



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 22, 2020 – 02:27 PM BST

PDB ID : 4K1Y  
Title : Crystal structure of Canavalia boliviana lectin in complex with Man1-3Man-OMe  
Authors : Bezerra, G.A.; Viertlmayr, R.; Moura, T.R.; Delatorre, P.; Rocha, B.A.M.; Cavada, B.S.; Gruber, K.  
Deposited on : 2013-04-07  
Resolution : 2.50 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

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

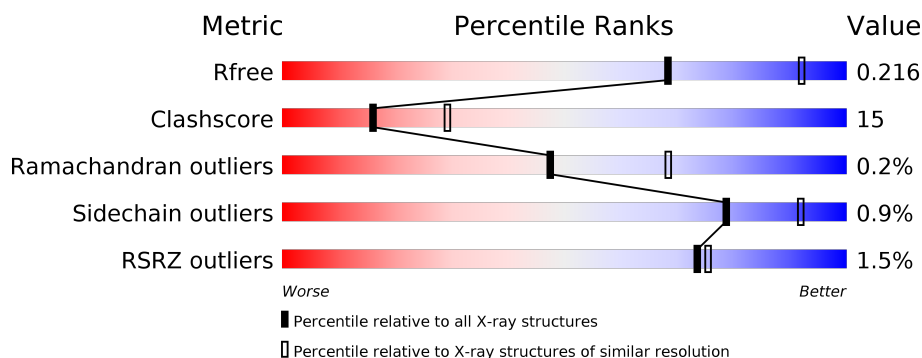
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.50 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.





Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	237	<div> <div>%</div> <div> <div></div> <div>73%</div> <div>25%</div> <div>.</div> </div> </div>
1	B	237	<div> <div>2%</div> <div> <div></div> <div>77%</div> <div>23%</div> </div> </div>
1	C	237	<div> <div>69%</div> <div>31%</div> </div>
1	D	237	<div> <div>3%</div> <div> <div></div> <div>76%</div> <div>23%</div> <div>.</div> </div> </div>
2	E	2	<div> <div>50%</div> <div>50%</div> </div>
2	F	2	<div> <div>100%</div> </div>

Continued on next page...

*Continued from previous page...*

Mol	Chain	Length	Quality of chain
2	G	2	 50%50%
2	H	2	 50%50%

## 2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 7529 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 Canavalia boliviana lectin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	237	Total	C	N	O	S	0	0	0
			1807	1138	305	362	2			
1	B	237	Total	C	N	O	S	0	0	0
			1807	1138	305	362	2			
1	C	237	Total	C	N	O	S	0	0	0
			1807	1138	305	362	2			
1	D	237	Total	C	N	O	S	0	0	0
			1807	1138	305	362	2			

- Molecule 2 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-methyl alpha-D-mannopyranoside.



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
2	E	2	Total	C	O	0	0	0
			24	13	11			
2	F	2	Total	C	O	0	0	0
			24	13	11			
2	G	2	Total	C	O	0	0	0
			24	13	11			
2	H	2	Total	C	O	0	0	0
			24	13	11			

- Molecule 3 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Mn	0	0
			1	1		

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total 1	Mn 1	0	0
3	D	1	Total 1	Mn 1	0	0
3	C	1	Total 1	Mn 1	0	0

- Molecule 4 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total 1	Ca 1	0	0
4	A	1	Total 1	Ca 1	0	0
4	D	1	Total 1	Ca 1	0	0
4	C	1	Total 1	Ca 1	0	0

- Molecule 5 is CADMIUM ION (three-letter code: CD) (formula: Cd).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	2	Total 2	Cd 2	0	0
5	A	2	Total 2	Cd 2	0	0
5	D	2	Total 2	Cd 2	0	0
5	C	3	Total 3	Cd 3	0	0

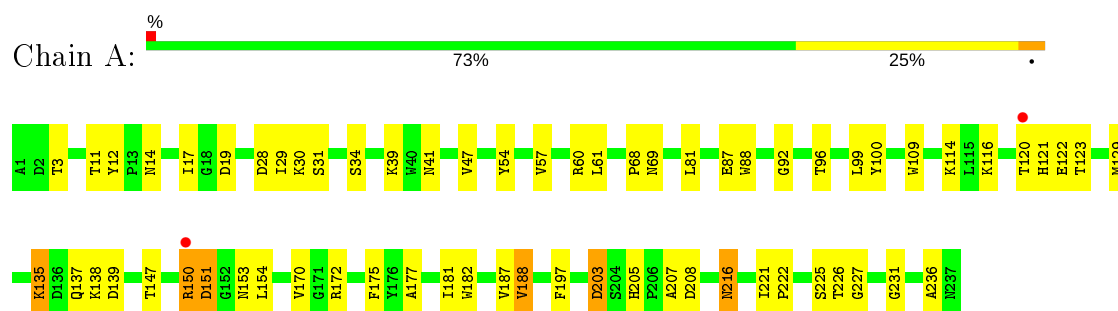
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	48	Total 48	O 48	0	0
6	B	45	Total 45	O 45	0	0
6	C	55	Total 55	O 55	0	0
6	D	40	Total 40	O 40	0	0

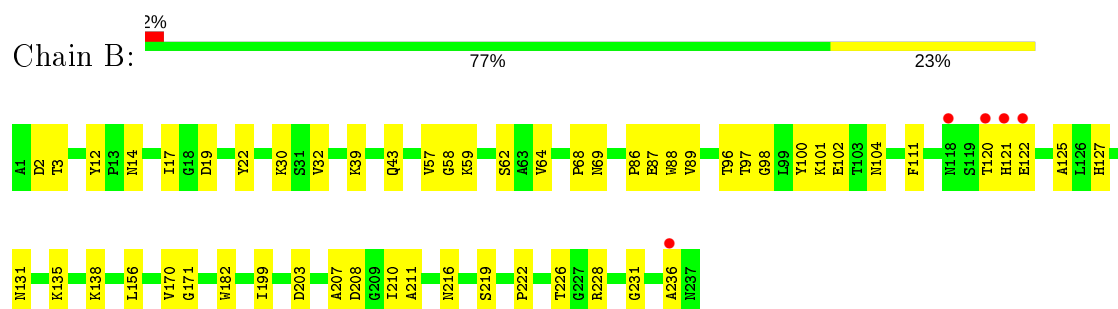
### 3 Residue-property plots

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.

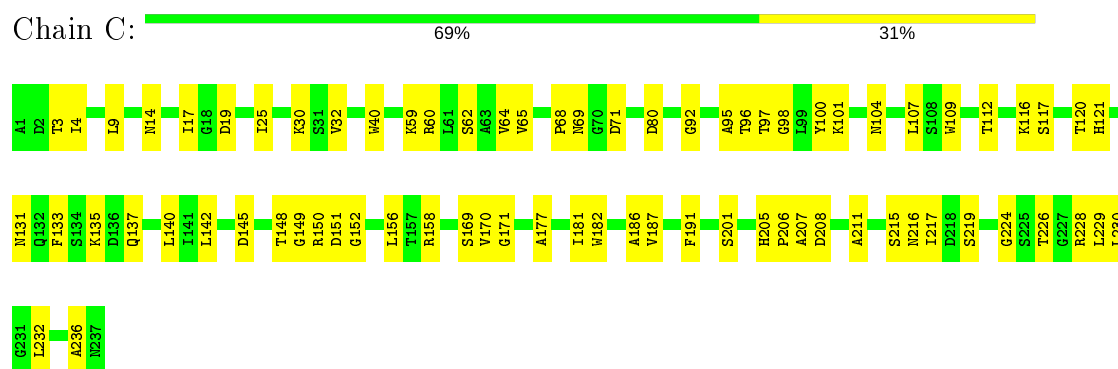
- Molecule 1: Canavalia boliviana lectin



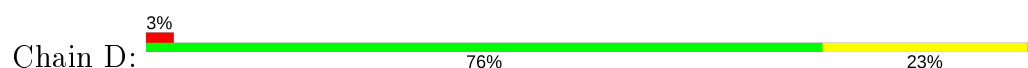
- Molecule 1: Canavalia boliviana lectin

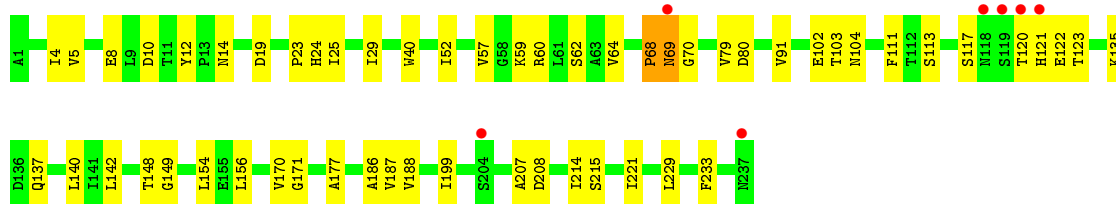


- Molecule 1: Canavalia boliviana lectin



- Molecule 1: Canavalia boliviana lectin





- Molecule 2: alpha-D-mannopyranose-(1-3)-methyl alpha-D-mannopyranoside

Chain E:  50%



- Molecule 2: alpha-D-mannopyranose-(1-3)-methyl alpha-D-mannopyranoside

Chain F:  100%




- Molecule 2: alpha-D-mannopyranose-(1-3)-methyl alpha-D-mannopyranoside

Chain G:  50%



- Molecule 2: alpha-D-mannopyranose-(1-3)-methyl alpha-D-mannopyranoside

Chain H:  50%



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	139.88Å 95.66Å 94.61Å 90.00° 132.29° 90.00°	Depositor
Resolution (Å)	40.94 – 2.50 40.94 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.9 (40.94-2.50) 98.7 (40.94-2.50)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.14	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.34 (at 2.51Å)	Xtriage
Refinement program	PHENIX 1.7 _650	Depositor
R, $R_{free}$	0.204 , 0.228 0.195 , 0.216	Depositor DCC
$R_{free}$ test set	1614 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	36.8	Xtriage
Anisotropy	0.108	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 19.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.44$ , $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	0.058 for -h+k-l,-l,-k 0.049 for -h-k-l,l,k 0.259 for -h-2*l,-k,l	Xtriage
Reported twinning fraction	0.296 for -h-2*l,-k,l	Depositor
Outliers	0 of 31960 reflections	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	7529	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.73% 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 [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: MAN, CA, MN, MMA, CD

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	0.28	0/1848	0.52	0/2515
1	B	0.27	0/1848	0.50	0/2515
1	C	0.29	0/1848	0.51	0/2515
1	D	0.27	0/1848	0.52	0/2515
All	All	0.28	0/7392	0.51	0/10060

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	D	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	D	68	PRO	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	A	1807	0	1756	61	0
1	B	1807	0	1756	57	0
1	C	1807	0	1756	64	0
1	D	1807	0	1756	53	0
2	E	24	0	23	3	0
2	F	24	0	23	7	0
2	G	24	0	23	2	0
2	H	24	0	23	1	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
5	A	2	0	0	0	0
5	B	2	0	0	0	0
5	C	3	0	0	0	0
5	D	2	0	0	0	0
6	A	48	0	0	3	0
6	B	45	0	0	2	0
6	C	55	0	0	4	0
6	D	40	0	0	1	0
All	All	7529	0	7116	210	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 15.

All (210) 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:D:69:ASN:HB3	1:D:70:GLY:HA3	1.36	1.07
1:D:69:ASN:HB3	1:D:70:GLY:CA	1.92	0.99
1:A:123:THR:H	1:B:131:ASN:HD22	0.98	0.95
1:C:131:ASN:HD22	1:D:123:THR:H	1.18	0.92
1:C:135:LYS:HD3	1:C:149:GLY:HA3	1.54	0.89
1:C:135:LYS:NZ	1:C:150:ARG:HG2	1.92	0.84
1:A:123:THR:N	1:B:131:ASN:HD22	1.76	0.83
1:C:68:PRO:O	1:C:69:ASN:HB3	1.81	0.81
1:C:120:THR:O	1:C:121:HIS:HB2	1.83	0.77
1:A:123:THR:H	1:B:131:ASN:ND2	1.81	0.76

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:69:ASN:CB	1:D:70:GLY:CA	2.64	0.76
1:B:100:TYR:HE1	2:F:1:MMA:C7	1.98	0.76
1:B:96:THR:HG22	1:B:170:VAL:HG23	1.68	0.75
1:B:121:HIS:HB2	1:B:122:GLU:HA	1.69	0.74
1:C:145:ASP:HB3	1:C:158:ARG:HG2	1.69	0.73
1:D:120:THR:HA	1:D:121:HIS:C	2.10	0.72
1:D:4:ILE:HD13	1:D:215:SER:HB3	1.72	0.71
1:B:100:TYR:CE1	2:F:1:MMA:C7	2.74	0.71
1:C:14:ASN:O	1:C:19:ASP:HB2	1.92	0.70
1:D:14:ASN:O	1:D:19:ASP:HB2	1.91	0.69
1:A:88:TRP:CG	1:B:138:LYS:HD2	2.28	0.69
1:D:187:VAL:HG23	1:D:188:VAL:HG23	1.75	0.69
1:B:14:ASN:O	1:B:19:ASP:HB2	1.94	0.68
1:B:120:THR:HA	1:B:121:HIS:C	2.15	0.67
1:D:137:GLN:HG2	1:D:140:LEU:HD12	1.76	0.66
1:C:131:ASN:ND2	1:D:123:THR:H	1.93	0.66
1:A:96:THR:HG22	1:A:170:VAL:HG23	1.76	0.66
1:A:151:ASP:OD2	6:A:426:HOH:O	2.14	0.65
1:A:57:VAL:HG13	1:C:64:VAL:HG23	1.79	0.64
1:C:68:PRO:O	1:C:69:ASN:CB	2.46	0.64
1:B:100:TYR:CE1	2:F:1:MMA:H71	2.32	0.64
1:C:135:LYS:CE	1:C:150:ARG:HG2	2.28	0.64
1:C:17:ILE:HD11	6:C:455:HOH:O	1.98	0.63
1:C:145:ASP:CB	1:C:158:ARG:HG2	2.28	0.63
1:A:12:TYR:CD1	2:E:2:MAN:H61	2.34	0.62
1:C:135:LYS:HZ1	1:C:150:ARG:HG2	1.63	0.62
1:B:17:ILE:HD13	1:B:228:ARG:HD2	1.81	0.62
1:C:131:ASN:HD22	1:D:123:THR:N	1.93	0.61
1:B:121:HIS:CB	1:B:122:GLU:HA	2.29	0.61
1:A:92:GLY:HA2	1:A:109:TRP:CH2	2.36	0.61
1:C:208:ASP:HB3	6:C:411:HOH:O	2.00	0.61
1:C:97:THR:OG1	1:C:169:SER:HB3	2.00	0.60
1:C:224:GLY:O	1:C:229:LEU:HD12	2.00	0.60
1:A:60:ARG:HB2	1:C:60:ARG:NH1	2.15	0.60
1:A:150:ARG:O	1:A:151:ASP:CG	2.40	0.60
1:B:62:SER:HB3	1:D:57:VAL:HG12	1.84	0.60
1:C:25:ILE:HG21	1:C:65:VAL:HG11	1.83	0.59
1:B:62:SER:HB3	1:D:57:VAL:CG1	2.32	0.59
1:C:120:THR:HA	6:C:430:HOH:O	2.02	0.59
1:A:121:HIS:HB2	1:A:122:GLU:HA	1.85	0.58
1:A:17:ILE:HG13	1:A:236:ALA:HB1	1.85	0.58

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:121:HIS:CB	1:A:122:GLU:HA	2.33	0.58
1:A:120:THR:HA	1:A:121:HIS:C	2.23	0.58
1:A:170:VAL:HB	1:A:226:THR:HG22	1.85	0.58
1:D:121:HIS:CB	1:D:122:GLU:HA	2.34	0.57
1:D:59:LYS:NZ	6:D:424:HOH:O	2.36	0.57
1:B:120:THR:HA	1:B:121:HIS:O	2.05	0.57
1:A:116:LYS:O	1:A:187:VAL:HG22	2.05	0.56
1:C:59:LYS:HD3	1:C:80:ASP:HB2	1.88	0.56
1:C:100:TYR:HD1	2:G:2:MAN:H62	1.70	0.56
1:D:12:TYR:HB2	1:D:207:ALA:HB2	1.87	0.56
1:D:148:THR:HG22	1:D:154:LEU:HD13	1.86	0.56
1:B:57:VAL:HG12	1:D:62:SER:HB3	1.88	0.56
1:A:28:ASP:HB3	1:A:31:SER:O	2.06	0.56
1:C:145:ASP:CG	1:C:158:ARG:HG2	2.26	0.55
1:B:3:THR:HG23	1:B:30:LYS:HD3	1.88	0.55
1:D:170:VAL:HG22	1:D:221:ILE:HD13	1.89	0.55
1:B:68:PRO:O	1:B:69:ASN:CG	2.44	0.55
1:C:4:ILE:HD13	1:C:215:SER:HB3	1.89	0.55
1:C:96:THR:HG22	1:C:170:VAL:HG23	1.90	0.54
1:D:121:HIS:HB2	1:D:122:GLU:HA	1.88	0.54
1:D:120:THR:HA	1:D:121:HIS:O	2.06	0.54
1:B:98:GLY:HA3	2:F:2:MAN:H4	1.89	0.54
1:B:57:VAL:HG13	1:D:64:VAL:HG23	1.90	0.54
1:C:116:LYS:O	1:C:187:VAL:HG22	2.07	0.54
1:A:208:ASP:OD2	1:A:227:GLY:HA2	2.08	0.54
1:B:86:PRO:HG2	1:B:89:VAL:HG12	1.89	0.53
1:C:228:ARG:O	1:C:230:LEU:HG	2.08	0.53
1:A:100:TYR:CE2	1:A:205:HIS:HB2	2.43	0.53
1:B:87:GLU:HG3	1:B:182:TRP:O	2.09	0.53
1:C:25:ILE:HG21	1:C:65:VAL:CG1	2.38	0.53
1:D:68:PRO:O	1:D:69:ASN:CB	2.56	0.53
1:A:150:ARG:O	1:A:151:ASP:CB	2.56	0.53
1:A:181:ILE:HG23	1:A:182:TRP:CD1	2.43	0.53
1:C:142:LEU:HD11	1:C:148:THR:HG23	1.91	0.52
1:C:216:ASN:OD1	1:C:219:SER:HB2	2.09	0.52
1:C:135:LYS:CD	1:C:149:GLY:HA3	2.32	0.52
1:A:181:ILE:HG23	1:A:182:TRP:HD1	1.75	0.52
1:C:150:ARG:O	1:C:151:ASP:OD1	2.27	0.52
1:B:97:THR:HB	1:B:101:LYS:HA	1.92	0.52
1:C:95:ALA:HB1	1:C:104:ASN:OD1	2.10	0.52
1:A:225:SER:OG	1:A:231:GLY:HA2	2.09	0.51

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:135:LYS:HE2	1:C:150:ARG:HG2	1.90	0.51
1:B:208:ASP:OD1	2:F:2:MAN:O4	2.23	0.51
1:B:216:ASN:OD1	1:B:219:SER:HB2	2.10	0.51
1:D:69:ASN:CB	1:D:70:GLY:HA2	2.41	0.50
1:B:102:GLU:HG2	1:B:207:ALA:O	2.11	0.50
1:C:120:THR:O	1:C:121:HIS:CB	2.55	0.50
1:C:117:SER:HA	1:C:186:ALA:HA	1.94	0.49
1:B:59:LYS:NZ	6:B:427:HOH:O	2.44	0.49
1:A:175:PHE:CE2	1:A:177:ALA:HB3	2.47	0.49
1:A:39:LYS:HE2	1:A:41:ASN:HD21	1.77	0.49
1:B:222:PRO:HD2	1:B:231:GLY:O	2.12	0.49
1:B:69:ASN:OD1	1:B:69:ASN:C	2.50	0.49
1:A:14:ASN:O	1:A:17:ILE:HG22	2.13	0.49
1:A:14:ASN:O	1:A:19:ASP:HB2	2.12	0.49
1:B:32:VAL:HG11	1:B:236:ALA:HA	1.95	0.49
1:C:150:ARG:O	1:C:151:ASP:CG	2.51	0.49
1:C:3:THR:HG23	1:C:30:LYS:HD3	1.94	0.49
1:C:98:GLY:HA3	2:G:2:MAN:H4	1.95	0.49
1:D:156:LEU:O	1:D:171:GLY:HA3	2.13	0.49
1:A:137:GLN:HG3	1:A:139:ASP:OD1	2.12	0.49
1:D:12:TYR:HB2	1:D:207:ALA:CB	2.43	0.49
1:A:147:THR:O	1:A:154:LEU:HD12	2.13	0.48
1:A:54:TYR:CE2	1:A:81:LEU:HD12	2.48	0.48
1:A:216:ASN:OD1	1:A:216:ASN:N	2.41	0.48
1:B:2:ASP:HA	1:B:216:ASN:HD21	1.79	0.48
1:C:32:VAL:HG11	1:C:236:ALA:HA	1.95	0.48
1:D:229:LEU:HD13	1:D:233:PHE:O	2.14	0.48
1:A:187:VAL:HG23	1:A:188:VAL:CG1	2.44	0.48
1:C:9:LEU:HB3	1:C:40:TRP:CZ3	2.48	0.48
1:A:120:THR:HA	1:A:121:HIS:O	2.14	0.47
1:B:12:TYR:HB2	1:B:207:ALA:HB2	1.96	0.47
1:C:135:LYS:HE2	1:C:150:ARG:CD	2.45	0.47
1:C:170:VAL:HB	1:C:226:THR:HG22	1.97	0.47
1:D:12:TYR:HD1	1:D:14:ASN:OD1	1.98	0.46
1:B:156:LEU:O	1:B:171:GLY:HA3	2.16	0.46
2:E:1:MMA:H2	2:E:2:MAN:H5	1.97	0.46
1:B:104:ASN:HD22	1:B:210:ILE:CG1	2.28	0.46
1:A:114:LYS:NZ	6:A:418:HOH:O	2.45	0.46
1:B:100:TYR:HE1	2:F:1:MMA:H72	1.80	0.46
1:C:101:LYS:HG3	6:C:431:HOH:O	2.16	0.46
1:B:64:VAL:HG23	1:D:57:VAL:HG13	1.96	0.46

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:156:LEU:O	1:C:171:GLY:HA3	2.16	0.46
1:B:207:ALA:HA	1:B:208:ASP:HA	1.77	0.46
1:A:12:TYR:CE1	2:E:2:MAN:H61	2.50	0.45
1:C:92:GLY:HA2	1:C:109:TRP:CH2	2.51	0.45
1:A:92:GLY:HA2	1:A:109:TRP:HH2	1.79	0.45
1:B:57:VAL:HG13	1:D:64:VAL:CG2	2.46	0.45
1:A:14:ASN:HA	6:A:436:HOH:O	2.17	0.45
1:A:87:GLU:HG3	1:A:182:TRP:O	2.16	0.45
1:B:210:ILE:HG22	1:B:211:ALA:N	2.32	0.44
1:D:111:PHE:CE2	1:D:113:SER:HB2	2.51	0.44
1:A:47:VAL:HA	1:A:197:PHE:O	2.18	0.44
1:A:129:MET:HE3	1:B:125:ALA:HB3	1.98	0.44
1:B:100:TYR:HD2	1:B:203:ASP:OD2	2.00	0.44
1:D:135:LYS:HD3	1:D:149:GLY:HA3	1.99	0.44
1:C:150:ARG:O	1:C:151:ASP:CB	2.65	0.44
1:A:203:ASP:OD1	1:A:203:ASP:N	2.48	0.44
1:A:3:THR:HG23	1:A:30:LYS:HD2	1.98	0.44
1:A:29:ILE:HG22	1:A:30:LYS:HG3	1.99	0.44
1:B:97:THR:HG22	1:B:207:ALA:O	2.18	0.44
1:B:57:VAL:CG1	1:D:62:SER:HB3	2.47	0.44
1:C:207:ALA:HB1	1:C:208:ASP:CG	2.38	0.44
1:D:69:ASN:CG	1:D:70:GLY:HA2	2.37	0.44
1:A:57:VAL:HG13	1:C:64:VAL:CG2	2.47	0.44
1:B:58:GLY:O	1:D:60:ARG:NH1	2.49	0.44
1:D:52:ILE:N	1:D:52:ILE:HD12	2.32	0.44
1:A:57:VAL:HG12	1:C:62:SER:HB3	1.99	0.43
1:B:100:TYR:CE1	2:F:1:MMA:H72	2.52	0.43
1:C:107:LEU:HD12	1:C:107:LEU:N	2.32	0.43
1:D:4:ILE:CD1	1:D:215:SER:HB3	2.46	0.43
1:A:28:ASP:OD1	1:A:34:SER:HA	2.18	0.43
1:B:64:VAL:CG2	1:D:57:VAL:HG13	2.48	0.43
1:D:208:ASP:OD1	2:H:2:MAN:O4	2.36	0.43
1:A:135:LYS:HD2	1:A:135:LYS:HA	1.78	0.43
1:A:54:TYR:HB2	1:A:61:LEU:HD12	2.00	0.43
1:C:137:GLN:HG2	1:C:140:LEU:HD12	2.00	0.43
1:A:54:TYR:CD2	1:A:81:LEU:HD12	2.54	0.43
1:C:181:ILE:HG23	1:C:182:TRP:CD1	2.53	0.43
1:C:97:THR:HG22	1:C:207:ALA:O	2.18	0.43
1:C:177:ALA:HB2	1:D:177:ALA:HB2	2.01	0.42
1:A:221:ILE:HA	1:A:222:PRO:HD3	1.91	0.42
1:A:57:VAL:CG1	1:C:64:VAL:HG23	2.46	0.42

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:117:SER:HA	1:D:186:ALA:HA	2.01	0.42
1:D:5:VAL:HG13	1:D:29:ILE:HD13	2.01	0.42
1:C:135:LYS:HD3	1:C:149:GLY:CA	2.36	0.42
1:D:91:VAL:HG12	1:D:214:ILE:HG12	2.02	0.42
1:B:135:LYS:HD3	1:B:135:LYS:HA	1.83	0.42
1:C:112:THR:O	1:C:191:PHE:HA	2.20	0.42
1:B:22:TYR:CD1	1:B:39:LYS:HG3	2.55	0.42
1:A:11:THR:OG1	1:A:207:ALA:HA	2.20	0.41
1:A:54:TYR:HB2	1:A:61:LEU:CD1	2.50	0.41
1:A:172:ARG:HG3	1:A:221:ILE:HD11	2.01	0.41
1:B:111:PHE:O	1:B:127:HIS:HA	2.20	0.41
1:D:103:THR:O	1:D:199:ILE:HA	2.20	0.41
1:A:151:ASP:OD2	1:A:153:ASN:HB2	2.21	0.41
1:B:64:VAL:HG23	1:D:57:VAL:CG1	2.50	0.41
1:C:133:PHE:O	1:C:152:GLY:HA2	2.20	0.41
1:D:10:ASP:HB3	1:D:24:HIS:CE1	2.56	0.41
1:B:57:VAL:CG1	1:D:64:VAL:HG23	2.49	0.41
1:D:59:LYS:HD3	1:D:80:ASP:HB2	2.03	0.41
1:B:14:ASN:HB2	1:B:17:ILE:HD11	2.02	0.41
1:A:138:LYS:HD2	1:B:88:TRP:HB3	2.02	0.41
1:B:170:VAL:HB	1:B:226:THR:HG22	2.02	0.41
1:D:23:PRO:HB2	1:D:40:TRP:O	2.21	0.41
1:A:187:VAL:HG23	1:A:188:VAL:HG13	2.02	0.41
1:A:68:PRO:O	1:A:69:ASN:CB	2.70	0.41
1:B:102:GLU:OE2	1:B:199:ILE:HD13	2.21	0.41
1:C:135:LYS:HE2	1:C:150:ARG:NE	2.36	0.41
1:D:142:LEU:HD11	1:D:148:THR:HG23	2.03	0.41
1:D:8:GLU:O	1:D:25:ILE:HA	2.21	0.41
1:A:69:ASN:C	1:A:69:ASN:OD1	2.59	0.40
1:A:99:LEU:HD13	1:A:99:LEU:C	2.42	0.40
1:C:100:TYR:CD2	1:C:205:HIS:HB2	2.57	0.40
1:D:102:GLU:OE2	1:D:104:ASN:ND2	2.49	0.40
1:D:79:VAL:HG22	1:D:80:ASP:N	2.35	0.40
1:C:201:SER:CB	1:C:206:PRO:HB3	2.52	0.40
1:C:211:ALA:CB	1:C:232:LEU:HD11	2.52	0.40
1:B:43:GLN:NE2	6:B:422:HOH:O	2.55	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	235/237 (99%)	223 (95%)	11 (5%)	1 (0%)	34	54
1	B	235/237 (99%)	228 (97%)	7 (3%)	0	100	100
1	C	235/237 (99%)	223 (95%)	12 (5%)	0	100	100
1	D	235/237 (99%)	225 (96%)	9 (4%)	1 (0%)	34	54
All	All	940/948 (99%)	899 (96%)	39 (4%)	2 (0%)	47	68

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	151	ASP
1	D	69	ASN

### 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	202/202 (100%)	197 (98%)	5 (2%)	47	73
1	B	202/202 (100%)	202 (100%)	0	100	100
1	C	202/202 (100%)	200 (99%)	2 (1%)	76	90
1	D	202/202 (100%)	202 (100%)	0	100	100
All	All	808/808 (100%)	801 (99%)	7 (1%)	78	92

All (7) residues with a non-rotameric sidechain are listed below:



Mol	Chain	Res	Type
1	A	135	LYS
1	A	150	ARG
1	A	188	VAL
1	A	203	ASP
1	A	216	ASN
1	C	71	ASP
1	C	217	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	41	ASN
1	A	43	GLN
1	A	83	ASN
1	A	132	GLN
1	A	205	HIS
1	B	43	GLN
1	B	104	ASN
1	B	131	ASN
1	B	132	GLN
1	B	166	GLN
1	B	237	ASN
1	C	118	ASN
1	C	131	ASN
1	C	132	GLN
1	C	237	ASN
1	D	43	GLN
1	D	216	ASN
1	D	237	ASN

### 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 ⓘ

8 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
2	MMA	E	1	2	13,13,13	1.38	2 (15%)	18,18,18	1.68	4 (22%)
2	MAN	E	2	2	11,11,12	0.61	0	15,15,17	1.00	0
2	MMA	F	1	2	13,13,13	1.26	1 (7%)	18,18,18	1.92	5 (27%)
2	MAN	F	2	2	11,11,12	1.10	2 (18%)	15,15,17	1.84	4 (26%)
2	MMA	G	1	2	13,13,13	1.39	2 (15%)	18,18,18	1.72	5 (27%)
2	MAN	G	2	2	11,11,12	1.01	1 (9%)	15,15,17	1.18	1 (6%)
2	MMA	H	1	2	13,13,13	0.85	0	18,18,18	1.50	3 (16%)
2	MAN	H	2	2	11,11,12	1.03	1 (9%)	15,15,17	2.00	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
2	MMA	E	1	2	-	0/4/24/24	0/1/1/1
2	MAN	E	2	2	-	0/2/19/22	0/1/1/1
2	MMA	F	1	2	-	2/4/24/24	0/1/1/1
2	MAN	F	2	2	-	0/2/19/22	0/1/1/1
2	MMA	G	1	2	-	0/4/24/24	0/1/1/1
2	MAN	G	2	2	-	0/2/19/22	0/1/1/1
2	MMA	H	1	2	-	0/4/24/24	0/1/1/1
2	MAN	H	2	2	-	0/2/19/22	0/1/1/1

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	G	1	MMA	O1-C1	3.41	1.46	1.40
2	E	1	MMA	O5-C1	3.08	1.49	1.41
2	F	1	MMA	C4-C5	-2.64	1.47	1.53
2	G	1	MMA	O5-C1	2.52	1.48	1.41
2	H	2	MAN	O5-C1	2.32	1.47	1.43
2	F	2	MAN	C2-C3	-2.24	1.49	1.52

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	2	MAN	C4-C3	-2.22	1.46	1.52
2	E	1	MMA	O1-C1	2.06	1.43	1.40
2	G	2	MAN	C2-C3	-2.01	1.49	1.52

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	2	MAN	O5-C5-C6	6.16	116.86	107.20
2	F	1	MMA	O5-C5-C6	-4.97	94.07	106.44
2	F	2	MAN	O5-C5-C6	4.60	114.41	107.20
2	E	1	MMA	C7-O1-C1	-4.16	106.85	113.27
2	F	1	MMA	C6-C5-C4	-4.01	103.60	113.00
2	H	1	MMA	C7-O1-C1	-3.73	107.52	113.27
2	E	1	MMA	C1-O5-C5	-3.28	107.25	113.69
2	G	1	MMA	C4-C3-C2	-3.20	105.24	110.82
2	F	1	MMA	O1-C1-C2	2.83	111.47	108.15
2	G	1	MMA	O5-C5-C6	2.72	113.19	106.44
2	H	1	MMA	C6-C5-C4	-2.66	106.76	113.00
2	F	1	MMA	C4-C3-C2	-2.65	106.19	110.82
2	F	2	MAN	O2-C2-C3	2.63	115.41	110.14
2	G	1	MMA	C7-O1-C1	-2.55	109.34	113.27
2	H	1	MMA	O4-C4-C5	-2.40	103.33	109.30
2	H	2	MAN	C6-C5-C4	-2.40	107.38	113.00
2	G	1	MMA	C6-C5-C4	-2.39	107.41	113.00
2	G	2	MAN	O2-C2-C3	2.36	114.86	110.14
2	H	2	MAN	C3-C4-C5	-2.35	106.04	110.24
2	E	1	MMA	O2-C2-C3	2.34	115.75	110.35
2	G	1	MMA	O5-C1-O1	2.23	116.14	110.97
2	F	1	MMA	O5-C1-C2	-2.23	105.63	110.35
2	F	2	MAN	C3-C4-C5	-2.18	106.36	110.24
2	F	2	MAN	O3-C3-C4	-2.12	105.45	110.35
2	E	1	MMA	O4-C4-C5	2.03	114.33	109.30

There are no chirality outliers.

All (2) torsion outliers are listed below:

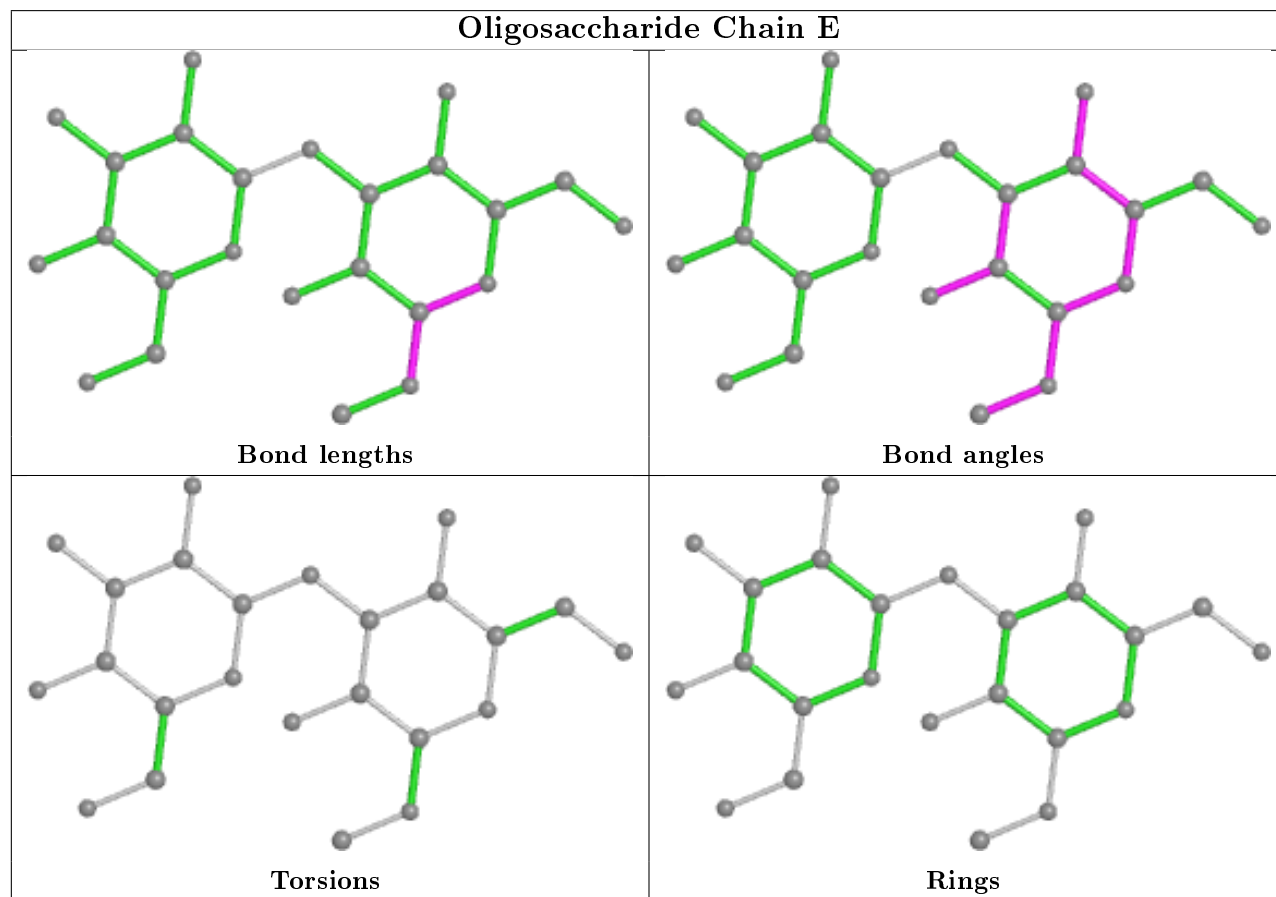
Mol	Chain	Res	Type	Atoms
2	F	1	MMA	O5-C1-O1-C7
2	F	1	MMA	C2-C1-O1-C7

There are no ring outliers.

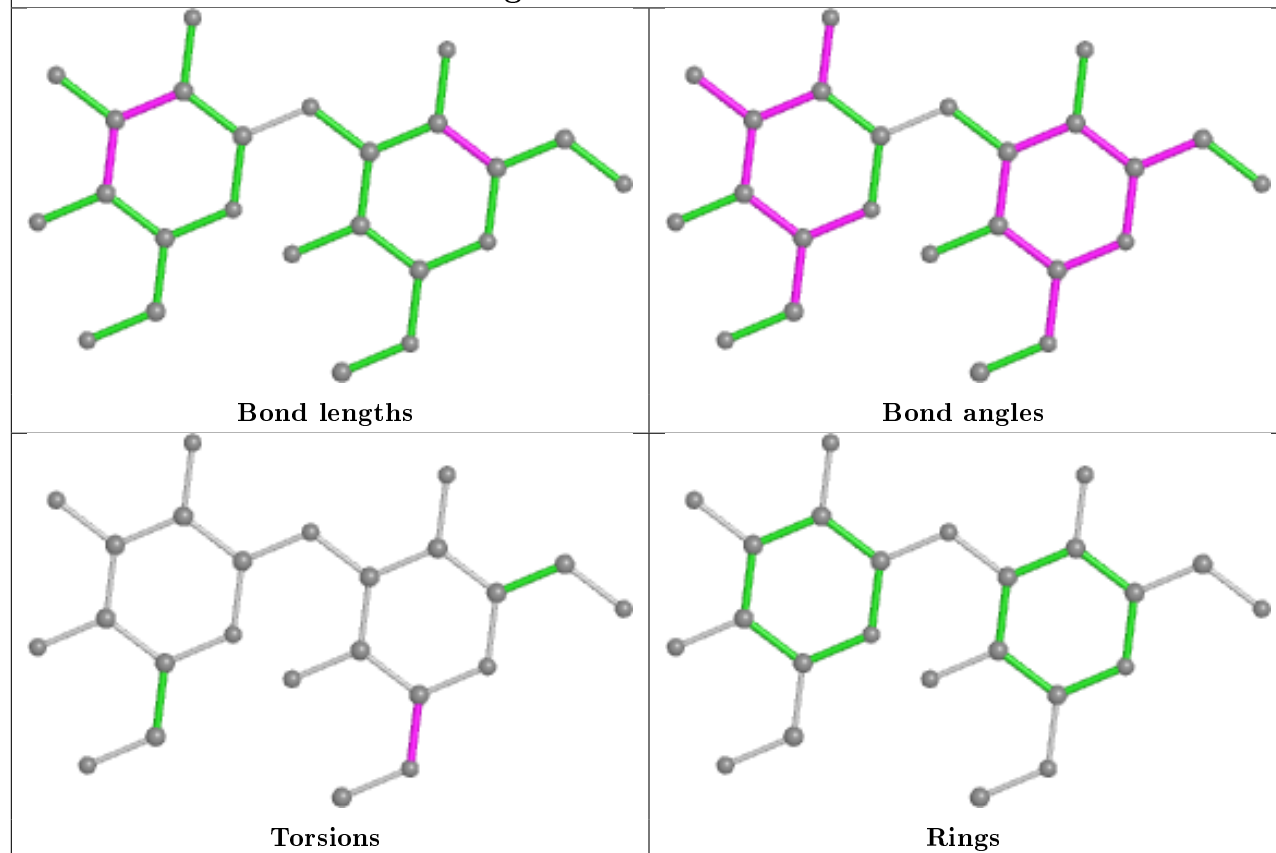
6 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	2	MAN	3	0
2	G	2	MAN	2	0
2	F	2	MAN	2	0
2	H	2	MAN	1	0
2	E	1	MMA	1	0
2	F	1	MMA	5	0

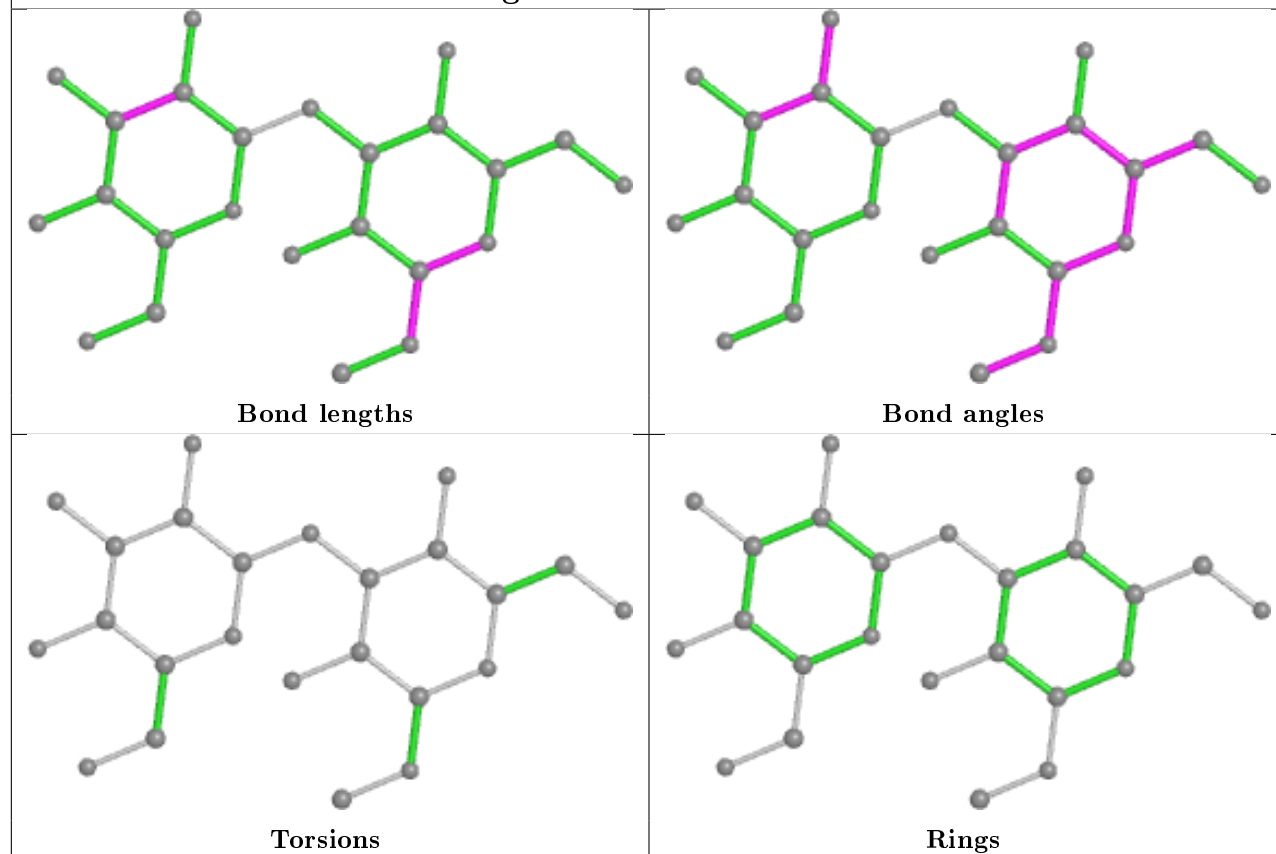
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

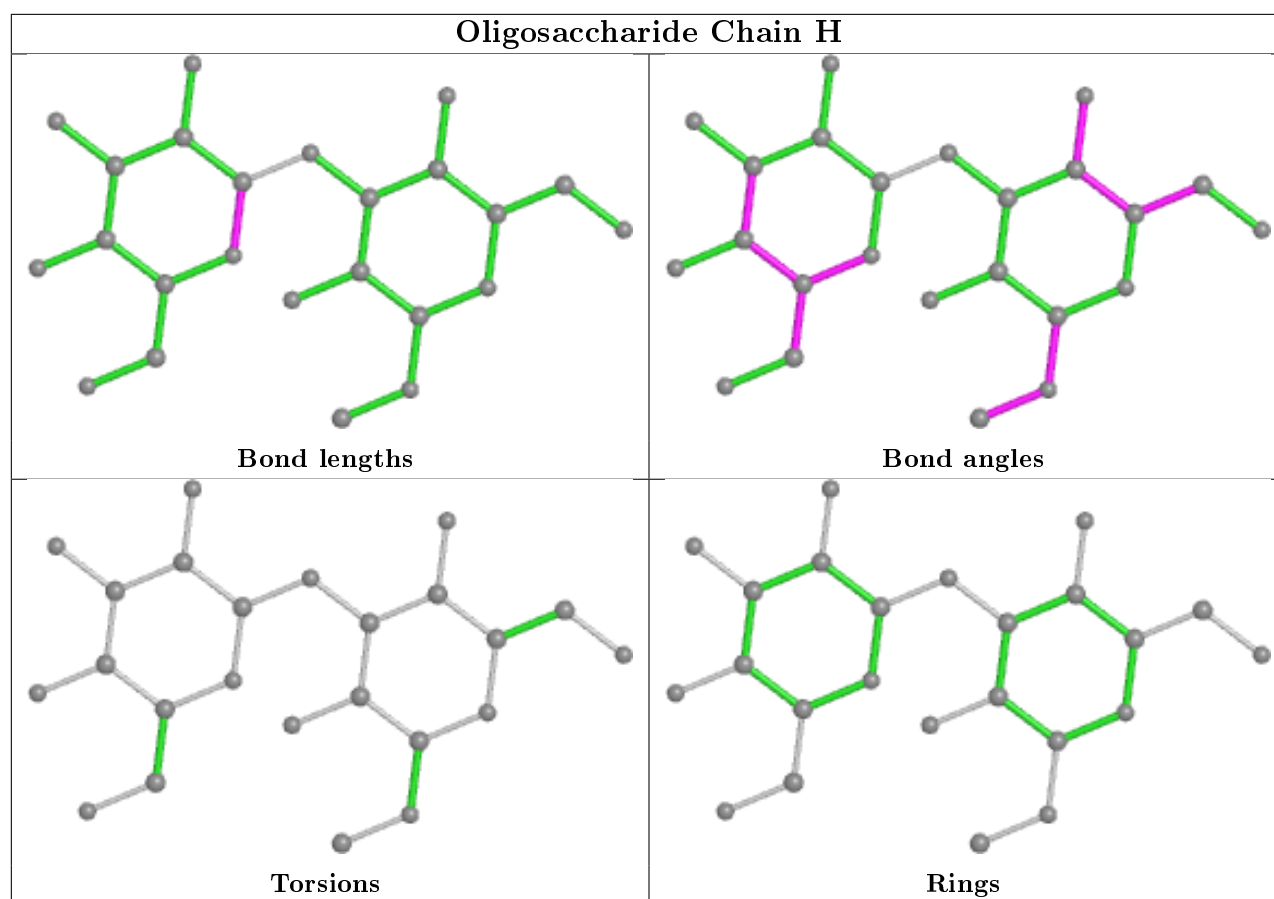


## Oligosaccharide Chain F



## Oligosaccharide Chain G





## 5.6 Ligand geometry [i](#)

Of 17 ligands modelled in this entry, 17 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	237/237 (100%)	-0.08	2 (0%) 86 87	19, 30, 45, 63	0
1	B	237/237 (100%)	0.01	5 (2%) 63 66	20, 30, 48, 67	0
1	C	237/237 (100%)	-0.13	0 100 100	19, 28, 45, 60	0
1	D	237/237 (100%)	0.10	7 (2%) 50 53	19, 32, 54, 63	0
All	All	948/948 (100%)	-0.03	14 (1%) 73 75	19, 30, 48, 67	0

All (14) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	120	THR	4.7
1	B	121	HIS	3.8
1	B	236	ALA	3.4
1	D	118	ASN	3.3
1	D	121	HIS	3.0
1	A	120	THR	3.0
1	D	204	SER	2.8
1	B	122	GLU	2.6
1	D	119	SER	2.4
1	B	120	THR	2.3
1	B	118	ASN	2.3
1	D	237	ASN	2.2
1	A	150	ARG	2.0
1	D	69	ASN	2.0

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

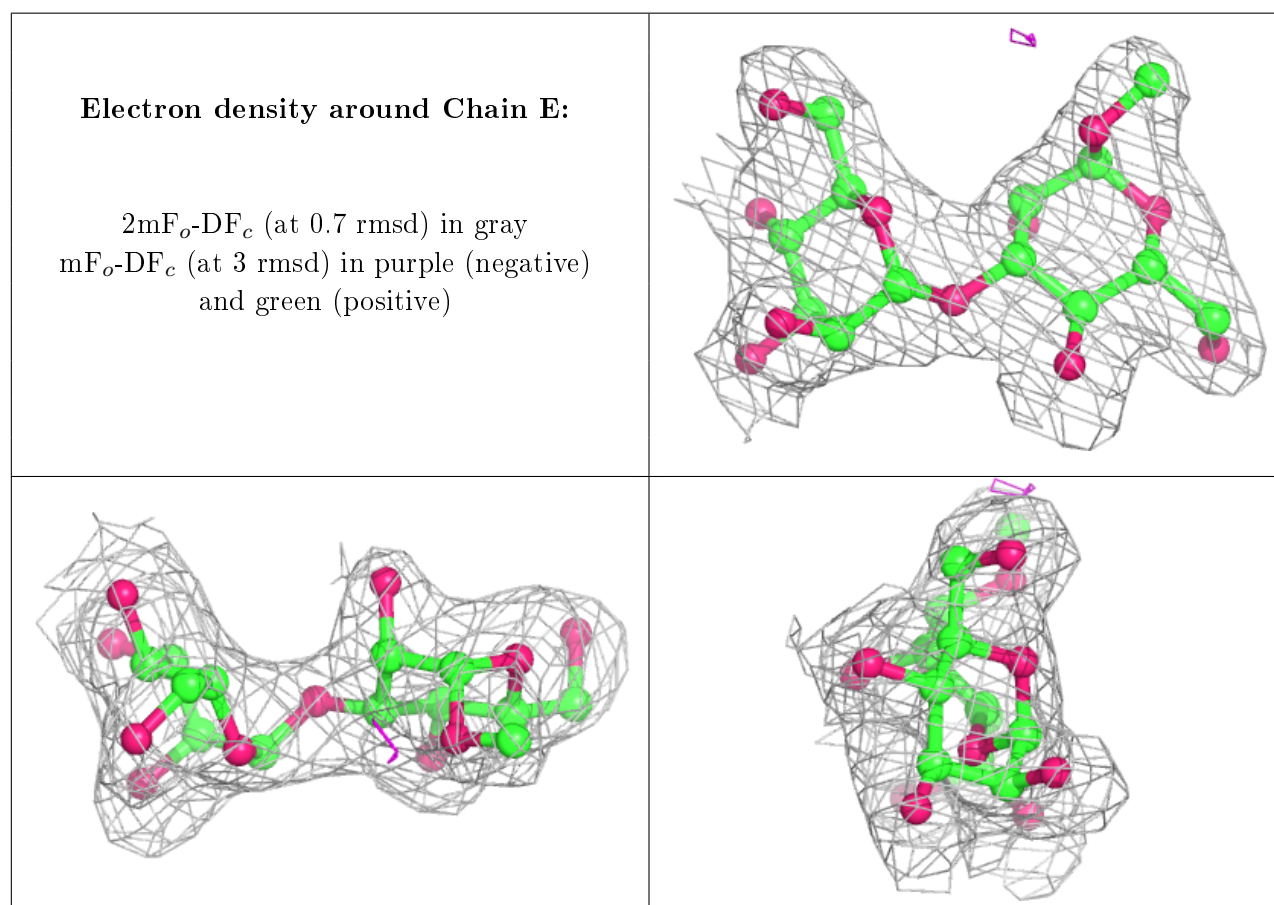
There are no non-standard protein/DNA/RNA residues in this entry.

## 6.3 Carbohydrates ⓘ

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	MMA	H	1	13/13	0.89	0.16	37,43,48,57	0
2	MMA	F	1	13/13	0.89	0.16	30,41,44,45	0
2	MAN	H	2	11/12	0.90	0.13	29,32,38,39	0
2	MMA	E	1	13/13	0.92	0.13	30,35,38,38	0
2	MAN	G	2	11/12	0.93	0.11	30,34,40,45	0
2	MAN	F	2	11/12	0.94	0.10	23,28,33,37	0
2	MMA	G	1	13/13	0.94	0.10	30,38,44,48	0
2	MAN	E	2	11/12	0.94	0.10	26,28,31,37	0

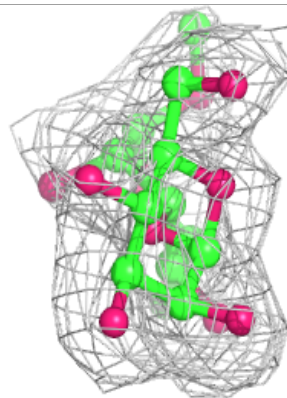
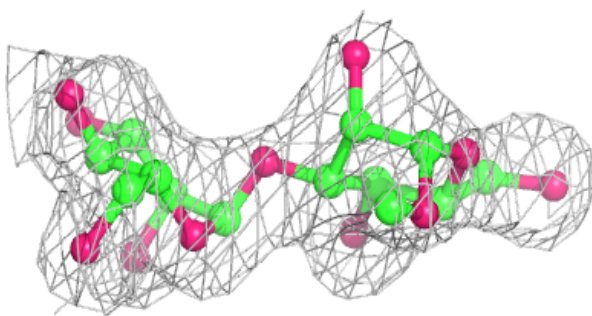
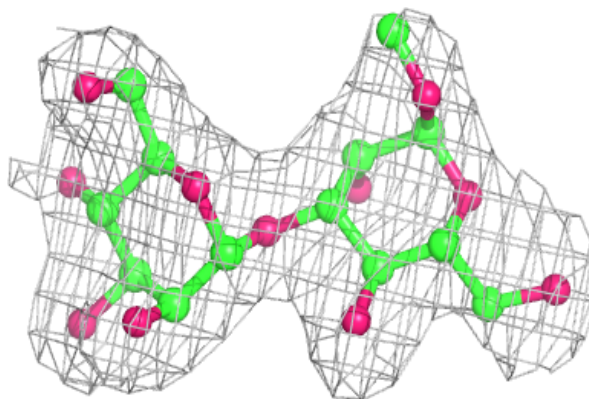
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.



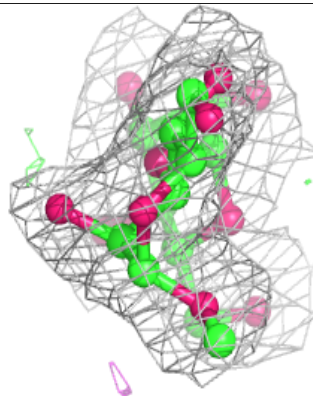
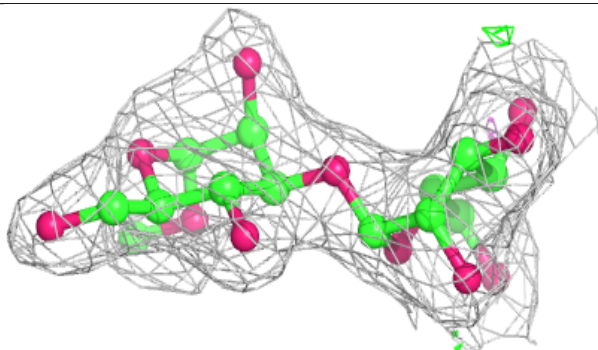
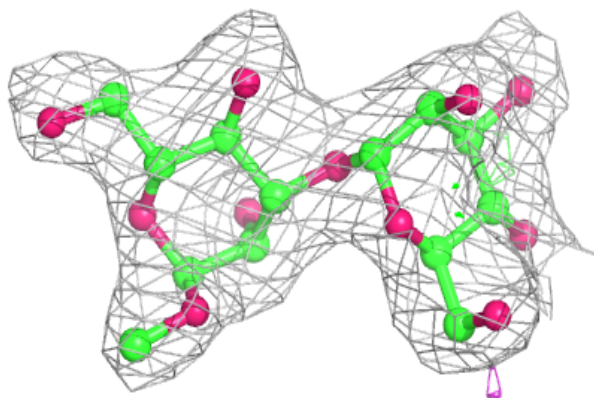


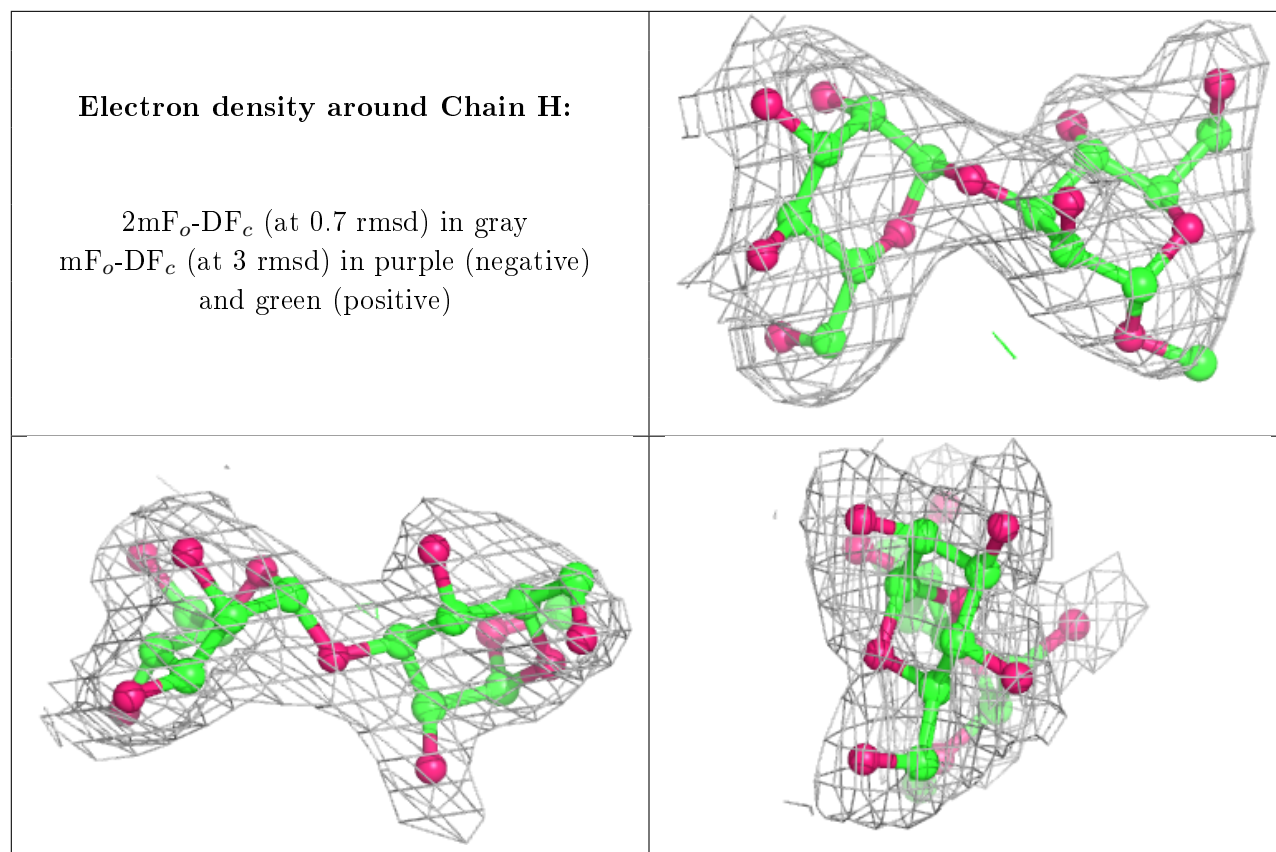
**Electron density around Chain F:**

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

**Electron density around Chain G:**

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





## 6.4 Ligands [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( $\text{\AA}^2$ )	Q<0.9
4	CA	C	302	1/1	0.80	0.14	32,32,32,32	0
4	CA	D	302	1/1	0.87	0.17	36,36,36,36	0
5	CD	C	305	1/1	0.90	0.07	83,83,83,83	1
5	CD	B	303	1/1	0.91	0.11	54,54,54,54	0
4	CA	B	302	1/1	0.94	0.17	30,30,30,30	0
5	CD	C	304	1/1	0.95	0.06	73,73,73,73	1
5	CD	D	304	1/1	0.95	0.04	86,86,86,86	1
5	CD	D	303	1/1	0.96	0.10	56,56,56,56	0
4	CA	A	302	1/1	0.96	0.12	29,29,29,29	0
3	MN	D	301	1/1	0.98	0.17	30,30,30,30	0
5	CD	A	303	1/1	0.99	0.11	45,45,45,45	0
5	CD	C	303	1/1	0.99	0.09	40,40,40,40	0
5	CD	B	304	1/1	0.99	0.04	57,57,57,57	1
3	MN	B	301	1/1	0.99	0.14	22,22,22,22	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	MN	A	301	1/1	0.99	0.17	23,23,23,23	0
3	MN	C	301	1/1	0.99	0.18	24,24,24,24	0
5	CD	A	304	1/1	0.99	0.05	61,61,61,61	1

## 6.5 Other polymers [i](#)

There are no such residues in this entry.