



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 06:57 AM UTC

PDB ID : 3FCU / pdb_00003fcu
Title : Structure of headpiece of integrin α IIBb3 in open conformation
Authors : Zhu, J.; Luo, B.-H.; Xiao, T.; Zhang, C.; Nishida, N.; Springer, T.A.
Deposited on : 2008-11-22
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

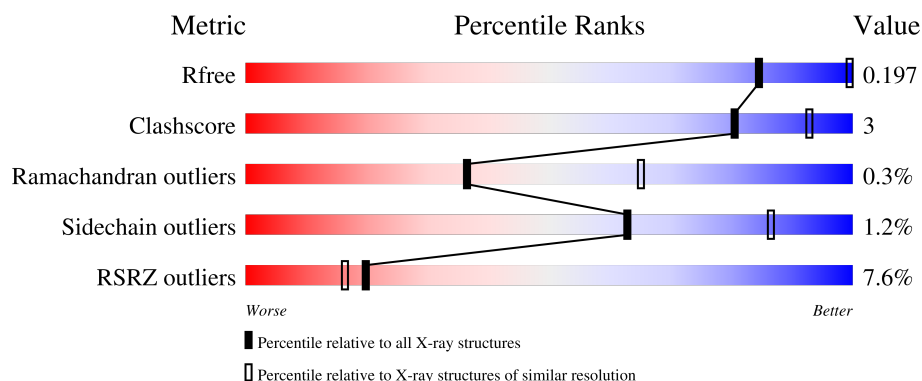
1 Overall quality at a glance

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))
R_{free}	180053	2481 (2.90-2.90)
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	A	457	4% 91% 9%
1	C	457	2% 94% 5%
1	E	457	2% 93% 5%
2	B	461	8% 92% 7%
2	D	461	13% 91% 8%

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Mol	Chain	Length	Quality of chain
2	F	461	
3	G	5	
3	I	5	
4	H	4	

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
3	MAN	G	3	X	-	-	-
3	MAN	I	3	X	-	-	-
4	MAN	H	3	X	-	-	-

2 Entry composition [i](#)

There are 9 unique types of molecules in this entry. The entry contains 21657 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.

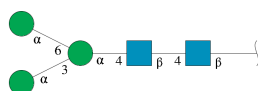
- Molecule 1 is a protein called Integrin, alpha 2b.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	457	Total	C	N	O	S	0	1	0
			3511	2230	606	667	8			
1	C	451	Total	C	N	O	S	0	2	0
			3477	2207	602	660	8			
1	E	452	Total	C	N	O	S	0	2	0
			3485	2213	603	661	8			

- Molecule 2 is a protein called Integrin beta-3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	455	Total	C	N	O	S	0	0	0
			3521	2196	601	692	32			
2	D	455	Total	C	N	O	S	0	0	0
			3521	2196	601	692	32			
2	F	455	Total	C	N	O	S	0	0	0
			3521	2196	601	692	32			

- Molecule 3 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-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	G	5	Total	C	N	O	0	0	0
			61	34	2	25			
3	I	5	Total	C	N	O	0	0	0
			61	34	2	25			

- Molecule 4 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-alpha-D-mannopyran

ose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.

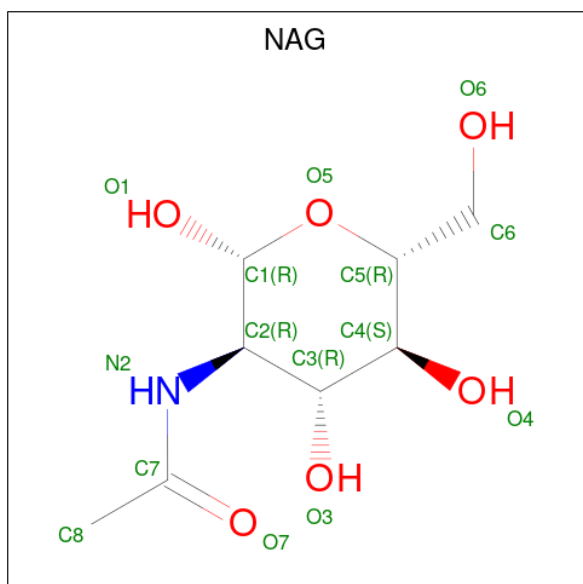


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	H	4	Total	C	N	O	0	0	0
			50	28	2	20			

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	4	Total	Ca	0	0
			4	4		
5	B	2	Total	Ca	0	0
			2	2		
5	C	4	Total	Ca	0	0
			4	4		
5	D	2	Total	Ca	0	0
			2	2		
5	E	4	Total	Ca	0	0
			4	4		
5	F	2	Total	Ca	0	0
			2	2		

- Molecule 6 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).

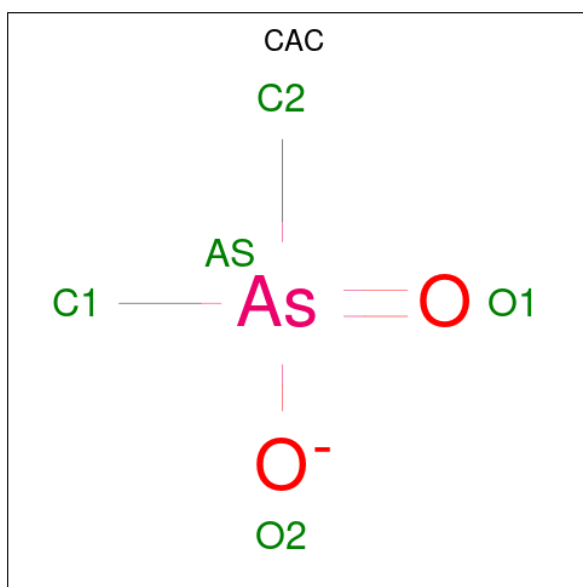


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total C N O 14 8 1 5	0	0
6	B	1	Total C N O 14 8 1 5	0	0
6	B	1	Total C N O 14 8 1 5	0	0
6	C	1	Total C N O 14 8 1 5	0	0
6	D	1	Total C N O 14 8 1 5	0	0
6	D	1	Total C N O 14 8 1 5	0	0
6	E	1	Total C N O 14 8 1 5	0	0
6	F	1	Total C N O 14 8 1 5	0	0

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total Mg 1 1	0	0
7	B	1	Total Mg 1 1	0	0
7	C	1	Total Mg 1 1	0	0
7	D	1	Total Mg 1 1	0	0
7	E	1	Total Mg 1 1	0	0
7	F	1	Total Mg 1 1	0	0

- Molecule 8 is CACODYLATE ION (CCD ID: CAC) (formula: C₂H₆AsO₂).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	B	1	Total	As	C	O	0	0
			5	1	2	2		
8	D	1	Total	As	C	O	0	0
			5	1	2	2		
8	F	1	Total	As	C	O	0	0
			5	1	2	2		

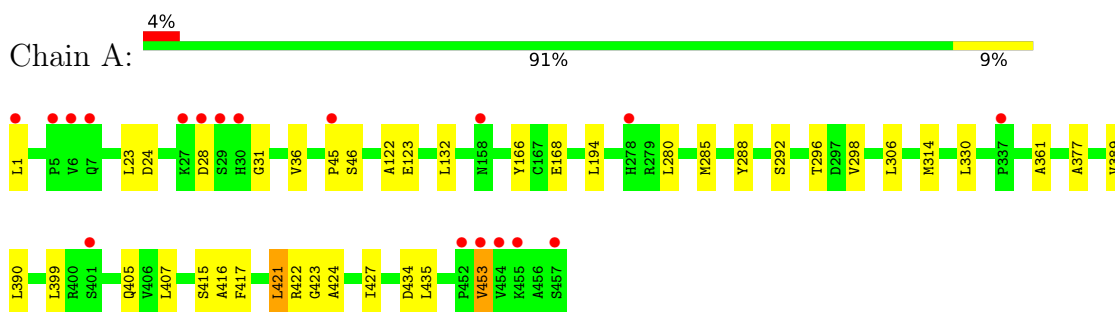
- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	191	Total	O	0	0
			191	191		
9	C	56	Total	O	0	0
			56	56		
9	E	51	Total	O	0	0
			51	51		

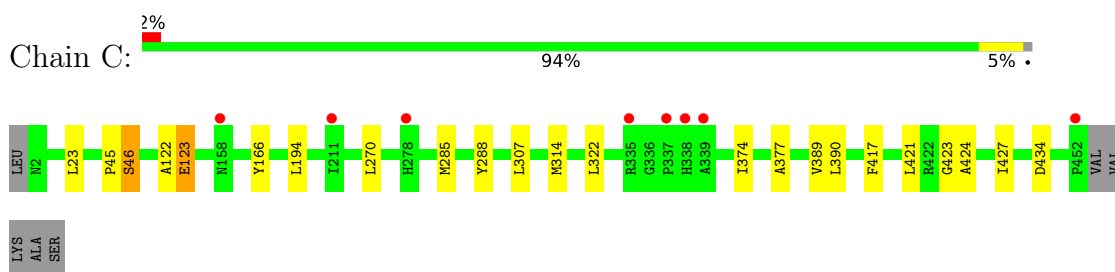
3 Residue-property plots [i](#)

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

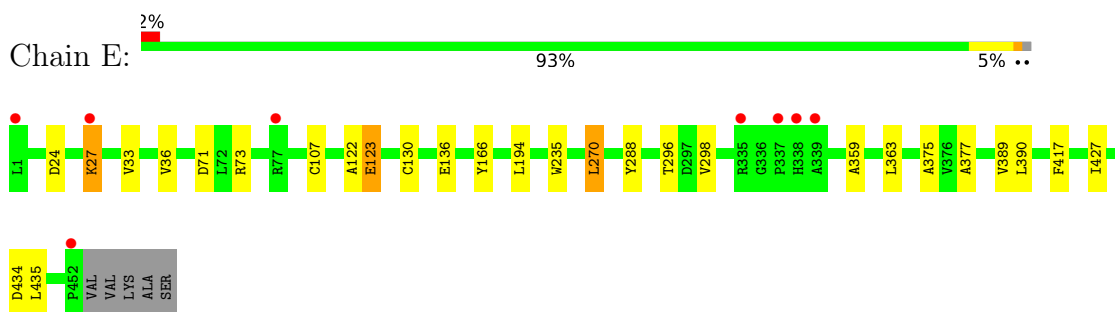
- Molecule 1: Integrin, alpha 2b



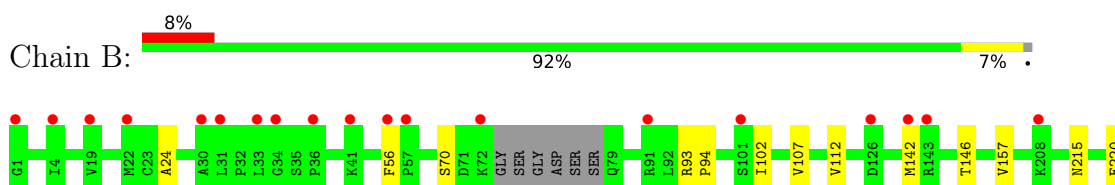
- Molecule 1: Integrin, alpha 2b

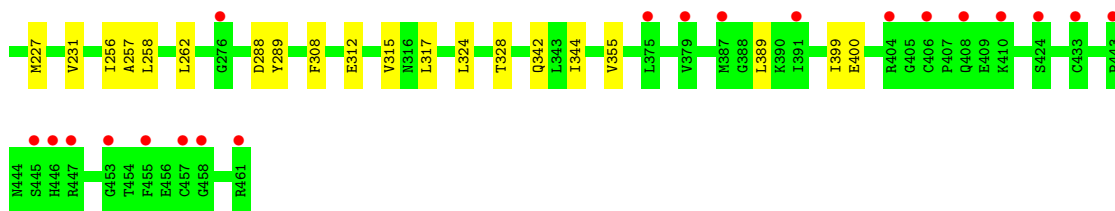


- Molecule 1: Integrin, alpha 2b

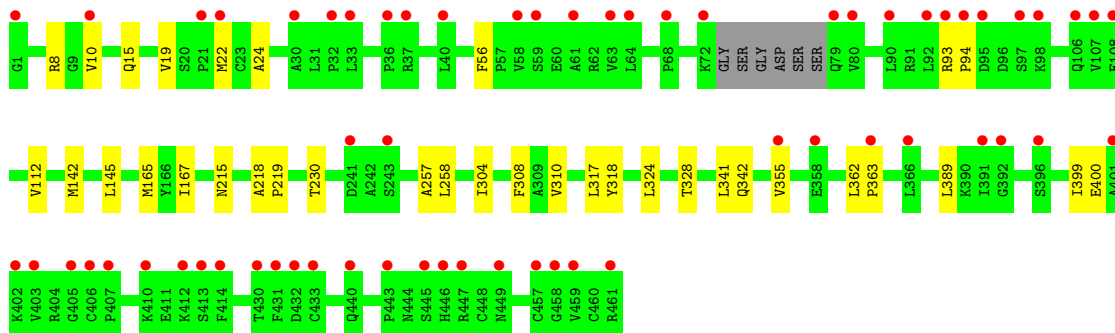
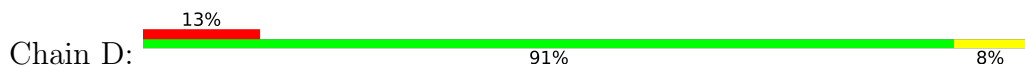


- Molecule 2: Integrin beta-3

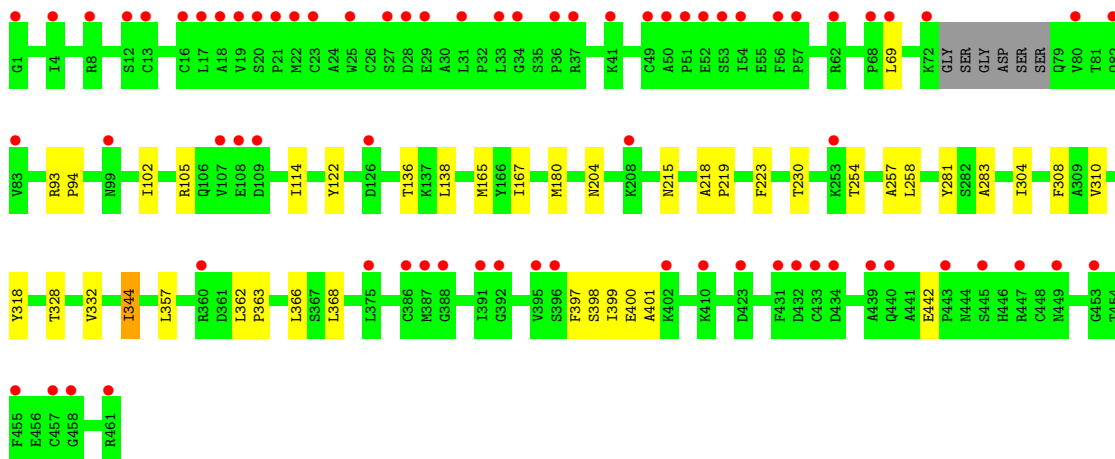
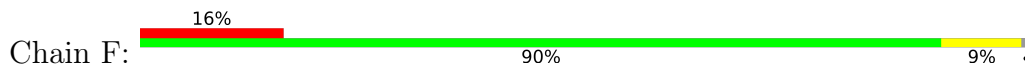




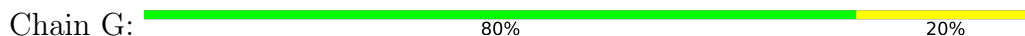
● Molecule 2: Integrin beta-3



● Molecule 2: Integrin beta-3



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



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

nose

Chain I:  80% 20%



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

Chain H:  75% 25%



4 Data and refinement statistics

Property	Value	Source
Space group	P 62	Depositor
Cell constants a, b, c, α , β , γ	332.09Å 332.09Å 88.29Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	44.59 – 2.90 44.59 – 2.90	Depositor EDS
% Data completeness (in resolution range)	95.2 (44.59-2.90) 95.4 (44.59-2.90)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	0.10	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.32 (at 2.90Å)	Xtriage
Refinement program	REFMAC 5.4.0066	Depositor
R, R_{free}	0.174 , 0.197 0.177 , 0.197	Depositor DCC
R_{free} test set	3098 reflections (2.49%)	wwPDB-VP
Wilson B-factor (Å ²)	63.7	Xtriage
Anisotropy	0.057	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 75.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.018 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	21657	wwPDB-VP
Average B, all atoms (Å ²)	70.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.65% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: CAC, MAN, MG, CA, NAG

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	0.45	0/3608	0.58	0/4916
1	C	0.44	0/3577	0.58	0/4873
1	E	0.44	0/3585	0.59	0/4884
2	B	0.43	0/3584	0.58	0/4858
2	D	0.43	0/3584	0.59	0/4858
2	F	0.43	0/3584	0.59	0/4858
All	All	0.44	0/21522	0.58	0/29247

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3511	0	3345	22	0
1	C	3477	0	3303	12	0
1	E	3485	0	3317	16	0
2	B	3521	0	3455	21	0
2	D	3521	0	3455	19	0
2	F	3521	0	3456	25	0
3	G	61	0	52	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	I	61	0	52	0	0
4	H	50	0	43	0	0
5	A	4	0	0	0	0
5	B	2	0	0	0	0
5	C	4	0	0	0	0
5	D	2	0	0	0	0
5	E	4	0	0	0	0
5	F	2	0	0	0	0
6	A	14	0	13	0	0
6	B	28	0	26	1	0
6	C	14	0	13	0	0
6	D	28	0	26	1	0
6	E	14	0	13	0	0
6	F	14	0	13	1	0
7	A	1	0	0	0	0
7	B	1	0	0	0	0
7	C	1	0	0	0	0
7	D	1	0	0	0	0
7	E	1	0	0	0	0
7	F	1	0	0	0	0
8	B	5	0	0	0	0
8	D	5	0	0	0	0
8	F	5	0	0	0	0
9	A	191	0	0	0	0
9	C	56	0	0	0	0
9	E	51	0	0	1	0
All	All	21657	0	20582	110	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 3.

All (110) 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:D:112:VAL:HG11	2:D:142:MET:HE2	1.57	0.85
1:A:427:ILE:HG22	1:A:434:ASP:OD1	1.91	0.70
2:B:112:VAL:HG11	2:B:142:MET:HE3	1.75	0.68
2:F:138:LEU:CD2	2:F:344:ILE:HD12	2.26	0.66
2:D:230:THR:HG23	2:D:304:ILE:HD12	1.79	0.63
2:D:8:ARG:HB2	2:D:10:VAL:HG13	1.80	0.62
2:F:138:LEU:HD23	2:F:344:ILE:HD12	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:427:ILE:HG22	1:C:434:ASP:OD1	2.03	0.59
1:E:427:ILE:HG22	1:E:434:ASP:OD1	2.03	0.59
2:F:400:GLU:HB2	6:F:3371:NAG:H83	1.86	0.58
2:F:223:PHE:CZ	2:F:254:THR:HG21	2.40	0.57
1:E:363:LEU:HD21	1:E:435:LEU:HD13	1.86	0.57
2:D:308:PHE:CE2	2:D:328:THR:HG21	2.40	0.57
2:B:142:MET:HE2	2:B:344:ILE:HG23	1.85	0.57
1:A:377:ALA:HB2	1:A:421:LEU:HD22	1.86	0.57
2:D:400:GLU:HB2	6:D:3371:NAG:H83	1.86	0.57
2:F:281:TYR:CE1	2:F:283:ALA:HB3	2.41	0.55
1:A:330:LEU:HD22	1:A:399:LEU:HD12	1.89	0.54
2:B:400:GLU:HB2	6:B:3371:NAG:H83	1.90	0.53
1:C:194:LEU:C	1:C:194:LEU:HD12	2.34	0.53
2:F:218:ALA:HB3	2:F:219:PRO:HD3	1.91	0.52
1:E:122:ALA:O	1:E:123:GLU:HB2	2.08	0.52
1:C:122:ALA:O	1:C:123:GLU:HB2	2.09	0.52
2:B:355:VAL:HG23	2:B:389:LEU:HD22	1.91	0.52
1:A:1:LEU:HD12	1:A:405:GLN:HG3	1.92	0.51
2:D:218:ALA:HB3	2:D:219:PRO:HD3	1.93	0.51
1:C:45:PRO:O	1:C:46:SER:CB	2.57	0.51
2:B:256:ILE:HD12	9:E:494:HOH:O	2.09	0.51
2:B:102:ILE:HG22	2:B:399:ILE:HD11	1.93	0.51
2:F:308:PHE:CE2	2:F:328:THR:HG21	2.45	0.51
1:C:377:ALA:HB2	1:C:421:LEU:HD11	1.93	0.50
1:A:285:MET:HE1	2:B:317:LEU:HD12	1.94	0.50
1:A:132:LEU:HD12	1:A:132:LEU:N	2.28	0.49
2:F:230:THR:HG23	2:F:304:ILE:HD12	1.93	0.49
2:D:112:VAL:HG21	2:D:142:MET:CE	2.42	0.49
1:E:235:TRP:HZ2	1:E:270:LEU:HD11	1.77	0.49
1:E:296:THR:HG23	1:E:298:VAL:HG13	1.94	0.49
1:C:389:VAL:HG23	1:C:417:PHE:CE2	2.47	0.48
2:B:142:MET:HE2	2:B:344:ILE:CG2	2.43	0.48
2:F:138:LEU:HD22	2:F:344:ILE:HD12	1.96	0.48
2:B:24:ALA:HB2	2:B:56:PHE:CD1	2.49	0.47
1:E:24:ASP:O	1:E:36:VAL:HG12	2.13	0.47
1:A:122:ALA:O	1:A:123:GLU:HB2	2.14	0.47
2:F:114:ILE:HD13	2:F:344:ILE:HD11	1.96	0.47
2:D:257:ALA:O	2:D:258:LEU:HB2	2.15	0.47
2:F:399:ILE:HD12	2:F:399:ILE:N	2.30	0.47
2:B:257:ALA:O	2:B:258:LEU:HB2	2.15	0.46
2:B:312:GLU:O	2:B:315:VAL:HG12	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:332:VAL:HG13	2:F:332:VAL:O	2.14	0.46
1:E:71:ASP:OD1	1:E:73:ARG:HD3	2.16	0.46
1:A:314:MET:HE1	2:B:324:LEU:HB3	1.97	0.46
2:D:15:GLN:O	2:D:19:VAL:HG23	2.15	0.46
1:E:390:LEU:HD12	1:E:390:LEU:N	2.31	0.46
1:C:390:LEU:HD12	1:C:390:LEU:N	2.31	0.46
2:D:112:VAL:CG1	2:D:142:MET:HE2	2.38	0.45
2:F:93:ARG:HB2	2:F:94:PRO:HD2	1.98	0.45
1:E:363:LEU:CD2	1:E:435:LEU:HD13	2.46	0.45
1:A:280:LEU:HD11	1:A:306:LEU:HD23	1.99	0.45
2:D:165:MET:HE3	2:D:167:ILE:HG22	1.99	0.45
2:B:112:VAL:HG11	2:B:142:MET:CE	2.45	0.45
2:B:308:PHE:CE2	2:B:328:THR:HG21	2.52	0.45
1:A:280:LEU:CD1	1:A:306:LEU:HD23	2.46	0.45
2:B:93:ARG:HB2	2:B:94:PRO:HD2	1.99	0.45
2:F:357:LEU:HD11	2:F:397:PHE:CD2	2.51	0.45
2:F:362:LEU:HD12	2:F:363:PRO:HD2	1.97	0.45
2:F:368:LEU:HD23	2:F:401:ALA:HA	1.98	0.44
1:E:363:LEU:HD11	1:E:375:ALA:HB2	1.99	0.44
2:D:355:VAL:HG23	2:D:389:LEU:HD22	2.00	0.44
2:D:93:ARG:HB2	2:D:94:PRO:HD2	1.99	0.44
2:B:70:SER:HB2	2:B:107:VAL:HG11	1.99	0.44
1:E:27:LYS:HG3	1:E:33:VAL:HG22	1.99	0.44
1:C:314:MET:HE3	1:C:322:LEU:HD13	1.99	0.44
2:F:102:ILE:CG2	2:F:397:PHE:HB2	2.48	0.43
1:A:390:LEU:HD12	1:A:390:LEU:N	2.33	0.43
2:B:142:MET:CE	2:B:344:ILE:HG23	2.48	0.43
1:E:194:LEU:HD12	1:E:194:LEU:C	2.42	0.43
1:A:24:ASP:O	1:A:36:VAL:HG12	2.18	0.43
2:F:69:LEU:HD13	2:F:105:ARG:HB2	2.00	0.43
2:D:310:VAL:HG11	2:D:318:TYR:CD2	2.53	0.43
1:C:307:LEU:HD11	1:C:374:ILE:HG21	2.01	0.43
1:E:107:CYS:HA	1:E:130:CYS:HA	2.00	0.43
1:C:285:MET:HE1	2:D:317:LEU:HD12	2.01	0.42
1:C:314:MET:HE1	2:D:324:LEU:HB3	2.02	0.42
2:F:310:VAL:HG11	2:F:318:TYR:CD2	2.53	0.42
2:B:157:VAL:O	2:B:220:GLU:HB3	2.19	0.42
1:A:194:LEU:HD12	1:A:194:LEU:C	2.44	0.42
1:A:415:SER:O	1:A:416:ALA:HB3	2.20	0.42
2:F:102:ILE:HG22	2:F:399:ILE:HD11	2.01	0.42
2:D:24:ALA:HB2	2:D:56:PHE:CD1	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:227:MET:O	2:B:231:VAL:HG22	2.19	0.41
1:A:389:VAL:HG23	1:A:417:PHE:CE2	2.55	0.41
1:E:389:VAL:HG23	1:E:417:PHE:CE2	2.55	0.41
1:A:296:THR:HG23	1:A:298:VAL:HG13	2.03	0.41
2:D:399:ILE:HD12	2:D:399:ILE:N	2.34	0.41
1:A:422:ARG:O	1:A:435:LEU:HD12	2.20	0.41
2:D:362:LEU:HD12	2:D:363:PRO:HD2	2.01	0.41
1:A:423:GLY:O	1:A:424:ALA:HB3	2.21	0.41
1:E:359:ALA:HB3	1:E:377:ALA:HB3	2.02	0.41
1:C:423:GLY:O	1:C:424:ALA:HB3	2.21	0.41
1:E:122:ALA:O	1:E:123:GLU:CB	2.69	0.41
2:F:363:PRO:HG2	2:F:366:LEU:HD12	2.03	0.41
1:A:168:GLU:OE1	2:B:262:LEU:O	2.39	0.40
1:A:361:ALA:HB2	1:A:421:LEU:HB3	2.01	0.40
1:A:377:ALA:HB2	1:A:421:LEU:CD2	2.50	0.40
2:B:288:ASP:OD1	2:B:289:TYR:N	2.54	0.40
2:F:165:MET:HE3	2:F:167:ILE:HG22	2.02	0.40
2:F:136:THR:HG22	2:F:204:ASN:OD1	2.21	0.40
2:F:257:ALA:O	2:F:258:LEU:HB2	2.21	0.40
1:A:405:GLN:NE2	1:A:407:LEU:HD21	2.36	0.40
2:F:122:TYR:CZ	2:F:180:MET:HE1	2.56	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	456/457 (100%)	435 (95%)	16 (4%)	5 (1%)	11	36
1	C	451/457 (99%)	436 (97%)	13 (3%)	2 (0%)	30	59
1	E	452/457 (99%)	440 (97%)	11 (2%)	1 (0%)	43	72
2	B	451/461 (98%)	437 (97%)	14 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	D	451/461 (98%)	435 (96%)	16 (4%)	0	100	100
2	F	451/461 (98%)	434 (96%)	17 (4%)	0	100	100
All	All	2712/2754 (98%)	2617 (96%)	87 (3%)	8 (0%)	36	65

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	46	SER
1	A	28	ASP
1	C	46	SER
1	A	31	GLY
1	E	123	GLU
1	C	123	GLU
1	A	45	PRO
1	A	453	VAL

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	365/364 (100%)	359 (98%)	6 (2%)	55	83
1	C	361/364 (99%)	357 (99%)	4 (1%)	65	88
1	E	362/364 (100%)	357 (99%)	5 (1%)	59	85
2	B	405/409 (99%)	402 (99%)	3 (1%)	76	92
2	D	405/409 (99%)	400 (99%)	5 (1%)	63	86
2	F	405/409 (99%)	401 (99%)	4 (1%)	68	89
All	All	2303/2319 (99%)	2276 (99%)	27 (1%)	63	86

All (27) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	23	LEU
1	A	166	TYR

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Mol	Chain	Res	Type
1	A	288	TYR
1	A	292	SER
1	A	421	LEU
1	A	453	VAL
2	B	146	THR
2	B	215	ASN
2	B	342	GLN
1	C	23	LEU
1	C	166	TYR
1	C	270	LEU
1	C	288	TYR
2	D	22	MET
2	D	145	LEU
2	D	215	ASN
2	D	341	LEU
2	D	342	GLN
1	E	27	LYS
1	E	136	GLU
1	E	166	TYR
1	E	270	LEU
1	E	288	TYR
2	F	215	ASN
2	F	344	ILE
2	F	398	SER
2	F	442	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (31) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	85	GLN
1	A	134	GLN
1	A	197	GLN
1	A	372	ASN
1	A	444	GLN
1	A	451	GLN
2	B	316	ASN
1	C	2	ASN
1	C	7	GLN
1	C	78	ASN
1	C	85	GLN
1	C	197	GLN
1	C	215	HIS

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Mol	Chain	Res	Type
1	C	219	GLN
1	C	275	GLN
1	C	443	ASN
1	C	444	GLN
2	D	316	ASN
2	D	319	GLN
2	D	428	GLN
1	E	30	HIS
1	E	85	GLN
1	E	134	GLN
1	E	197	GLN
1	E	372	ASN
1	E	395	GLN
1	E	444	GLN
2	F	316	ASN
2	F	342	GLN
2	F	428	GLN
2	F	449	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 ⓘ

14 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	G	1	2,3	14,14,15	0.53	0	17,19,21	0.95	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	NAG	G	2	3	14,14,15	0.54	0	17,19,21	0.56	0
3	MAN	G	3	3	11,11,12	0.59	0	15,15,17	0.65	0
3	MAN	G	4	3	11,11,12	0.57	0	15,15,17	0.62	0
3	MAN	G	5	3	11,11,12	0.54	0	15,15,17	0.65	0
4	NAG	H	1	2,4	14,14,15	0.56	0	17,19,21	0.87	1 (5%)
4	NAG	H	2	4	14,14,15	0.44	0	17,19,21	0.88	0
4	MAN	H	3	4	11,11,12	0.57	0	15,15,17	0.47	0
4	MAN	H	4	4	11,11,12	0.56	0	15,15,17	0.55	0
3	NAG	I	1	2,3	14,14,15	0.57	0	17,19,21	0.85	1 (5%)
3	NAG	I	2	3	14,14,15	0.51	0	17,19,21	0.59	0
3	MAN	I	3	3	11,11,12	0.55	0	15,15,17	0.51	0
3	MAN	I	4	3	11,11,12	0.52	0	15,15,17	0.61	0
3	MAN	I	5	3	11,11,12	0.53	0	15,15,17	0.67	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	G	1	2,3	-	0/6/23/26	0/1/1/1
3	NAG	G	2	3	-	1/6/23/26	0/1/1/1
3	MAN	G	3	3	1/1/4/5	2/2/19/22	0/1/1/1
3	MAN	G	4	3	-	1/2/19/22	0/1/1/1
3	MAN	G	5	3	-	2/2/19/22	0/1/1/1
4	NAG	H	1	2,4	-	2/6/23/26	0/1/1/1
4	NAG	H	2	4	-	1/6/23/26	0/1/1/1
4	MAN	H	3	4	1/1/4/5	0/2/19/22	0/1/1/1
4	MAN	H	4	4	-	0/2/19/22	0/1/1/1
3	NAG	I	1	2,3	-	0/6/23/26	0/1/1/1
3	NAG	I	2	3	-	0/6/23/26	0/1/1/1
3	MAN	I	3	3	1/1/4/5	0/2/19/22	0/1/1/1
3	MAN	I	4	3	-	0/2/19/22	0/1/1/1
3	MAN	I	5	3	-	2/2/19/22	0/1/1/1

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	G	1	NAG	C1-O5-C5	2.98	116.17	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	H	1	NAG	C1-O5-C5	2.56	115.62	112.19
3	I	1	NAG	C1-O5-C5	2.12	115.03	112.19

All (3) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	G	3	MAN	C1
3	I	3	MAN	C1
4	H	3	MAN	C1

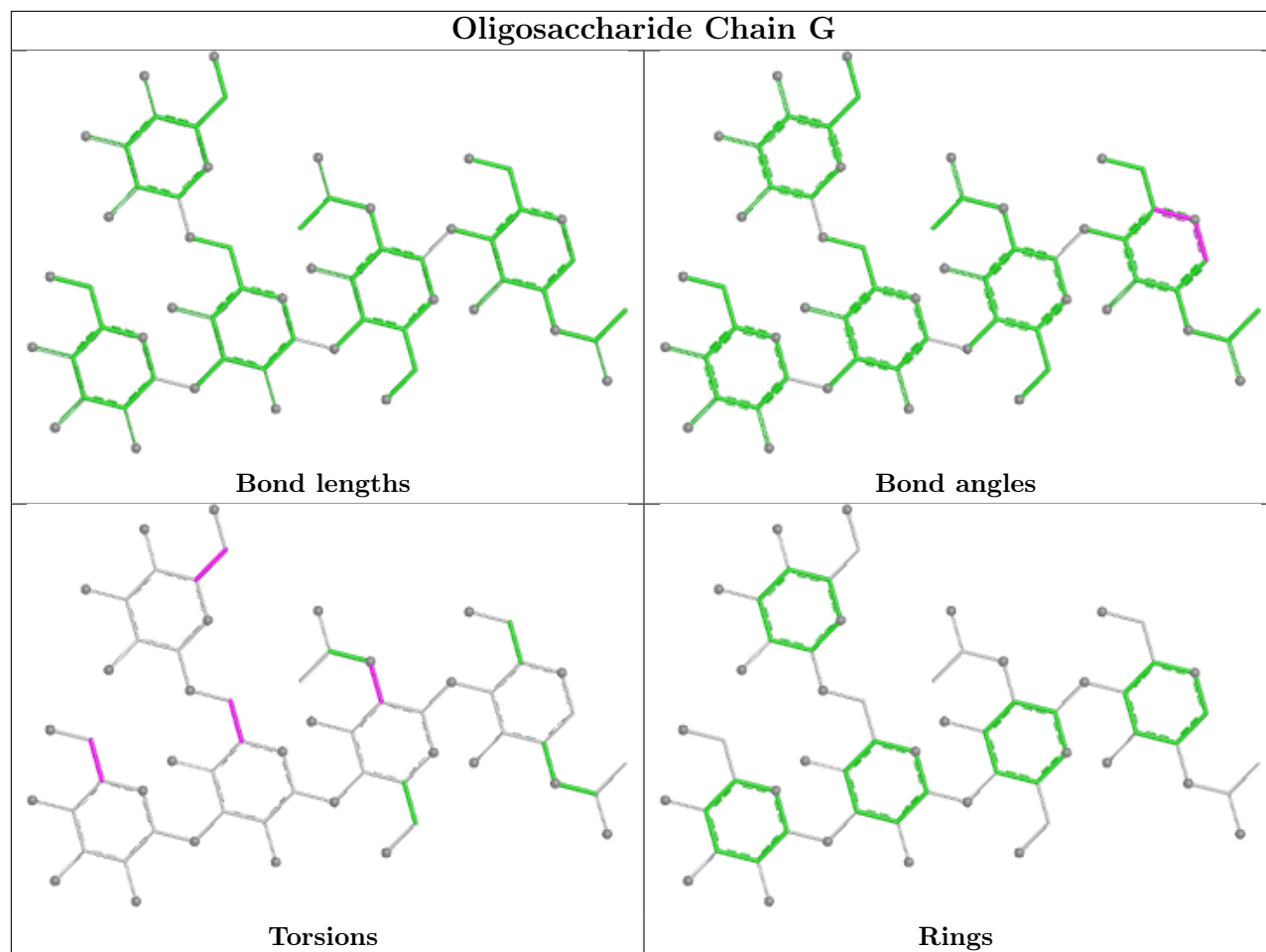
All (11) torsion outliers are listed below:

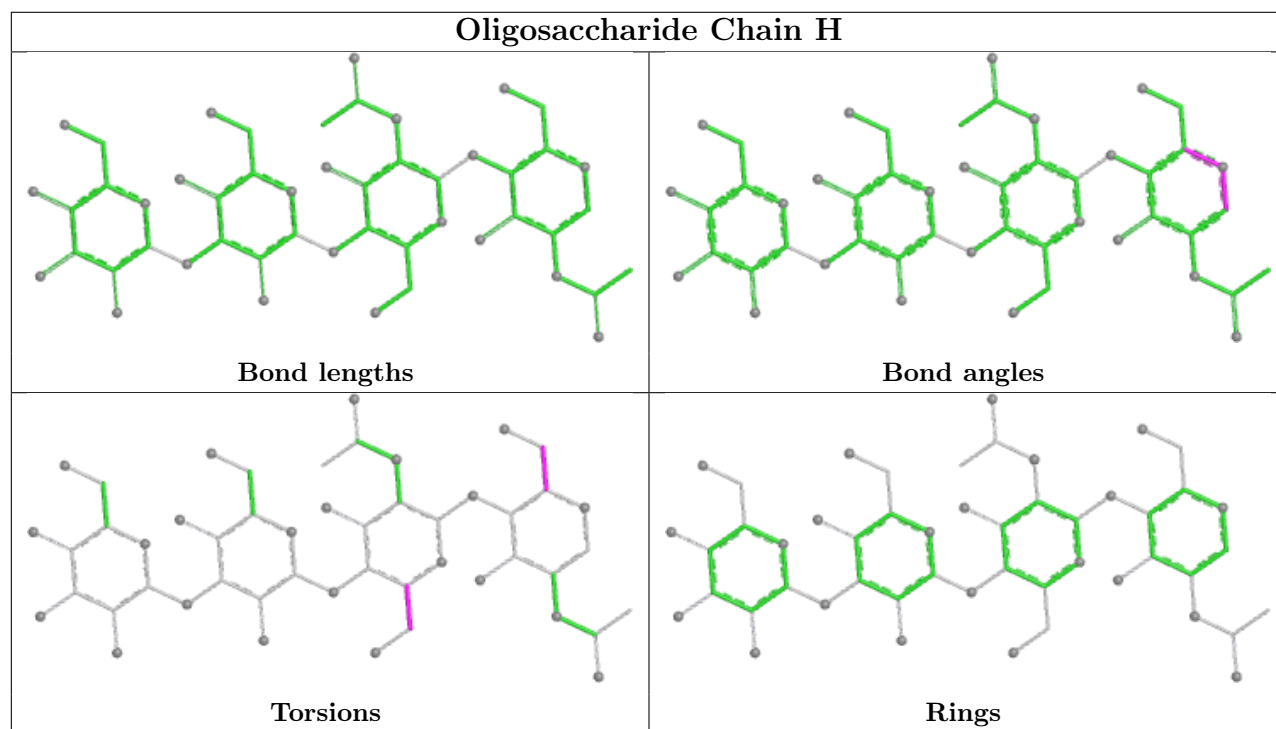
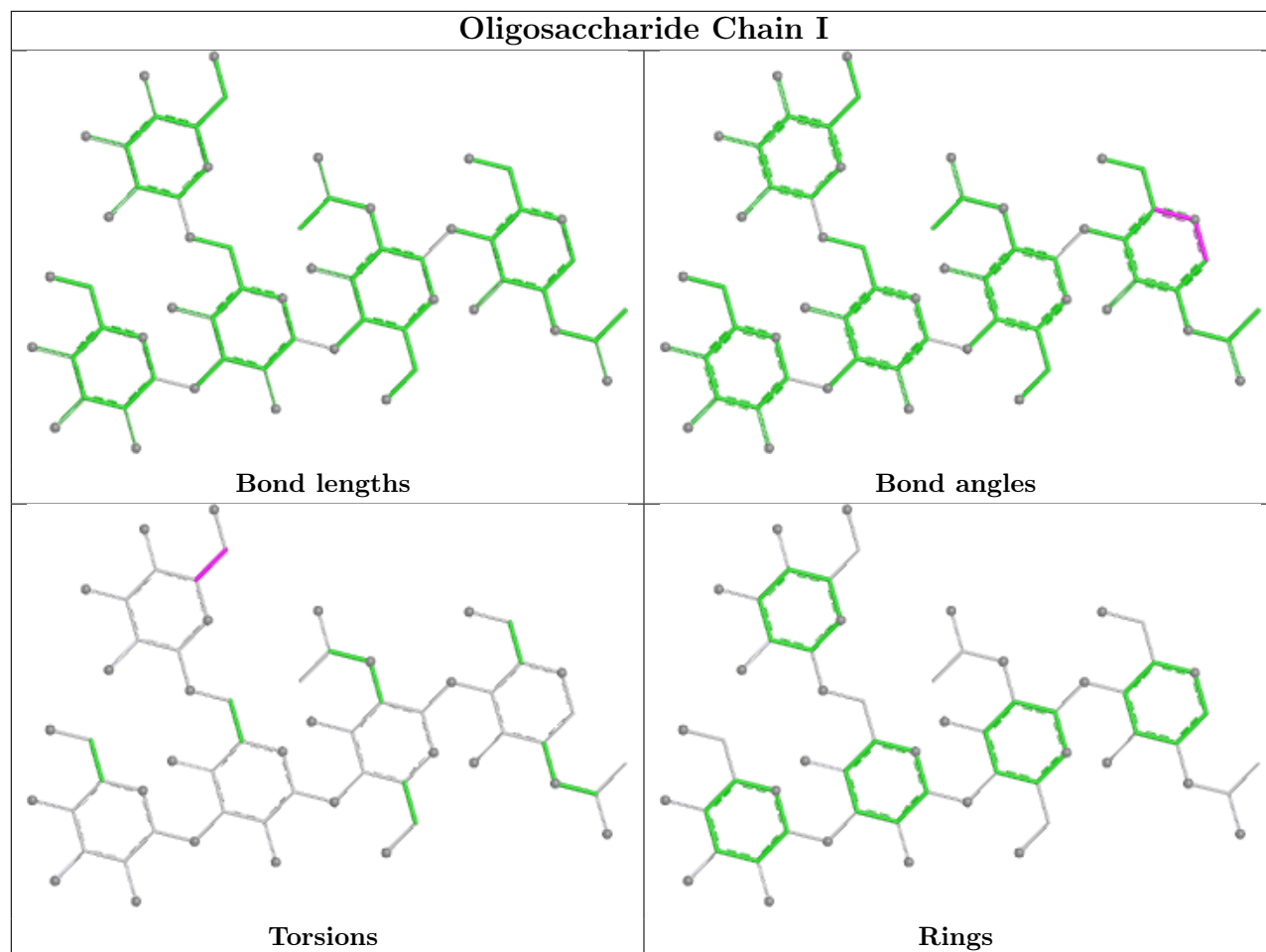
Mol	Chain	Res	Type	Atoms
3	I	5	MAN	O5-C5-C6-O6
3	I	5	MAN	C4-C5-C6-O6
3	G	5	MAN	O5-C5-C6-O6
3	G	5	MAN	C4-C5-C6-O6
4	H	1	NAG	O5-C5-C6-O6
4	H	1	NAG	C4-C5-C6-O6
3	G	3	MAN	C4-C5-C6-O6
3	G	3	MAN	O5-C5-C6-O6
3	G	4	MAN	C4-C5-C6-O6
4	H	2	NAG	O5-C5-C6-O6
3	G	2	NAG	C1-C2-N2-C7

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

Of 35 ligands modelled in this entry, 24 are monoatomic - leaving 11 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
6	NAG	E	3015	1	14,14,15	0.64	0	17,19,21	0.64	0
6	NAG	D	3099	2	14,14,15	0.66	0	17,19,21	0.73	0
8	CAC	D	462	-	2,4,4	2.79	2 (100%)	4,6,6	1.38	0
8	CAC	F	462	-	2,4,4	2.73	2 (100%)	4,6,6	1.41	0
6	NAG	C	3015	1	14,14,15	0.47	0	17,19,21	0.68	0
6	NAG	A	3015	1	14,14,15	0.61	0	17,19,21	0.61	0
6	NAG	F	3371	2	14,14,15	0.51	0	17,19,21	0.64	0
8	CAC	B	462	-	2,4,4	2.75	2 (100%)	4,6,6	1.56	0
6	NAG	B	3371	2	14,14,15	0.48	0	17,19,21	0.60	0
6	NAG	D	3371	2	14,14,15	0.46	0	17,19,21	0.61	0
6	NAG	B	3099	2	14,14,15	0.57	0	17,19,21	0.58	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
6	NAG	E	3015	1	-	2/6/23/26	0/1/1/1
6	NAG	D	3099	2	-	2/6/23/26	0/1/1/1
6	NAG	C	3015	1	-	1/6/23/26	0/1/1/1
6	NAG	A	3015	1	-	2/6/23/26	0/1/1/1
6	NAG	F	3371	2	-	0/6/23/26	0/1/1/1
6	NAG	B	3371	2	-	0/6/23/26	0/1/1/1
6	NAG	D	3371	2	-	0/6/23/26	0/1/1/1
6	NAG	B	3099	2	-	2/6/23/26	0/1/1/1

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	D	462	CAC	AS-C1	2.93	1.97	1.90
8	B	462	CAC	AS-C2	2.89	1.97	1.90
8	F	462	CAC	AS-C1	2.83	1.97	1.90
8	D	462	CAC	AS-C2	2.65	1.96	1.90
8	F	462	CAC	AS-C2	2.63	1.96	1.90
8	B	462	CAC	AS-C1	2.61	1.96	1.90

There are no bond angle outliers.

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	E	3015	NAG	O5-C5-C6-O6
6	B	3099	NAG	O5-C5-C6-O6
6	A	3015	NAG	O5-C5-C6-O6
6	E	3015	NAG	C4-C5-C6-O6
6	A	3015	NAG	C4-C5-C6-O6
6	B	3099	NAG	C4-C5-C6-O6
6	D	3099	NAG	C4-C5-C6-O6
6	D	3099	NAG	O5-C5-C6-O6
6	C	3015	NAG	O5-C5-C6-O6

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	F	3371	NAG	1	0
6	B	3371	NAG	1	0
6	D	3371	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	A	457/457 (100%)	0.09	18 (3%) 43 35	27, 52, 90, 144	1 (0%)
1	C	451/457 (98%)	0.11	8 (1%) 67 59	30, 52, 85, 133	2 (0%)
1	E	452/457 (98%)	-0.10	8 (1%) 67 59	27, 52, 85, 133	2 (0%)
2	B	455/461 (98%)	0.66	39 (8%) 16 13	45, 80, 125, 139	1 (0%)
2	D	455/461 (98%)	0.74	62 (13%) 7 5	45, 80, 125, 139	1 (0%)
2	F	455/461 (98%)	0.97	72 (15%) 5 4	45, 80, 124, 139	1 (0%)
All	All	2725/2754 (98%)	0.41	207 (7%) 20 16	27, 60, 122, 144	8 (0%)

All (207) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	453	VAL	6.7
1	A	454	VAL	6.3
2	F	21	PRO	5.9
1	A	457	SER	4.9
2	F	439	ALA	4.9
2	D	433	CYS	4.5
2	D	431	PHE	4.3
1	A	455	LYS	4.2
2	F	20	SER	4.1
2	F	107	VAL	4.0
1	E	1	LEU	3.9
1	C	337	PRO	3.9
1	C	452	PRO	3.9
2	F	410	LYS	3.9
2	F	22	MET	3.9
2	D	410	LYS	3.8
2	D	107	VAL	3.8
2	F	41	LYS	3.8
1	A	6	VAL	3.7

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Mol	Chain	Res	Type	RSRZ
2	B	30	ALA	3.7
2	D	93	ARG	3.7
1	E	452	PRO	3.7
2	B	1	GLY	3.6
2	F	458	GLY	3.6
1	A	1	LEU	3.5
1	A	7	GLN	3.4
2	D	92	LEU	3.4
2	D	432	ASP	3.4
2	F	51	PRO	3.4
2	F	455	PHE	3.4
2	B	33	LEU	3.3
1	E	77[A]	ARG	3.3
2	B	447	ARG	3.3
2	D	458	GLY	3.2
2	D	94	PRO	3.2
2	F	4	ILE	3.2
2	D	33	LEU	3.2
2	D	446	HIS	3.2
2	B	142	MET	3.2
2	F	68	PRO	3.2
2	D	108	GLU	3.1
2	B	445	SER	3.1
2	B	446	HIS	3.0
2	F	17	LEU	3.0
2	F	108	GLU	3.0
2	D	405	GLY	3.0
2	D	30	ALA	3.0
2	F	19	VAL	3.0
1	E	335	ARG	2.9
2	B	453	GLY	2.9
1	A	337	PRO	2.9
2	B	4	ILE	2.9
2	F	433	CYS	2.9
2	F	34	GLY	2.9
1	A	28	ASP	2.9
2	B	424	SER	2.9
1	C	335	ARG	2.8
2	B	19	VAL	2.8
2	B	72	LYS	2.8
2	F	13	CYS	2.8
1	E	337	PRO	2.8

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Mol	Chain	Res	Type	RSRZ
2	B	408	GLN	2.8
2	F	80	VAL	2.8
2	F	33	LEU	2.8
2	F	69	LEU	2.8
1	C	278[A]	HIS	2.8
2	B	443	PRO	2.8
2	D	403	VAL	2.7
2	F	83	VAL	2.7
2	F	56	PHE	2.7
2	B	461	ARG	2.7
2	D	79	GLN	2.7
2	F	82	GLN	2.7
2	D	64	LEU	2.7
2	D	72	LYS	2.7
2	B	34	GLY	2.7
2	F	440	GLN	2.7
2	B	458	GLY	2.7
2	D	363	PRO	2.7
1	C	339	ALA	2.6
2	D	32	PRO	2.6
2	F	423	ASP	2.6
2	D	445	SER	2.6
1	A	5	PRO	2.6
2	D	443	PRO	2.6
2	F	1	GLY	2.6
2	F	57	PRO	2.6
2	B	410	LYS	2.6
2	D	58	VAL	2.6
2	B	455	PHE	2.6
2	D	430	THR	2.5
2	F	432	ASP	2.5
2	F	25	TRP	2.5
2	F	8	ARG	2.5
2	F	447	ARG	2.5
2	D	22	MET	2.5
2	D	407	PRO	2.5
2	F	54	ILE	2.5
2	F	208	LYS	2.5
2	B	375	LEU	2.4
2	D	95	ASP	2.4
2	D	355	VAL	2.4
2	D	414	PHE	2.4

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Mol	Chain	Res	Type	RSRZ
2	D	98	LYS	2.4
2	D	449	ASN	2.4
2	B	457	CYS	2.4
2	D	106	GLN	2.4
2	D	401	ALA	2.4
1	A	278[A]	HIS	2.4
2	F	387	MET	2.4
2	F	375	LEU	2.4
2	B	208	LYS	2.4
2	F	62	ARG	2.4
2	F	434	ASP	2.4
2	D	21	PRO	2.4
2	B	126	ASP	2.3
2	D	406	CYS	2.3
1	A	29	SER	2.3
2	B	101	SER	2.3
2	D	97	SER	2.3
2	D	243	SER	2.3
2	B	276	GLY	2.3
2	D	1	GLY	2.3
1	C	211	ILE	2.3
1	A	45	PRO	2.3
2	D	37	ARG	2.3
2	D	68	PRO	2.3
2	B	56	PHE	2.3
2	B	22	MET	2.3
2	B	31	LEU	2.3
2	F	253	LYS	2.3
2	F	431	PHE	2.2
1	E	339	ALA	2.2
2	D	412	LYS	2.2
2	F	402	LYS	2.2
1	A	30	HIS	2.2
2	F	49	CYS	2.2
2	F	395	VAL	2.2
2	D	61	ALA	2.2
2	F	18	ALA	2.2
2	B	41	LYS	2.2
2	D	90	LEU	2.2
2	B	91	ARG	2.2
2	D	461	ARG	2.2
2	D	10	VAL	2.2

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Mol	Chain	Res	Type	RSRZ
2	F	23	CYS	2.2
1	C	158	ASN	2.2
2	F	360	ARG	2.2
2	F	126	ASP	2.2
2	F	16	CYS	2.2
2	F	457	CYS	2.2
2	D	392	GLY	2.2
2	D	413	SER	2.2
2	D	402	LYS	2.2
2	D	80	VAL	2.2
2	F	443	PRO	2.2
2	F	72	LYS	2.2
2	F	50	ALA	2.2
1	E	27	LYS	2.1
2	D	40	LEU	2.1
2	F	12	SER	2.1
2	F	27	SER	2.1
2	B	404	ARG	2.1
2	F	37	ARG	2.1
2	B	391	ILE	2.1
1	E	338	HIS	2.1
2	D	63	VAL	2.1
2	D	241	ASP	2.1
1	A	401	SER	2.1
2	D	391	ILE	2.1
2	D	396	SER	2.1
2	F	386	CYS	2.1
2	F	391	ILE	2.1
2	F	396	SER	2.1
2	F	445	SER	2.1
2	B	387	MET	2.1
2	D	36	PRO	2.1
2	D	366	LEU	2.1
2	F	388	GLY	2.1
2	F	392	GLY	2.1
2	F	453	GLY	2.1
2	B	406	CYS	2.1
2	B	433	CYS	2.1
2	F	36	PRO	2.1
2	F	449	ASN	2.1
2	F	31	LEU	2.1
2	D	358	GLU	2.1

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Mol	Chain	Res	Type	RSRZ
2	D	59	SER	2.0
1	C	338	HIS	2.0
2	B	379	VAL	2.0
2	B	36	PRO	2.0
1	A	158	ASN	2.0
2	D	447	ARG	2.0
2	D	440	GLN	2.0
2	D	459	VAL	2.0
2	F	53	SER	2.0
1	A	452	PRO	2.0
2	B	57	PRO	2.0
2	D	457	CYS	2.0
2	B	143	ARG	2.0
2	F	99	ASN	2.0
2	F	461	ARG	2.0
2	F	28	ASP	2.0
2	F	29	GLU	2.0
2	F	52	GLU	2.0
2	F	109	ASP	2.0
1	A	27	LYS	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.

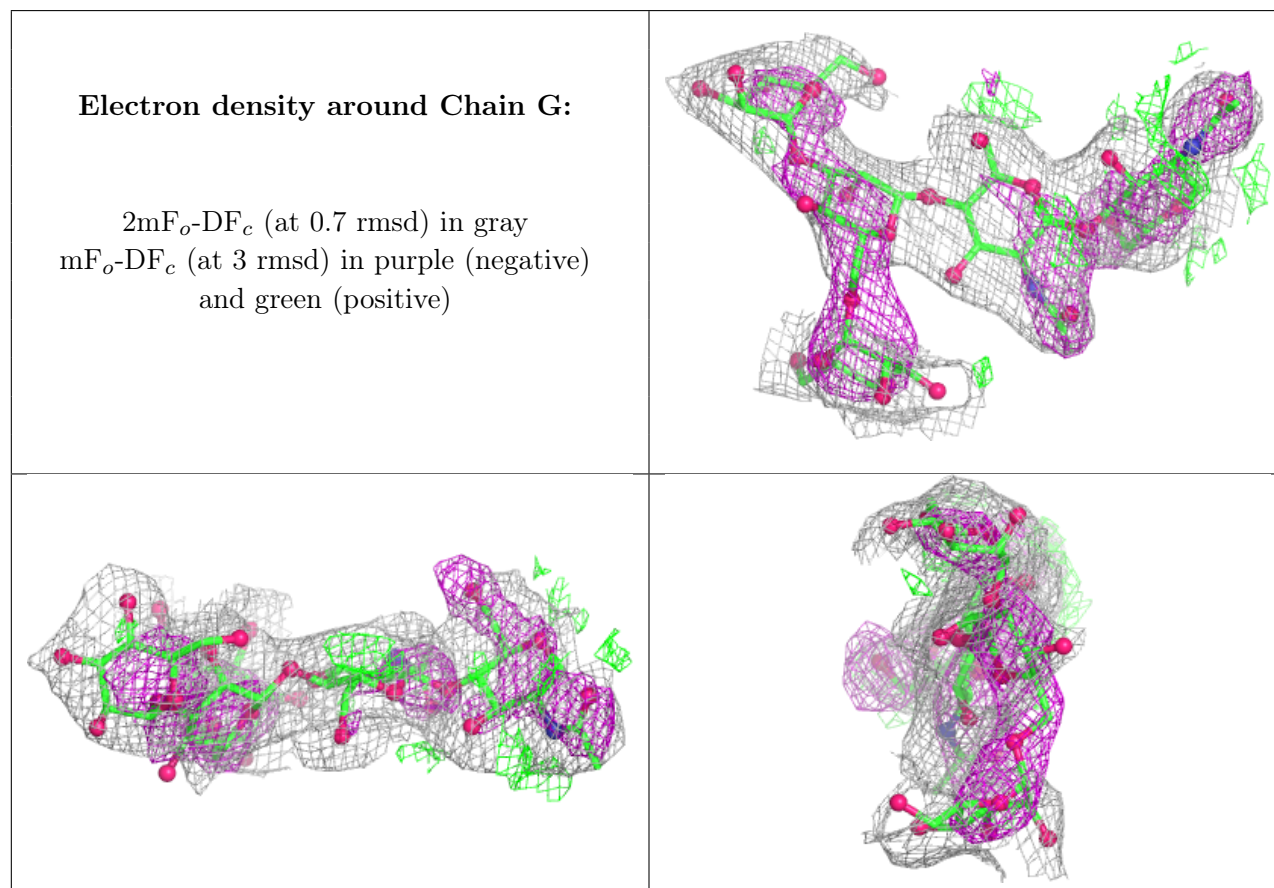
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	MAN	I	5	11/12	0.14	0.23	144,146,147,147	0
3	MAN	G	5	11/12	0.25	0.22	147,148,149,149	0
4	MAN	H	3	11/12	0.57	0.16	106,114,118,119	0
3	MAN	G	3	11/12	0.63	0.16	118,126,137,144	0
3	MAN	I	3	11/12	0.64	0.15	118,123,135,142	0
3	MAN	I	4	11/12	0.69	0.17	111,117,120,121	0
4	NAG	H	2	14/15	0.71	0.17	89,94,99,103	0
3	MAN	G	4	11/12	0.72	0.15	119,125,127,127	0

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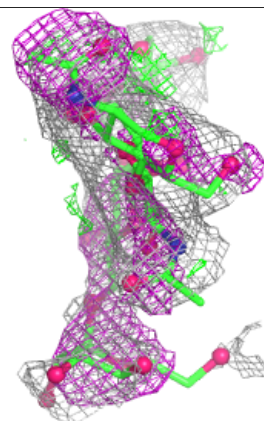
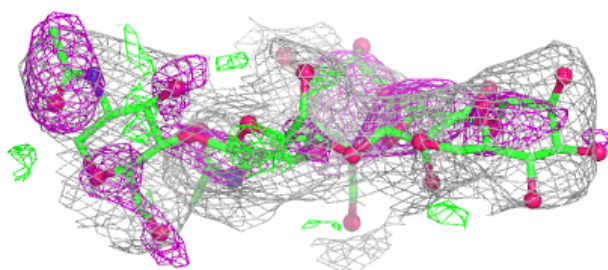
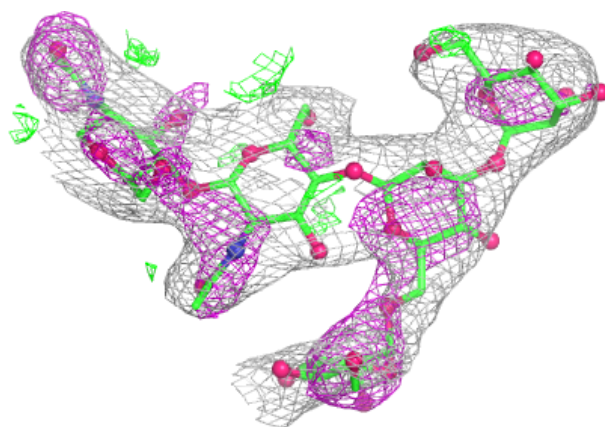
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	MAN	H	4	11/12	0.75	0.13	106,113,114,115	0
3	NAG	I	2	14/15	0.78	0.16	89,98,102,110	0
3	NAG	G	2	14/15	0.83	0.14	80,86,96,108	0
3	NAG	G	1	14/15	0.90	0.13	55,62,65,72	0
4	NAG	H	1	14/15	0.92	0.11	49,59,68,80	0
3	NAG	I	1	14/15	0.92	0.12	52,62,73,78	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.

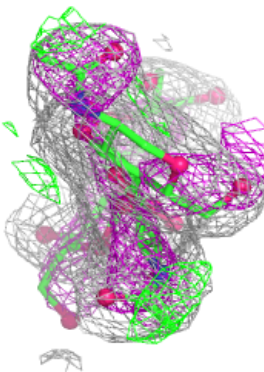
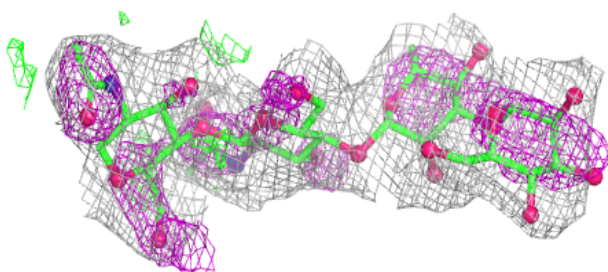
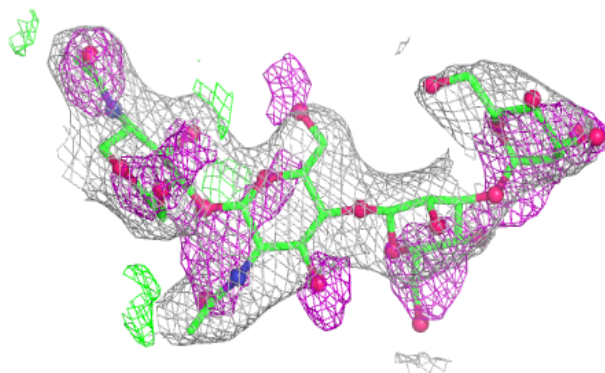


Electron density around Chain I:

$2mF_o-DF_c$ (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)



6.4 Ligands

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
6	NAG	A	3015	14/15	0.32	0.28	118,126,129,131	0
6	NAG	D	3099	14/15	0.40	0.18	128,131,135,135	0
6	NAG	B	3099	14/15	0.56	0.18	131,136,139,141	0
6	NAG	C	3015	14/15	0.57	0.18	117,124,126,127	0
6	NAG	D	3371	14/15	0.63	0.17	92,111,115,115	0
6	NAG	F	3371	14/15	0.66	0.16	117,123,126,127	0
6	NAG	B	3371	14/15	0.70	0.14	112,118,120,120	0
6	NAG	E	3015	14/15	0.71	0.24	104,106,108,108	14
7	MG	E	458	1/1	0.90	0.14	68,68,68,68	0
7	MG	A	458	1/1	0.91	0.11	61,61,61,61	0
8	CAC	F	462	5/5	0.91	0.30	122,122,124,126	0
8	CAC	B	462	5/5	0.92	0.30	103,106,109,109	0
5	CA	B	2002	1/1	0.93	0.07	72,72,72,72	0
8	CAC	D	462	5/5	0.94	0.27	91,96,99,101	0
7	MG	B	2001	1/1	0.95	0.07	39,39,39,39	0
5	CA	F	2002	1/1	0.96	0.04	66,66,66,66	0
7	MG	C	458	1/1	0.97	0.13	72,72,72,72	0
5	CA	D	2002	1/1	0.97	0.05	74,74,74,74	0
7	MG	F	2001	1/1	0.97	0.05	37,37,37,37	0
5	CA	C	2006	1/1	0.98	0.05	63,63,63,63	0
5	CA	C	2007	1/1	0.98	0.09	78,78,78,78	0
5	CA	A	2005	1/1	0.98	0.05	66,66,66,66	0
5	CA	C	2005	1/1	0.98	0.04	43,43,43,43	0
5	CA	E	2006	1/1	0.99	0.03	62,62,62,62	0
5	CA	E	2007	1/1	0.99	0.15	65,65,65,65	0
5	CA	A	2006	1/1	0.99	0.06	61,61,61,61	0
5	CA	F	2003	1/1	0.99	0.10	42,42,42,42	0
5	CA	A	2007	1/1	0.99	0.13	74,74,74,74	0
7	MG	D	2001	1/1	0.99	0.04	43,43,43,43	0
5	CA	A	2004	1/1	0.99	0.03	56,56,56,56	0
5	CA	B	2003	1/1	0.99	0.06	37,37,37,37	0
5	CA	D	2003	1/1	0.99	0.05	40,40,40,40	0
5	CA	E	2004	1/1	0.99	0.04	57,57,57,57	0
5	CA	E	2005	1/1	0.99	0.03	42,42,42,42	0
5	CA	C	2004	1/1	1.00	0.01	53,53,53,53	0

6.5 Other polymers [i](#)

There are no such residues in this entry.