1-O5-C5	2.88	116.04	112.19
4	F	9	MAN	C1-C2-C3	2.68	113.55	109.64
3	D	1	NAG	O5-C1-C2	-2.60	107.27	111.29
2	C	2	NAG	C1-O5-C5	2.53	115.58	112.19
4	F	9	MAN	C3-C4-C5	2.52	114.81	110.23
4	F	1	NAG	O5-C5-C6	2.36	112.25	107.66
4	F	6	MAN	C1-O5-C5	2.08	114.97	112.19
2	C	1	NAG	O5-C1-C2	-2.07	108.08	111.29

There are no chirality outliers.

All (22) torsion outliers are listed below:

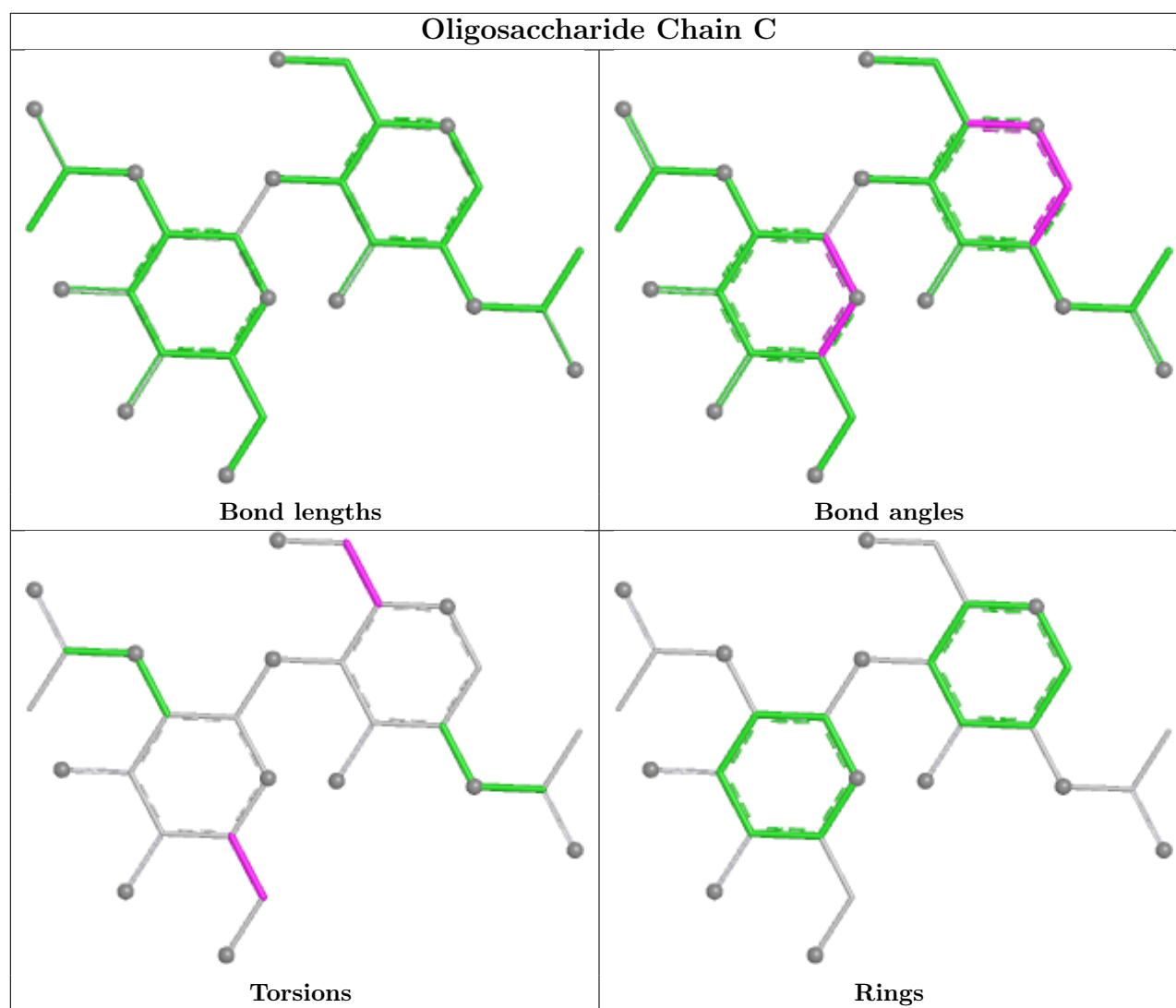
Mol	Chain	Res	Type	Atoms
2	E	1	NAG	O5-C5-C6-O6
3	D	3	BMA	O5-C5-C6-O6
3	D	5	MAN	O5-C5-C6-O6
2	C	2	NAG	O5-C5-C6-O6
2	E	1	NAG	C4-C5-C6-O6
3	D	3	BMA	C4-C5-C6-O6
4	F	8	MAN	C4-C5-C6-O6
4	F	8	MAN	O5-C5-C6-O6
3	D	5	MAN	C4-C5-C6-O6
4	F	7	MAN	C4-C5-C6-O6
3	D	2	NAG	O5-C5-C6-O6
2	C	2	NAG	C4-C5-C6-O6
4	F	7	MAN	O5-C5-C6-O6
4	F	9	MAN	O5-C5-C6-O6
3	D	2	NAG	C4-C5-C6-O6
4	F	5	MAN	O5-C5-C6-O6
2	C	1	NAG	C4-C5-C6-O6
4	F	9	MAN	C4-C5-C6-O6
2	C	1	NAG	O5-C5-C6-O6
3	D	1	NAG	O5-C5-C6-O6
2	E	1	NAG	C1-C2-N2-C7
4	F	5	MAN	C4-C5-C6-O6

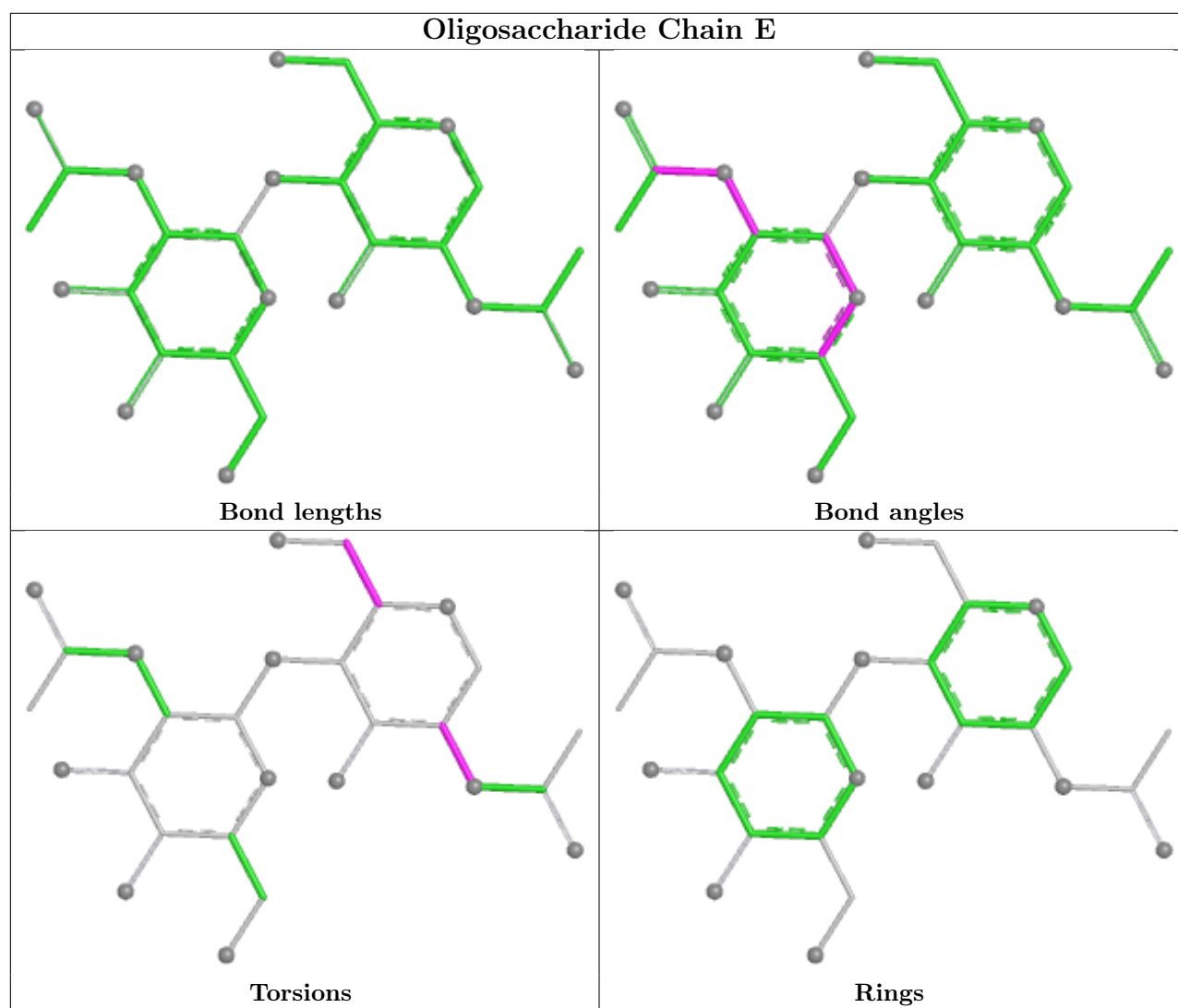
There are no ring outliers.

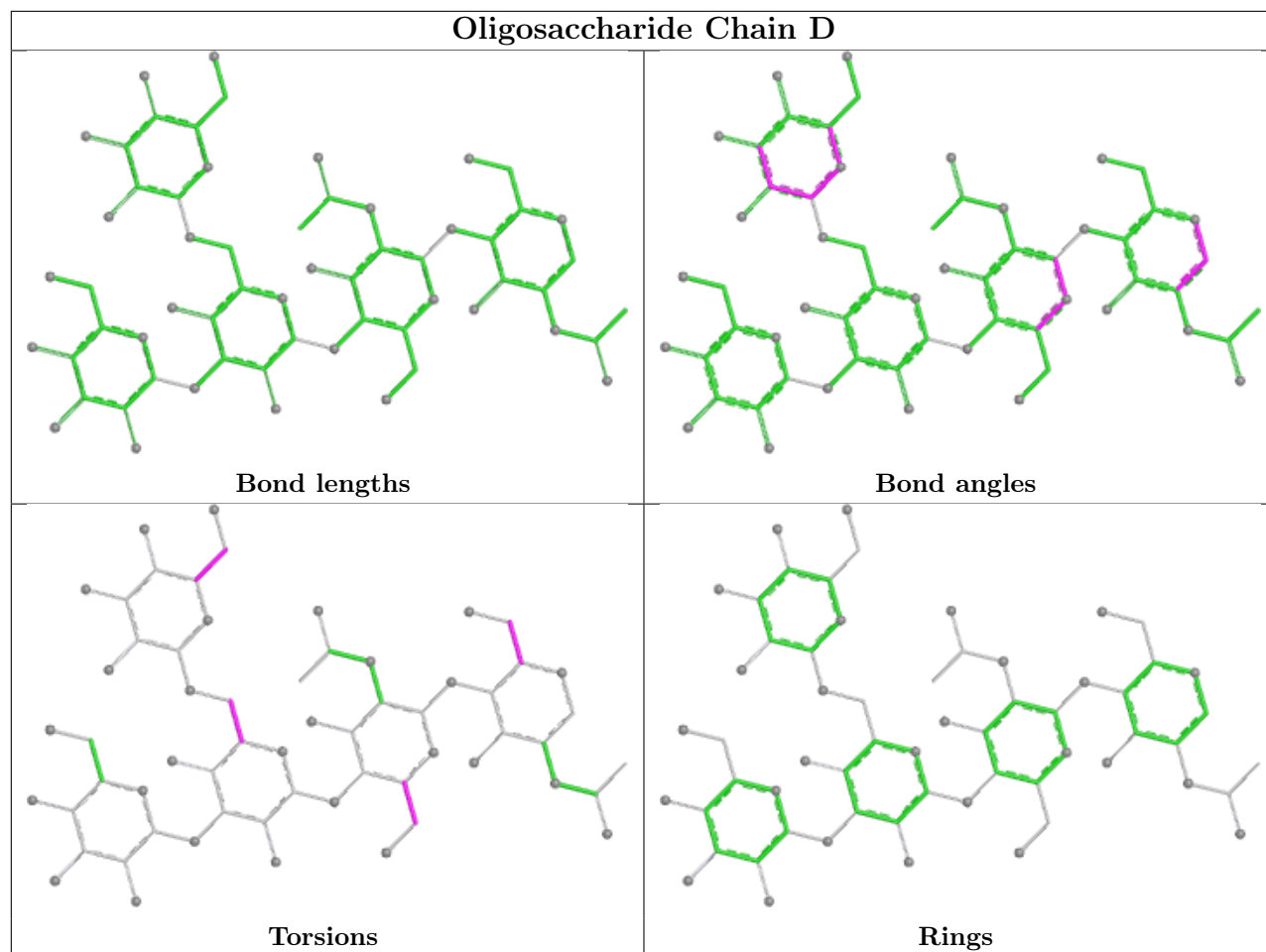
5 monomers are involved in 5 short contacts:

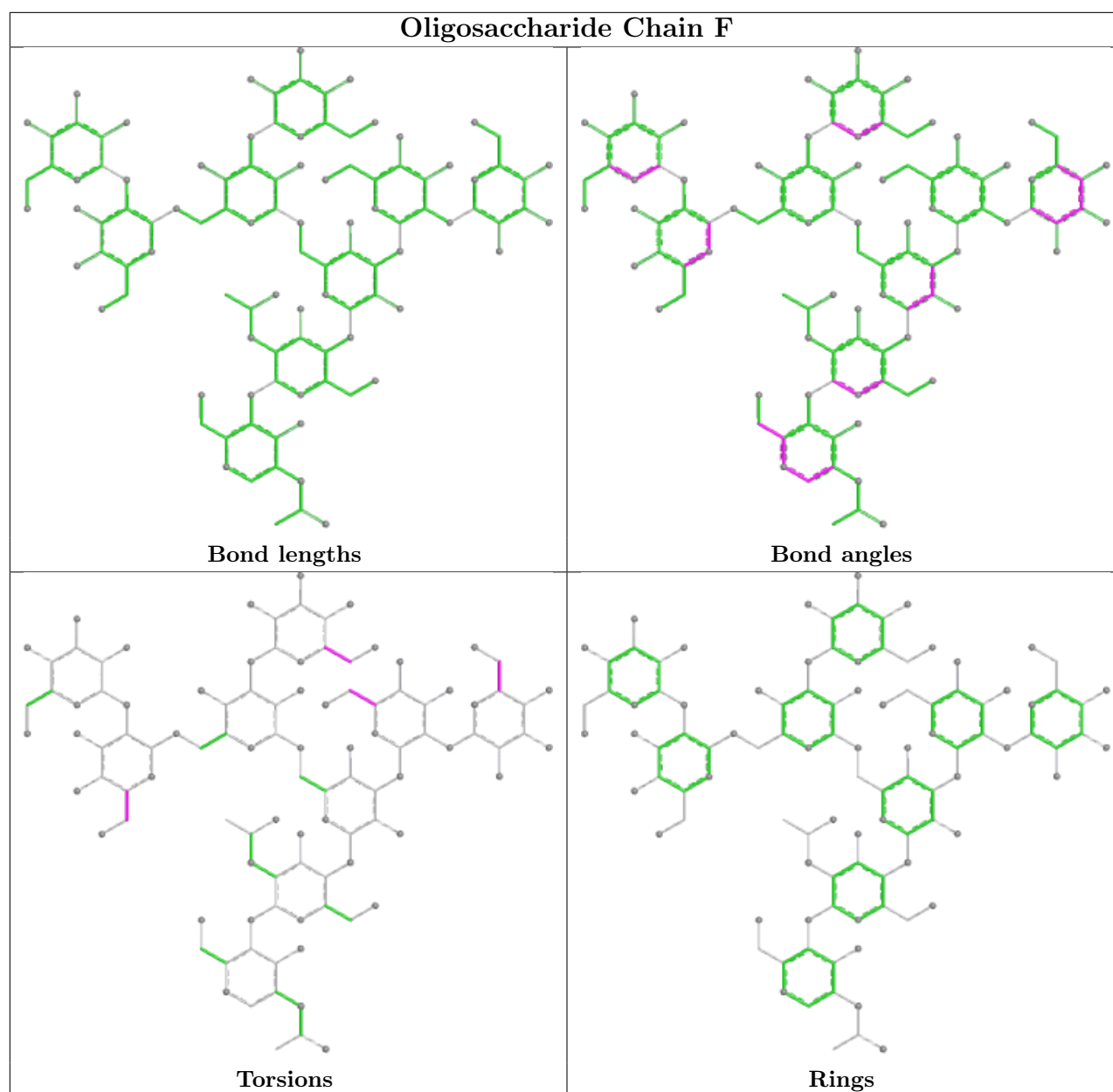
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	3	BMA	2	0
4	F	5	MAN	1	0
4	F	3	BMA	1	0
3	D	5	MAN	2	0
2	E	1	NAG	1	0

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](#)

10 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	GOL	B	915	-	5,5,5	0.33	0	5,5,5	0.39	0
8	TLA	B	917	-	9,9,9	1.19	0	12,12,12	1.20	1 (8%)
5	NAG	B	901	1	14,14,15	0.46	0	17,19,21	0.86	1 (5%)
6	GOL	B	913	-	5,5,5	0.36	0	5,5,5	0.27	0
6	GOL	A	909	-	5,5,5	0.23	0	5,5,5	0.23	0
6	GOL	B	914	-	5,5,5	0.36	0	5,5,5	0.24	0
6	GOL	B	916	-	5,5,5	0.37	0	5,5,5	0.70	0
7	IDJ	A	910	-	11,12,12	1.18	0	12,17,17	2.23	2 (16%)
7	IDJ	B	918	-	11,12,12	1.12	0	12,17,17	1.93	2 (16%)
5	NAG	A	901	1	14,14,15	0.56	0	17,19,21	1.16	1 (5%)

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
6	GOL	B	915	-	-	3/4/4/4	-
8	TLA	B	917	-	-	8/12/12/12	-
5	NAG	B	901	1	-	2/6/23/26	0/1/1/1
6	GOL	B	913	-	-	0/4/4/4	-
6	GOL	A	909	-	-	2/4/4/4	-
6	GOL	B	914	-	-	4/4/4/4	-
6	GOL	B	916	-	-	0/4/4/4	-
7	IDJ	A	910	-	-	0/3/21/21	0/1/1/1
7	IDJ	B	918	-	-	0/3/21/21	0/1/1/1
5	NAG	A	901	1	-	1/6/23/26	0/1/1/1

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	910	IDJ	C1-C2-C3	5.29	116.72	110.25
7	B	918	IDJ	C1-C2-C3	4.93	116.28	110.25
7	A	910	IDJ	C2-C3-C4	4.74	119.19	110.86
7	B	918	IDJ	C2-C3-C4	3.56	117.11	110.86
5	A	901	NAG	C1-O5-C5	3.24	116.53	112.19
8	B	917	TLA	O41-C4-C3	2.60	120.54	113.31
5	B	901	NAG	C1-O5-C5	2.40	115.41	112.19

There are no chirality outliers.

All (20) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	909	GOL	O1-C1-C2-O2
6	A	909	GOL	O1-C1-C2-C3
8	B	917	TLA	C2-C3-C4-O4
8	B	917	TLA	C2-C3-C4-O41
8	B	917	TLA	O3-C3-C4-O4
8	B	917	TLA	O3-C3-C4-O41
5	B	901	NAG	O5-C5-C6-O6
5	B	901	NAG	C4-C5-C6-O6
8	B	917	TLA	C1-C2-C3-O3
6	B	914	GOL	O1-C1-C2-O2
8	B	917	TLA	O2-C2-C3-C4
8	B	917	TLA	O2-C2-C3-O3
6	B	914	GOL	O1-C1-C2-C3
6	B	914	GOL	C1-C2-C3-O3
6	B	915	GOL	C1-C2-C3-O3
6	B	914	GOL	O2-C2-C3-O3
8	B	917	TLA	C1-C2-C3-C4
6	B	915	GOL	O2-C2-C3-O3
6	B	915	GOL	O1-C1-C2-O2
5	A	901	NAG	C4-C5-C6-O6

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	909	GOL	2	0
6	B	914	GOL	2	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	595/627 (94%)	0.03	10 (1%) 69 67	34, 52, 81, 105	0
1	B	612/627 (97%)	-0.14	12 (1%) 65 62	19, 47, 76, 112	4 (0%)
All	All	1207/1254 (96%)	-0.06	22 (1%) 67 65	19, 49, 79, 112	4 (0%)

All (22) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	639	LEU	4.9
1	A	64	TYR	4.1
1	A	431	ALA	3.6
1	B	339	SER	3.6
1	B	338	THR	3.4
1	B	61	ALA	3.3
1	A	338	THR	3.3
1	A	340	ALA	3.0
1	B	337	THR	3.0
1	A	337	THR	2.6
1	B	642	PRO	2.5
1	B	429	GLY	2.4
1	B	28	ALA	2.4
1	B	340	ALA	2.3
1	B	39	ALA	2.2
1	B	252	ALA	2.2
1	A	588	ASP	2.2
1	A	577	CYS	2.1
1	B	341	PHE	2.1
1	A	146	LYS	2.1
1	B	431	ALA	2.1
1	A	28	ALA	2.0

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

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

6.3 Carbohydrates ⓘ

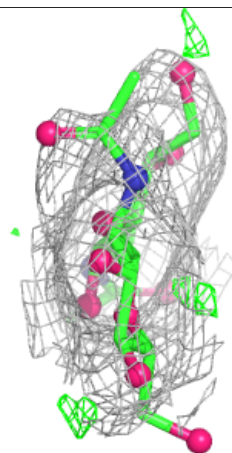
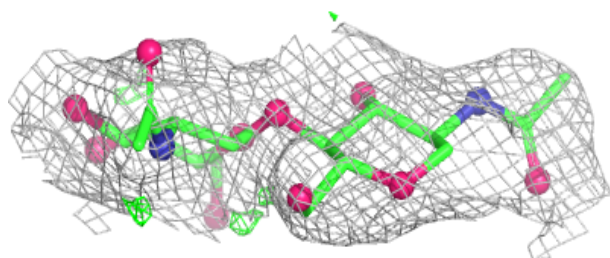
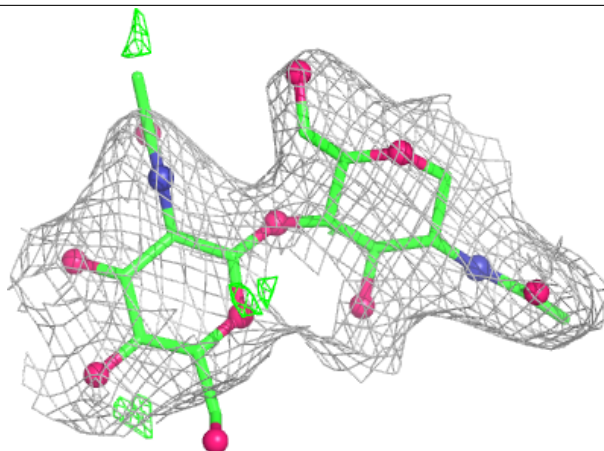
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	MAN	D	4	11/12	0.57	0.16	98,102,105,107	0
4	MAN	F	9	11/12	0.60	0.17	78,89,91,92	0
2	NAG	C	2	14/15	0.73	0.14	94,102,109,115	0
4	MAN	F	5	11/12	0.77	0.14	92,99,103,105	0
4	MAN	F	7	11/12	0.78	0.14	80,89,92,95	0
3	MAN	D	5	11/12	0.81	0.11	75,82,85,91	0
2	NAG	E	2	14/15	0.82	0.12	75,77,80,81	0
4	MAN	F	6	11/12	0.85	0.13	85,93,100,101	0
4	MAN	F	4	11/12	0.87	0.10	69,76,84,90	0
4	MAN	F	8	11/12	0.88	0.10	70,73,76,83	0
3	NAG	D	2	14/15	0.90	0.11	53,61,68,74	0
2	NAG	C	1	14/15	0.91	0.10	56,64,70,83	0
2	NAG	E	1	14/15	0.93	0.08	53,59,64,71	0
4	NAG	F	2	14/15	0.93	0.09	42,43,49,49	0
3	BMA	D	3	11/12	0.94	0.07	74,78,83,93	0
3	NAG	D	1	14/15	0.94	0.12	56,58,61,63	0
4	BMA	F	3	11/12	0.94	0.09	50,53,61,61	0
4	NAG	F	1	14/15	0.97	0.07	40,41,44,45	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.

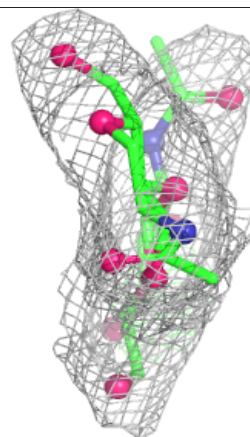
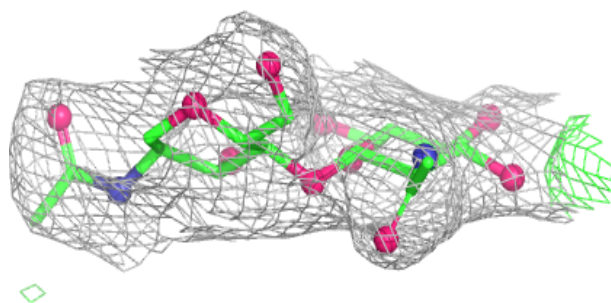
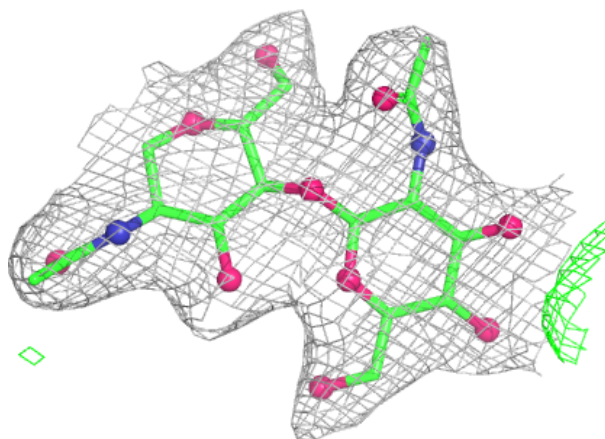
Electron density around Chain C:

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



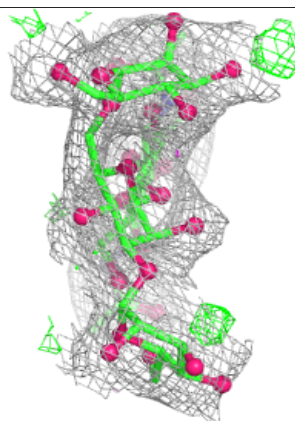
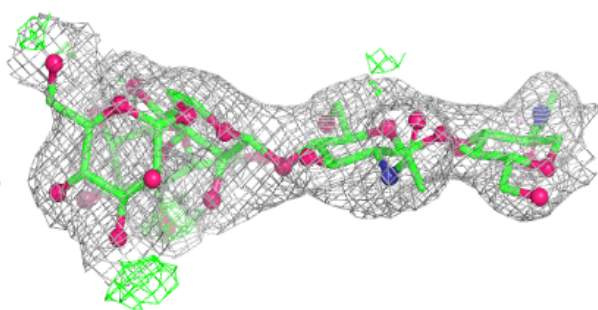
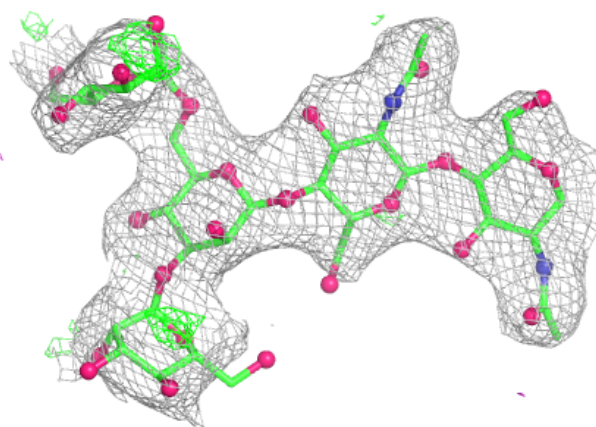
Electron density around Chain E:

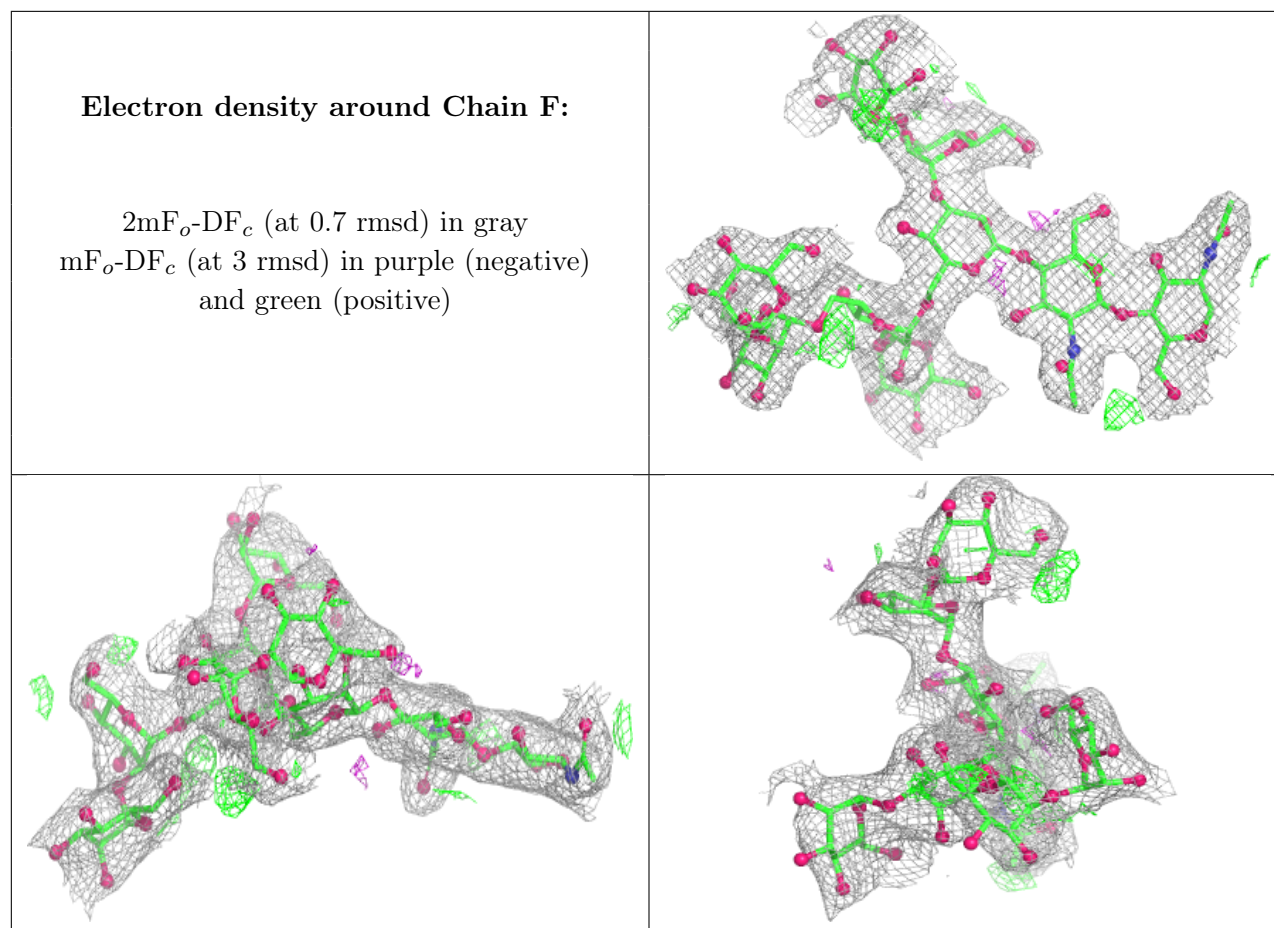
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around Chain D:

$2mF_o-DF_c$ (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
5	NAG	A	901	14/15	0.67	0.16	87,95,99,99	0
7	IDJ	A	910	12/12	0.86	0.14	82,86,88,89	0
7	IDJ	B	918	12/12	0.86	0.12	69,73,75,77	0
6	GOL	B	913	6/6	0.87	0.18	55,62,64,65	0
8	TLA	B	917	10/10	0.89	0.10	63,66,70,71	0
6	GOL	A	909	6/6	0.91	0.10	50,52,54,56	0
5	NAG	B	901	14/15	0.91	0.10	55,58,61,62	0
6	GOL	B	916	6/6	0.91	0.14	41,45,47,51	0
6	GOL	B	915	6/6	0.92	0.11	51,52,53,54	0
6	GOL	B	914	6/6	0.93	0.14	51,57,57,58	0

6.5 Other polymers [i](#)

There are no such residues in this entry.