



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 7, 2020 – 12:28 PM BST

PDB ID : 4YH6
Title : Crystal structure of IL1RAPL1 ectodomain
Authors : Yamagata, A.; Fukai, S.
Deposited on : 2015-02-27
Resolution : 3.00 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.13.1
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.13.1

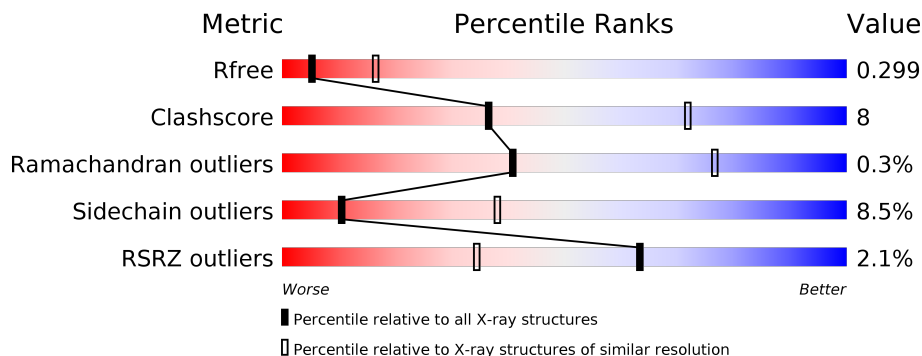
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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.




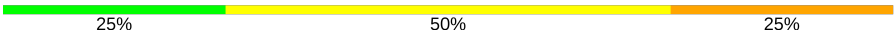
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (3.00-3.00)

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 on 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	348	<div style="display: flex; align-items: center;"> <div style="width: 2%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 66%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 21%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 10%; height: 10px; background-color: orange; margin-right: 5px;"></div> <div style="width: 1%; height: 10px; background-color: grey; margin-right: 5px;"></div> </div> <p style="font-size: small; margin-top: 5px;">2% 66% 21% 10%</p>
1	B	348	<div style="display: flex; align-items: center;"> <div style="width: 2%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 66%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 20%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 12%; height: 10px; background-color: orange; margin-right: 5px;"></div> <div style="width: 1%; height: 10px; background-color: grey; margin-right: 5px;"></div> </div> <p style="font-size: small; margin-top: 5px;">2% 66% 20% 12%</p>
2	C	3	<div style="display: flex; align-items: center;"> <div style="width: 33%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 33%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 33%; height: 10px; background-color: orange; margin-right: 5px;"></div> </div> <p style="font-size: small; margin-top: 5px;">33% 33% 33%</p>
2	F	3	<div style="display: flex; align-items: center;"> <div style="width: 67%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 33%; height: 10px; background-color: orange; margin-right: 5px;"></div> </div> <p style="font-size: small; margin-top: 5px;">67% 33%</p>
3	D	5	<div style="display: flex; align-items: center;"> <div style="width: 40%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 60%; height: 10px; background-color: orange; margin-right: 5px;"></div> </div> <p style="font-size: small; margin-top: 5px;">40% 60%</p>
3	E	5	<div style="display: flex; align-items: center;"> <div style="width: 40%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 40%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 20%; height: 10px; background-color: orange; margin-right: 5px;"></div> </div> <p style="font-size: small; margin-top: 5px;">40% 40% 20%</p>

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Mol	Chain	Length	Quality of chain
3	G	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	E	5	-	-	-	X

2 Entry composition i

There are 5 unique types of molecules in this entry. The entry contains 5288 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 Interleukin-1 receptor accessory protein-like 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	313	2519	1606	414	483	16	0	0	0
1	B	305	2444	1557	402	469	16	0	0	0

There are 28 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	12	ALA	-	expression tag	UNP P59823
A	13	GLN	-	expression tag	UNP P59823
A	14	PRO	-	expression tag	UNP P59823
A	15	ALA	-	expression tag	UNP P59823
A	16	ALA	-	expression tag	UNP P59823
A	17	ARG	-	expression tag	UNP P59823
A	18	ASP	-	expression tag	UNP P59823
A	353	LYS	-	expression tag	UNP P59823
A	354	HIS	-	expression tag	UNP P59823
A	355	HIS	-	expression tag	UNP P59823
A	356	HIS	-	expression tag	UNP P59823
A	357	HIS	-	expression tag	UNP P59823
A	358	HIS	-	expression tag	UNP P59823
A	359	HIS	-	expression tag	UNP P59823
B	12	ALA	-	expression tag	UNP P59823
B	13	GLN	-	expression tag	UNP P59823
B	14	PRO	-	expression tag	UNP P59823
B	15	ALA	-	expression tag	UNP P59823
B	16	ALA	-	expression tag	UNP P59823
B	17	ARG	-	expression tag	UNP P59823
B	18	ASP	-	expression tag	UNP P59823
B	353	LYS	-	expression tag	UNP P59823
B	354	HIS	-	expression tag	UNP P59823
B	355	HIS	-	expression tag	UNP P59823
B	356	HIS	-	expression tag	UNP P59823

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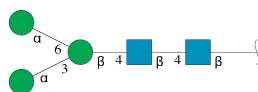
Chain	Residue	Modelled	Actual	Comment	Reference
B	357	HIS	-	expression tag	UNP P59823
B	358	HIS	-	expression tag	UNP P59823
B	359	HIS	-	expression tag	UNP P59823

- Molecule 2 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.



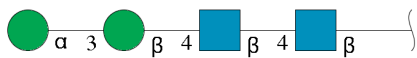
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
2	C	3	39	22	2	15	0	0	0
2	F	3	39	22	2	15	0	0	0

- Molecule 3 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



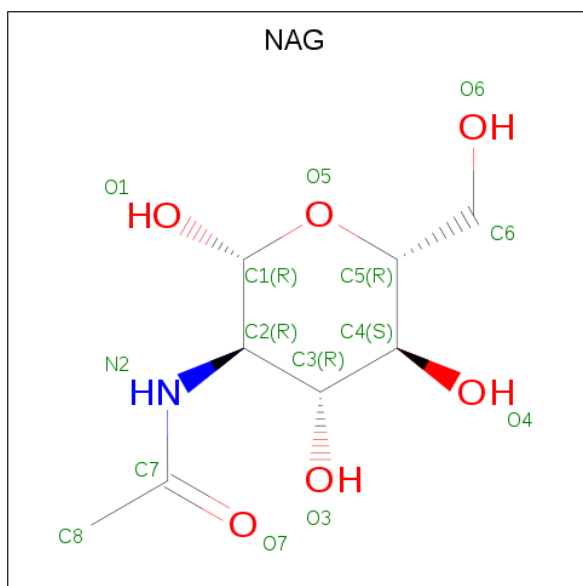
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
3	D	5	61	34	2	25	0	0	0
3	E	5	61	34	2	25	0	0	0
3	G	5	61	34	2	25	0	0	0

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



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

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



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



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

Chain F: 67% 33%



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

Chain D: 40% 60%



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

Chain E: 40% 40% 20%



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

Chain G: 40% 60%



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

Chain H: 25% 50% 25%



4 Data and refinement statistics

Property	Value	Source
Space group	P 42 21 2	Depositor
Cell constants a, b, c, α , β , γ	102.45Å 102.45Å 222.71Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.85 – 3.00 40.85 – 2.90	Depositor EDS
% Data completeness (in resolution range)	97.7 (40.85-3.00) 97.1 (40.85-2.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.12	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.83 (at 2.90Å)	Xtrriage
Refinement program	PHENIX (phenix.refine: 1.9_1692)	Depositor
R, R_{free}	0.263 , 0.298 0.264 , 0.299	Depositor DCC
R_{free} test set	1328 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å ²)	46.1	Xtrriage
Anisotropy	0.239	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 51.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.38$, $\langle L^2 \rangle = 0.21$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.82	EDS
Total number of atoms	5288	wwPDB-VP
Average B, all atoms (Å ²)	67.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.48% 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: BMA, NAG, 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	0.22	0/2571	0.44	0/3469
1	B	0.23	0/2492	0.43	0/3360
All	All	0.22	0/5063	0.43	0/6829

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

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	2519	0	2475	38	0
1	B	2444	0	2412	40	0
2	C	39	0	34	2	0
2	F	39	0	34	1	0
3	D	61	0	52	2	0
3	E	61	0	52	1	0
3	G	61	0	52	0	0
4	H	50	0	43	2	0
5	A	14	0	13	1	0
All	All	5288	0	5167	83	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 8.

All (83) 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:A:295:GLU:HB2	1:A:298:VAL:HG12	1.57	0.86
1:A:79:SER:HB3	1:A:86:GLU:HG3	1.59	0.83
1:B:182:TYR:HB2	1:B:215:THR:HG23	1.74	0.69
1:B:76:TRP:HB2	1:B:89:ILE:HD11	1.75	0.68
1:A:76:TRP:HB2	1:A:89:ILE:HD11	1.79	0.64
1:B:137:GLU:O	1:B:145:ASN:ND2	2.31	0.63
1:B:32:THR:OG1	1:B:127:MET:SD	2.57	0.61
1:A:155:GLU:OE2	1:A:158:LYS:NZ	2.34	0.61
1:B:92:ASP:OD2	3:E:4:MAN:O2	2.20	0.58
4:H:1:NAG:H3	4:H:1:NAG:H83	1.86	0.56
1:A:67:ALA:HB1	1:A:72:LEU:HD12	1.87	0.55
2:F:1:NAG:H3	2:F:1:NAG:H83	1.88	0.55
1:B:331:ASN:HD22	1:B:348:LEU:HD23	1.70	0.55
1:B:150:TYR:HB2	1:B:229:THR:HB	1.88	0.55
1:A:122:ASN:HB3	1:A:125:TYR:H	1.71	0.55
1:A:179:ILE:HD11	1:A:198:ARG:HA	1.88	0.55
1:B:240:LYS:HD3	1:B:241:PRO:HD2	1.88	0.55
1:B:304:ARG:HH22	4:H:1:NAG:H83	1.71	0.54
2:C:1:NAG:O3	2:C:2:NAG:O5	2.21	0.54
1:B:297:ARG:NH1	1:B:328:ASP:OD2	2.38	0.54
1:A:297:ARG:HB3	1:A:322:ASP:O	2.08	0.54
1:B:149:LYS:NZ	1:B:230:GLU:OE1	2.38	0.54
1:A:193:SER:HA	1:A:204:LYS:HE2	1.91	0.52
1:A:215:THR:HB	1:A:228:THR:HB	1.92	0.52
1:B:45:VAL:HA	1:B:108:THR:HG23	1.92	0.51
1:A:256:GLU:HB3	1:A:351:LYS:HG3	1.92	0.51
1:B:241:PRO:HG2	1:B:343:ARG:NH2	2.26	0.50
1:B:44:LEU:HD21	1:B:145:ASN:HB2	1.93	0.50
1:A:241:PRO:HG2	1:A:343:ARG:NH2	2.27	0.50
1:B:48:PRO:HD3	1:B:223:PHE:HB3	1.93	0.50
1:B:182:TYR:HE1	1:B:217:GLU:HB2	1.77	0.50
1:A:33:ASP:OD1	1:A:34:TRP:N	2.45	0.49
1:A:194:ILE:HG13	1:A:203:ILE:HG12	1.94	0.49
1:B:55:LEU:HD11	1:B:127:MET:HB3	1.95	0.49
1:A:226:ARG:NH2	5:A:404:NAG:O7	2.45	0.48
1:A:307:LYS:HG2	1:A:314:GLU:HB3	1.95	0.48
1:B:139:ASP:OD1	1:B:139:ASP:N	2.41	0.48
1:A:291:GLU:O	1:A:294:ASP:HB2	2.12	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:122:ASN:HD22	1:A:125:TYR:HB3	1.79	0.48
1:A:289:PHE:N	1:A:292:ASP:OD2	2.41	0.48
3:D:3:BMA:H4	3:D:5:MAN:H2	1.97	0.47
1:B:155:GLU:HG2	1:B:236:PRO:HA	1.97	0.47
1:B:179:ILE:HD12	1:B:199:ASP:HA	1.96	0.47
1:A:43:VAL:HG21	1:A:49:VAL:HG21	1.97	0.46
1:A:72:LEU:HB3	1:A:120:ILE:HG22	1.96	0.46
1:B:157:SER:HA	1:B:205:GLU:HG2	1.97	0.46
1:A:271:PHE:CZ	1:A:336:VAL:HG13	2.50	0.46
1:B:194:ILE:HG12	1:B:203:ILE:HG12	1.98	0.46
1:A:263:ALA:HB3	1:A:321:VAL:HB	1.98	0.46
1:B:43:VAL:HG11	1:B:49:VAL:HG21	1.98	0.46
1:B:167:ILE:HD11	1:B:218:LEU:HD22	1.97	0.46
1:A:85:PHE:HA	1:B:153:LYS:NZ	2.32	0.45
1:A:138:ASN:HB2	1:A:142:LEU:O	2.17	0.45
2:C:1:NAG:H83	2:C:1:NAG:H3	1.98	0.45
1:B:91:PHE:CE2	1:B:98:LYS:HE3	2.52	0.45
1:B:51:ILE:HD11	1:B:133:LEU:HD13	1.98	0.45
1:A:50:ARG:HD3	1:A:104:TRP:CE2	2.53	0.44
1:A:246:TYR:O	1:A:268:ARG:N	2.47	0.44
1:A:91:PHE:CE2	1:A:98:LYS:HB2	2.52	0.44
1:B:191:ARG:HG3	1:B:191:ARG:H	1.60	0.44
1:B:119:VAL:HG22	1:B:128:LYS:HB2	1.98	0.44
1:B:272:GLY:HA2	1:B:312:GLU:HG2	2.00	0.44
1:B:76:TRP:CZ3	1:B:118:CYS:HB2	2.52	0.44
1:A:106:ARG:HA	1:A:107:PRO:HA	1.79	0.44
1:B:294:ASP:OD2	1:B:297:ARG:NE	2.51	0.44
1:A:44:LEU:O	1:A:47:GLU:HG2	2.18	0.43
1:B:92:ASP:OD1	1:B:93:GLY:N	2.43	0.43
1:B:43:VAL:HG21	1:B:49:VAL:HG22	2.01	0.43
1:A:265:LEU:HD22	1:A:347:VAL:HG11	2.01	0.43
1:A:52:LYS:HE3	1:A:57:TYR:CZ	2.53	0.42
1:A:266:THR:HA	1:A:318:SER:HA	2.02	0.42
1:B:89:ILE:HG13	1:B:89:ILE:H	1.43	0.42
1:B:144:TYR:HB2	1:B:228:THR:HG21	2.01	0.42
1:B:215:THR:HB	1:B:228:THR:HB	2.01	0.42
1:A:95:ARG:NH1	1:A:107:PRO:O	2.48	0.41
3:D:3:BMA:H3	3:D:4:MAN:H2	1.61	0.41
1:B:33:ASP:OD1	1:B:34:TRP:N	2.54	0.41
1:A:43:VAL:HG23	1:A:135:VAL:HG22	2.01	0.41
1:A:48:PRO:HD3	1:A:223:PHE:HB3	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:122:ASN:HB3	1:B:125:TYR:H	1.86	0.41
1:A:350:HIS:CG	1:A:351:LYS:H	2.38	0.41
1:A:76:TRP:CZ3	1:A:118:CYS:HB3	2.56	0.41
1:B:246:TYR:HA	1:B:247:PRO:HA	1.92	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	307/348 (88%)	293 (95%)	13 (4%)	1 (0%)	41	76
1	B	295/348 (85%)	284 (96%)	10 (3%)	1 (0%)	41	76
All	All	602/696 (86%)	577 (96%)	23 (4%)	2 (0%)	41	76

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	198	ARG
1	A	91	PHE

5.3.2 Protein sidechains [i](#)

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.

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	281/309 (91%)	257 (92%)	24 (8%)	10	38
1	B	274/309 (89%)	251 (92%)	23 (8%)	11	38
All	All	555/618 (90%)	508 (92%)	47 (8%)	10	38

All (47) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	32	THR
1	A	43	VAL
1	A	50	ARG
1	A	61	ARG
1	A	62	THR
1	A	106	ARG
1	A	156	LEU
1	A	167	ILE
1	A	179	ILE
1	A	180	LEU
1	A	199	ASP
1	A	210	ASP
1	A	215	THR
1	A	228	THR
1	A	229	THR
1	A	231	LEU
1	A	239	ASP
1	A	246	TYR
1	A	252	LEU
1	A	255	GLN
1	A	256	GLU
1	A	280	LEU
1	A	293	LEU
1	A	340	ASN
1	B	32	THR
1	B	49	VAL
1	B	50	ARG
1	B	66	LEU
1	B	79	SER
1	B	89	ILE
1	B	121	ARG
1	B	153	LYS

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Mol	Chain	Res	Type
1	B	171	LEU
1	B	172	LEU
1	B	177	PRO
1	B	199	ASP
1	B	215	THR
1	B	228	THR
1	B	229	THR
1	B	231	LEU
1	B	232	THR
1	B	246	TYR
1	B	262	SER
1	B	280	LEU
1	B	293	LEU
1	B	318	SER
1	B	340	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	331	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

25 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	1,2	14,14,15	0.73	1 (7%)	17,19,21	1.71	3 (17%)
2	NAG	C	2	2	14,14,15	0.28	0	17,19,21	0.80	0
2	BMA	C	3	2	11,11,12	0.72	0	15,15,17	0.72	0
3	NAG	D	1	1,3	14,14,15	0.23	0	17,19,21	0.42	0
3	NAG	D	2	3	14,14,15	0.25	0	17,19,21	0.39	0
3	BMA	D	3	3	11,11,12	0.87	1 (9%)	15,15,17	0.72	0
3	MAN	D	4	3	11,11,12	1.34	2 (18%)	15,15,17	1.95	5 (33%)
3	MAN	D	5	3	11,11,12	0.83	1 (9%)	15,15,17	0.91	1 (6%)
3	NAG	E	1	1,3	14,14,15	0.28	0	17,19,21	0.44	0
3	NAG	E	2	3	14,14,15	0.19	0	17,19,21	0.47	0
3	BMA	E	3	3	11,11,12	1.23	1 (9%)	15,15,17	1.33	2 (13%)
3	MAN	E	4	3	11,11,12	1.02	1 (9%)	15,15,17	1.03	1 (6%)
3	MAN	E	5	3	11,11,12	0.85	1 (9%)	15,15,17	1.65	4 (26%)
2	NAG	F	1	1,2	14,14,15	0.51	0	17,19,21	1.29	2 (11%)
2	NAG	F	2	2	14,14,15	0.39	0	17,19,21	0.44	0
2	BMA	F	3	2	11,11,12	0.67	0	15,15,17	0.73	0
3	NAG	G	1	1,3	14,14,15	0.49	0	17,19,21	0.49	0
3	NAG	G	2	3	14,14,15	0.28	0	17,19,21	0.55	0
3	BMA	G	3	3	11,11,12	1.04	1 (9%)	15,15,17	1.90	4 (26%)
3	MAN	G	4	3	11,11,12	0.70	1 (9%)	15,15,17	1.60	3 (20%)
3	MAN	G	5	3	11,11,12	0.78	0	15,15,17	1.18	2 (13%)
4	NAG	H	1	1,4	14,14,15	0.39	0	17,19,21	1.29	2 (11%)
4	NAG	H	2	4	14,14,15	0.44	0	17,19,21	0.43	0
4	BMA	H	3	4	11,11,12	1.34	3 (27%)	15,15,17	1.27	2 (13%)
4	MAN	H	4	4	11,11,12	0.74	0	15,15,17	1.36	2 (13%)

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	1,2	-	5/6/23/26	0/1/1/1
2	NAG	C	2	2	-	4/6/23/26	0/1/1/1
2	BMA	C	3	2	-	1/2/19/22	0/1/1/1
3	NAG	D	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	D	2	3	-	2/6/23/26	0/1/1/1
3	BMA	D	3	3	-	1/2/19/22	0/1/1/1

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

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	4	MAN	C1-C2	3.13	1.59	1.52
3	E	3	BMA	O3-C3	2.70	1.49	1.43
3	D	4	MAN	C2-C3	2.68	1.56	1.52
3	G	3	BMA	C1-C2	2.66	1.58	1.52
3	E	5	MAN	C1-C2	2.59	1.58	1.52
4	H	3	BMA	O5-C1	-2.55	1.39	1.43
2	C	1	NAG	O5-C1	2.45	1.47	1.43
4	H	3	BMA	C4-C5	2.37	1.58	1.53
3	D	5	MAN	O5-C1	-2.28	1.40	1.43
3	E	4	MAN	C1-C2	2.12	1.57	1.52
3	G	4	MAN	C1-C2	2.11	1.57	1.52
4	H	3	BMA	C4-C3	2.08	1.57	1.52
3	D	3	BMA	O5-C1	-2.03	1.40	1.43

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	G	3	BMA	C1-O5-C5	4.46	118.23	112.19
3	D	4	MAN	C1-C2-C3	4.44	115.12	109.67
2	C	1	NAG	C2-N2-C7	4.41	129.19	122.90
2	F	1	NAG	C2-N2-C7	4.35	129.09	122.90
2	C	1	NAG	C1-O5-C5	4.35	118.08	112.19
4	H	1	NAG	C2-N2-C7	4.35	129.09	122.90
3	E	5	MAN	C1-O5-C5	3.96	117.56	112.19
4	H	4	MAN	C1-O5-C5	3.94	117.53	112.19
3	G	3	BMA	O5-C1-C2	3.84	116.69	110.77
3	G	4	MAN	C1-O5-C5	3.60	117.07	112.19
3	E	3	BMA	O3-C3-C2	3.52	116.73	109.99
3	D	4	MAN	O5-C1-C2	3.47	116.12	110.77
3	G	4	MAN	O5-C1-C2	3.28	115.84	110.77
3	G	5	MAN	C1-O5-C5	3.24	116.59	112.19
3	E	5	MAN	O5-C1-C2	3.19	115.69	110.77
4	H	3	BMA	C3-C4-C5	2.86	115.33	110.24
3	D	4	MAN	C1-O5-C5	2.81	115.99	112.19
3	E	4	MAN	C1-O5-C5	2.64	115.77	112.19
3	G	3	BMA	C3-C4-C5	-2.57	105.66	110.24
3	D	4	MAN	O2-C2-C3	-2.51	105.11	110.14
2	C	1	NAG	C1-C2-N2	2.47	114.70	110.49
4	H	3	BMA	C2-C3-C4	2.31	114.89	110.89
3	E	3	BMA	C1-C2-C3	-2.30	106.84	109.67
3	E	5	MAN	C1-C2-C3	2.26	112.45	109.67
3	G	3	BMA	C1-C2-C3	2.24	112.42	109.67
3	G	4	MAN	O2-C2-C3	-2.24	105.66	110.14
2	F	1	NAG	C1-C2-N2	2.22	114.28	110.49
3	D	5	MAN	O2-C2-C3	-2.22	105.69	110.14
3	G	5	MAN	O2-C2-C3	-2.20	105.72	110.14
3	E	5	MAN	O2-C2-C3	-2.20	105.73	110.14
4	H	4	MAN	O2-C2-C3	-2.17	105.78	110.14
4	H	1	NAG	C1-C2-N2	2.09	114.06	110.49
3	D	4	MAN	O5-C5-C4	-2.04	105.87	110.83

There are no chirality outliers.

All (52) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	G	3	BMA	C4-C5-C6-O6
2	C	1	NAG	C4-C5-C6-O6
2	F	1	NAG	O5-C5-C6-O6
3	D	2	NAG	O5-C5-C6-O6
3	G	3	BMA	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
3	E	2	NAG	O5-C5-C6-O6
3	E	1	NAG	O5-C5-C6-O6
2	C	1	NAG	O5-C5-C6-O6
3	E	1	NAG	C4-C5-C6-O6
3	D	2	NAG	C4-C5-C6-O6
3	G	4	MAN	O5-C5-C6-O6
2	F	1	NAG	C4-C5-C6-O6
3	E	1	NAG	C8-C7-N2-C2
3	E	1	NAG	O7-C7-N2-C2
2	F	2	NAG	C8-C7-N2-C2
2	F	2	NAG	O7-C7-N2-C2
2	F	1	NAG	C8-C7-N2-C2
2	F	1	NAG	O7-C7-N2-C2
2	C	2	NAG	C8-C7-N2-C2
2	C	2	NAG	O7-C7-N2-C2
2	C	1	NAG	C8-C7-N2-C2
2	C	1	NAG	O7-C7-N2-C2
4	H	1	NAG	C8-C7-N2-C2
4	H	1	NAG	O7-C7-N2-C2
3	G	4	MAN	C4-C5-C6-O6
4	H	3	BMA	C4-C5-C6-O6
4	H	2	NAG	O5-C5-C6-O6
3	E	2	NAG	C4-C5-C6-O6
4	H	1	NAG	O5-C5-C6-O6
4	H	1	NAG	C4-C5-C6-O6
3	G	1	NAG	O5-C5-C6-O6
3	D	3	BMA	O5-C5-C6-O6
3	D	1	NAG	C4-C5-C6-O6
3	E	4	MAN	O5-C5-C6-O6
4	H	2	NAG	C4-C5-C6-O6
3	D	1	NAG	O5-C5-C6-O6
2	C	3	BMA	O5-C5-C6-O6
2	F	3	BMA	O5-C5-C6-O6
4	H	3	BMA	O5-C5-C6-O6
3	E	5	MAN	C4-C5-C6-O6
2	F	2	NAG	C4-C5-C6-O6
2	C	2	NAG	C4-C5-C6-O6
2	F	2	NAG	O5-C5-C6-O6
3	G	1	NAG	C1-C2-N2-C7
3	E	3	BMA	C4-C5-C6-O6
2	C	2	NAG	O5-C5-C6-O6
2	C	1	NAG	C3-C2-N2-C7

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Mol	Chain	Res	Type	Atoms
4	H	1	NAG	C3-C2-N2-C7
3	E	5	MAN	O5-C5-C6-O6
3	E	3	BMA	O5-C5-C6-O6
3	G	1	NAG	C4-C5-C6-O6
2	F	1	NAG	C3-C2-N2-C7

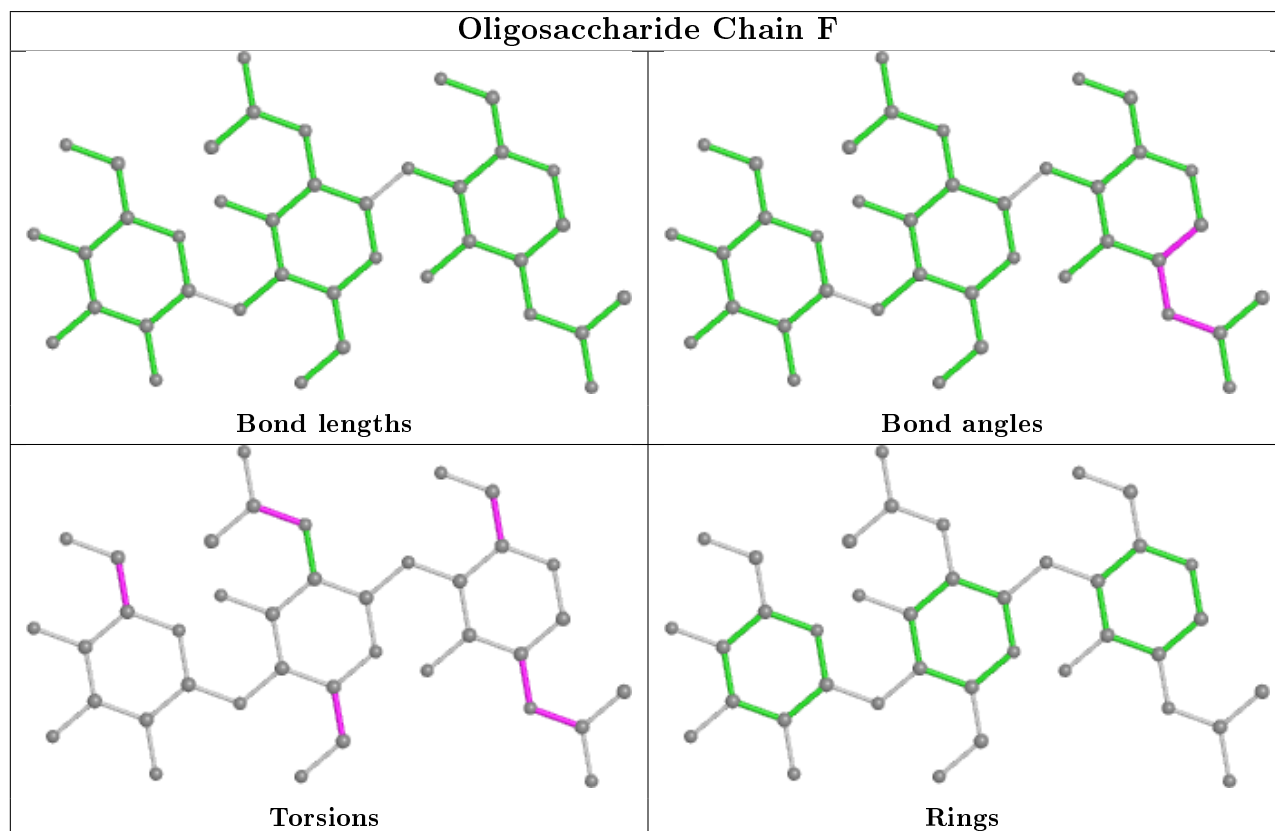
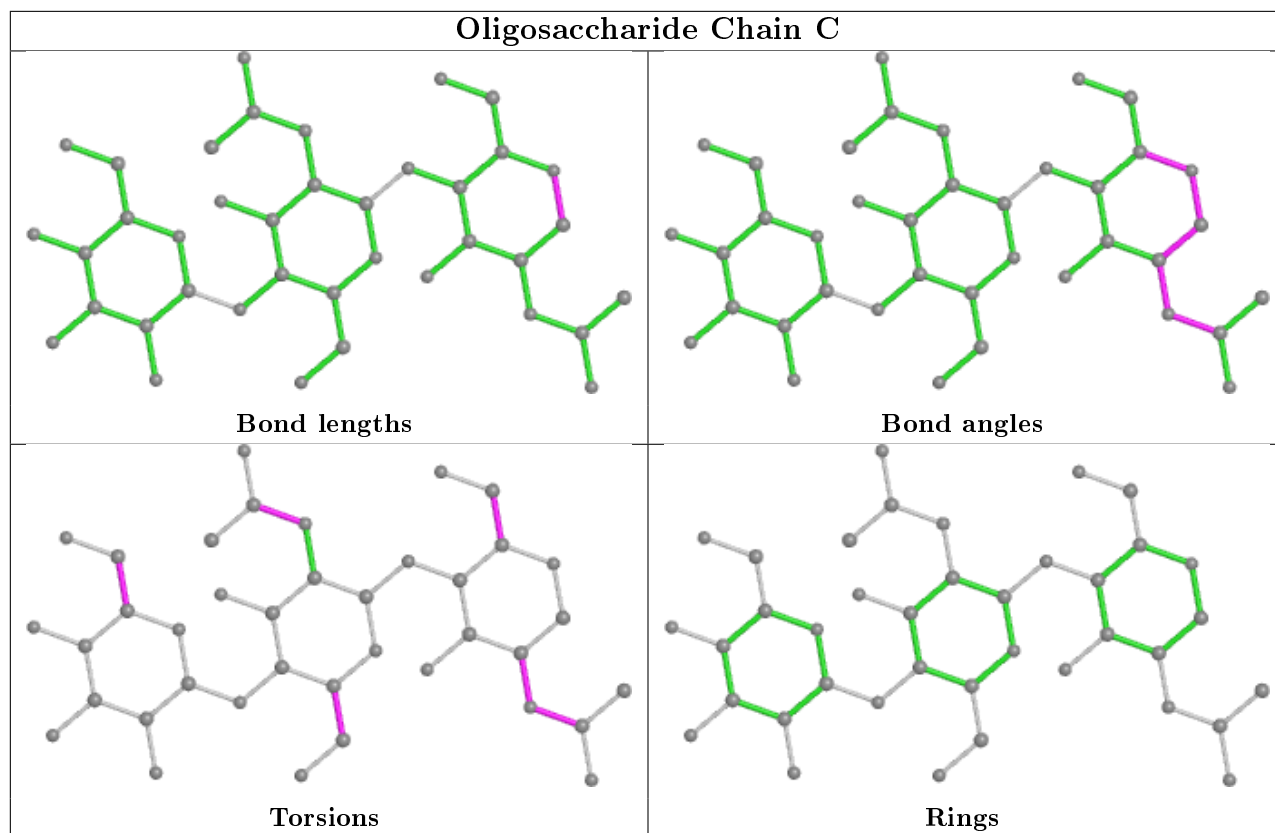
All (3) ring outliers are listed below:

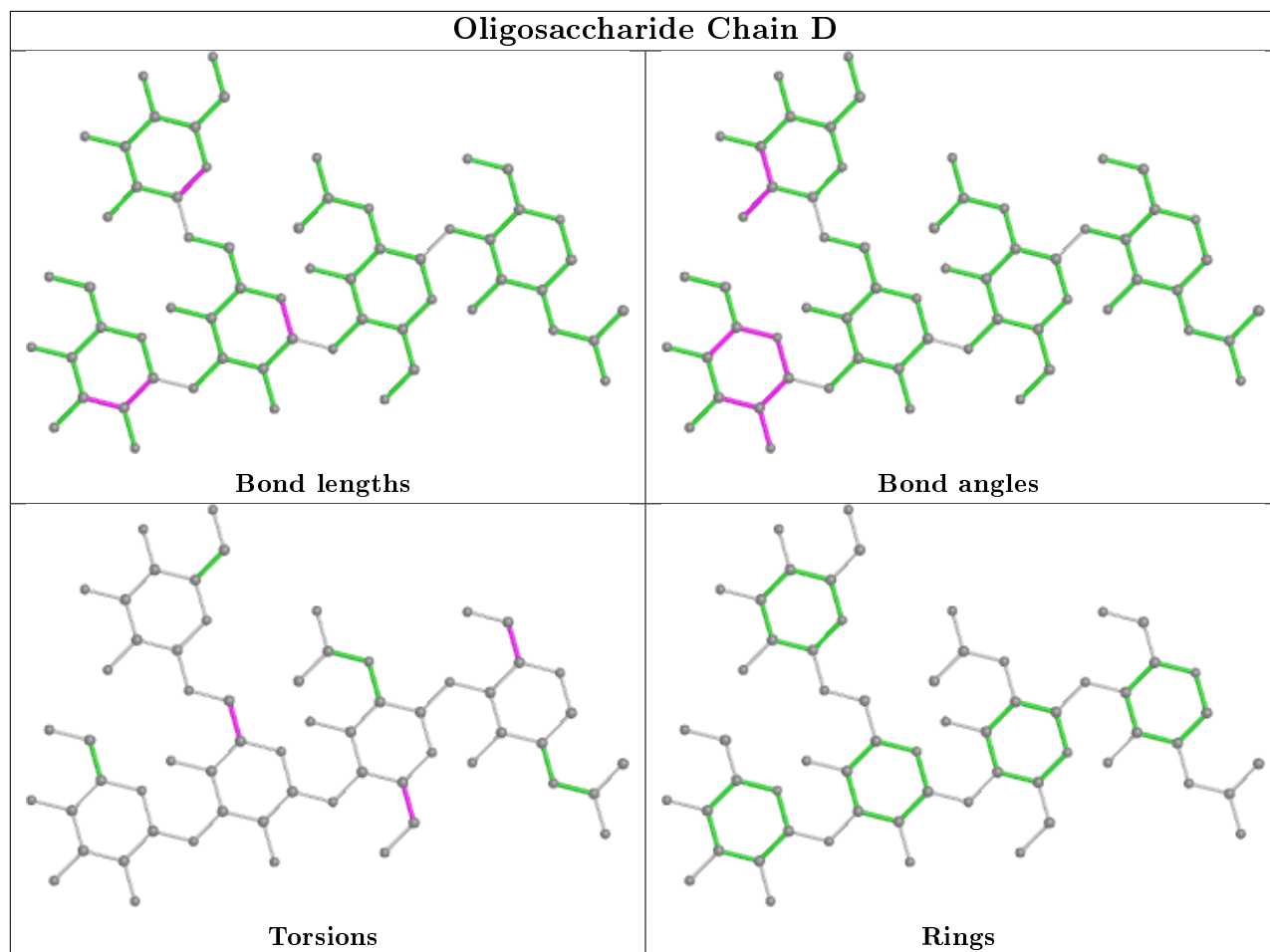
Mol	Chain	Res	Type	Atoms
3	G	5	MAN	C1-C2-C3-C4-C5-O5
3	E	4	MAN	C1-C2-C3-C4-C5-O5
4	H	4	MAN	C1-C2-C3-C4-C5-O5

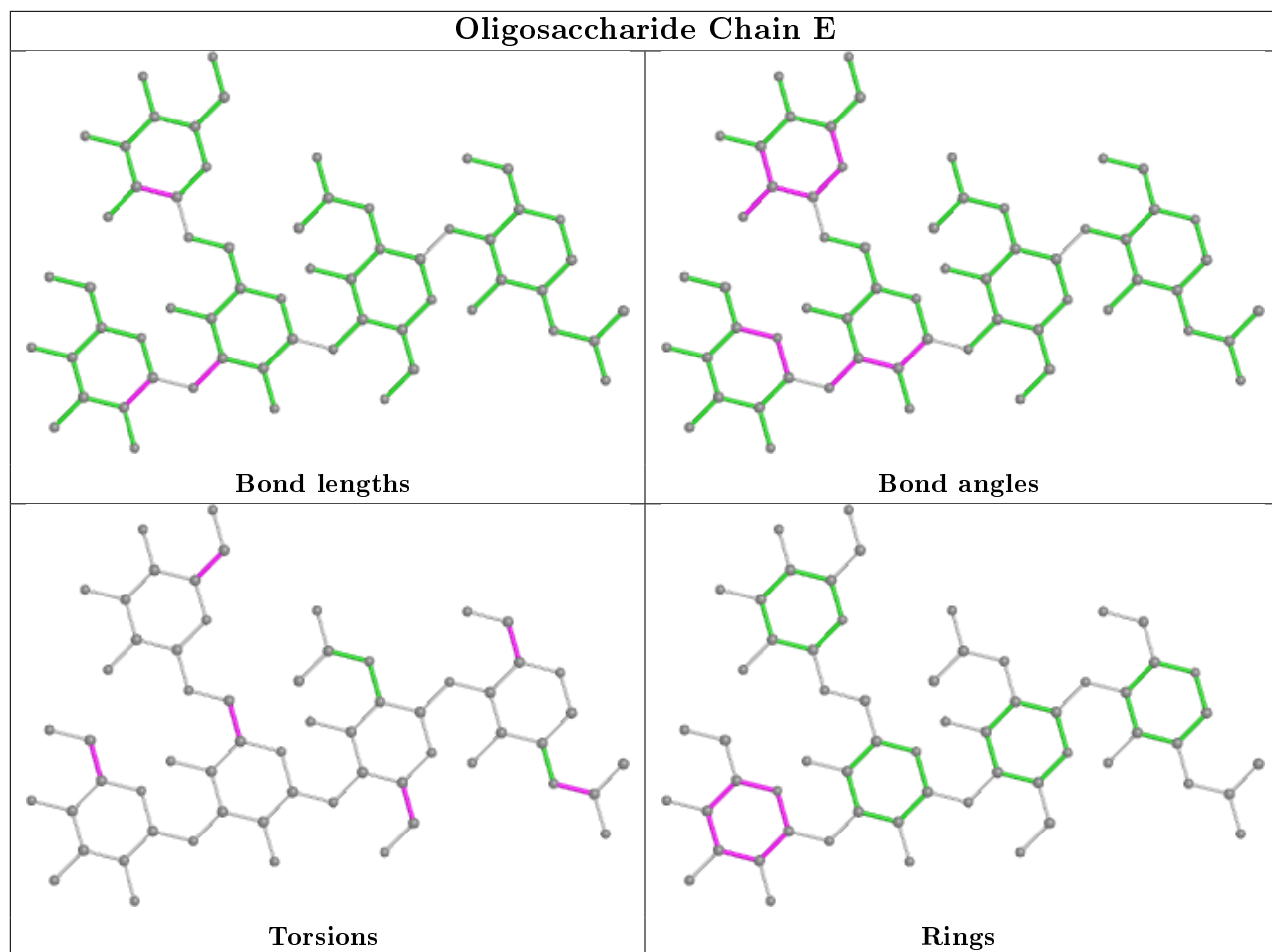
8 monomers are involved in 8 short contacts:

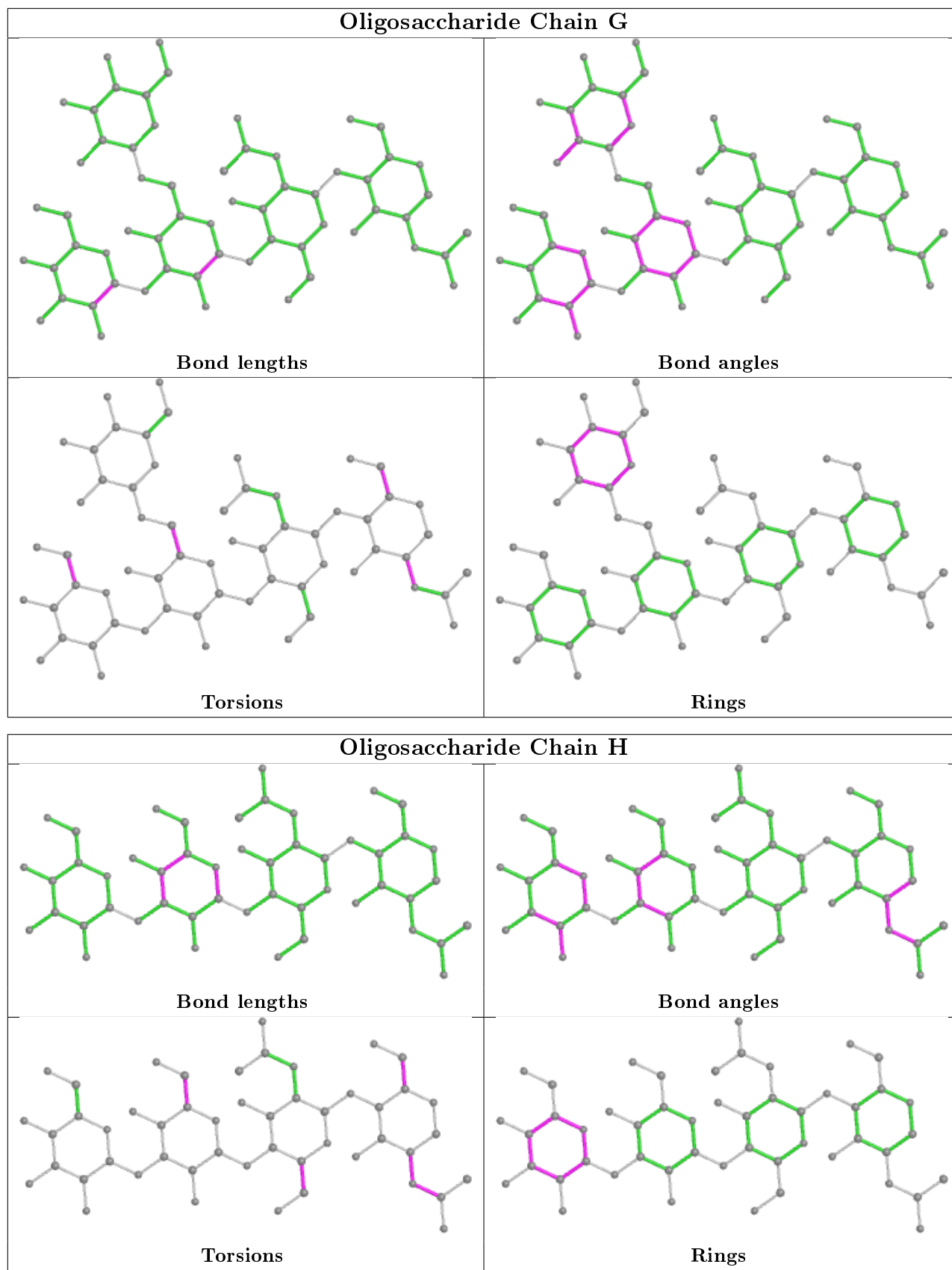
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	E	4	MAN	1	0
3	D	5	MAN	1	0
3	D	4	MAN	1	0
2	F	1	NAG	1	0
3	D	3	BMA	2	0
2	C	2	NAG	1	0
2	C	1	NAG	2	0
4	H	1	NAG	2	0

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](#)

1 ligand is modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	NAG	A	404	1	14,14,15	0.22	0	17,19,21	0.37	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
5	NAG	A	404	1	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	404	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	313/348 (89%)	-0.07	7 (2%) 62 33	33, 73, 113, 143	0
1	B	305/348 (87%)	-0.35	6 (1%) 65 36	16, 48, 104, 163	0
All	All	618/696 (88%)	-0.21	13 (2%) 63 34	16, 61, 110, 163	0

All (13) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	34	TRP	4.6
1	B	69	SER	4.1
1	B	55	LEU	3.8
1	A	61	ARG	3.5
1	A	138	ASN	3.1
1	A	185	CYS	3.0
1	A	195	VAL	2.9
1	B	178	GLU	2.7
1	A	35	SER	2.6
1	B	33	ASP	2.6
1	A	194	ILE	2.5
1	A	59	TYR	2.5
1	B	54	ALA	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,

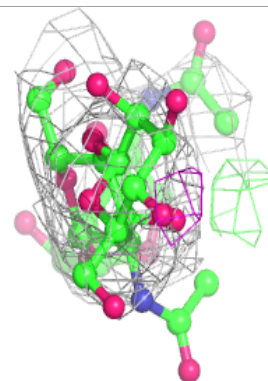
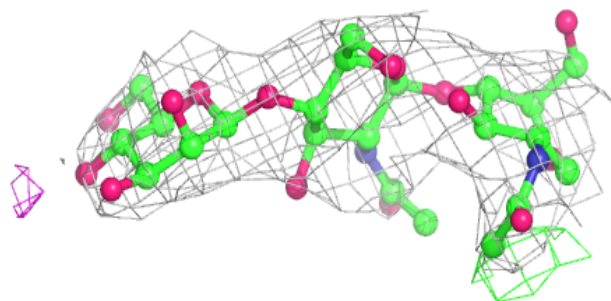
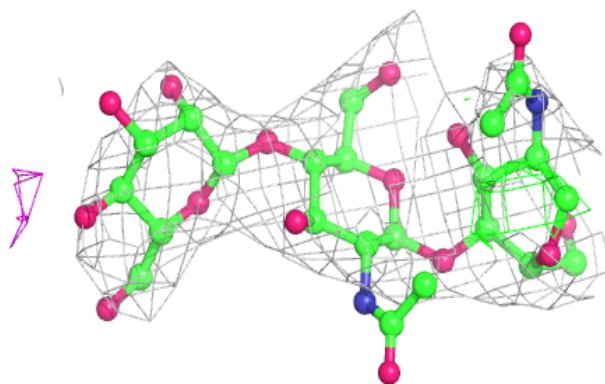
median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	MAN	D	4	11/12	0.47	0.33	122,148,154,157	0
3	BMA	D	3	11/12	0.69	0.20	129,135,145,147	0
4	MAN	H	4	11/12	0.73	0.31	98,123,129,131	0
3	MAN	E	5	11/12	0.73	0.47	138,143,144,146	0
3	MAN	G	5	11/12	0.75	0.33	80,122,134,139	0
3	MAN	D	5	11/12	0.76	0.16	93,111,116,122	0
3	NAG	G	2	14/15	0.77	0.23	53,87,108,133	0
3	MAN	G	4	11/12	0.79	0.23	78,97,124,134	0
3	BMA	G	3	11/12	0.79	0.22	119,140,147,158	0
3	MAN	E	4	11/12	0.81	0.35	133,142,162,164	0
2	BMA	F	3	11/12	0.82	0.24	43,63,85,87	0
4	NAG	H	2	14/15	0.87	0.18	58,73,93,96	0
4	BMA	H	3	11/12	0.87	0.16	34,67,110,117	0
2	NAG	C	1	14/15	0.88	0.22	38,60,80,86	0
2	NAG	C	2	14/15	0.88	0.28	64,96,123,124	0
3	NAG	D	1	14/15	0.90	0.19	36,69,79,80	0
3	BMA	E	3	11/12	0.90	0.16	117,121,127,129	0
2	NAG	F	1	14/15	0.90	0.15	54,67,91,96	0
2	BMA	C	3	11/12	0.90	0.34	95,102,109,109	0
2	NAG	F	2	14/15	0.90	0.34	68,77,84,87	0
3	NAG	D	2	14/15	0.90	0.17	73,100,118,130	0
3	NAG	E	2	14/15	0.91	0.20	69,105,122,123	0
3	NAG	E	1	14/15	0.91	0.23	48,70,75,76	0
4	NAG	H	1	14/15	0.93	0.19	13,48,57,58	0
3	NAG	G	1	14/15	0.96	0.19	6,41,90,98	0

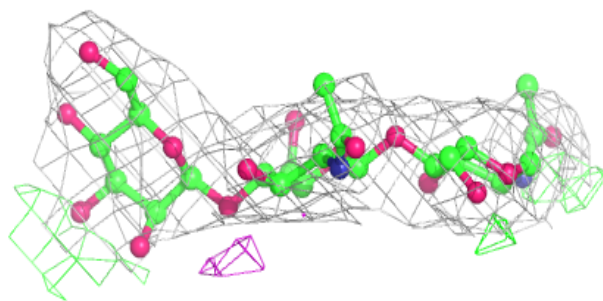
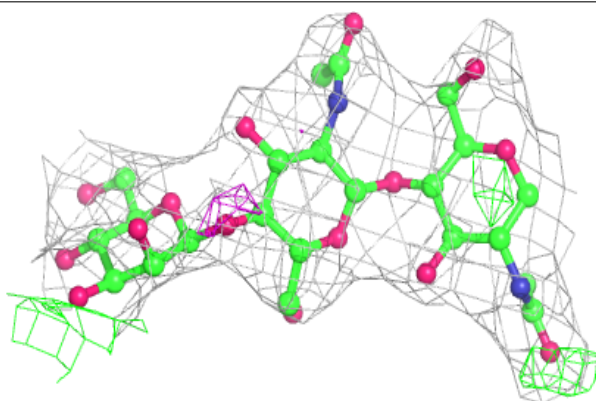
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around Chain C:

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

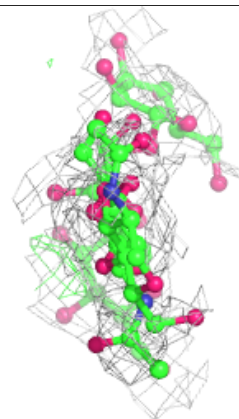
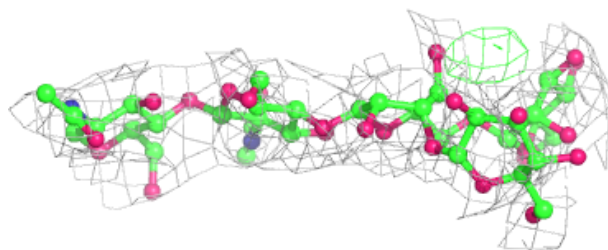
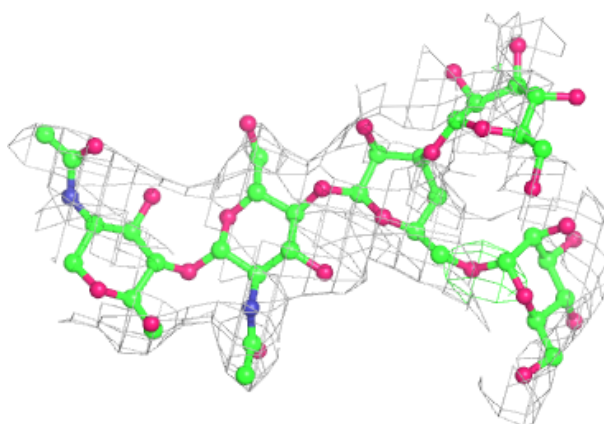
**Electron density around Chain F:**

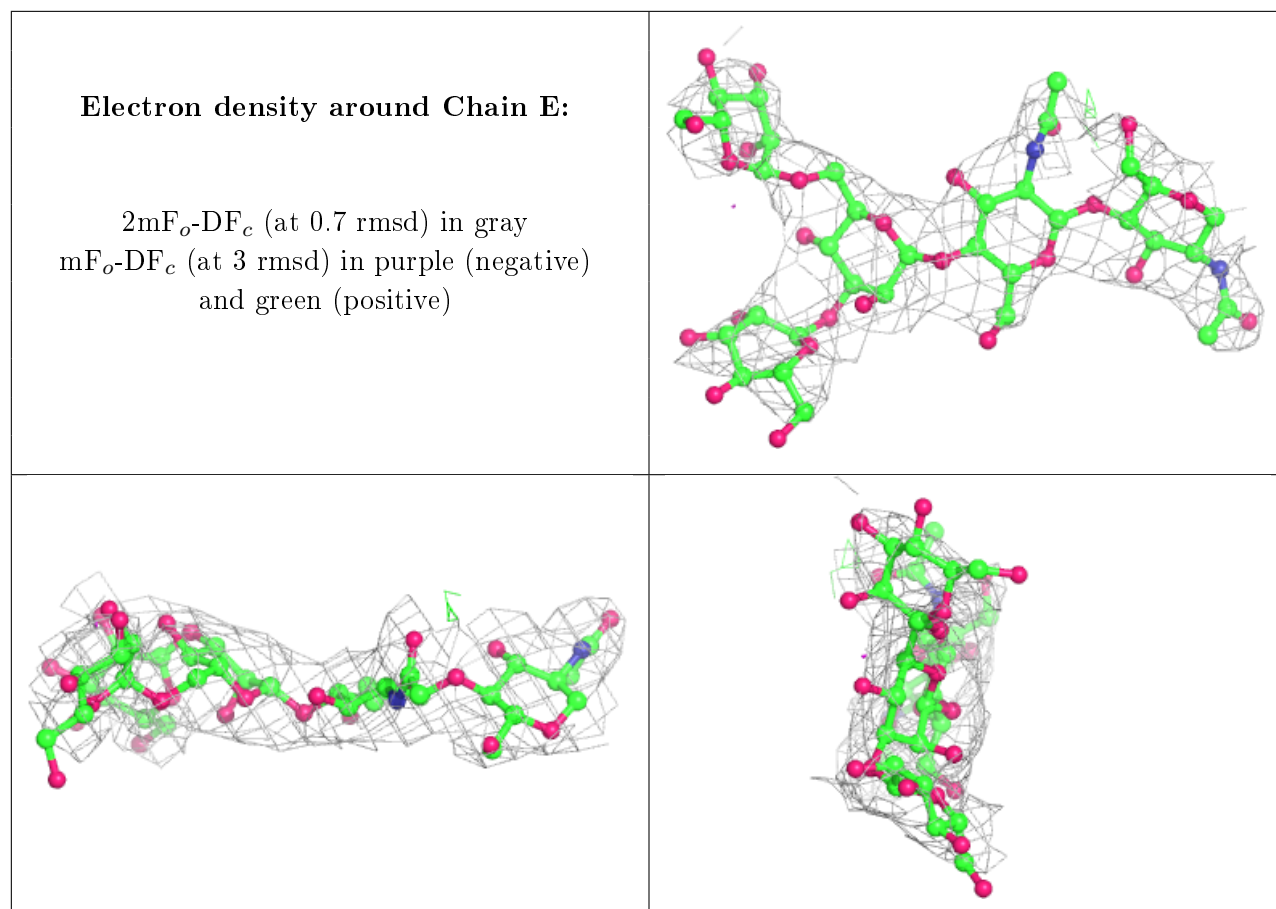
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around Chain D:

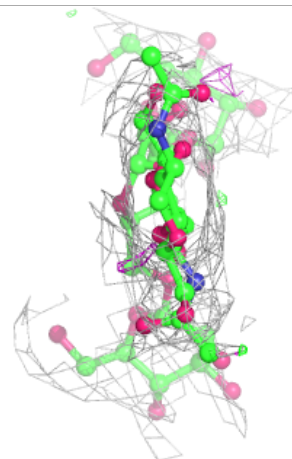
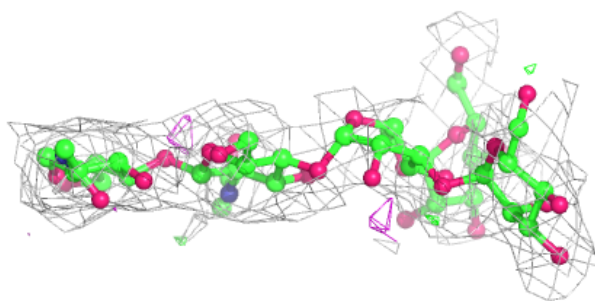
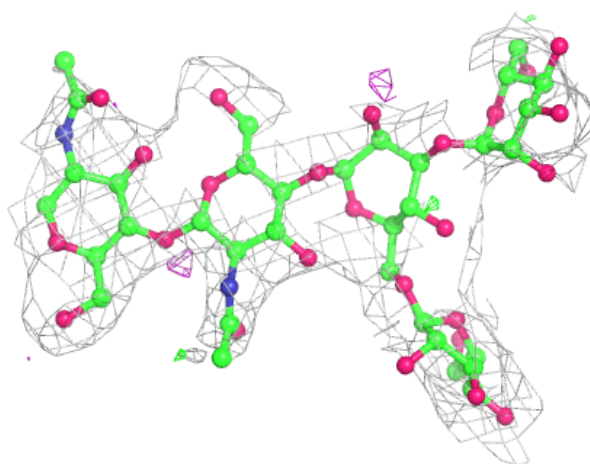
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

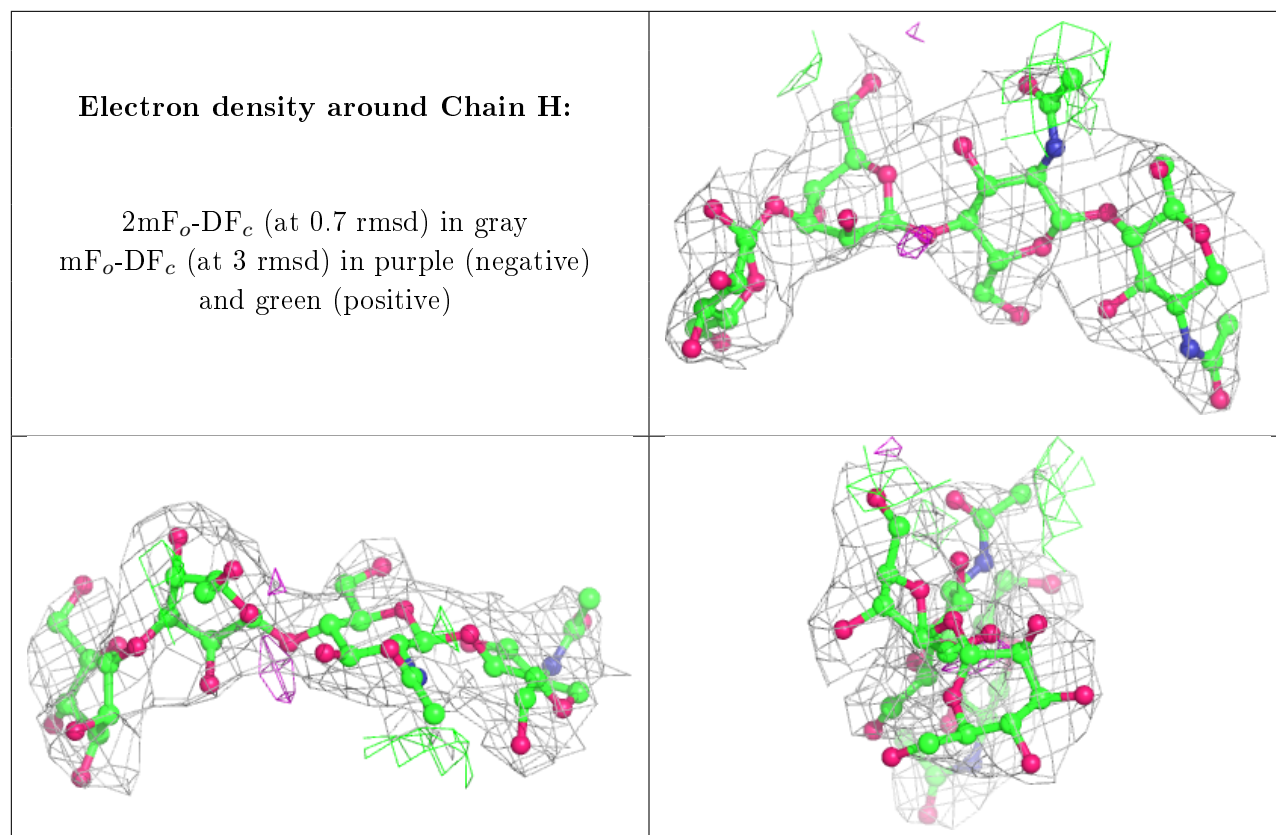




Electron density around Chain G:

$2mF_o-DF_c$ (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
5	NAG	A	404	14/15	0.77	0.31	107,116,132,133	0

6.5 Other polymers [i](#)

There are no such residues in this entry.