



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 06:18 AM UTC

PDB ID : 8YXI / pdb_00008yxi
Title : Crystal structure of SFTSV Gn in complex with a neutralizing antibody 40C10
Authors : Yang, P.; Guo, Y.; Zhang, N.
Deposited on : 2024-04-02
Resolution : 2.40 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

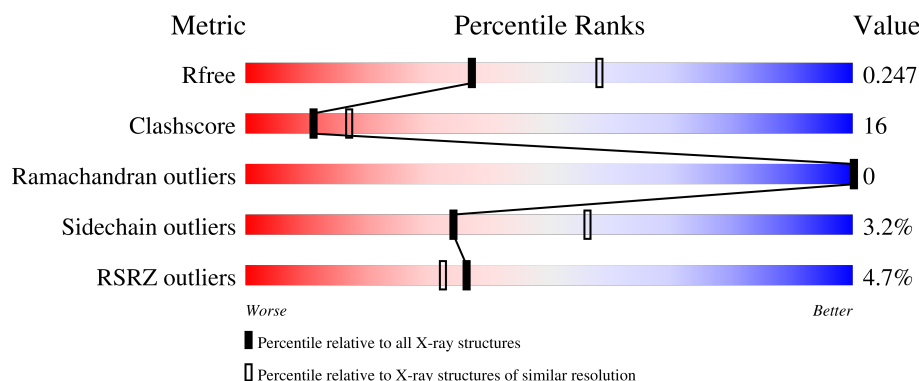
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

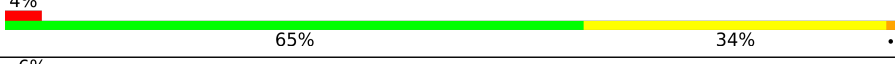
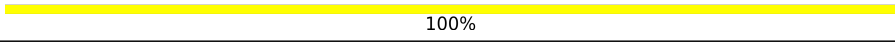
The reported resolution of this entry is 2.40 Å.

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	4912 (2.40-2.40)
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (2.40-2.40)

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 $\leq 5\%$. 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	C	222	
2	B	212	
3	A	347	
4	D	3	
5	E	2	

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 6192 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 heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	C	218	Total	C	N	O	S	0	0	0
			1652	1048	266	332	6			

- Molecule 2 is a protein called light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	212	Total	C	N	O	S	0	0	0
			1654	1042	274	332	6			

- Molecule 3 is a protein called Envelopment polyprotein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	A	321	Total	C	N	O	S	0	0	0
			2464	1540	426	472	26			

There are 26 discrepancies between the modelled and reference sequences:

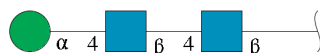
Chain	Residue	Modelled	Actual	Comment	Reference
A	322	GLY	-	expression tag	UNP A0A2Z4HIM0
A	323	LEU	-	expression tag	UNP A0A2Z4HIM0
A	324	ASN	-	expression tag	UNP A0A2Z4HIM0
A	325	ASP	-	expression tag	UNP A0A2Z4HIM0
A	326	ILE	-	expression tag	UNP A0A2Z4HIM0
A	327	PHE	-	expression tag	UNP A0A2Z4HIM0
A	328	GLU	-	expression tag	UNP A0A2Z4HIM0
A	329	ALA	-	expression tag	UNP A0A2Z4HIM0
A	330	GLN	-	expression tag	UNP A0A2Z4HIM0
A	331	LYS	-	expression tag	UNP A0A2Z4HIM0
A	332	ILE	-	expression tag	UNP A0A2Z4HIM0
A	333	GLU	-	expression tag	UNP A0A2Z4HIM0
A	334	TRP	-	expression tag	UNP A0A2Z4HIM0
A	335	HIS	-	expression tag	UNP A0A2Z4HIM0

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Chain	Residue	Modelled	Actual	Comment	Reference
A	336	GLU	-	expression tag	UNP A0A2Z4HIM0
A	337	ALA	-	expression tag	UNP A0A2Z4HIM0
A	338	ALA	-	expression tag	UNP A0A2Z4HIM0
A	339	ALA	-	expression tag	UNP A0A2Z4HIM0
A	340	HIS	-	expression tag	UNP A0A2Z4HIM0
A	341	HIS	-	expression tag	UNP A0A2Z4HIM0
A	342	HIS	-	expression tag	UNP A0A2Z4HIM0
A	343	HIS	-	expression tag	UNP A0A2Z4HIM0
A	344	HIS	-	expression tag	UNP A0A2Z4HIM0
A	345	HIS	-	expression tag	UNP A0A2Z4HIM0
A	346	HIS	-	expression tag	UNP A0A2Z4HIM0
A	347	HIS	-	expression tag	UNP A0A2Z4HIM0

- Molecule 4 is an oligosaccharide called 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
4	D	3	Total	C	N	O	0	0	0
			39	22	2	15			

- Molecule 5 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
5	E	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	C	116	Total	O	0	0
			116	116		

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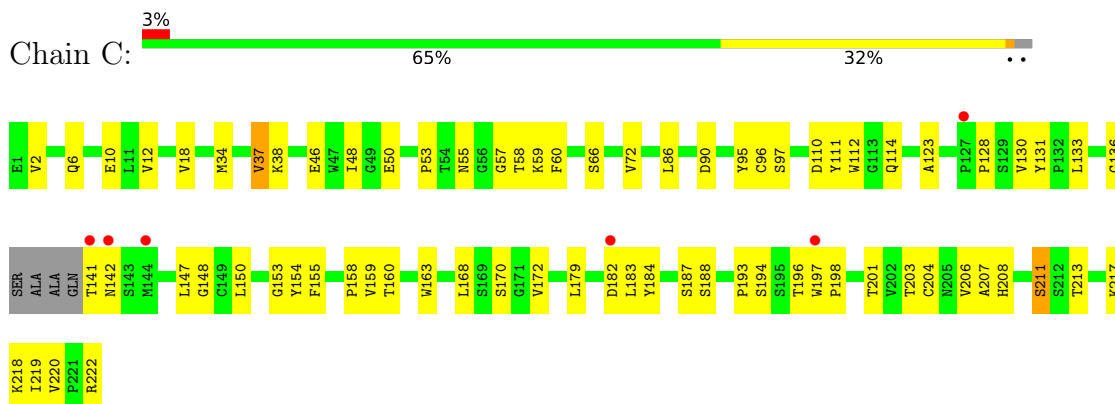
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	95	Total 95	O 95	0	0
6	A	144	Total 144	O 144	0	0

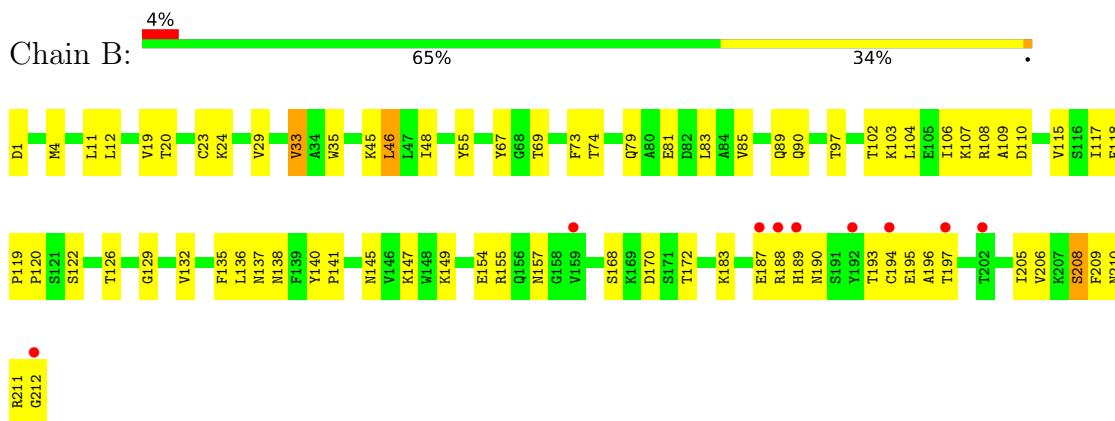
3 Residue-property plots

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

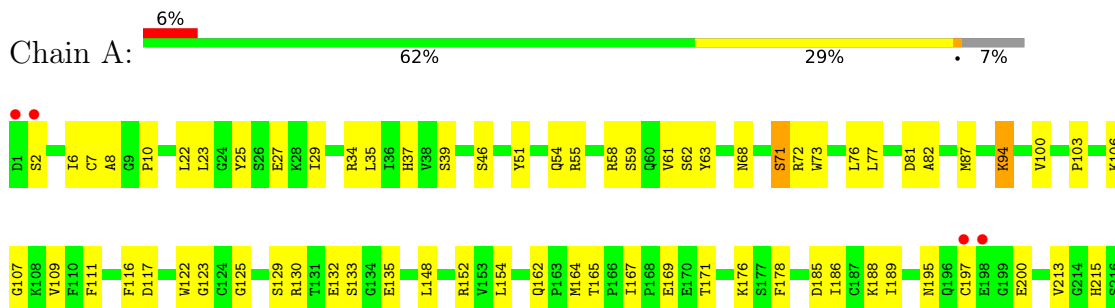
- Molecule 1: heavy chain

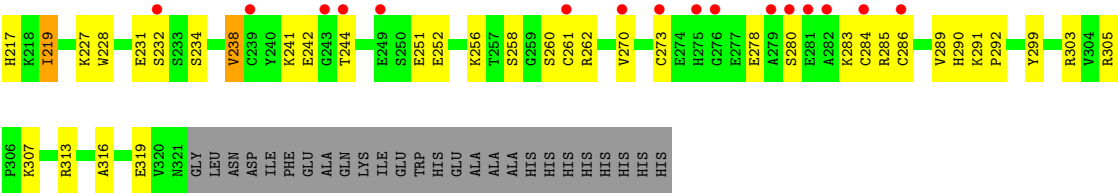


- Molecule 2: light chain



- Molecule 3: Envelopment polypeptide





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



● Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	195.75Å 65.91Å 73.74Å 90.00° 105.38° 90.00°	Depositor
Resolution (Å)	36.63 – 2.40 36.63 – 2.40	Depositor EDS
% Data completeness (in resolution range)	99.5 (36.63-2.40) 99.5 (36.63-2.40)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.39 (at 2.39Å)	Xtriage
Refinement program	PHENIX (1.20.1_4487: ???)	Depositor
R, R_{free}	0.206 , 0.249 0.205 , 0.247	Depositor DCC
R_{free} test set	1697 reflections (4.75%)	wwPDB-VP
Wilson B-factor (Å ²)	32.1	Xtriage
Anisotropy	0.298	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 37.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	6192	wwPDB-VP
Average B, all atoms (Å ²)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.71% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: MAN, 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	C	0.47	0/1697	0.65	0/2318
2	B	0.47	0/1694	0.64	0/2304
3	A	0.44	0/2526	0.63	0/3407
All	All	0.46	0/5917	0.64	0/8029

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	C	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	60	PHE	Peptide

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	C	1652	0	1601	55	1
2	B	1654	0	1581	57	1
3	A	2464	0	2356	78	0
4	D	39	0	34	0	0
5	E	28	0	25	1	0
6	A	144	0	0	7	0
6	B	95	0	0	7	0
6	C	116	0	0	6	0
All	All	6192	0	5597	186	1

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 16.

All (186) 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)
3:A:262:ARG:NH1	6:A:401:HOH:O	2.04	0.87
3:A:6:ILE:HD12	3:A:238:VAL:HB	1.56	0.87
3:A:303:ARG:NH1	6:A:402:HOH:O	2.10	0.82
1:C:128:PRO:HB3	1:C:154:TYR:HB3	1.60	0.81
3:A:8:ALA:O	3:A:34:ARG:NH1	2.17	0.77
1:C:136:GLY:HA3	1:C:222:ARG:HD3	1.71	0.73
1:C:53:PRO:HA	1:C:72:VAL:HG21	1.72	0.72
2:B:29:VAL:HG11	2:B:90:GLN:HG3	1.72	0.71
3:A:242:GLU:OE2	3:A:285:ARG:HD3	1.93	0.68
1:C:208:HIS:ND1	1:C:211:SER:OG	2.24	0.67
2:B:35:TRP:HB2	2:B:48:ILE:HB	1.77	0.67
1:C:130:VAL:HG21	1:C:206:VAL:HG11	1.78	0.66
3:A:68:ASN:HD22	3:A:71:SER:H	1.45	0.64
2:B:67:TYR:O	6:B:302:HOH:O	2.15	0.64
1:C:172:VAL:O	6:C:302:HOH:O	2.15	0.64
2:B:189:HIS:O	2:B:212:GLY:HA2	1.98	0.63
3:A:2:SER:HB3	3:A:72:ARG:HA	1.79	0.63
3:A:178:PHE:HD2	3:A:299:TYR:CZ	2.17	0.63
1:C:147:LEU:HB3	1:C:219:ILE:HD13	1.82	0.62
1:C:147:LEU:HD22	1:C:219:ILE:HG21	1.81	0.62
2:B:81:GLU:H	2:B:81:GLU:CD	2.08	0.62
2:B:108:ARG:NH1	2:B:109:ALA:O	2.32	0.62
3:A:68:ASN:ND2	3:A:71:SER:H	1.97	0.62
3:A:278:GLU:OE1	6:A:403:HOH:O	2.15	0.61
3:A:280:SER:HB3	3:A:283:LYS:HD3	1.83	0.60
3:A:103:PRO:HB3	3:A:154:LEU:HD21	1.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:110:ASP:OD1	2:B:141:PRO:HD3	2.01	0.60
1:C:201:THR:HB	1:C:218:LYS:HD2	1.84	0.59
2:B:155:ARG:NE	2:B:157:ASN:OD1	2.35	0.59
2:B:145:ASN:HB3	2:B:197:THR:HB	1.84	0.59
1:C:2:VAL:HG11	1:C:111:TYR:CD1	2.38	0.59
2:B:196:ALA:HB3	2:B:205:ILE:HB	1.84	0.59
2:B:120:PRO:HD3	2:B:132:VAL:HG22	1.86	0.58
6:A:529:HOH:O	5:E:1:NAG:O6	2.17	0.58
3:A:261:CYS:SG	3:A:283:LYS:HE2	2.44	0.58
1:C:10:GLU:HG2	1:C:18:VAL:CG2	2.34	0.58
2:B:89:GLN:NE2	6:B:310:HOH:O	2.37	0.58
2:B:190:ASN:OD1	2:B:210:ASN:HB3	2.05	0.57
3:A:231:GLU:CD	3:A:305:ARG:HH12	2.13	0.57
1:C:50:GLU:OE2	1:C:59:LYS:NZ	2.27	0.57
3:A:234:SER:HB2	3:A:256:LYS:HE3	1.87	0.57
2:B:12:LEU:HG	2:B:107:LYS:HB2	1.87	0.57
1:C:10:GLU:HG2	1:C:18:VAL:HG21	1.88	0.56
1:C:222:ARG:CZ	2:B:119:PRO:HG2	2.36	0.56
2:B:149:LYS:HB2	2:B:193:THR:HB	1.87	0.56
3:A:107:GLY:O	3:A:152:ARG:HD2	2.06	0.56
2:B:137:ASN:HB3	2:B:138:ASN:OD1	2.06	0.56
2:B:170:ASP:OD1	2:B:172:THR:OG1	2.14	0.56
3:A:169:GLU:HG2	3:A:215:HIS:CD2	2.42	0.55
3:A:133:SER:OG	3:A:135:GLU:HG2	2.07	0.54
1:C:128:PRO:HD2	1:C:213:THR:HG21	1.90	0.54
2:B:129:GLY:HA3	6:B:358:HOH:O	2.06	0.54
1:C:18:VAL:HG12	1:C:86:LEU:HD11	1.88	0.54
3:A:2:SER:O	3:A:59:SER:HB2	2.08	0.54
3:A:238:VAL:O	3:A:286:CYS:HA	2.08	0.54
2:B:83:LEU:HD21	2:B:106:ILE:HG12	1.90	0.53
3:A:258:SER:OG	3:A:260:SER:OG	2.16	0.53
1:C:142:ASN:O	1:C:194:SER:OG	2.12	0.53
1:C:218:LYS:HG2	1:C:220:VAL:HG13	1.90	0.53
1:C:222:ARG:NH2	2:B:120:PRO:O	2.41	0.53
2:B:35:TRP:CD2	2:B:73:PHE:HB2	2.44	0.52
3:A:87:MET:O	3:A:307:LYS:HE3	2.08	0.52
3:A:122:TRP:HB3	3:A:130:ARG:NH2	2.24	0.52
1:C:187:SER:HG	2:B:135:PHE:HE1	1.57	0.52
3:A:165:THR:HB	3:A:305:ARG:HB3	1.92	0.52
3:A:94:LYS:HB2	6:A:476:HOH:O	2.08	0.52
3:A:261:CYS:HB3	3:A:284:CYS:O	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:111:PHE:HB3	3:A:154:LEU:HB3	1.93	0.51
1:C:38:LYS:HB2	1:C:48:ILE:HD11	1.91	0.51
2:B:195:GLU:HG2	2:B:206:VAL:HG22	1.92	0.51
2:B:126:THR:O	6:B:303:HOH:O	2.19	0.51
1:C:6:GLN:O	1:C:114:GLN:NE2	2.38	0.51
2:B:147:LYS:HB3	2:B:195:GLU:HB2	1.93	0.51
3:A:116:PHE:HB2	3:A:189:ILE:HG22	1.91	0.51
1:C:12:VAL:HG21	1:C:86:LEU:HD13	1.92	0.51
1:C:34:MET:CE	1:C:96:CYS:HB2	2.41	0.51
2:B:33:VAL:HA	2:B:89:GLN:O	2.10	0.50
2:B:183:LYS:HE2	2:B:187:GLU:OE2	2.11	0.50
3:A:61:VAL:HG22	3:A:62:SER:O	2.11	0.50
1:C:86:LEU:HA	1:C:90:ASP:OD2	2.11	0.50
1:C:197:TRP:O	1:C:198:PRO:C	2.55	0.50
2:B:211:ARG:NH2	6:B:316:HOH:O	2.44	0.50
3:A:185:ASP:HB2	3:A:319:GLU:HG2	1.94	0.50
3:A:228:TRP:CE3	3:A:292:PRO:HG2	2.47	0.50
3:A:35:LEU:HD23	3:A:37:HIS:HE1	1.77	0.49
1:C:111:TYR:OH	6:C:301:HOH:O	2.14	0.49
1:C:163:TRP:CZ3	1:C:219:ILE:HD11	2.48	0.49
2:B:35:TRP:CE2	2:B:73:PHE:HB2	2.47	0.49
3:A:185:ASP:HA	3:A:319:GLU:HG2	1.95	0.49
3:A:68:ASN:ND2	3:A:71:SER:OG	2.39	0.49
3:A:132:GLU:O	3:A:132:GLU:OE2	2.30	0.49
3:A:111:PHE:HA	3:A:154:LEU:O	2.13	0.48
1:C:2:VAL:HG21	1:C:111:TYR:CZ	2.47	0.48
3:A:10:PRO:HB3	3:A:34:ARG:HD3	1.95	0.48
1:C:163:TRP:CZ3	1:C:204:CYS:HB3	2.48	0.48
2:B:188:ARG:NH1	2:B:189:HIS:CE1	2.81	0.48
3:A:73:TRP:CG	3:A:292:PRO:HD3	2.47	0.48
1:C:153:GLY:HA2	1:C:183:LEU:HB3	1.96	0.48
3:A:82:ALA:HB1	3:A:87:MET:HB2	1.94	0.48
3:A:6:ILE:HG23	3:A:7:CYS:SG	2.55	0.47
3:A:63:TYR:CZ	3:A:71:SER:HB3	2.49	0.47
3:A:176:LYS:HE2	3:A:217:HIS:NE2	2.30	0.47
3:A:219:ILE:HG13	3:A:219:ILE:O	2.14	0.47
2:B:81:GLU:CD	2:B:81:GLU:N	2.72	0.47
3:A:58:ARG:O	3:A:61:VAL:HG12	2.15	0.47
3:A:188:LYS:NZ	3:A:200:GLU:OE2	2.37	0.47
1:C:130:VAL:CG2	1:C:206:VAL:HG11	2.45	0.47
1:C:148:GLY:HA2	1:C:188:SER:O	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1:ASP:HB3	6:B:338:HOH:O	2.14	0.47
2:B:140:TYR:CG	2:B:141:PRO:HA	2.51	0.46
3:A:290:HIS:HB2	6:A:527:HOH:O	2.14	0.46
3:A:35:LEU:HD23	3:A:37:HIS:CE1	2.50	0.46
2:B:45:LYS:HG3	6:B:321:HOH:O	2.14	0.46
2:B:190:ASN:O	2:B:210:ASN:HA	2.14	0.46
3:A:10:PRO:HD3	3:A:34:ARG:HA	1.98	0.46
1:C:222:ARG:NH2	2:B:119:PRO:HG2	2.30	0.46
3:A:106:LYS:HB2	3:A:132:GLU:HA	1.96	0.46
1:C:37:VAL:HG22	1:C:95:TYR:HB2	1.96	0.46
1:C:46:GLU:OE2	6:C:303:HOH:O	2.21	0.46
2:B:108:ARG:HG2	2:B:109:ALA:N	2.31	0.46
3:A:22:LEU:HD13	3:A:27:GLU:HB3	1.97	0.46
3:A:46:SER:O	3:A:125:GLY:HA2	2.16	0.46
2:B:210:ASN:O	2:B:211:ARG:HB2	2.16	0.46
3:A:319:GLU:O	3:A:319:GLU:HG3	2.15	0.45
2:B:103:LYS:HE3	2:B:104:LEU:O	2.16	0.45
3:A:186:ILE:O	3:A:195:ASN:HB2	2.17	0.45
1:C:222:ARG:HA	6:C:345:HOH:O	2.16	0.45
1:C:193:PRO:HG2	1:C:196:THR:OG1	2.17	0.45
3:A:39:SER:HB3	3:A:51:TYR:HA	1.99	0.45
3:A:54:GLN:O	3:A:55:ARG:HB2	2.17	0.45
3:A:100:VAL:HB	3:A:313:ARG:HG2	1.98	0.45
3:A:283:LYS:HA	3:A:283:LYS:HD2	1.60	0.45
2:B:11:LEU:HD13	2:B:19:VAL:HG13	1.99	0.45
3:A:54:GLN:HG3	3:A:55:ARG:HD2	1.98	0.45
1:C:34:MET:HE1	1:C:96:CYS:HB2	1.98	0.44
2:B:117:ILE:HD12	2:B:194:CYS:HB2	1.99	0.44
3:A:232:SER:OG	3:A:270:VAL:HG11	2.17	0.44
1:C:131:TYR:HB2	1:C:150:LEU:HB3	1.98	0.44
3:A:227:LYS:HD2	3:A:227:LYS:HA	1.86	0.44
1:C:133:LEU:HB3	2:B:118:PHE:CD2	2.53	0.44
2:B:188:ARG:HH12	2:B:189:HIS:CE1	2.36	0.44
1:C:55:ASN:HB2	1:C:57:GLY:H	1.82	0.44
1:C:217:LYS:HD3	1:C:217:LYS:HA	1.82	0.44
3:A:25:TYR:O	3:A:29:ILE:HG12	2.17	0.44
2:B:46:LEU:HD13	2:B:55:TYR:HB2	2.00	0.44
3:A:261:CYS:O	3:A:273:CYS:HB2	2.18	0.44
1:C:160:THR:OG1	1:C:207:ALA:HB3	2.18	0.44
3:A:164:MET:HE1	3:A:213:VAL:O	2.18	0.44
1:C:158:PRO:HG3	6:C:409:HOH:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:55:ASN:CB	1:C:57:GLY:H	2.31	0.43
2:B:24:LYS:HA	2:B:69:THR:O	2.18	0.43
3:A:77:LEU:HD22	3:A:81:ASP:HB3	1.98	0.43
1:C:203:THR:HG23	1:C:217:LYS:C	2.43	0.43
3:A:58:ARG:NH2	3:A:76:LEU:O	2.51	0.43
3:A:23:LEU:H	3:A:23:LEU:HD22	1.84	0.43
1:C:123:ALA:HB3	1:C:155:PHE:CE2	2.53	0.43
1:C:163:TRP:CH2	1:C:219:ILE:HD11	2.54	0.43
2:B:115:VAL:HG13	2:B:136:LEU:HG	2.01	0.43
2:B:119:PRO:HB3	2:B:209:PHE:CZ	2.54	0.43
3:A:87:MET:HE1	3:A:162:GLN:C	2.44	0.42
3:A:185:ASP:CA	3:A:319:GLU:HG2	2.49	0.42
1:C:50:GLU:HG2	1:C:59:LYS:HB2	2.01	0.42
1:C:179:LEU:HB2	1:C:184:TYR:CE1	2.54	0.42
2:B:103:LYS:HD2	2:B:103:LYS:HA	1.81	0.42
3:A:289:VAL:HG23	3:A:291:LYS:HG2	2.02	0.42
3:A:117:ASP:HA	3:A:217:HIS:HA	2.01	0.42
3:A:167:ILE:HD12	3:A:171:THR:HG22	2.00	0.42
1:C:12:VAL:HG21	1:C:86:LEU:CD1	2.49	0.42
2:B:4:MET:HE3	2:B:23:CYS:SG	2.60	0.42
2:B:119:PRO:HB3	2:B:209:PHE:CE2	2.54	0.42
2:B:79:GLN:HB3	2:B:81:GLU:OE1	2.19	0.42
3:A:307:LYS:NZ	6:A:423:HOH:O	2.52	0.42
2:B:12:LEU:HD21	2:B:107:LYS:HG3	2.02	0.42
3:A:46:SER:OG	3:A:123:GLY:HA3	2.20	0.42
3:A:107:GLY:HA2	3:A:129:SER:OG	2.20	0.42
3:A:186:ILE:HG23	3:A:316:ALA:HB1	2.02	0.41
3:A:252:GLU:HG2	3:A:256:LYS:HD2	2.01	0.41
1:C:141:THR:HG21	6:C:334:HOH:O	2.20	0.41
1:C:50:GLU:O	1:C:58:THR:HA	2.20	0.41
2:B:136:LEU:HD12	2:B:136:LEU:N	2.36	0.41
2:B:85:VAL:HA	2:B:102:THR:O	2.20	0.41
2:B:193:THR:HA	2:B:208:SER:HB3	2.03	0.40
2:B:19:VAL:O	2:B:74:THR:HA	2.22	0.40
1:C:110:ASP:OD2	1:C:112:TRP:NE1	2.53	0.40
3:A:241:LYS:HE3	3:A:251:GLU:OE2	2.21	0.40
3:A:109:VAL:HG21	3:A:148:LEU:HD13	2.03	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:182:ASP:OD2	2:B:188:ARG:NH1[2_657]	2.14	0.06

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	C	214/222 (96%)	204 (95%)	10 (5%)	0	100	100
2	B	210/212 (99%)	200 (95%)	10 (5%)	0	100	100
3	A	319/347 (92%)	303 (95%)	16 (5%)	0	100	100
All	All	743/781 (95%)	707 (95%)	36 (5%)	0	100	100

There are no Ramachandran outliers to report.

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	C	189/191 (99%)	182 (96%)	7 (4%)	30	51
2	B	185/186 (100%)	177 (96%)	8 (4%)	26	44
3	A	275/297 (93%)	269 (98%)	6 (2%)	45	67
All	All	649/674 (96%)	628 (97%)	21 (3%)	34	56

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	37	VAL
1	C	66	SER
1	C	97	SER
1	C	159	VAL
1	C	168	LEU
1	C	170	SER
1	C	211	SER
2	B	20	THR
2	B	33	VAL
2	B	46	LEU
2	B	97	THR
2	B	122	SER
2	B	154	GLU
2	B	168	SER
2	B	208	SER
3	A	71	SER
3	A	94	LYS
3	A	197	CYS
3	A	219	ILE
3	A	238	VAL
3	A	244	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	3	GLN
1	C	5	GLN
1	C	39	GLN
1	C	55	ASN
2	B	38	GLN
2	B	89	GLN
2	B	189	HIS
3	A	47	GLN
3	A	68	ASN
3	A	215	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

5 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	$\# Z > 2$
4	NAG	D	1	4,3	14,14,15	0.75	1 (7%)	17,19,21	0.54	0
4	NAG	D	2	4	14,14,15	0.62	1 (7%)	17,19,21	0.75	1 (5%)
4	MAN	D	3	4	11,11,12	1.22	1 (9%)	15,15,17	0.92	1 (6%)
5	NAG	E	1	5,3	14,14,15	0.45	0	17,19,21	0.68	1 (5%)
5	NAG	E	2	5	14,14,15	0.53	0	17,19,21	0.42	0

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

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

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	1	NAG	O5-C1	-2.56	1.39	1.43
4	D	3	MAN	C4-C5	2.27	1.57	1.53
4	D	2	NAG	O5-C1	-2.21	1.40	1.43

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	3	MAN	O2-C2-C3	-2.67	104.63	110.15
5	E	1	NAG	C1-O5-C5	-2.13	109.33	112.19
4	D	2	NAG	O4-C4-C5	-2.04	104.31	109.32

There are no chirality outliers.

All (10) torsion outliers are listed below:

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

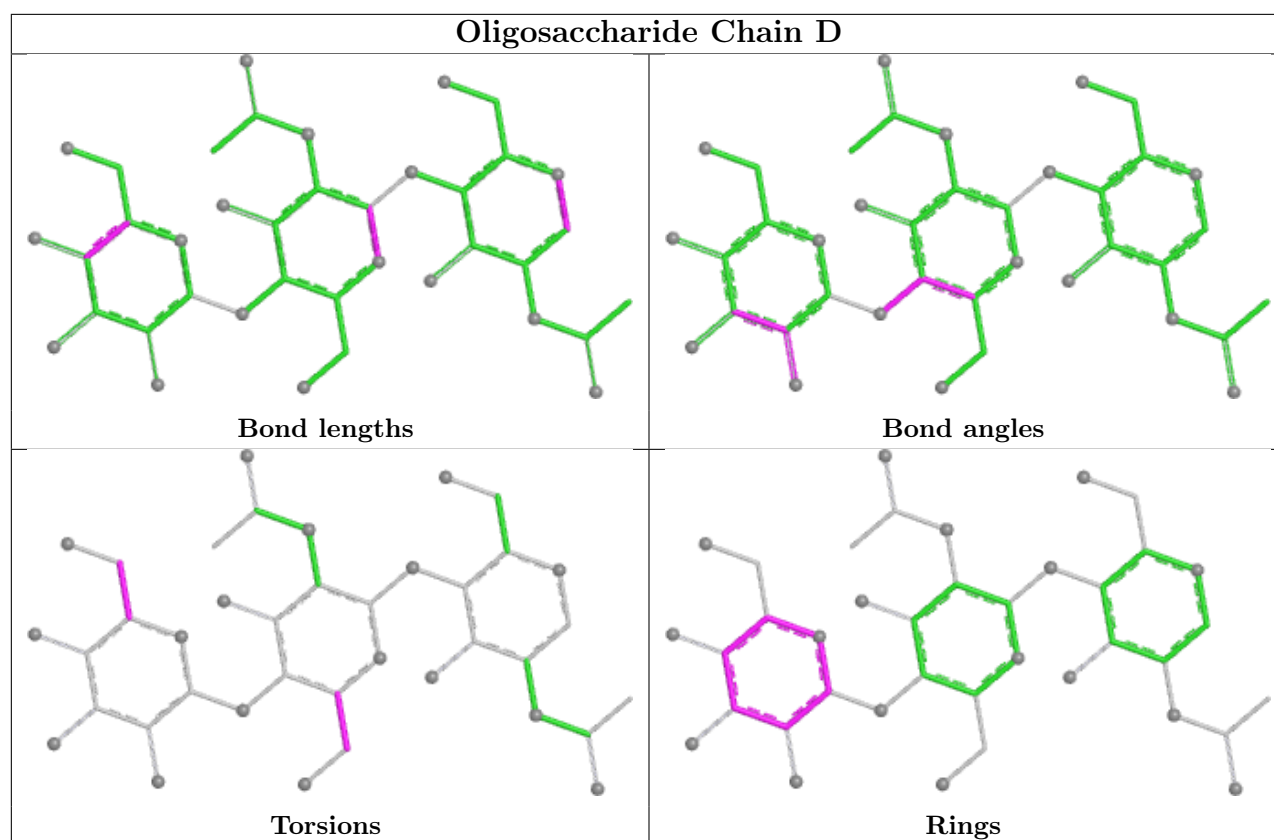
All (1) ring outliers are listed below:

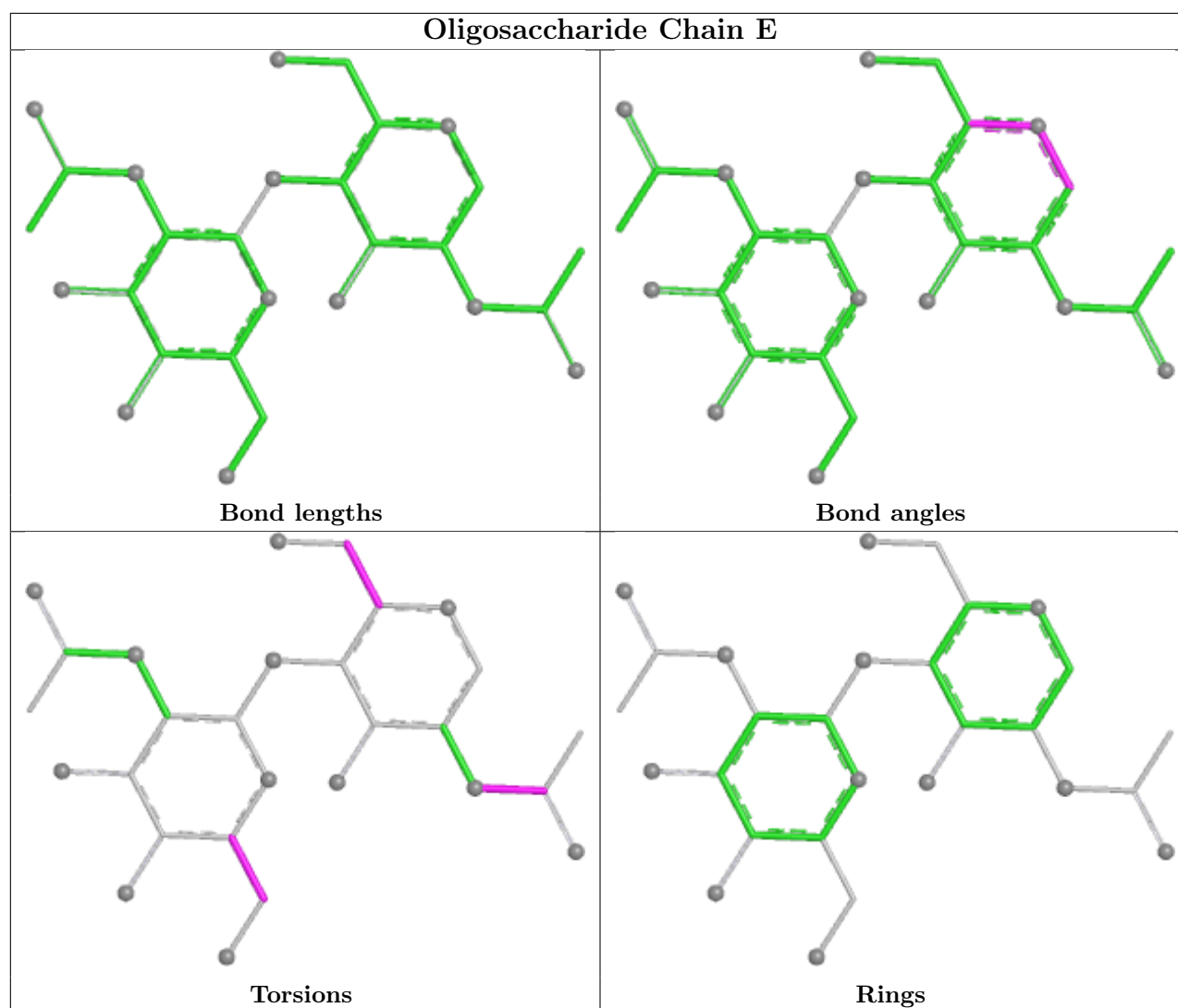
Mol	Chain	Res	Type	Atoms
4	D	3	MAN	C1-C2-C3-C4-C5-O5

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	E	1	NAG	1	0

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





5.6 Ligand geometry [i](#)

There are no ligands in this entry.

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	C	218/222 (98%)	0.26	6 (2%)	55	51	22, 35, 55, 72	0
2	B	212/212 (100%)	0.49	9 (4%)	40	36	20, 41, 66, 75	0
3	A	321/347 (92%)	0.37	20 (6%)	26	23	19, 35, 70, 166	0
All	All	751/781 (96%)	0.37	35 (4%)	36	32	19, 36, 65, 166	0

All (35) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	A	279	ALA	7.0
3	A	282	ALA	6.5
3	A	280	SER	5.9
3	A	270	VAL	4.3
3	A	281	GLU	4.3
3	A	1	ASP	3.7
1	C	182	ASP	3.4
3	A	243	GLY	3.3
3	A	198	GLU	3.3
1	C	127	PRO	3.0
2	B	194	CYS	3.0
2	B	202	THR	2.9
1	C	197	TRP	2.8
3	A	273	CYS	2.7
2	B	197	THR	2.5
3	A	2	SER	2.5
3	A	261	CYS	2.5
3	A	284	CYS	2.5
1	C	144	MET	2.5
3	A	197	CYS	2.4
3	A	286	CYS	2.4
3	A	275	HIS	2.4
1	C	141	THR	2.4

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Mol	Chain	Res	Type	RSRZ
3	A	276	GLY	2.4
2	B	189	HIS	2.4
2	B	188	ARG	2.4
1	C	142	ASN	2.3
2	B	159	VAL	2.3
2	B	212	GLY	2.2
3	A	249	GLU	2.2
3	A	232	SER	2.2
3	A	239	CYS	2.2
2	B	187	GLU	2.2
3	A	244	THR	2.0
2	B	192	TYR	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](#)

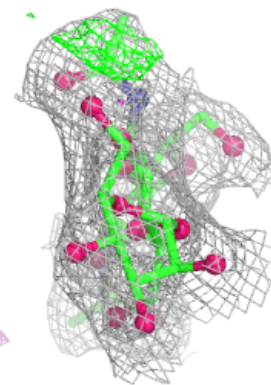
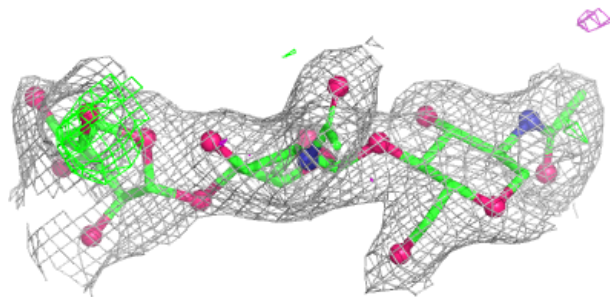
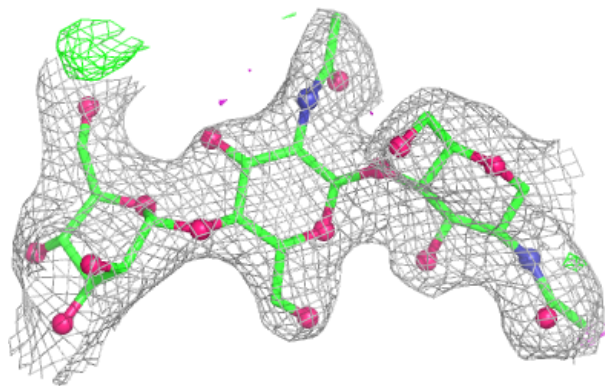
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

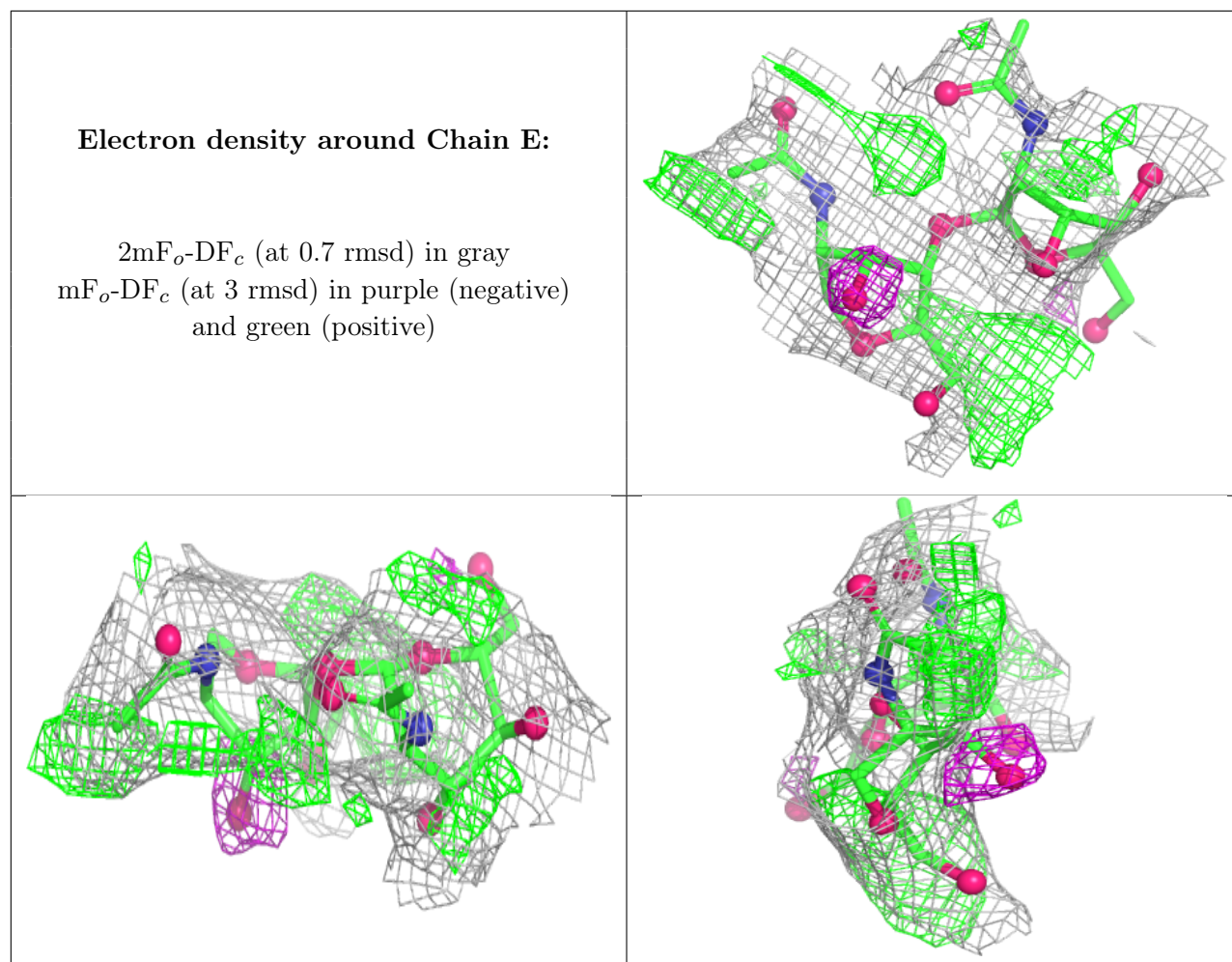
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	NAG	E	1	14/15	0.43	0.24	54,63,78,82	0
5	NAG	E	2	14/15	0.52	0.23	80,82,87,88	0
4	MAN	D	3	11/12	0.82	0.10	48,53,60,60	0
4	NAG	D	2	14/15	0.89	0.12	29,41,51,58	0
4	NAG	D	1	14/15	0.94	0.09	23,28,35,35	0

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

Electron density around Chain D:

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





6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.