



# Full wwPDB X-ray Structure Validation Report ⓘ

Apr 4, 2026 – 10:36 PM UTC

PDB ID : 9OWF / pdb\_00009owf  
Title : X-ray crystal structure of Zika virus envelope glycoprotein in complex with Fab of F25.S02  
Authors : Hurlburt, N.K.; Pancera, M.  
Deposited on : 2025-06-02  
Resolution : 2.30 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](mailto: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>.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

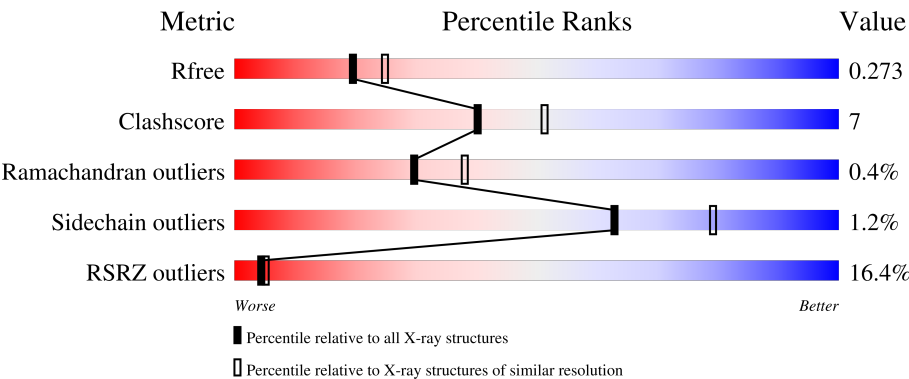
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:  
*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.30 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	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (2.30-2.30)

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  $\geq 3$ , 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	404	<div><div>9%</div><div>85%</div><div>14%</div><div>.</div></div>
1	B	404	<div><div>12%</div><div>89%</div><div>10%</div><div>.</div></div>
2	C	238	<div><div>27%</div><div>73%</div><div>18%</div><div>8%</div><div>.</div></div>
2	H	238	<div><div>16%</div><div>70%</div><div>18%</div><div>11%</div><div>.</div></div>
3	D	217	<div><div>22%</div><div>90%</div><div>7%</div><div>.</div></div>

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Mol	Chain	Length	Quality of chain
3	L	217	
4	E	6	
5	F	5	

## 2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 26033 atoms, of which 12882 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 Genome polyprotein.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	404	Total	C	H	N	O	S	0	0	0
			6097	1924	3013	539	595	26			
1	B	404	Total	C	H	N	O	S	0	0	0
			6063	1924	2979	539	595	26			

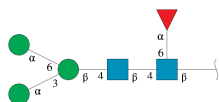
- Molecule 2 is a protein called F25.S02 heavy chain.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	C	220	Total	C	H	N	O	S	0	0	0
			3273	1049	1619	279	319	7			
2	H	212	Total	C	H	N	O	S	0	0	0
			3181	1021	1573	271	309	7			

- Molecule 3 is a protein called F25.S02 light chain.

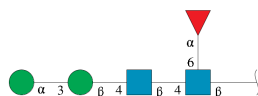
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
3	D	211	Total	C	H	N	O	S	0	0	0
			3097	985	1524	263	319	6			
3	L	212	Total	C	H	N	O	S	0	0	0
			3109	988	1530	264	321	6			

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



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
4	E	6	Total	C	H	N	O		0	0	0
			138	40	67	2	29				

- Molecule 5 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-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	H	N	O	0	0	0
			117	34	57	2	24			

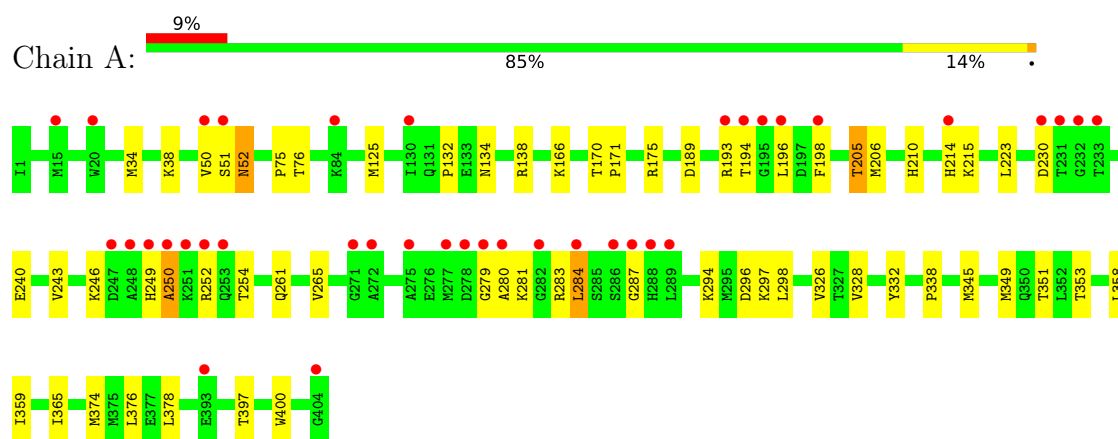
- Molecule 6 is water.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	122	Total	H	O	0	0
			262	140	122		
6	B	104	Total	H	O	0	0
			236	132	104		
6	C	31	Total	H	O	0	0
			63	32	31		
6	D	58	Total	H	O	0	0
			118	60	58		
6	H	43	Total	H	O	0	0
			101	58	43		
6	L	80	Total	H	O	0	0
			178	98	80		

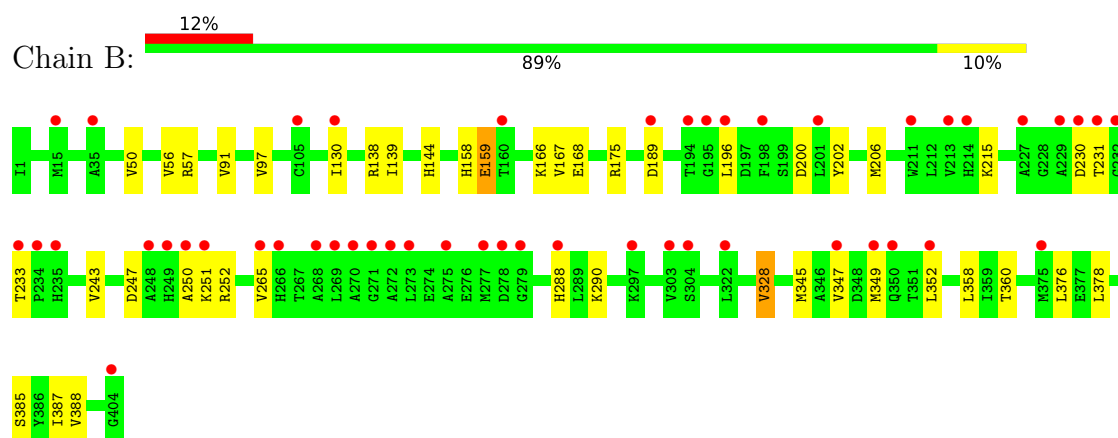
### 3 Residue-property plots [i](#)

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.

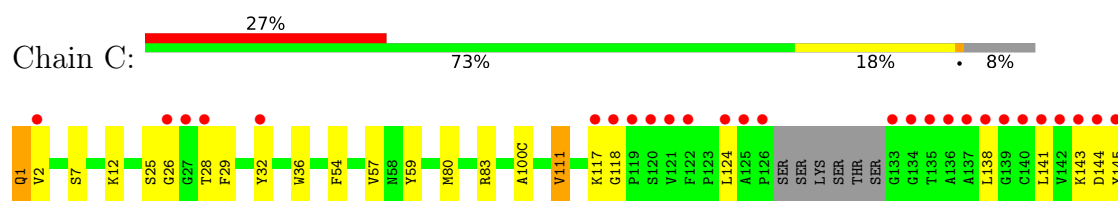
- Molecule 1: Genome polypeptide

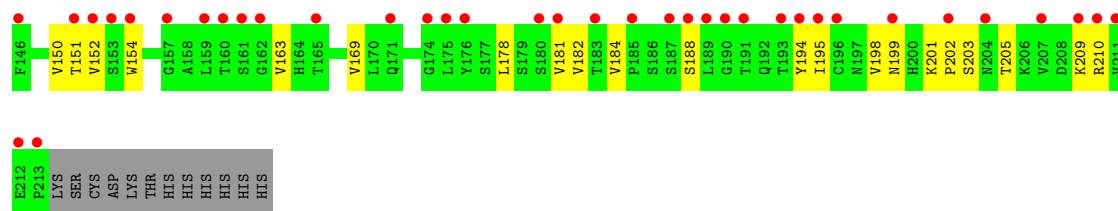


- Molecule 1: Genome polypeptide

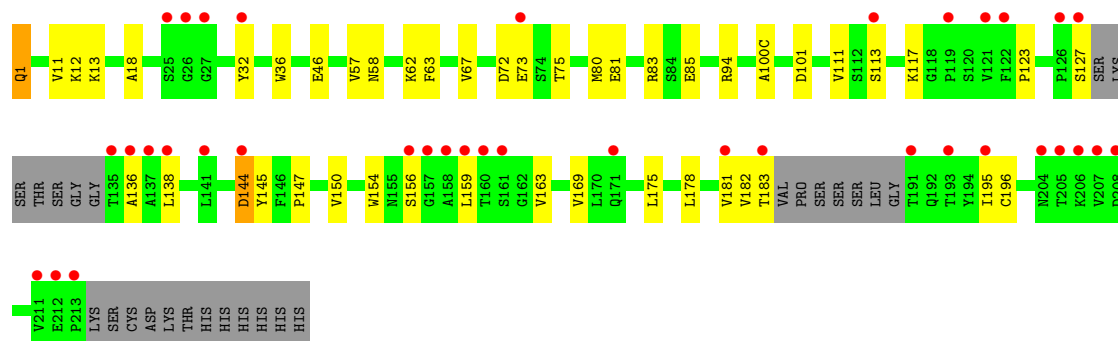


- Molecule 2: F25.S02 heavy chain

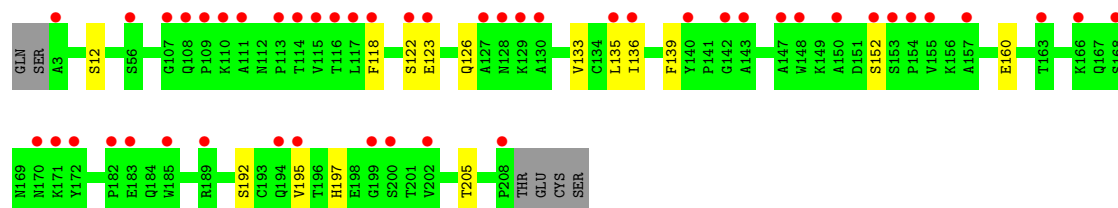
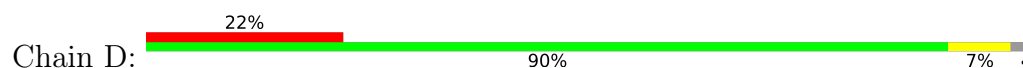




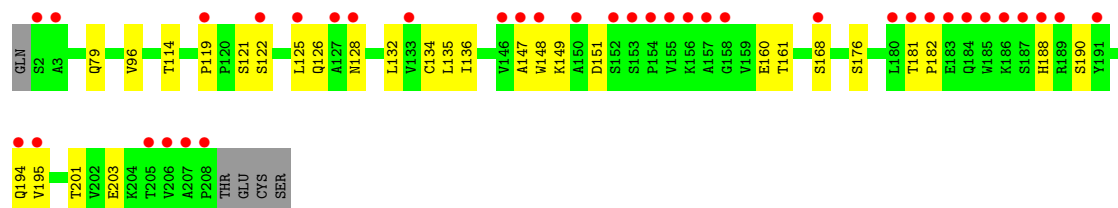
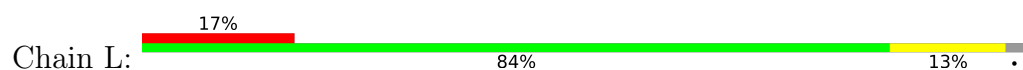
• Molecule 2: F25.S02 heavy chain



• Molecule 3: F25.S02 light chain



• Molecule 3: F25.S02 light chain




• Molecule 4: alpha-D-mannopyranose-(1-3)-[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





- Molecule 5: alpha-D-mannopyranose-(1-3)-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:  80% 20%





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	117.86Å 117.86Å 346.10Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.70 – 2.30 48.70 – 2.30	Depositor EDS
% Data completeness (in resolution range)	99.3 (48.70-2.30) 99.2 (48.70-2.30)	Depositor EDS
$R_{merge}$	0.16	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.43 (at 2.29Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, $R_{free}$	0.225 , 0.274 0.226 , 0.273	Depositor DCC
$R_{free}$ test set	5420 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	43.9	Xtriage
Anisotropy	0.164	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.38 , 51.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	26033	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	75.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.32% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: MAN, BMA, NAG, FUC, PCA

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	0.19	0/3149	0.41	0/4266
1	B	0.20	0/3149	0.41	0/4266
2	C	0.18	0/1688	0.39	0/2300
2	H	0.18	0/1640	0.40	1/2233 (0.0%)
3	D	0.18	0/1613	0.40	0/2201
3	L	0.20	0/1619	0.46	0/2209
All	All	0.19	0/12858	0.41	1/17475 (0.0%)

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	1
1	B	0	1
2	H	0	1
All	All	0	3

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	1	PCA	O-C-N	-6.33	112.86	123.00

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	252	ARG	Sidechain
1	B	252	ARG	Sidechain
2	H	1	PCA	Mainchain

## 5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3084	3013	3012	45	0
1	B	3084	2979	3012	32	0
2	C	1654	1619	1618	40	0
2	H	1608	1573	1571	30	0
3	D	1573	1524	1523	13	0
3	L	1579	1530	1528	16	0
4	E	71	67	61	2	0
5	F	60	57	52	1	0
6	A	122	140	0	0	0
6	B	104	132	0	0	0
6	C	31	32	0	1	0
6	D	58	60	0	0	0
6	H	43	58	0	0	0
6	L	80	98	0	0	0
All	All	13151	12882	12377	165	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 7.

All (165) 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:D:123:GLU:OE1	3:D:123:GLU:N	2.11	0.84
2:H:145:TYR:CE2	2:H:150:VAL:HG23	2.15	0.82
2:C:141:LEU:HD11	2:C:143:LYS:HD2	1.62	0.81
1:A:194:THR:HG23	1:A:287:GLY:HA3	1.64	0.79
1:B:56:VAL:HG21	1:B:202:TYR:HE1	1.48	0.78
2:H:169:VAL:HG21	3:L:160:GLU:HB3	1.70	0.74
2:H:85:GLU:N	2:H:85:GLU:OE2	2.19	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:163:VAL:HG22	2:C:182:VAL:HG12	1.72	0.72
2:H:32:TYR:CE2	5:F:1:NAG:H83	2.26	0.71
2:C:181:VAL:HG11	3:D:135:LEU:CD1	2.22	0.70
1:B:200:ASP:OD2	1:B:200:ASP:O	2.11	0.68
1:B:175:ARG:HG3	1:B:189:ASP:OD1	1.94	0.68
1:A:51:SER:HA	1:A:281:LYS:HE3	1.76	0.67
1:A:206:MET:HE1	1:A:265:VAL:CG1	2.23	0.67
2:H:181:VAL:HG21	3:L:135:LEU:CD1	2.25	0.66
1:A:294:LYS:HZ3	1:A:297:LYS:HD3	1.61	0.65
1:A:38:LYS:NZ	1:A:298:LEU:O	2.25	0.65
2:C:169:VAL:HG21	3:D:160:GLU:HB3	1.77	0.65
2:H:163:VAL:HG12	2:H:182:VAL:HG22	1.79	0.64
1:B:230:ASP:O	1:B:231:THR:OG1	2.15	0.64
1:B:139:ILE:HB	1:B:167:VAL:HG13	1.81	0.62
2:C:28:THR:OG1	2:C:29:PHE:N	2.33	0.61
1:A:52:ASN:O	1:A:52:ASN:OD1	2.20	0.59
1:A:194:THR:HG22	1:A:196:LEU:HD22	1.84	0.58
3:L:119:PRO:HA	3:L:132:LEU:HD23	1.85	0.58
1:B:247:ASP:OD2	1:B:247:ASP:O	2.22	0.58
1:A:230:ASP:O	1:A:230:ASP:OD1	2.22	0.58
1:B:175:ARG:CG	1:B:189:ASP:OD1	2.51	0.58
1:B:56:VAL:HG21	1:B:202:TYR:CE1	2.37	0.57
2:H:13:LYS:NZ	2:H:113:SER:O	2.39	0.56
2:C:188:SER:OG	2:C:194:TYR:OH	2.16	0.56
3:L:181:THR:HB	3:L:182:PRO:CD	2.36	0.55
1:A:328:VAL:HG13	1:A:376:LEU:HG	1.88	0.55
1:A:279:GLY:O	1:A:280:ALA:HB3	2.08	0.54
2:H:117:LYS:NZ	2:H:144:ASP:O	2.31	0.54
2:C:138:LEU:CD1	2:C:182:VAL:HG22	2.37	0.54
1:A:125:MET:HE1	1:A:265:VAL:HG21	1.91	0.53
1:B:349:MET:HE3	1:B:352:LEU:HD21	1.89	0.53
2:H:11:VAL:HB	2:H:147:PRO:HG3	1.90	0.53
1:A:223:LEU:HD21	1:A:261:GLN:HG3	1.90	0.53
2:C:83:ARG:O	2:C:111:VAL:HG11	2.08	0.53
2:C:152:VAL:HG12	2:C:198:VAL:HG23	1.92	0.52
1:B:144:HIS:HB3	1:B:360:THR:HG23	1.92	0.52
2:H:156:SER:O	2:H:156:SER:OG	2.20	0.52
1:A:249:HIS:O	1:A:250:ALA:HB2	2.09	0.52
3:L:161:THR:OG1	3:L:176:SER:OG	2.24	0.52
1:A:132:PRO:O	1:A:171:PRO:HG2	2.10	0.51
1:A:246:LYS:O	1:A:254:THR:HG22	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1:PCA:OE	4:E:1:NAG:H82	2.10	0.50
1:A:338:PRO:HA	1:A:365:ILE:O	2.11	0.50
1:A:294:LYS:NZ	1:A:297:LYS:HD3	2.25	0.50
1:A:284:LEU:HD23	1:A:284:LEU:N	2.27	0.50
3:D:122:SER:OG	3:D:123:GLU:OE1	2.19	0.50
2:H:63:PHE:HB3	2:H:67:VAL:HG12	1.94	0.50
1:A:50:VAL:O	1:A:281:LYS:HG3	2.12	0.50
1:A:175:ARG:NE	1:A:189:ASP:OD2	2.45	0.50
1:B:158:HIS:O	1:B:159:GLU:CB	2.59	0.50
1:A:51:SER:HA	1:A:281:LYS:CE	2.40	0.49
1:B:288:HIS:NE2	1:B:290:LYS:HE2	2.27	0.49
2:C:141:LEU:CD1	2:C:143:LYS:HD2	2.39	0.49
2:C:57:VAL:HG11	2:C:59:TYR:CZ	2.48	0.49
2:C:201:LYS:N	2:C:202:PRO:HD2	2.29	0.48
1:A:34:MET:HE1	1:A:359:ILE:HA	1.96	0.47
1:B:175:ARG:CD	1:B:189:ASP:OD1	2.62	0.47
3:L:151:ASP:HB2	3:L:188:HIS:ND1	2.29	0.47
1:B:202:TYR:CE2	1:B:215:LYS:HB2	2.49	0.47
3:L:136:ILE:HG12	3:L:195:VAL:HG21	1.95	0.47
3:L:149:LYS:NZ	3:L:203:GLU:OE2	2.47	0.47
1:A:206:MET:HE1	1:A:265:VAL:HG11	1.93	0.47
2:H:72:ASP:HB3	2:H:75:THR:HG22	1.95	0.47
2:H:63:PHE:HB3	2:H:67:VAL:CG1	2.45	0.47
3:L:147:ALA:HB3	3:L:194:GLN:HG2	1.97	0.47
2:C:182:VAL:HG23	2:C:184:VAL:HG13	1.96	0.46
1:B:158:HIS:O	1:B:159:GLU:HB2	2.14	0.46
3:D:139:PHE:HB2	3:D:197:HIS:CD2	2.49	0.46
3:L:181:THR:HB	3:L:182:PRO:HD3	1.95	0.46
1:A:249:HIS:O	1:A:250:ALA:CB	2.64	0.46
2:C:151:THR:HG22	2:C:199:ASN:HB3	1.97	0.46
2:C:178:LEU:C	2:C:178:LEU:HD12	2.40	0.46
1:A:296:ASP:OD1	1:A:297:LYS:HG3	2.16	0.46
2:C:117:LYS:HD3	2:C:118:GLY:O	2.16	0.46
2:H:12:LYS:O	2:H:111:VAL:HA	2.16	0.45
2:C:141:LEU:C	2:C:141:LEU:HD13	2.41	0.45
2:C:138:LEU:HD12	2:C:138:LEU:O	2.16	0.45
2:C:124:LEU:HD22	3:D:118:PHE:CB	2.46	0.45
1:B:57:ARG:HG3	1:B:57:ARG:HH11	1.80	0.45
2:C:12:LYS:O	2:C:111:VAL:HA	2.17	0.45
2:C:181:VAL:HG11	3:D:135:LEU:HD12	1.99	0.45
2:H:63:PHE:O	2:H:67:VAL:HG12	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:196:LEU:HD21	1:A:198:PHE:HE1	1.82	0.45
1:A:138:ARG:HE	1:A:166:LYS:HD2	1.81	0.44
1:A:332:TYR:HB2	1:A:365:ILE:CD1	2.47	0.44
1:A:351:THR:HG23	1:A:353:THR:H	1.82	0.44
3:L:128:ASN:O	3:L:128:ASN:CG	2.60	0.44
1:A:349:MET:HE2	1:A:397:THR:HG21	1.99	0.44
2:H:18:ALA:O	2:H:81:GLU:HA	2.18	0.44
2:C:2:VAL:HG22	2:C:25:SER:OG	2.17	0.44
1:A:193:ARG:NE	1:A:193:ARG:HA	2.32	0.44
2:H:36:TRP:CE2	2:H:80:MET:HB2	2.52	0.44
1:B:358:LEU:HD22	1:B:378:LEU:HD23	2.00	0.44
1:A:283:ARG:C	1:A:284:LEU:HD23	2.43	0.44
2:C:145:TYR:CE1	2:C:150:VAL:HG23	2.52	0.44
2:H:136:ALA:O	2:H:183:THR:HA	2.18	0.44
2:C:182:VAL:HG23	2:C:184:VAL:CG1	2.48	0.43
3:D:192:SER:OG	3:D:205:THR:OG1	2.33	0.43
2:C:25:SER:OG	2:C:26:GLY:N	2.50	0.43
2:H:73:GLU:OE1	2:H:73:GLU:N	2.41	0.43
2:H:123:PRO:HD2	3:L:121:SER:OG	2.18	0.43
1:A:374:MET:HE1	1:A:376:LEU:HB3	2.00	0.43
3:L:122:SER:O	3:L:126:GLN:HG3	2.19	0.43
1:B:200:ASP:HA	1:B:215:LYS:HD2	1.99	0.43
2:C:32:TYR:CE2	4:E:1:NAG:H83	2.53	0.43
1:A:196:LEU:H	1:A:196:LEU:HD23	1.83	0.43
3:D:122:SER:O	3:D:126:GLN:HG2	2.19	0.43
1:A:374:MET:C	1:A:374:MET:SD	3.01	0.43
2:C:36:TRP:CE2	2:C:80:MET:HB2	2.53	0.43
1:A:326:VAL:HG21	1:A:400:TRP:CE2	2.54	0.43
1:B:97:VAL:HG11	2:C:54:PHE:CE1	2.54	0.43
1:B:250:ALA:C	1:B:251:LYS:HD2	2.44	0.43
2:C:138:LEU:HD12	2:C:182:VAL:HG22	2.00	0.42
1:B:206:MET:HE1	1:B:265:VAL:CG1	2.49	0.42
1:A:196:LEU:HD23	1:A:196:LEU:N	2.35	0.42
1:A:205:THR:HB	1:A:210:HIS:CD2	2.55	0.42
1:B:91:VAL:HG11	1:B:243:VAL:HG21	2.01	0.42
3:L:134:CYS:HB2	3:L:148:TRP:CH2	2.55	0.42
2:C:141:LEU:HD23	3:D:133:VAL:HG21	2.00	0.42
2:C:184:VAL:HG11	2:C:194:TYR:CE1	2.54	0.42
1:A:51:SER:HB3	1:A:134:ASN:HB3	2.02	0.42
1:B:196:LEU:HD12	1:B:196:LEU:N	2.34	0.42
2:H:46:GLU:OE2	2:H:62:LYS:NZ	2.44	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:345:MET:HE3	1:B:387:ILE:CG1	2.49	0.42
1:B:206:MET:HE1	1:B:265:VAL:HB	2.01	0.42
1:B:349:MET:HE1	1:B:388:VAL:CG2	2.49	0.42
2:C:117:LYS:HD3	2:C:117:LYS:C	2.45	0.42
2:C:209:LYS:HG3	2:C:210:ARG:N	2.35	0.42
2:H:83:ARG:HB3	2:H:85:GLU:OE2	2.20	0.41
3:L:195:VAL:O	3:L:201:THR:HA	2.20	0.41
1:A:196:LEU:HG	1:A:198:PHE:CE1	2.55	0.41
2:C:169:VAL:CG2	3:D:160:GLU:HB3	2.48	0.41
1:B:138:ARG:HD2	1:B:166:LYS:HD2	2.01	0.41
2:H:138:LEU:HD12	2:H:138:LEU:C	2.45	0.41
1:B:175:ARG:NE	1:B:189:ASP:OD1	2.52	0.41
1:B:288:HIS:CD2	1:B:288:HIS:C	2.98	0.41
1:A:240:GLU:HA	1:A:243:VAL:HG22	2.02	0.41
3:L:121:SER:O	3:L:125:LEU:HG	2.21	0.41
2:C:203:SER:OG	2:C:205:THR:HG23	2.21	0.41
3:D:136:ILE:HG12	3:D:195:VAL:HG21	2.01	0.41
1:A:358:LEU:CD2	1:A:378:LEU:HD23	2.51	0.41
2:C:154:TRP:CE3	2:C:195:ILE:O	2.74	0.41
2:H:57:VAL:C	2:H:58:ASN:HD22	2.29	0.41
1:A:75:PRO:C	1:A:76:THR:HG23	2.46	0.40
1:A:214:HIS:HD2	1:A:215:LYS:N	2.19	0.40
2:H:154:TRP:HA	2:H:195:ILE:O	2.21	0.40
2:H:159:LEU:HD21	2:H:182:VAL:HG11	2.03	0.40
2:H:72:ASP:OD2	2:H:75:THR:HG22	2.22	0.40
2:C:138:LEU:HD12	2:C:138:LEU:C	2.47	0.40
2:H:117:LYS:HE3	2:H:175:LEU:CD2	2.52	0.40
1:A:345:MET:HE3	1:A:345:MET:HB2	1.95	0.40
1:B:138:ARG:HD3	1:B:168:GLU:OE2	2.22	0.40
1:B:328:VAL:HG22	1:B:376:LEU:HG	2.04	0.40
2:H:178:LEU:C	2:H:178:LEU:HD12	2.46	0.40
1:B:50:VAL:HG21	1:B:130:ILE:HD11	2.03	0.40
2:C:7:SER:HB2	6:C:305:HOH:O	2.21	0.40
2:C:181:VAL:HG11	3:D:135:LEU:HD11	1.98	0.40
2:H:94:ARG:HD2	2:H:101:ASP:OD1	2.21	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	402/404 (100%)	391 (97%)	9 (2%)	2 (0%)	24	31
1	B	402/404 (100%)	386 (96%)	15 (4%)	1 (0%)	43	55
2	C	216/238 (91%)	209 (97%)	5 (2%)	2 (1%)	14	17
2	H	206/238 (87%)	198 (96%)	6 (3%)	2 (1%)	12	15
3	D	209/217 (96%)	205 (98%)	4 (2%)	0	100	100
3	L	210/217 (97%)	201 (96%)	9 (4%)	0	100	100
All	All	1645/1718 (96%)	1590 (97%)	48 (3%)	7 (0%)	30	38

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	52	ASN
1	A	250	ALA
1	B	159	GLU
2	C	144	ASP
2	C	100(C)	ALA
2	H	100(C)	ALA
2	H	144	ASP

### 5.3.2 Protein sidechains

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	337/337 (100%)	334 (99%)	3 (1%)	70	84

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	337/337 (100%)	333 (99%)	4 (1%)	63	79
2	C	181/199 (91%)	180 (99%)	1 (1%)	78	89
2	H	176/199 (88%)	174 (99%)	2 (1%)	65	81
3	D	177/183 (97%)	175 (99%)	2 (1%)	65	81
3	L	178/183 (97%)	173 (97%)	5 (3%)	38	56
All	All	1386/1438 (96%)	1369 (99%)	17 (1%)	63	79

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	170	THR
1	A	205	THR
1	A	284	LEU
1	B	233	THR
1	B	328	VAL
1	B	347	VAL
1	B	385	SER
2	C	111	VAL
3	D	12	SER
3	D	152	SER
2	H	127	SER
2	H	196	CYS
3	L	79	GLN
3	L	96	VAL
3	L	114	THR
3	L	168	SER
3	L	190	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	77	GLN
1	A	147	GLN
1	A	214	HIS
1	B	147	GLN
1	B	226	HIS
1	B	253	GLN
1	B	323	HIS
2	C	39	GLN

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Mol	Chain	Res	Type
3	D	37	GLN
3	D	38	GLN
3	D	188	HIS
2	H	192	GLN
3	L	37	GLN
3	L	126	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

2 non-standard protein/DNA/RNA residues 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	PCA	C	1	2	7,8,9	1.92	1 (14%)	9,10,12	2.15	5 (55%)
2	PCA	H	1	2	7,8,9	1.91	1 (14%)	9,10,12	2.00	4 (44%)

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	PCA	C	1	2	-	0/0/11/13	0/1/1/1
2	PCA	H	1	2	-	0/0/11/13	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	1	PCA	CD-N	4.97	1.46	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	1	PCA	CD-N	4.93	1.46	1.34

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	1	PCA	CB-CA-N	2.99	111.47	103.24
2	H	1	PCA	CB-CA-N	2.97	111.42	103.24
2	C	1	PCA	CA-N-CD	-2.84	103.86	113.58
2	C	1	PCA	OE-CD-CG	-2.81	121.71	126.72
2	H	1	PCA	CA-N-CD	-2.80	103.97	113.58
2	H	1	PCA	OE-CD-CG	-2.71	121.89	126.72
2	C	1	PCA	CB-CA-C	-2.60	109.08	112.66
2	H	1	PCA	CG-CD-N	2.53	114.57	108.39
2	C	1	PCA	CG-CD-N	2.52	114.56	108.39

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	1	PCA	1	0

## 5.5 Carbohydrates

11 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	E	1	1,4	14,14,15	0.48	0	17,19,21	0.56	0
4	NAG	E	2	4	14,14,15	0.32	0	17,19,21	0.50	0
4	BMA	E	3	4	11,11,12	0.61	0	15,15,17	0.76	0
4	MAN	E	4	4	11,11,12	0.73	0	15,15,17	1.11	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	MAN	E	5	4	11,11,12	0.72	0	15,15,17	0.94	1 (6%)
4	FUC	E	6	4	10,10,11	0.74	0	14,14,16	0.61	0
5	NAG	F	1	1,5	14,14,15	0.41	0	17,19,21	0.51	0
5	NAG	F	2	5	14,14,15	0.31	0	17,19,21	0.48	0
5	BMA	F	3	5	11,11,12	0.60	0	15,15,17	0.68	0
5	MAN	F	4	5	11,11,12	0.80	0	15,15,17	0.76	0
5	FUC	F	5	5	10,10,11	0.69	0	14,14,16	0.63	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	E	1	1,4	-	1/6/23/26	0/1/1/1
4	NAG	E	2	4	-	0/6/23/26	0/1/1/1
4	BMA	E	3	4	-	0/2/19/22	0/1/1/1
4	MAN	E	4	4	-	0/2/19/22	0/1/1/1
4	MAN	E	5	4	-	2/2/19/22	0/1/1/1
4	FUC	E	6	4	-	-	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	-	0/2/19/22	0/1/1/1
5	MAN	F	4	5	-	0/2/19/22	0/1/1/1
5	FUC	F	5	5	-	-	0/1/1/1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	E	4	MAN	C1-O5-C5	3.39	116.73	112.19
4	E	5	MAN	C1-O5-C5	2.57	115.63	112.19

There are no chirality outliers.

All (4) torsion outliers are listed below:

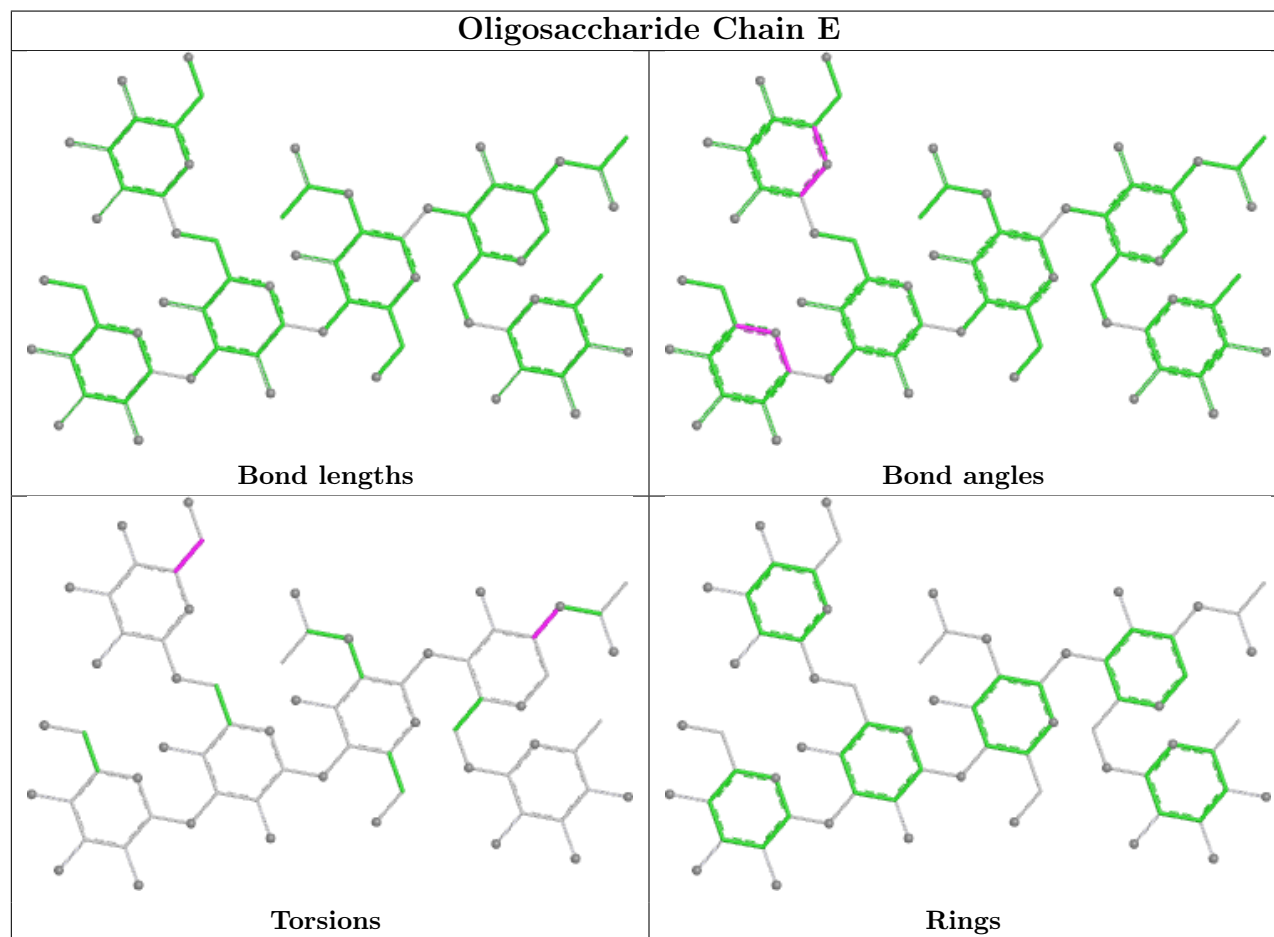
Mol	Chain	Res	Type	Atoms
4	E	1	NAG	C1-C2-N2-C7
5	F	1	NAG	C1-C2-N2-C7
4	E	5	MAN	C4-C5-C6-O6
4	E	5	MAN	O5-C5-C6-O6

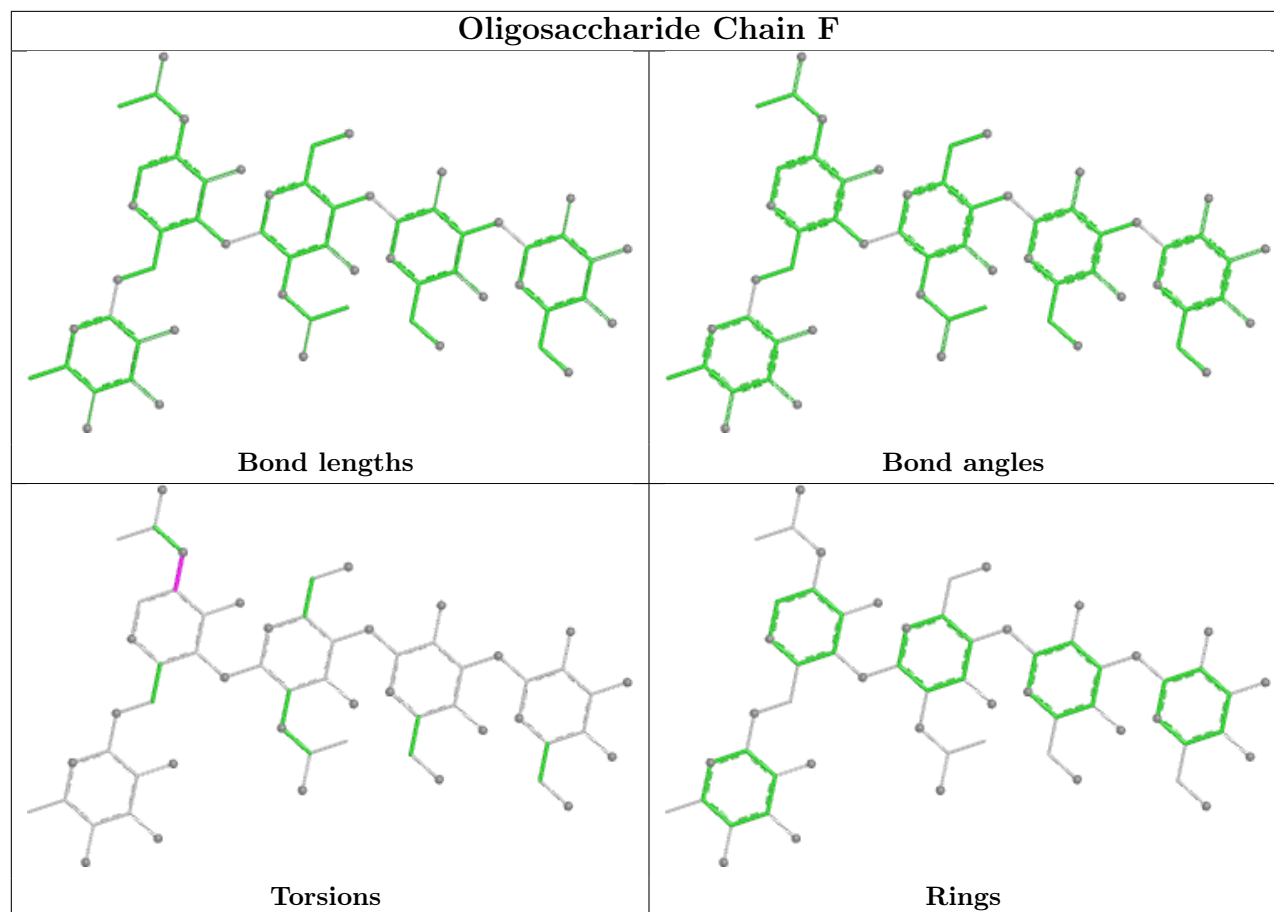
There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	F	1	NAG	1	0
4	E	1	NAG	2	0

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





## 5.6 Ligand geometry [i](#)

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	404/404 (100%)	0.75	38 (9%) 14 15	40, 66, 111, 150	0
1	B	404/404 (100%)	0.88	49 (12%) 8 9	41, 65, 111, 158	0
2	C	219/238 (92%)	1.34	64 (29%) 1 1	42, 80, 134, 211	0
2	H	211/238 (88%)	1.04	37 (17%) 4 4	37, 78, 123, 135	0
3	D	211/217 (97%)	1.13	48 (22%) 2 2	42, 86, 126, 154	0
3	L	212/217 (97%)	0.78	37 (17%) 4 4	37, 59, 132, 168	0
All	All	1661/1718 (96%)	0.95	273 (16%) 4 5	37, 69, 125, 211	0

All (273) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	C	195	ILE	9.3
1	B	234	PRO	9.1
3	L	2	SER	7.8
3	L	208	PRO	6.9
1	B	404	GLY	6.5
2	H	136	ALA	6.3
1	B	233	THR	6.3
3	D	109	PRO	6.2
1	B	229	ALA	5.6
2	C	133	GLY	5.5
1	A	404	GLY	5.3
2	C	126	PRO	5.3
1	A	250	ALA	5.3
1	B	231	THR	5.3
1	A	284	LEU	5.1
2	H	26	GLY	5.1
1	A	232	GLY	5.1
3	D	3	ALA	5.0
2	C	27	GLY	5.0

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Mol	Chain	Res	Type	RSRZ
3	L	207	ALA	5.0
1	B	232	GLY	4.9
2	C	26	GLY	4.9
1	A	249	HIS	4.9
1	A	231	THR	4.8
1	B	270	ALA	4.8
2	H	127	SER	4.8
2	H	211	VAL	4.8
1	B	230	ASP	4.8
2	C	213	PRO	4.8
2	H	135	THR	4.7
2	H	158	ALA	4.6
2	H	213	PRO	4.6
1	A	248	ALA	4.5
1	A	194	THR	4.4
3	L	181	THR	4.4
2	C	211	VAL	4.4
2	C	119	PRO	4.3
2	C	193	THR	4.3
1	A	196	LEU	4.3
1	A	50	VAL	4.2
3	L	180	LEU	4.1
1	B	278	ASP	4.1
3	L	186	LYS	4.0
3	L	182	PRO	4.0
1	B	196	LEU	4.0
1	B	227	ALA	4.0
1	B	272	ALA	3.9
3	L	122	SER	3.9
1	B	279	GLY	3.9
1	A	247	ASP	3.9
2	C	210	ARG	3.9
1	B	248	ALA	3.9
2	C	28	THR	3.8
3	L	189	ARG	3.8
2	C	194	TYR	3.7
2	C	191	THR	3.7
2	C	181	VAL	3.7
2	H	193	THR	3.7
2	H	208	ASP	3.7
3	D	202	VAL	3.6
1	A	251	LYS	3.6

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Mol	Chain	Res	Type	RSRZ
3	L	185	TRP	3.6
1	B	269	LEU	3.6
1	B	105	CYS	3.6
3	L	184	GLN	3.5
1	A	51	SER	3.5
3	D	208	PRO	3.5
2	C	121	VAL	3.5
2	H	137	ALA	3.5
3	D	118	PHE	3.4
3	L	133	VAL	3.4
1	A	198	PHE	3.4
3	L	183	GLU	3.4
2	H	159	LEU	3.4
3	D	157	ALA	3.4
3	D	154	PRO	3.3
3	D	108	GLN	3.3
3	D	155	VAL	3.3
1	B	195	GLY	3.3
3	L	152	SER	3.3
3	D	129	LYS	3.3
1	B	160	THR	3.3
1	B	288	HIS	3.2
1	B	198	PHE	3.2
2	C	154	TRP	3.2
1	A	288	HIS	3.2
1	A	287	GLY	3.2
2	C	162	GLY	3.2
2	C	183	THR	3.2
1	B	266	HIS	3.2
3	L	154	PRO	3.2
1	A	282	GLY	3.1
2	C	137	ALA	3.1
3	L	150	ALA	3.1
2	H	32	TYR	3.1
2	H	183	THR	3.1
2	C	190	GLY	3.1
2	C	135	THR	3.1
2	H	113	SER	3.1
1	B	271	GLY	3.1
1	A	280	ALA	3.1
3	L	3	ALA	3.1
2	H	138	LEU	3.1

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Mol	Chain	Res	Type	RSRZ
3	D	123	GLU	3.0
1	B	214	HIS	3.0
3	D	195	VAL	3.0
2	C	32	TYR	3.0
1	B	249	HIS	3.0
2	C	136	ALA	3.0
1	A	233	THR	3.0
1	A	195	GLY	3.0
2	H	157	GLY	3.0
3	D	113	PRO	3.0
1	A	275	ALA	2.9
3	D	150	ALA	2.9
3	D	114	THR	2.9
1	A	278	ASP	2.9
2	C	118	GLY	2.9
3	D	117	LEU	2.9
2	H	121	VAL	2.9
2	C	189	LEU	2.8
2	C	122	PHE	2.8
2	H	207	VAL	2.8
2	C	199	ASN	2.8
2	H	25	SER	2.8
3	D	122	SER	2.8
3	L	156	LYS	2.8
2	H	195	ILE	2.8
2	C	204	ASN	2.8
2	C	157	GLY	2.8
3	D	56	SER	2.8
3	D	127	ALA	2.8
2	C	2	VAL	2.8
2	C	151	THR	2.7
2	H	161	SER	2.7
2	C	140	CYS	2.7
1	A	252	ARG	2.7
1	B	268	ALA	2.7
3	L	127	ALA	2.7
1	B	235	HIS	2.7
1	B	303	VAL	2.7
1	A	271	GLY	2.7
2	C	185	PRO	2.7
2	C	196	CYS	2.7
1	B	15	MET	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	375	MET	2.7
1	B	130	ILE	2.7
2	H	206	LYS	2.7
3	D	200	SER	2.7
1	A	289	LEU	2.7
1	B	251	LYS	2.7
3	D	147	ALA	2.6
1	B	350	GLN	2.6
2	H	122	PHE	2.6
1	B	213	VAL	2.6
2	H	181	VAL	2.6
2	H	191	THR	2.6
3	D	116	THR	2.6
3	L	157	ALA	2.6
1	B	194	THR	2.6
1	B	277	MET	2.6
2	C	134	GLY	2.6
3	L	155	VAL	2.6
2	C	180	SER	2.6
2	C	174	GLY	2.6
3	D	107	GLY	2.6
3	D	152	SER	2.6
3	D	194	GLN	2.5
1	B	273	LEU	2.5
3	D	189	ARG	2.5
3	D	172	TYR	2.5
1	A	214	HIS	2.5
1	A	286	SER	2.5
2	C	152	VAL	2.5
2	H	212	GLU	2.5
1	B	275	ALA	2.5
3	D	166	LYS	2.5
1	A	130	ILE	2.5
3	D	185	TRP	2.5
2	C	212	GLU	2.4
2	H	156	SER	2.4
2	C	176	TYR	2.4
1	B	349	MET	2.4
2	C	144	ASP	2.4
3	D	128	ASN	2.4
2	H	27	GLY	2.4
2	C	143	LYS	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	277	MET	2.4
1	B	211	TRP	2.4
3	D	110	LYS	2.4
1	A	15	MET	2.4
1	B	322	LEU	2.4
2	C	159	LEU	2.4
3	L	125	LEU	2.4
3	D	170	ASN	2.4
2	C	124	LEU	2.4
2	C	138	LEU	2.4
2	C	171	GLN	2.4
1	A	20	TRP	2.4
2	H	126	PRO	2.3
2	C	209	LYS	2.3
2	H	160	THR	2.3
3	D	148	TRP	2.3
3	L	147	ALA	2.3
1	B	347	VAL	2.3
3	L	188	HIS	2.3
3	L	195	VAL	2.3
3	L	191	TYR	2.3
2	C	120	SER	2.3
2	C	207	VAL	2.3
2	H	119	PRO	2.3
1	A	193	ARG	2.3
1	A	84	LYS	2.3
1	B	352	LEU	2.2
2	C	141	LEU	2.2
2	C	175	LEU	2.2
3	D	115	VAL	2.3
3	D	142	GLY	2.2
3	D	199	GLY	2.2
2	H	171	GLN	2.2
2	C	161	SER	2.2
3	D	153	SER	2.2
1	B	297	LYS	2.2
2	C	188	SER	2.2
3	L	153	SER	2.2
1	B	201	LEU	2.2
3	D	135	LEU	2.2
2	C	202	PRO	2.2
3	D	182	PRO	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	304	SER	2.2
2	C	153	SER	2.2
2	C	187	SER	2.2
3	L	205	THR	2.2
2	H	144	ASP	2.1
3	L	146	VAL	2.1
3	D	183	GLU	2.1
1	A	253	GLN	2.1
1	A	279	GLY	2.1
2	H	141	LEU	2.1
3	D	171	LYS	2.1
3	L	128	ASN	2.1
3	L	148	TRP	2.1
2	C	146	PHE	2.1
2	C	160	THR	2.1
1	B	250	ALA	2.1
3	D	143	ALA	2.1
3	L	168	SER	2.1
2	H	73	GLU	2.1
2	C	142	VAL	2.1
3	L	187	SER	2.1
1	A	272	ALA	2.1
3	D	136	ILE	2.1
3	D	140	TYR	2.1
3	L	206	VAL	2.1
3	L	158	GLY	2.1
3	D	163	THR	2.0
3	D	168	SER	2.0
1	A	393	GLU	2.0
1	B	35	ALA	2.0
2	C	125	ALA	2.0
3	D	130	ALA	2.0
2	H	204	ASN	2.0
3	L	119	PRO	2.0
2	C	145	TYR	2.0
1	B	265	VAL	2.0
2	C	139	GLY	2.0
2	C	165	THR	2.0
2	H	205	THR	2.0
3	D	111	ALA	2.0
3	L	194	GLN	2.0
1	A	230	ASP	2.0

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Mol	Chain	Res	Type	RSRZ
1	B	189	ASP	2.0
2	C	117	LYS	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains [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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
2	PCA	C	1	8/9	0.90	0.20	68,80,96,99	0
2	PCA	H	1	8/9	0.91	0.22	63,70,81,85	0

## 6.3 Carbohydrates [i](#)

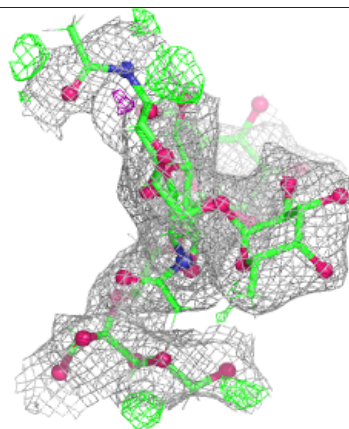
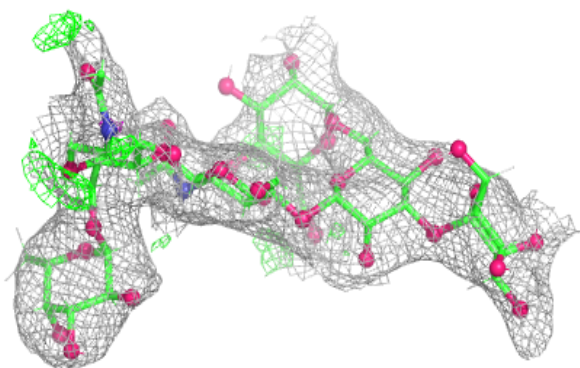
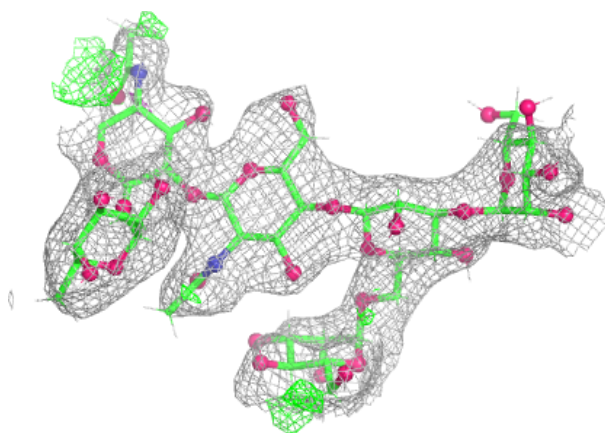
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
4	NAG	E	1	14/15	-	-	72,89,107,110	0
4	NAG	E	2	14/15	-	-	77,85,102,103	0
4	BMA	E	3	11/12	-	-	88,101,118,119	0
4	MAN	E	4	11/12	-	-	94,105,122,126	0
4	MAN	E	5	11/12	-	-	97,114,133,134	0
4	FUC	E	6	10/11	-	-	69,83,95,102	0
5	NAG	F	1	14/15	-	-	61,81,97,98	0
5	NAG	F	2	14/15	-	-	59,71,85,89	0
5	BMA	F	3	11/12	-	-	77,91,108,119	0
5	MAN	F	4	11/12	-	-	71,95,117,122	0
5	FUC	F	5	10/11	-	-	59,71,83,97	0

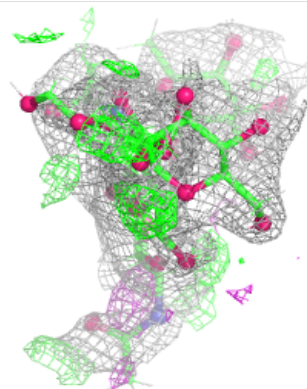
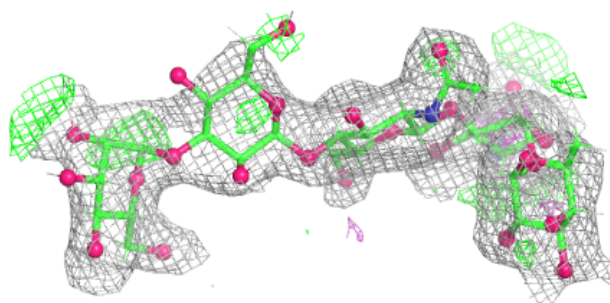
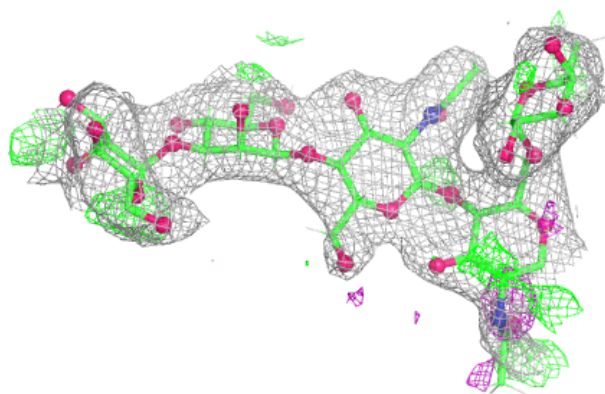
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

**Electron density around Chain 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)



## 6.4 Ligands [i](#)

There are no ligands in this entry.

## 6.5 Other polymers [i](#)

There are no such residues in this entry.