



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 01:57 PM UTC

PDB ID : 4NEH / pdb_00004neh
Title : An internal ligand-bound, metastable state of a leukocyte integrin, aXb2
Authors : Sen, M.; Yuki, K.; Springer, T.A.
Deposited on : 2013-10-29
Resolution : 2.75 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

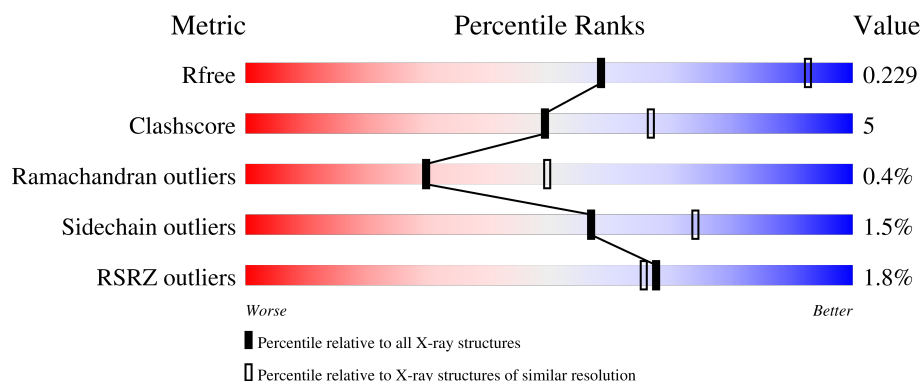
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.75 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	1009 (2.76-2.76)
Clashscore	190562	1044 (2.76-2.76)
Ramachandran outliers	187476	1024 (2.76-2.76)
Sidechain outliers	187428	1024 (2.76-2.76)
RSRZ outliers	180081	1009 (2.76-2.76)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	1094	 2% 84% 15% ..
2	B	686	 2% 80% 16% ..
3	C	2	 100%
3	F	2	 100%
3	G	2	 50% 50%

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Mol	Chain	Length	Quality of chain
3	H	2	 100%
4	D	3	 67% 33%
5	E	7	 14% 86%

2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 14175 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 Integrin alpha-X.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	1084	8457	5355	1461	1602	39	0	11	1

There are 17 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	42	ASP	ASN	conflict	UNP P20702
A	368	ASP	SER	conflict	UNP P20702
A	678	THR	ASN	conflict	UNP P20702
A	885	SER	ASN	conflict	UNP P20702
A	920	CYS	ASN	conflict	UNP P20702
A	1083	PRO	-	expression tag	UNP P20702
A	1084	GLY	-	expression tag	UNP P20702
A	1085	PRO	-	expression tag	UNP P20702
A	1086	ALA	-	expression tag	UNP P20702
A	1087	ALA	-	expression tag	UNP P20702
A	1088	LEU	-	expression tag	UNP P20702
A	1089	GLN	-	expression tag	UNP P20702
A	1090	THR	-	expression tag	UNP P20702
A	1091	LEU	-	expression tag	UNP P20702
A	1092	PHE	-	expression tag	UNP P20702
A	1093	GLN	-	expression tag	UNP P20702
A	1094	GLY	-	expression tag	UNP P20702

- Molecule 2 is a protein called Integrin beta-2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	668	5153	3173	919	995	66	0	6	2

There are 15 discrepancies between the modelled and reference sequences:

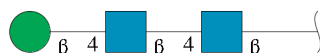
Chain	Residue	Modelled	Actual	Comment	Reference
B	190	ASP	ASN	conflict	UNP P05107
B	232	LYS	ASN	conflict	UNP P05107
B	674	CYS	VAL	conflict	UNP P05107
B	675	GLY	-	expression tag	UNP P05107
B	676	GLY	-	expression tag	UNP P05107
B	677	PRO	-	expression tag	UNP P05107
B	678	ALA	-	expression tag	UNP P05107
B	679	ALA	-	expression tag	UNP P05107
B	680	LEU	-	expression tag	UNP P05107
B	681	GLN	-	expression tag	UNP P05107
B	682	THR	-	expression tag	UNP P05107
B	683	LEU	-	expression tag	UNP P05107
B	684	PHE	-	expression tag	UNP P05107
B	685	GLN	-	expression tag	UNP P05107
B	686	GLY	-	expression tag	UNP P05107

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



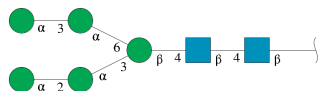
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	C	2	Total	C	N	O	0	0	0
			28	16	2	10			
3	F	2	Total	C	N	O	0	0	0
			28	16	2	10			
3	G	2	Total	C	N	O	0	0	0
			28	16	2	10			
3	H	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 4 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
4	D	3	Total	C	N	O	0	0	0
			39	22	2	15			

- Molecule 5 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[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.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	E	7	Total	C	N	O	0	0	0
			83	46	2	35			

- Molecule 6 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	3	Total	Ca	0	0
			3	3		
6	B	2	Total	Ca	0	0
			2	2		

- Molecule 7 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	1	Total	Mg	0	0
			1	1		
7	B	1	Total	Mg	0	0
			1	1		

- Molecule 8 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).



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

- Molecule 9 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	1	Total	Cl	0	0
			1	1		

- Molecule 10 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	1	Total	Na	0	0
			1	1		

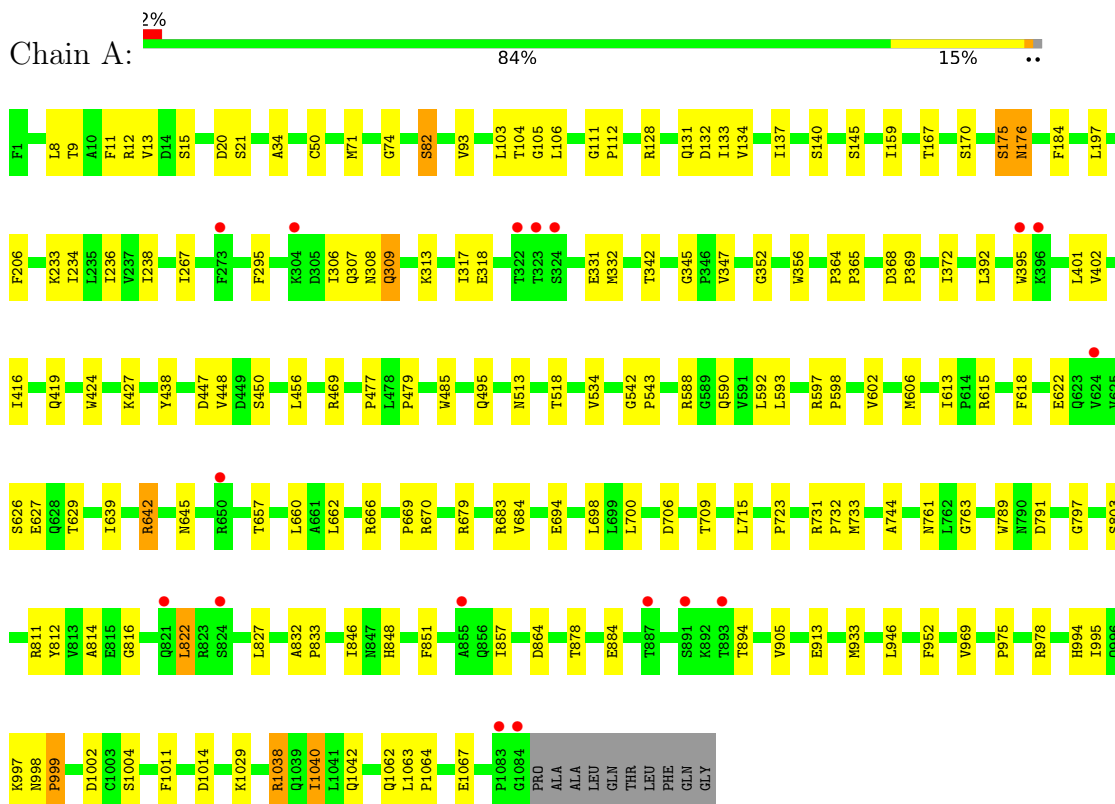
- Molecule 11 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	A	222	Total	O	0	0
			222	222		
11	B	86	Total	O	0	0
			86	86		

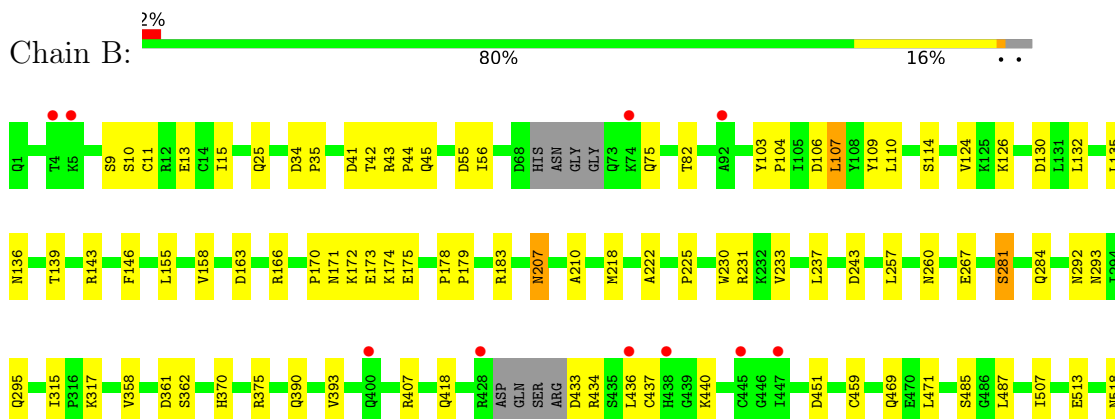
3 Residue-property plots

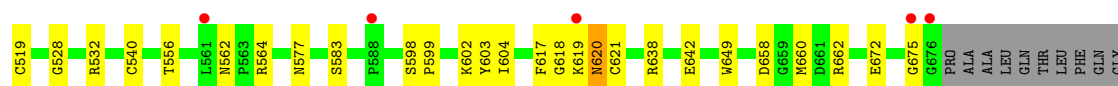
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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



• Molecule 2: Integrin beta-2



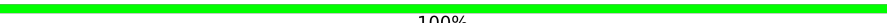


- Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain C:  100%



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

Chain F:  100%



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

Chain G:  50%



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

Chain H:  100%



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

Chain D:  67%



- Molecule 5: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[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 E:  14%



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	126.97Å 131.44Å 190.48Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	45.66 – 2.75 45.66 – 2.75	Depositor EDS
% Data completeness (in resolution range)	97.7 (45.66-2.75) 97.7 (45.66-2.75)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.34 (at 2.77Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.2_1309)	Depositor
R, R_{free}	0.193 , 0.225 0.196 , 0.229	Depositor DCC
R_{free} test set	4044 reflections (4.85%)	wwPDB-VP
Wilson B-factor (Å ²)	68.7	Xtriage
Anisotropy	0.349	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 69.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.015 for k,h,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	14175	wwPDB-VP
Average B, all atoms (Å ²)	85.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.84% 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: CL, BMA, NAG, NA, MAN, CA, MG

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	0.28	0/8679	0.81	11/11790 (0.1%)
2	B	0.27	0/5264	0.74	5/7103 (0.1%)
All	All	0.27	0/13943	0.79	16/18893 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	3

There are no bond length outliers.

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	82[A]	SER	CA-C-N	-15.44	100.53	119.84
1	A	82[A]	SER	C-N-CA	-15.44	100.53	119.84
1	A	82[B]	SER	CA-C-N	-15.44	100.53	119.84
1	A	82[B]	SER	C-N-CA	-15.44	100.53	119.84
1	A	542	GLY	CA-C-N	8.80	130.84	119.84
1	A	542	GLY	C-N-CA	8.80	130.84	119.84
1	A	176	ASN	N-CA-C	-5.72	106.35	113.38
1	A	822	LEU	N-CA-C	-5.36	106.11	113.30
1	A	34	ALA	CA-C-N	5.28	125.09	119.28
1	A	34	ALA	C-N-CA	5.28	125.09	119.28
1	A	309	GLN	N-CA-C	5.26	118.31	110.52
2	B	619	LYS	CA-C-N	5.26	127.85	120.28
2	B	619	LYS	C-N-CA	5.26	127.85	120.28
2	B	315	ILE	CA-C-N	5.12	124.29	118.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	315	ILE	C-N-CA	5.12	124.29	118.97
2	B	583	SER	CB-CA-C	-5.04	110.78	116.63

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	622	GLU	Peptide
1	A	82[A]	SER	Peptide
1	A	82[B]	SER	Peptide

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	8457	0	8289	94	0
2	B	5153	0	4960	61	0
3	C	28	0	25	0	0
3	F	28	0	25	0	0
3	G	28	0	25	0	0
3	H	28	0	25	0	0
4	D	39	0	34	0	0
5	E	83	0	70	0	0
6	A	3	0	0	0	0
6	B	2	0	0	0	0
7	A	1	0	0	0	0
7	B	1	0	0	0	0
8	A	14	0	13	0	0
9	A	1	0	0	1	0
10	A	1	0	0	0	0
11	A	222	0	0	4	0
11	B	86	0	0	2	0
All	All	14175	0	13466	148	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 5.

All (148) 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)
2:B:222:ALA:O	2:B:292:ASN:ND2	2.21	0.73
2:B:41:ASP:OD2	2:B:45:GLN:NE2	2.23	0.71
2:B:293[B]:ASN:OD1	2:B:407:ARG:NH2	2.27	0.66
1:A:723:PRO:HG3	1:A:731:ARG:HE	1.61	0.65
2:B:132:LEU:O	2:B:136:ASN:ND2	2.30	0.64
1:A:995:ILE:HG21	1:A:1040:ILE:HG23	1.81	0.62
2:B:260:ASN:O	2:B:284:GLN:NE2	2.33	0.62
1:A:12:ARG:HG2	1:A:590:GLN:HG2	1.82	0.61
1:A:427:LYS:NZ	11:A:1242:HOH:O	2.34	0.61
2:B:618:GLY:C	2:B:620:ASN:H	2.10	0.60
1:A:318:GLU:OE1	2:B:114:SER:HB2	2.02	0.59
2:B:163:ASP:OD1	2:B:166:ARG:NH2	2.36	0.58
1:A:332:MET:HE1	2:B:155:LEU:HD22	1.85	0.58
1:A:761:ASN:ND2	1:A:791:ASP:O	2.37	0.57
1:A:13:VAL:HG12	1:A:15:SER:H	1.68	0.57
2:B:361:ASP:HB2	2:B:390:GLN:HB3	1.85	0.57
2:B:658:ASP:O	2:B:662:ARG:NH1	2.38	0.57
1:A:645[B]:ASN:ND2	11:A:1366:HOH:O	2.39	0.56
1:A:669:PRO:HB3	1:A:679:ARG:HD3	1.89	0.55
1:A:307:GLN:HB2	1:A:309:GLN:HG3	1.89	0.55
1:A:159:ILE:HD12	1:A:197:LEU:HD11	1.89	0.54
2:B:434:ARG:C	2:B:436:LEU:H	2.15	0.54
1:A:342:THR:OG1	1:A:345:GLY:O	2.20	0.54
1:A:352:GLY:HA2	1:A:356:TRP:CD1	2.43	0.53
1:A:994[A]:HIS:HA	1:A:997:LYS:HE2	1.91	0.53
1:A:978:ARG:HD3	1:A:1014:ASP:HB2	1.91	0.53
1:A:469:ARG:HD3	1:A:495:GLN:HG2	1.90	0.53
2:B:231:ARG:HB2	2:B:233:VAL:HG22	1.92	0.52
2:B:82:THR:HG22	2:B:418:GLN:HB3	1.91	0.52
2:B:556:THR:HG23	2:B:577:ASN:HD21	1.75	0.52
2:B:513:GLU:OE2	2:B:513:GLU:N	2.37	0.51
1:A:479:PRO:HD3	1:A:485:TRP:CD1	2.46	0.51
1:A:71:MET:HG2	1:A:93:VAL:HG22	1.91	0.51
1:A:103:LEU:HD22	2:B:155:LEU:HB3	1.93	0.51
1:A:994[B]:HIS:HA	1:A:997:LYS:HE2	1.94	0.50
1:A:236:ILE:HG23	1:A:267:ILE:HD13	1.94	0.50
1:A:606:MET:HB2	1:A:744:ALA:HB2	1.94	0.49
1:A:134:VAL:HG22	1:A:170:SER:HB3	1.94	0.49
1:A:21:SER:OG	1:A:74:GLY:O	2.24	0.49
2:B:358:VAL:HG22	2:B:393:VAL:HG22	1.94	0.49
1:A:848:HIS:ND1	2:B:485[A]:SER:HB2	2.27	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:562:ASN:HD21	2:B:564:ARG:HB2	1.78	0.49
1:A:626:SER:OG	1:A:627:GLU:N	2.41	0.49
1:A:8:LEU:HD21	1:A:592:LEU:HD23	1.94	0.48
1:A:295:PHE:HZ	1:A:306:ILE:HD11	1.78	0.48
2:B:218:MET:HG2	2:B:237:LEU:HD21	1.94	0.48
1:A:372:ILE:HG12	1:A:424:TRP:CG	2.47	0.48
1:A:602:VAL:HG22	1:A:639:ILE:HG12	1.95	0.48
1:A:456:LEU:HA	1:A:477:PRO:HA	1.95	0.48
1:A:666:ARG:NH2	1:A:706:ASP:OD2	2.46	0.48
1:A:913:GLU:OE2	2:B:638:ARG:HB2	2.13	0.48
1:A:905:VAL:HG21	1:A:946:LEU:HD22	1.96	0.48
1:A:128:ARG:NH2	1:A:308:ASN:OD1	2.47	0.48
1:A:816:GLY:HA2	1:A:822:LEU:HB3	1.96	0.48
2:B:183[A]:ARG:NH2	11:B:863:HOH:O	2.44	0.48
1:A:332:MET:O	1:A:352:GLY:HA3	2.14	0.47
1:A:419:GLN:HE21	1:A:424:TRP:NE1	2.13	0.47
1:A:233:LYS:NZ	11:A:1320:HOH:O	2.31	0.47
1:A:1040:ILE:HG22	1:A:1042:GLN:H	1.79	0.47
2:B:281:SER:HB3	2:B:284:GLN:HB2	1.97	0.47
2:B:469:GLN:C	2:B:471:LEU:H	2.23	0.47
1:A:347:VAL:HG11	1:A:401:LEU:HD21	1.97	0.46
1:A:797:GLY:HA3	1:A:884:GLU:HG3	1.97	0.46
2:B:295:GLN:HG2	2:B:317:LYS:HB3	1.97	0.46
1:A:662:LEU:HD11	1:A:698:LEU:HD22	1.97	0.46
2:B:25:GLN:HG2	2:B:55:ASP:HB2	1.97	0.46
1:A:933:MET:HG2	1:A:1029:LYS:HG3	1.96	0.46
1:A:175:SER:OG	1:A:176:ASN:N	2.49	0.46
2:B:602:LYS:HE3	2:B:603:TYR:CZ	2.51	0.46
1:A:402:VAL:HG22	1:A:416:ILE:HG12	1.98	0.45
1:A:952:PHE:HB2	1:A:1011:PHE:HB2	1.97	0.45
1:A:313:LYS:NZ	1:A:331:GLU:OE2	2.35	0.45
2:B:10:SER:OG	2:B:11:CYS:N	2.49	0.45
2:B:487:LEU:HB3	2:B:507:ILE:HD13	1.96	0.45
1:A:1063:LEU:HD12	1:A:1064:PRO:HD2	1.98	0.45
2:B:604:ILE:HD13	2:B:642:GLU:HB2	1.97	0.45
1:A:629:THR:HB	1:A:700:LEU:HB2	1.99	0.45
1:A:851:PHE:HE1	1:A:857:ILE:HG12	1.82	0.45
2:B:126:LYS:NZ	2:B:130:ASP:OD2	2.41	0.45
1:A:588:ARG:NH2	11:A:1354:HOH:O	2.49	0.45
1:A:803:SER:HB3	1:A:878:THR:OG1	2.16	0.45
1:A:827:LEU:HD21	1:A:846:ILE:HG12	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:104:THR:OG1	1:A:105:GLY:N	2.50	0.45
2:B:618:GLY:C	2:B:620:ASN:N	2.76	0.44
1:A:513:ASN:OD1	1:A:513:ASN:N	2.51	0.44
2:B:433:ASP:HB3	2:B:436:LEU:HD12	2.00	0.44
1:A:811:ARG:HD3	1:A:864:ASP:OD2	2.17	0.44
1:A:133:ILE:HG12	1:A:234:ILE:HB	2.00	0.44
1:A:642:ARG:HA	1:A:642:ARG:HE	1.83	0.44
1:A:1038:ARG:HA	1:A:1038:ARG:HD2	1.57	0.44
1:A:812:TYR:CE2	1:A:814:ALA:HB2	2.53	0.43
2:B:178:PRO:HA	2:B:179:PRO:HD3	1.90	0.43
1:A:763:GLY:HA3	1:A:789:TRP:CE2	2.53	0.43
2:B:210:ALA:HB1	2:B:243:ASP:OD2	2.18	0.43
2:B:43:ARG:N	2:B:44:PRO:HD2	2.34	0.43
1:A:71:MET:HE3	1:A:106:LEU:HB3	2.00	0.43
1:A:448:VAL:HA	1:A:518:THR:HB	2.01	0.43
1:A:598:PRO:HG2	1:A:732:PRO:HA	2.01	0.43
1:A:998:ASN:HA	1:A:999:PRO:HD3	1.86	0.43
1:A:1062:GLN:HG2	1:A:1067:GLU:HA	2.01	0.42
2:B:110:LEU:HD12	2:B:110:LEU:HA	1.79	0.42
1:A:20:ASP:OD2	2:B:257:LEU:HD12	2.19	0.42
1:A:683:ARG:NE	1:A:694:GLU:OE2	2.29	0.42
2:B:158:VAL:HG22	2:B:207:ASN:HB2	2.02	0.42
2:B:528:GLY:HA3	2:B:532:ARG:HD2	2.01	0.42
1:A:317:ILE:HD11	2:B:170:PRO:HD3	2.00	0.42
1:A:342:THR:HA	1:A:392:LEU:HD22	2.00	0.42
1:A:597:ARG:NH2	1:A:733:MET:HB3	2.33	0.42
2:B:42:THR:HB	2:B:44:PRO:HD2	2.01	0.42
2:B:103:TYR:O	2:B:139:THR:HG23	2.19	0.42
2:B:519:CYS:HB3	2:B:540:CYS:SG	2.60	0.42
1:A:131:GLN:HG3	1:A:167:THR:HG23	2.01	0.42
2:B:9:SER:OG	2:B:13:GLU:OE1	2.31	0.42
1:A:419:GLN:HG3	1:A:424:TRP:CE2	2.54	0.42
2:B:104:PRO:HB2	2:B:233:VAL:HG11	2.01	0.42
1:A:447:ASP:OD2	1:A:450:SER:HA	2.20	0.42
2:B:109:TYR:O	2:B:146:PHE:HB2	2.19	0.42
1:A:670:ARG:NH1	1:A:709:THR:O	2.41	0.41
2:B:11:CYS:O	2:B:15:ILE:HG12	2.20	0.41
2:B:437:CYS:O	2:B:459:CYS:HB2	2.20	0.41
1:A:132:ASP:HB3	1:A:184:PHE:CZ	2.56	0.41
1:A:295:PHE:CZ	1:A:306:ILE:HD11	2.55	0.41
1:A:660:LEU:HD21	1:A:715:LEU:HD12	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:225:PRO:HA	2:B:230:TRP:HD1	1.86	0.41
2:B:34:ASP:HA	2:B:35:PRO:HD3	1.82	0.41
1:A:111:GLY:HA2	1:A:112:PRO:HD3	1.92	0.41
2:B:362:SER:HB2	2:B:370:HIS:HB2	2.02	0.41
2:B:649:TRP:HB2	2:B:672:GLU:HB2	2.02	0.41
1:A:832:ALA:HA	1:A:833:PRO:HD3	1.86	0.41
1:A:1002:ASP:OD1	1:A:1004:SER:OG	2.32	0.41
1:A:137:ILE:HG22	1:A:238:ILE:HD12	2.02	0.41
2:B:440:LYS:HB3	2:B:451:ASP:OD2	2.21	0.41
2:B:617:PHE:HA	2:B:620:ASN:HB3	2.03	0.41
1:A:11:PHE:CE1	1:A:50:CYS:HB3	2.56	0.41
2:B:107:LEU:HB2	2:B:135:LEU:HD13	2.03	0.41
2:B:231:ARG:C	2:B:233:VAL:H	2.29	0.41
1:A:9:THR:HB	1:A:593:LEU:HB3	2.02	0.40
1:A:176:ASN:HB3	1:A:206:PHE:HB2	2.03	0.40
1:A:364:PRO:HA	1:A:365:PRO:HD3	1.95	0.40
1:A:613:ILE:HG21	1:A:618[B]:PHE:CE2	2.56	0.40
2:B:598:SER:HA	2:B:599:PRO:HD3	1.78	0.40
1:A:140:SER:HB2	9:A:1120:CL:CL	2.59	0.40
1:A:368:ASP:HA	1:A:369:PRO:HD3	1.91	0.40
1:A:613:ILE:HG21	1:A:618[B]:PHE:HE2	1.87	0.40
1:A:615:ARG:HA	1:A:618[A]:PHE:CE1	2.57	0.40
2:B:106:ASP:OD1	2:B:143:ARG:HB2	2.21	0.40
2:B:375:ARG:HD3	11:B:848:HOH:O	2.21	0.40
1:A:657:THR:HG23	1:A:684:VAL:HG22	2.04	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	1093/1094 (100%)	1044 (96%)	44 (4%)	5 (0%)	24 43

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	668/686 (97%)	637 (95%)	29 (4%)	2 (0%)	36	56
All	All	1761/1780 (99%)	1681 (96%)	73 (4%)	7 (0%)	30	50

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	145	SER
1	A	543	PRO
2	B	621	CYS
1	A	175	SER
1	A	975	PRO
2	B	675	GLY
1	A	999	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	932/932 (100%)	924 (99%)	8 (1%)	70	82
2	B	582/590 (99%)	567 (97%)	15 (3%)	40	63
All	All	1514/1522 (100%)	1491 (98%)	23 (2%)	57	74

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

Mol	Chain	Res	Type
1	A	395	TRP
1	A	438	TYR
1	A	534	VAL
1	A	642	ARG
1	A	894	THR
1	A	969	VAL
1	A	1038	ARG
1	A	1040	ILE
2	B	56	ILE

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Mol	Chain	Res	Type
2	B	75	GLN
2	B	107	LEU
2	B	124	VAL
2	B	171	ASN
2	B	172	LYS
2	B	173	GLU
2	B	174	LYS
2	B	175	GLU
2	B	207	ASN
2	B	267	GLU
2	B	281	SER
2	B	518	ASN
2	B	620	ASN
2	B	660	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	192	ASN
1	A	214	GLN
1	A	378	ASN
1	A	399	GLN
1	A	419	GLN
1	A	538	HIS
1	A	692	HIS
1	A	912	HIS
1	A	996	GLN
1	A	1066	GLN
2	B	75	GLN
2	B	287	HIS
2	B	518	ASN
2	B	577	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 ⓘ

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
3	NAG	C	1	1,3	14,14,15	0.61	0	17,19,21	0.48	0
3	NAG	C	2	3	14,14,15	0.28	0	17,19,21	0.40	0
4	NAG	D	1	1,4	14,14,15	0.23	0	17,19,21	0.52	0
4	NAG	D	2	4	14,14,15	0.24	0	17,19,21	0.59	0
4	BMA	D	3	4	11,11,12	0.67	0	15,15,17	1.49	2 (13%)
5	NAG	E	1	5,1	14,14,15	0.84	1 (7%)	17,19,21	0.49	0
5	NAG	E	2	5	14,14,15	0.22	0	17,19,21	0.38	0
5	BMA	E	3	5	11,11,12	0.86	1 (9%)	15,15,17	1.04	1 (6%)
5	MAN	E	4	5	11,11,12	0.65	0	15,15,17	1.28	2 (13%)
5	MAN	E	5	5	11,11,12	0.69	0	15,15,17	0.99	1 (6%)
5	MAN	E	6	5	11,11,12	0.71	0	15,15,17	1.16	3 (20%)
5	MAN	E	7	5	11,11,12	0.80	1 (9%)	15,15,17	1.08	2 (13%)
3	NAG	F	1	1,3	14,14,15	0.47	0	17,19,21	0.65	0
3	NAG	F	2	3	14,14,15	0.52	0	17,19,21	0.52	0
3	NAG	G	1	3,2	14,14,15	0.39	0	17,19,21	0.73	1 (5%)
3	NAG	G	2	3	14,14,15	0.41	0	17,19,21	0.56	0
3	NAG	H	1	3,2	14,14,15	0.35	0	17,19,21	0.68	0
3	NAG	H	2	3	14,14,15	0.36	0	17,19,21	0.44	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
3	NAG	C	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	C	2	3	-	2/6/23/26	0/1/1/1
4	NAG	D	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	D	2	4	-	2/6/23/26	0/1/1/1

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

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	E	1	NAG	O5-C1	-3.03	1.38	1.43
5	E	7	MAN	C1-C2	2.14	1.57	1.52
5	E	3	BMA	O5-C1	-2.06	1.40	1.43

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	3	BMA	C1-O5-C5	3.89	117.40	112.19
5	E	4	MAN	C1-O5-C5	3.40	116.75	112.19
5	E	6	MAN	C1-O5-C5	2.74	115.86	112.19
5	E	3	BMA	C1-O5-C5	2.71	115.81	112.19
5	E	5	MAN	C1-O5-C5	2.51	115.54	112.19
3	G	1	NAG	C1-O5-C5	2.39	115.39	112.19
5	E	7	MAN	C1-O5-C5	2.28	115.24	112.19
5	E	7	MAN	O2-C2-C3	-2.25	105.48	110.15
4	D	3	BMA	O2-C2-C3	-2.23	105.52	110.15
5	E	4	MAN	O2-C2-C3	-2.18	105.64	110.15
5	E	6	MAN	O3-C3-C2	2.09	114.32	110.05
5	E	6	MAN	O2-C2-C3	-2.08	105.84	110.15

There are no chirality outliers.

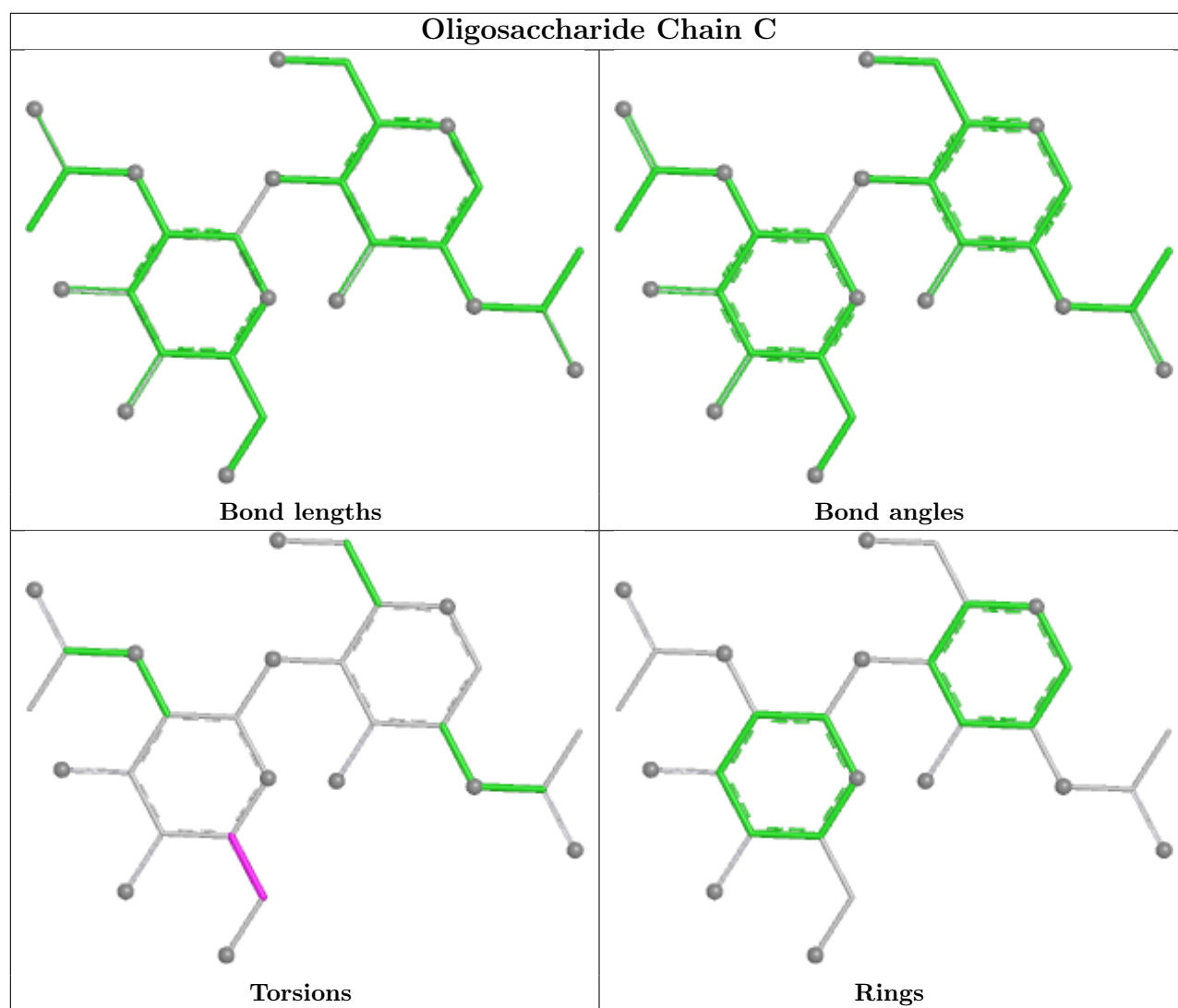
All (18) torsion outliers are listed below:

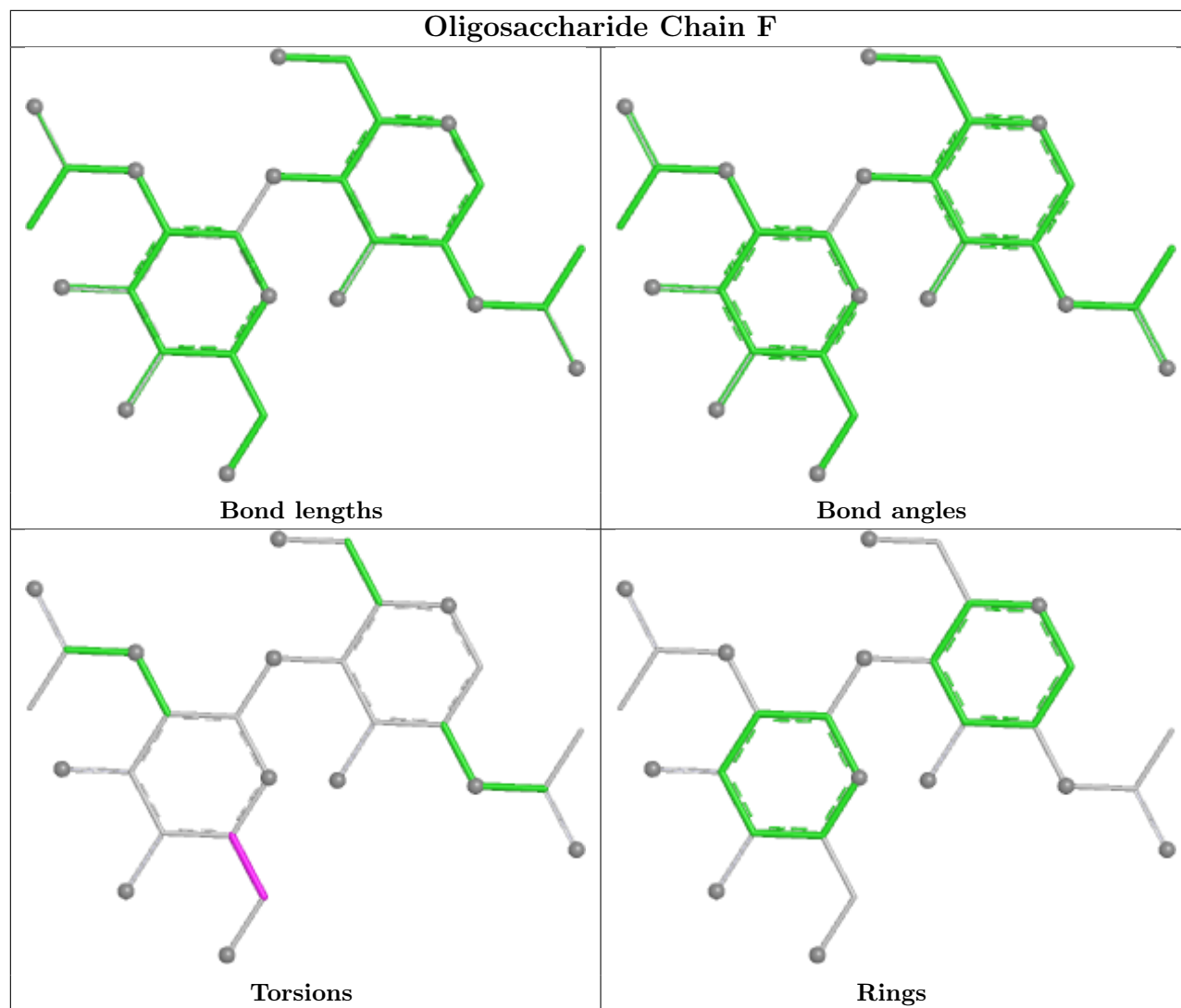
Mol	Chain	Res	Type	Atoms
3	H	1	NAG	O5-C5-C6-O6
4	D	3	BMA	O5-C5-C6-O6
3	C	2	NAG	C4-C5-C6-O6
5	E	2	NAG	O5-C5-C6-O6
3	H	1	NAG	C4-C5-C6-O6
3	C	2	NAG	O5-C5-C6-O6
5	E	2	NAG	C4-C5-C6-O6
4	D	3	BMA	C4-C5-C6-O6
4	D	2	NAG	O5-C5-C6-O6
3	G	1	NAG	O5-C5-C6-O6
3	G	2	NAG	O5-C5-C6-O6
5	E	6	MAN	O5-C5-C6-O6
5	E	5	MAN	O5-C5-C6-O6
3	H	2	NAG	O5-C5-C6-O6
4	D	2	NAG	C4-C5-C6-O6
3	G	1	NAG	C4-C5-C6-O6
3	F	2	NAG	O5-C5-C6-O6
3	G	2	NAG	C4-C5-C6-O6

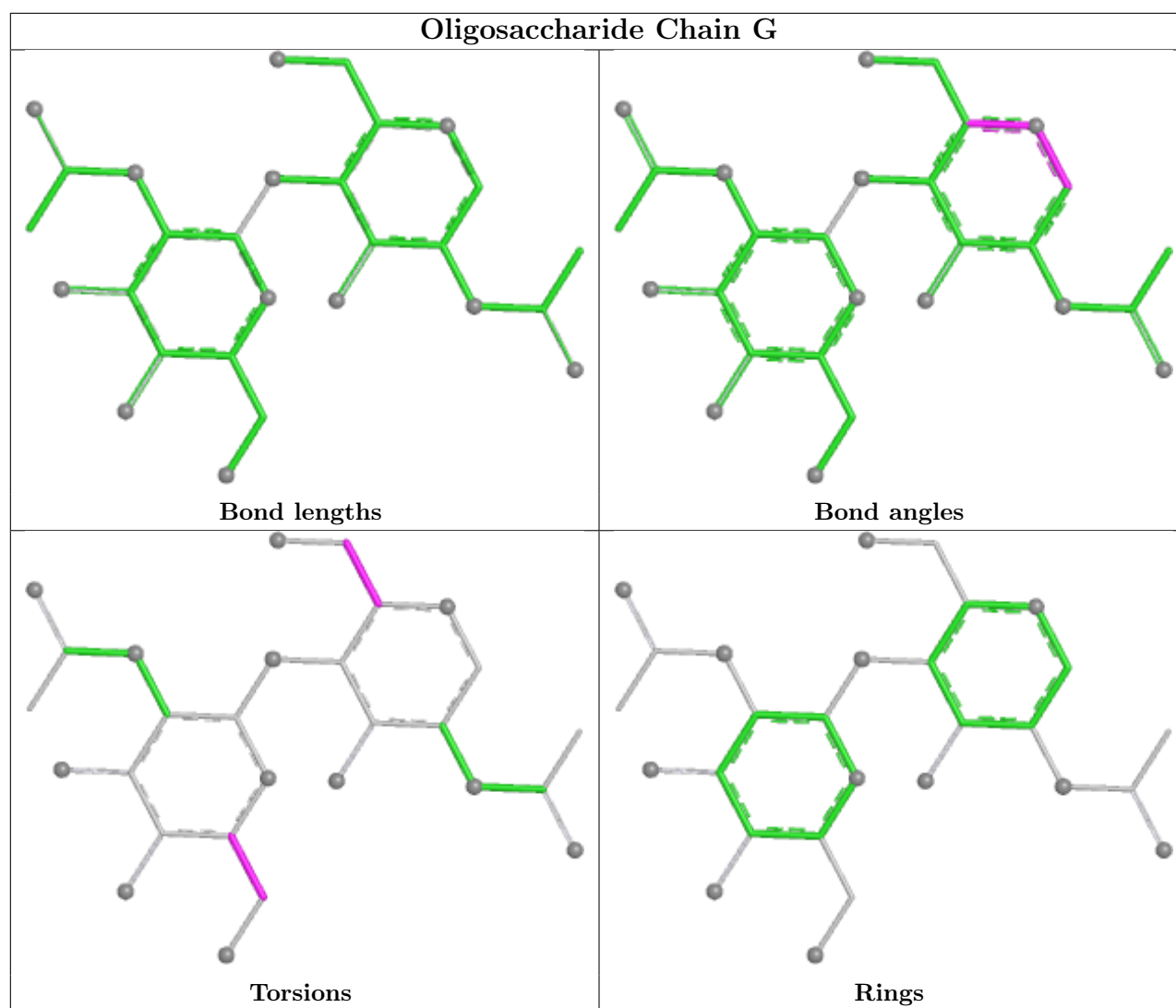
There are no ring outliers.

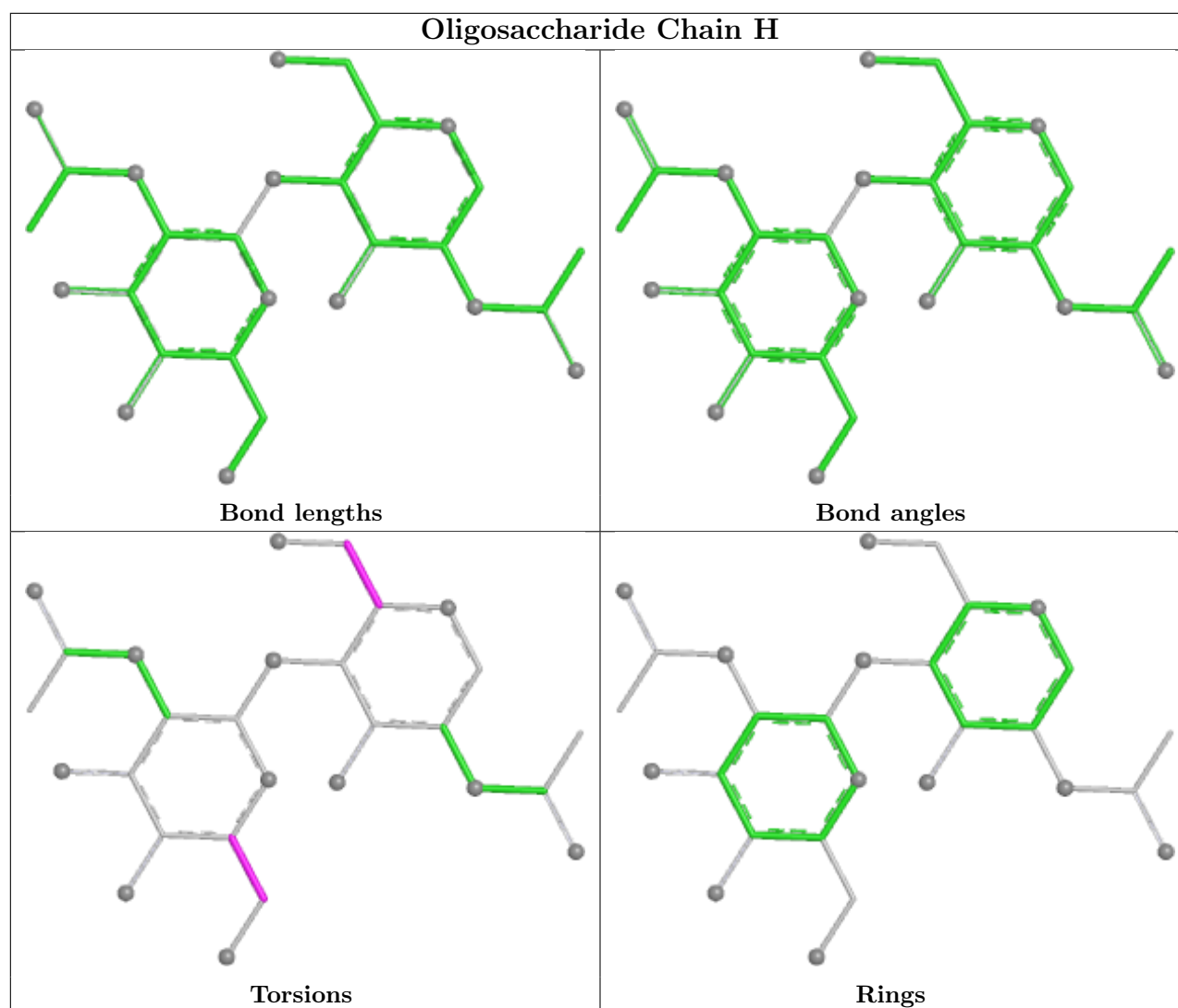
No monomer is involved in short contacts.

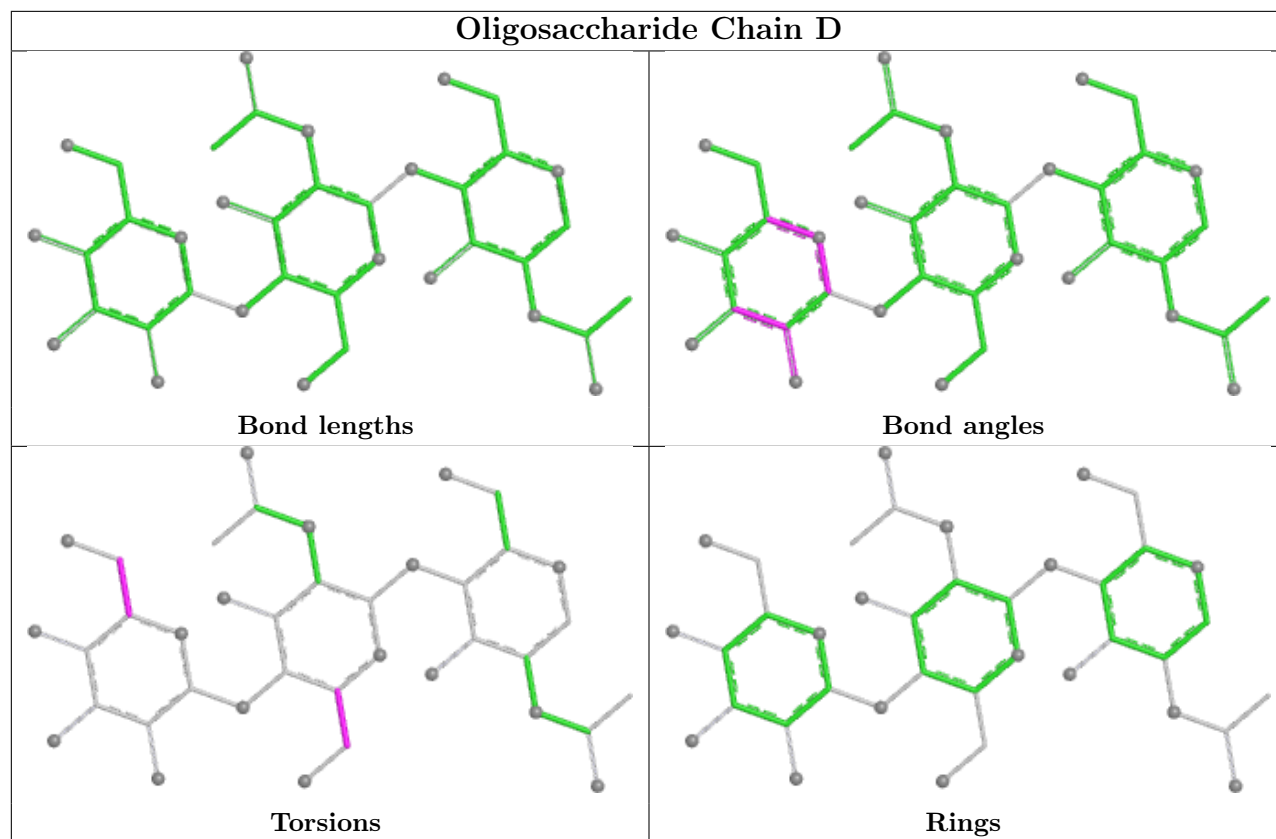
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

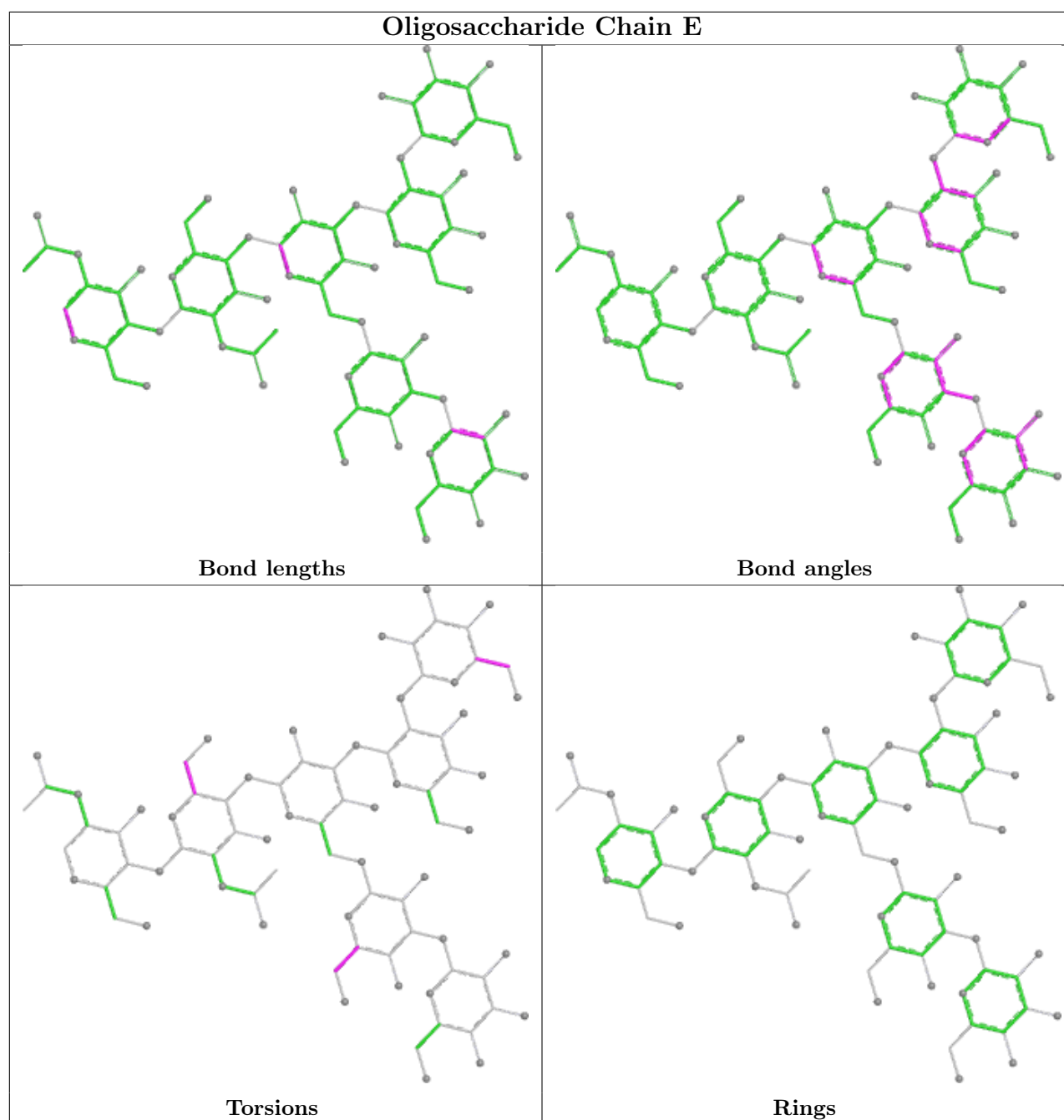












5.6 Ligand geometry [i](#)

Of 10 ligands modelled in this entry, 9 are monoatomic - leaving 1 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
8	NAG	A	1119	1	14,14,15	0.57	0	17,19,21	0.56	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
8	NAG	A	1119	1	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	A	1119	NAG	O5-C5-C6-O6
8	A	1119	NAG	C4-C5-C6-O6

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [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	1084/1094 (99%)	-0.15	17 (1%) 70 69	30, 70, 143, 274	11 (1%)
2	B	668/686 (97%)	0.06	15 (2%) 62 60	37, 90, 168, 230	7 (1%)
All	All	1752/1780 (98%)	-0.07	32 (1%) 67 65	30, 76, 159, 274	18 (1%)

All (32) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	428	ARG	7.6
1	A	1084	GLY	7.0
2	B	676	GLY	6.4
1	A	1083	PRO	4.9
1	A	891	SER	4.2
2	B	561	LEU	3.9
1	A	893	THR	3.4
1	A	322	THR	3.4
1	A	824	SER	3.3
1	A	821	GLN	3.2
2	B	445	CYS	3.1
1	A	650	ARG	2.9
1	A	395	TRP	2.9
2	B	400	GLN	2.9
2	B	447	ILE	2.8
2	B	4	THR	2.8
1	A	855	ALA	2.7
2	B	675	GLY	2.6
2	B	74	LYS	2.5
2	B	436	LEU	2.5
1	A	396	LYS	2.4
1	A	624	VAL	2.4
2	B	619	LYS	2.3
2	B	588	PRO	2.3

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Mol	Chain	Res	Type	RSRZ
2	B	92	ALA	2.3
1	A	323	THR	2.3
1	A	304	LYS	2.2
1	A	324	SER	2.2
1	A	273	PHE	2.2
2	B	438	HIS	2.1
1	A	887	THR	2.1
2	B	5	LYS	2.1

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

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

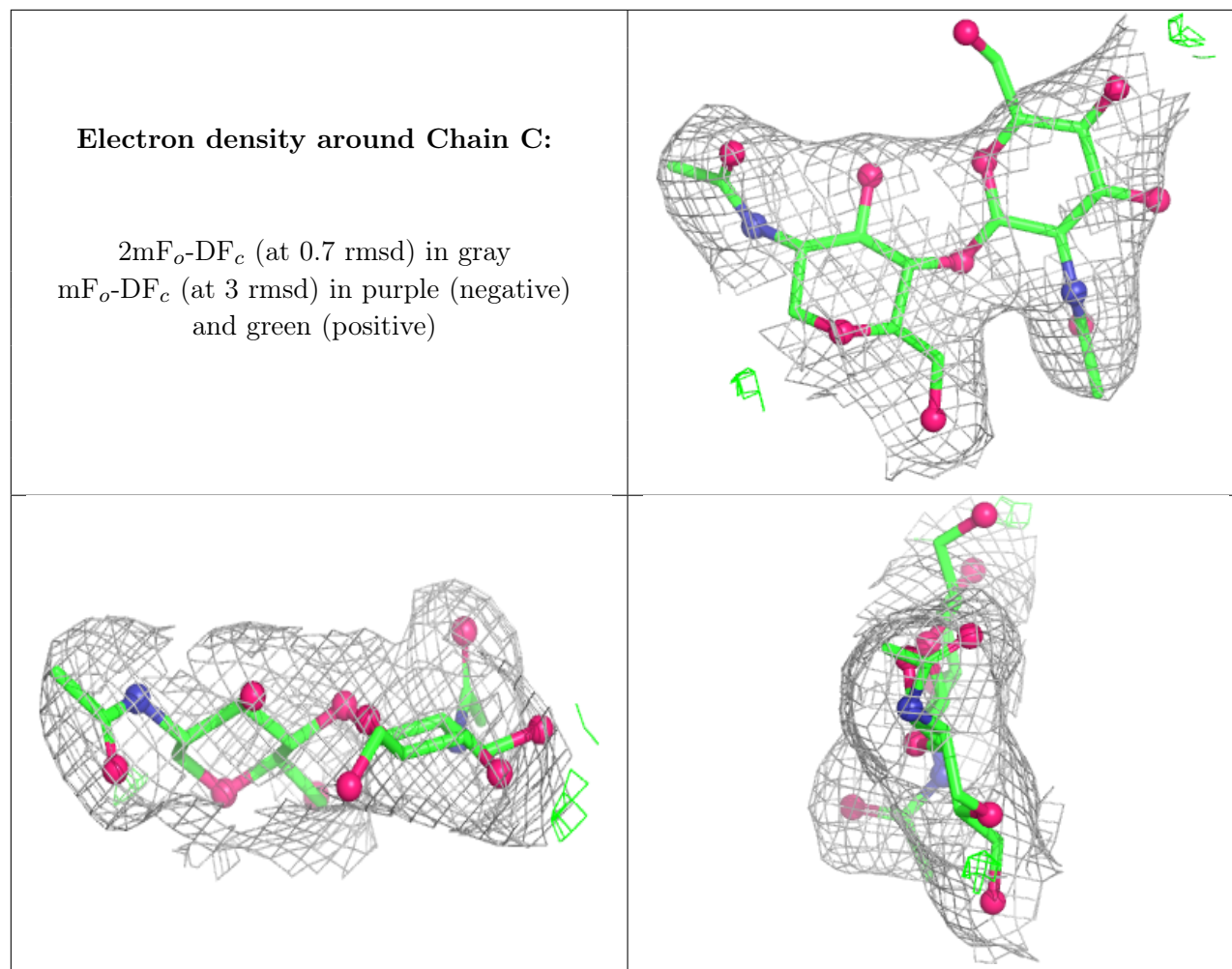
6.3 Carbohydrates [i](#)

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($\text{\AA}^2$)	Q<0.9
4	BMA	D	3	11/12	0.08	0.17	136,171,177,177	0
5	MAN	E	5	11/12	0.38	0.14	146,156,174,181	0
5	MAN	E	6	11/12	0.49	0.15	164,171,177,183	0
5	MAN	E	7	11/12	0.65	0.13	158,169,191,196	0
5	BMA	E	3	11/12	0.70	0.12	106,123,165,169	0
3	NAG	G	2	14/15	0.72	0.14	143,154,167,176	0
3	NAG	F	2	14/15	0.72	0.10	105,127,133,139	0
3	NAG	H	2	14/15	0.73	0.11	148,162,179,182	0
3	NAG	C	2	14/15	0.75	0.12	85,118,155,161	0
4	NAG	D	2	14/15	0.78	0.11	90,117,135,159	0
3	NAG	H	1	14/15	0.84	0.09	100,105,121,121	0
5	NAG	E	2	14/15	0.90	0.09	60,85,111,121	0
5	MAN	E	4	11/12	0.91	0.09	107,117,127,131	0
4	NAG	D	1	14/15	0.91	0.11	59,85,92,111	0
3	NAG	G	1	14/15	0.92	0.10	80,106,119,120	0
3	NAG	F	1	14/15	0.93	0.07	66,86,100,113	0
3	NAG	C	1	14/15	0.95	0.06	56,75,93,99	0
5	NAG	E	1	14/15	0.96	0.07	37,53,61,86	0

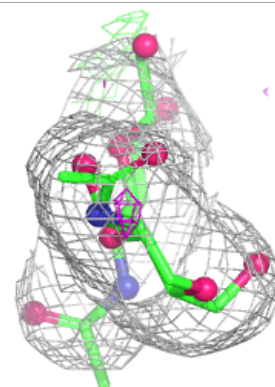
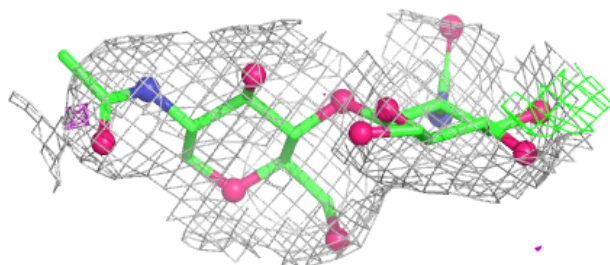
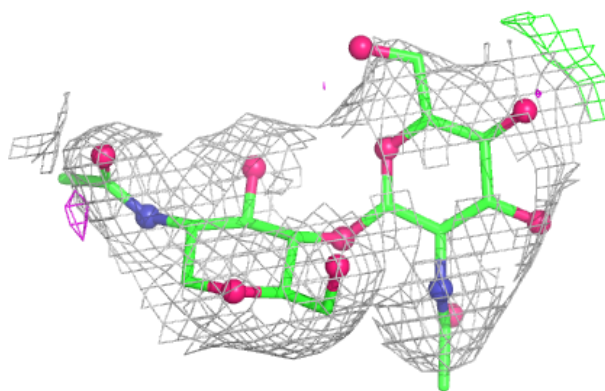
The following is a graphical depiction of the model fit to experimental electron density for oligosac-

charide. Each fit is shown from different orientation to approximate a three-dimensional view.

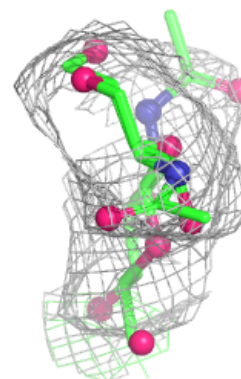
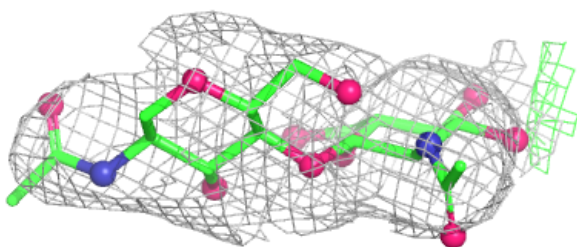
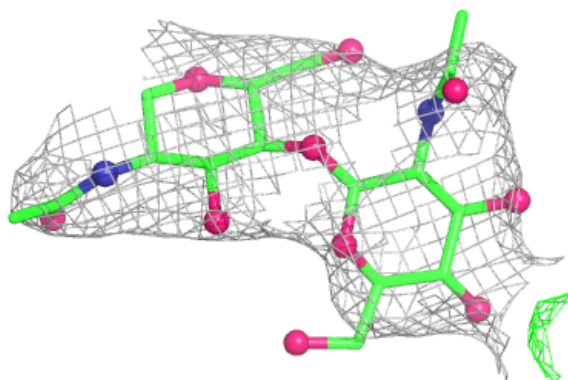


Electron density around Chain F:

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

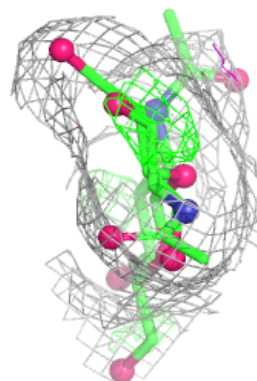
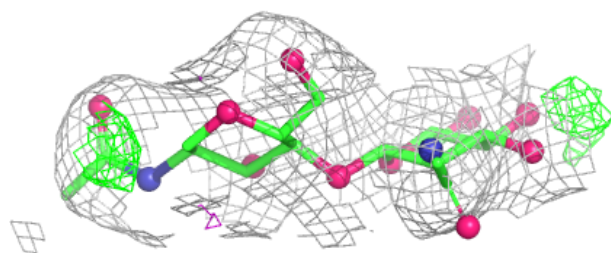
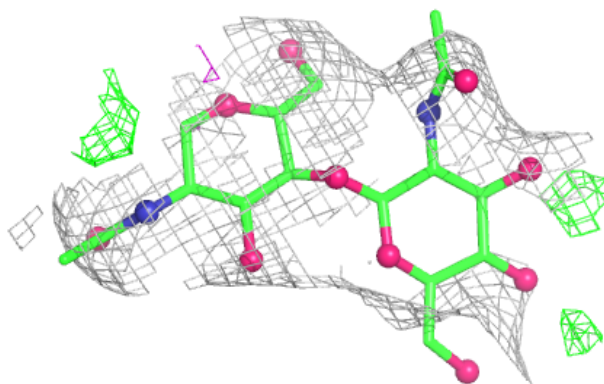
**Electron density around Chain G:**

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

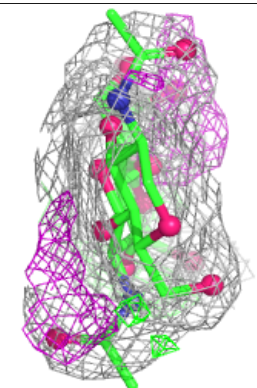
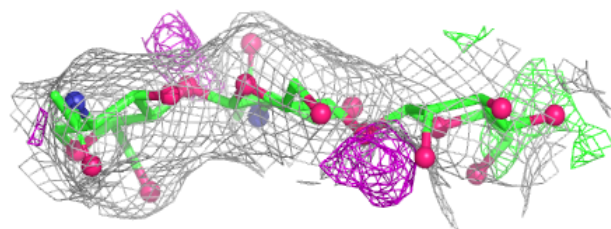
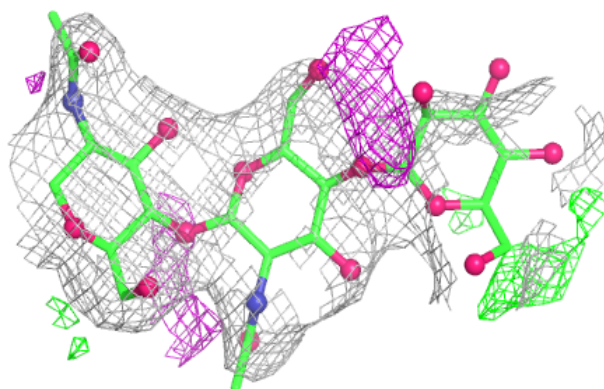


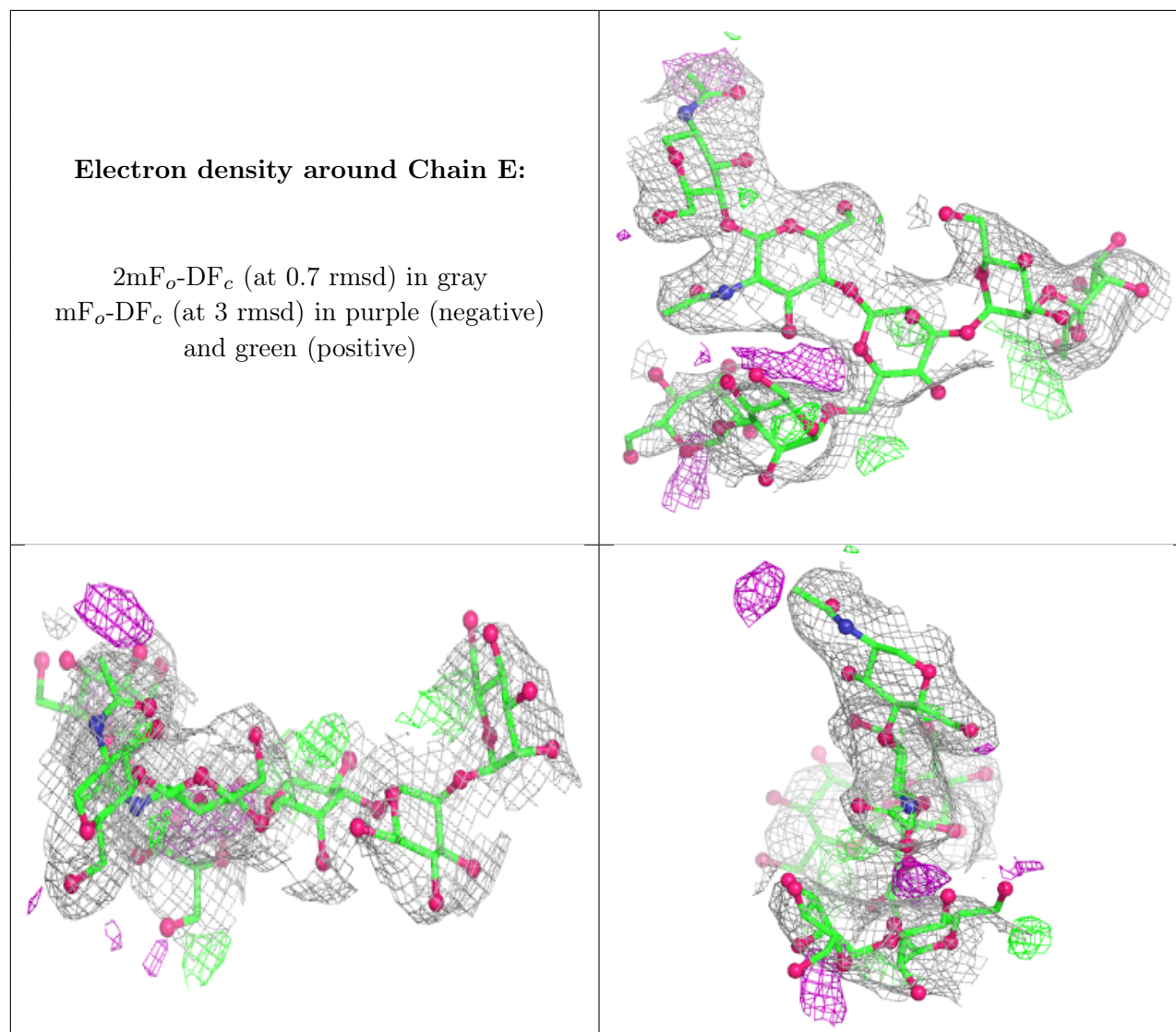
Electron density around Chain H:

$2mF_o-DF_c$ (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(Å ²)	Q<0.9
8	NAG	A	1119	14/15	0.64	0.18	152,172,178,181	0
9	CL	A	1120	1/1	0.91	0.08	82,82,82,82	0
10	NA	A	1121	1/1	0.95	0.17	77,77,77,77	0
6	CA	A	1104	1/1	0.96	0.11	143,143,143,143	0
6	CA	B	702	1/1	0.99	0.05	100,100,100,100	0
6	CA	B	701	1/1	0.99	0.03	48,48,48,48	0
7	MG	B	703	1/1	1.00	0.01	46,46,46,46	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
6	CA	A	1103	1/1	1.00	0.04	54,54,54,54	0
6	CA	A	1101	1/1	1.00	0.01	46,46,46,46	0
7	MG	A	1102	1/1	1.00	0.02	69,69,69,69	0

6.5 Other polymers [i](#)

There are no such residues in this entry.