



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 05:05 AM UTC

PDB ID : 1V2I / pdb_00001v2i
Title : Structure of the hemagglutinin-neuraminidase from human parainfluenza virus type III
Authors : Lawrence, M.C.; Borg, N.A.; Streltsov, V.A.; Pilling, P.A.; Epa, V.C.; Varghese, J.N.; McKimm-Breschkin, J.L.; Colman, P.M.
Deposited on : 2003-10-16
Resolution : 2.20 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

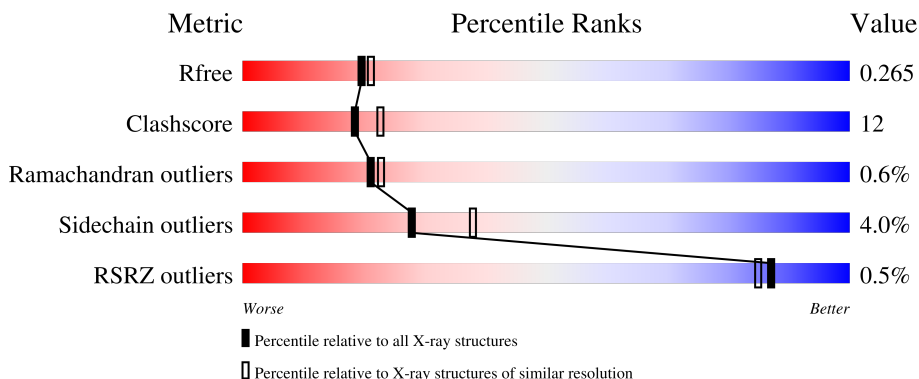
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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	6164 (2.20-2.20)
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (2.20-2.20)

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	431	73% 24% .
1	B	431	71% 26% .
2	C	5	20% 60% 20%
3	D	2	50% 50%
3	E	2	100%

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
4	NAG	A	3081	X	-	-	-

2 Entry composition [i](#)

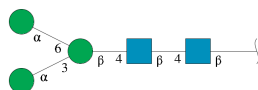
There are 7 unique types of molecules in this entry. The entry contains 7301 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 hemagglutinin-neuraminidase glycoprotein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	431	Total	C	N	O	S	0	1	0
			3382	2142	581	639	20			
1	B	431	Total	C	N	O	S	0	0	0
			3376	2138	579	639	20			

- Molecule 2 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
2	C	5	Total	C	N	O	0	0	0
			61	34	2	25			

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



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

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).



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

- Molecule 5 is CALCIUM ION (CCD ID: CA) (formula: Ca).

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

- Molecule 6 is PHOSPHATE ION (CCD ID: PO4) (formula: O₄P).



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

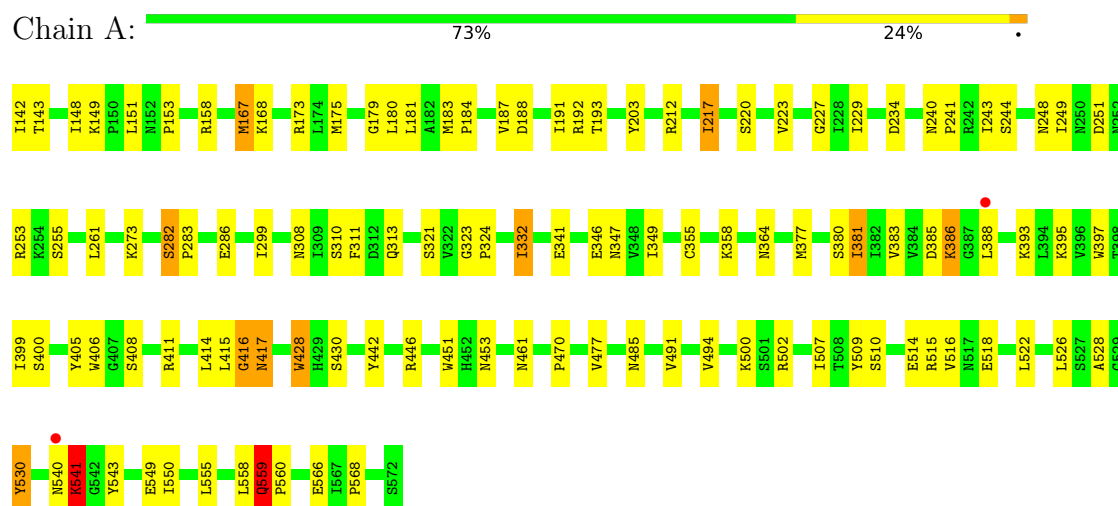
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	172	Total	O	0	0
			172	172		
7	B	200	Total	O	0	0
			200	200		

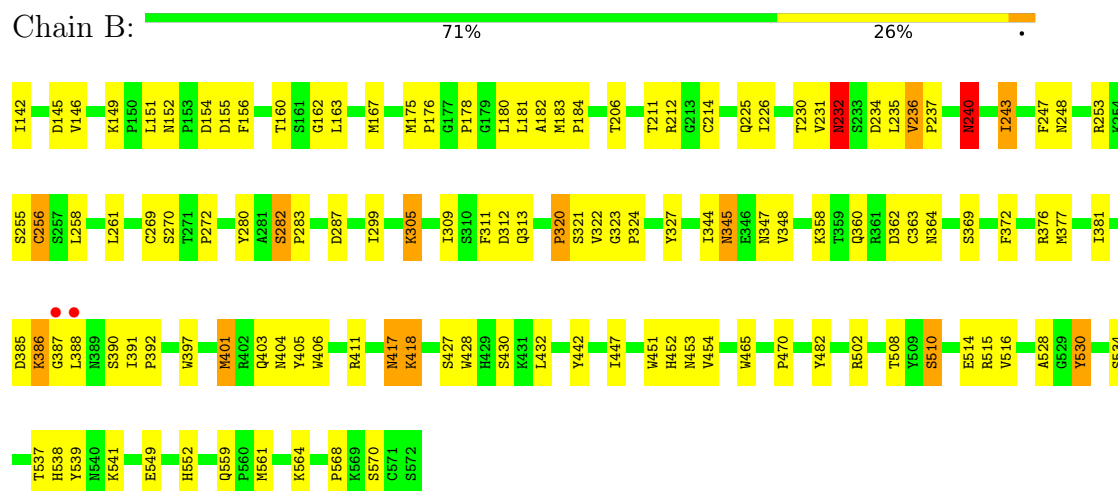
3 Residue-property plots

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.

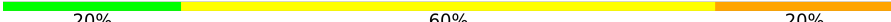
- Molecule 1: hemagglutinin-neuraminidase glycoprotein



- Molecule 1: hemagglutinin-neuraminidase glycoprotein



- Molecule 2: 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 C:  20% 60% 20%

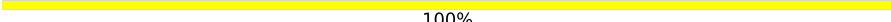


- Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain D:  50% 50%



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

Chain E:  100%



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	83.50Å 93.78Å 105.20Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	18.30 – 2.20 18.30 – 2.20	Depositor EDS
% Data completeness (in resolution range)	94.5 (18.30-2.20) 94.3 (18.30-2.20)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	0.15	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.06 (at 2.21Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.185 , 0.259 0.192 , 0.265	Depositor DCC
R_{free} test set	4020 reflections (9.99%)	wwPDB-VP
Wilson B-factor (Å ²)	31.6	Xtriage
Anisotropy	0.394	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 47.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	7301	wwPDB-VP
Average B, all atoms (Å ²)	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.71% 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: CA, NAG, PO4, BMA, MAN

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	0.68	0/3468	1.11	20/4730 (0.4%)
1	B	0.67	1/3457 (0.0%)	1.15	25/4715 (0.5%)
All	All	0.67	1/6925 (0.0%)	1.13	45/9445 (0.5%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	401	MET	SD-CE	-7.32	1.61	1.79

All (45) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	516	VAL	N-CA-C	8.76	119.59	111.45
1	B	454	VAL	N-CA-C	8.50	119.12	111.81
1	A	541	LYS	N-CA-C	-8.17	93.39	110.80
1	B	324	PRO	N-CA-C	7.11	122.69	111.38
1	A	332	ILE	N-CA-C	-6.96	98.55	108.58
1	A	516	VAL	N-CA-C	6.64	117.63	111.45
1	A	408	SER	N-CA-C	6.38	116.88	107.88
1	A	324	PRO	N-CA-C	6.33	120.91	111.41
1	A	514	GLU	N-CA-C	6.33	118.81	108.55
1	B	256	CYS	N-CA-C	6.28	119.35	110.50
1	A	193	THR	CB-CA-C	-6.24	106.77	111.20
1	A	282	SER	N-CA-C	6.22	117.50	109.72
1	A	509	TYR	N-CA-C	-6.01	97.50	108.02
1	B	390	SER	N-CA-C	6.01	118.80	109.60
1	B	232	ASN	N-CA-C	5.98	121.33	113.20
1	B	369	SER	CA-C-N	5.88	125.75	119.28
1	B	369	SER	C-N-CA	5.88	125.75	119.28
1	B	240	ASN	CA-C-N	5.88	125.81	119.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	240	ASN	C-N-CA	5.88	125.81	119.76
1	B	418	LYS	N-CA-C	5.87	119.29	109.95
1	A	234	ASP	N-CA-C	-5.84	105.34	112.88
1	B	211	THR	N-CA-C	5.72	117.52	111.28
1	A	430	SER	N-CA-C	5.72	119.52	112.54
1	A	417	ASN	N-CA-CB	-5.64	107.74	114.17
1	A	428	TRP	N-CA-C	5.63	118.18	111.71
1	B	404	ASN	N-CA-C	5.62	117.95	109.23
1	A	559	GLN	N-CA-C	5.59	119.24	108.45
1	A	299	ILE	N-CA-C	5.58	116.77	108.46
1	B	282	SER	N-CA-C	5.49	117.58	109.62
1	B	514	GLU	N-CA-C	5.44	117.36	108.55
1	B	305	LYS	N-CA-C	-5.43	102.49	110.52
1	A	179	GLY	N-CA-C	-5.42	101.45	111.04
1	B	320	PRO	N-CA-C	-5.39	102.98	111.34
1	A	491	VAL	N-CA-C	5.38	116.45	108.65
1	A	286	GLU	N-CA-C	-5.31	102.62	110.48
1	A	149	LYS	N-CA-C	5.30	112.90	108.13
1	B	508	THR	N-CA-C	5.20	117.29	109.23
1	B	299	ILE	N-CA-C	5.14	116.12	108.46
1	B	312	ASP	N-CA-C	-5.14	105.86	111.82
1	B	388	LEU	N-CA-C	5.14	121.74	110.80
1	B	530	TYR	N-CA-C	5.11	117.50	110.35
1	B	214	CYS	N-CA-C	-5.08	106.76	113.17
1	B	430	SER	N-CA-C	5.07	118.72	112.54
1	B	428	TRP	N-CA-C	5.07	117.54	111.71
1	A	321	SER	N-CA-C	5.07	119.22	113.19

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	3382	0	3349	74	0
1	B	3376	0	3345	95	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	61	0	52	2	0
3	D	28	0	25	1	0
3	E	28	0	25	0	0
4	A	28	0	26	1	0
4	B	14	0	13	0	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
6	A	5	0	0	0	0
6	B	5	0	0	0	0
7	A	172	0	0	4	0
7	B	200	0	0	6	0
All	All	7301	0	6835	165	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 12.

All (165) 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:417:ASN:HD22	1:B:417:ASN:H	1.15	0.92
1:B:510:SER:HB2	1:B:515:ARG:HA	1.57	0.87
1:B:417:ASN:H	1:B:417:ASN:ND2	1.77	0.81
1:A:142:ILE:HG13	1:A:143:THR:HG23	1.62	0.79
1:A:347:ASN:HD22	1:A:364:ASN:HD21	1.27	0.79
1:A:248:ASN:HB3	1:A:251:ASP:OD2	1.86	0.76
1:B:417:ASN:HD22	1:B:417:ASN:N	1.81	0.76
1:B:403:GLN:HE21	1:B:447:ILE:H	1.31	0.76
1:A:446:ARG:HH11	1:A:446:ARG:HB3	1.52	0.74
1:A:358:LYS:HD2	1:A:470:PRO:HG2	1.72	0.71
1:A:183:MET:HE2	1:B:181:LEU:H	1.56	0.71
1:B:360:GLN:HE21	1:B:364:ASN:ND2	1.89	0.70
1:A:241:PRO:HG2	7:B:5308:HOH:O	1.91	0.70
1:A:386:LYS:N	1:A:386:LYS:HD3	2.07	0.69
1:A:310:SER:OG	1:A:395:LYS:HG2	1.93	0.69
1:B:182:ALA:H	1:B:225:GLN:HE22	1.41	0.69
1:B:360:GLN:HE21	1:B:364:ASN:HD21	1.39	0.69
1:A:446:ARG:HB3	1:A:446:ARG:NH1	2.06	0.68
1:A:217:ILE:H	1:A:217:ILE:HD13	1.60	0.67
1:B:231:VAL:CG1	1:B:235:LEU:HA	2.26	0.66
1:B:427:SER:HB3	7:B:5235:HOH:O	1.95	0.66
1:A:541:LYS:HE3	1:A:541:LYS:HA	1.79	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:231:VAL:HG13	1:B:235:LEU:HA	1.78	0.65
1:B:184:PRO:HD3	1:B:559:GLN:OE1	1.97	0.64
1:A:261:LEU:HB2	1:A:332:ILE:HD11	1.79	0.64
1:A:142:ILE:HG23	1:A:143:THR:H	1.62	0.63
1:B:212:ARG:O	1:B:212:ARG:HG3	2.01	0.61
1:A:212:ARG:HH11	1:A:212:ARG:HG2	1.66	0.61
1:B:231:VAL:HG11	1:B:235:LEU:HD23	1.81	0.61
1:B:451:TRP:CH2	1:B:453:ASN:HB2	2.36	0.61
1:A:151:LEU:C	1:A:151:LEU:HD23	2.28	0.59
1:B:149:LYS:HE3	7:B:5353:HOH:O	2.03	0.59
1:B:403:GLN:NE2	1:B:447:ILE:H	1.99	0.59
1:A:243:ILE:HD12	1:A:244:SER:H	1.68	0.59
1:A:323:GLY:HA3	1:A:411:ARG:HB3	1.85	0.59
1:B:162:GLY:C	1:B:163:LEU:HD22	2.30	0.56
1:B:175:MET:HE1	1:B:237:PRO:HD2	1.87	0.56
1:A:349:ILE:HG13	7:A:5289:HOH:O	2.05	0.56
1:A:451:TRP:CZ2	2:C:2:NAG:H5	2.40	0.56
1:B:552:HIS:HE1	7:B:5384:HOH:O	1.88	0.55
1:B:226:ILE:HB	1:B:243:ILE:HD13	1.88	0.55
1:A:173:ARG:NH2	7:A:5329:HOH:O	2.38	0.55
1:A:180:LEU:HD23	1:B:182:ALA:HA	1.89	0.55
1:B:243:ILE:HD12	1:B:243:ILE:N	2.22	0.55
1:B:386:LYS:CG	1:B:387:GLY:N	2.69	0.55
1:B:386:LYS:HG2	1:B:387:GLY:N	2.21	0.54
1:A:530:TYR:C	1:A:530:TYR:CD2	2.85	0.54
1:B:167:MET:HE2	1:B:568:PRO:HA	1.89	0.54
1:A:142:ILE:HG23	1:A:143:THR:N	2.22	0.54
1:B:451:TRP:CZ2	1:B:453:ASN:HB2	2.43	0.54
1:A:515:ARG:HD2	1:A:518:GLU:OE1	2.07	0.53
1:A:428:TRP:CD2	1:A:470:PRO:HA	2.44	0.53
1:B:175:MET:HE2	1:B:564:LYS:CB	2.39	0.53
1:A:167:MET:HG2	1:A:568:PRO:O	2.10	0.52
1:A:510:SER:HB2	1:A:515:ARG:HA	1.91	0.52
1:B:167:MET:HG2	1:B:570:SER:HB2	1.91	0.52
1:B:226:ILE:HB	1:B:243:ILE:CD1	2.39	0.52
1:B:323:GLY:HA3	1:B:411:ARG:HB3	1.92	0.51
1:B:152:ASN:ND2	1:B:155:ASP:OD2	2.43	0.51
1:A:386:LYS:N	1:A:386:LYS:CD	2.72	0.50
1:B:175:MET:CE	1:B:564:LYS:HB2	2.40	0.50
1:A:148:ILE:HD13	1:A:229:ILE:HG22	1.94	0.50
1:B:358:LYS:HA	1:B:362:ASP:OD2	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:283:PRO:HB3	1:A:341:GLU:CD	2.35	0.50
1:B:348:VAL:HG12	1:B:401:MET:HB3	1.94	0.50
1:B:175:MET:HE2	1:B:564:LYS:HB2	1.94	0.50
1:B:386:LYS:CG	1:B:387:GLY:H	2.24	0.49
1:B:417:ASN:ND2	1:B:417:ASN:N	2.46	0.49
1:A:451:TRP:CH2	1:A:453:ASN:HB2	2.47	0.49
1:B:151:LEU:HD23	1:B:151:LEU:C	2.38	0.49
1:A:415:LEU:O	1:A:416:GLY:C	2.55	0.49
4:A:3081:NAG:H83	4:A:3081:NAG:O3	2.13	0.49
1:B:372:PHE:HA	7:B:5267:HOH:O	2.11	0.49
1:B:377:MET:HG3	1:B:406:TRP:CZ2	2.47	0.49
1:B:232:ASN:ND2	1:B:236:VAL:H	2.10	0.49
1:B:376:ARG:CG	1:B:401:MET:HE1	2.43	0.49
1:B:385:ASP:O	1:B:392:PRO:HA	2.13	0.49
1:B:386:LYS:HB2	1:B:392:PRO:HB3	1.95	0.49
1:B:311:PHE:HB3	1:B:313:GLN:O	2.13	0.48
1:A:192:ARG:HH11	1:A:192:ARG:HG3	1.77	0.48
1:A:347:ASN:ND2	1:A:364:ASN:HD21	2.02	0.48
1:B:432:LEU:HD23	1:B:452:HIS:CD2	2.49	0.48
1:B:502:ARG:HB3	1:B:528:ALA:O	2.14	0.48
1:B:530:TYR:C	1:B:530:TYR:CD2	2.92	0.48
1:A:555:LEU:HD12	1:B:561:MET:HE1	1.96	0.47
1:B:397:TRP:CD2	1:B:442:TYR:HB3	2.49	0.47
1:B:269:CYS:HA	1:B:320:PRO:HG2	1.96	0.47
1:B:377:MET:HG3	1:B:406:TRP:CE2	2.49	0.47
1:B:405:TYR:O	1:B:406:TRP:C	2.57	0.47
1:A:383:VAL:HG12	1:A:385:ASP:OD1	2.15	0.47
1:A:183:MET:HE1	1:B:181:LEU:HB2	1.95	0.47
1:B:255:SER:O	1:B:320:PRO:HB2	2.15	0.47
1:B:287:ASP:CG	1:B:305:LYS:HD2	2.40	0.47
1:A:184:PRO:HG3	1:A:191:ILE:HG13	1.97	0.47
1:A:526:LEU:HD11	1:A:550:ILE:HG23	1.97	0.47
1:B:261:LEU:HG	1:B:327:TYR:CE1	2.50	0.47
1:B:537:THR:HA	1:B:541:LYS:O	2.15	0.47
1:B:538:HIS:O	1:B:539:TYR:HB2	2.15	0.47
1:B:232:ASN:HD21	1:B:236:VAL:HB	1.79	0.46
1:A:377:MET:HG3	1:A:406:TRP:CZ2	2.51	0.46
1:B:321:SER:O	1:B:322:VAL:HB	2.15	0.46
1:B:151:LEU:HD11	1:B:156:PHE:CD2	2.51	0.46
1:A:381:ILE:CD1	1:A:399:ILE:HD11	2.47	0.45
1:A:393:LYS:HG2	7:A:5265:HOH:O	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:223:VAL:HG21	1:B:178:PRO:HB3	1.99	0.45
1:A:515:ARG:CD	1:A:518:GLU:OE1	2.64	0.45
1:B:232:ASN:C	1:B:232:ASN:HD22	2.25	0.45
1:A:181:LEU:H	1:B:183:MET:CE	2.29	0.45
1:A:397:TRP:CD2	1:A:442:TYR:HB3	2.52	0.45
1:B:391:ILE:HG23	1:B:392:PRO:HD2	1.98	0.45
1:B:175:MET:HG3	1:B:564:LYS:O	2.17	0.44
1:A:428:TRP:CG	1:A:470:PRO:HA	2.52	0.44
1:A:153:PRO:HB3	1:A:485:ASN:C	2.42	0.44
1:A:451:TRP:CZ2	1:A:453:ASN:HB2	2.53	0.44
1:A:502:ARG:HB3	1:A:528:ALA:O	2.17	0.44
1:B:154:ASP:OD1	1:B:418:LYS:NZ	2.50	0.44
1:B:280:TYR:CD1	1:B:372:PHE:HD2	2.36	0.44
1:B:482:TYR:CD1	1:B:534:SER:HA	2.52	0.44
2:C:1:NAG:O6	2:C:2:NAG:H82	2.18	0.44
1:B:145:ASP:OD1	1:B:230:THR:HG22	2.18	0.44
1:A:323:GLY:HA2	7:A:5260:HOH:O	2.17	0.44
1:B:256:CYS:O	1:B:322:VAL:HA	2.18	0.44
1:B:465:TRP:C	1:B:465:TRP:CD1	2.96	0.43
1:A:175:MET:HE1	1:A:543:TYR:CD2	2.53	0.43
1:A:227:GLY:HA3	1:A:240:ASN:O	2.18	0.43
1:B:391:ILE:HD12	1:B:391:ILE:N	2.32	0.43
1:A:346:GLU:OE2	1:A:400:SER:OG	2.32	0.43
1:B:167:MET:CG	1:B:570:SER:HB2	2.48	0.43
1:B:182:ALA:H	1:B:225:GLN:NE2	2.14	0.43
1:B:348:VAL:HG22	1:B:364:ASN:HD22	1.82	0.43
1:B:381:ILE:HD13	1:B:381:ILE:HA	1.88	0.43
1:A:217:ILE:HG12	1:A:217:ILE:O	2.18	0.43
1:A:273:LYS:HA	1:A:273:LYS:HD3	1.76	0.42
1:B:287:ASP:OD1	1:B:305:LYS:HD2	2.19	0.42
1:A:549:GLU:OE2	1:A:560:PRO:HG3	2.20	0.42
1:B:344:ILE:HG22	1:B:345:ASN:N	2.34	0.42
1:A:251:ASP:OD2	1:A:253:ARG:NH1	2.51	0.42
1:B:391:ILE:HG23	1:B:392:PRO:CD	2.49	0.42
1:A:220:SER:O	1:A:249:ILE:HA	2.20	0.42
1:B:282:SER:HA	1:B:283:PRO:HD3	1.95	0.42
1:A:405:TYR:O	1:A:406:TRP:C	2.62	0.42
1:A:192:ARG:HG3	1:A:192:ARG:NH1	2.35	0.42
1:A:203:TYR:CD1	1:A:203:TYR:C	2.97	0.42
1:A:355:CYS:HB3	1:A:358:LYS:HG3	2.01	0.42
1:A:243:ILE:HD12	1:B:240:ASN:ND2	2.34	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:282:SER:HA	1:A:283:PRO:HD3	1.91	0.41
1:A:559:GLN:HA	1:A:560:PRO:HD3	1.75	0.41
3:D:1:NAG:H61	3:D:2:NAG:C8	2.50	0.41
1:A:311:PHE:HB3	1:A:313:GLN:O	2.20	0.41
1:B:253:ARG:HG3	7:B:5314:HOH:O	2.19	0.41
1:A:541:LYS:HE2	1:A:566:GLU:OE1	2.19	0.41
1:A:212:ARG:HG2	1:A:212:ARG:NH1	2.34	0.41
1:B:163:LEU:HD22	1:B:163:LEU:N	2.36	0.41
1:A:187:VAL:O	1:A:188:ASP:HB2	2.21	0.41
1:B:176:PRO:O	1:B:236:VAL:HG11	2.20	0.41
1:B:270:SER:OG	1:B:272:PRO:HD3	2.20	0.41
1:B:344:ILE:CG2	1:B:345:ASN:N	2.84	0.41
1:B:347:ASN:HA	1:B:364:ASN:HD21	1.86	0.41
1:A:446:ARG:HH11	1:A:446:ARG:CB	2.29	0.41
1:B:206:THR:HB	1:B:258:LEU:HD11	2.03	0.41
1:B:309:ILE:HB	1:B:311:PHE:CE1	2.56	0.41
1:B:247:PHE:O	1:B:248:ASN:C	2.64	0.40
1:A:494:VAL:HG22	1:A:507:ILE:HG12	2.03	0.40
1:B:363:CYS:SG	1:B:470:PRO:HG3	2.61	0.40
1:A:243:ILE:CD1	1:A:244:SER:H	2.34	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	430/431 (100%)	394 (92%)	33 (8%)	3 (1%)	18	19
1	B	429/431 (100%)	396 (92%)	31 (7%)	2 (0%)	24	27
All	All	859/862 (100%)	790 (92%)	64 (8%)	5 (1%)	21	23

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	386	LYS
1	B	234	ASP
1	A	416	GLY
1	A	522	LEU
1	A	540	ASN

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	391/390 (100%)	372 (95%)	19 (5%)	22	29
1	B	390/390 (100%)	378 (97%)	12 (3%)	35	48
All	All	781/780 (100%)	750 (96%)	31 (4%)	28	38

All (31) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	158	ARG
1	A	167	MET
1	A	168	LYS
1	A	217	ILE
1	A	255	SER
1	A	308	ASN
1	A	380	SER
1	A	381	ILE
1	A	386	LYS
1	A	388	LEU
1	A	414	LEU
1	A	417	ASN
1	A	461	ASN
1	A	477	VAL
1	A	500	LYS
1	A	530	TYR
1	A	541	LYS
1	A	558	LEU
1	A	559	GLN

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Mol	Chain	Res	Type
1	B	142	ILE
1	B	146	VAL
1	B	160	THR
1	B	180	LEU
1	B	232	ASN
1	B	236	VAL
1	B	240	ASN
1	B	243	ILE
1	B	345	ASN
1	B	417	ASN
1	B	510	SER
1	B	549	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	250	ASN
1	A	262	ASN
1	A	347	ASN
1	A	453	ASN
1	A	461	ASN
1	A	504	ASN
1	A	540	ASN
1	A	552	HIS
1	B	225	GLN
1	B	232	ASN
1	B	240	ASN
1	B	245	HIS
1	B	345	ASN
1	B	347	ASN
1	B	360	GLN
1	B	364	ASN
1	B	403	GLN
1	B	417	ASN
1	B	461	ASN
1	B	552	HIS

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	NAG	C	1	2,1	14,14,15	0.53	0	17,19,21	0.85	0
2	NAG	C	2	2	14,14,15	0.58	0	17,19,21	0.79	1 (5%)
2	BMA	C	3	2	11,11,12	0.54	0	15,15,17	0.70	0
2	MAN	C	4	2	11,11,12	0.45	0	15,15,17	0.67	1 (6%)
2	MAN	C	5	2	11,11,12	0.70	0	15,15,17	0.87	1 (6%)
3	NAG	D	1	3,1	14,14,15	0.57	0	17,19,21	0.78	1 (5%)
3	NAG	D	2	3	14,14,15	0.58	0	17,19,21	0.72	0
3	NAG	E	1	3,1	14,14,15	0.71	0	17,19,21	1.08	1 (5%)
3	NAG	E	2	3	14,14,15	0.58	0	17,19,21	1.02	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
2	NAG	C	1	2,1	-	4/6/23/26	0/1/1/1
2	NAG	C	2	2	-	1/6/23/26	0/1/1/1
2	BMA	C	3	2	-	0/2/19/22	0/1/1/1
2	MAN	C	4	2	-	0/2/19/22	0/1/1/1
2	MAN	C	5	2	-	0/2/19/22	0/1/1/1
3	NAG	D	1	3,1	-	2/6/23/26	0/1/1/1
3	NAG	D	2	3	-	3/6/23/26	0/1/1/1
3	NAG	E	1	3,1	-	4/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	E	2	3	-	4/6/23/26	0/1/1/1

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	5	MAN	C1-O5-C5	2.78	115.91	112.19
3	E	2	NAG	C2-N2-C7	-2.74	119.23	122.90
3	E	1	NAG	C3-C4-C5	2.51	114.78	110.23
3	D	1	NAG	C2-N2-C7	-2.26	119.88	122.90
2	C	4	MAN	C1-O5-C5	2.23	115.17	112.19
2	C	2	NAG	C2-N2-C7	-2.13	120.04	122.90

There are no chirality outliers.

All (18) torsion outliers are listed below:

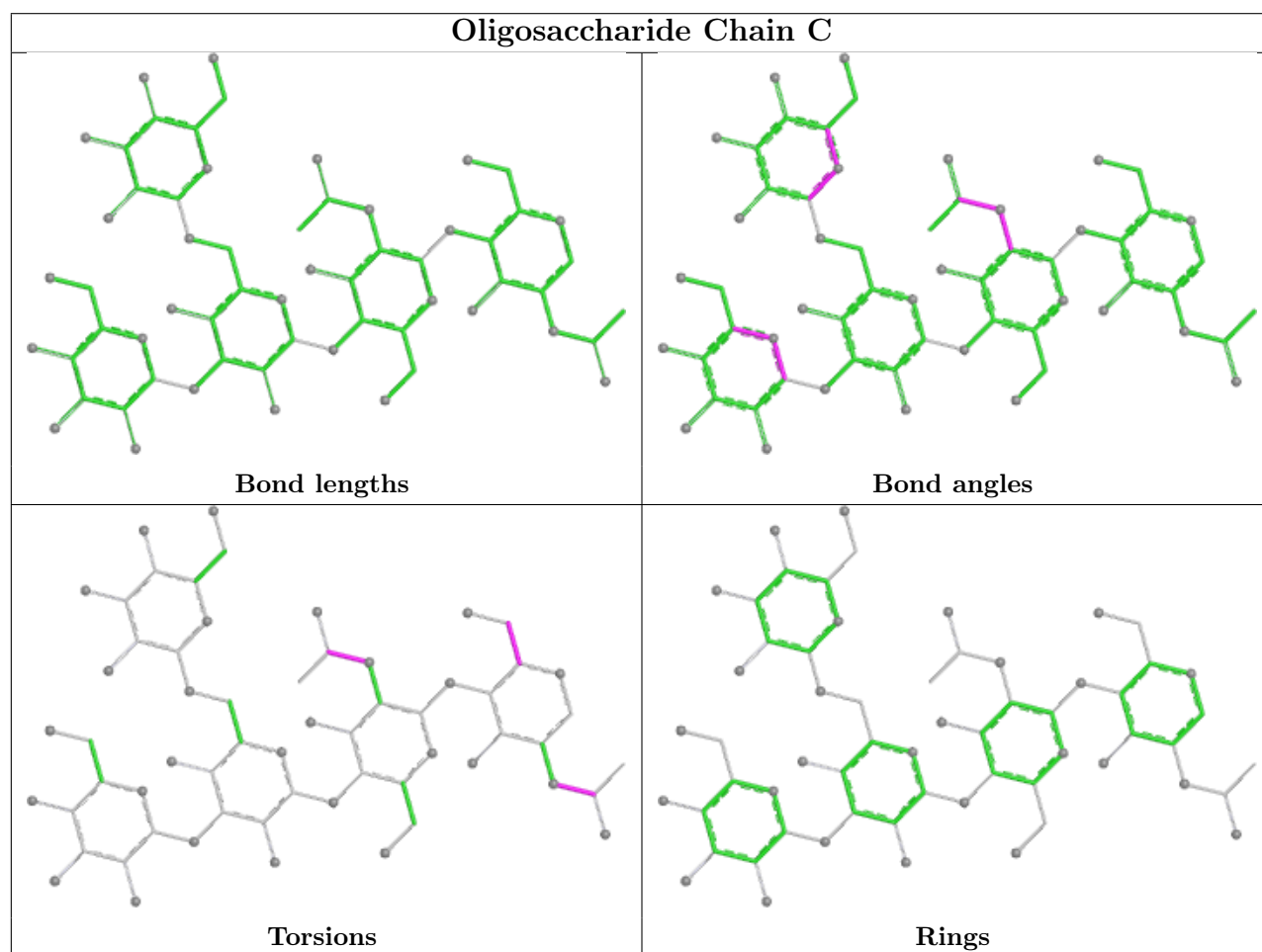
Mol	Chain	Res	Type	Atoms
3	D	1	NAG	C8-C7-N2-C2
3	D	1	NAG	O7-C7-N2-C2
3	E	2	NAG	C8-C7-N2-C2
3	E	2	NAG	O7-C7-N2-C2
3	E	1	NAG	C8-C7-N2-C2
3	E	1	NAG	O7-C7-N2-C2
3	E	1	NAG	O5-C5-C6-O6
2	C	1	NAG	O5-C5-C6-O6
3	E	1	NAG	C4-C5-C6-O6
2	C	1	NAG	C4-C5-C6-O6
3	D	2	NAG	C8-C7-N2-C2
3	D	2	NAG	O5-C5-C6-O6
2	C	1	NAG	C8-C7-N2-C2
3	D	2	NAG	O7-C7-N2-C2
2	C	1	NAG	O7-C7-N2-C2
3	E	2	NAG	C4-C5-C6-O6
3	E	2	NAG	O5-C5-C6-O6
2	C	2	NAG	C8-C7-N2-C2

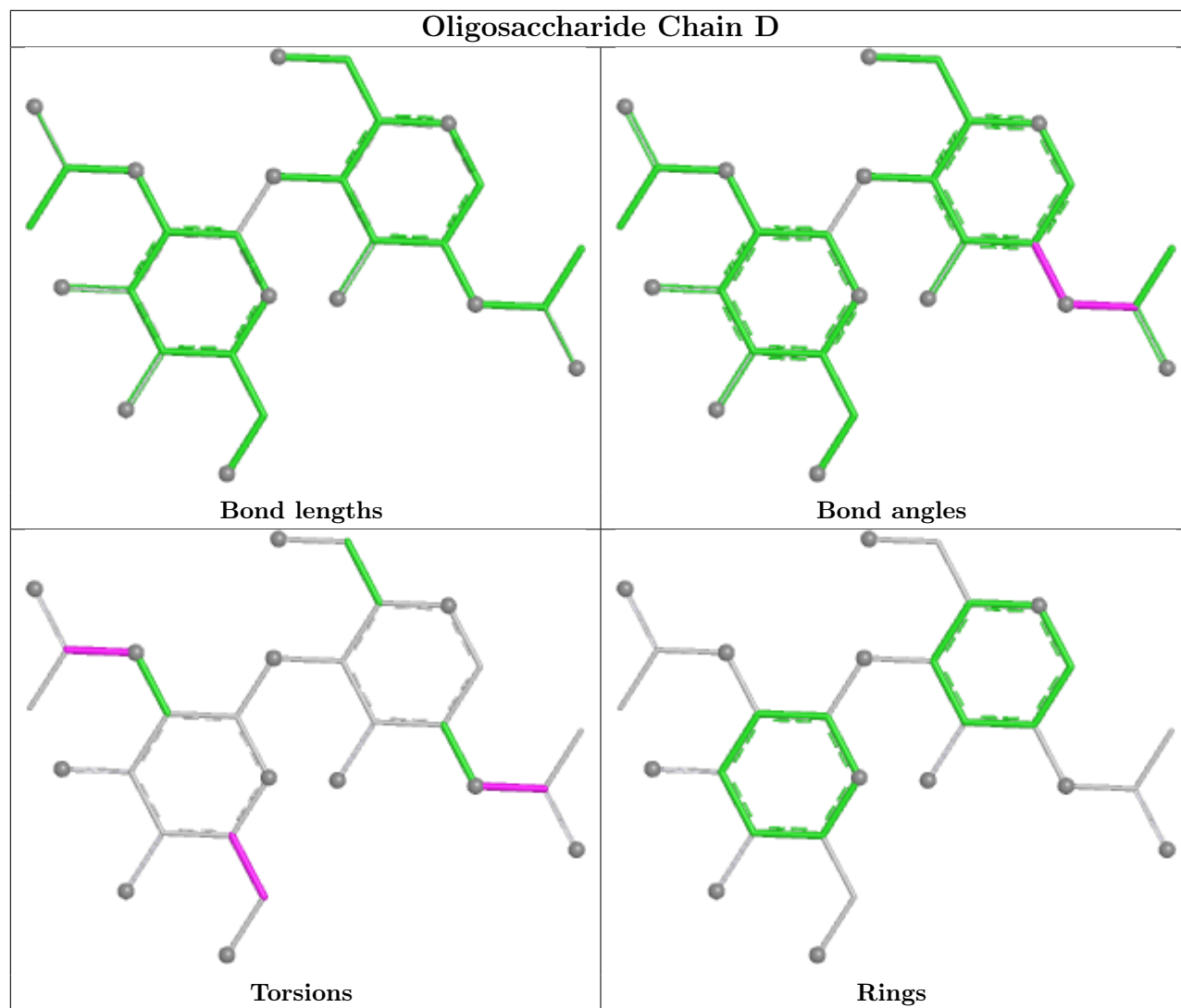
There are no ring outliers.

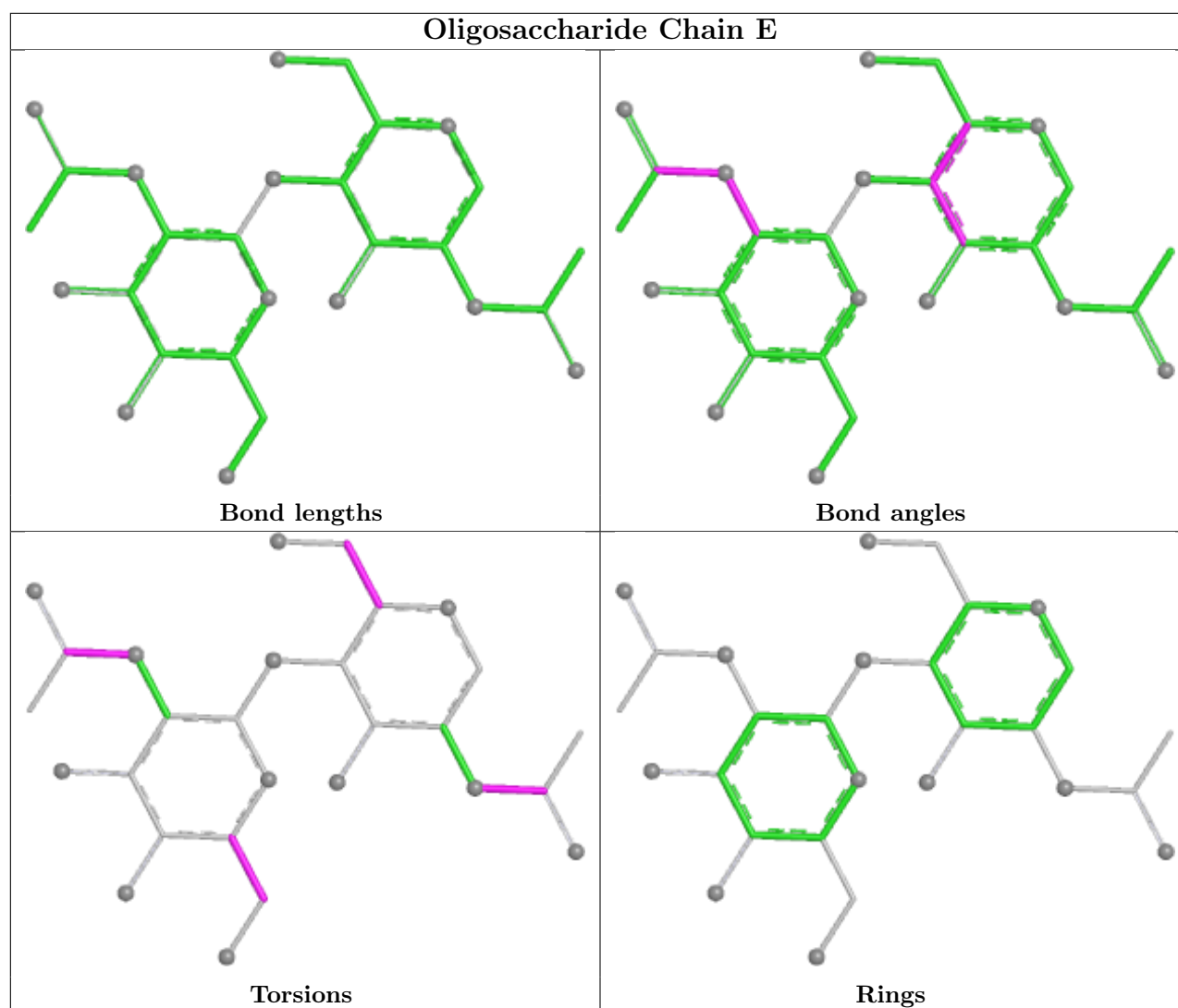
4 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	1	NAG	1	0
3	D	1	NAG	1	0
2	C	2	NAG	2	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](#)

Of 7 ligands modelled in this entry, 2 are monoatomic - leaving 5 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	NAG	B	3081	1	14,14,15	0.64	0	17,19,21	0.91	2 (11%)
6	PO4	A	2001	-	4,4,4	1.63	0	6,6,6	0.53	0
4	NAG	A	3081	1	14,14,15	0.74	1 (7%)	17,19,21	0.89	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	PO4	B	2002	-	4,4,4	1.54	1 (25%)	6,6,6	0.46	0
4	NAG	A	5231	1	14,14,15	0.72	0	17,19,21	0.76	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
4	NAG	B	3081	1	-	2/6/23/26	0/1/1/1
4	NAG	A	5231	1	-	2/6/23/26	0/1/1/1
4	NAG	A	3081	1	1/1/5/7	2/6/23/26	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	2002	PO4	P-O3	-2.11	1.48	1.54
4	A	3081	NAG	C1-C2	2.09	1.55	1.52

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	3081	NAG	C2-N2-C7	-2.18	119.97	122.90
4	A	3081	NAG	C1-C2-N2	-2.07	107.17	110.43
4	B	3081	NAG	C4-C3-C2	-2.01	108.07	111.02

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	A	3081	NAG	C1

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	3081	NAG	C8-C7-N2-C2
4	A	3081	NAG	O7-C7-N2-C2
4	B	3081	NAG	O5-C5-C6-O6
4	A	5231	NAG	C8-C7-N2-C2
4	A	5231	NAG	O7-C7-N2-C2
4	B	3081	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
4	A	3081	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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	431/431 (100%)	-0.48	2 (0%) 87 85	16, 29, 53, 85	1 (0%)
1	B	431/431 (100%)	-0.37	2 (0%) 87 85	18, 30, 60, 99	1 (0%)
All	All	862/862 (100%)	-0.42	4 (0%) 87 85	16, 30, 56, 99	2 (0%)

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	388	LEU	4.5
1	B	388	LEU	3.1
1	B	387	GLY	2.7
1	A	540	ASN	2.5

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.

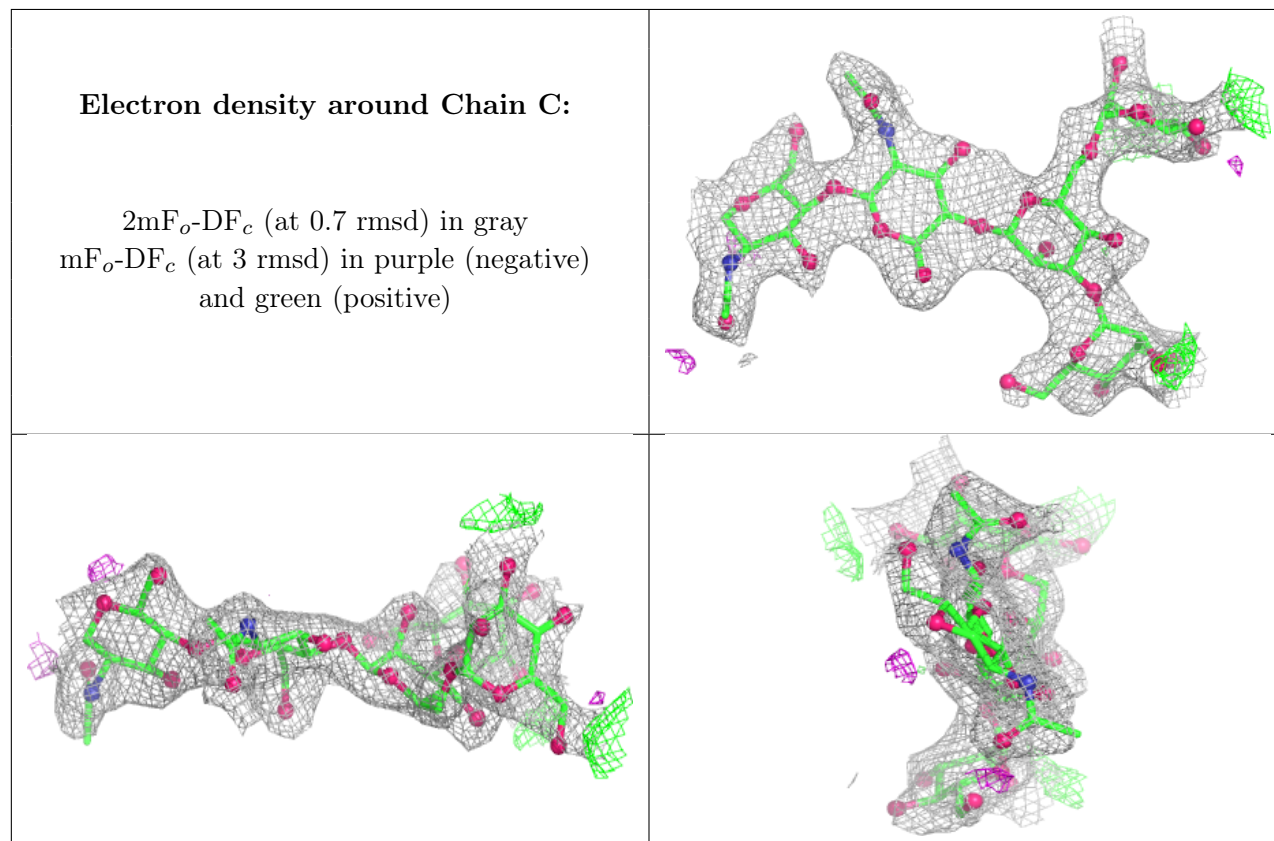
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	NAG	E	1	14/15	0.70	0.12	54,61,68,72	0
3	NAG	E	2	14/15	0.70	0.11	83,87,88,89	0
2	MAN	C	5	11/12	0.75	0.15	70,73,75,76	0
3	NAG	D	1	14/15	0.78	0.10	57,60,64,65	0
2	MAN	C	4	11/12	0.82	0.11	54,58,60,61	0

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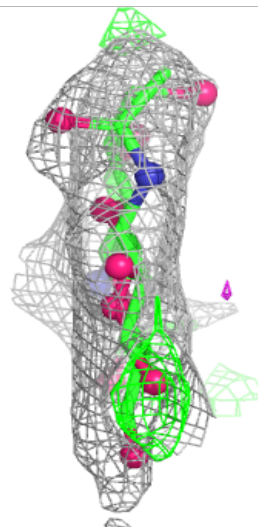
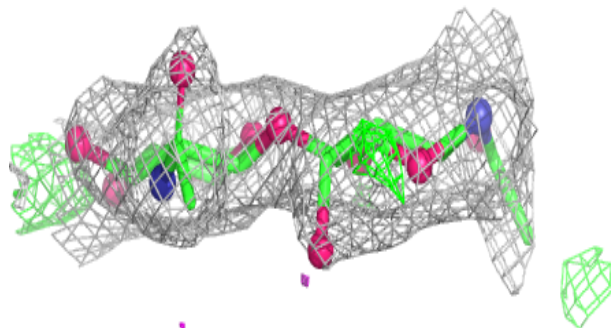
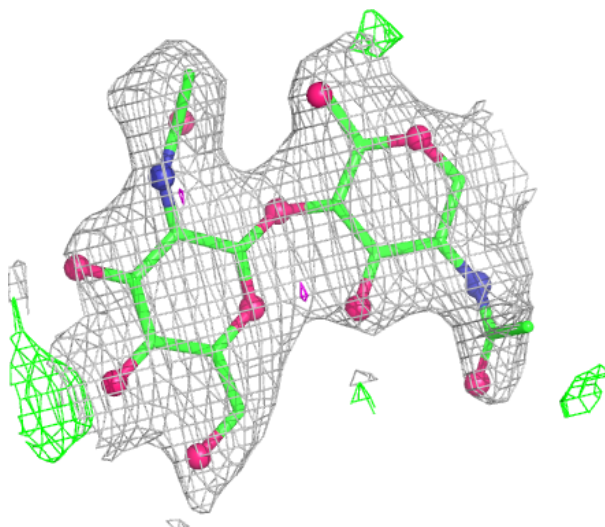
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	NAG	D	2	14/15	0.83	0.09	60,63,67,68	0
2	BMA	C	3	11/12	0.87	0.09	48,52,57,67	0
2	NAG	C	2	14/15	0.89	0.09	41,51,56,59	0
2	NAG	C	1	14/15	0.90	0.09	45,50,54,57	0

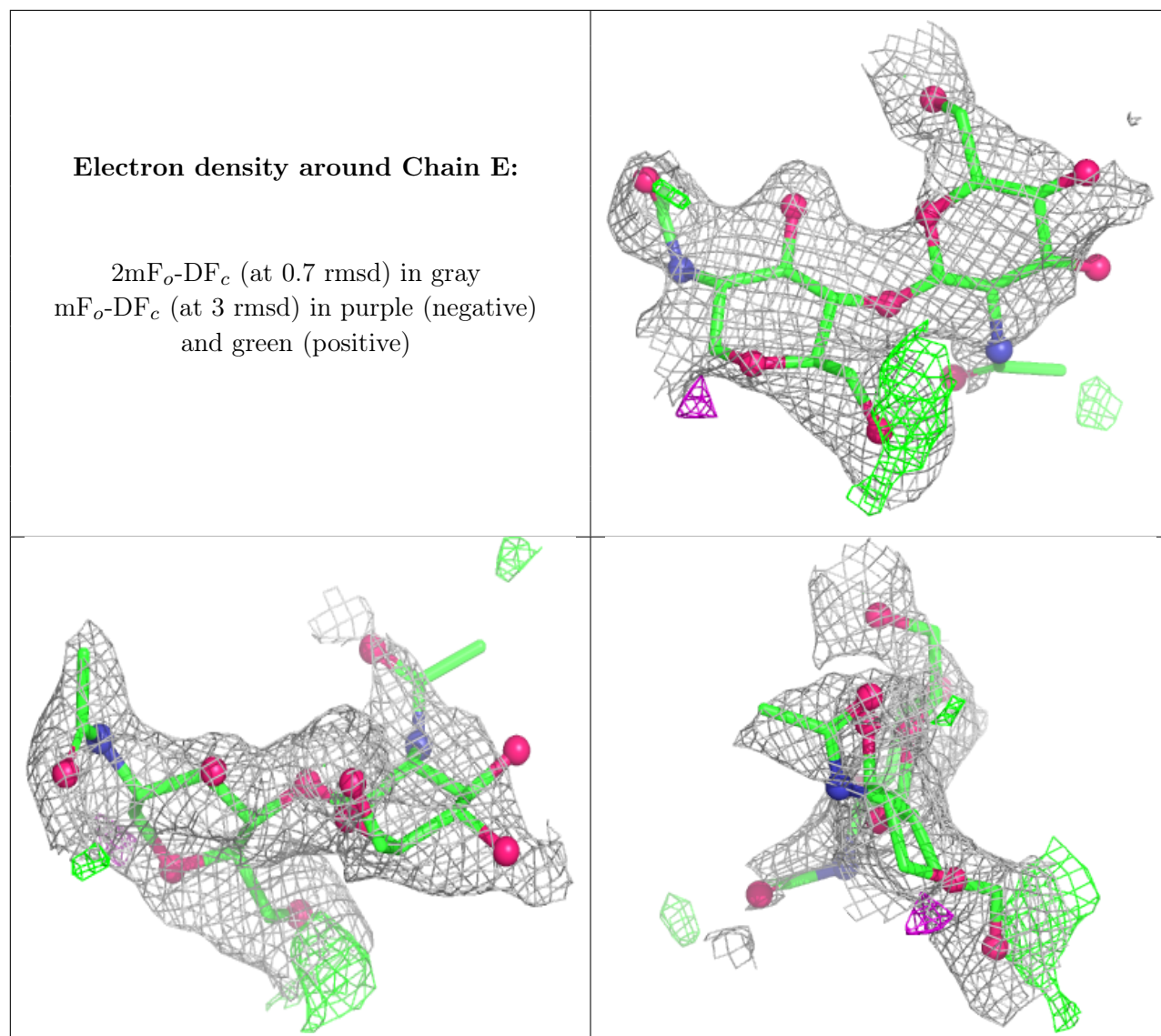
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.



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)





6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	NAG	A	3081	14/15	0.67	0.11	73,77,79,80	0
4	NAG	A	5231	14/15	0.74	0.11	59,67,73,73	0
4	NAG	B	3081	14/15	0.82	0.09	49,52,60,65	0
6	PO4	A	2001	5/5	0.96	0.06	35,41,42,44	0
6	PO4	B	2002	5/5	0.96	0.07	28,30,40,43	0
5	CA	A	1001	1/1	0.97	0.03	27,27,27,27	0
5	CA	B	1002	1/1	0.99	0.03	28,28,28,28	0

6.5 Other polymers [i](#)

There are no such residues in this entry.