



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 8, 2020 – 12:20 PM BST

PDB ID : 2P2K
Title : Crystal structure of a lectin from Canavalia gladiata seeds (CGL) in complex with man1-4man-OMe
Authors : Moreno, F.B.M.B.; Bezerra, G.A.; Oliveira, T.M.; Souza, E.P.; Rocha, B.A.M.; Benevides, G.B.; Delatorre, P.; Cavada, B.S.; de Azevedo Jr., W.F.
Deposited on : 2007-03-07
Resolution : 1.98 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 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

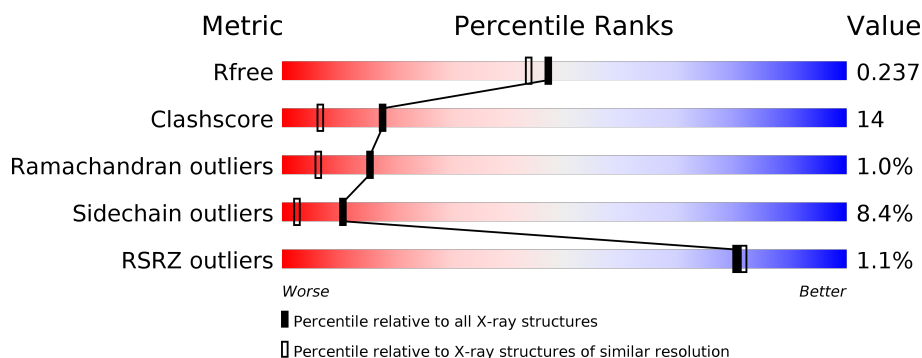
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.98 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	11647 (2.00-1.96)
Clashscore	141614	1014 (1.98-1.98)
Ramachandran outliers	138981	1006 (1.98-1.98)
Sidechain outliers	138945	1006 (1.98-1.98)
RSRZ outliers	127900	11410 (2.00-1.96)

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 ≥ 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>76% 20% ...</div> </div>
1	B	237	<div> <div></div> <div>73% 22% ...</div> </div>
1	C	237	<div> <div></div> <div>67% 29% ...</div> </div>
1	D	237	<div> <div></div> <div>64% 28% 6% ..</div> </div>
2	E	2	<div> <div></div> <div>100%</div> </div>
2	F	2	<div> <div></div> <div>100%</div> </div>

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Mol	Chain	Length	Quality of chain
2	G	2	 100%
2	H	2	 50%50%

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
2	MMA	E	1	X	-	-	-
2	MMA	F	1	X	-	-	-
2	MMA	G	1	X	-	-	-
2	MMA	H	1	X	-	-	-

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 7697 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 gladiata lectin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	234	Total	C	N	O	S	0	0	0
			1779	1123	298	356	2			
1	B	234	Total	C	N	O	S	0	0	0
			1782	1125	298	357	2			
1	C	234	Total	C	N	O	S	0	0	0
			1779	1123	298	356	2			
1	D	234	Total	C	N	O	S	0	0	0
			1782	1125	298	357	2			

- Molecule 2 is an oligosaccharide called alpha-D-mannopyranose-(1-4)-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		

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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

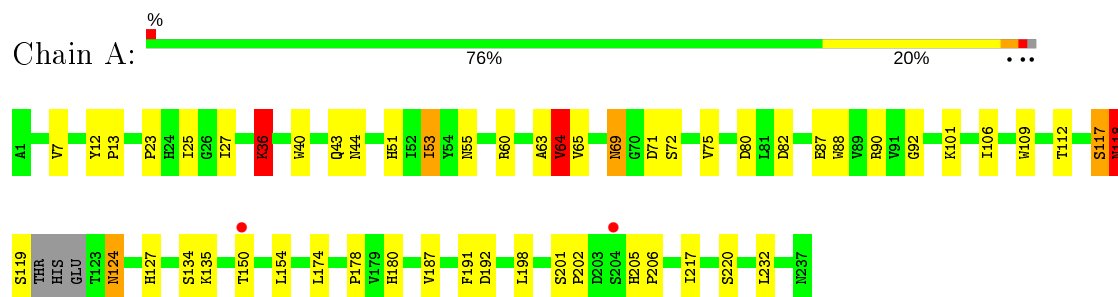
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	145	Total 145	O 145	0	0
5	B	144	Total 144	O 144	0	0
5	C	84	Total 84	O 84	0	0
5	D	98	Total 98	O 98	0	0

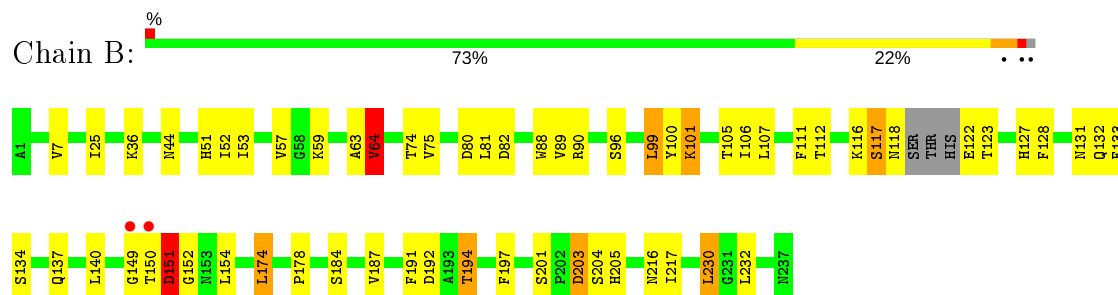
3 Residue-property plots

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.

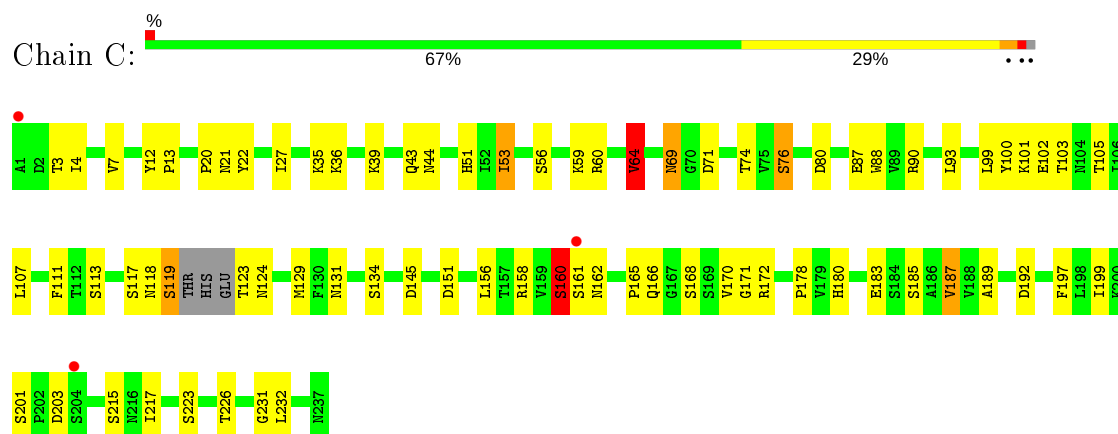
- Molecule 1: *Canavalia gladiata* lectin



- Molecule 1: *Canavalia gladiata* lectin

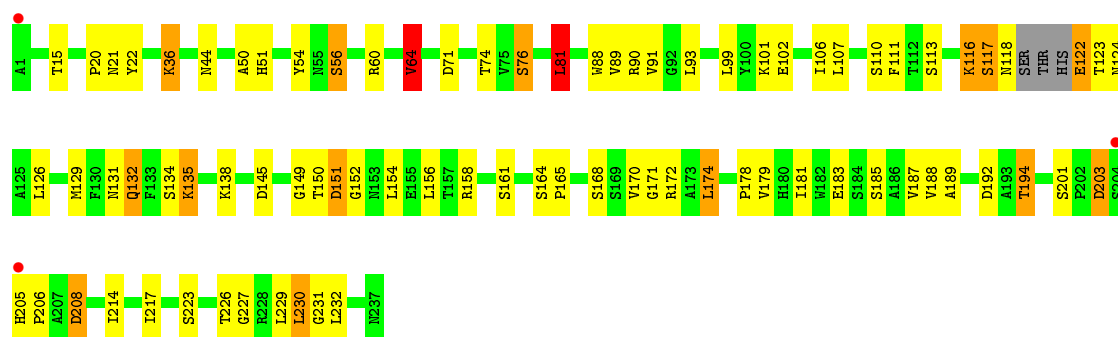


- Molecule 1: *Canavalia gladiata* lectin



- Molecule 1: *Canavalia gladiata* lectin





- Molecule 2: alpha-D-mannopyranose-(1-4)-methyl alpha-D-mannopyranoside

Chain E: 100%

MVA1
MAN2

- Molecule 2: alpha-D-mannopyranose-(1-4)-methyl alpha-D-mannopyranoside

Chain F: 100%

MVA1
MAN2

- Molecule 2: alpha-D-mannopyranose-(1-4)-methyl alpha-D-mannopyranoside

Chain G: 100%

MVA1
MAN2

- Molecule 2: alpha-D-mannopyranose-(1-4)-methyl alpha-D-mannopyranoside

Chain H: 50% 50%

MVA1
MAN2

4 Data and refinement statistics

Property	Value	Source
Space group	P 32	Depositor
Cell constants a, b, c, α , β , γ	68.93Å 68.93Å 160.44Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	39.84 – 1.98 39.83 – 1.98	Depositor EDS
% Data completeness (in resolution range)	99.6 (39.84-1.98) 99.5 (39.83-1.98)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	6.80	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.31 (at 1.98Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.182 , 0.236 0.184 , 0.237	Depositor DCC
R_{free} test set	2983 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å ²)	19.2	Xtriage
Anisotropy	0.012	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 18.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.027 for -h,-k,l 0.486 for h,-h-k,-l 0.028 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	7697	wwPDB-VP
Average B, all atoms (Å ²)	18.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.16% 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: CA, MN, MMA, MAN

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	0.92	2/1819 (0.1%)	0.97	4/2476 (0.2%)
1	B	0.95	2/1822 (0.1%)	1.02	6/2480 (0.2%)
1	C	0.92	1/1820 (0.1%)	1.12	6/2479 (0.2%)
1	D	0.86	2/1822 (0.1%)	1.01	10/2480 (0.4%)
All	All	0.91	7/7283 (0.1%)	1.03	26/9915 (0.3%)

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	B	0	2
1	C	0	1
1	D	0	1
All	All	0	4

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	119	SER	C-N	18.07	1.75	1.34
1	B	101	LYS	CE-NZ	7.33	1.67	1.49
1	D	36	LYS	CE-NZ	6.54	1.65	1.49
1	D	36	LYS	CB-CG	6.53	1.70	1.52
1	B	89	VAL	CB-CG1	5.69	1.64	1.52
1	A	36	LYS	CE-NZ	5.19	1.62	1.49
1	A	36	LYS	CD-CE	5.10	1.64	1.51

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	119	SER	O-C-N	-24.89	82.87	122.70
1	C	119	SER	CA-C-N	16.08	152.57	117.20
1	C	119	SER	C-N-CA	10.68	148.39	121.70
1	D	230	LEU	N-CA-C	-10.22	83.40	111.00
1	D	36	LYS	CD-CE-NZ	9.30	133.09	111.70
1	C	64	VAL	CB-CA-C	-8.54	95.17	111.40
1	D	229	LEU	C-N-CA	8.32	142.50	121.70
1	A	64	VAL	CB-CA-C	-8.29	95.65	111.40
1	D	64	VAL	CB-CA-C	-8.01	96.18	111.40
1	B	64	VAL	CB-CA-C	-7.82	96.55	111.40
1	D	174	LEU	CA-CB-CG	7.67	132.95	115.30
1	A	64	VAL	CG1-CB-CG2	7.26	122.52	110.90
1	B	151	ASP	N-CA-C	7.19	130.40	111.00
1	B	174	LEU	CA-CB-CG	7.12	131.68	115.30
1	D	229	LEU	O-C-N	-6.78	111.86	122.70
1	C	64	VAL	CG1-CB-CG2	6.15	120.74	110.90
1	D	64	VAL	CG1-CB-CG2	5.99	120.48	110.90
1	D	229	LEU	CA-C-N	5.95	130.29	117.20
1	D	229	LEU	N-CA-C	5.91	126.94	111.00
1	B	151	ASP	N-CA-CB	-5.80	100.16	110.60
1	D	81	LEU	CB-CG-CD1	5.68	120.65	111.00
1	A	60	ARG	NE-CZ-NH2	-5.46	117.57	120.30
1	A	60	ARG	NE-CZ-NH1	5.46	123.03	120.30
1	C	21	ASN	CB-CA-C	5.33	121.05	110.40
1	B	64	VAL	CG1-CB-CG2	5.10	119.05	110.90
1	B	101	LYS	CD-CE-NZ	-5.03	100.13	111.70

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	116	LYS	Peptide
1	B	149	GLY	Peptide
1	C	160	SER	Peptide
1	D	116	LYS	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	1779	0	1730	40	0
1	B	1782	0	1731	48	0
1	C	1779	0	1730	56	0
1	D	1782	0	1730	62	0
2	E	24	0	23	0	0
2	F	24	0	23	0	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	145	0	0	3	0
5	B	144	0	0	6	0
5	C	84	0	0	8	0
5	D	98	0	0	7	0
All	All	7697	0	7013	194	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 14.

All (194) 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:C:119:SER:C	1:C:123:THR:N	1.75	1.36
1:D:150:THR:HA	1:D:152:GLY:H	1.00	1.12
1:B:150:THR:HA	1:B:152:GLY:H	0.96	1.10
1:B:64:VAL:HG13	1:B:74:THR:HG22	1.33	1.09
1:A:53:ILE:CD1	5:C:483:HOH:O	2.02	1.08
1:D:64:VAL:HG13	1:D:74:THR:HG22	1.34	1.06
1:D:117:SER:HB3	1:D:118:ASN:HA	1.05	1.02
1:B:150:THR:HA	1:B:152:GLY:N	1.76	1.00
1:B:203:ASP:O	1:B:205:HIS:N	1.96	0.96
1:D:117:SER:HB3	1:D:118:ASN:CA	1.95	0.95
1:B:74:THR:HG23	5:B:493:HOH:O	1.62	0.95
1:D:117:SER:CB	1:D:118:ASN:HA	1.95	0.94
1:A:53:ILE:HD11	5:C:483:HOH:O	1.67	0.93
1:C:119:SER:O	1:C:123:THR:N	2.02	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:150:THR:HA	1:D:152:GLY:N	1.85	0.90
1:A:205:HIS:HD2	1:A:206:PRO:O	1.55	0.89
1:C:44:ASN:HD21	1:C:201:SER:H	1.20	0.88
1:A:118:ASN:HB3	5:A:486:HOH:O	1.73	0.88
1:B:134:SER:H	1:B:137:GLN:NE2	1.76	0.83
1:B:117:SER:CB	1:B:118:ASN:HA	2.08	0.82
1:A:118:ASN:OD1	1:A:119:SER:N	2.13	0.81
1:D:150:THR:CA	1:D:152:GLY:H	1.90	0.81
1:A:205:HIS:CD2	1:A:206:PRO:O	2.34	0.81
1:A:44:ASN:HD21	1:A:201:SER:H	1.27	0.81
1:C:88:TRP:HB3	1:C:217:ILE:HD11	1.62	0.81
1:D:99:LEU:HD12	2:H:1:MMA:H4	1.61	0.81
1:B:194:THR:HG22	5:B:532:HOH:O	1.83	0.78
1:A:51:HIS:HB2	1:A:64:VAL:HG23	1.64	0.77
1:C:166:GLN:HG3	5:C:474:HOH:O	1.84	0.77
1:D:44:ASN:HD21	1:D:201:SER:H	1.36	0.74
1:A:36:LYS:HD2	1:A:75:VAL:HG23	1.70	0.74
1:A:124:ASN:HD21	1:B:132:GLN:H	1.35	0.73
1:B:117:SER:HB3	1:B:118:ASN:HA	1.69	0.73
1:B:194:THR:CG2	5:B:532:HOH:O	2.35	0.73
1:B:36:LYS:HE3	5:B:492:HOH:O	1.90	0.72
1:B:203:ASP:C	1:B:205:HIS:H	1.92	0.72
1:D:150:THR:HB	1:D:151:ASP:HA	1.70	0.72
1:C:53:ILE:C	1:C:53:ILE:HD13	2.10	0.71
1:B:117:SER:HB2	1:B:187:VAL:HG12	1.70	0.71
1:A:53:ILE:HD12	5:C:483:HOH:O	1.78	0.71
1:C:107:LEU:O	5:C:401:HOH:O	2.11	0.68
1:A:44:ASN:HD21	1:A:201:SER:N	1.91	0.68
1:D:205:HIS:HD2	1:D:206:PRO:O	1.77	0.68
1:B:80:ASP:OD1	1:B:82:ASP:HB2	1.95	0.66
1:A:117:SER:HA	1:A:187:VAL:HG22	1.78	0.66
1:B:64:VAL:HG13	1:B:74:THR:CG2	2.21	0.66
1:A:90:ARG:NH1	1:A:217:ILE:HG23	2.11	0.65
1:C:124:ASN:ND2	1:D:131:ASN:H	1.94	0.65
1:B:99:LEU:HD13	1:B:100:TYR:CZ	2.32	0.65
1:A:178:PRO:HB3	1:A:217:ILE:CD1	2.27	0.64
1:D:122:GLU:HG2	5:D:493:HOH:O	1.98	0.64
1:C:131:ASN:O	5:C:401:HOH:O	2.15	0.64
1:C:156:LEU:O	1:C:171:GLY:HA3	1.98	0.63
1:C:51:HIS:HB2	1:C:64:VAL:HG23	1.81	0.63
5:B:457:HOH:O	1:D:194:THR:HG21	1.97	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:44:ASN:ND2	1:D:201:SER:H	1.96	0.63
1:C:160:SER:O	1:C:162:ASN:N	2.31	0.63
1:B:134:SER:H	1:B:137:GLN:HE21	1.46	0.63
1:D:122:GLU:CG	5:D:493:HOH:O	2.48	0.62
1:B:51:HIS:HB2	1:B:64:VAL:HG23	1.82	0.62
1:D:36:LYS:HE3	5:D:481:HOH:O	1.98	0.62
1:D:51:HIS:HB2	1:D:64:VAL:HG23	1.80	0.61
1:C:88:TRP:HB3	1:C:217:ILE:CD1	2.28	0.61
1:D:178:PRO:HB3	1:D:217:ILE:HD11	1.82	0.61
1:C:7:VAL:HG22	1:C:27:ILE:CD1	2.32	0.60
1:C:56:SER:CB	1:C:189:ALA:H	2.15	0.59
1:B:117:SER:HB3	1:B:118:ASN:CA	2.32	0.59
1:B:53:ILE:HD13	5:D:458:HOH:O	2.01	0.59
1:D:201:SER:OG	1:D:203:ASP:HB2	2.03	0.59
1:D:20:PRO:HB2	1:D:22:TYR:CZ	2.38	0.58
1:B:194:THR:HG21	5:D:459:HOH:O	2.02	0.58
1:A:25:ILE:HD12	1:A:75:VAL:HG12	1.86	0.58
1:D:88:TRP:HB3	1:D:217:ILE:CD1	2.34	0.57
1:A:88:TRP:HB3	1:A:217:ILE:HD11	1.87	0.57
1:C:53:ILE:O	1:C:53:ILE:HD13	2.04	0.56
1:A:36:LYS:HD2	1:A:75:VAL:CG2	2.34	0.56
1:D:99:LEU:HD12	5:D:401:HOH:O	2.05	0.56
1:B:88:TRP:HB3	1:B:217:ILE:HD11	1.87	0.56
1:D:64:VAL:HG13	1:D:74:THR:CG2	2.22	0.56
1:B:25:ILE:HD12	1:B:75:VAL:HG12	1.86	0.56
1:C:20:PRO:HB2	1:C:22:TYR:CZ	2.41	0.56
1:B:137:GLN:HG2	1:B:140:LEU:HD12	1.88	0.56
1:C:69:ASN:HD21	1:C:71:ASP:HB2	1.71	0.56
1:B:134:SER:N	1:B:137:GLN:NE2	2.52	0.55
1:B:44:ASN:HD21	1:B:201:SER:H	1.52	0.55
1:B:44:ASN:HD21	1:B:201:SER:N	2.04	0.55
1:C:145:ASP:HB3	1:C:158:ARG:HG2	1.88	0.55
1:D:56:SER:CB	1:D:189:ALA:H	2.20	0.55
1:D:111:PHE:CE2	1:D:113:SER:HB2	2.42	0.55
1:C:60:ARG:HD3	1:C:76:SER:OG	2.07	0.55
1:D:88:TRP:HB3	1:D:217:ILE:HD11	1.89	0.55
1:C:100:TYR:HD2	2:G:2:MAN:H62	1.71	0.55
1:D:60:ARG:HD3	1:D:76:SER:OG	2.07	0.55
1:A:178:PRO:HB3	1:A:217:ILE:HD11	1.88	0.55
1:B:90:ARG:NH1	1:B:217:ILE:CG2	2.70	0.54
1:A:44:ASN:ND2	1:A:201:SER:H	2.02	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:44:ASN:ND2	1:C:201:SER:H	1.97	0.53
1:D:90:ARG:NH1	1:D:217:ILE:HG23	2.24	0.52
1:D:145:ASP:HB3	1:D:158:ARG:HG2	1.91	0.52
1:A:124:ASN:ND2	1:B:131:ASN:H	2.07	0.52
1:D:178:PRO:HB3	1:D:217:ILE:CD1	2.39	0.52
1:B:178:PRO:HB3	1:B:217:ILE:CD1	2.40	0.51
1:A:43:GLN:HE22	1:A:69:ASN:HD21	1.57	0.51
1:D:156:LEU:O	1:D:171:GLY:HA3	2.10	0.51
1:C:99:LEU:HD22	2:G:1:MMA:H4	1.92	0.51
1:C:59:LYS:HD3	1:C:80:ASP:HB2	1.92	0.51
1:C:35:LYS:O	1:C:36:LYS:HG2	2.10	0.51
1:D:116:LYS:O	1:D:187:VAL:N	2.44	0.50
1:A:127:HIS:HB3	1:B:127:HIS:HB3	1.93	0.50
1:C:90:ARG:NH1	1:C:217:ILE:HG23	2.26	0.50
1:C:4:ILE:HD13	1:C:215:SER:HB3	1.93	0.50
1:C:43:GLN:HE22	1:C:69:ASN:ND2	2.09	0.50
1:B:99:LEU:HD13	1:B:100:TYR:CE2	2.46	0.49
1:A:112:THR:O	1:A:191:PHE:HA	2.11	0.49
1:B:105:THR:O	1:B:197:PHE:HA	2.12	0.49
1:B:90:ARG:NH1	1:B:217:ILE:HG22	2.27	0.49
1:B:122:GLU:OE2	1:B:123:THR:OG1	2.31	0.49
1:C:102:GLU:C	1:C:165:PRO:HB3	2.33	0.49
1:C:119:SER:HB3	1:D:131:ASN:HB3	1.95	0.48
1:D:54:TYR:CE1	1:D:81:LEU:HD22	2.48	0.48
1:C:124:ASN:HD21	1:D:132:GLN:H	1.61	0.48
5:A:436:HOH:O	1:C:74:THR:HG21	2.14	0.48
1:C:76:SER:HB3	5:C:471:HOH:O	2.12	0.48
1:D:91:VAL:HG12	1:D:214:ILE:HG12	1.95	0.48
1:B:96:SER:OG	1:B:230:LEU:HA	2.13	0.48
1:C:187:VAL:HG11	5:C:402:HOH:O	2.13	0.48
1:D:170:VAL:HG21	1:D:231:GLY:HA2	1.94	0.48
1:D:170:VAL:HB	1:D:226:THR:HG22	1.96	0.48
1:A:51:HIS:O	1:A:63:ALA:HA	2.14	0.47
1:A:69:ASN:HD21	1:A:71:ASP:HB3	1.79	0.47
1:C:170:VAL:HB	1:C:226:THR:HG22	1.97	0.47
1:B:7:VAL:HG21	1:B:52:ILE:HG12	1.96	0.47
1:B:57:VAL:HG21	1:D:64:VAL:HG22	1.96	0.46
1:C:12:TYR:HA	1:C:13:PRO:HD3	1.77	0.46
1:D:54:TYR:CD1	1:D:81:LEU:HD22	2.51	0.46
1:A:7:VAL:HG22	1:A:27:ILE:HD12	1.97	0.46
1:B:118:ASN:OD1	5:B:401:HOH:O	2.21	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:110:SER:HB3	1:D:129:MET:HG3	1.98	0.46
1:C:43:GLN:HE22	1:C:69:ASN:HD21	1.63	0.46
1:A:92:GLY:HA2	1:A:109:TRP:CH2	2.50	0.46
1:C:158:ARG:HB2	1:C:166:GLN:HB3	1.98	0.46
1:C:178:PRO:HB3	1:C:217:ILE:CD1	2.46	0.45
1:A:12:TYR:HA	1:A:13:PRO:HD3	1.83	0.45
1:C:217:ILE:CD1	1:D:138:LYS:HD2	2.46	0.45
1:A:80:ASP:OD1	1:A:82:ASP:HB2	2.17	0.45
1:B:133:PHE:HA	1:B:137:GLN:NE2	2.31	0.45
1:C:111:PHE:CE2	1:C:113:SER:HB2	2.51	0.45
1:C:22:TYR:CD2	1:C:39:LYS:HE3	2.52	0.45
1:C:107:LEU:N	1:C:107:LEU:HD12	2.31	0.45
1:A:69:ASN:ND2	1:A:71:ASP:H	2.15	0.45
1:D:205:HIS:CD2	1:D:206:PRO:O	2.65	0.44
1:D:102:GLU:C	1:D:165:PRO:HB3	2.38	0.44
1:C:36:LYS:HE3	1:C:76:SER:O	2.18	0.44
1:A:106:ILE:HB	1:A:154:LEU:HB3	2.00	0.43
1:B:112:THR:O	1:B:191:PHE:HA	2.18	0.43
1:A:174:LEU:HD12	1:A:174:LEU:N	2.32	0.43
1:D:208:ASP:OD2	1:D:227:GLY:HA2	2.19	0.43
1:B:51:HIS:O	1:B:63:ALA:HA	2.19	0.43
1:C:87:GLU:HG3	1:C:180:HIS:CD2	2.54	0.43
1:D:106:ILE:HB	1:D:154:LEU:HB3	2.01	0.43
1:D:15:THR:HG21	1:D:21:ASN:HD22	1.84	0.43
1:C:105:THR:O	1:C:197:PHE:HA	2.19	0.43
1:D:116:LYS:HG3	1:D:188:VAL:HB	2.01	0.43
1:C:129:MET:HE3	1:D:123:THR:HB	2.01	0.42
1:A:90:ARG:NH1	1:A:217:ILE:CG2	2.80	0.42
1:D:88:TRP:HB3	1:D:217:ILE:HD12	2.01	0.42
1:A:65:VAL:O	1:A:72:SER:HA	2.20	0.42
5:A:511:HOH:O	1:C:118:ASN:HA	2.20	0.42
1:D:50:ALA:O	1:D:194:THR:HA	2.20	0.42
1:C:170:VAL:HG21	1:C:231:GLY:HA2	2.00	0.42
1:D:126:LEU:CD2	1:D:179:VAL:HG22	2.49	0.42
1:C:53:ILE:C	1:C:53:ILE:CD1	2.84	0.42
1:A:69:ASN:C	1:A:69:ASN:HD22	2.22	0.42
1:C:124:ASN:HA	1:D:129:MET:O	2.20	0.42
1:A:198:LEU:HD23	1:A:198:LEU:C	2.39	0.41
1:D:135:LYS:HG3	1:D:149:GLY:O	2.20	0.41
1:B:59:LYS:HD3	1:B:80:ASP:HA	2.02	0.41
1:D:150:THR:CB	1:D:151:ASP:HA	2.44	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:149:GLY:HA2	1:D:150:THR:O	2.21	0.41
1:A:87:GLU:HG2	1:A:180:HIS:CD2	2.55	0.41
1:A:55:ASN:HD21	1:C:53:ILE:HD12	1.85	0.41
1:C:93:LEU:O	1:C:172:ARG:HA	2.21	0.41
1:D:93:LEU:O	1:D:172:ARG:HA	2.20	0.41
1:C:103:THR:O	1:C:199:ILE:HA	2.20	0.41
1:C:3:THR:O	1:C:215:SER:HA	2.21	0.41
1:D:15:THR:CG2	1:D:21:ASN:HD22	2.33	0.41
1:B:106:ILE:HB	1:B:154:LEU:HB3	2.02	0.40
1:D:89:VAL:HG22	1:D:181:ILE:HB	2.03	0.40
1:B:187:VAL:HG21	5:D:436:HOH:O	2.21	0.40
1:D:107:LEU:HD12	1:D:107:LEU:N	2.36	0.40
1:B:64:VAL:CG1	1:B:74:THR:HG22	2.25	0.40
1:A:23:PRO:HB2	1:A:40:TRP:O	2.22	0.40
1:B:111:PHE:HB3	1:B:128:PHE:CZ	2.56	0.40
1:C:129:MET:O	1:D:124:ASN:HA	2.20	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	230/237 (97%)	219 (95%)	9 (4%)	2 (1%)	17	8
1	B	230/237 (97%)	219 (95%)	8 (4%)	3 (1%)	12	4
1	C	232/237 (98%)	219 (94%)	11 (5%)	2 (1%)	17	8
1	D	230/237 (97%)	219 (95%)	9 (4%)	2 (1%)	17	8
All	All	922/948 (97%)	876 (95%)	37 (4%)	9 (1%)	15	6

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	151	ASP
1	B	204	SER
1	C	161	SER
1	C	203	ASP
1	D	203	ASP
1	B	203	ASP
1	A	202	PRO
1	D	151	ASP
1	A	118	ASN

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	199/202 (98%)	185 (93%)	14 (7%)	15	6
1	B	199/202 (98%)	185 (93%)	14 (7%)	15	6
1	C	199/202 (98%)	183 (92%)	16 (8%)	12	3
1	D	199/202 (98%)	176 (88%)	23 (12%)	5	1
All	All	796/808 (98%)	729 (92%)	67 (8%)	11	2

All (67) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	36	LYS
1	A	53	ILE
1	A	64	VAL
1	A	69	ASN
1	A	101	LYS
1	A	117	SER
1	A	118	ASN
1	A	124	ASN
1	A	134	SER
1	A	135	LYS
1	A	150	THR
1	A	192	ASP
1	A	220	SER

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Mol	Chain	Res	Type
1	A	232	LEU
1	B	64	VAL
1	B	81	LEU
1	B	99	LEU
1	B	101	LYS
1	B	107	LEU
1	B	117	SER
1	B	151	ASP
1	B	174	LEU
1	B	184	SER
1	B	192	ASP
1	B	194	THR
1	B	216	ASN
1	B	230	LEU
1	B	232	LEU
1	C	53	ILE
1	C	64	VAL
1	C	69	ASN
1	C	76	SER
1	C	101	LYS
1	C	117	SER
1	C	134	SER
1	C	151	ASP
1	C	160	SER
1	C	168	SER
1	C	183	GLU
1	C	185	SER
1	C	187	VAL
1	C	192	ASP
1	C	223	SER
1	C	232	LEU
1	D	56	SER
1	D	64	VAL
1	D	71	ASP
1	D	76	SER
1	D	81	LEU
1	D	101	LYS
1	D	117	SER
1	D	122	GLU
1	D	132	GLN
1	D	134	SER
1	D	135	LYS

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Mol	Chain	Res	Type
1	D	161	SER
1	D	164	SER
1	D	168	SER
1	D	174	LEU
1	D	183	GLU
1	D	185	SER
1	D	192	ASP
1	D	194	THR
1	D	208	ASP
1	D	223	SER
1	D	230	LEU
1	D	232	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	21	ASN
1	A	41	ASN
1	A	44	ASN
1	A	69	ASN
1	A	83	ASN
1	A	104	ASN
1	A	124	ASN
1	A	166	GLN
1	A	205	HIS
1	B	41	ASN
1	B	44	ASN
1	B	104	ASN
1	B	118	ASN
1	B	137	GLN
1	B	166	GLN
1	C	41	ASN
1	C	44	ASN
1	C	69	ASN
1	C	124	ASN
1	C	131	ASN
1	D	21	ASN
1	D	44	ASN
1	D	104	ASN
1	D	132	GLN
1	D	205	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

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	0.61	0	18,18,18	3.70	7 (38%)
2	MAN	E	2	2	11,11,12	0.71	0	15,15,17	1.36	2 (13%)
2	MMA	F	1	2	13,13,13	0.69	0	18,18,18	3.73	7 (38%)
2	MAN	F	2	2	11,11,12	0.82	0	15,15,17	1.53	2 (13%)
2	MMA	G	1	2	13,13,13	0.98	1 (7%)	18,18,18	1.39	2 (11%)
2	MAN	G	2	2	11,11,12	0.97	1 (9%)	15,15,17	1.16	2 (13%)
2	MMA	H	1	2	13,13,13	0.95	1 (7%)	18,18,18	1.27	3 (16%)
2	MAN	H	2	2	11,11,12	1.00	1 (9%)	15,15,17	1.26	2 (13%)

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	1/1/5/5	1/4/24/24	0/1/1/1
2	MAN	E	2	2	-	0/2/19/22	0/1/1/1
2	MMA	F	1	2	1/1/5/5	1/4/24/24	0/1/1/1
2	MAN	F	2	2	-	0/2/19/22	0/1/1/1
2	MMA	G	1	2	1/1/5/5	4/4/24/24	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	MAN	G	2	2	-	0/2/19/22	0/1/1/1
2	MMA	H	1	2	1/1/5/5	4/4/24/24	0/1/1/1
2	MAN	H	2	2	-	0/2/19/22	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	1	MMA	O1-C1	2.56	1.44	1.40
2	H	2	MAN	C2-C3	2.49	1.56	1.52
2	G	1	MMA	O1-C1	2.47	1.44	1.40
2	G	2	MAN	C2-C3	2.14	1.55	1.52

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	1	MMA	O1-C1-C2	10.10	119.98	108.15
2	E	1	MMA	O1-C1-C2	9.01	118.71	108.15
2	E	1	MMA	C1-O5-C5	-7.44	99.09	113.69
2	E	1	MMA	C1-C2-C3	-7.26	94.88	110.00
2	F	1	MMA	C1-C2-C3	-7.18	95.05	110.00
2	F	1	MMA	C1-O5-C5	-6.95	100.05	113.69
2	F	2	MAN	C1-O5-C5	4.04	117.67	112.19
2	G	1	MMA	O5-C5-C4	3.95	116.87	109.69
2	E	1	MMA	O6-C6-C5	-3.88	97.97	111.29
2	E	1	MMA	O5-C1-O1	3.35	118.75	110.97
2	E	2	MAN	C1-O5-C5	3.27	116.62	112.19
2	F	1	MMA	O2-C2-C1	3.20	117.82	110.05
2	E	1	MMA	O2-C2-C1	3.08	117.54	110.05
2	E	2	MAN	O2-C2-C1	-2.88	103.26	109.15
2	F	1	MMA	O2-C2-C3	-2.65	104.22	110.35
2	H	1	MMA	C3-C4-C5	2.60	114.87	110.24
2	F	1	MMA	O6-C6-C5	-2.57	102.48	111.29
2	H	2	MAN	O3-C3-C4	2.50	116.13	110.35
2	E	1	MMA	O5-C5-C6	2.50	112.65	106.44
2	H	1	MMA	O1-C1-C2	2.46	111.04	108.15
2	F	1	MMA	O5-C1-O1	2.42	116.58	110.97
2	H	2	MAN	C1-C2-C3	2.21	112.39	109.67
2	H	1	MMA	O5-C1-C2	-2.21	105.67	110.35
2	G	2	MAN	O3-C3-C4	2.12	115.26	110.35
2	F	2	MAN	O3-C3-C2	-2.11	105.95	109.99
2	G	2	MAN	O2-C2-C3	2.10	114.34	110.14
2	G	1	MMA	C1-O5-C5	2.07	117.75	113.69

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	G	1	MMA	C1
2	F	1	MMA	C1
2	E	1	MMA	C1
2	H	1	MMA	C1

All (10) torsion outliers are listed below:

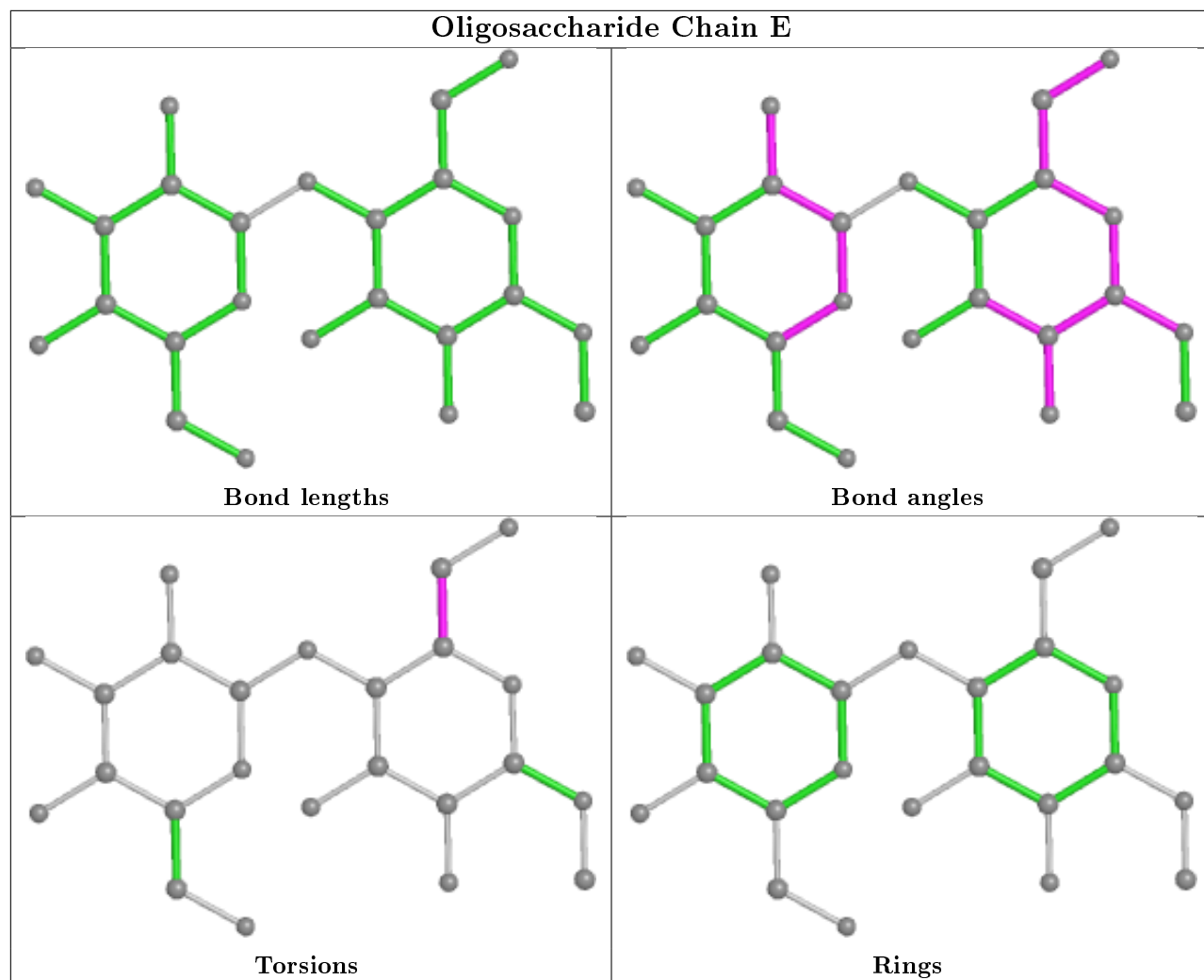
Mol	Chain	Res	Type	Atoms
2	G	1	MMA	O5-C1-O1-C7
2	H	1	MMA	O5-C1-O1-C7
2	G	1	MMA	C2-C1-O1-C7
2	H	1	MMA	C2-C1-O1-C7
2	G	1	MMA	C4-C5-C6-O6
2	H	1	MMA	C4-C5-C6-O6
2	G	1	MMA	O5-C5-C6-O6
2	H	1	MMA	O5-C5-C6-O6
2	F	1	MMA	C4-C5-C6-O6
2	E	1	MMA	C4-C5-C6-O6

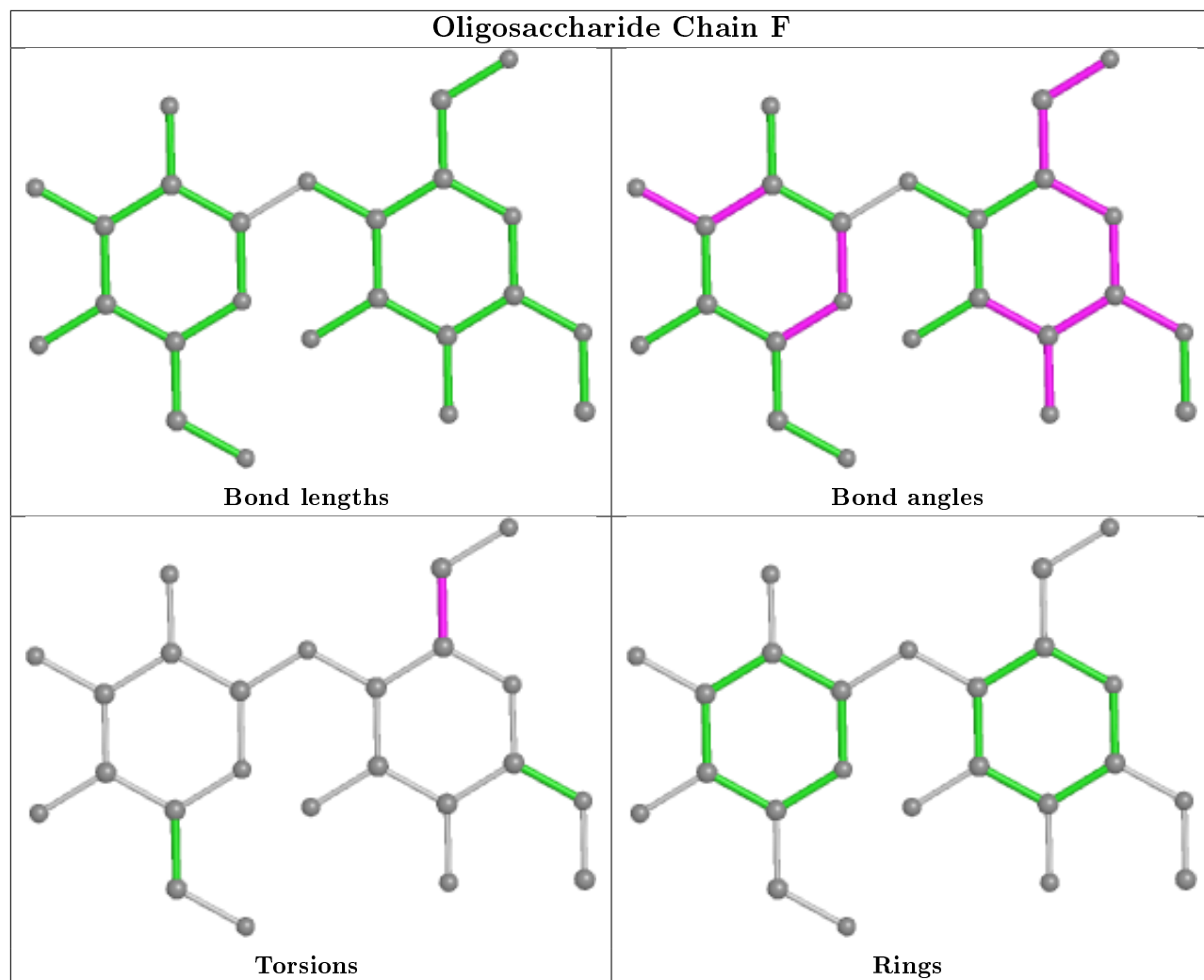
There are no ring outliers.

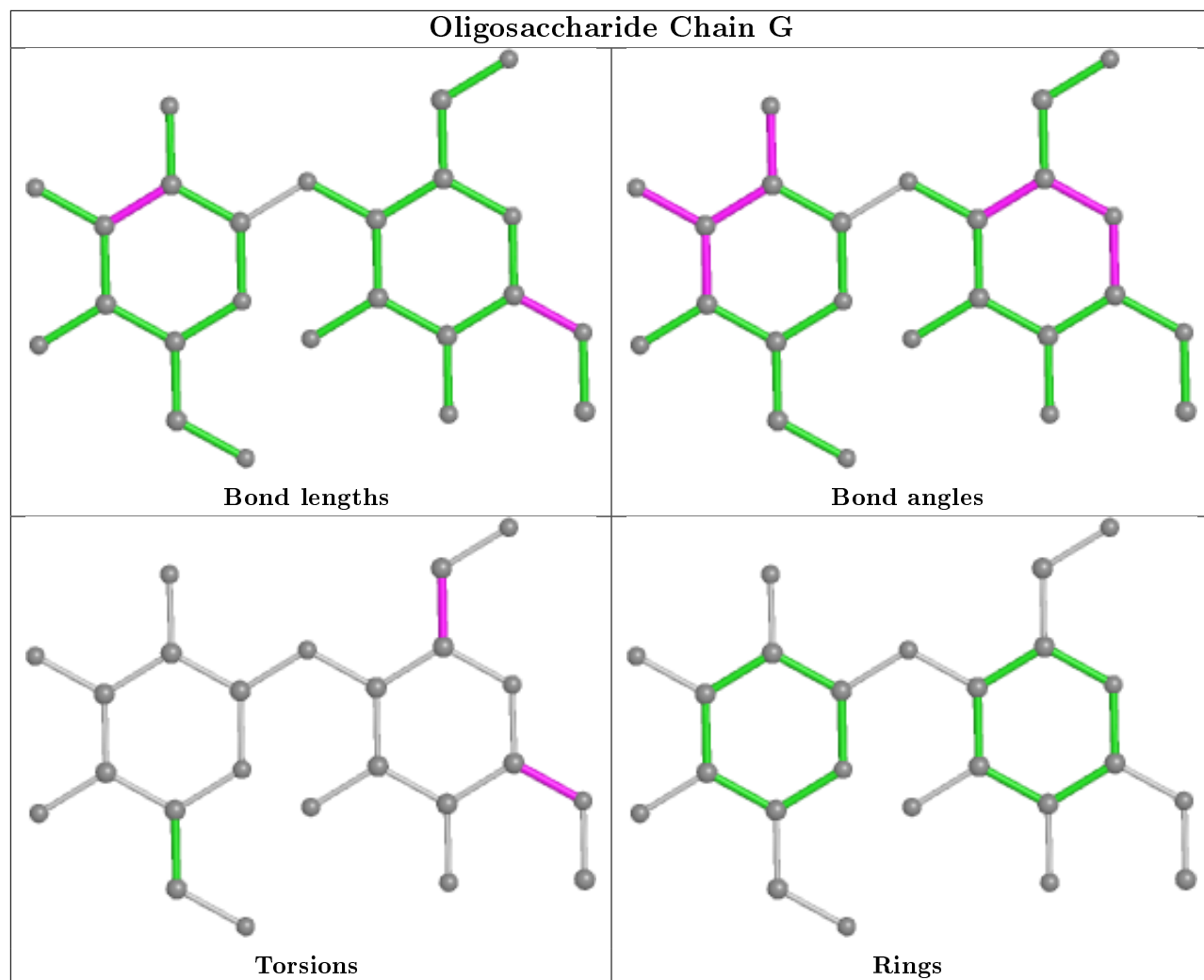
3 monomers are involved in 3 short contacts:

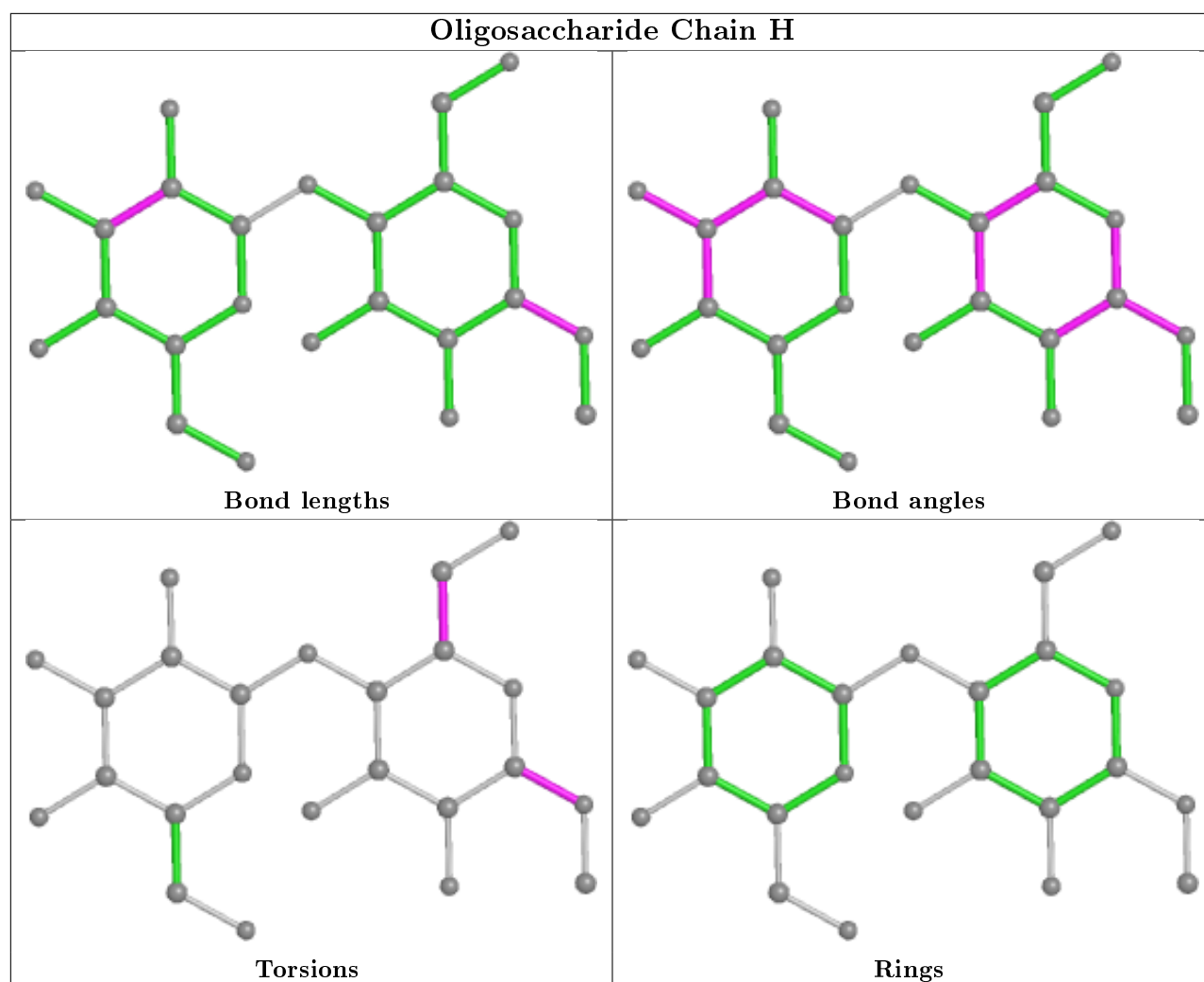
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	G	2	MAN	1	0
2	G	1	MMA	1	0
2	H	1	MMA	1	0

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









5.6 Ligand geometry [i](#)

Of 8 ligands modelled in this entry, 8 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 ⓘ

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, 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	234/237 (98%)	-0.41	2 (0%) 84 85	8, 14, 29, 46	6 (2%)
1	B	234/237 (98%)	-0.38	2 (0%) 84 85	9, 14, 28, 42	4 (1%)
1	C	234/237 (98%)	-0.15	3 (1%) 77 78	11, 20, 37, 45	6 (2%)
1	D	234/237 (98%)	-0.18	3 (1%) 77 78	9, 20, 36, 45	6 (2%)
All	All	936/948 (98%)	-0.28	10 (1%) 80 82	8, 17, 32, 46	22 (2%)

All (10) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	204	SER	5.9
1	B	149	GLY	3.3
1	D	1	ALA	2.9
1	A	204	SER	2.8
1	D	205	HIS	2.6
1	D	204	SER	2.3
1	C	1	ALA	2.2
1	A	150	THR	2.2
1	B	150	THR	2.1
1	C	161	SER	2.0

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

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

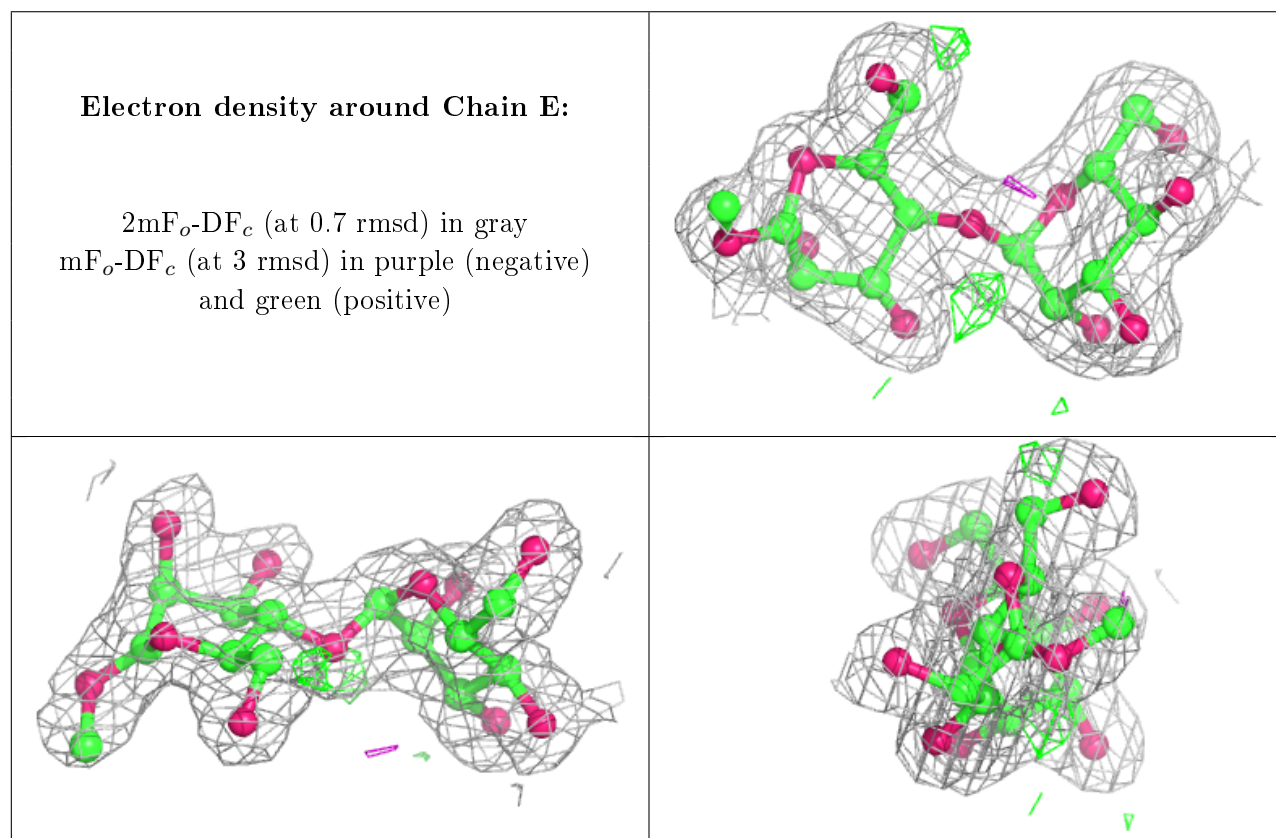
6.3 Carbohydrates [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,

median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists the number of atoms with occupancy less than 0.9.

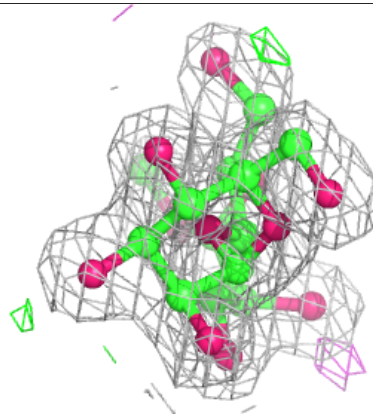
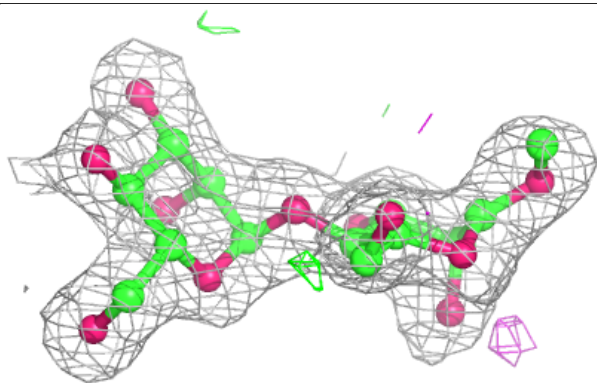
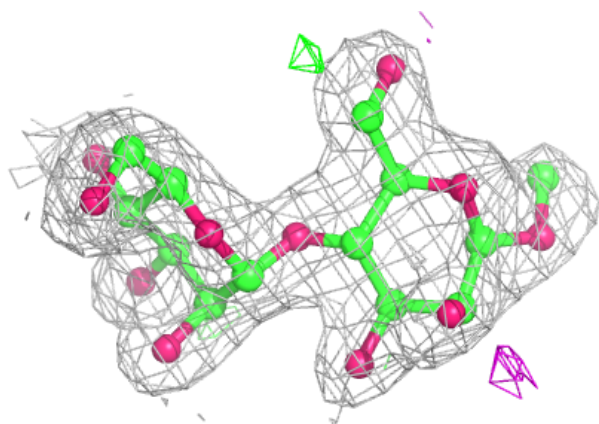
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	MMA	G	1	13/13	0.75	0.36	40,52,58,59	0
2	MMA	H	1	13/13	0.88	0.30	42,53,59,60	0
2	MAN	G	2	11/12	0.90	0.12	19,29,33,34	0
2	MAN	H	2	11/12	0.92	0.12	21,27,32,33	0
2	MMA	E	1	13/13	0.96	0.09	18,21,26,28	0
2	MMA	F	1	13/13	0.96	0.10	18,24,26,27	0
2	MAN	E	2	11/12	0.98	0.08	8,13,15,16	0
2	MAN	F	2	11/12	0.98	0.07	9,14,16,18	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.

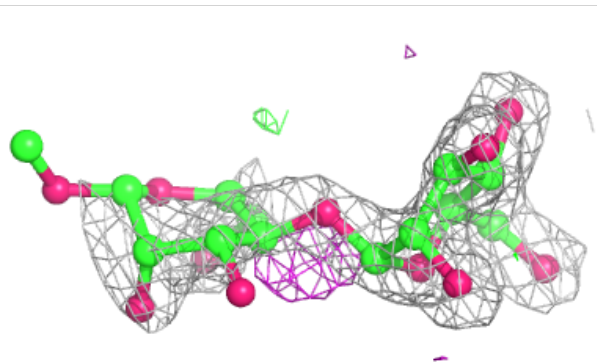
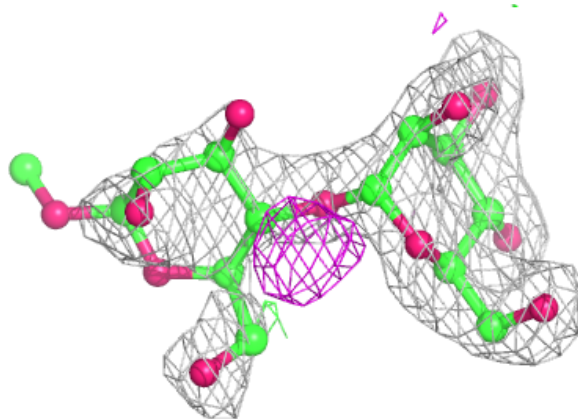


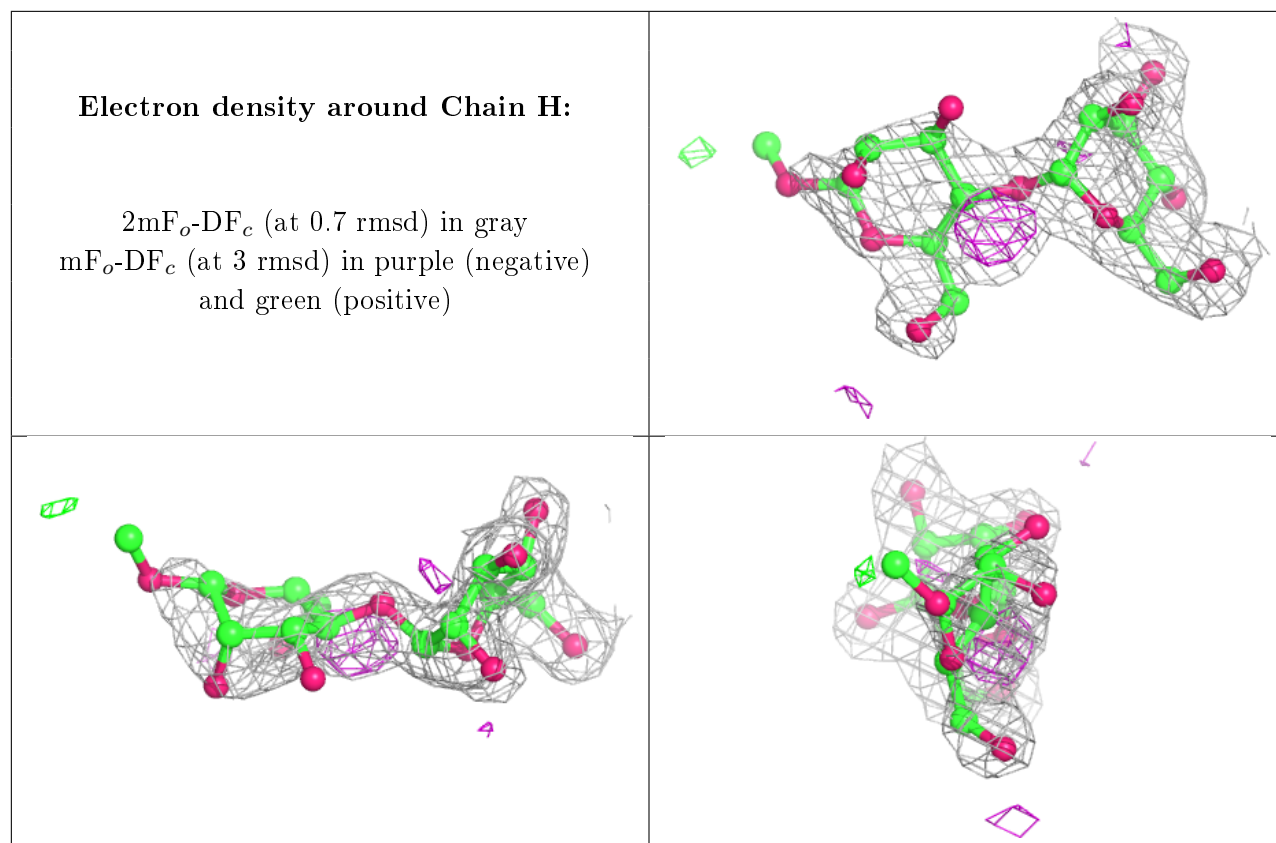
Electron density around Chain F:

$2mF_o - DF_c$ (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, 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(\AA^2)	Q<0.9
3	MN	A	301	1/1	0.99	0.08	16,16,16,16	0
4	CA	C	302	1/1	0.99	0.06	17,17,17,17	0
3	MN	B	301	1/1	0.99	0.08	16,16,16,16	0
3	MN	D	301	1/1	0.99	0.04	21,21,21,21	0
3	MN	C	301	1/1	0.99	0.04	21,21,21,21	0
4	CA	A	302	1/1	1.00	0.04	12,12,12,12	0
4	CA	B	302	1/1	1.00	0.06	11,11,11,11	0
4	CA	D	302	1/1	1.00	0.06	17,17,17,17	0

6.5 Other polymers [i](#)

There are no such residues in this entry.