



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 10:52 AM UTC

PDB ID : 3C5X / pdb_00003c5x
Title : Crystal structure of the precursor membrane protein- envelope protein heterodimer from the dengue 2 virus at low pH
Authors : Li, L.
Deposited on : 2008-02-01
Resolution : 2.20 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

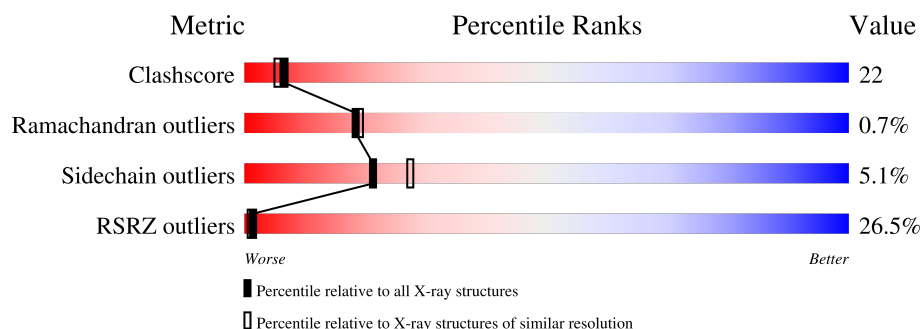
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

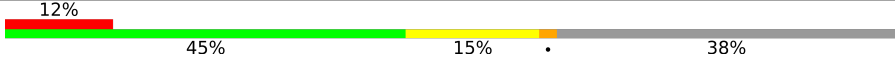
The reported resolution of this entry is 2.20 Å.

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))
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (2.20-2.20)

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

Mol	Chain	Length	Quality of chain
1	A	402	
2	C	130	
3	B	2	
4	D	5	

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
4	NAG	D	2	-	-	X	-
4	BMA	D	4	X	-	-	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 3860 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 Envelope protein E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	390	Total	C	N	O	S	0	0	0
			3047	1926	525	569	27			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-7	GLY	-	expression tag	UNP O09234
A	-6	GLU	-	expression tag	UNP O09234
A	-5	ASN	-	expression tag	UNP O09234
A	-4	LEU	-	expression tag	UNP O09234
A	-3	TYR	-	expression tag	UNP O09234
A	-2	PHE	-	expression tag	UNP O09234
A	-1	GLN	-	expression tag	UNP O09234
A	0	GLY	-	expression tag	UNP O09234

- Molecule 2 is a protein called prM.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	81	Total	C	N	O	S	0	0	0
			640	396	106	128	10			

There are 3 discrepancies between the modelled and reference sequences:

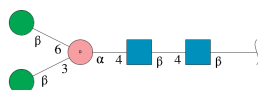
Chain	Residue	Modelled	Actual	Comment	Reference
C	87	SER	ARG	engineered mutation	UNP O09234
C	88	THR	ARG	engineered mutation	UNP O09234
C	91	SER	ARG	engineered mutation	UNP O09234

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



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

- Molecule 4 is an oligosaccharide called beta-D-mannopyranose-(1-3)-[beta-D-mannopyranose-(1-6)]alpha-D-altropyranose-(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	5	Total	C	N	O	0	0	0
			61	34	2	25			

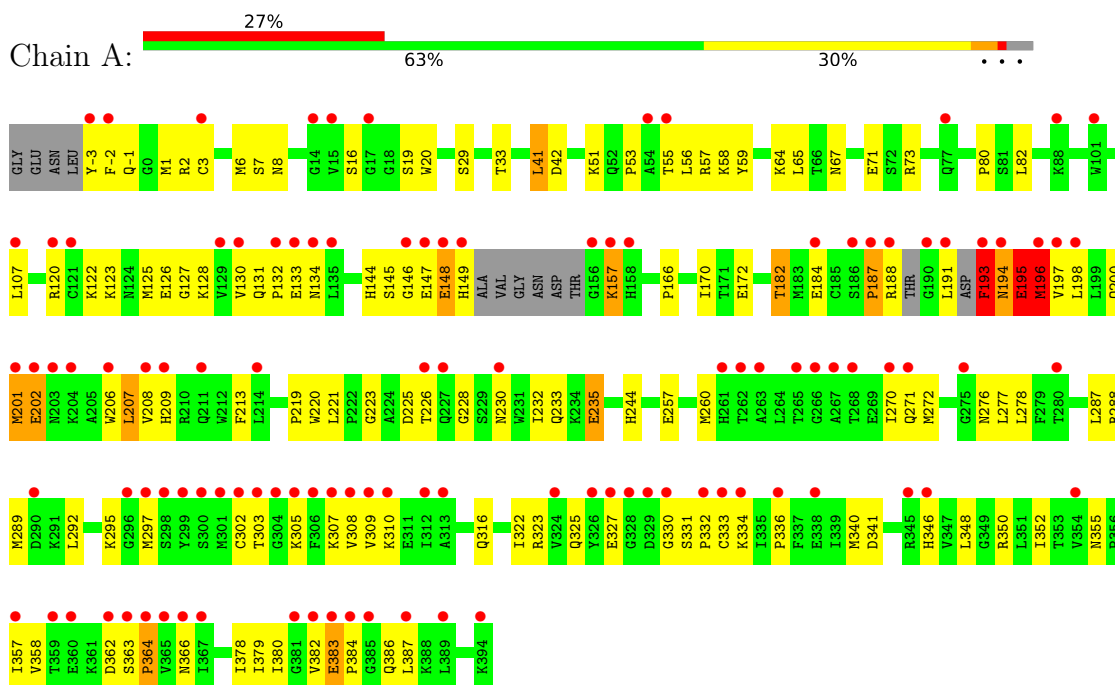
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	61	Total	O	0	0
			61	61		
5	C	23	Total	O	0	0
			23	23		

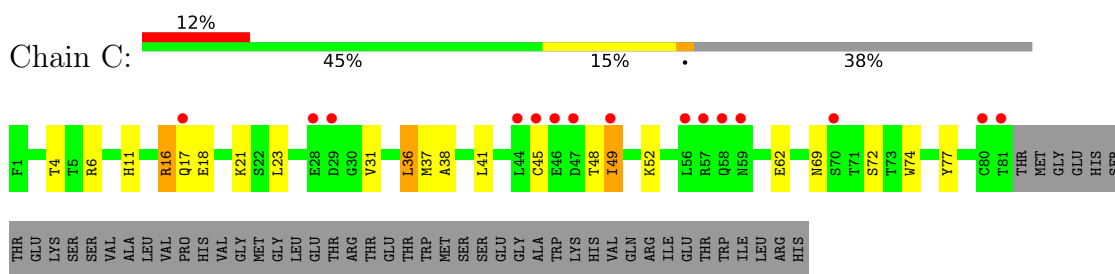
3 Residue-property plots [i](#)

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: Envelope protein E



• Molecule 2: prM



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



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

Chain D:



MAG1
MAG2
SHD3
BM14
BM15

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	71.21Å 108.59Å 108.74Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.20 50.00 – 2.21	Depositor EDS
% Data completeness (in resolution range)	100.0 (50.00-2.20) 98.1 (50.00-2.21)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.74 (at 2.20Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.253 , 0.275 0.248 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	45.1	Xtriage
Anisotropy	0.561	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 38.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.016 for -h,l,k	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	3860	wwPDB-VP
Average B, all atoms (Å ²)	55.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.04% 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, SHD, NDG

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	0.39	0/3108	0.97	10/4189 (0.2%)
2	C	0.76	2/652 (0.3%)	0.85	0/883
All	All	0.47	2/3760 (0.1%)	0.95	10/5072 (0.2%)

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

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

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	49	ILE	C-N	-14.09	1.14	1.33
2	C	49	ILE	C-O	6.51	1.30	1.24

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	195	GLU	N-CA-C	17.49	148.06	110.80
1	A	196	MET	N-CA-CB	-10.97	91.74	110.83
1	A	352	ILE	N-CA-C	-10.90	102.44	111.81
1	A	196	MET	N-CA-C	-8.08	96.22	109.40
1	A	195	GLU	CB-CA-C	-7.99	94.51	110.42
1	A	297	MET	N-CA-C	-6.98	104.57	113.23
1	A	384	PRO	N-CA-C	5.92	127.50	112.10
1	A	244	HIS	N-CA-C	-5.47	101.44	109.81
1	A	148	GLU	N-CA-C	-5.22	103.64	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	226	THR	N-CA-C	-5.20	107.60	114.31

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	193	PHE	Peptide
1	A	194	ASN	Peptide
1	A	362	ASP	Peptide

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3047	0	3047	135	0
2	C	640	0	609	21	0
3	B	28	0	24	5	0
4	D	61	0	46	11	0
5	A	61	0	0	6	0
5	C	23	0	0	0	0
All	All	3860	0	3726	162	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 22.

All (162) 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:195:GLU:CG	1:A:195:GLU:O	1.87	1.20
2:C:31:VAL:HG21	4:D:2:NAG:C8	1.72	1.19
2:C:31:VAL:CG2	4:D:2:NAG:H81	1.74	1.18
1:A:195:GLU:O	1:A:195:GLU:HG2	1.57	0.98
1:A:195:GLU:O	1:A:195:GLU:HG3	1.62	0.97
1:A:309:VAL:HG21	1:A:364:PRO:HB3	1.50	0.93
1:A:198:LEU:HD13	1:A:277:LEU:HD13	1.51	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:149:HIS:HB3	1:A:157:LYS:HD2	1.52	0.92
1:A:57:ARG:HD2	1:A:220:TRP:CE3	2.10	0.86
1:A:201:MET:HE1	1:A:257:GLU:HG3	1.59	0.85
1:A:157:LYS:HD3	1:A:157:LYS:H	1.41	0.84
1:A:149:HIS:HB3	1:A:157:LYS:CD	2.12	0.79
1:A:148:GLU:OE1	1:A:364:PRO:HG2	1.84	0.77
1:A:172:GLU:OE2	1:A:182:THR:HB	1.83	0.77
2:C:31:VAL:HG21	4:D:2:NAG:H81	0.84	0.76
1:A:196:MET:HE3	1:A:207:LEU:HD12	1.69	0.74
2:C:49:ILE:HD11	2:C:77:TYR:CZ	2.25	0.72
1:A:332:PRO:HA	1:A:358:VAL:O	1.89	0.71
1:A:170:ILE:CD1	1:A:184:GLU:HB2	2.20	0.71
2:C:16:ARG:O	2:C:16:ARG:HD3	1.90	0.71
1:A:7:SER:HB3	1:A:316:GLN:HE22	1.55	0.70
1:A:221:LEU:HD13	1:A:228:GLY:HA2	1.74	0.70
1:A:271:GLN:HG3	1:A:278:LEU:HB2	1.74	0.69
1:A:201:MET:HB2	1:A:206:TRP:HZ3	1.56	0.69
1:A:120:ARG:HD3	1:A:122:LYS:NZ	2.08	0.68
1:A:195:GLU:OE2	1:A:209:HIS:CE1	2.46	0.67
1:A:303:THR:OG1	5:A:1457:HOH:O	2.01	0.67
1:A:170:ILE:HD13	1:A:184:GLU:HB2	1.77	0.66
1:A:333:CYS:O	1:A:357:ILE:HG23	1.96	0.66
1:A:132:PRO:HG3	1:A:193:PHE:HD2	1.61	0.65
1:A:157:LYS:H	1:A:157:LYS:CD	2.10	0.65
1:A:331:SER:HA	1:A:332:PRO:C	2.22	0.65
1:A:309:VAL:HG21	1:A:364:PRO:CB	2.26	0.64
1:A:42:ASP:OD1	1:A:144:HIS:HD2	1.80	0.64
1:A:41:LEU:HD21	1:A:292:LEU:HD11	1.79	0.64
1:A:130:VAL:HG23	1:A:193:PHE:CD2	2.33	0.64
1:A:123:LYS:HE2	1:A:202:GLU:OE1	1.98	0.64
1:A:221:LEU:CD1	1:A:228:GLY:HA2	2.29	0.63
4:D:1:NAG:H61	4:D:2:NAG:C1	2.28	0.63
2:C:4:THR:HG23	2:C:11:HIS:HB3	1.81	0.62
1:A:127:GLY:HA3	1:A:213:PHE:CZ	2.35	0.61
1:A:383:GLU:HG2	1:A:386:GLN:CB	2.30	0.61
1:A:51:LYS:HG2	1:A:276:ASN:ND2	2.16	0.61
1:A:382:VAL:HG12	5:A:1459:HOH:O	1.99	0.61
1:A:3:CYS:HA	1:A:6:MET:HE3	1.83	0.60
1:A:134:ASN:O	5:A:1450:HOH:O	2.16	0.60
1:A:303:THR:HG22	1:A:303:THR:O	2.02	0.60
1:A:148:GLU:O	1:A:149:HIS:HB2	1.99	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:-3:TYR:HD2	1:A:148:GLU:OE2	1.85	0.59
1:A:235:GLU:H	1:A:235:GLU:CD	2.09	0.59
1:A:120:ARG:HD3	1:A:122:LYS:HZ1	1.67	0.59
1:A:323:ARG:HG3	1:A:366:ASN:OD1	2.03	0.59
1:A:8:ASN:HB2	1:A:29:SER:HB3	1.85	0.58
1:A:-2:PHE:HB3	1:A:148:GLU:HG2	1.84	0.58
1:A:131:GLN:HB3	1:A:133:GLU:HG2	1.86	0.58
1:A:307:LYS:HD3	1:A:327:GLU:OE2	2.04	0.57
1:A:383:GLU:HG2	1:A:386:GLN:HB3	1.85	0.57
1:A:157:LYS:HD3	1:A:157:LYS:N	2.14	0.57
2:C:31:VAL:CG2	4:D:2:NAG:C8	2.54	0.57
1:A:-3:TYR:N	1:A:1:MET:SD	2.77	0.57
1:A:322:ILE:HD11	1:A:378:ILE:HD13	1.86	0.56
1:A:334:LYS:HG2	5:A:1456:HOH:O	2.05	0.56
2:C:69:ASN:C	2:C:69:ASN:OD1	2.49	0.56
1:A:182:THR:HG23	1:A:288:ARG:HB3	1.88	0.55
2:C:49:ILE:HD11	2:C:77:TYR:OH	2.05	0.55
1:A:287:LEU:HD11	1:A:289:MET:HE2	1.89	0.55
1:A:260:MET:HA	1:A:260:MET:HE2	1.89	0.55
1:A:302:CYS:HB2	1:A:336:PRO:HD3	1.88	0.55
1:A:197:VAL:HG12	1:A:198:LEU:N	2.21	0.55
1:A:-2:PHE:HB3	1:A:366:ASN:HD22	1.72	0.54
1:A:148:GLU:HG2	1:A:366:ASN:ND2	2.21	0.54
1:A:-3:TYR:CD2	1:A:148:GLU:OE2	2.60	0.54
1:A:230:ASN:N	1:A:230:ASN:HD22	2.04	0.54
2:C:31:VAL:HG11	4:D:2:NAG:O7	2.08	0.54
2:C:31:VAL:O	4:D:1:NAG:H3	2.08	0.53
1:A:197:VAL:CG1	1:A:198:LEU:N	2.72	0.53
2:C:52:LYS:HD2	2:C:72:SER:OG	2.08	0.53
1:A:132:PRO:HG3	1:A:193:PHE:CD2	2.42	0.53
4:D:2:NAG:O3	4:D:3:SHD:C2	2.57	0.52
1:A:8:ASN:CB	1:A:29:SER:HB3	2.40	0.52
1:A:340:MET:CE	1:A:379:ILE:HG13	2.39	0.52
1:A:20:TRP:NE1	1:A:288:ARG:NH2	2.58	0.52
1:A:-2:PHE:CB	1:A:366:ASN:HD22	2.23	0.51
1:A:59:TYR:CD1	1:A:220:TRP:HB3	2.46	0.51
2:C:16:ARG:HD3	2:C:16:ARG:C	2.34	0.51
1:A:-2:PHE:CD2	1:A:366:ASN:ND2	2.78	0.51
1:A:145:SER:OG	1:A:147:GLU:HB2	2.12	0.50
1:A:73:ARG:HG3	1:A:80:PRO:HB3	1.92	0.50
1:A:194:ASN:O	1:A:195:GLU:CB	2.60	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:383:GLU:HG2	1:A:386:GLN:HB2	1.93	0.49
3:B:1:NAG:H61	3:B:2:NDG:H8C3	1.95	0.49
1:A:170:ILE:HD12	1:A:184:GLU:HB2	1.95	0.49
1:A:131:GLN:HB3	1:A:133:GLU:CG	2.44	0.48
1:A:219:PRO:HA	1:A:232:ILE:O	2.14	0.48
1:A:232:ILE:O	1:A:233:GLN:HB2	2.13	0.48
1:A:230:ASN:N	1:A:230:ASN:ND2	2.61	0.48
1:A:41:LEU:CD2	1:A:292:LEU:HD11	2.44	0.48
1:A:363:SER:O	1:A:364:PRO:C	2.56	0.48
1:A:123:LYS:CE	1:A:202:GLU:OE1	2.62	0.48
1:A:196:MET:HE3	1:A:207:LEU:CD1	2.42	0.47
1:A:309:VAL:CG2	1:A:325:GLN:HB2	2.44	0.47
1:A:330:GLY:O	1:A:333:CYS:HB3	2.13	0.47
1:A:225:ASP:OD2	1:A:228:GLY:N	2.45	0.47
1:A:133:GLU:O	1:A:166:PRO:HG2	2.15	0.47
1:A:195:GLU:OE2	1:A:209:HIS:ND1	2.48	0.47
3:B:1:NAG:H61	3:B:2:NDG:O7	2.15	0.47
2:C:31:VAL:CB	4:D:2:NAG:H81	2.39	0.47
1:A:16:SER:HB3	1:A:19:SER:OG	2.15	0.47
3:B:1:NAG:O3	3:B:2:NDG:O5	2.33	0.47
1:A:71:GLU:HG3	1:A:80:PRO:HB2	1.97	0.47
1:A:272:MET:HB2	1:A:276:ASN:O	2.15	0.47
1:A:198:LEU:CD2	1:A:270:ILE:HG13	2.46	0.46
1:A:341:ASP:HB3	1:A:348:LEU:HD11	1.97	0.46
1:A:-2:PHE:HD1	1:A:146:GLY:HA2	1.80	0.46
1:A:71:GLU:HB2	1:A:82:LEU:HD21	1.98	0.46
2:C:36:LEU:HD22	2:C:38:ALA:H	1.81	0.46
1:A:157:LYS:O	1:A:157:LYS:HG2	2.16	0.45
1:A:198:LEU:HD13	1:A:277:LEU:CD1	2.36	0.45
1:A:309:VAL:HG22	1:A:325:GLN:HB2	1.99	0.45
1:A:201:MET:HB2	1:A:206:TRP:CZ3	2.45	0.45
2:C:31:VAL:CB	4:D:2:NAG:C8	2.93	0.45
1:A:308:VAL:HG12	1:A:310:LYS:O	2.17	0.45
1:A:191:LEU:HD23	1:A:191:LEU:HA	1.86	0.45
1:A:59:TYR:CE1	1:A:220:TRP:HB3	2.52	0.44
2:C:45:CYS:O	2:C:48:THR:HG23	2.18	0.44
1:A:147:GLU:OE2	1:A:295:LYS:NZ	2.45	0.44
1:A:149:HIS:HB3	1:A:157:LYS:CE	2.47	0.44
1:A:193:PHE:CD1	1:A:193:PHE:N	2.83	0.44
1:A:302:CYS:SG	1:A:334:LYS:O	2.75	0.44
1:A:197:VAL:N	1:A:208:VAL:O	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2:ARG:HG2	1:A:6:MET:HE2	2.00	0.44
1:A:33:THR:HG21	1:A:287:LEU:HD21	1.99	0.44
2:C:6:ARG:HD3	2:C:74:TRP:CD2	2.52	0.44
1:A:148:GLU:CG	1:A:366:ASN:ND2	2.81	0.43
1:A:67:ASN:OD1	3:B:1:NAG:C1	2.66	0.43
1:A:187:PRO:O	1:A:188:ARG:HB2	2.18	0.43
1:A:383:GLU:H	1:A:383:GLU:HG3	1.54	0.43
1:A:125:MET:HE1	1:A:260:MET:SD	2.58	0.43
3:B:1:NAG:H61	3:B:2:NDG:C7	2.48	0.43
1:A:51:LYS:HG2	1:A:276:ASN:HD22	1.83	0.43
1:A:64:LYS:HG2	1:A:65:LEU:N	2.32	0.43
1:A:107:LEU:HD12	5:A:1423:HOH:O	2.20	0.42
1:A:148:GLU:HG2	1:A:366:ASN:HD22	1.84	0.42
1:A:53:PRO:HG2	1:A:128:LYS:HD3	2.01	0.42
1:A:380:ILE:HB	1:A:387:LEU:HB2	2.00	0.42
1:A:55:THR:O	1:A:223:GLY:HA3	2.19	0.42
1:A:383:GLU:HG3	5:A:1459:HOH:O	2.19	0.42
1:A:128:LYS:HD2	1:A:200:GLN:OE1	2.20	0.42
1:A:148:GLU:CD	1:A:323:ARG:HE	2.27	0.42
1:A:120:ARG:HD3	1:A:122:LYS:HZ3	1.83	0.41
1:A:196:MET:HA	1:A:208:VAL:O	2.21	0.41
1:A:195:GLU:OE2	1:A:209:HIS:HE1	2.03	0.41
1:A:355:ASN:HD21	1:A:357:ILE:HD11	1.84	0.41
1:A:149:HIS:CB	1:A:157:LYS:HD2	2.37	0.41
1:A:157:LYS:CD	1:A:157:LYS:N	2.79	0.41
2:C:17:GLN:N	2:C:17:GLN:CD	2.79	0.41
1:A:-2:PHE:HB3	1:A:366:ASN:ND2	2.34	0.40
2:C:18:GLU:O	2:C:21:LYS:HG2	2.20	0.40
1:A:58:LYS:HG2	1:A:126:GLU:HG2	2.04	0.40
1:A:383:GLU:N	1:A:386:GLN:HB2	2.37	0.40
2:C:31:VAL:HG11	4:D:2:NAG:C7	2.51	0.40
1:A:130:VAL:HG23	1:A:193:PHE:CG	2.55	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

of similar resolution.

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	382/402 (95%)	365 (96%)	14 (4%)	3 (1%)	16	16
2	C	79/130 (61%)	74 (94%)	5 (6%)	0	100	100
All	All	461/532 (87%)	439 (95%)	19 (4%)	3 (1%)	18	19

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	195	GLU
1	A	187	PRO
1	A	364	PRO

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	339/348 (97%)	324 (96%)	15 (4%)	25	34
2	C	75/118 (64%)	69 (92%)	6 (8%)	11	13
All	All	414/466 (89%)	393 (95%)	21 (5%)	21	27

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

Mol	Chain	Res	Type
1	A	-1	GLN
1	A	41	LEU
1	A	56	LEU
1	A	157	LYS
1	A	182	THR
1	A	193	PHE
1	A	196	MET
1	A	201	MET
1	A	202	GLU

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Mol	Chain	Res	Type
1	A	207	LEU
1	A	235	GLU
1	A	305	LYS
1	A	346	HIS
1	A	350	ARG
1	A	383	GLU
2	C	16	ARG
2	C	23	LEU
2	C	36	LEU
2	C	37	MET
2	C	41	LEU
2	C	62	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	-1	GLN
1	A	144	HIS
1	A	209	HIS
1	A	227	GLN
1	A	230	ASN
1	A	233	GLN
1	A	242	ASN
1	A	256	GLN
1	A	276	ASN
1	A	316	GLN
1	A	355	ASN
1	A	366	ASN
2	C	17	GLN

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 ⓘ

7 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	NAG	B	1	3	14,14,15	0.61	0	17,19,21	0.74	0
3	NDG	B	2	3	14,14,15	0.60	0	17,19,21	0.99	2 (11%)
4	NAG	D	1	4,2	14,14,15	0.85	1 (7%)	17,19,21	1.40	1 (5%)
4	NAG	D	2	4	14,14,15	0.56	0	17,19,21	1.73	4 (23%)
4	SHD	D	3	4	11,11,12	1.68	3 (27%)	15,15,17	5.82	5 (33%)
4	BMA	D	4	4	11,11,12	0.87	1 (9%)	15,15,17	1.12	2 (13%)
4	BMA	D	5	4	11,11,12	0.48	0	15,15,17	1.56	3 (20%)

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

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

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	3	SHD	C2-C3	-3.86	1.46	1.52
4	D	3	SHD	O3-C3	-2.55	1.36	1.43
4	D	3	SHD	C4-C3	2.48	1.58	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	1	NAG	C1-C2	2.09	1.55	1.52
4	D	4	BMA	O5-C5	2.03	1.47	1.43

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	3	SHD	O2-C2-C3	-18.42	71.99	110.15
4	D	3	SHD	O4-C4-C3	9.59	132.98	110.38
4	D	3	SHD	C1-C2-C3	6.25	118.74	109.64
4	D	3	SHD	O3-C3-C4	-5.22	98.08	110.38
4	D	2	NAG	C3-C4-C5	-4.21	102.59	110.23
4	D	1	NAG	C4-C3-C2	-3.76	105.51	111.02
4	D	5	BMA	C1-C2-C3	3.42	114.62	109.64
4	D	4	BMA	C1-O5-C5	3.13	116.38	112.19
4	D	5	BMA	C6-C5-C4	-2.91	105.87	113.02
4	D	2	NAG	C4-C3-C2	-2.91	106.76	111.02
4	D	5	BMA	C1-O5-C5	2.81	115.95	112.19
4	D	4	BMA	C1-C2-C3	2.49	113.26	109.64
4	D	2	NAG	C6-C5-C4	2.40	118.91	113.02
4	D	2	NAG	C1-O5-C5	2.23	115.18	112.19
3	B	2	NDG	C1-O5-C5	2.12	115.03	112.19
4	D	3	SHD	C3-C4-C5	2.12	114.07	110.23
3	B	2	NDG	O5-C1-C2	-2.04	108.13	111.29

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	D	4	BMA	C1

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	1	NAG	C8-C7-N2-C2
3	B	1	NAG	O7-C7-N2-C2
3	B	2	NDG	C1-C2-N2-C7
3	B	2	NDG	C8-C7-N2-C2
3	B	2	NDG	O7-C7-N2-C2
4	D	3	SHD	C4-C5-C6-O6
3	B	2	NDG	O5-C5-C6-O6
4	D	3	SHD	O5-C5-C6-O6
4	D	1	NAG	O5-C5-C6-O6
4	D	1	NAG	C4-C5-C6-O6

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

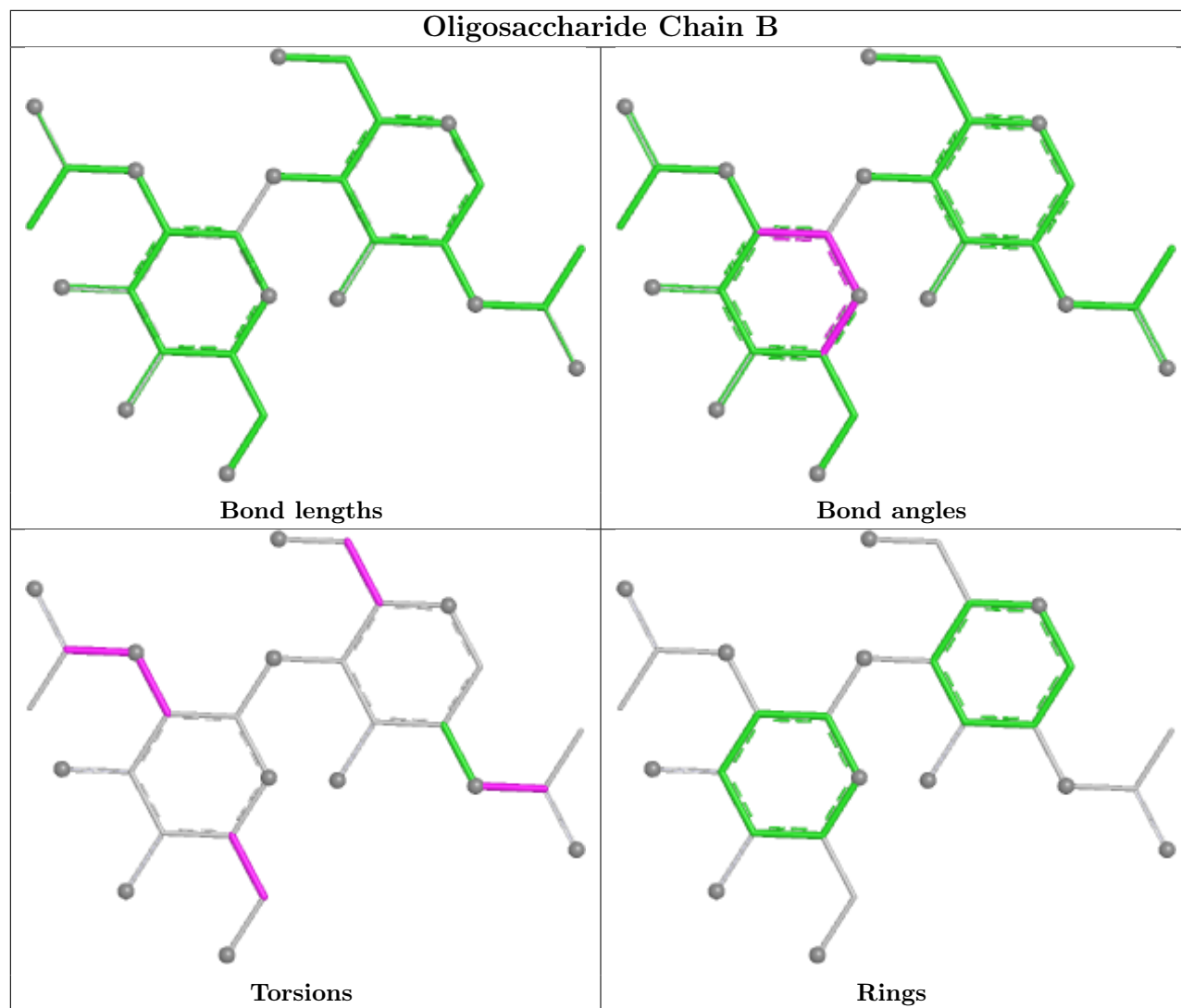
All (1) ring outliers are listed below:

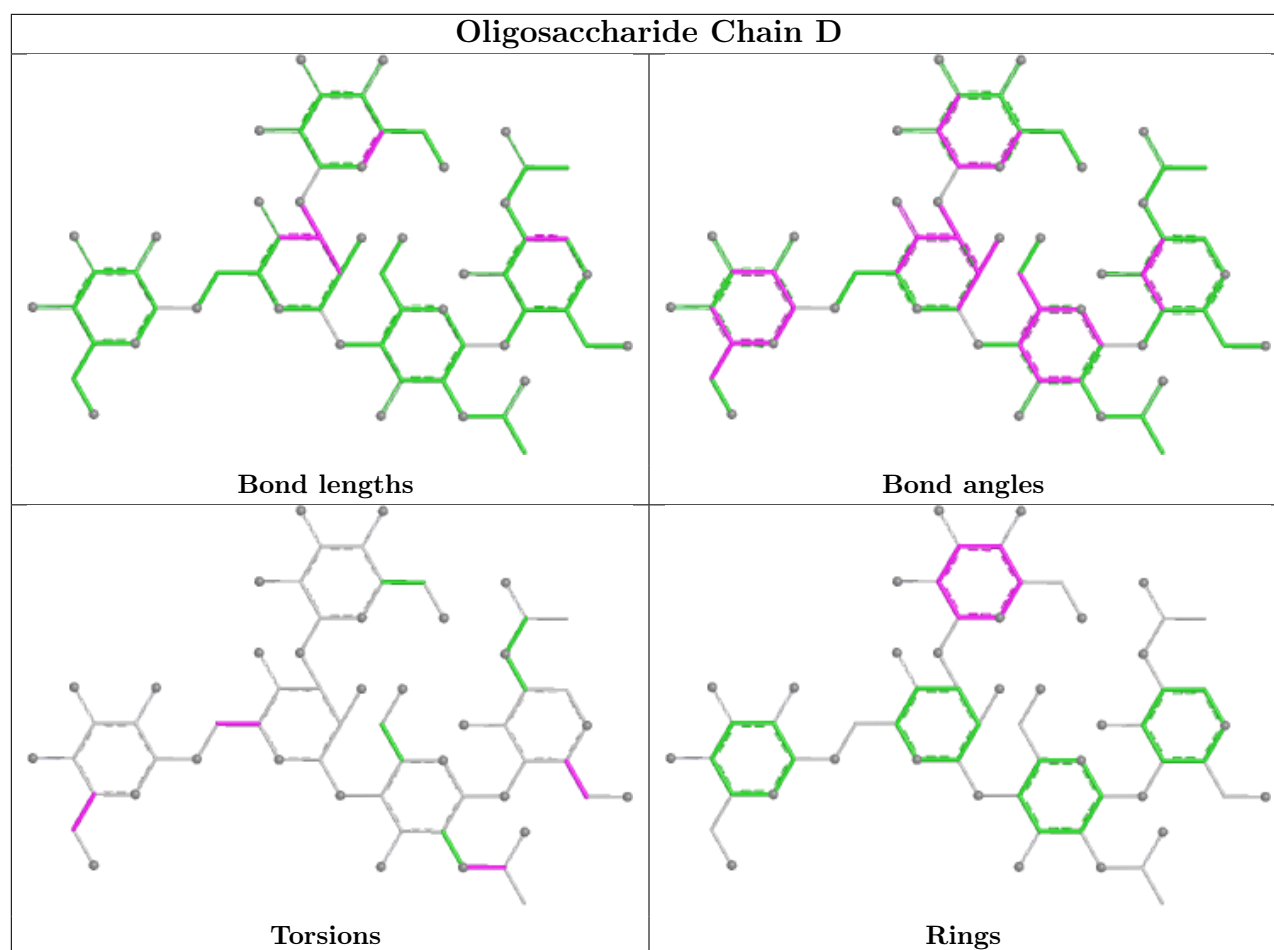
Mol	Chain	Res	Type	Atoms
4	D	4	BMA	C1-C2-C3-C4-C5-O5

5 monomers are involved in 16 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	1	NAG	2	0
4	D	3	SHD	1	0
3	B	2	NDG	4	0
3	B	1	NAG	5	0
4	D	2	NAG	10	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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
2	C	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	C	49:ILE	C	50:THR	N	1.14

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	390/402 (97%)	1.48	110 (28%)  	30, 52, 87, 113	0
2	C	81/130 (62%)	0.97	15 (18%)  	22, 41, 73, 97	0
All	All	471/532 (88%)	1.39	125 (26%)  	22, 50, 85, 113	0

All (125) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	303	THR	7.7
1	A	193	PHE	6.5
1	A	309	VAL	6.1
1	A	-3	TYR	6.1
1	A	333	CYS	5.5
1	A	366	ASN	4.9
1	A	382	VAL	4.9
1	A	191	LEU	4.8
1	A	365	VAL	4.8
1	A	148	GLU	4.7
1	A	190	GLY	4.7
1	A	297	MET	4.6
1	A	363	SER	4.5
1	A	326	TYR	4.5
1	A	302	CYS	4.4
1	A	362	ASP	4.4
1	A	226	THR	4.4
1	A	328	GLY	4.3
1	A	194	ASN	4.3
1	A	381	GLY	4.2
1	A	149	HIS	4.2
2	C	57	ARG	4.2
1	A	336	PRO	4.1
1	A	383	GLU	4.0

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Mol	Chain	Res	Type	RSRZ
1	A	-2	PHE	4.0
1	A	296	GLY	3.9
1	A	157	LYS	3.9
1	A	301	MET	3.9
1	A	299	TYR	3.8
1	A	346	HIS	3.8
1	A	360	GLU	3.8
2	C	80	CYS	3.8
1	A	107	LEU	3.8
1	A	201	MET	3.7
1	A	324	VAL	3.7
1	A	196	MET	3.7
1	A	203	ASN	3.7
2	C	58	GLN	3.7
2	C	81	THR	3.7
1	A	304	GLY	3.6
2	C	45	CYS	3.6
1	A	271	GLN	3.6
1	A	306	PHE	3.6
1	A	188	ARG	3.5
1	A	330	GLY	3.5
1	A	267	ALA	3.4
1	A	329	ASP	3.4
1	A	312	ILE	3.3
1	A	184	GLU	3.3
1	A	298	SER	3.3
1	A	156	GLY	3.2
2	C	46	GLU	3.2
1	A	132	PRO	3.2
1	A	364	PRO	3.2
1	A	3	CYS	3.1
1	A	147	GLU	3.1
1	A	385	GLY	3.1
1	A	204	LYS	3.1
1	A	359	THR	3.1
2	C	56	LEU	3.0
1	A	266	GLY	3.0
1	A	158	HIS	3.0
1	A	268	THR	3.0
1	A	146	GLY	3.0
1	A	206	TRP	3.0
1	A	202	GLU	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	187	PRO	3.0
1	A	384	PRO	3.0
1	A	387	LEU	2.9
1	A	197	VAL	2.9
1	A	357	ILE	2.9
1	A	133	GLU	2.9
1	A	134	ASN	2.9
1	A	15	VAL	2.9
1	A	307	LYS	2.8
2	C	47	ASP	2.8
1	A	334	LYS	2.8
2	C	29	ASP	2.8
1	A	77	GLN	2.8
1	A	209	HIS	2.7
2	C	28	GLU	2.7
1	A	265	THR	2.7
1	A	394	LYS	2.7
1	A	332	PRO	2.6
1	A	300	SER	2.6
1	A	130	VAL	2.6
1	A	261	HIS	2.6
1	A	338	GLU	2.5
1	A	262	THR	2.5
1	A	198	LEU	2.5
1	A	327	GLU	2.5
1	A	121	CYS	2.5
1	A	280	THR	2.5
1	A	275	GLY	2.5
2	C	70	SER	2.4
1	A	305	LYS	2.4
1	A	14	GLY	2.4
1	A	345	ARG	2.4
1	A	55	THR	2.3
1	A	308	VAL	2.3
1	A	135	LEU	2.3
1	A	263	ALA	2.3
1	A	186	SER	2.3
1	A	214	LEU	2.3
1	A	389	LEU	2.2
1	A	88	LYS	2.2
1	A	129	VAL	2.2
1	A	290	ASP	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	120	ARG	2.2
2	C	44	LEU	2.2
1	A	313	ALA	2.2
1	A	354	VAL	2.2
1	A	310	LYS	2.2
2	C	49	ILE	2.1
1	A	211	GLN	2.1
1	A	227	GLN	2.1
1	A	101	TRP	2.1
1	A	230	ASN	2.1
1	A	208	VAL	2.1
1	A	17	GLY	2.1
2	C	17	GLN	2.0
1	A	54	ALA	2.0
2	C	59	ASN	2.0
1	A	270	ILE	2.0
1	A	367	ILE	2.0

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

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

6.3 Carbohydrates ⓘ

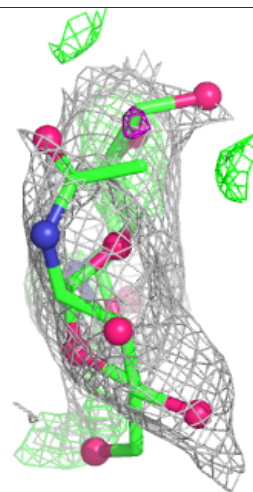
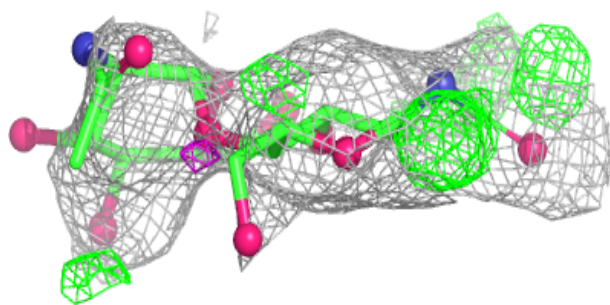
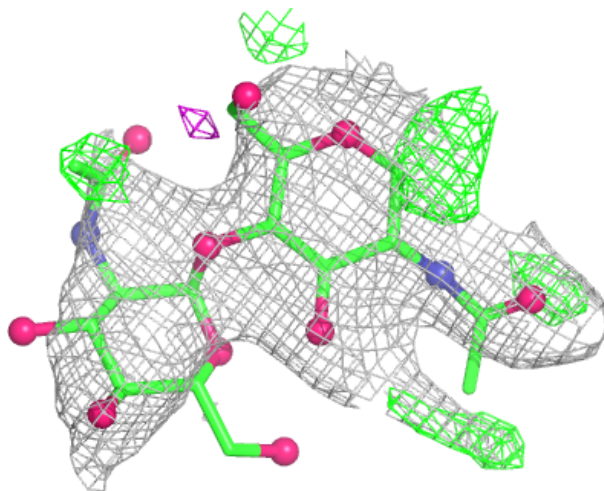
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

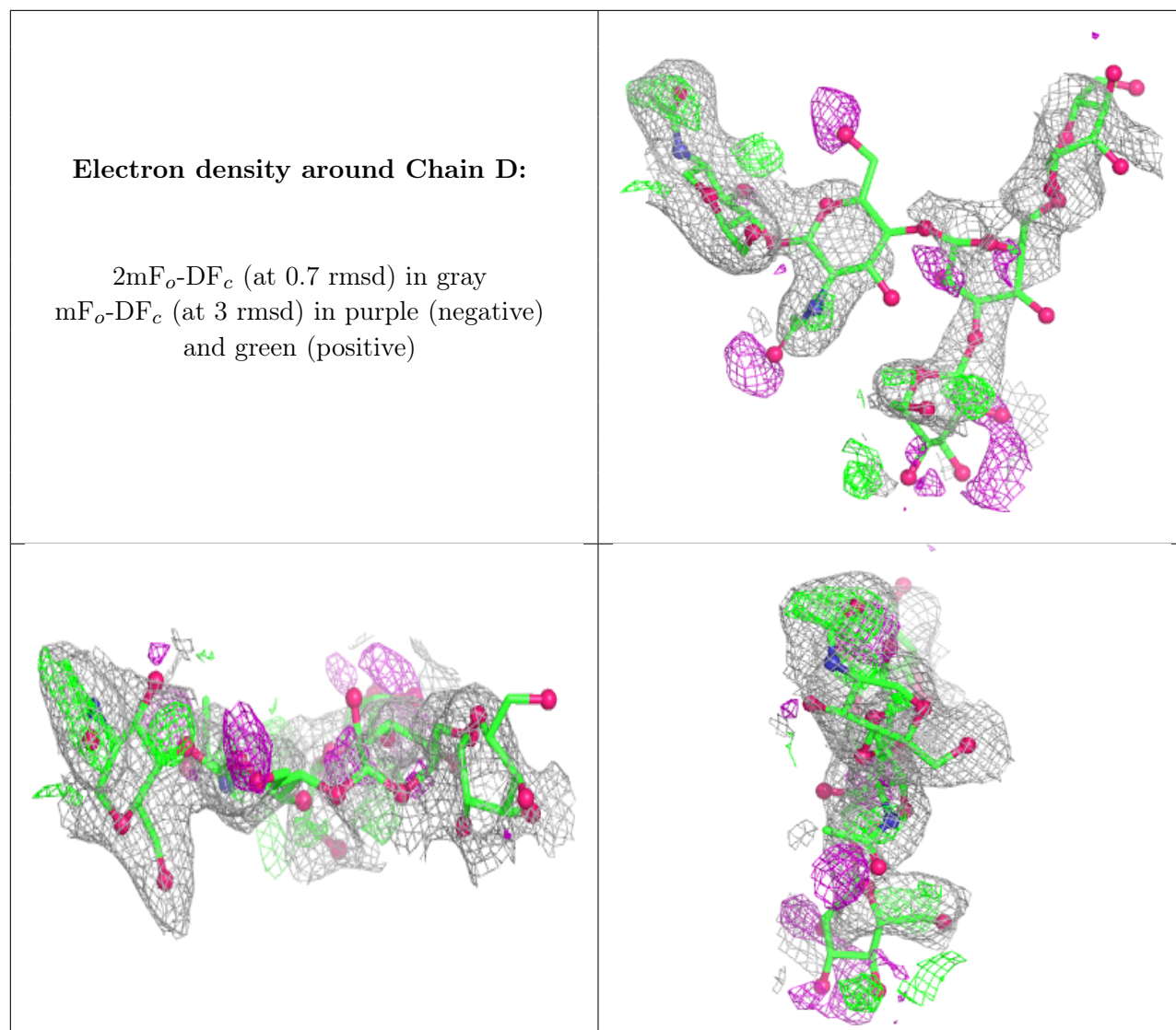
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	NAG	B	1	14/15	-	-	79,84,91,108	0
3	NDG	B	2	14/15	-	-	118,132,133,133	0
4	BMA	D	5	11/12	0.39	0.20	138,141,142,142	0
4	SHD	D	3	11/12	0.57	0.23	124,127,130,135	0
4	BMA	D	4	11/12	0.60	0.39	119,120,121,122	0
4	NAG	D	2	14/15	0.68	0.33	104,119,121,124	0
4	NAG	D	1	14/15	0.76	0.20	64,69,76,93	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)





6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.