



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 01:15 PM UTC

PDB ID : 1E03 / pdb_00001e03
Title : PLASMA ALPHA ANTITHROMBIN-III AND PENTASACCHARIDE
Authors : McCoy, A.J.; Jin, L.; Abrahams, J.-P.; Skinner, R.; Carrell, R.W.
Deposited on : 2000-03-09
Resolution : 2.90 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

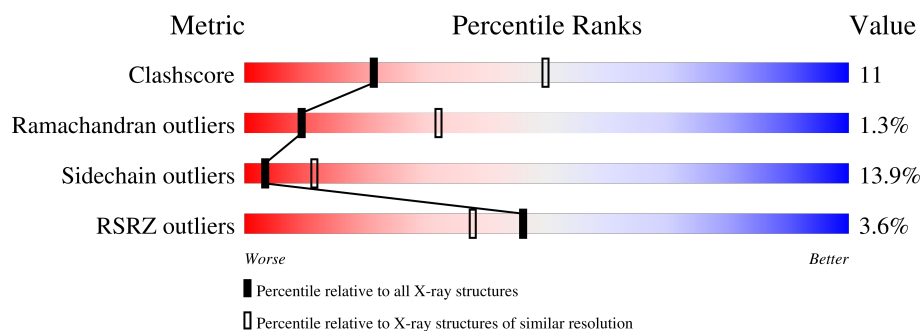
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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.



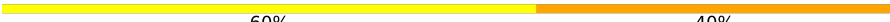
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)
RSRZ outliers	180081	2481 (2.90-2.90)

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	I	432	3% 58% 31% 6% ..
1	L	432	4% 64% 28% 5% ..
2	A	2	100%
3	B	3	33% 67%
3	C	3	67% 33%
3	D	3	33% 67%
4	E	5	80% 20%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
4	F	5	

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	NAG	A	2	X	-	-	-
4	GU1	E	4	-	-	X	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 7001 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 ANTITHROMBIN-III.

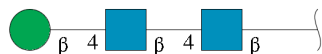
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	I	418	Total	C	N	O	S	0	0	0
			3279	2090	546	626	17			
1	L	423	Total	C	N	O	S	0	0	0
			3335	2122	560	635	18			

- 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	A	2	Total	C	N	O	0	0	0
			28	16	2	10			

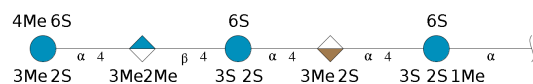
- Molecule 3 is an oligosaccharide called beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	B	3	Total	C	N	O	0	0	0
			39	22	2	15			
3	C	3	Total	C	N	O	0	0	0
			39	22	2	15			
3	D	3	Total	C	N	O	0	0	0
			39	22	2	15			

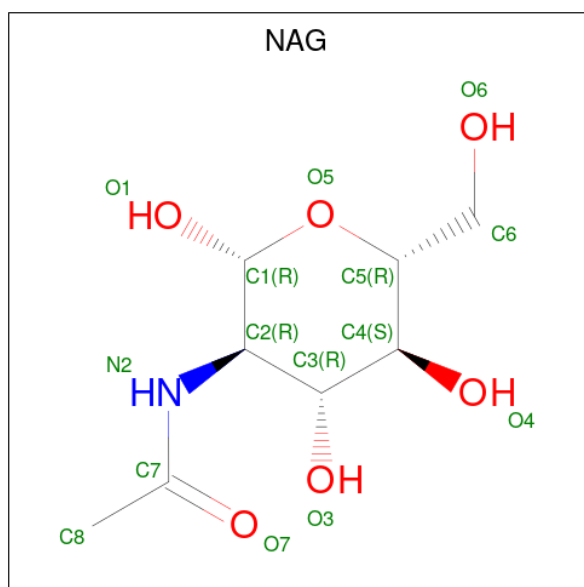
- Molecule 4 is an oligosaccharide called 3,4-di-O-methyl-2,6-di-O-sulfo-alpha-D-glucopyranos

e-(1-4)-2,3-di-O-methyl-beta-D-glucopyranuronic acid-(1-4)-2,3,6-tri-O-sulfo-alpha-D-glucopyranose-(1-4)-3-O-methyl-2-O-sulfo-alpha-L-idopyranuronic acid-(1-4)-methyl 2,3,6-tri-O-sulfo-alpha-D-glucopyranoside.



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
4	E	5	Total	C	O	S	0	0
			100	36	55	9		
4	F	5	Total	C	O	S	0	0
			100	36	55	9		

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



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

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	I	6	Total	O	0	0
			6	6		

Continued on next page...

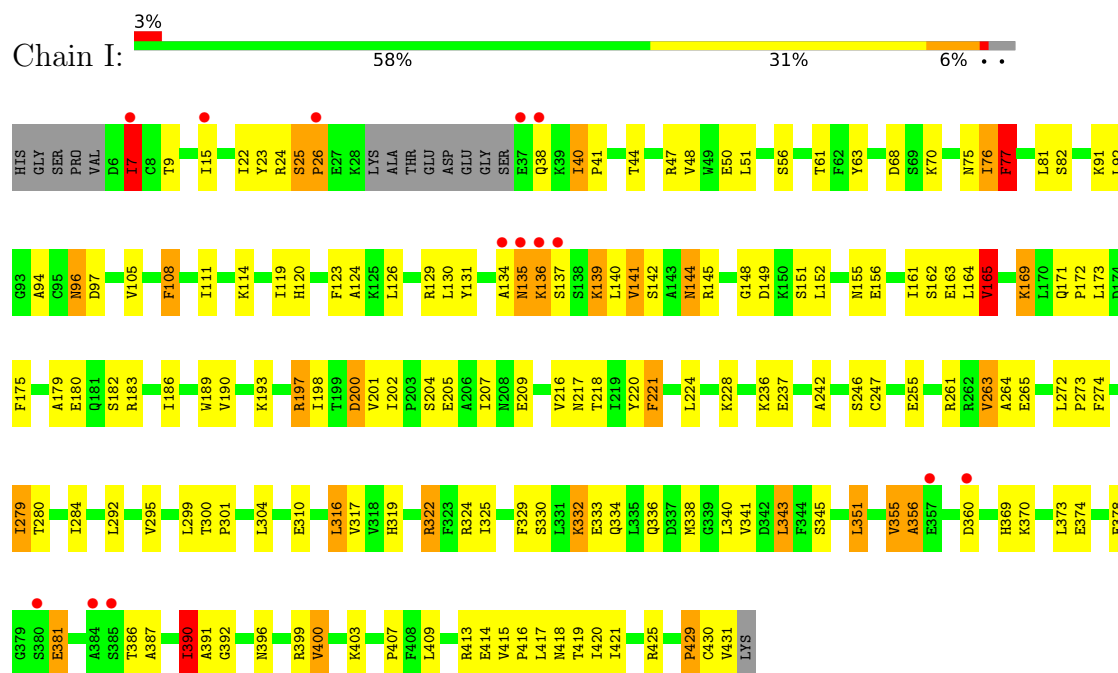
Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	L	8	Total	O	0	0
			8	8		

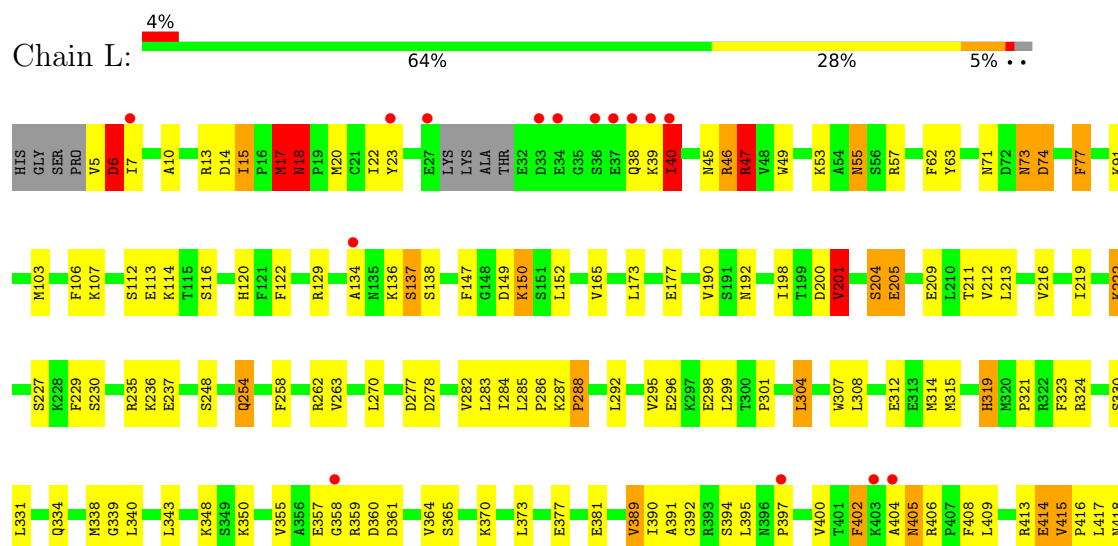
3 Residue-property plots

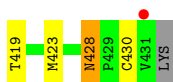
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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



• Molecule 1: ANTITHROMBIN-III





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

Chain A: 100%



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

Chain B: 33% 67%



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

Chain C: 67% 33%



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

Chain D: 33% 67%



- Molecule 4: 3,4-di-O-methyl-2,6-di-O-sulfo-alpha-D-glucopyranose-(1-4)-2,3-di-O-methyl-beta-D-glucopyranuronic acid-(1-4)-2,3,6-tri-O-sulfo-alpha-D-glucopyranose-(1-4)-3-O-methyl-2-O-sulfo-alpha-L-idopyranuronic acid-(1-4)-methyl 2,3,6-tri-O-sulfo-alpha-D-glucopyranoside

Chain E: 80% 20%



- Molecule 4: 3,4-di-O-methyl-2,6-di-O-sulfo-alpha-D-glucopyranose-(1-4)-2,3-di-O-methyl-beta-D-glucopyranuronic acid-(1-4)-2,3,6-tri-O-sulfo-alpha-D-glucopyranose-(1-4)-3-O-methyl-2-O-sulfo-alpha-L-idopyranuronic acid-(1-4)-methyl 2,3,6-tri-O-sulfo-alpha-D-glucopyranoside

Chain F: 60% 40%

Z9L1	Z9K2	G063	G014	Z9H5
------	------	------	------	------

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	70.51Å 87.07Å 97.35Å 90.00° 108.88° 90.00°	Depositor
Resolution (Å)	20.00 – 2.90 20.00 – 2.90	Depositor EDS
% Data completeness (in resolution range)	94.2 (20.00-2.90) 94.2 (20.00-2.90)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.87 (at 2.88Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.199 , 0.252 (Not available) , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	45.6	Xtriage
Anisotropy	0.353	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 58.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.023 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	7001	wwPDB-VP
Average B, all atoms (Å ²)	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.65% 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: NAG, GU6, Z9H, Z9L, BMA, Z9K, GU1

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	I	0.62	0/3345	1.49	35/4531 (0.8%)
1	L	0.63	0/3401	1.51	41/4601 (0.9%)
All	All	0.63	0/6746	1.50	76/9132 (0.8%)

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	L	0	1

There are no bond length outliers.

All (76) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	200	ASP	CA-CB-CG	10.85	123.45	112.60
1	L	40	ILE	CB-CA-C	-9.49	101.57	110.88
1	L	137	SER	N-CA-C	-9.20	100.95	112.72
1	L	405	ASN	N-CA-C	8.87	124.17	110.42
1	I	40	ILE	N-CA-C	8.37	117.57	107.61
1	I	165	VAL	N-CA-C	7.67	120.68	111.09
1	I	26	PRO	N-CA-C	7.67	124.00	113.65
1	L	122	PHE	CA-CB-CG	-7.44	106.36	113.80
1	L	200	ASP	N-CA-C	7.19	118.89	110.41
1	I	38	GLN	N-CA-C	7.18	120.38	108.96
1	I	242	ALA	N-CA-C	7.14	121.63	112.34
1	L	323	PHE	N-CA-C	7.10	118.54	108.74
1	L	17	MET	N-CA-C	7.06	123.64	114.75
1	I	221	PHE	CA-CB-CG	6.99	120.79	113.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	192	ASN	OD1-CG-ND2	6.90	129.50	122.60
1	I	295	VAL	N-CA-CB	6.59	117.82	110.51
1	L	10	ALA	N-CA-C	6.58	118.82	110.33
1	L	201	VAL	CB-CA-C	-6.54	103.32	111.70
1	I	155	ASN	CA-CB-CG	6.53	119.13	112.60
1	I	387	ALA	CA-C-O	-6.53	113.80	121.44
1	L	222	LYS	N-CA-CB	6.48	120.63	110.71
1	L	47	ARG	CD-NE-CZ	6.47	133.47	124.40
1	L	301	PRO	CA-C-N	6.46	128.84	120.44
1	L	301	PRO	C-N-CA	6.46	128.84	120.44
1	I	94	ALA	N-CA-C	6.39	119.04	110.35
1	L	258	PHE	CA-CB-CG	6.33	120.13	113.80
1	I	25	SER	CA-C-N	6.13	126.03	119.28
1	I	25	SER	C-N-CA	6.13	126.03	119.28
1	I	151	SER	N-CA-C	6.13	119.86	112.38
1	L	402	PHE	CA-CB-CG	6.07	119.87	113.80
1	I	193	LYS	N-CA-C	6.06	118.68	111.71
1	L	219	ILE	N-CA-CB	6.03	121.32	111.44
1	I	108	PHE	CA-CB-CG	5.95	119.75	113.80
1	I	135	ASN	OD1-CG-ND2	5.89	128.49	122.60
1	L	404	ALA	CA-C-O	-5.84	114.80	121.58
1	I	414	GLU	N-CA-C	-5.83	100.49	109.76
1	I	247	CYS	N-CA-CB	-5.74	102.31	111.62
1	L	14	ASP	CA-CB-CG	5.66	118.26	112.60
1	L	150	LYS	N-CA-C	5.65	118.99	111.75
1	L	415	VAL	N-CA-C	5.64	121.06	108.88
1	I	23	TYR	CA-C-O	5.63	126.57	120.32
1	L	112	SER	N-CA-C	5.62	117.55	110.24
1	I	322	ARG	N-CA-CB	5.61	119.41	110.16
1	I	7	ILE	N-CA-C	5.61	121.00	109.34
1	I	343	LEU	N-CA-C	5.59	118.09	111.33
1	L	402	PHE	N-CA-C	5.52	118.36	110.24
1	L	134	ALA	N-CA-C	5.50	122.53	110.80
1	I	180	GLU	N-CA-C	5.49	117.26	111.28
1	L	408	PHE	CA-CB-CG	5.48	119.28	113.80
1	L	216	VAL	N-CA-C	5.46	116.34	108.48
1	L	389	VAL	N-CA-CB	5.45	117.58	111.21
1	L	405	ASN	O-C-N	-5.42	116.91	123.03
1	I	329	PHE	CA-CB-CG	5.41	119.21	113.80
1	I	40	ILE	CA-C-O	5.38	122.84	119.51
1	L	73	ASN	N-CA-CB	-5.37	102.33	110.92
1	L	413	ARG	N-CA-C	5.36	118.44	110.14

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	68	ASP	N-CA-C	5.28	118.51	111.75
1	L	177	GLU	CB-CA-C	5.28	119.05	110.24
1	I	156	GLU	N-CA-C	5.27	117.93	111.82
1	I	396	ASN	CA-CB-CG	5.27	117.87	112.60
1	L	339	GLY	N-CA-C	5.25	121.99	114.64
1	L	55	ASN	CA-CB-CG	5.21	117.81	112.60
1	L	414	GLU	N-CA-CB	5.18	118.88	110.43
1	L	47	ARG	N-CA-C	5.18	117.59	111.33
1	I	23	TYR	N-CA-C	5.17	117.50	108.76
1	I	77	PHE	N-CA-CB	5.15	119.19	110.49
1	I	263	VAL	CA-C-O	5.09	127.14	120.78
1	I	390	ILE	CB-CA-C	-5.06	104.95	111.53
1	L	106	PHE	CA-CB-CG	-5.06	108.74	113.80
1	I	413	ARG	N-CA-C	5.05	116.86	109.24
1	I	200	ASP	N-CA-C	5.02	118.51	111.74
1	L	278	ASP	CA-CB-CG	5.01	117.61	112.60
1	L	277	ASP	CA-C-N	5.01	127.93	120.31
1	L	277	ASP	C-N-CA	5.01	127.93	120.31
1	L	343	LEU	N-CA-C	5.01	118.16	111.75
1	L	77	PHE	N-CA-CB	5.00	118.84	110.59

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	L	6	ASP	Mainchain

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	I	3279	0	3200	78	0
1	L	3335	0	3278	62	0
2	A	28	0	25	0	0
3	B	39	0	34	1	0
3	C	39	0	34	2	0
3	D	39	0	34	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	E	100	0	16	6	0
4	F	100	0	16	6	0
5	I	14	0	13	1	0
5	L	14	0	13	0	0
6	I	6	0	0	0	0
6	L	8	0	0	1	0
All	All	7001	0	6663	149	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 (149) 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:F:5:Z9H:O9	4:F:5:Z9H:C8	1.90	1.17
4:F:4:GU1:H82	4:F:5:Z9H:C1	1.85	1.07
4:F:5:Z9H:C8	4:F:5:Z9H:S2	2.64	0.85
4:E:4:GU1:C8	4:E:4:GU1:O2	2.31	0.79
1:L:129:ARG:HD3	1:L:417:LEU:HD21	1.65	0.79
4:F:5:Z9H:C7	4:F:5:Z9H:O3	2.34	0.75
1:I:144:ASN:HB3	1:I:217:ASN:HA	1.70	0.74
4:E:4:GU1:O2	4:E:4:GU1:H83	1.89	0.73
1:I:141:VAL:HG23	1:I:220:TYR:HB3	1.71	0.73
1:L:120:HIS:HB3	1:L:165:VAL:HG11	1.71	0.70
1:L:20:MET:HE2	3:C:1:NAG:H4	1.73	0.69
1:I:415:VAL:HB	1:I:416:PRO:HD3	1.77	0.65
1:I:183:ARG:NH2	1:I:204:SER:HA	2.12	0.64
1:I:218:THR:HG22	1:I:370:LYS:HB3	1.80	0.64
1:L:7:ILE:HD12	1:L:15:ILE:HD13	1.79	0.63
1:L:211:THR:HA	1:L:391:ALA:O	1.99	0.62
1:L:270:LEU:HD23	1:L:283:LEU:HD12	1.80	0.62
1:L:428:ASN:HD21	1:L:430:CYS:HB2	1.63	0.62
1:L:415:VAL:HB	1:L:416:PRO:HD3	1.82	0.61
1:I:274:PHE:HD2	1:I:279:ILE:HG22	1.65	0.61
1:I:264:ALA:O	1:I:265:GLU:HB2	2.00	0.61
1:I:48:VAL:HG13	1:I:126:LEU:HB2	1.84	0.60
1:L:20:MET:HB2	3:C:1:NAG:H61	1.85	0.58
1:L:198:ILE:HG23	1:L:370:LYS:HG2	1.86	0.58
4:E:4:GU1:H72	4:E:4:GU1:H82	1.86	0.58
1:L:49:TRP:CZ2	1:L:53:LYS:HD2	2.39	0.58
1:L:365:SER:HB3	1:L:392:GLY:H	1.69	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:202:ILE:HD13	1:I:207:ILE:HD11	1.86	0.56
4:F:5:Z9H:C8	4:F:5:Z9H:O2	2.49	0.56
4:E:4:GU1:H82	4:E:4:GU1:C7	2.36	0.56
1:L:222:LYS:HD2	1:L:381:GLU:HG3	1.89	0.55
1:I:292:LEU:HD11	1:I:409:LEU:HG	1.89	0.55
1:I:139:LYS:NZ	1:I:197:ARG:HH22	2.05	0.55
3:D:1:NAG:H62	3:D:2:NAG:N2	2.22	0.54
1:I:25:SER:HB2	1:I:26:PRO:CD	2.38	0.54
1:I:134:ALA:HA	1:I:279:ILE:HD13	1.90	0.54
1:I:22:ILE:HD12	1:I:24:ARG:HE	1.72	0.53
1:I:124:ALA:HB2	1:I:165:VAL:HG22	1.90	0.53
1:I:190:VAL:HG11	1:I:201:VAL:HG21	1.91	0.53
1:I:130:LEU:HD13	1:I:421:ILE:HD11	1.90	0.53
1:I:91:LYS:HD2	1:I:119:ILE:HG21	1.90	0.52
1:L:57:ARG:HB2	1:L:107:LYS:HG3	1.90	0.52
1:L:284:ILE:HB	1:L:409:LEU:HB2	1.91	0.52
1:I:163:GLU:HB2	1:I:169:LYS:HG2	1.92	0.52
1:I:204:SER:O	1:I:205:GLU:HB2	2.09	0.51
1:I:77:PHE:CZ	1:I:373:LEU:HB2	2.46	0.51
1:I:390:ILE:HA	1:L:319:HIS:HB2	1.92	0.51
1:I:319:HIS:HB2	1:I:403:LYS:HA	1.91	0.50
1:L:17:MET:O	1:L:18:ASN:C	2.54	0.50
1:L:295:VAL:HG13	1:L:307:TRP:HH2	1.76	0.50
1:I:44:THR:HG21	1:I:417:LEU:HD13	1.93	0.50
1:I:135:ASN:O	1:I:136:LYS:C	2.55	0.50
1:I:148:GLY:O	1:I:172:PRO:HA	2.12	0.50
1:I:273:PRO:HA	1:I:280:THR:HG22	1.94	0.50
1:I:7:ILE:HG23	1:I:164:LEU:HG	1.94	0.49
1:L:77:PHE:CE2	1:L:373:LEU:HB2	2.47	0.49
1:L:63:TYR:HE2	1:L:296:GLU:HG2	1.77	0.49
3:B:1:NAG:H62	3:B:2:NAG:N2	2.28	0.49
1:I:391:ALA:O	1:L:321:PRO:HD3	2.12	0.49
1:I:25:SER:CB	1:I:26:PRO:CD	2.90	0.49
1:I:300:THR:HB	1:I:301:PRO:HD2	1.94	0.49
1:L:55:ASN:HB2	6:L:2001:HOH:O	2.12	0.49
1:L:364:VAL:HG22	1:L:390:ILE:HD13	1.95	0.48
1:I:198:ILE:HD11	1:I:220:TYR:HB2	1.96	0.48
1:I:139:LYS:HZ2	1:I:197:ARG:HH22	1.60	0.48
1:I:70:LYS:HD3	1:I:76:ILE:HD13	1.96	0.48
1:I:75:ASN:HB3	1:I:325:ILE:HG12	1.96	0.47
1:I:108:PHE:O	1:I:111:ILE:HG12	2.14	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:186:ILE:HG21	1:I:202:ILE:HD12	1.95	0.47
1:L:149:ASP:HB3	1:L:152:LEU:HD12	1.94	0.47
4:E:4:GU1:C8	4:E:4:GU1:C7	2.91	0.47
1:L:355:VAL:HG21	1:L:359:ARG:HB3	1.96	0.47
1:I:316:LEU:HB3	1:I:400:VAL:HG12	1.96	0.47
1:I:392:GLY:HA3	1:L:321:PRO:HG3	1.96	0.47
1:L:38:GLN:O	1:L:39:LYS:C	2.57	0.47
1:L:40:ILE:H	1:L:40:ILE:HG13	1.51	0.47
1:L:282:VAL:HG21	1:L:308:LEU:HD21	1.97	0.47
1:I:56:SER:HA	1:I:420:ILE:HD12	1.96	0.47
1:I:131:TYR:HD1	1:I:140:LEU:HD23	1.79	0.47
1:L:428:ASN:HD22	1:L:428:ASN:C	2.23	0.46
4:E:4:GU1:O2	4:E:4:GU1:H82	2.14	0.46
1:I:198:ILE:HG23	1:I:370:LYS:HG2	1.97	0.46
1:L:39:LYS:NZ	1:L:46:ARG:HH22	2.13	0.46
1:I:201:VAL:HG11	1:I:216:VAL:HG13	1.98	0.46
1:L:152:LEU:HD13	1:L:212:VAL:HG13	1.97	0.46
1:L:395:LEU:O	1:L:397:PRO:HD3	2.15	0.46
1:I:47:ARG:O	1:I:50:GLU:HG2	2.16	0.46
1:L:299:LEU:HD11	1:L:304:LEU:HD12	1.98	0.46
1:I:51:LEU:HD21	1:I:123:PHE:CD2	2.51	0.45
1:L:57:ARG:CB	1:L:107:LYS:HG3	2.46	0.45
1:L:71:ASN:O	1:L:74:ASP:HB2	2.16	0.45
1:I:131:TYR:HE2	5:I:821:NAG:H82	1.81	0.45
1:L:359:ARG:HG2	1:L:361:ASP:OD1	2.17	0.45
1:I:105:VAL:HG21	1:I:340:LEU:HB2	1.97	0.45
1:I:224:LEU:HD12	1:I:378:GLU:O	2.17	0.45
1:I:92:LEU:HD21	1:I:161:ILE:HG21	1.99	0.45
1:L:103:MET:HA	1:L:103:MET:HE2	1.98	0.45
1:L:45:ASN:O	1:L:46:ARG:C	2.58	0.45
1:L:190:VAL:HG11	1:L:201:VAL:CG2	2.46	0.45
1:I:120:HIS:CD2	1:I:120:HIS:H	2.34	0.45
1:I:263:VAL:HB	1:I:264:ALA:H	1.60	0.45
1:L:47:ARG:NH1	1:L:114:LYS:HB3	2.32	0.44
1:L:286:PRO:HG3	1:L:292:LEU:HD13	1.97	0.44
1:L:204:SER:O	1:L:205:GLU:HB2	2.17	0.44
1:L:287:LYS:O	1:L:288:PRO:C	2.59	0.44
1:L:40:ILE:HD11	1:L:46:ARG:NE	2.32	0.44
1:I:145:ARG:HB2	1:I:189:TRP:CH2	2.53	0.44
1:L:40:ILE:HD11	1:L:46:ARG:HE	1.83	0.44
1:I:261:ARG:HG3	1:I:263:VAL:HG13	1.98	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:324:ARG:CG	1:I:374:GLU:HG3	2.49	0.43
1:I:343:LEU:HD11	1:I:351:LEU:HD21	1.99	0.43
1:L:71:ASN:OD1	1:L:73:ASN:HB2	2.18	0.43
1:I:274:PHE:CD2	1:I:279:ILE:HG22	2.49	0.43
1:I:149:ASP:HA	1:I:173:LEU:O	2.18	0.43
1:I:236:LYS:HD2	1:I:236:LYS:HA	1.91	0.43
1:L:62:PHE:HD1	1:L:338:MET:HE1	1.84	0.43
1:I:40:ILE:HA	1:I:41:PRO:HD3	1.89	0.43
1:I:139:LYS:O	1:I:221:PHE:HA	2.19	0.43
1:L:147:PHE:HB3	1:L:173:LEU:HD12	2.01	0.43
1:L:314:MET:HE3	1:L:314:MET:HB2	1.90	0.42
1:I:198:ILE:HG21	1:I:218:THR:HG21	2.01	0.42
1:I:63:TYR:OH	1:I:425:ARG:HB2	2.18	0.42
1:I:355:VAL:O	1:I:356:ALA:C	2.62	0.42
1:I:130:LEU:HD11	1:I:419:THR:HG21	2.01	0.42
1:I:175:PHE:O	1:I:209:GLU:HA	2.19	0.42
1:L:17:MET:O	1:L:17:MET:HG2	2.20	0.42
1:I:152:LEU:HD22	1:I:360:ASP:OD2	2.20	0.42
1:I:7:ILE:H	1:I:7:ILE:HD13	1.83	0.42
1:I:217:ASN:O	1:I:369:HIS:HA	2.20	0.42
1:L:338:MET:HE3	1:L:338:MET:HB2	1.86	0.42
1:L:405:ASN:OD1	1:L:406:ARG:N	2.53	0.42
1:L:40:ILE:HG23	1:L:49:TRP:CG	2.56	0.41
1:I:197:ARG:NH2	1:I:381:GLU:OE2	2.53	0.41
1:L:17:MET:HE3	1:L:17:MET:HB3	1.99	0.41
1:I:332:LYS:O	1:I:336:GLN:HG3	2.20	0.41
1:L:229:PHE:CD2	1:L:254:GLN:HB2	2.56	0.41
1:I:299:LEU:HD12	1:I:299:LEU:HA	1.92	0.41
1:I:391:ALA:HB2	1:L:285:LEU:HD21	2.02	0.41
1:I:76:ILE:HG22	1:I:77:PHE:H	1.85	0.41
1:I:332:LYS:O	1:I:333:GLU:C	2.64	0.41
1:I:119:ILE:O	1:I:123:PHE:HD2	2.04	0.41
1:I:292:LEU:HD21	1:I:425:ARG:HG3	2.02	0.41
1:L:13:ARG:HG3	4:F:3:GU6:S2	2.61	0.41
1:L:229:PHE:HB2	1:L:377:GLU:HA	2.02	0.41
1:L:324:ARG:HA	1:L:373:LEU:O	2.20	0.41
1:L:62:PHE:CD1	1:L:338:MET:HE1	2.56	0.41
1:I:96:ASN:HB3	1:I:97:ASP:H	1.66	0.40
1:I:255:GLU:HG2	1:I:317:VAL:HG22	2.03	0.40
1:L:5:VAL:HB	1:L:6:ASP:H	1.59	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	I	414/432 (96%)	371 (90%)	36 (9%)	7 (2%)	7	26
1	L	419/432 (97%)	376 (90%)	39 (9%)	4 (1%)	12	39
All	All	833/864 (96%)	747 (90%)	75 (9%)	11 (1%)	9	32

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	I	136	LYS
1	I	179	ALA
1	I	356	ALA
1	L	357	GLU
1	L	358	GLY
1	I	77	PHE
1	I	332	LYS
1	L	18	ASN
1	L	288	PRO
1	I	407	PRO
1	I	429	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	I	356/383 (93%)	308 (86%)	48 (14%)	4	12
1	L	365/383 (95%)	313 (86%)	52 (14%)	3	11

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	721/766 (94%)	621 (86%)	100 (14%)	3 11

All (100) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	I	7	ILE
1	I	9	THR
1	I	15	ILE
1	I	61	THR
1	I	76	ILE
1	I	81	LEU
1	I	82	SER
1	I	96	ASN
1	I	114	LYS
1	I	129	ARG
1	I	137	SER
1	I	139	LYS
1	I	141	VAL
1	I	142	SER
1	I	144	ASN
1	I	162	SER
1	I	165	VAL
1	I	169	LYS
1	I	171	GLN
1	I	182	SER
1	I	197	ARG
1	I	200	ASP
1	I	228	LYS
1	I	237	GLU
1	I	246	SER
1	I	272	LEU
1	I	279	ILE
1	I	284	ILE
1	I	304	LEU
1	I	310	GLU
1	I	316	LEU
1	I	322	ARG
1	I	330	SER
1	I	334	GLN
1	I	338	MET
1	I	341	VAL
1	I	345	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	I	351	LEU
1	I	355	VAL
1	I	381	GLU
1	I	386	THR
1	I	390	ILE
1	I	399	ARG
1	I	400	VAL
1	I	418	ASN
1	I	429	PRO
1	I	430	CYS
1	I	431	VAL
1	L	6	ASP
1	L	15	ILE
1	L	17	MET
1	L	18	ASN
1	L	22	ILE
1	L	23	TYR
1	L	40	ILE
1	L	46	ARG
1	L	47	ARG
1	L	74	ASP
1	L	91	LYS
1	L	113	GLU
1	L	116	SER
1	L	136	LYS
1	L	137	SER
1	L	138	SER
1	L	150	LYS
1	L	201	VAL
1	L	204	SER
1	L	205	GLU
1	L	209	GLU
1	L	213	LEU
1	L	227	SER
1	L	230	SER
1	L	235	ARG
1	L	236	LYS
1	L	237	GLU
1	L	248	SER
1	L	254	GLN
1	L	262	ARG
1	L	263	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	L	298	GLU
1	L	304	LEU
1	L	312	GLU
1	L	315	MET
1	L	319	HIS
1	L	330	SER
1	L	331	LEU
1	L	334	GLN
1	L	340	LEU
1	L	348	LYS
1	L	350	LYS
1	L	360	ASP
1	L	389	VAL
1	L	394	SER
1	L	400	VAL
1	L	402	PHE
1	L	414	GLU
1	L	418	ASN
1	L	419	THR
1	L	423	MET
1	L	428	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	I	65	HIS
1	I	73	ASN
1	I	120	HIS
1	I	319	HIS
1	I	428	ASN
1	L	64	GLN
1	L	118	GLN
1	L	127	ASN
1	L	396	ASN
1	L	428	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 ⓘ

21 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	A	1	2,1	14,14,15	1.71	2 (14%)	17,19,21	3.69	4 (23%)
2	NAG	A	2	2	14,14,15	1.65	3 (21%)	17,19,21	1.63	4 (23%)
3	NAG	B	1	3,1	14,14,15	1.28	1 (7%)	17,19,21	0.80	0
3	NAG	B	2	3	14,14,15	1.38	1 (7%)	17,19,21	1.54	3 (17%)
3	BMA	B	3	3	11,11,12	0.99	1 (9%)	15,15,17	0.89	0
3	NAG	C	1	3,1	14,14,15	1.30	1 (7%)	17,19,21	0.96	1 (5%)
3	NAG	C	2	3	14,14,15	1.60	4 (28%)	17,19,21	2.88	7 (41%)
3	BMA	C	3	3	11,11,12	0.94	1 (9%)	15,15,17	1.00	0
3	NAG	D	1	3,1	14,14,15	1.34	2 (14%)	17,19,21	1.81	5 (29%)
3	NAG	D	2	3	14,14,15	1.30	1 (7%)	17,19,21	2.21	4 (23%)
3	BMA	D	3	3	11,11,12	1.04	2 (18%)	15,15,17	1.18	1 (6%)
4	Z9L	E	1	4	25,25,25	1.03	1 (4%)	34,39,39	1.43	4 (11%)
4	Z9K	E	2	4	17,17,18	1.32	2 (11%)	17,25,27	1.18	1 (5%)
4	GU6	E	3	4	23,23,24	1.48	3 (13%)	28,36,38	1.67	3 (10%)
4	GU1	E	4	4	14,14,15	1.03	1 (7%)	15,19,21	1.03	1 (6%)
4	Z9H	E	5	4	21,21,22	1.01	1 (4%)	26,31,33	0.94	1 (3%)
4	Z9L	F	1	4	25,25,25	1.11	1 (4%)	34,39,39	1.00	1 (2%)
4	Z9K	F	2	4	17,17,18	1.29	2 (11%)	17,25,27	1.07	2 (11%)
4	GU6	F	3	4	23,23,24	1.30	3 (13%)	28,36,38	0.93	0
4	GU1	F	4	4	14,14,15	1.06	2 (14%)	15,19,21	1.16	2 (13%)
4	Z9H	F	5	4	21,21,22	0.97	0	26,31,33	1.02	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
2	NAG	A	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	A	2	2	1/1/5/7	0/6/23/26	0/1/1/1
3	NAG	B	1	3,1	-	1/6/23/26	0/1/1/1
3	NAG	B	2	3	-	1/6/23/26	0/1/1/1
3	BMA	B	3	3	-	0/2/19/22	0/1/1/1
3	NAG	C	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	C	2	3	-	3/6/23/26	0/1/1/1
3	BMA	C	3	3	-	2/2/19/22	0/1/1/1
3	NAG	D	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	D	2	3	-	2/6/23/26	0/1/1/1
3	BMA	D	3	3	-	1/2/19/22	0/1/1/1
4	Z9L	E	1	4	-	5/18/38/38	0/1/1/1
4	Z9K	E	2	4	-	0/11/28/31	0/1/1/1
4	GU6	E	3	4	-	5/16/33/36	0/1/1/1
4	GU1	E	4	4	-	1/8/25/28	0/1/1/1
4	Z9H	E	5	4	-	5/15/32/35	0/1/1/1
4	Z9L	F	1	4	-	6/18/38/38	0/1/1/1
4	Z9K	F	2	4	-	0/11/28/31	0/1/1/1
4	GU6	F	3	4	-	5/16/33/36	0/1/1/1
4	GU1	F	4	4	-	2/8/25/28	0/1/1/1
4	Z9H	F	5	4	-	7/15/32/35	0/1/1/1

All (35) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	E	3	GU6	O2-C2	-4.44	1.40	1.47
2	A	1	NAG	O5-C5	-4.31	1.35	1.43
3	C	2	NAG	O7-C7	-3.94	1.14	1.23
3	B	2	NAG	O7-C7	-3.84	1.14	1.23
3	D	2	NAG	O7-C7	-3.80	1.14	1.23
3	B	1	NAG	O7-C7	-3.71	1.14	1.23
3	C	1	NAG	O7-C7	-3.71	1.14	1.23
2	A	2	NAG	O7-C7	-3.68	1.15	1.23
2	A	1	NAG	O7-C7	-3.66	1.15	1.23
3	D	1	NAG	O7-C7	-3.61	1.15	1.23
4	F	2	Z9K	C1-C2	3.17	1.56	1.51

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	2	NAG	O5-C1	-3.12	1.38	1.43
4	F	3	GU6	C1-C2	3.03	1.56	1.51
4	E	2	Z9K	C1-C2	2.98	1.56	1.51
2	A	2	NAG	C1-C2	-2.87	1.48	1.52
3	C	2	NAG	C4-C3	2.57	1.59	1.52
3	C	2	NAG	C3-C2	-2.41	1.47	1.52
3	C	2	NAG	C2-N2	-2.35	1.42	1.46
4	E	3	GU6	O6-S6	2.31	1.63	1.56
4	E	1	Z9L	O6-S1	2.30	1.63	1.56
4	E	2	Z9K	O2-C2	-2.27	1.44	1.47
3	C	3	BMA	C1-C2	2.27	1.57	1.52
3	D	3	BMA	C1-C2	2.22	1.57	1.52
3	B	3	BMA	C1-C2	2.22	1.57	1.52
4	F	3	GU6	O6-S6	2.20	1.62	1.56
4	E	3	GU6	O3-C3	-2.19	1.41	1.46
4	F	1	Z9L	O6-S1	2.18	1.62	1.56
4	E	5	Z9H	C1-C2	2.17	1.55	1.51
4	F	2	Z9K	O2-C2	-2.12	1.44	1.47
4	F	3	GU6	O3-C3	-2.12	1.41	1.46
4	E	4	GU1	C4-C5	2.10	1.56	1.53
3	D	1	NAG	O5-C5	-2.09	1.39	1.43
4	F	4	GU1	C1-C2	2.06	1.54	1.51
4	F	4	GU1	C4-C5	2.05	1.56	1.53
3	D	3	BMA	O5-C1	-2.05	1.40	1.43

All (44) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1	NAG	C1-O5-C5	13.04	129.66	112.19
4	E	3	GU6	O2-C2-C3	6.87	114.26	106.65
2	A	1	NAG	C4-C3-C2	-5.76	102.58	111.02
3	C	2	NAG	C2-N2-C7	5.70	130.54	122.90
3	C	2	NAG	C1-C2-N2	5.22	118.65	110.43
3	D	2	NAG	C1-O5-C5	5.11	119.04	112.19
3	C	2	NAG	C1-O5-C5	4.94	118.81	112.19
3	C	2	NAG	C4-C3-C2	-4.67	104.17	111.02
3	D	2	NAG	C4-C3-C2	-4.45	104.50	111.02
2	A	2	NAG	O5-C1-C2	4.30	117.94	111.29
3	B	2	NAG	C1-O5-C5	4.21	117.83	112.19
4	E	1	Z9L	O2-C2-C1	4.16	113.17	107.58
3	D	2	NAG	O5-C1-C2	4.00	117.47	111.29
3	D	1	NAG	O5-C1-C2	-3.89	105.28	111.29

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	3	BMA	C1-C2-C3	-3.69	104.27	109.64
2	A	1	NAG	C1-C2-N2	3.58	116.07	110.43
2	A	2	NAG	C4-C3-C2	-3.51	105.87	111.02
4	E	2	Z9K	O6-C6-O10	-3.20	116.81	124.08
3	C	2	NAG	O4-C4-C5	3.15	117.08	109.32
4	E	1	Z9L	O1-C1-C2	3.04	113.46	107.85
3	D	1	NAG	C3-C4-C5	2.95	115.57	110.23
3	D	1	NAG	C1-C2-N2	2.89	114.98	110.43
3	C	2	NAG	O4-C4-C3	-2.78	103.81	110.38
3	D	2	NAG	O4-C4-C5	2.76	116.12	109.32
3	D	1	NAG	C4-C3-C2	-2.70	107.06	111.02
3	D	1	NAG	O5-C5-C6	-2.70	102.42	107.66
4	E	3	GU6	C3-O3-S3	-2.66	112.66	119.04
4	F	1	Z9L	C4-C3-C2	-2.66	105.75	111.72
4	F	4	GU1	O6B-C6-O6A	-2.63	118.12	124.08
4	E	1	Z9L	O5-C5-C4	2.54	114.27	109.70
4	F	4	GU1	C4-C3-C2	-2.51	105.36	110.93
4	E	4	GU1	O6B-C6-O6A	-2.41	118.62	124.08
4	E	5	Z9H	O2-C2-C3	2.34	109.25	106.65
3	C	1	NAG	O4-C4-C5	2.33	115.07	109.32
2	A	1	NAG	O5-C5-C6	2.30	112.15	107.66
3	B	2	NAG	C4-C3-C2	-2.27	107.69	111.02
3	C	2	NAG	O5-C5-C6	-2.27	103.25	107.66
4	F	2	Z9K	O6-C6-O10	-2.24	119.00	124.08
4	F	2	Z9K	O5-C1-C2	2.19	113.95	109.51
3	B	2	NAG	O4-C4-C3	-2.18	105.24	110.38
2	A	2	NAG	C1-C2-N2	2.17	113.85	110.43
4	E	1	Z9L	C4-C3-C2	-2.13	106.94	111.72
2	A	2	NAG	C3-C4-C5	2.01	113.88	110.23
4	E	3	GU6	O18-S3-O16	2.00	115.56	108.56

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	A	2	NAG	C1

All (46) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	2	NAG	C3-C2-N2-C7
4	E	1	Z9L	C4-C5-C6-O6
4	E	1	Z9L	O5-C5-C6-O6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
4	E	3	GU6	C1-C2-O2-S2
4	E	3	GU6	C6-O6-S6-O19
4	E	5	Z9H	C4-C5-C6-O6
4	E	5	Z9H	O5-C5-C6-O6
4	E	5	Z9H	C6-O6-S1-O8
4	E	5	Z9H	C6-O6-S1-O12
4	F	3	GU6	O5-C5-C6-O6
4	F	5	Z9H	C4-C5-C6-O6
4	F	5	Z9H	O5-C5-C6-O6
4	E	4	GU1	C2-C3-O3-C8
4	F	5	Z9H	C2-C3-O3-C8
4	E	1	Z9L	C2-C1-O1-C7
3	C	2	NAG	O5-C5-C6-O6
4	F	4	GU1	C4-C3-O3-C8
3	C	2	NAG	C4-C5-C6-O6
4	E	1	Z9L	O5-C1-O1-C7
4	F	5	Z9H	C3-C4-O4-C7
3	C	3	BMA	O5-C5-C6-O6
4	E	3	GU6	C6-O6-S6-O21
4	F	5	Z9H	C6-O6-S1-O8
4	F	5	Z9H	C6-O6-S1-O12
4	F	1	Z9L	C2-O2-S3-O13
4	F	1	Z9L	C2-O2-S3-O14
4	E	5	Z9H	C6-O6-S1-O7
4	F	5	Z9H	C6-O6-S1-O7
3	D	2	NAG	O5-C5-C6-O6
4	E	3	GU6	C6-O6-S6-O20
4	F	1	Z9L	C2-O2-S3-O12
3	D	2	NAG	C4-C5-C6-O6
4	F	1	Z9L	C6-O6-S1-O15
4	F	1	Z9L	C6-O6-S1-O7
4	F	3	GU6	C6-O6-S6-O20
4	F	3	GU6	C6-O6-S6-O21
4	F	1	Z9L	C6-O6-S1-O11
4	F	3	GU6	C4-C5-C6-O6
4	E	1	Z9L	C2-O2-S3-O12
3	B	2	NAG	O5-C5-C6-O6
4	F	3	GU6	C6-O6-S6-O19
3	D	3	BMA	O5-C5-C6-O6
3	B	1	NAG	C1-C2-N2-C7
3	C	3	BMA	C4-C5-C6-O6
4	E	3	GU6	C2-O2-S2-O13

Continued on next page...

Continued from previous page...

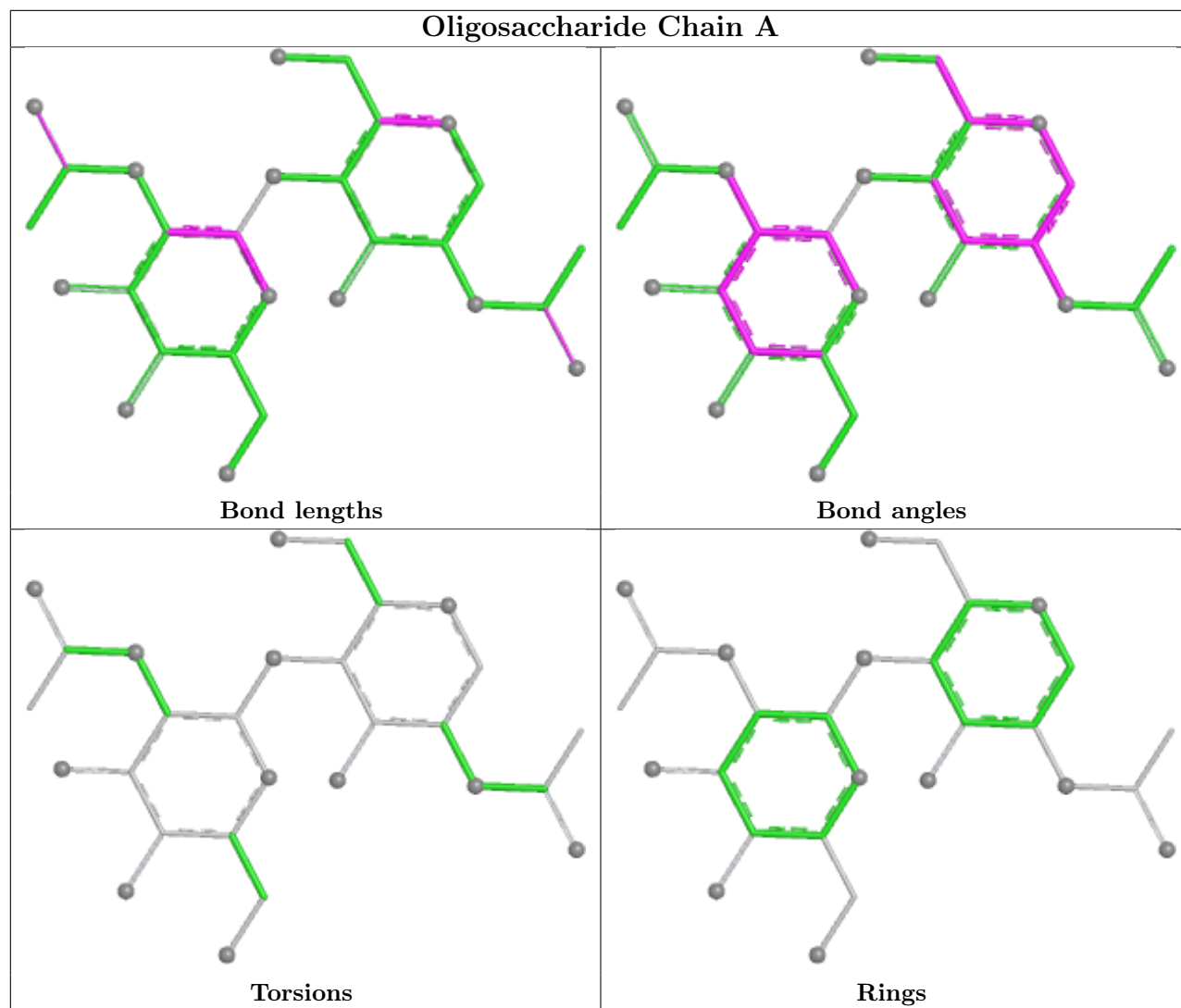
Mol	Chain	Res	Type	Atoms
4	F	4	GU1	C1-C2-O2-C7

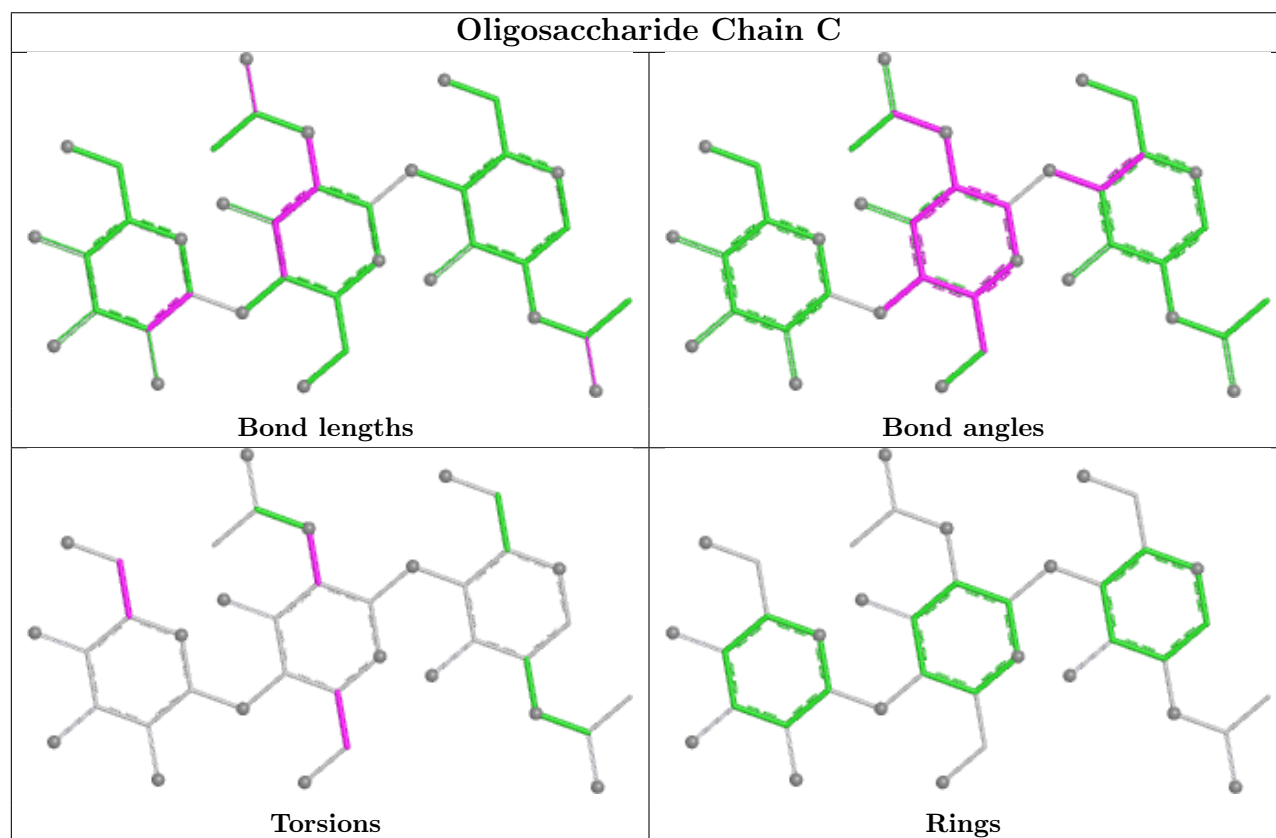
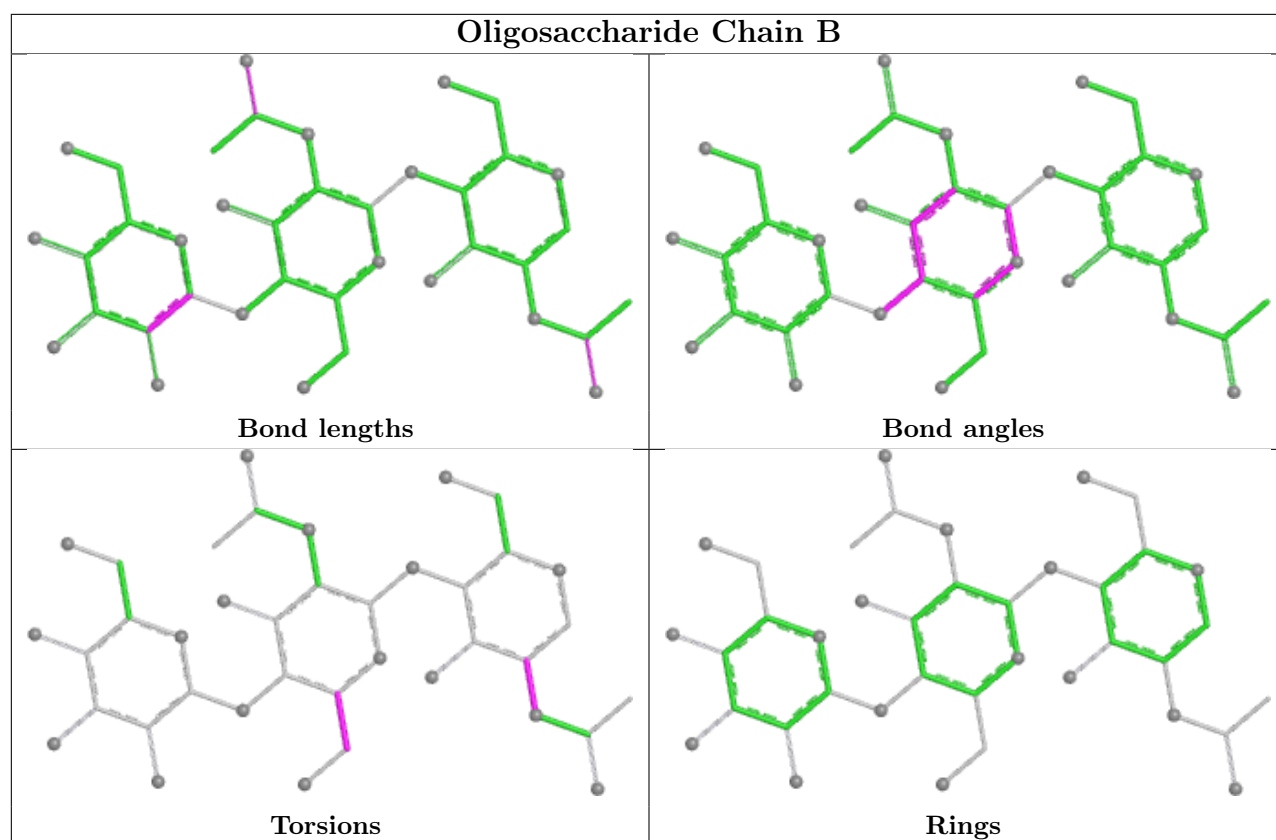
There are no ring outliers.

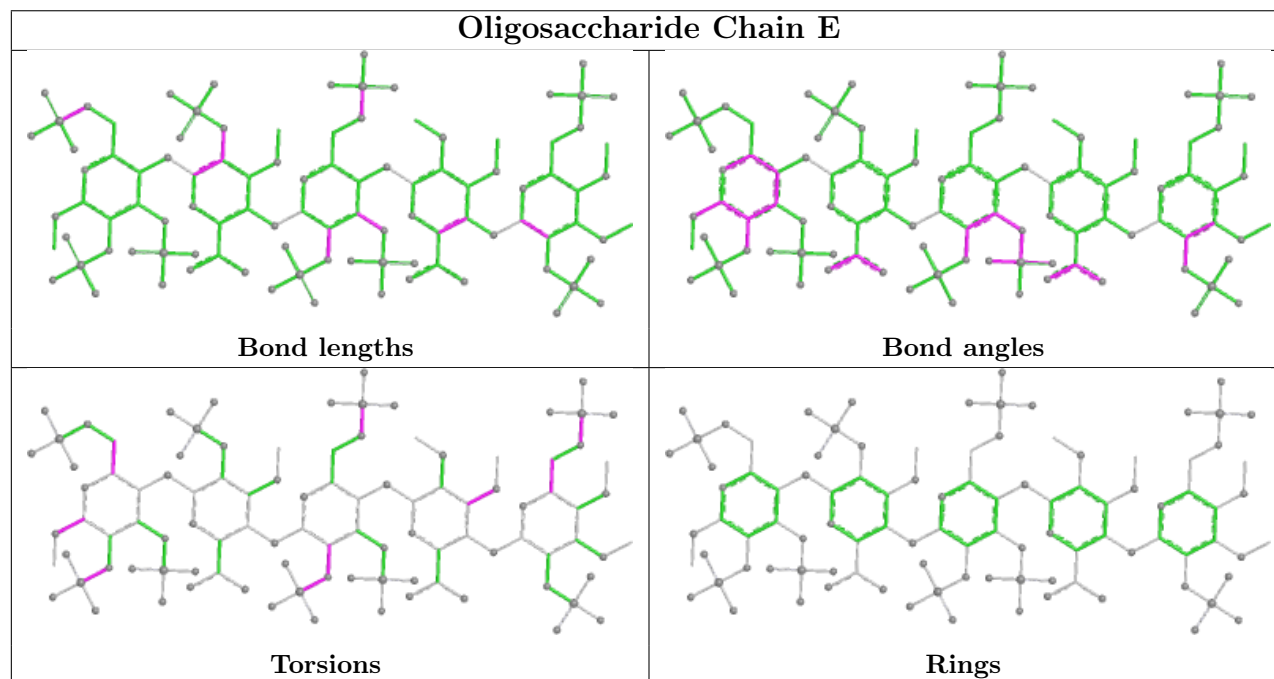
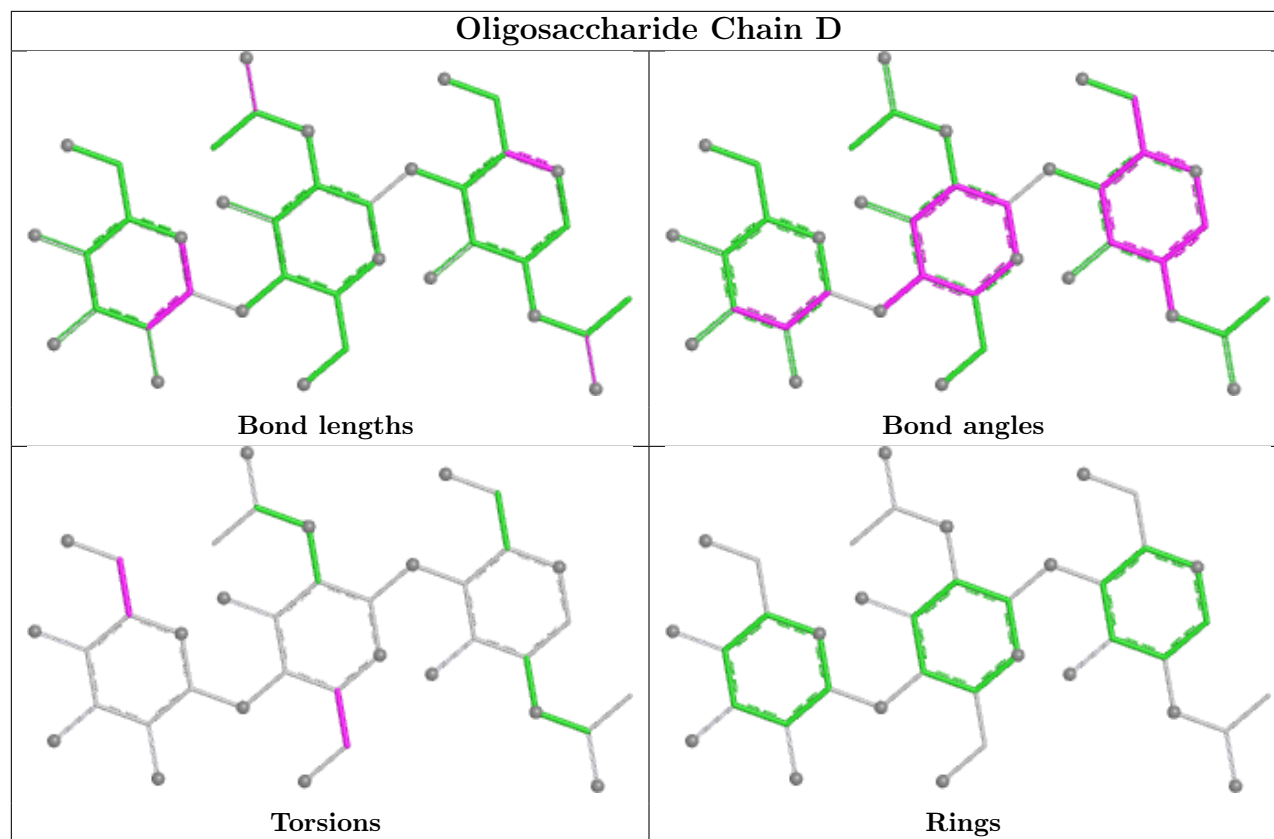
9 monomers are involved in 16 short contacts:

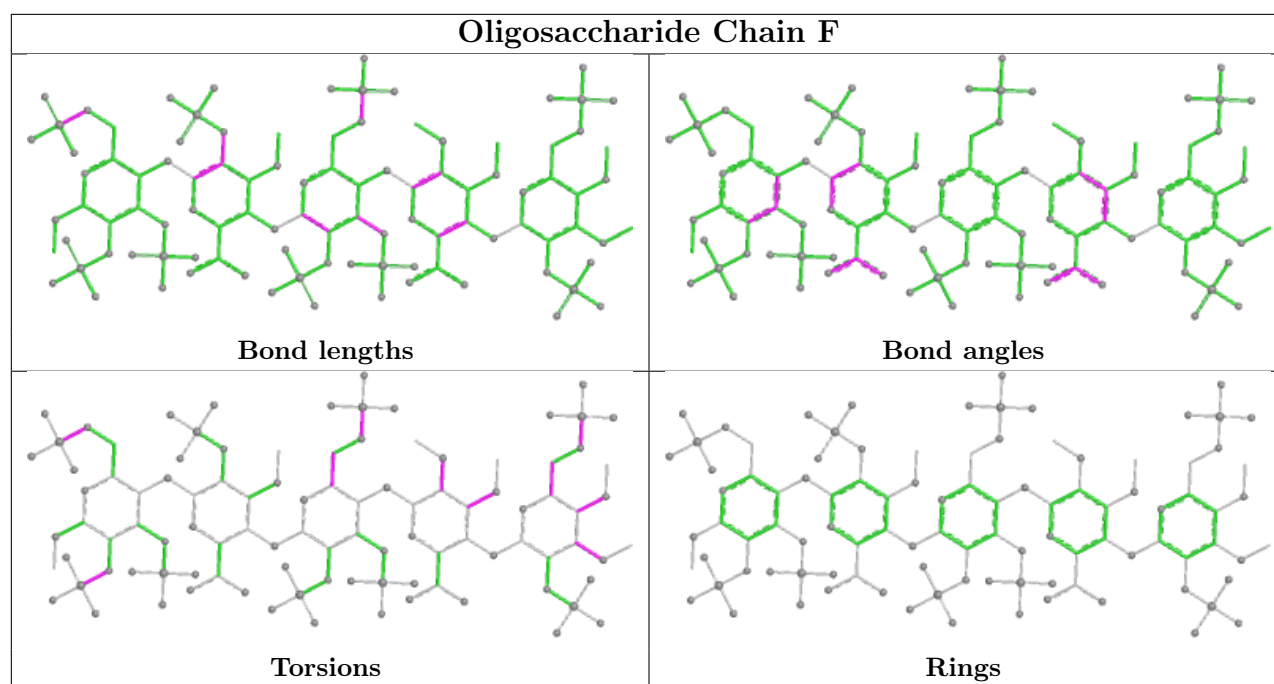
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	F	4	GU1	1	0
3	B	2	NAG	1	0
4	E	4	GU1	6	0
4	F	3	GU6	1	0
3	C	1	NAG	2	0
3	D	1	NAG	1	0
4	F	5	Z9H	5	0
3	B	1	NAG	1	0
3	D	2	NAG	1	0

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](#)

2 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$
5	NAG	L	801	1	14,14,15	1.37	2 (14%)	17,19,21	1.83	1 (5%)
5	NAG	I	821	1	14,14,15	1.29	1 (7%)	17,19,21	0.89	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
5	NAG	L	801	1	-	2/6/23/26	0/1/1/1
5	NAG	I	821	1	-	0/6/23/26	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	L	801	NAG	O7-C7	-3.75	1.14	1.23
5	I	821	NAG	O7-C7	-3.71	1.14	1.23
5	L	801	NAG	O5-C5	-2.07	1.39	1.43

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	L	801	NAG	C1-O5-C5	6.62	121.05	112.19
5	I	821	NAG	O5-C1-C2	-2.01	108.19	111.29

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	L	801	NAG	O5-C5-C6-O6
5	L	801	NAG	C4-C5-C6-O6

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	I	821	NAG	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	I	418/432 (96%)	0.06	14 (3%)	49 40	13, 43, 90, 126	0
1	L	423/432 (97%)	-0.09	16 (3%)	44 36	11, 33, 86, 133	0
All	All	841/864 (97%)	-0.02	30 (3%)	46 38	11, 38, 90, 133	0

All (30) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	L	38	GLN	4.5
1	I	385	SER	4.2
1	I	384	ALA	3.6
1	I	137	SER	3.4
1	L	431	VAL	3.3
1	L	39	LYS	3.3
1	L	37	GLU	3.1
1	L	40	ILE	3.0
1	L	36	SER	2.9
1	L	358	GLY	2.9
1	L	397	PRO	2.8
1	L	134	ALA	2.8
1	L	404	ALA	2.6
1	L	7	ILE	2.5
1	I	136	LYS	2.4
1	L	23	TYR	2.4
1	I	380	SER	2.4
1	I	357	GLU	2.4
1	I	134	ALA	2.4
1	I	38	GLN	2.4
1	I	360	ASP	2.3
1	I	7	ILE	2.3
1	L	403	LYS	2.3
1	L	34	GLU	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	I	26	PRO	2.2
1	L	33	ASP	2.1
1	I	135	ASN	2.1
1	I	15	ILE	2.0
1	L	27	GLU	2.0
1	I	37	GLU	2.0

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

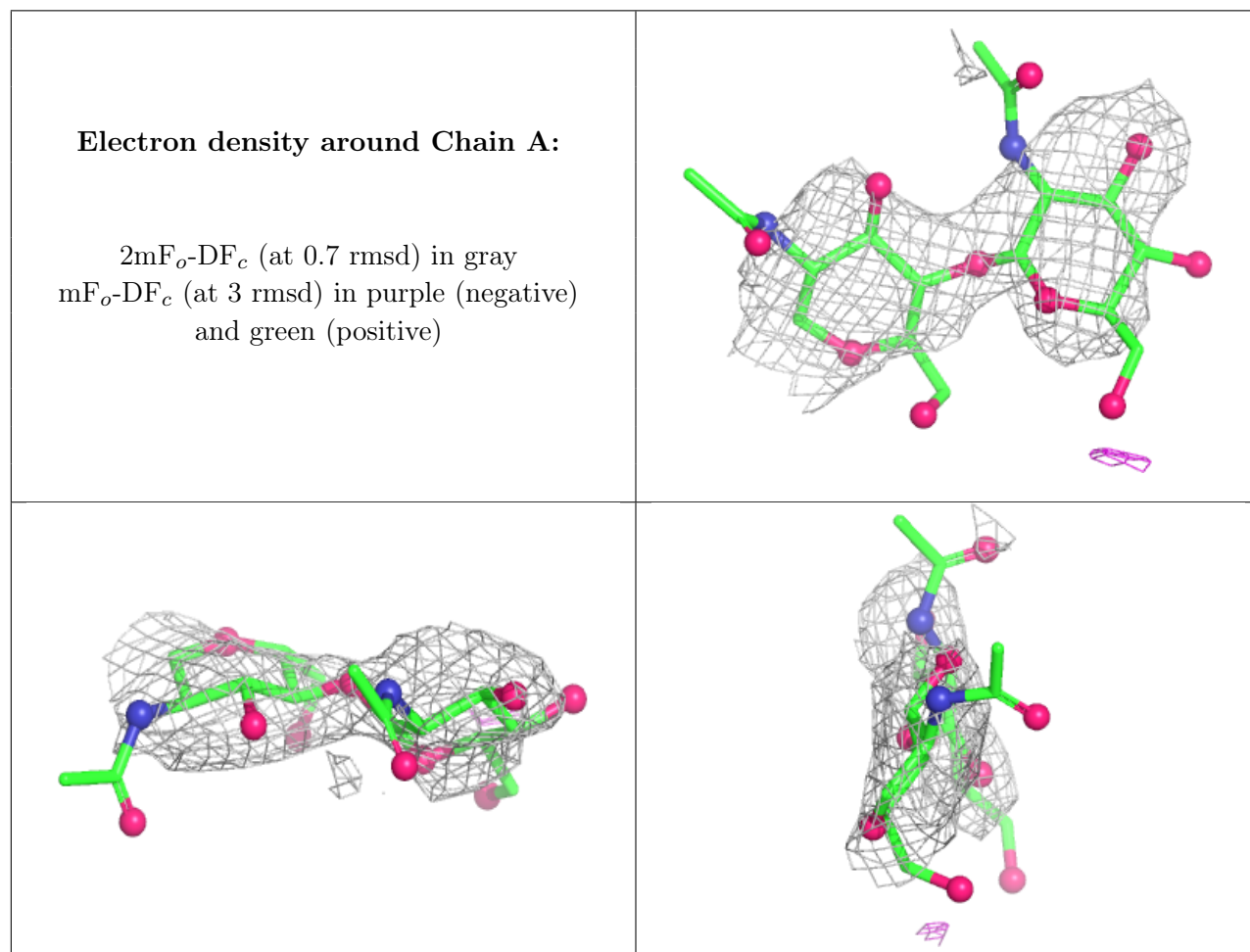
There are no non-standard protein/DNA/RNA residues in this entry.

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.

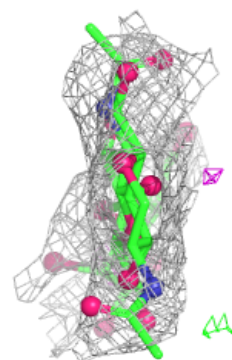
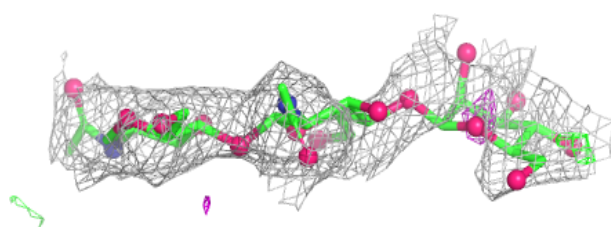
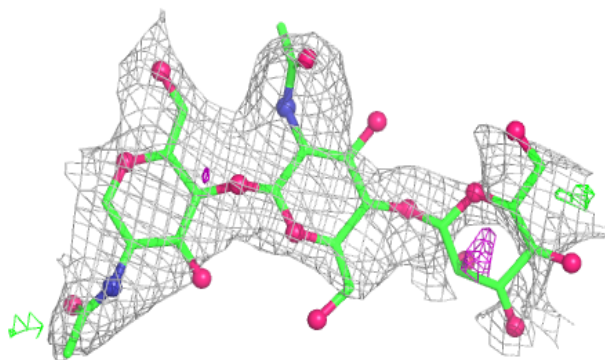
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	NAG	A	1	14/15	-	-	116,122,125,125	0
2	NAG	A	2	14/15	-	-	127,128,131,132	0
3	NAG	B	1	14/15	-	-	63,68,81,94	0
3	NAG	B	2	14/15	-	-	106,112,123,132	0
3	BMA	B	3	11/12	-	-	141,145,146,147	0
3	BMA	D	3	11/12	0.21	0.15	116,117,118,118	0
3	NAG	C	1	14/15	0.54	0.16	74,81,91,94	0
3	BMA	C	3	11/12	-	-	109,109,110,111	0
3	NAG	C	2	14/15	0.57	0.13	94,100,105,107	0
3	NAG	D	2	14/15	0.76	0.12	113,119,122,123	0
3	NAG	D	1	14/15	0.89	0.10	85,95,98,106	0
4	Z9L	E	1	25/25	-	-	49,57,66,69	0
4	Z9K	E	2	17/18	-	-	64,69,76,77	0
4	GU6	E	3	23/24	-	-	61,66,77,77	0
4	GU1	E	4	14/15	-	-	49,54,57,57	0
4	Z9H	E	5	21/22	-	-	42,56,60,61	0
4	Z9L	F	1	25/25	-	-	29,37,42,43	0
4	Z9K	F	2	17/18	-	-	29,34,43,45	0
4	GU6	F	3	23/24	-	-	29,36,41,43	0
4	GU1	F	4	14/15	-	-	39,46,48,49	0
4	Z9H	F	5	21/22	-	-	27,51,54,56	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.

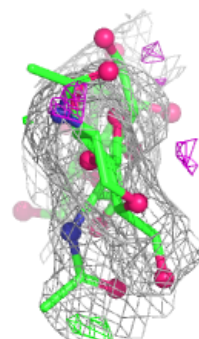
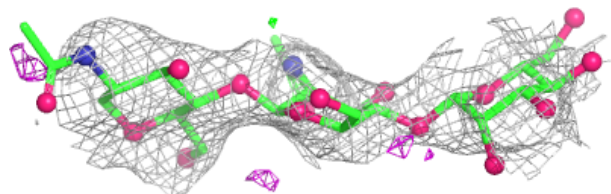
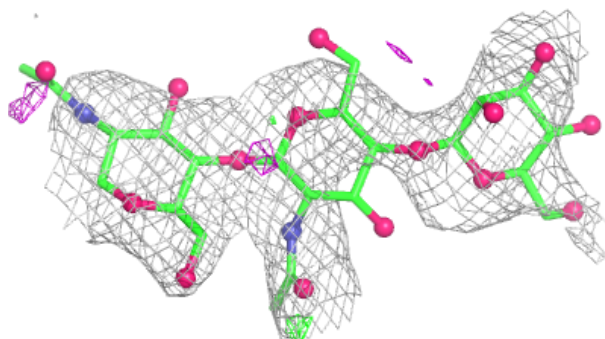


Electron density around Chain B:

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

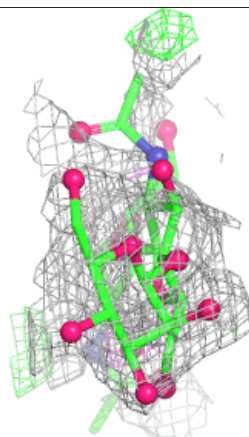
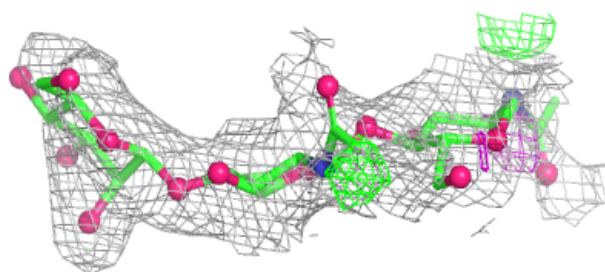
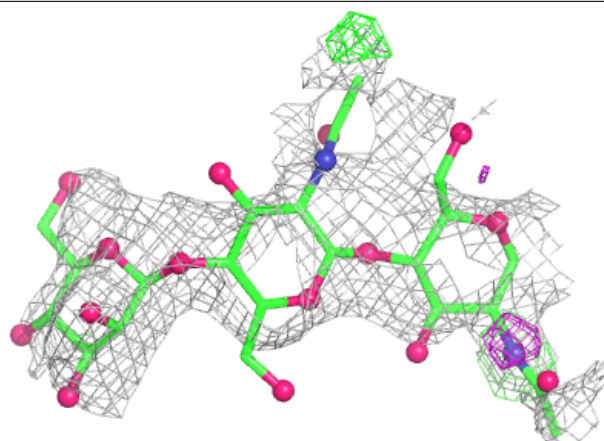
**Electron density around Chain C:**

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

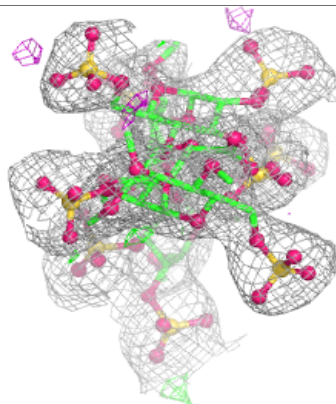
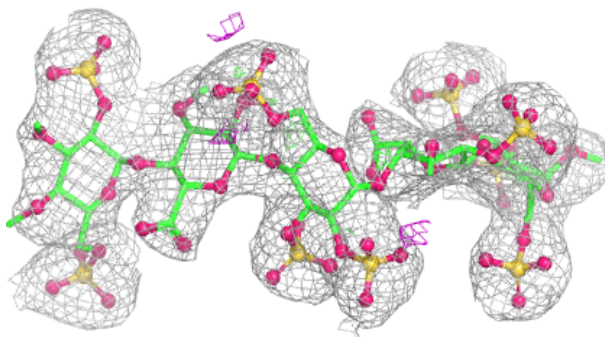
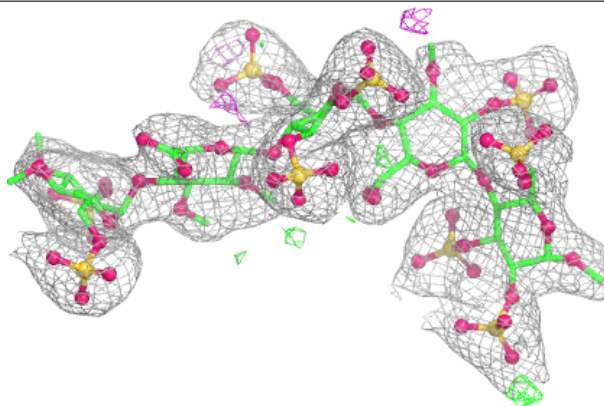


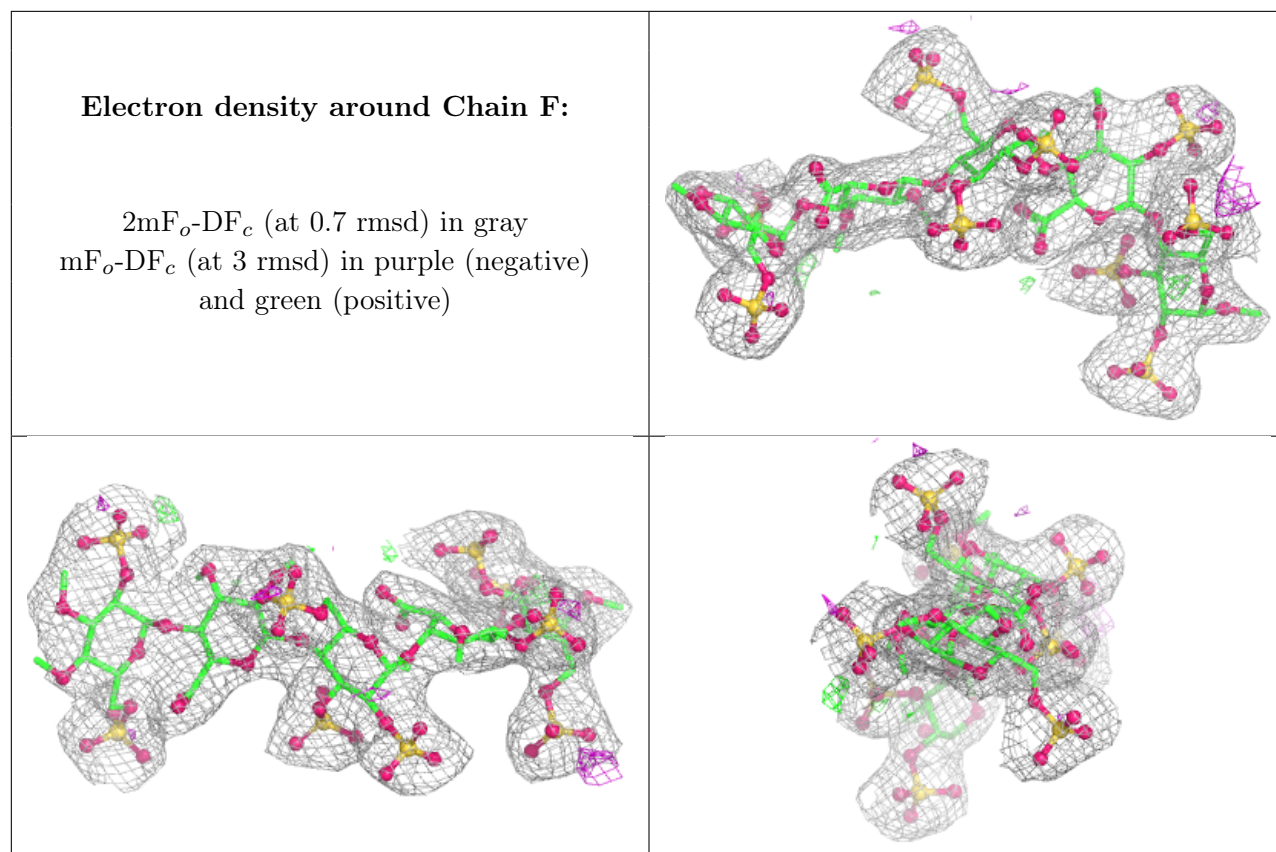
Electron density around Chain D:

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

**Electron density around Chain E:**

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





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	I	821	14/15	0.54	0.16	125,127,130,131	0
5	NAG	L	801	14/15	0.68	0.15	103,110,114,114	0

6.5 Other polymers [i](#)

There are no such residues in this entry.