Full wwPDB X-ray Structure Validation Report (i)

Jan 26, 2023 – 12:24 pm GMT

PDB ID	:	8C6I
Title	:	TMEM2 ectodomain
Authors	:	Hohenester, E.
Deposited on	:	2023-01-11
Resolution	:	3.50 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 (i) 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 (1)) were used in the production of this report:

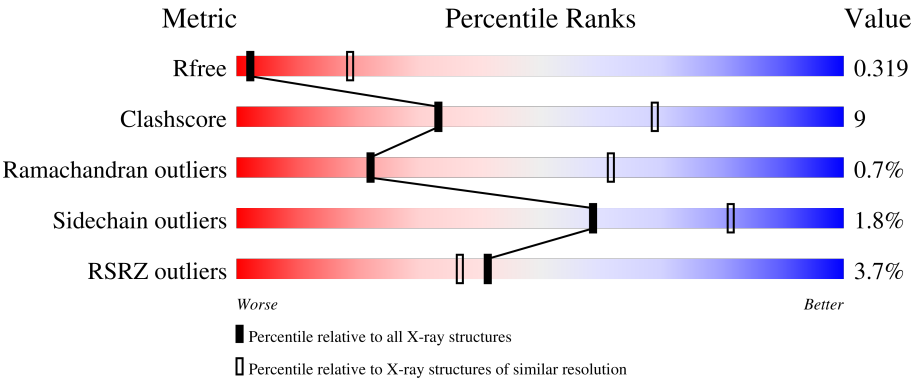
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.31.3
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.3

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 3.50 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	1659 (3.60-3.40)
Clashscore	141614	1036 (3.58-3.42)
Ramachandran outliers	138981	1005 (3.58-3.42)
Sidechain outliers	138945	1006 (3.58-3.42)
RSRZ outliers	127900	1559 (3.60-3.40)

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 <=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	1301	4% 76% 21%
2	B	4	50% 25% 25%
2	D	4	25% 50% 25%
3	C	2	50% 50%
3	H	2	50% 50%

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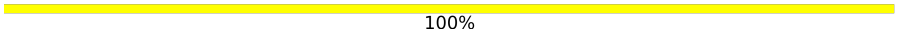
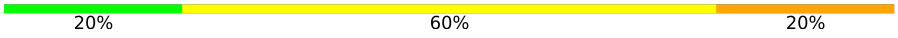
Mol	Chain	Length	Quality of chain
4	E	3	
5	F	5	
6	G	4	

2 Entry composition (i)

There are 9 unique types of molecules in this entry. The entry contains 10327 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 Cell surface hyaluronidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1270	Total	C	N	O	S	0	0	0
			9992	6320	1746	1880	46			

There are 23 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	83	ALA	-	expression tag	UNP Q9UHN6
A	84	PRO	-	expression tag	UNP Q9UHN6
A	85	LEU	-	expression tag	UNP Q9UHN6
A	86	VAL	-	expression tag	UNP Q9UHN6
A	87	HIS	-	expression tag	UNP Q9UHN6
A	88	HIS	-	expression tag	UNP Q9UHN6
A	89	HIS	-	expression tag	UNP Q9UHN6
A	90	HIS	-	expression tag	UNP Q9UHN6
A	91	HIS	-	expression tag	UNP Q9UHN6
A	92	HIS	-	expression tag	UNP Q9UHN6
A	93	ALA	-	expression tag	UNP Q9UHN6
A	94	LEU	-	expression tag	UNP Q9UHN6
A	95	ASP	-	expression tag	UNP Q9UHN6
A	96	GLU	-	expression tag	UNP Q9UHN6
A	97	ASN	-	expression tag	UNP Q9UHN6
A	98	LEU	-	expression tag	UNP Q9UHN6
A	99	TYR	-	expression tag	UNP Q9UHN6
A	100	PHE	-	expression tag	UNP Q9UHN6
A	101	GLN	-	expression tag	UNP Q9UHN6
A	102	GLY	-	expression tag	UNP Q9UHN6
A	103	ALA	-	expression tag	UNP Q9UHN6
A	104	LEU	-	expression tag	UNP Q9UHN6
A	105	ALA	-	expression tag	UNP Q9UHN6

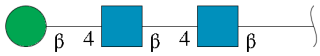
- Molecule 2 is an oligosaccharide called alpha-D-mannopyranose-(1-6)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.

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

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

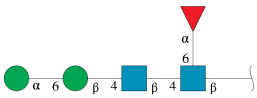
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	C	2	Total	C	N	O	0	0	0
			28	16	2	10			
3	H	2	Total	C	N	O	0	0	0
			28	16	2	10			

- 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	E	3	Total	C	N	O	0	0	0
			39	22	2	15			

- Molecule 5 is an oligosaccharide called alpha-D-mannopyranose-(1-6)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
5	F	5	Total C N O 60 34 2 24	0	0	0

- Molecule 6 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
6	G	4	Total C N O 50 28 2 20	0	0	0

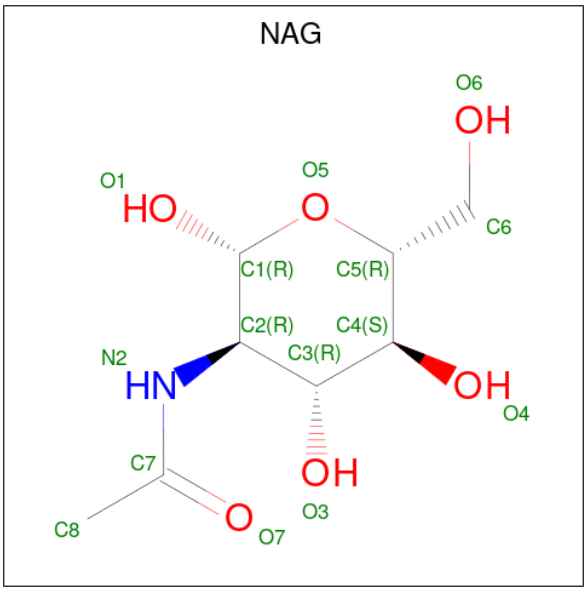
- Molecule 7 is NICKEL (II) ION (three-letter code: NI) (formula: Ni).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total Ni 1 1	0	0

- Molecule 8 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

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

- Molecule 9 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



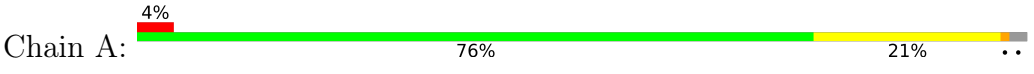
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	A	1	Total C N O 14 8 1 5	0	0
9	A	1	Total C N O 14 8 1 5	0	0

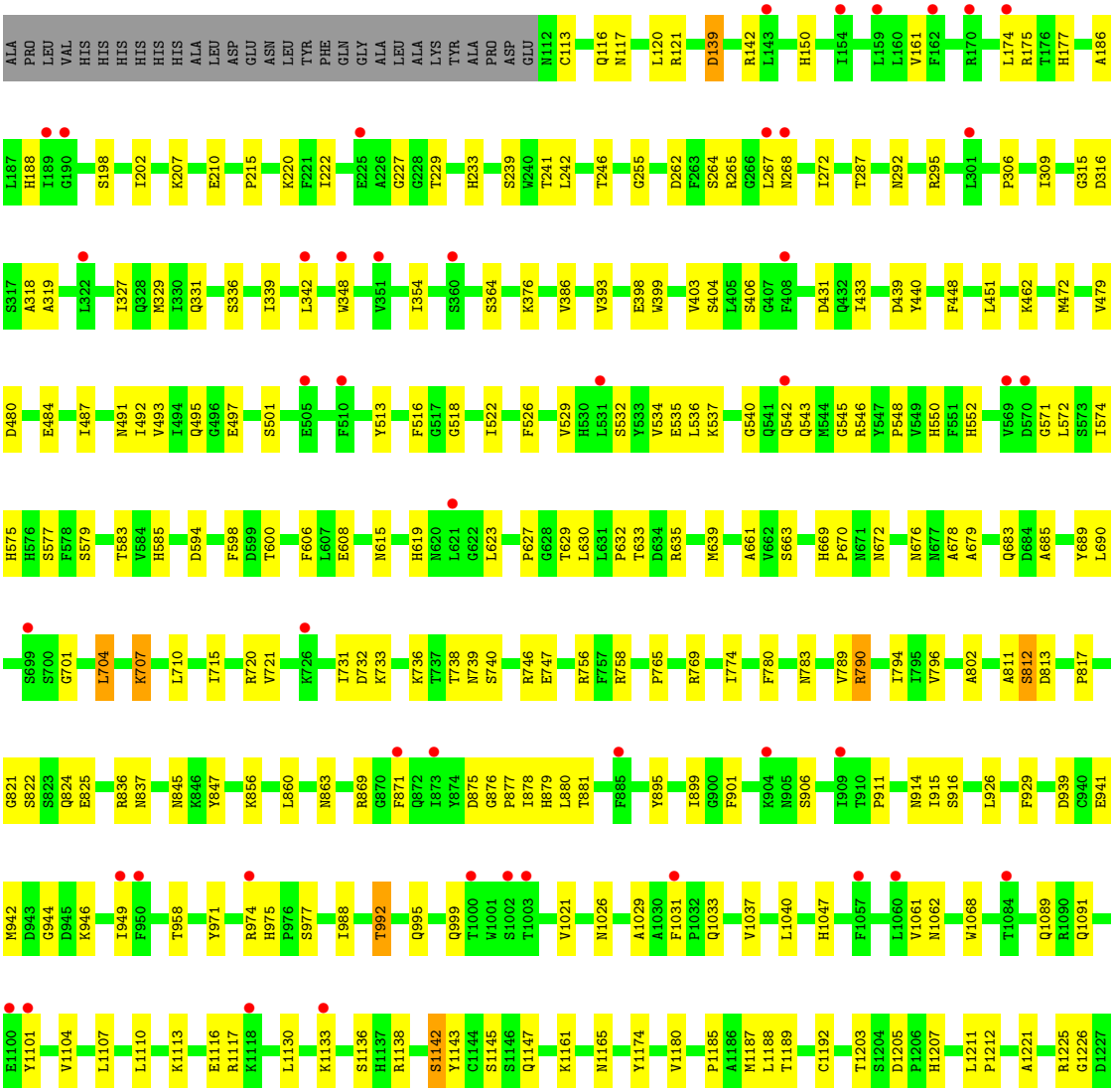
3 Residue-property plots (i)

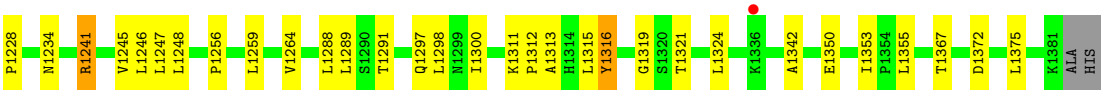
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

Chain A:





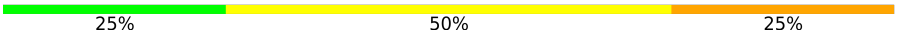


• Molecule 2: alpha-D-mannopyranose-(1-6)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain B:

• Molecule 2: 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:



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

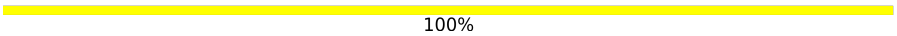
Chain C:

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

Chain H:

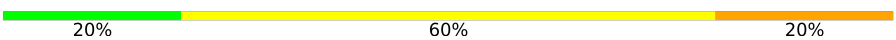
• Molecule 4: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain E:



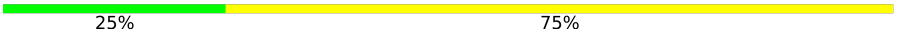
• Molecule 5: alpha-D-mannopyranose-(1-6)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain F:



• Molecule 6: 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 G:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 42 21 2	Depositor
Cell constants a, b, c, α, β, γ	184.76Å 184.76Å 105.40Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	91.55 – 3.50 92.38 – 3.50	Depositor EDS
% Data completeness (in resolution range)	99.8 (91.55-3.50) 100.0 (92.38-3.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.08 (at 3.49Å)	Xtriage
Refinement program	PHENIX 1.18	Depositor
R, R_{free}	0.265 , 0.319 0.265 , 0.319	Depositor DCC
R_{free} test set	1123 reflections (4.76%)	wwPDB-VP
Wilson B-factor (Å^2)	121.6	Xtriage
Anisotropy	0.232	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 65.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.38$, $< L^2 > = 0.22$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.90	EDS
Total number of atoms	10327	wwPDB-VP
Average B, all atoms (Å^2)	113.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.62% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: MAN, BMA, NAG, FUC, NI, CL

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	0.27	0/10231	0.47	0/13855

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	9992	0	9746	171	0
2	B	50	0	43	2	0
2	D	50	0	43	4	0
3	C	28	0	25	4	0
3	H	28	0	25	0	0
4	E	39	0	34	2	0
5	F	60	0	52	3	0
6	G	50	0	43	1	0
7	A	1	0	0	0	0
8	A	1	0	0	0	0
9	A	28	0	26	0	0
All	All	10327	0	10037	176	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 9.

All (176) 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:999:GLN:HG2	1:A:1033:GLN:HB3	1.61	0.82
1:A:769:ARG:NH1	1:A:821:GLY:O	2.16	0.78
1:A:789:VAL:HG11	1:A:794:ILE:HG21	1.68	0.73
1:A:220:LYS:NZ	1:A:497:GLU:O	2.22	0.72
1:A:265:ARG:HG3	1:A:316:ASP:HB3	1.74	0.70
1:A:227:GLY:H	1:A:526:PHE:HA	1.55	0.69
1:A:220:LYS:NZ	1:A:516:PHE:O	2.27	0.67
1:A:484:GLU:OE1	1:A:720:ARG:NH1	2.27	0.67
1:A:255:GLY:HA3	4:E:1:NAG:H81	1.76	0.66
1:A:876:GLY:HA2	1:A:878:ILE:HG13	1.76	0.66
1:A:1212:PRO:HG2	1:A:1234:ASN:HA	1.77	0.65
1:A:946:LYS:NZ	1:A:1021:VAL:O	2.29	0.65
1:A:756:ARG:NH1	1:A:813:ASP:OD1	2.29	0.64
1:A:120:LEU:HB3	1:A:142:ARG:HB2	1.79	0.64
1:A:627:PRO:HG3	1:A:683:GLN:HG2	1.79	0.64
1:A:265:ARG:HA	1:A:316:ASP:H	1.62	0.63
1:A:999:GLN:NE2	1:A:1033:GLN:OE1	2.30	0.63
1:A:856:LYS:HE2	4:E:2:NAG:H83	1.81	0.62
1:A:1026:ASN:HB3	1:A:1029:ALA:HB3	1.80	0.62
1:A:113:CYS:HB2	1:A:116:GLN:HB2	1.82	0.62
1:A:633:THR:HB	1:A:661:ALA:HB3	1.81	0.61
1:A:995:GLN:NE2	1:A:1062:ASN:OD1	2.34	0.61
1:A:879:HIS:HB2	3:C:1:NAG:H83	1.83	0.61
1:A:1247:LEU:HD12	1:A:1289:LEU:HD12	1.82	0.60
1:A:710:LEU:HD23	1:A:758:ARG:HG3	1.83	0.60
3:C:2:NAG:H3	3:C:2:NAG:H83	1.84	0.59
1:A:518:GLY:O	1:A:540:GLY:N	2.33	0.59
1:A:739:ASN:OD1	6:G:1:NAG:N2	2.35	0.59
1:A:552:HIS:HA	1:A:585:HIS:HB3	1.85	0.58
1:A:161:VAL:HG22	1:A:188:HIS:HB2	1.86	0.57
1:A:689:TYR:HB2	1:A:731:ILE:HG12	1.85	0.57
1:A:207:LYS:HB2	1:A:210:GLU:HB2	1.86	0.57
1:A:790:ARG:HB2	1:A:811:ALA:HB3	1.85	0.57
1:A:318:ALA:HB3	1:A:342:LEU:HD21	1.86	0.57
1:A:306:PRO:HA	1:A:354:ILE:HG22	1.87	0.56
1:A:439:ASP:OD2	1:A:845:ASN:ND2	2.38	0.56
1:A:545:GLY:O	1:A:550:HIS:ND1	2.38	0.56
2:B:1:NAG:H3	2:B:1:NAG:H83	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:881:THR:HA	1:A:916:SER:O	2.06	0.56
1:A:479:VAL:HG21	1:A:802:ALA:HB2	1.87	0.56
1:A:679:ALA:HB3	1:A:721:VAL:HG12	1.88	0.56
1:A:1319:GLY:HA2	1:A:1342:ALA:HA	1.88	0.55
1:A:327:ILE:HG23	1:A:339:ILE:HG13	1.88	0.55
1:A:1226:GLY:O	1:A:1241:ARG:NH1	2.35	0.55
1:A:583:THR:HG23	1:A:606:PHE:HD2	1.72	0.54
1:A:1138:ARG:NH1	1:A:1142:SER:O	2.41	0.54
1:A:542:GLN:OE1	1:A:629:THR:OG1	2.22	0.54
1:A:789:VAL:HG12	1:A:794:ILE:HD13	1.90	0.54
1:A:1161:LYS:HZ1	5:F:4:MAN:H3	1.73	0.54
1:A:1104:VAL:HG21	1:A:1110:LEU:HB2	1.89	0.54
1:A:386:VAL:HG11	1:A:1313:ALA:HB2	1.90	0.54
1:A:480:ASP:O	1:A:720:ARG:NH2	2.41	0.54
1:A:598:PHE:HD1	1:A:623:LEU:HB2	1.72	0.54
1:A:120:LEU:HD13	1:A:142:ARG:HB2	1.90	0.54
1:A:1324:LEU:HD23	1:A:1353:ILE:HD11	1.89	0.53
1:A:117:ASN:HB3	1:A:120:LEU:HG	1.89	0.53
1:A:958:THR:HB	1:A:988:ILE:HD13	1.90	0.53
1:A:1211:LEU:HB2	1:A:1355:LEU:HD11	1.90	0.53
1:A:1248:LEU:HB2	1:A:1288:LEU:HB2	1.91	0.53
1:A:1248:LEU:HB3	1:A:1259:LEU:HD11	1.91	0.53
1:A:1161:LYS:NZ	5:F:4:MAN:H3	2.24	0.52
1:A:704:LEU:HD13	1:A:707:LYS:HB3	1.90	0.52
1:A:1047:HIS:HB3	1:A:1165:ASN:HA	1.90	0.52
1:A:246:THR:HG23	1:A:472:MET:HA	1.90	0.52
1:A:811:ALA:O	1:A:824:GLN:NE2	2.43	0.52
1:A:198:SER:O	1:A:491:ASN:HB2	2.10	0.52
1:A:319:ALA:HB2	1:A:342:LEU:HG	1.91	0.51
1:A:1113:LYS:HB3	1:A:1116:GLU:HB2	1.92	0.51
1:A:1101:TYR:CZ	1:A:1117:ARG:HD2	2.46	0.51
1:A:1245:VAL:HG22	1:A:1291:THR:HG22	1.93	0.50
3:C:1:NAG:H61	3:C:2:NAG:C7	2.40	0.50
1:A:472:MET:HE3	1:A:837:ASN:HA	1.92	0.50
1:A:492:ILE:HG22	1:A:534:VAL:HG13	1.93	0.50
1:A:267:LEU:HD12	1:A:287:THR:HG21	1.93	0.50
1:A:264:SER:O	1:A:315:GLY:HA3	2.12	0.50
1:A:732:ASP:OD1	1:A:733:LYS:N	2.36	0.50
1:A:812:SER:HB3	1:A:875:ASP:HB3	1.94	0.50
2:D:1:NAG:O3	2:D:2:NAG:N2	2.40	0.50
1:A:774:ILE:HB	1:A:796:VAL:HG22	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:817:PRO:HD3	1:A:1143:TYR:CD2	2.47	0.49
1:A:376:LYS:HA	1:A:398:GLU:HB3	1.94	0.49
1:A:439:ASP:CG	1:A:845:ASN:HD21	2.16	0.49
1:A:899:ILE:HD13	1:A:915:ILE:HD13	1.93	0.49
1:A:939:ASP:HB3	1:A:941:GLU:HB2	1.94	0.49
1:A:669:HIS:O	1:A:672:ASN:ND2	2.44	0.49
1:A:1091:GLN:NE2	2:D:1:NAG:H62	2.27	0.49
1:A:1091:GLN:HE22	2:D:1:NAG:H62	1.76	0.49
1:A:1147:GLN:NE2	2:D:2:NAG:O6	2.45	0.49
1:A:992:THR:HB	1:A:1040:LEU:HD12	1.95	0.49
1:A:227:GLY:N	1:A:526:PHE:HA	2.26	0.49
1:A:241:THR:OG1	1:A:242:LEU:N	2.45	0.49
1:A:121:ARG:HH21	1:A:139:ASP:HA	1.78	0.48
1:A:1107:LEU:HD22	1:A:1174:TYR:CE1	2.47	0.48
1:A:906:SER:HA	1:A:944:GLY:H	1.77	0.48
1:A:663:SER:HA	1:A:685:ALA:O	2.13	0.48
1:A:911:PRO:HB3	1:A:949:ILE:HD13	1.96	0.48
1:A:1311:LYS:O	1:A:1313:ALA:N	2.46	0.48
1:A:272:ILE:HB	1:A:309:ILE:HB	1.95	0.48
1:A:736:LYS:NZ	1:A:738:THR:O	2.40	0.48
1:A:1246:LEU:HD13	1:A:1264:VAL:HG22	1.96	0.48
1:A:433:ILE:HG13	1:A:448:PHE:HB2	1.96	0.47
1:A:440:TYR:HB3	1:A:783:ASN:HD21	1.80	0.47
1:A:577:SER:HB2	1:A:600:THR:HG22	1.97	0.47
1:A:292:ASN:HA	1:A:295:ARG:HD2	1.96	0.47
1:A:571:GLY:HA2	1:A:594:ASP:O	2.15	0.47
1:A:895:TYR:HD2	1:A:929:PHE:CZ	2.33	0.47
1:A:926:LEU:HD12	1:A:926:LEU:HA	1.82	0.47
1:A:264:SER:OG	1:A:268:ASN:OD1	2.29	0.46
1:A:715:ILE:HD13	1:A:1375:LEU:HD22	1.96	0.46
1:A:1061:VAL:HG13	1:A:1143:TYR:HB3	1.96	0.46
1:A:1315:LEU:H	1:A:1315:LEU:HD23	1.80	0.46
1:A:480:ASP:HB2	1:A:1203:THR:HA	1.98	0.46
1:A:522:ILE:HG21	1:A:529:VAL:HG21	1.98	0.46
1:A:710:LEU:HD13	1:A:765:PRO:HD3	1.97	0.46
1:A:825:GLU:HG3	1:A:879:HIS:HB3	1.97	0.46
1:A:1228:PRO:HB3	1:A:1241:ARG:CZ	2.45	0.46
1:A:121:ARG:NH2	1:A:139:ASP:HA	2.31	0.46
1:A:1315:LEU:HG	1:A:1316:TYR:H	1.81	0.46
1:A:635:ARG:HB3	1:A:639:MET:HB2	1.98	0.45
1:A:1068:TRP:HB3	1:A:1133:LYS:HG3	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1372:ASP:OD1	1:A:1372:ASP:N	2.46	0.45
1:A:822:SER:O	1:A:877:PRO:HD2	2.17	0.45
1:A:233:HIS:ND1	1:A:532:SER:OG	2.47	0.45
1:A:995:GLN:HG2	1:A:1037:VAL:HG22	1.99	0.45
1:A:1256:PRO:HB3	2:B:1:NAG:H2	1.99	0.45
1:A:150:HIS:O	1:A:177:HIS:HB2	2.17	0.44
1:A:399:TRP:CZ3	1:A:404:SER:HB3	2.52	0.44
1:A:534:VAL:HB	1:A:572:LEU:HD22	1.99	0.44
1:A:906:SER:HB3	1:A:942:MET:SD	2.57	0.44
1:A:678:ALA:HA	1:A:720:ARG:O	2.18	0.44
1:A:736:LYS:CD	1:A:746:ARG:HB2	2.47	0.44
1:A:975:HIS:HB2	1:A:1180:VAL:HG22	1.99	0.44
1:A:339:ILE:HD13	1:A:348:TRP:CH2	2.53	0.44
1:A:615:ASN:ND2	1:A:672:ASN:OD1	2.39	0.44
1:A:871:PHE:HZ	1:A:878:ILE:HG21	1.81	0.44
1:A:543:GLN:HB3	1:A:546:ARG:HG3	2.00	0.43
1:A:1136:SER:HB2	1:A:1145:SER:HB2	2.00	0.43
1:A:431:ASP:HB3	1:A:487:ILE:HD11	2.00	0.43
1:A:493:VAL:HG22	1:A:535:GLU:HB3	1.99	0.43
1:A:869:ARG:HH12	1:A:901:PHE:N	2.14	0.43
1:A:174:LEU:HD12	1:A:175:ARG:H	1.84	0.43
1:A:732:ASP:CG	1:A:790:ARG:HD2	2.39	0.43
1:A:575:HIS:HA	1:A:598:PHE:O	2.18	0.43
1:A:1205:ASP:HB2	1:A:1207:HIS:CE1	2.54	0.43
5:F:4:MAN:O4	5:F:4:MAN:O6	2.31	0.43
1:A:121:ARG:O	1:A:142:ARG:N	2.42	0.43
1:A:1221:ALA:O	1:A:1225:ARG:HG3	2.19	0.42
1:A:670:PRO:O	1:A:672:ASN:N	2.50	0.42
1:A:451:LEU:HB2	1:A:462:LYS:HB3	2.01	0.42
1:A:619:HIS:HA	1:A:676:ASN:O	2.20	0.42
1:A:880:LEU:HB3	1:A:915:ILE:HG12	2.01	0.42
1:A:186:ALA:HA	1:A:229:THR:HB	2.02	0.42
1:A:495:GLN:HA	1:A:537:LYS:O	2.20	0.42
1:A:239:SER:OG	1:A:594:ASP:HB3	2.19	0.42
1:A:812:SER:N	1:A:875:ASP:OD2	2.52	0.42
1:A:879:HIS:HB2	3:C:1:NAG:C8	2.49	0.41
1:A:1187:MET:HE2	1:A:1189:THR:HG23	2.02	0.41
1:A:548:PRO:HD3	1:A:579:SER:O	2.20	0.41
1:A:836:ARG:NH2	1:A:1350:GLU:HB3	2.36	0.41
1:A:309:ILE:HG21	1:A:393:VAL:HG21	2.02	0.41
1:A:975:HIS:CE1	1:A:977:SER:HB2	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1298:LEU:HD12	1:A:1298:LEU:HA	1.76	0.41
1:A:348:TRP:HD1	1:A:364:SER:O	2.03	0.41
1:A:1089:GLN:NE2	1:A:1147:GLN:O	2.49	0.41
1:A:202:ILE:HG21	1:A:222:ILE:HD11	2.03	0.41
1:A:331:GLN:HG2	1:A:336:SER:O	2.21	0.41
1:A:632:PRO:HG3	1:A:747:GLU:OE1	2.20	0.41
1:A:780:PHE:HA	1:A:802:ALA:O	2.21	0.41
1:A:847:TYR:HB2	1:A:860:LEU:O	2.20	0.41
1:A:971:TYR:HA	1:A:974:ARG:HD3	2.03	0.41
1:A:536:LEU:HB2	1:A:574:ILE:HG12	2.03	0.40
1:A:501:SER:HA	1:A:513:TYR:HA	2.03	0.40
1:A:1187:MET:HE2	1:A:1187:MET:HB3	1.94	0.40
1:A:1298:LEU:C	1:A:1300:ILE:H	2.25	0.40
1:A:399:TRP:HA	1:A:403:VAL:O	2.21	0.40
1:A:1315:LEU:H	1:A:1315:LEU:CD2	2.33	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	1268/1301 (98%)	1141 (90%)	118 (9%)	9 (1%)	22 61

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	812	SER
1	A	215	PRO
1	A	630	LEU
1	A	608	GLU
1	A	1185	PRO
1	A	1312	PRO

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Mol	Chain	Res	Type
1	A	139	ASP
1	A	1297	GLN
1	A	701	GLY

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.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	1093/1117 (98%)	1073 (98%)	20 (2%)	59 81

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	262	ASP
1	A	329	MET
1	A	406	SER
1	A	690	LEU
1	A	704	LEU
1	A	707	LYS
1	A	740	SER
1	A	790	ARG
1	A	863	ASN
1	A	914	ASN
1	A	992	THR
1	A	1031	PHE
1	A	1130	LEU
1	A	1142	SER
1	A	1188	LEU
1	A	1192	CYS
1	A	1241	ARG
1	A	1316	TYR
1	A	1321	THR
1	A	1367	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	845	ASN
1	A	995	GLN
1	A	1091	GLN

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)

24 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	B	1	2,1	14,14,15	0.51	0	17,19,21	1.39	2 (11%)
2	NAG	B	2	2	14,14,15	0.50	0	17,19,21	0.49	0
2	BMA	B	3	2	11,11,12	0.79	0	15,15,17	0.85	0
2	MAN	B	4	2	11,11,12	0.84	0	15,15,17	0.97	1 (6%)
3	NAG	C	1	3,1	14,14,15	0.61	0	17,19,21	0.56	0
3	NAG	C	2	3	14,14,15	0.62	0	17,19,21	1.33	1 (5%)
2	NAG	D	1	2,1	14,14,15	0.20	0	17,19,21	0.48	0
2	NAG	D	2	2	14,14,15	0.66	1 (7%)	17,19,21	0.66	0
2	BMA	D	3	2	11,11,12	0.74	0	15,15,17	0.86	0
2	MAN	D	4	2	11,11,12	0.76	1 (9%)	15,15,17	1.18	2 (13%)
4	NAG	E	1	4,1	14,14,15	0.60	0	17,19,21	0.96	0
4	NAG	E	2	4	14,14,15	0.53	0	17,19,21	0.56	0
4	BMA	E	3	4	11,11,12	0.98	1 (9%)	15,15,17	0.84	0
5	NAG	F	1	1,5	14,14,15	0.34	0	17,19,21	0.54	0
5	NAG	F	2	5	14,14,15	0.36	0	17,19,21	0.83	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
5	BMA	F	3	5	11,11,12	0.88	1 (9%)	15,15,17	0.90	0
5	MAN	F	4	5	11,11,12	1.23	1 (9%)	15,15,17	1.69	4 (26%)
5	FUC	F	5	5	10,10,11	0.74	0	14,14,16	1.23	3 (21%)
6	NAG	G	1	1,6	14,14,15	0.47	0	17,19,21	0.41	0
6	NAG	G	2	6	14,14,15	0.30	0	17,19,21	0.62	0
6	BMA	G	3	6	11,11,12	1.36	3 (27%)	15,15,17	1.10	2 (13%)
6	MAN	G	4	6	11,11,12	1.12	2 (18%)	15,15,17	1.63	2 (13%)
3	NAG	H	1	3,1	14,14,15	0.20	0	17,19,21	0.58	0
3	NAG	H	2	3	14,14,15	0.93	2 (14%)	17,19,21	0.65	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

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

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

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	F	4	MAN	C1-C2	3.60	1.60	1.52
6	G	3	BMA	C1-C2	2.70	1.58	1.52
6	G	4	MAN	C1-C2	2.55	1.58	1.52
3	H	2	NAG	C1-C2	2.47	1.56	1.52
4	E	3	BMA	C1-C2	2.36	1.57	1.52
3	H	2	NAG	O5-C1	2.32	1.47	1.43
2	D	2	NAG	C1-C2	2.29	1.55	1.52
6	G	4	MAN	O5-C5	2.28	1.48	1.43
6	G	3	BMA	O3-C3	2.20	1.48	1.43
5	F	3	BMA	C1-C2	2.12	1.57	1.52
2	D	4	MAN	C1-C2	2.12	1.57	1.52
6	G	3	BMA	C2-C3	2.06	1.55	1.52

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	G	4	MAN	C1-O5-C5	5.36	119.45	112.19
3	C	2	NAG	C2-N2-C7	4.36	129.11	122.90
2	B	1	NAG	C2-N2-C7	4.31	129.04	122.90
5	F	4	MAN	C1-C2-C3	3.63	114.13	109.67
5	F	4	MAN	C1-O5-C5	3.30	116.66	112.19
2	D	4	MAN	C1-O5-C5	3.16	116.48	112.19
6	G	3	BMA	C1-C2-C3	2.60	112.86	109.67
5	F	4	MAN	O5-C1-C2	2.54	114.69	110.77
5	F	5	FUC	O2-C2-C1	2.51	114.28	109.15
6	G	4	MAN	O2-C2-C3	-2.49	105.16	110.14
5	F	4	MAN	O2-C2-C3	-2.28	105.56	110.14
5	F	2	NAG	C1-O5-C5	2.28	115.28	112.19
5	F	5	FUC	O5-C5-C4	2.27	113.60	109.52
2	D	4	MAN	O2-C2-C3	-2.24	105.65	110.14
2	B	1	NAG	C1-C2-N2	2.15	114.17	110.49
6	G	3	BMA	O2-C2-C3	-2.08	105.97	110.14
2	B	4	MAN	O2-C2-C3	-2.07	105.98	110.14
5	F	5	FUC	C1-O5-C5	2.02	117.35	112.78

There are no chirality outliers.

All (38) torsion outliers are listed below:

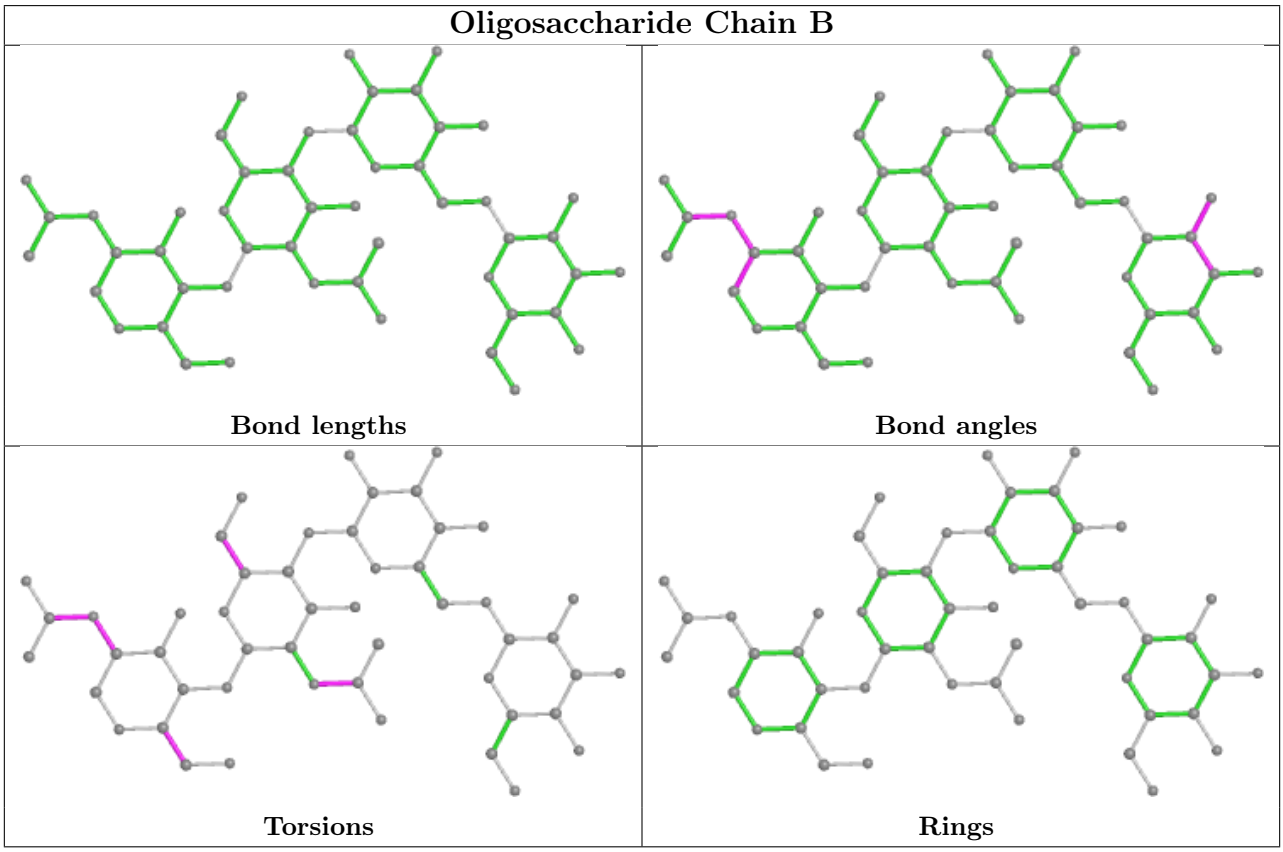
Mol	Chain	Res	Type	Atoms
2	D	2	NAG	O5-C5-C6-O6
2	D	3	BMA	O5-C5-C6-O6
5	F	4	MAN	O5-C5-C6-O6
2	D	3	BMA	C4-C5-C6-O6
4	E	2	NAG	O5-C5-C6-O6
2	D	2	NAG	C4-C5-C6-O6
5	F	3	BMA	C4-C5-C6-O6
4	E	2	NAG	C4-C5-C6-O6
2	B	1	NAG	C8-C7-N2-C2
2	B	1	NAG	O7-C7-N2-C2
2	B	2	NAG	C8-C7-N2-C2
2	B	2	NAG	O7-C7-N2-C2
3	C	2	NAG	C8-C7-N2-C2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

There are no ring outliers.

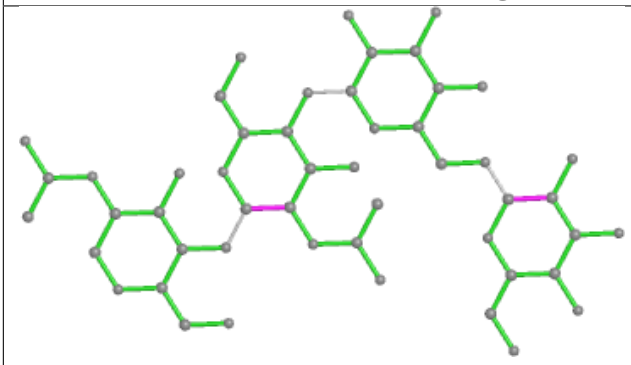
9 monomers are involved in 16 short contacts:

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

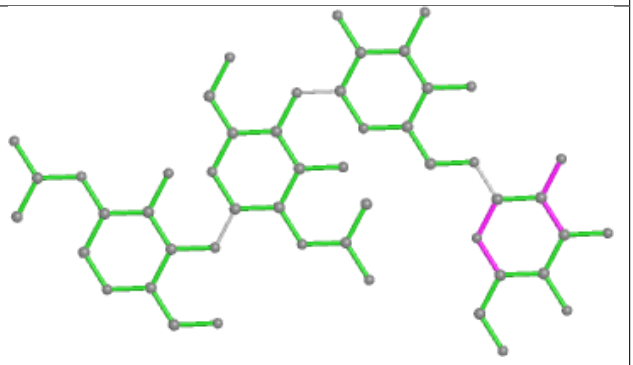
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.



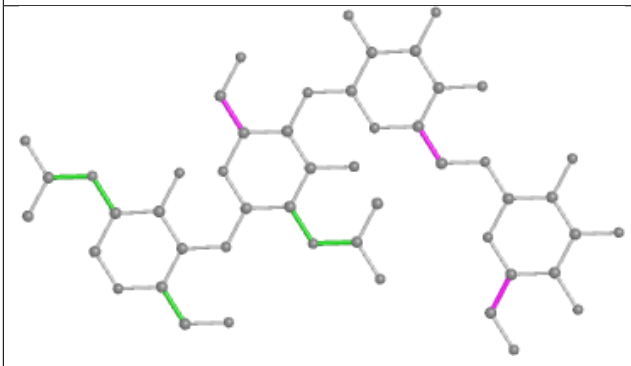
Oligosaccharide Chain D



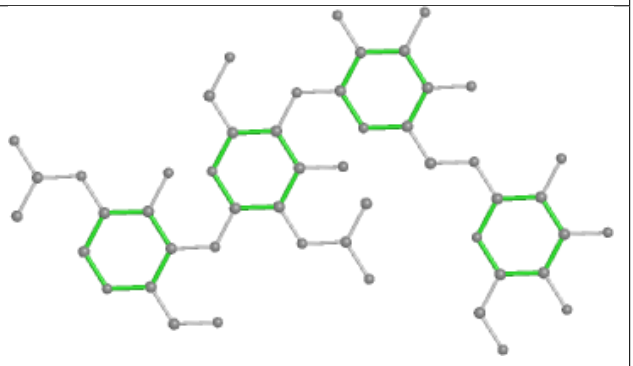
Bond lengths



Bond angles

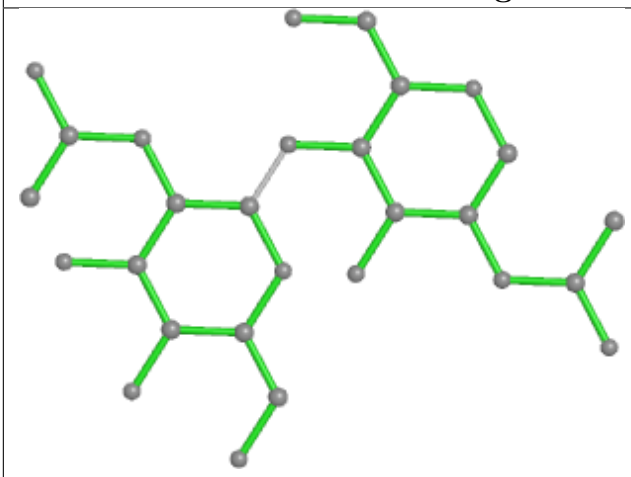


Torsions

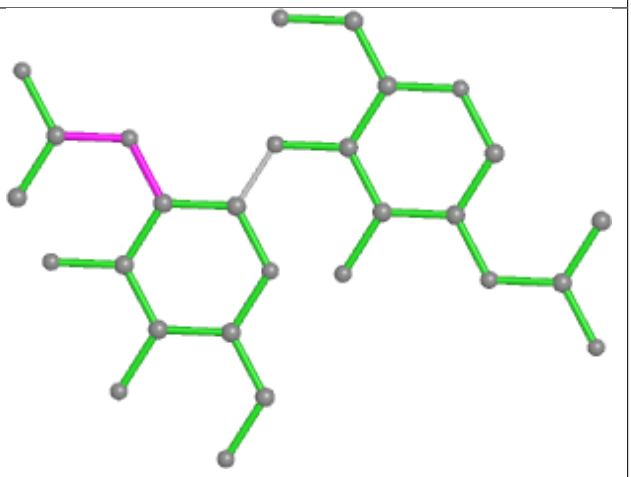


Rings

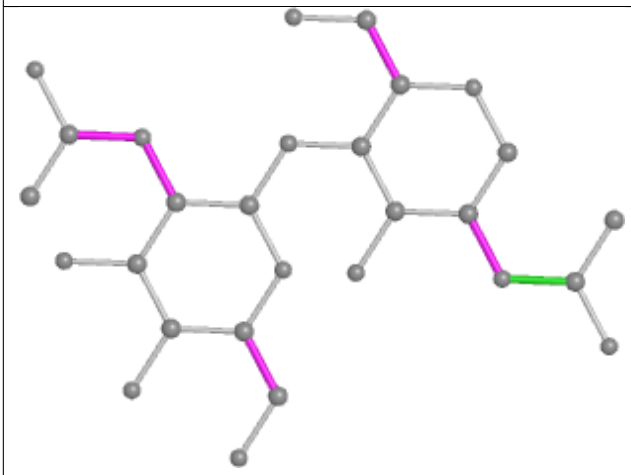
Oligosaccharide Chain C



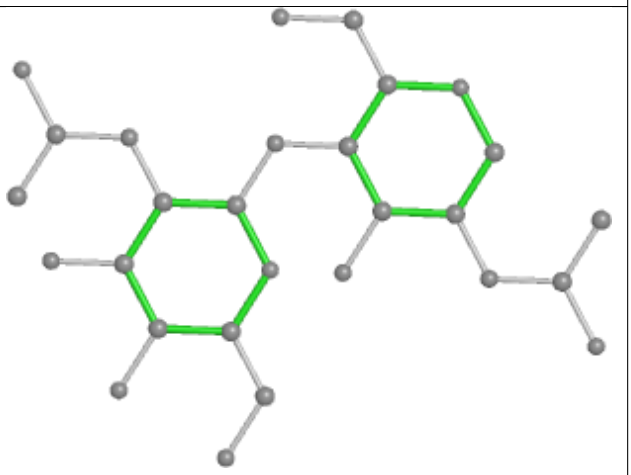
Bond lengths



Bond angles

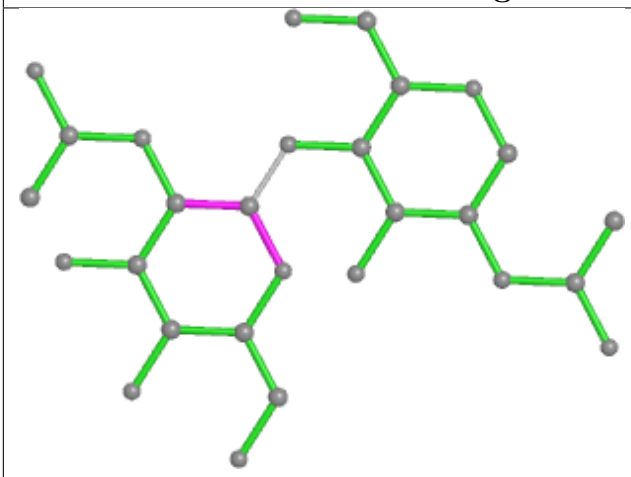


Torsions

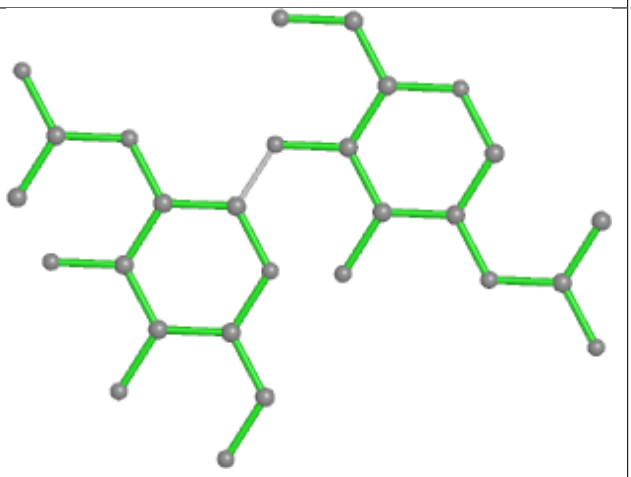


Rings

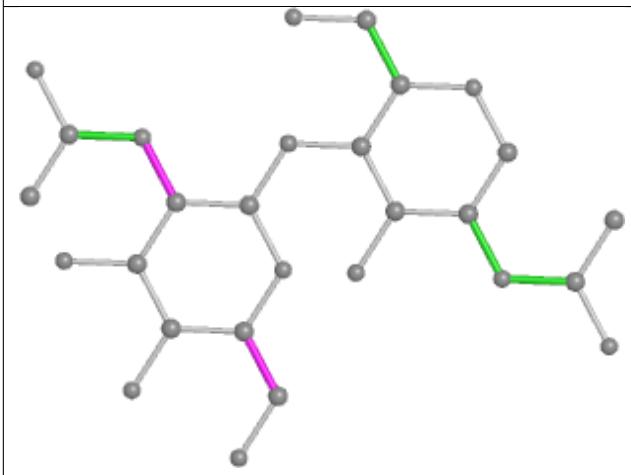
Oligosaccharide Chain H



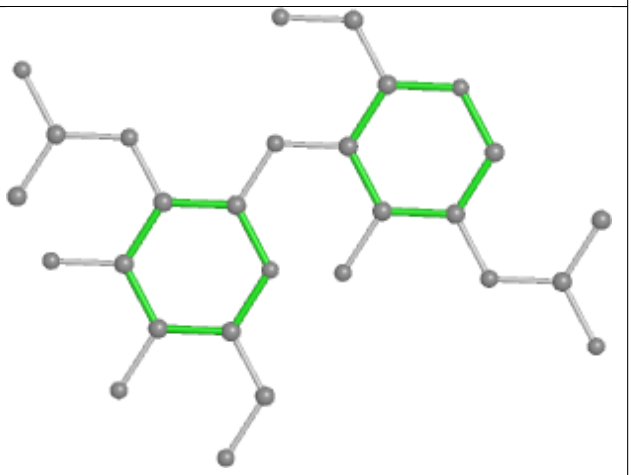
Bond lengths



Bond angles

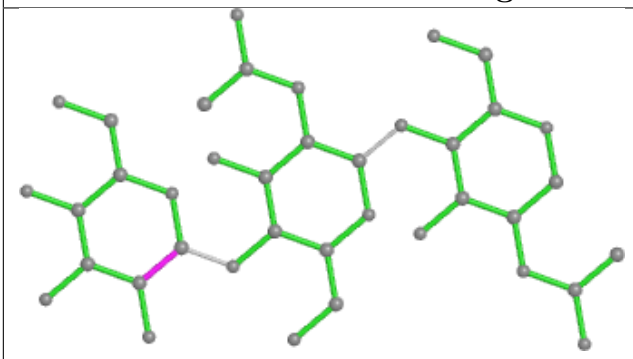


Torsions

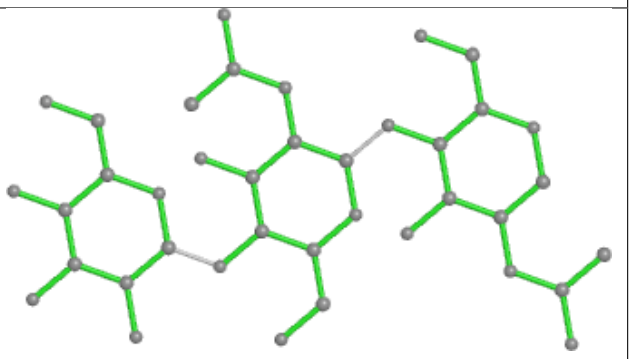


Rings

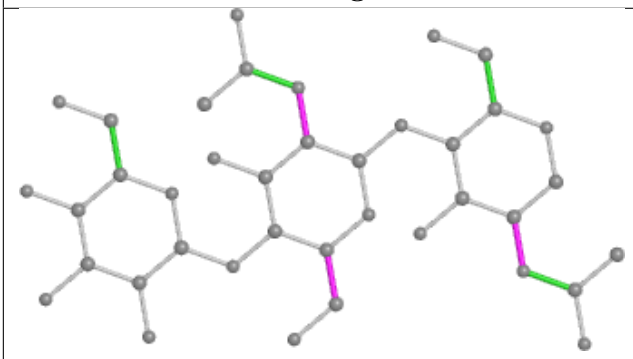
Oligosaccharide Chain E



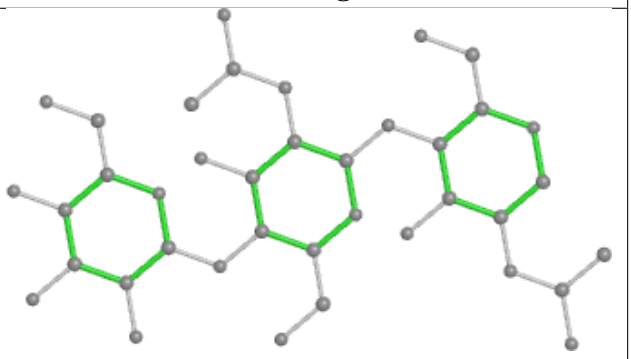
Bond lengths



Bond angles

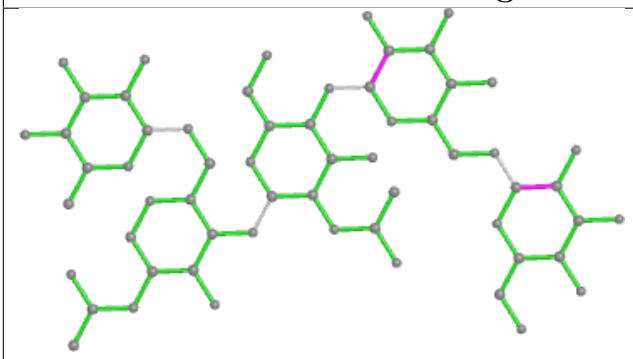


Torsions

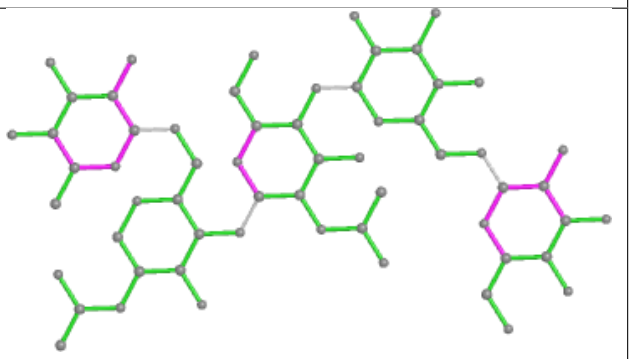


Rings

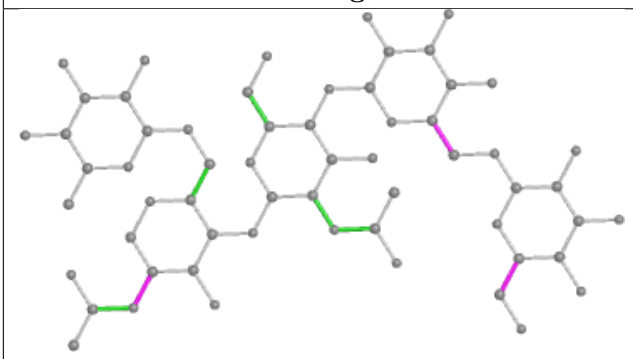
Oligosaccharide Chain F



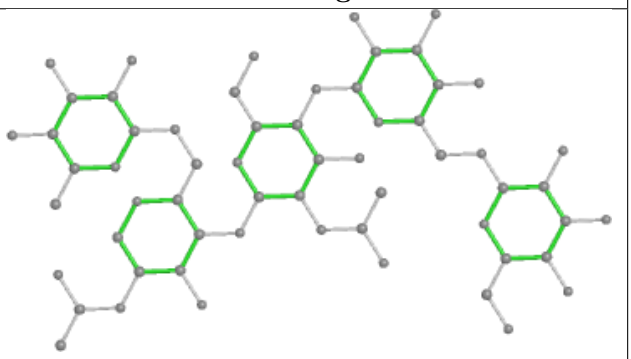
Bond lengths



Bond angles

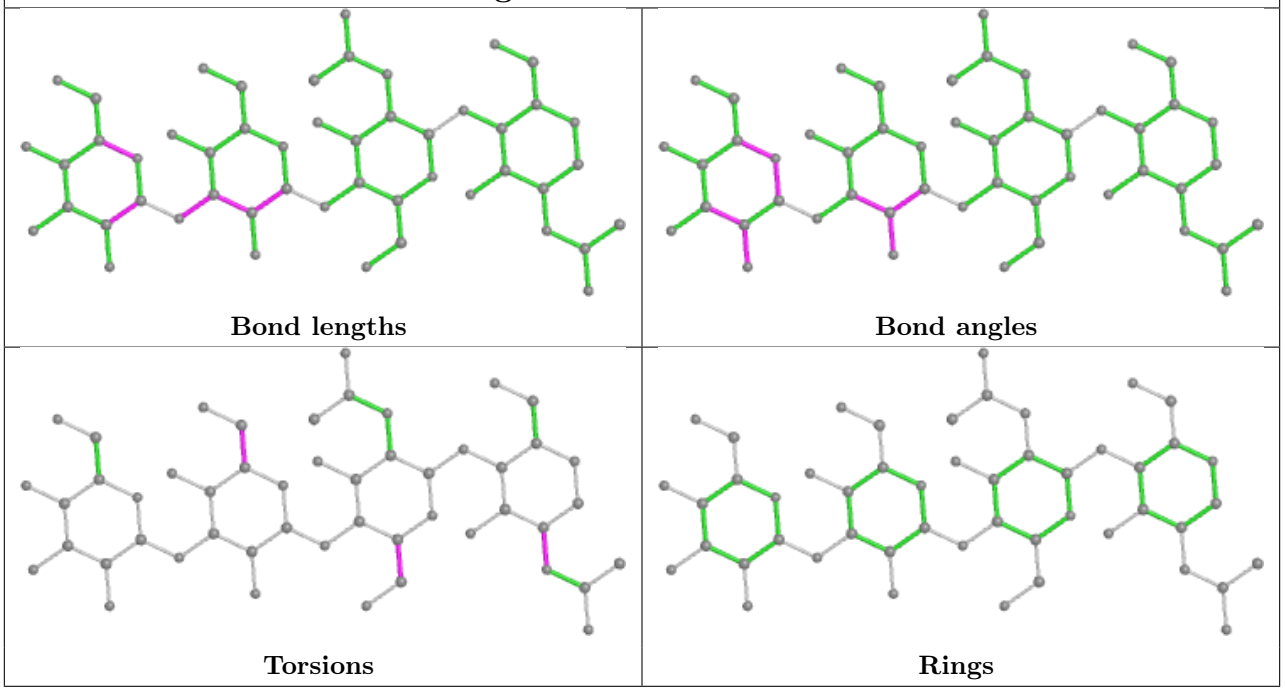


Torsions



Rings

Oligosaccharide Chain G



5.6 Ligand geometry (i)

Of 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 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	$\#\|Z\| > 2$
9	NAG	A	9904	1	14,14,15	0.46	0	17,19,21	0.46	0
9	NAG	A	9903	1	14,14,15	0.36	0	17,19,21	0.48	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
9	NAG	A	9904	1	-	2/6/23/26	0/1/1/1
9	NAG	A	9903	1	-	3/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	A	9904	NAG	C4-C5-C6-O6
9	A	9904	NAG	O5-C5-C6-O6
9	A	9903	NAG	O5-C5-C6-O6
9	A	9903	NAG	C4-C5-C6-O6
9	A	9903	NAG	C1-C2-N2-C7

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

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, 95^{th} 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	1270/1301 (97%)	0.51	47 (3%) 41 37	91, 113, 133, 144	0

All (47) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	342	LEU	4.3
1	A	189	ILE	3.5
1	A	542	GLN	3.4
1	A	267	LEU	3.1
1	A	162	PHE	3.0
1	A	904	LYS	3.0
1	A	1060	LEU	2.9
1	A	190	GLY	2.9
1	A	225	GLU	2.8
1	A	1003	THR	2.8
1	A	873	ILE	2.8
1	A	322	LEU	2.8
1	A	1002	SER	2.7
1	A	726	LYS	2.7
1	A	170	ARG	2.7
1	A	1031	PHE	2.6
1	A	950	PHE	2.6
1	A	505	GLU	2.5
1	A	1084	THR	2.5
1	A	1133	LYS	2.4
1	A	348	TRP	2.4
1	A	871	PHE	2.4
1	A	974	ARG	2.3
1	A	1118	LYS	2.3
1	A	408	PHE	2.3
1	A	569	VAL	2.3
1	A	570	ASP	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	909	ILE	2.2
1	A	1057	PHE	2.2
1	A	1000	THR	2.2
1	A	268	ASN	2.2
1	A	1101	TYR	2.2
1	A	510	PHE	2.2
1	A	159	LEU	2.2
1	A	621	LEU	2.2
1	A	174	LEU	2.2
1	A	301	LEU	2.2
1	A	949	ILE	2.1
1	A	699	SER	2.1
1	A	143	LEU	2.1
1	A	885	PHE	2.1
1	A	1100	GLU	2.1
1	A	531	LEU	2.0
1	A	360	SER	2.0
1	A	351	VAL	2.0
1	A	154	ILE	2.0
1	A	1336	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, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	NAG	H	2	14/15	0.56	0.35	134,134,134,134	0
5	BMA	F	3	11/12	0.68	0.20	134,134,134,134	0
6	NAG	G	1	14/15	0.70	0.31	112,112,112,112	0
2	MAN	B	4	11/12	0.77	0.22	133,133,133,133	0
3	NAG	H	1	14/15	0.79	0.21	128,128,128,128	0
5	FUC	F	5	10/11	0.79	0.32	128,128,128,128	0
4	NAG	E	2	14/15	0.79	0.23	126,126,126,126	0
2	NAG	B	2	14/15	0.80	0.20	124,124,124,124	0

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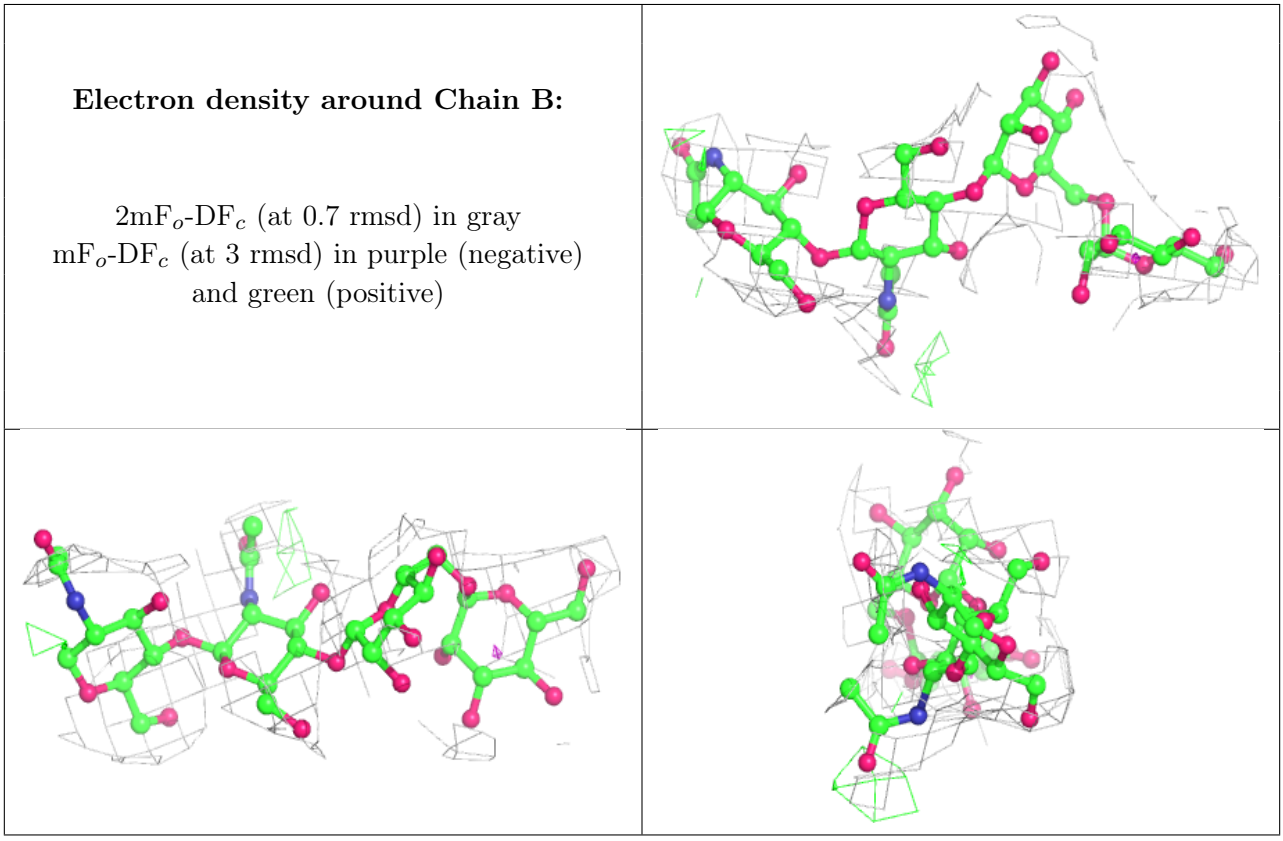
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	BMA	D	3	11/12	0.80	0.18	134,134,134,134	0
2	MAN	D	4	11/12	0.81	0.20	136,136,136,136	0
5	MAN	F	4	11/12	0.81	0.24	136,136,136,136	0
6	MAN	G	4	11/12	0.81	0.18	122,122,122,122	0
2	NAG	D	1	14/15	0.82	0.24	119,119,119,119	0
4	BMA	E	3	11/12	0.83	0.20	132,132,132,132	0
2	BMA	B	3	11/12	0.83	0.19	131,131,131,131	0
5	NAG	F	2	14/15	0.84	0.24	129,129,129,129	0
3	NAG	C	2	14/15	0.85	0.18	114,114,114,114	0
4	NAG	E	1	14/15	0.85	0.28	118,118,118,118	0
2	NAG	D	2	14/15	0.86	0.18	125,125,125,125	0
6	BMA	G	3	11/12	0.87	0.15	117,117,117,117	0
3	NAG	C	1	14/15	0.87	0.18	109,109,109,109	0
5	NAG	F	1	14/15	0.90	0.21	126,126,126,126	0
2	NAG	B	1	14/15	0.90	0.28	116,116,116,116	0
6	NAG	G	2	14/15	0.91	0.26	114,114,114,114	0

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

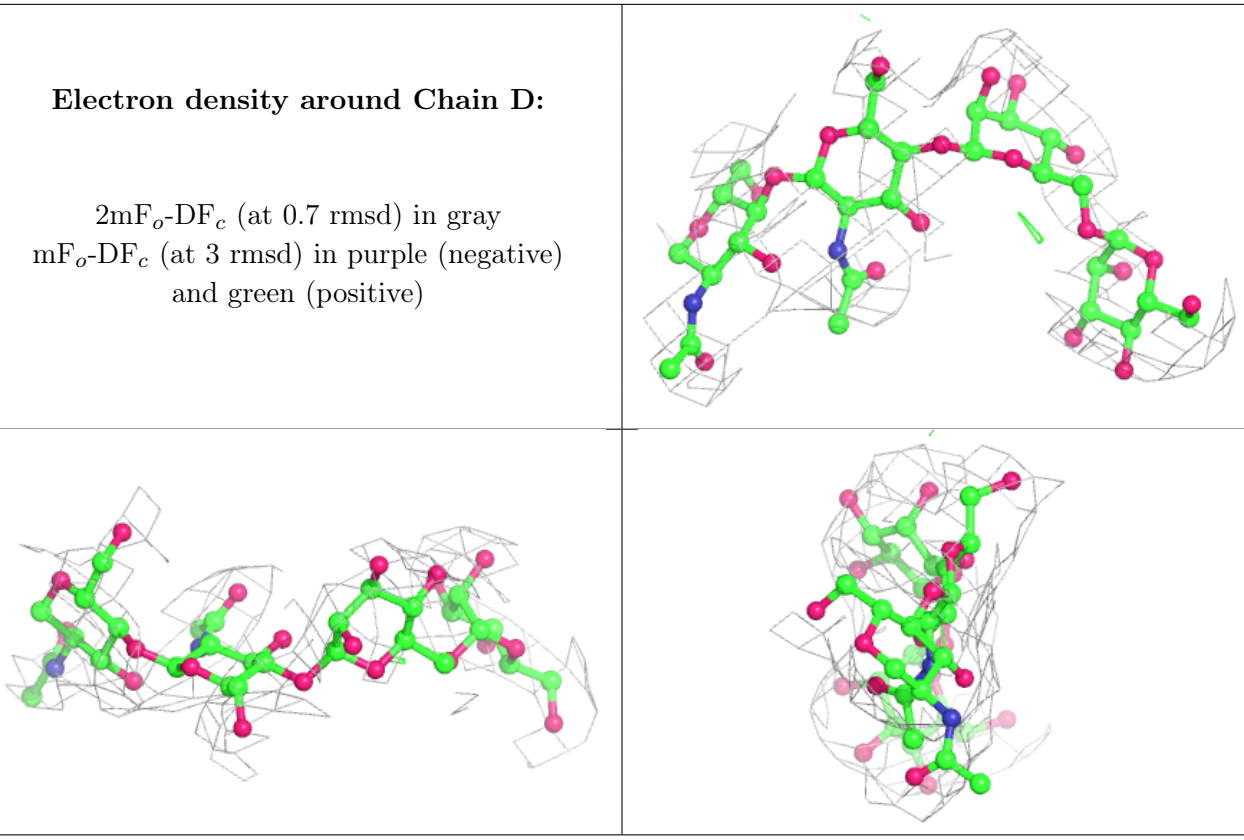
Electron density around Chain B:

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



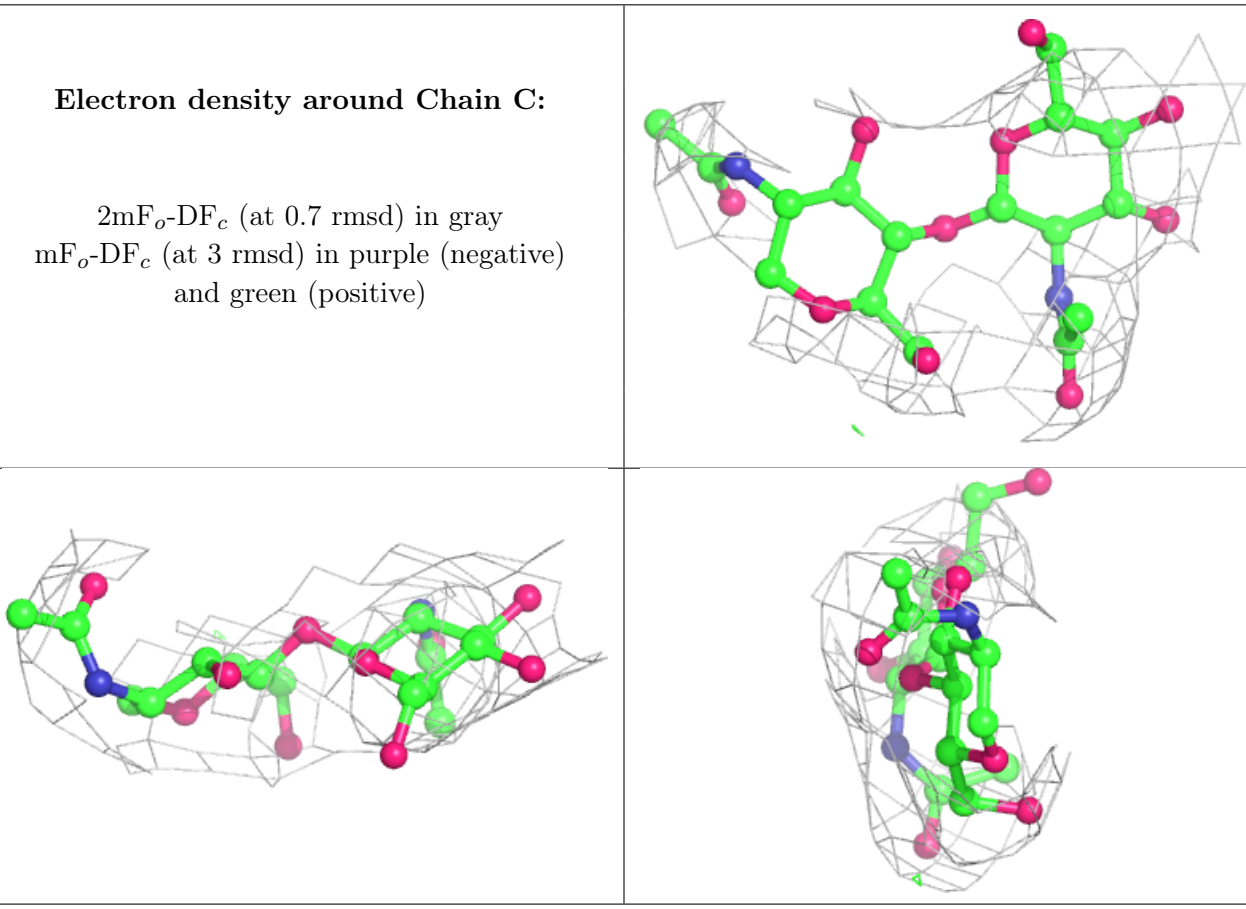
Electron density around Chain D:

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



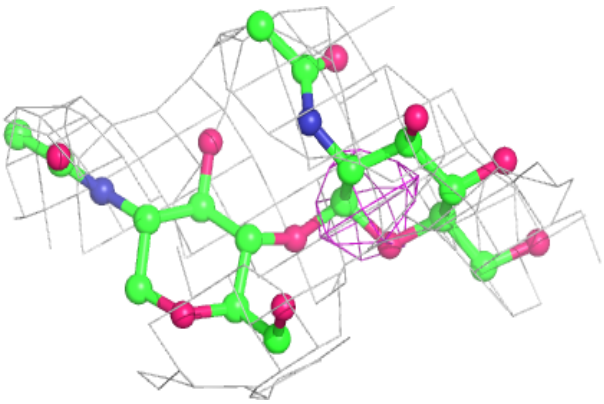
Electron density around Chain C:

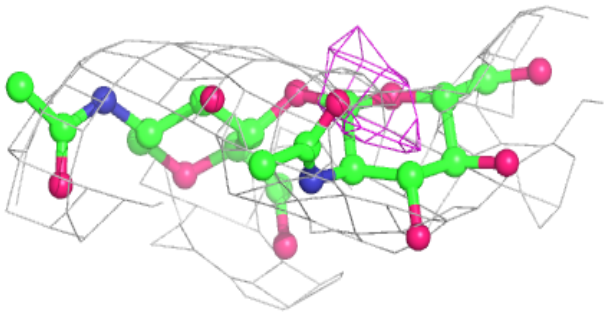
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

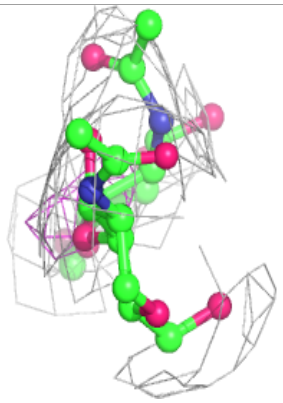


Electron density around Chain H:

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

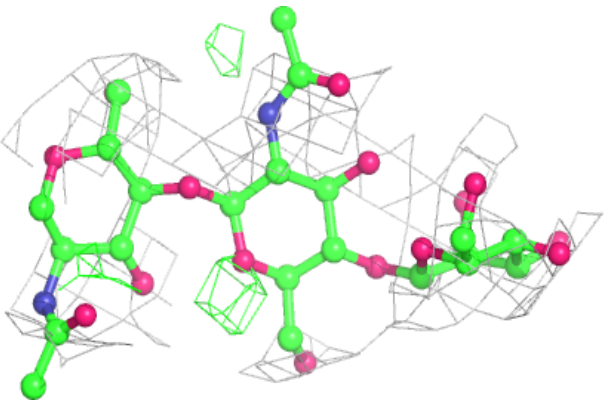


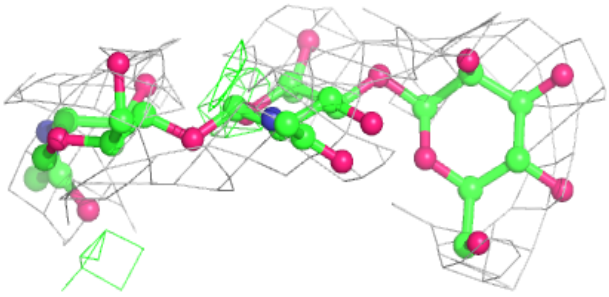


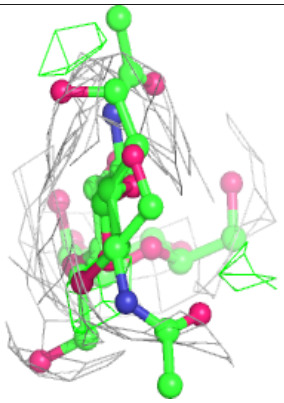


Electron density around Chain E:

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

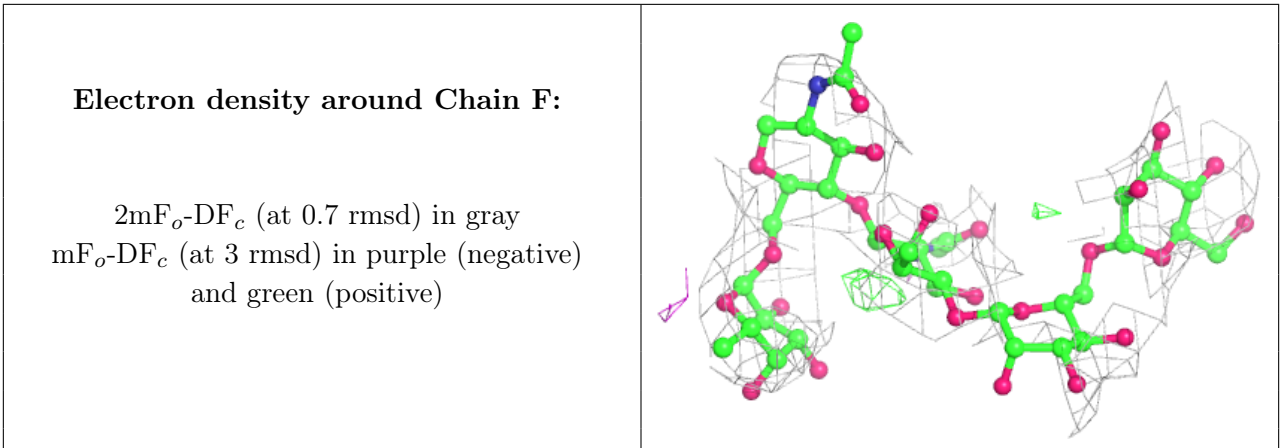






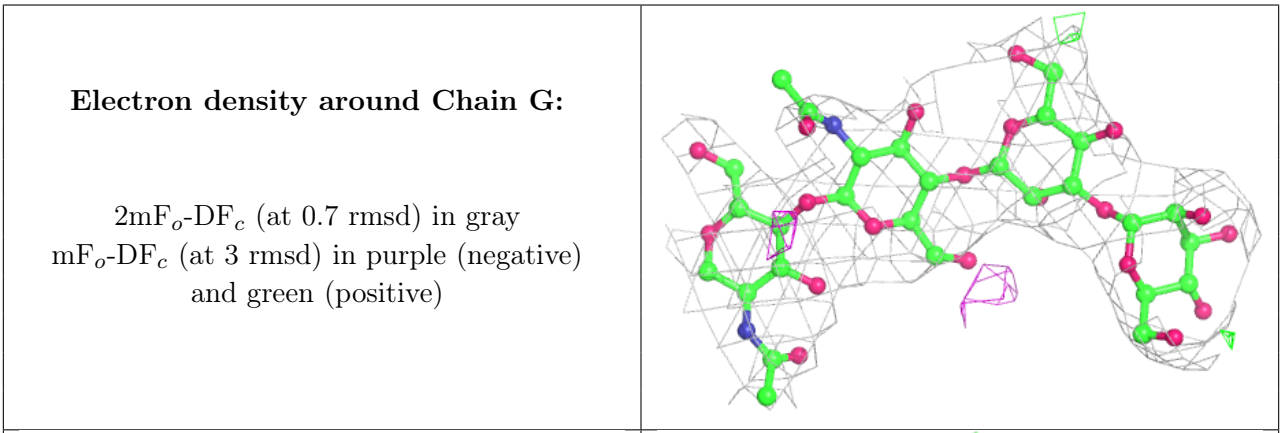
Electron density around Chain F:

$2mF_o$-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 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

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, 95^{th} 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
9	NAG	A	9903	14/15	0.72	0.30	138,138,138,138	0
9	NAG	A	9904	14/15	0.82	0.25	111,111,111,111	0
8	CL	A	9902	1/1	0.85	0.47	106,106,106,106	0
7	NI	A	9901	1/1	0.94	0.17	111,111,111,111	0

6.5 Other polymers

There are no such residues in this entry.