



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 9, 2020 – 10:13 AM BST

PDB ID : 1PC8  
Title : Crystal Structure of a novel form of mistletoe lectin from Himalayan Viscum album L. at 3.8Å resolution  
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Deposited on : 2003-05-16  
Resolution : 3.80 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.

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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

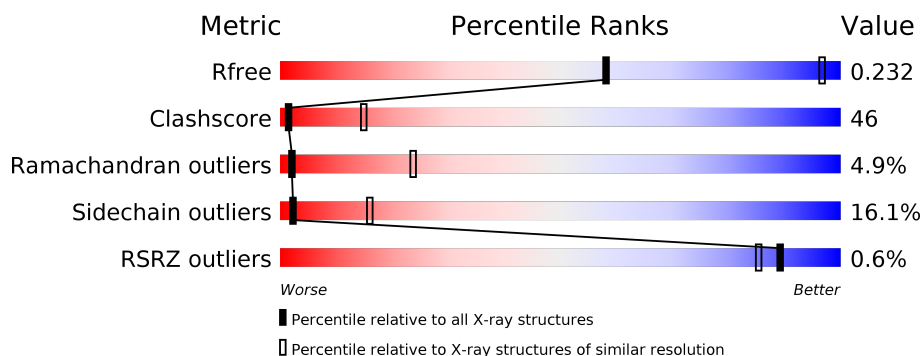
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.80 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	1212 (4.00-3.60)
Clashscore	141614	1288 (4.00-3.60)
Ramachandran outliers	138981	1243 (4.00-3.60)
Sidechain outliers	138945	1237 (4.00-3.60)
RSRZ outliers	127900	1121 (4.00-3.60)

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	240	<div> <div>37%</div> <div>50%</div> <div>11%</div> <div>.</div> </div>
2	B	255	<div> <div>%</div> <div>42%</div> <div>42%</div> <div>14%</div> <div>.</div> </div>
3	C	2	<div> <div>50%</div> <div>50%</div> </div>
3	E	2	<div> <div>50%</div> <div>50%</div> </div>
4	D	3	<div> <div>33%</div> <div>67%</div> </div>

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
3	NAG	C	1	X	-	-	-
3	NAG	C	2	-	-	-	X
3	NAG	E	1	-	-	-	X
3	NAG	E	2	-	-	-	X

## 2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 3935 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 Himalayan mistletoe ribosome-inactivating protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	240	Total	C	N	O	S	0	0	0
			1875	1191	319	361	4			

- Molecule 2 is a protein called Himalayan mistletoe ribosome-inactivating protein.

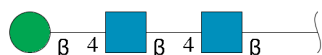
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	255	Total	C	N	O	S	0	0	0
			1938	1199	343	384	12			

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



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

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	D	3	Total	C	N	O	0	0	0
			39	22	2	15			

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula:  $C_8H_{15}NO_6$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O	0	0
			14	8	1	5		

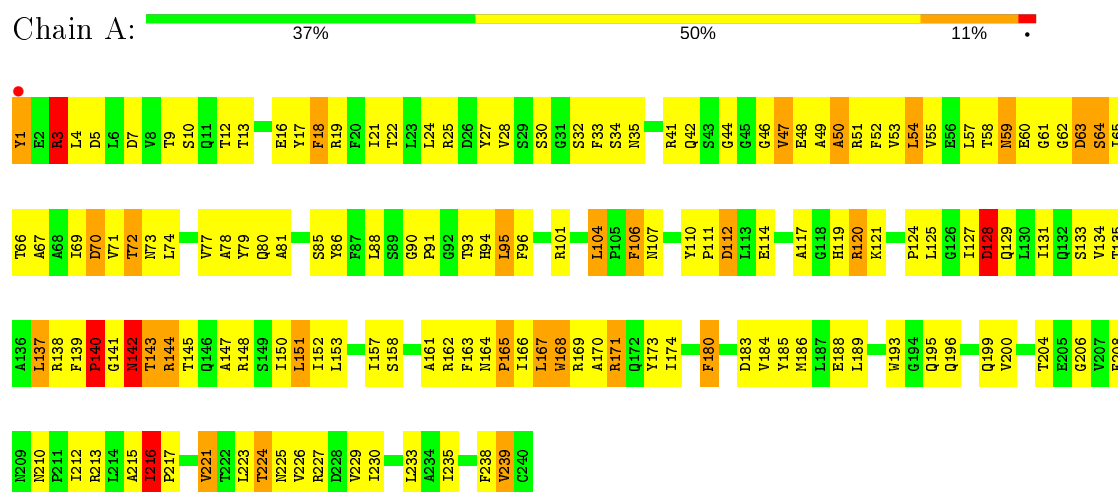
- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	8	Total O	0	0
			8 8		
6	B	5	Total O	0	0
			5 5		

### 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: Himalayan mistletoe ribosome-inactivating protein



- Molecule 2: Himalayan mistletoe ribosome-inactivating protein



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





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

Chain E:



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

Chain D:



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 65 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	109.18Å 109.18Å 309.44Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	20.00 – 3.80 32.44 – 3.80	Depositor EDS
% Data completeness (in resolution range)	100.0 (20.00-3.80) 99.6 (32.44-3.80)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.18	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.03 (at 3.75Å)	Xtriage
Refinement program	REFMAC 5.0	Depositor
R, $R_{free}$	0.228 , 0.271 0.222 , 0.232	Depositor DCC
$R_{free}$ test set	584 reflections (5.11%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	68.5	Xtriage
Anisotropy	0.189	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 77.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.88	EDS
Total number of atoms	3935	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	62.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.61% 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: BMA, NAG

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	A	1.08	1/1913 (0.1%)	1.10	11/2602 (0.4%)
2	B	1.22	2/1978 (0.1%)	1.20	21/2697 (0.8%)
All	All	1.15	3/3891 (0.1%)	1.15	32/5299 (0.6%)

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
2	B	0	1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	44	GLN	N-CA	7.79	1.61	1.46
2	B	57	ASN	C-N	6.74	1.45	1.33
1	A	221	VAL	CB-CG2	-5.11	1.42	1.52

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	39	ASN	CB-CA-C	-12.72	84.97	110.40
2	B	21	ARG	NE-CZ-NH1	-11.22	114.69	120.30
2	B	44	GLN	N-CA-C	9.38	136.32	111.00
2	B	57	ASN	CA-C-N	-8.46	99.28	116.20
2	B	21	ARG	NE-CZ-NH2	8.38	124.49	120.30
2	B	57	ASN	O-C-N	7.70	136.29	123.20
2	B	167	ASP	CB-CG-OD2	7.68	125.21	118.30
1	A	142	ASN	CB-CA-C	7.65	125.70	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	3	ARG	NE-CZ-NH2	-7.53	116.53	120.30
1	A	140	PRO	N-CA-C	7.49	131.56	112.10
2	B	24	ASP	CB-CG-OD2	7.45	125.00	118.30
1	A	3	ARG	NE-CZ-NH1	7.30	123.95	120.30
2	B	19	ASP	CB-CG-OD2	7.30	124.87	118.30
2	B	44	GLN	N-CA-CB	-7.14	97.74	110.60
1	A	7	ASP	CB-CG-OD2	7.02	124.62	118.30
2	B	22	ASP	CB-CG-OD2	6.79	124.42	118.30
1	A	63	ASP	CB-CG-OD2	6.69	124.32	118.30
1	A	5	ASP	CB-CG-OD2	6.61	124.25	118.30
1	A	70	ASP	CB-CG-OD2	6.60	124.24	118.30
1	A	128	ASP	CB-CG-OD2	6.36	124.02	118.30
1	A	112	ASP	CB-CG-OD2	6.36	124.02	118.30
2	B	192	ASP	CB-CG-OD2	6.15	123.83	118.30
2	B	146	ASP	CB-CG-OD2	6.13	123.82	118.30
2	B	40	ASN	N-CA-C	6.00	127.19	111.00
2	B	13	ARG	CA-C-N	-5.88	104.27	117.20
2	B	184	ASP	CB-CG-OD2	5.74	123.47	118.30
1	A	3	ARG	CG-CD-NE	-5.55	100.14	111.80
2	B	13	ARG	NE-CZ-NH1	5.51	123.06	120.30
2	B	121	ASP	CB-CG-OD2	5.46	123.22	118.30
2	B	229	ASP	CB-CG-OD2	5.43	123.19	118.30
2	B	21	ARG	CG-CD-NE	5.22	122.77	111.80
2	B	165	GLN	O-C-N	-5.09	114.56	122.70

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	39	ASN	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	1875	0	1850	195	0
2	B	1938	0	1851	164	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	28	0	25	1	0
3	E	28	0	25	2	0
4	D	39	0	34	5	0
5	A	14	0	13	0	0
6	A	8	0	0	1	0
6	B	5	0	0	0	0
All	All	3935	0	3798	358	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 46.

All (358) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:216:ILE:CG2	1:A:217:PRO:HD2	1.51	1.40
1:A:216:ILE:HG22	1:A:217:PRO:CD	1.56	1.35
1:A:52:PHE:CD2	1:A:95:LEU:HD11	1.79	1.18
1:A:216:ILE:HD11	1:A:221:VAL:CG2	1.74	1.16
2:B:189:SER:HB2	2:B:240:ILE:HD11	1.25	1.13
1:A:93:THR:HG22	1:A:94:HIS:H	1.13	1.09
1:A:70:ASP:OD1	1:A:72:THR:HG23	1.53	1.08
1:A:139:PHE:HB3	1:A:140:PRO:HD2	1.38	1.04
2:B:198:ASN:N	2:B:198:ASN:HD22	1.51	1.04
1:A:225:ASN:HD22	1:A:227:ARG:H	1.04	0.99
1:A:25:ARG:HG3	1:A:235:ILE:HD11	1.43	0.99
1:A:86:TYR:HB3	1:A:104:LEU:HD21	1.45	0.98
2:B:224:ASN:HD22	2:B:225:GLY:N	1.61	0.98
1:A:59:ASN:OD1	1:A:63:ASP:HB2	1.64	0.98
2:B:198:ASN:H	2:B:198:ASN:ND2	1.59	0.98
1:A:48:GLU:HG2	1:A:49:ALA:H	1.28	0.97
2:B:121:ASP:OD1	2:B:123:THR:HG23	1.63	0.97
2:B:20:VAL:HG21	2:B:74:ILE:HD12	1.44	0.97
1:A:52:PHE:CE2	1:A:95:LEU:HD11	2.02	0.95
1:A:215:ALA:O	1:A:216:ILE:HG12	1.68	0.92
1:A:215:ALA:C	1:A:216:ILE:HG12	1.90	0.91
2:B:194:VAL:HG12	2:B:194:VAL:O	1.70	0.90
1:A:110:TYR:HB3	1:A:111:PRO:HD3	1.55	0.88
1:A:93:THR:CG2	1:A:94:HIS:H	1.81	0.88
2:B:226:LEU:HD12	2:B:226:LEU:N	1.89	0.88
2:B:224:ASN:HD22	2:B:225:GLY:H	1.22	0.88
2:B:195:ALA:HA	2:B:239:ILE:HG23	1.57	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:216:ILE:HD11	1:A:221:VAL:HG23	1.55	0.86
2:B:121:ASP:H	2:B:126:GLN:HE22	0.91	0.86
1:A:225:ASN:ND2	1:A:227:ARG:H	1.73	0.86
2:B:166:ASN:N	2:B:166:ASN:HD22	1.74	0.85
2:B:189:SER:CB	2:B:240:ILE:HD11	2.06	0.85
1:A:94:HIS:O	1:A:95:LEU:HB2	1.75	0.84
2:B:121:ASP:H	2:B:126:GLN:NE2	1.76	0.83
1:A:141:GLY:O	1:A:142:ASN:HB3	1.81	0.81
1:A:32:SER:C	1:A:33:PHE:HD1	1.84	0.81
1:A:216:ILE:HD11	1:A:221:VAL:HG21	1.62	0.81
2:B:244:THR:HG23	2:B:246:LYS:H	1.44	0.79
2:B:21:ARG:HD3	2:B:32:GLN:NE2	1.97	0.79
4:D:2:NAG:H3	4:D:2:NAG:H83	1.65	0.78
2:B:166:ASN:HD22	2:B:166:ASN:H	1.30	0.78
1:A:93:THR:HG22	1:A:94:HIS:N	1.97	0.76
1:A:52:PHE:CE2	1:A:95:LEU:CD1	2.68	0.76
2:B:121:ASP:N	2:B:126:GLN:HE22	1.76	0.75
1:A:139:PHE:CB	1:A:140:PRO:HD2	2.11	0.75
1:A:110:TYR:O	1:A:114:GLU:HG2	1.86	0.75
1:A:61:GLY:O	1:A:63:ASP:N	2.20	0.75
2:B:117:VAL:HG23	2:B:117:VAL:O	1.88	0.74
1:A:27:TYR:O	1:A:27:TYR:CD1	2.40	0.73
2:B:139:VAL:HG12	2:B:255:PRO:HA	1.71	0.73
2:B:5:GLU:OE2	2:B:49:LYS:HD3	1.89	0.72
2:B:224:ASN:HB2	2:B:226:LEU:HD13	1.70	0.72
2:B:92:ASN:N	2:B:92:ASN:OD1	2.19	0.72
2:B:98:PRO:O	2:B:99:ARG:C	2.28	0.72
1:A:212:ILE:HB	1:A:223:LEU:HD12	1.71	0.72
1:A:65:ILE:HD11	1:A:137:LEU:HB3	1.70	0.71
1:A:138:ARG:HG3	1:A:139:PHE:CE1	2.26	0.71
1:A:180:PHE:HD1	1:A:180:PHE:H	1.37	0.71
1:A:94:HIS:O	1:A:95:LEU:CB	2.37	0.71
2:B:221:ASN:HB3	2:B:224:ASN:HD21	1.56	0.70
2:B:76:ASP:OD1	2:B:76:ASP:C	2.29	0.70
2:B:57:ASN:C	2:B:57:ASN:OD1	2.30	0.70
2:B:31:ILE:HD13	2:B:61:LEU:HD12	1.74	0.70
2:B:100:SER:OG	2:B:102:LEU:HG	1.91	0.69
1:A:188:GLU:OE1	1:A:215:ALA:N	2.22	0.69
1:A:59:ASN:HD21	1:A:63:ASP:N	1.90	0.69
2:B:231:ALA:O	2:B:232:ASN:HB2	1.93	0.69
2:B:76:ASP:OD1	2:B:78:ASN:N	2.26	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:117:ALA:HB2	1:A:147:ALA:HB1	1.73	0.68
1:A:158:SER:O	1:A:161:ALA:HB3	1.93	0.68
2:B:67:THR:O	2:B:70:VAL:HG22	1.93	0.68
2:B:3:ALA:O	2:B:4:SER:HB2	1.94	0.68
2:B:241:TYR:CG	2:B:242:PRO:HD2	2.29	0.68
1:A:53:VAL:HG12	1:A:69:ILE:HB	1.77	0.67
2:B:8:VAL:HG12	2:B:9:ARG:N	2.09	0.67
2:B:90:TRP:CH2	2:B:96:ILE:HD12	2.29	0.67
1:A:164:ASN:O	1:A:168:TRP:HB2	1.94	0.66
1:A:77:VAL:O	1:A:88:LEU:HG	1.95	0.66
2:B:226:LEU:CD1	2:B:226:LEU:N	2.57	0.66
1:A:104:LEU:HD22	1:A:104:LEU:N	2.10	0.66
2:B:198:ASN:N	2:B:198:ASN:ND2	2.22	0.66
2:B:57:ASN:O	2:B:57:ASN:OD1	2.15	0.65
1:A:34:SER:O	1:A:35:ASN:HB2	1.97	0.65
2:B:193:SER:O	2:B:194:VAL:HG23	1.96	0.65
2:B:8:VAL:HG12	2:B:9:ARG:O	1.96	0.65
1:A:19:ARG:O	1:A:22:THR:HB	1.95	0.65
2:B:20:VAL:CG2	2:B:74:ILE:HD12	2.22	0.65
2:B:198:ASN:H	2:B:198:ASN:HD22	0.75	0.64
1:A:120:ARG:H	1:A:120:ARG:HD3	1.61	0.64
2:B:124:LEU:HD12	2:B:205:GLY:HA2	1.79	0.64
1:A:158:SER:O	1:A:161:ALA:N	2.30	0.64
1:A:33:PHE:CD1	1:A:33:PHE:N	2.62	0.64
1:A:33:PHE:HD1	1:A:33:PHE:N	1.96	0.64
1:A:79:TYR:CZ	1:A:137:LEU:HD22	2.32	0.64
1:A:48:GLU:HG2	1:A:49:ALA:N	2.08	0.64
1:A:95:LEU:O	1:A:96:PHE:CD1	2.50	0.64
1:A:21:ILE:HG21	1:A:167:LEU:HD23	1.80	0.64
2:B:101:ASN:O	2:B:102:LEU:HD23	1.98	0.64
1:A:216:ILE:CB	1:A:217:PRO:HD2	2.24	0.63
4:D:1:NAG:O3	4:D:2:NAG:N2	2.32	0.63
1:A:208:PHE:HB2	1:A:224:THR:O	1.98	0.63
1:A:59:ASN:HB3	1:A:134:VAL:HG21	1.81	0.63
2:B:96:ILE:HG22	2:B:97:ASN:N	2.13	0.63
2:B:121:ASP:C	2:B:121:ASP:OD1	2.37	0.63
2:B:224:ASN:CB	2:B:226:LEU:HD13	2.28	0.63
1:A:141:GLY:O	1:A:142:ASN:CB	2.45	0.63
1:A:18:PHE:HD1	1:A:171:ARG:CZ	2.11	0.63
1:A:110:TYR:CB	1:A:111:PRO:HD3	2.29	0.62
2:B:244:THR:HG22	2:B:249:GLN:CD	2.20	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:162:ARG:HD3	1:A:193:TRP:CE2	2.34	0.62
1:A:12:THR:OG1	1:A:13:THR:N	2.31	0.61
2:B:166:ASN:ND2	2:B:166:ASN:H	1.98	0.61
2:B:51:ASP:OD1	2:B:52:GLY:N	2.33	0.61
1:A:125:LEU:HB2	1:A:180:PHE:CE1	2.36	0.61
1:A:225:ASN:HD22	1:A:227:ARG:N	1.87	0.61
1:A:49:ALA:O	1:A:51:ARG:N	2.32	0.61
1:A:58:THR:HG23	1:A:64:SER:OG	2.00	0.61
1:A:165:PRO:O	1:A:166:ILE:C	2.38	0.61
1:A:215:ALA:C	1:A:216:ILE:CG1	2.68	0.61
2:B:34:TRP:CG	2:B:35:PRO:HD2	2.35	0.60
1:A:58:THR:HG23	1:A:64:SER:CB	2.32	0.60
1:A:46:GLY:HA3	1:A:51:ARG:HH11	1.67	0.60
2:B:193:SER:O	2:B:194:VAL:CG2	2.49	0.60
1:A:85:SER:C	1:A:86:TYR:CD1	2.75	0.60
2:B:120:LEU:HD12	2:B:121:ASP:N	2.17	0.60
2:B:224:ASN:HB2	2:B:226:LEU:CD1	2.32	0.60
1:A:55:VAL:CG1	1:A:67:ALA:HB3	2.32	0.59
2:B:26:HIS:O	2:B:27:ASP:C	2.39	0.59
1:A:17:TYR:CZ	1:A:21:ILE:HD11	2.38	0.59
1:A:199:GLN:OE1	1:A:210:ASN:HB2	2.03	0.59
2:B:129:LEU:C	2:B:129:LEU:CD1	2.71	0.59
2:B:241:TYR:CD2	2:B:242:PRO:HD2	2.38	0.58
2:B:157:TRP:HZ3	2:B:237:GLN:HG2	1.68	0.58
2:B:21:ARG:HH21	2:B:32:GLN:HE21	1.52	0.58
1:A:49:ALA:C	1:A:51:ARG:H	2.07	0.58
2:B:221:ASN:HD22	2:B:221:ASN:C	2.07	0.58
2:B:172:TYR:HB3	2:B:174:ASP:OD1	2.03	0.58
2:B:189:SER:HB2	2:B:240:ILE:CD1	2.17	0.58
2:B:11:VAL:HG12	2:B:12:GLY:N	2.18	0.58
2:B:96:ILE:CG2	2:B:97:ASN:N	2.66	0.58
1:A:27:TYR:C	1:A:27:TYR:CD1	2.77	0.58
1:A:52:PHE:CD2	1:A:95:LEU:CD1	2.71	0.58
1:A:4:LEU:HD23	1:A:54:LEU:HB3	1.86	0.57
1:A:59:ASN:HD21	1:A:63:ASP:H	1.50	0.57
2:B:34:TRP:CG	2:B:35:PRO:CD	2.86	0.57
1:A:226:VAL:O	1:A:230:ILE:HG13	2.04	0.57
2:B:194:VAL:CG1	2:B:194:VAL:O	2.45	0.57
2:B:98:PRO:O	2:B:100:SER:N	2.38	0.57
2:B:224:ASN:CG	2:B:226:LEU:HD13	2.25	0.57
2:B:225:GLY:C	2:B:226:LEU:HD12	2.24	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:34:TRP:CD1	2:B:35:PRO:HD2	2.39	0.57
2:B:221:ASN:ND2	2:B:221:ASN:C	2.58	0.57
1:A:55:VAL:HG13	1:A:67:ALA:HB3	1.86	0.56
2:B:121:ASP:CG	2:B:123:THR:HG23	2.25	0.56
1:A:65:ILE:CD1	1:A:137:LEU:HB3	2.35	0.56
1:A:117:ALA:HB2	1:A:147:ALA:CB	2.35	0.56
1:A:142:ASN:O	1:A:145:THR:N	2.38	0.56
1:A:163:PHE:CE1	1:A:189:LEU:HB3	2.40	0.56
1:A:1:TYR:HE2	1:A:4:LEU:HG	1.71	0.56
2:B:12:GLY:O	2:B:15:GLY:N	2.30	0.55
1:A:10:SER:HA	1:A:131:ILE:HD11	1.88	0.55
2:B:67:THR:O	2:B:68:ALA:C	2.45	0.55
1:A:148:ARG:O	1:A:151:LEU:HB3	2.07	0.55
1:A:133:SER:O	1:A:137:LEU:HB2	2.06	0.55
1:A:46:GLY:HA3	1:A:51:ARG:NH1	2.22	0.55
2:B:197:ILE:HD12	2:B:238:ILE:HG22	1.88	0.55
1:A:79:TYR:CE1	1:A:86:TYR:HB2	2.42	0.55
1:A:138:ARG:O	1:A:139:PHE:CD1	2.60	0.55
1:A:52:PHE:CG	1:A:95:LEU:HD11	2.36	0.54
2:B:76:ASP:OD1	2:B:77:CYS:N	2.40	0.54
2:B:229:ASP:OD1	2:B:230:VAL:N	2.41	0.54
2:B:42:PRO:HG2	3:E:1:NAG:O7	2.08	0.54
1:A:170:ALA:O	1:A:173:TYR:N	2.40	0.54
2:B:56:SER:O	2:B:57:ASN:HB3	2.06	0.54
1:A:142:ASN:O	1:A:143:THR:C	2.45	0.54
1:A:238:PHE:CD1	1:A:239:VAL:N	2.76	0.54
2:B:197:ILE:CD1	2:B:238:ILE:HG22	2.38	0.54
2:B:20:VAL:O	2:B:20:VAL:HG22	2.08	0.54
2:B:11:VAL:CG1	2:B:12:GLY:N	2.72	0.53
2:B:158:VAL:HG23	2:B:158:VAL:O	2.07	0.53
1:A:106:PHE:HB2	1:A:112:ASP:OD2	2.08	0.53
1:A:18:PHE:O	1:A:19:ARG:C	2.46	0.53
1:A:204:THR:HG21	2:B:6:PRO:HD3	1.90	0.53
2:B:181:GLN:HA	2:B:181:GLN:OE1	2.08	0.53
2:B:45:LEU:CD1	2:B:45:LEU:N	2.71	0.53
1:A:129:GLN:HB3	1:A:152:ILE:HD13	1.90	0.53
1:A:53:VAL:CG1	1:A:69:ILE:HB	2.39	0.53
1:A:199:GLN:HE21	1:A:199:GLN:HA	1.75	0.52
2:B:129:LEU:HD13	2:B:129:LEU:C	2.29	0.52
2:B:20:VAL:HB	2:B:74:ILE:HD11	1.91	0.52
1:A:162:ARG:HB2	1:A:163:PHE:CD2	2.44	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:46:GLY:HA2	1:A:48:GLU:OE1	2.10	0.52
1:A:77:VAL:HG23	1:A:78:ALA:N	2.25	0.52
1:A:65:ILE:HG22	1:A:66:THR:N	2.25	0.51
2:B:14:ASN:HD22	2:B:178:ARG:HH22	1.58	0.51
1:A:199:GLN:NE2	1:A:199:GLN:HA	2.26	0.51
1:A:164:ASN:N	1:A:165:PRO:CD	2.73	0.51
2:B:30:GLN:NE2	2:B:114:THR:HG21	2.26	0.51
2:B:117:VAL:CG2	2:B:117:VAL:O	2.57	0.51
1:A:124:PRO:O	1:A:129:GLN:HG2	2.11	0.51
1:A:157:ILE:HG22	1:A:158:SER:N	2.25	0.51
2:B:148:CYS:O	2:B:158:VAL:HA	2.10	0.51
2:B:20:VAL:HG13	2:B:43:ASN:CB	2.41	0.51
1:A:104:LEU:H	1:A:104:LEU:HD22	1.76	0.51
1:A:59:ASN:C	1:A:59:ASN:HD22	2.14	0.51
2:B:44:GLN:C	2:B:45:LEU:HD12	2.31	0.51
1:A:106:PHE:CA	1:A:112:ASP:OD2	2.60	0.50
1:A:48:GLU:CG	1:A:49:ALA:H	2.07	0.50
2:B:211:TRP:CZ3	2:B:221:ASN:HB2	2.46	0.50
1:A:227:ARG:HH22	2:B:93:GLY:HA2	1.76	0.50
2:B:174:ASP:OD1	2:B:176:SER:OG	2.29	0.50
1:A:104:LEU:CD2	1:A:104:LEU:N	2.74	0.50
1:A:106:PHE:CB	1:A:112:ASP:OD2	2.60	0.50
1:A:17:TYR:CD2	1:A:174:ILE:HD12	2.45	0.50
2:B:42:PRO:CG	3:E:1:NAG:O7	2.60	0.50
1:A:143:THR:O	1:A:144:ARG:C	2.48	0.49
1:A:184:VAL:O	1:A:185:TYR:C	2.50	0.49
2:B:29:ASN:O	2:B:73:MET:HB2	2.12	0.49
1:A:104:LEU:H	1:A:104:LEU:CD2	2.26	0.49
1:A:188:GLU:OE1	1:A:215:ALA:HB3	2.13	0.49
2:B:185:GLN:HB3	2:B:199:ILE:CG2	2.42	0.49
1:A:79:TYR:CZ	1:A:137:LEU:CD2	2.95	0.49
1:A:13:THR:HG23	1:A:16:GLU:OE2	2.12	0.49
2:B:189:SER:O	2:B:189:SER:OG	2.19	0.49
2:B:20:VAL:CG1	2:B:43:ASN:HA	2.43	0.49
1:A:79:TYR:CE2	1:A:137:LEU:HD22	2.48	0.48
1:A:142:ASN:O	1:A:145:THR:HG22	2.13	0.48
2:B:115:LEU:HD22	2:B:115:LEU:N	2.28	0.48
2:B:124:LEU:CD1	2:B:205:GLY:HA2	2.42	0.48
1:A:150:ILE:O	1:A:153:LEU:HB2	2.14	0.48
1:A:195:GLN:O	1:A:196:GLN:C	2.52	0.48
1:A:58:THR:HG23	1:A:64:SER:HB2	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:7:THR:C	2:B:8:VAL:HG23	2.33	0.48
1:A:1:TYR:CE2	1:A:4:LEU:HG	2.48	0.48
1:A:124:PRO:O	1:A:125:LEU:HD23	2.14	0.48
1:A:128:ASP:O	1:A:131:ILE:N	2.47	0.48
1:A:51:ARG:HD2	1:A:51:ARG:O	2.13	0.48
1:A:158:SER:O	1:A:161:ALA:CB	2.62	0.48
1:A:9:THR:O	1:A:9:THR:HG23	2.14	0.48
2:B:75:PHE:CD1	2:B:76:ASP:N	2.82	0.48
1:A:106:PHE:HA	1:A:112:ASP:OD2	2.14	0.47
1:A:25:ARG:HG3	1:A:235:ILE:CD1	2.30	0.47
1:A:226:VAL:HG12	1:A:226:VAL:O	2.14	0.47
1:A:57:LEU:HD12	1:A:57:LEU:N	2.29	0.47
2:B:88:GLN:HE21	2:B:98:PRO:HG3	1.79	0.47
2:B:8:VAL:CG1	2:B:9:ARG:N	2.76	0.47
1:A:127:ILE:O	1:A:128:ASP:C	2.53	0.47
1:A:238:PHE:CD1	1:A:238:PHE:C	2.88	0.47
1:A:238:PHE:HD1	1:A:239:VAL:N	2.12	0.47
1:A:151:LEU:HD13	1:A:151:LEU:C	2.35	0.47
1:A:167:LEU:O	1:A:168:TRP:C	2.53	0.47
2:B:226:LEU:HB2	2:B:240:ILE:CG2	2.45	0.47
2:B:241:TYR:CD2	2:B:242:PRO:CD	2.97	0.47
2:B:29:ASN:HD22	2:B:30:GLN:H	1.61	0.47
1:A:88:LEU:N	1:A:88:LEU:HD23	2.29	0.47
2:B:16:MET:CE	2:B:35:PRO:HG3	2.44	0.46
2:B:29:ASN:ND2	2:B:30:GLN:H	2.12	0.46
2:B:90:TRP:CZ2	2:B:96:ILE:HD12	2.50	0.46
1:A:81:ALA:HB1	1:A:138:ARG:HD2	1.97	0.46
1:A:165:PRO:O	1:A:167:LEU:N	2.48	0.46
1:A:3:ARG:CZ	6:A:1010:HOH:O	2.64	0.46
1:A:78:ALA:HB1	1:A:86:TYR:O	2.15	0.46
2:B:34:TRP:CD2	2:B:35:PRO:HD2	2.50	0.46
1:A:10:SER:H	1:A:12:THR:CG2	2.29	0.46
1:A:85:SER:O	1:A:86:TYR:CD1	2.68	0.46
2:B:241:TYR:CD2	2:B:242:PRO:HG2	2.51	0.46
2:B:90:TRP:CH2	2:B:96:ILE:CD1	2.98	0.46
1:A:21:ILE:HD12	1:A:167:LEU:HD22	1.98	0.46
2:B:119:THR:O	2:B:120:LEU:C	2.50	0.46
1:A:61:GLY:C	1:A:63:ASP:H	2.17	0.46
2:B:57:ASN:C	2:B:59:SER:H	2.19	0.46
2:B:46:TRP:N	2:B:46:TRP:CD1	2.83	0.45
2:B:202:CYS:C	2:B:204:GLY:N	2.69	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:216:ILE:HG22	1:A:217:PRO:HD2	0.64	0.45
2:B:129:LEU:HD13	2:B:130:ALA:N	2.32	0.45
2:B:239:ILE:HG22	2:B:240:ILE:N	2.32	0.45
2:B:224:ASN:ND2	2:B:225:GLY:H	2.02	0.45
2:B:250:MET:C	2:B:251:TRP:CD1	2.89	0.45
1:A:199:GLN:CA	1:A:199:GLN:HE21	2.28	0.45
2:B:244:THR:HG22	2:B:249:GLN:NE2	2.31	0.45
2:B:3:ALA:O	2:B:4:SER:CB	2.65	0.45
1:A:119:HIS:ND1	1:A:121:LYS:HE2	2.31	0.45
1:A:10:SER:HB2	1:A:60:GLU:HG2	1.99	0.45
1:A:107:ASN:N	1:A:112:ASP:OD2	2.44	0.45
1:A:124:PRO:C	1:A:125:LEU:HD23	2.37	0.45
1:A:170:ALA:O	1:A:171:ARG:C	2.54	0.45
2:B:101:ASN:C	2:B:102:LEU:HD23	2.37	0.45
2:B:188:THR:CG2	2:B:189:SER:N	2.78	0.45
2:B:81:VAL:O	2:B:82:ARG:C	2.55	0.45
1:A:230:ILE:O	1:A:230:ILE:HG22	2.17	0.45
1:A:142:ASN:C	1:A:144:ARG:N	2.68	0.44
1:A:24:LEU:O	1:A:28:VAL:HG22	2.17	0.44
1:A:150:ILE:O	1:A:153:LEU:N	2.50	0.44
2:B:185:GLN:C	2:B:202:CYS:SG	2.96	0.44
1:A:133:SER:O	1:A:134:VAL:C	2.54	0.44
2:B:124:LEU:O	2:B:125:GLY:C	2.54	0.44
1:A:21:ILE:HG21	1:A:167:LEU:CD2	2.47	0.44
4:D:1:NAG:O3	4:D:2:NAG:C7	2.65	0.44
1:A:18:PHE:CD1	1:A:171:ARG:CZ	2.97	0.44
2:B:124:LEU:HD12	2:B:205:GLY:CA	2.45	0.44
2:B:21:ARG:HH21	2:B:32:GLN:NE2	2.16	0.44
1:A:183:ASP:O	1:A:184:VAL:C	2.53	0.44
1:A:50:ALA:O	1:A:71:VAL:HG21	2.18	0.44
2:B:139:VAL:HG12	2:B:255:PRO:CA	2.46	0.44
2:B:162:VAL:HG12	2:B:163:SER:H	1.80	0.44
1:A:95:LEU:O	1:A:96:PHE:CG	2.71	0.44
2:B:61:LEU:HD23	2:B:87:TRP:CE2	2.53	0.44
1:A:213:ARG:HG3	1:A:213:ARG:O	2.18	0.43
2:B:92:ASN:OD1	3:C:1:NAG:O5	2.32	0.43
1:A:21:ILE:O	1:A:22:THR:C	2.57	0.43
2:B:169:TRP:CZ3	2:B:187:LEU:HD13	2.53	0.43
2:B:19:ASP:C	2:B:19:ASP:OD1	2.57	0.43
2:B:45:LEU:N	2:B:45:LEU:HD12	2.33	0.43
1:A:54:LEU:HA	1:A:54:LEU:HD12	1.67	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:7:THR:C	2:B:8:VAL:CG2	2.87	0.43
1:A:169:ARG:O	1:A:170:ALA:C	2.56	0.43
1:A:70:ASP:O	1:A:71:VAL:C	2.57	0.43
1:A:163:PHE:CD1	1:A:189:LEU:HB3	2.53	0.43
2:B:186:CYS:O	2:B:187:LEU:C	2.56	0.43
2:B:231:ALA:O	2:B:232:ASN:CB	2.64	0.43
1:A:165:PRO:O	1:A:168:TRP:N	2.52	0.42
2:B:226:LEU:CB	2:B:240:ILE:CG2	2.97	0.42
1:A:204:THR:HG21	2:B:4:SER:O	2.19	0.42
2:B:98:PRO:C	2:B:100:SER:N	2.72	0.42
2:B:115:LEU:HD22	2:B:115:LEU:H	1.84	0.42
1:A:47:VAL:O	1:A:47:VAL:HG12	2.20	0.42
2:B:193:SER:C	2:B:194:VAL:HG23	2.39	0.42
1:A:147:ALA:O	1:A:148:ARG:C	2.58	0.42
2:B:226:LEU:HB3	2:B:240:ILE:HG22	2.02	0.42
2:B:22:ASP:O	2:B:23:ASP:C	2.54	0.42
4:D:2:NAG:H3	4:D:2:NAG:C8	2.43	0.42
1:A:10:SER:O	1:A:12:THR:HG23	2.19	0.42
2:B:165:GLN:HG2	2:B:165:GLN:H	1.58	0.42
2:B:7:THR:HA	2:B:47:THR:HA	2.00	0.42
2:B:114:THR:O	2:B:116:THR:HG22	2.20	0.42
1:A:65:ILE:CG2	1:A:66:THR:N	2.83	0.42
1:A:169:ARG:NH1	1:A:186:MET:HE3	2.35	0.41
1:A:200:VAL:HG12	1:A:200:VAL:O	2.19	0.41
1:A:49:ALA:C	1:A:51:ARG:N	2.73	0.41
2:B:132:ASN:HD22	4:D:1:NAG:C7	2.32	0.41
1:A:51:ARG:NE	1:A:72:THR:CG2	2.83	0.41
1:A:169:ARG:HE	1:A:173:TYR:HE2	1.69	0.41
1:A:167:LEU:O	1:A:169:ARG:N	2.53	0.41
1:A:167:LEU:C	1:A:169:ARG:N	2.73	0.41
2:B:110:ILE:O	2:B:111:LYS:C	2.57	0.41
1:A:135:THR:O	1:A:138:ARG:N	2.50	0.41
2:B:231:ALA:HB3	2:B:237:GLN:H	1.86	0.41
1:A:74:LEU:N	1:A:74:LEU:HD22	2.36	0.41
2:B:20:VAL:HG13	2:B:43:ASN:HB2	2.03	0.41
2:B:202:CYS:O	2:B:204:GLY:N	2.54	0.41
1:A:227:ARG:CZ	2:B:129:LEU:HD22	2.51	0.41
2:B:20:VAL:HB	2:B:74:ILE:CD1	2.51	0.41
1:A:166:ILE:HD11	1:A:186:MET:HG3	2.03	0.40
1:A:135:THR:C	1:A:137:LEU:N	2.74	0.40
1:A:110:TYR:CB	1:A:111:PRO:CD	2.99	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:233:LEU:HD12	1:A:233:LEU:HA	1.56	0.40
1:A:164:ASN:HB3	2:B:252:LEU:HD13	2.02	0.40
2:B:99:ARG:HB2	2:B:99:ARG:HH11	1.87	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	238/240 (99%)	176 (74%)	49 (21%)	13 (6%)	2	22
2	B	253/255 (99%)	208 (82%)	34 (13%)	11 (4%)	2	26
All	All	491/495 (99%)	384 (78%)	83 (17%)	24 (5%)	2	24

All (24) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	47	VAL
1	A	50	ALA
1	A	90	GLY
1	A	91	PRO
1	A	140	PRO
1	A	216	ILE
2	B	165	GLN
2	B	193	SER
2	B	232	ASN
1	A	62	GLY
2	B	4	SER
2	B	39	ASN
1	A	165	PRO
1	A	206	GLY
2	B	162	VAL

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Mol	Chain	Res	Type
2	B	194	VAL
2	B	231	ALA
1	A	44	GLY
2	B	27	ASP
1	A	73	ASN
2	B	98	PRO
2	B	197	ILE
1	A	30	SER
1	A	239	VAL

### 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	205/205 (100%)	177 (86%)	28 (14%)	3	22
2	B	211/211 (100%)	172 (82%)	39 (18%)	1	11
All	All	416/416 (100%)	349 (84%)	67 (16%)	2	16

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

Mol	Chain	Res	Type
1	A	1	TYR
1	A	3	ARG
1	A	18	PHE
1	A	41	ARG
1	A	42	GLN
1	A	54	LEU
1	A	59	ASN
1	A	64	SER
1	A	72	THR
1	A	80	GLN
1	A	95	LEU
1	A	101	ARG
1	A	104	LEU
1	A	106	PHE

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Mol	Chain	Res	Type
1	A	120	ARG
1	A	128	ASP
1	A	137	LEU
1	A	142	ASN
1	A	143	THR
1	A	144	ARG
1	A	151	LEU
1	A	167	LEU
1	A	168	TRP
1	A	171	ARG
1	A	180	PHE
1	A	216	ILE
1	A	224	THR
1	A	229	VAL
2	B	1	CYS
2	B	6	PRO
2	B	16	MET
2	B	19	ASP
2	B	20	VAL
2	B	23	ASP
2	B	50	ARG
2	B	51	ASP
2	B	57	ASN
2	B	73	MET
2	B	76	ASP
2	B	83	GLU
2	B	92	ASN
2	B	99	ARG
2	B	101	ASN
2	B	107	SER
2	B	116	THR
2	B	118	GLN
2	B	119	THR
2	B	120	LEU
2	B	129	LEU
2	B	132	ASN
2	B	134	THR
2	B	155	SER
2	B	160	THR
2	B	164	GLN
2	B	165	GLN
2	B	166	ASN

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Mol	Chain	Res	Type
2	B	167	ASP
2	B	176	SER
2	B	182	ASN
2	B	183	GLN
2	B	192	ASP
2	B	198	ASN
2	B	207	SER
2	B	216	GLU
2	B	221	ASN
2	B	224	ASN
2	B	232	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	42	GLN
1	A	59	ASN
1	A	115	GLN
1	A	199	GLN
1	A	225	ASN
2	B	14	ASN
2	B	29	ASN
2	B	30	GLN
2	B	32	GLN
2	B	39	ASN
2	B	101	ASN
2	B	118	GLN
2	B	126	GLN
2	B	145	ASN
2	B	164	GLN
2	B	166	ASN
2	B	182	ASN
2	B	198	ASN
2	B	221	ASN
2	B	224	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 ⓘ

7 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z  > 2$	Counts	RMSZ	# $ Z  > 2$
3	NAG	C	1	3,2	14,14,15	1.10	1 (7%)	17,19,21	2.35	4 (23%)
3	NAG	C	2	3	14,14,15	0.41	0	17,19,21	2.31	6 (35%)
4	NAG	D	1	2,4	14,14,15	1.58	2 (14%)	17,19,21	2.88	3 (17%)
4	NAG	D	2	4	14,14,15	1.75	1 (7%)	17,19,21	4.21	11 (64%)
4	BMA	D	3	4	11,11,12	0.78	0	15,15,17	1.89	3 (20%)
3	NAG	E	1	3,2	14,14,15	0.94	0	17,19,21	2.73	8 (47%)
3	NAG	E	2	3	14,14,15	0.71	0	17,19,21	1.14	2 (11%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	C	1	3,2	1/1/5/7	2/6/23/26	0/1/1/1
3	NAG	C	2	3	-	6/6/23/26	0/1/1/1
4	NAG	D	1	2,4	-	2/6/23/26	0/1/1/1
4	NAG	D	2	4	-	5/6/23/26	0/1/1/1
4	BMA	D	3	4	-	1/2/19/22	0/1/1/1
3	NAG	E	1	3,2	-	1/6/23/26	0/1/1/1
3	NAG	E	2	3	-	0/6/23/26	0/1/1/1

All (4) bond length outliers are listed below:



Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	2	NAG	C1-C2	5.36	1.60	1.52
4	D	1	NAG	C3-C2	-2.90	1.46	1.52
4	D	1	NAG	O5-C1	-2.65	1.39	1.43
3	C	1	NAG	O4-C4	-2.55	1.37	1.43

All (37) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	2	NAG	C1-C2-N2	12.62	132.05	110.49
4	D	1	NAG	O4-C4-C3	-8.61	90.44	110.35
3	E	1	NAG	O4-C4-C3	-7.63	92.70	110.35
4	D	1	NAG	O5-C1-C2	-6.71	100.69	111.29
4	D	2	NAG	O5-C5-C4	-6.46	95.10	110.83
3	C	1	NAG	O4-C4-C5	-5.93	94.58	109.30
3	C	2	NAG	C1-C2-N2	-5.60	100.92	110.49
4	D	2	NAG	O4-C4-C3	4.54	120.84	110.35
3	C	1	NAG	O5-C5-C6	4.38	114.07	107.20
3	C	1	NAG	C4-C3-C2	-4.24	104.80	111.02
4	D	3	BMA	O5-C5-C6	4.12	113.66	107.20
4	D	3	BMA	C1-C2-C3	-4.10	104.62	109.67
3	C	2	NAG	C1-O5-C5	-4.06	106.70	112.19
3	C	2	NAG	O5-C5-C6	4.00	113.48	107.20
4	D	2	NAG	C2-N2-C7	-3.94	117.30	122.90
4	D	2	NAG	C4-C3-C2	-3.49	105.91	111.02
4	D	2	NAG	O5-C5-C6	3.35	112.46	107.20
3	E	1	NAG	O4-C4-C5	3.29	117.46	109.30
3	E	1	NAG	O5-C5-C6	3.18	112.19	107.20
3	E	1	NAG	O3-C3-C2	3.17	116.02	109.47
3	E	1	NAG	C3-C4-C5	3.12	115.81	110.24
3	C	1	NAG	C2-N2-C7	-2.87	118.82	122.90
4	D	3	BMA	C3-C4-C5	2.79	115.21	110.24
4	D	2	NAG	C3-C4-C5	-2.77	105.30	110.24
4	D	2	NAG	C1-O5-C5	-2.65	108.60	112.19
4	D	2	NAG	O7-C7-C8	-2.65	117.14	122.06
4	D	2	NAG	O5-C1-C2	2.64	115.46	111.29
3	E	1	NAG	C6-C5-C4	-2.61	106.88	113.00
4	D	1	NAG	C1-C2-N2	2.60	114.93	110.49
3	C	2	NAG	C6-C5-C4	-2.53	107.08	113.00
3	E	1	NAG	C1-O5-C5	-2.52	108.77	112.19
3	E	2	NAG	C2-N2-C7	-2.52	119.32	122.90
4	D	2	NAG	C8-C7-N2	2.41	120.18	116.10
3	E	1	NAG	O5-C1-C2	-2.39	107.51	111.29
3	C	2	NAG	C4-C3-C2	2.36	114.48	111.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	2	NAG	O5-C1-C2	-2.08	108.01	111.29
3	C	2	NAG	C2-N2-C7	2.00	125.75	122.90

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	C	1	NAG	C1

All (17) torsion outliers are listed below:

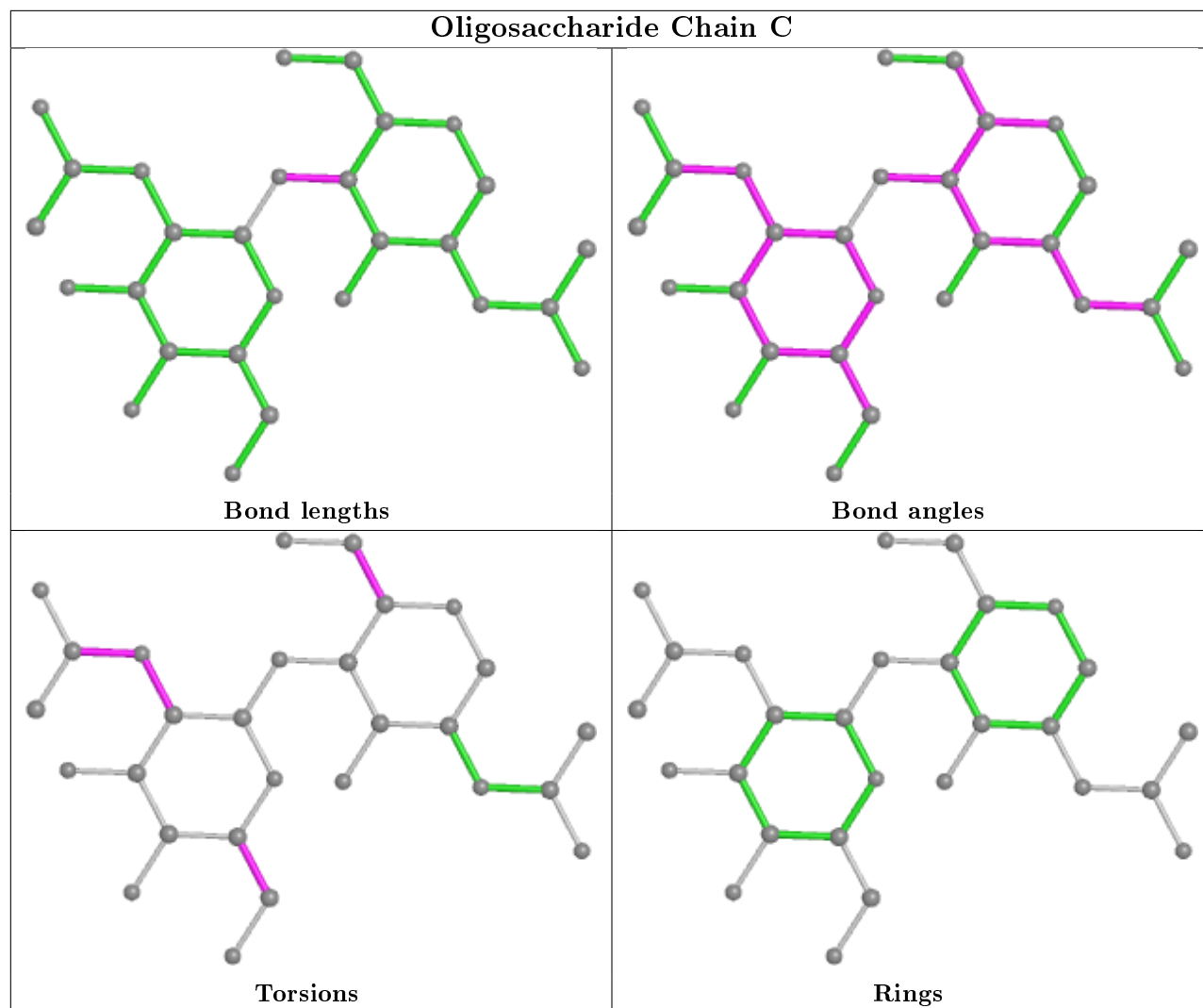
Mol	Chain	Res	Type	Atoms
4	D	2	NAG	O5-C5-C6-O6
3	C	2	NAG	O5-C5-C6-O6
3	C	1	NAG	O5-C5-C6-O6
3	C	2	NAG	C1-C2-N2-C7
4	D	1	NAG	C4-C5-C6-O6
3	C	1	NAG	C4-C5-C6-O6
4	D	2	NAG	C8-C7-N2-C2
4	D	2	NAG	O7-C7-N2-C2
4	D	1	NAG	O5-C5-C6-O6
4	D	2	NAG	C4-C5-C6-O6
3	E	1	NAG	O5-C5-C6-O6
4	D	3	BMA	O5-C5-C6-O6
3	C	2	NAG	C3-C2-N2-C7
3	C	2	NAG	C4-C5-C6-O6
3	C	2	NAG	C8-C7-N2-C2
3	C	2	NAG	O7-C7-N2-C2
4	D	2	NAG	C3-C2-N2-C7

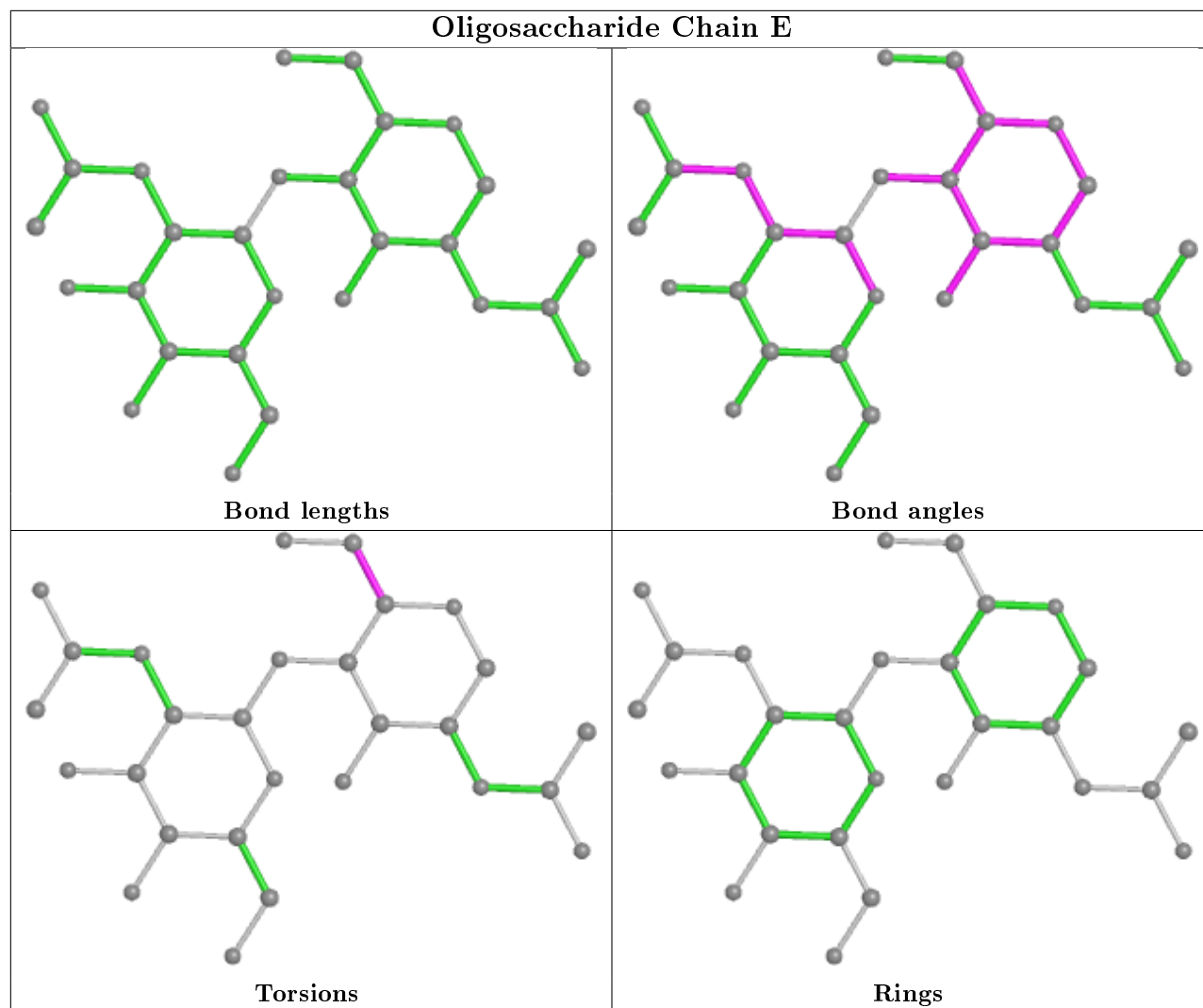
There are no ring outliers.

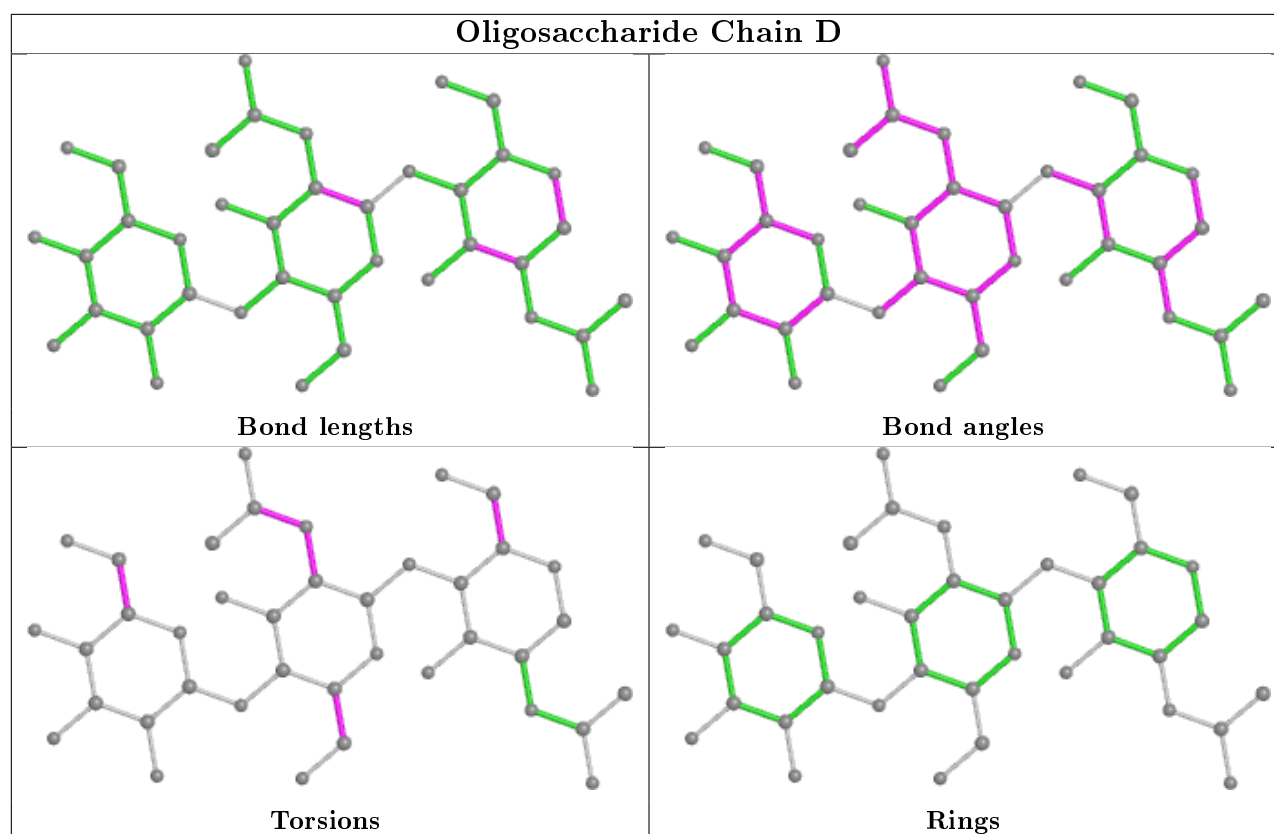
4 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	E	1	NAG	2	0
4	D	2	NAG	4	0
4	D	1	NAG	3	0
3	C	1	NAG	1	0

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







## 5.6 Ligand geometry [i](#)

1 ligand is 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	$\# Z  > 2$
5	NAG	A	1002	1	14,14,15	0.58	0	17,19,21	1.45	1 (5%)

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
5	NAG	A	1002	1	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
5	A	1002	NAG	C1-O5-C5	4.08	117.72	112.19

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	1002	NAG	O5-C5-C6-O6
5	A	1002	NAG	C4-C5-C6-O6

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	240/240 (100%)	-0.53	1 (0%) 92 89	27, 62, 100, 127	0
2	B	255/255 (100%)	-0.54	2 (0%) 86 81	27, 50, 91, 115	0
All	All	495/495 (100%)	-0.54	3 (0%) 89 85	27, 55, 97, 127	0

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1	TYR	2.2
2	B	40	ASN	2.1
2	B	232	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 [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.

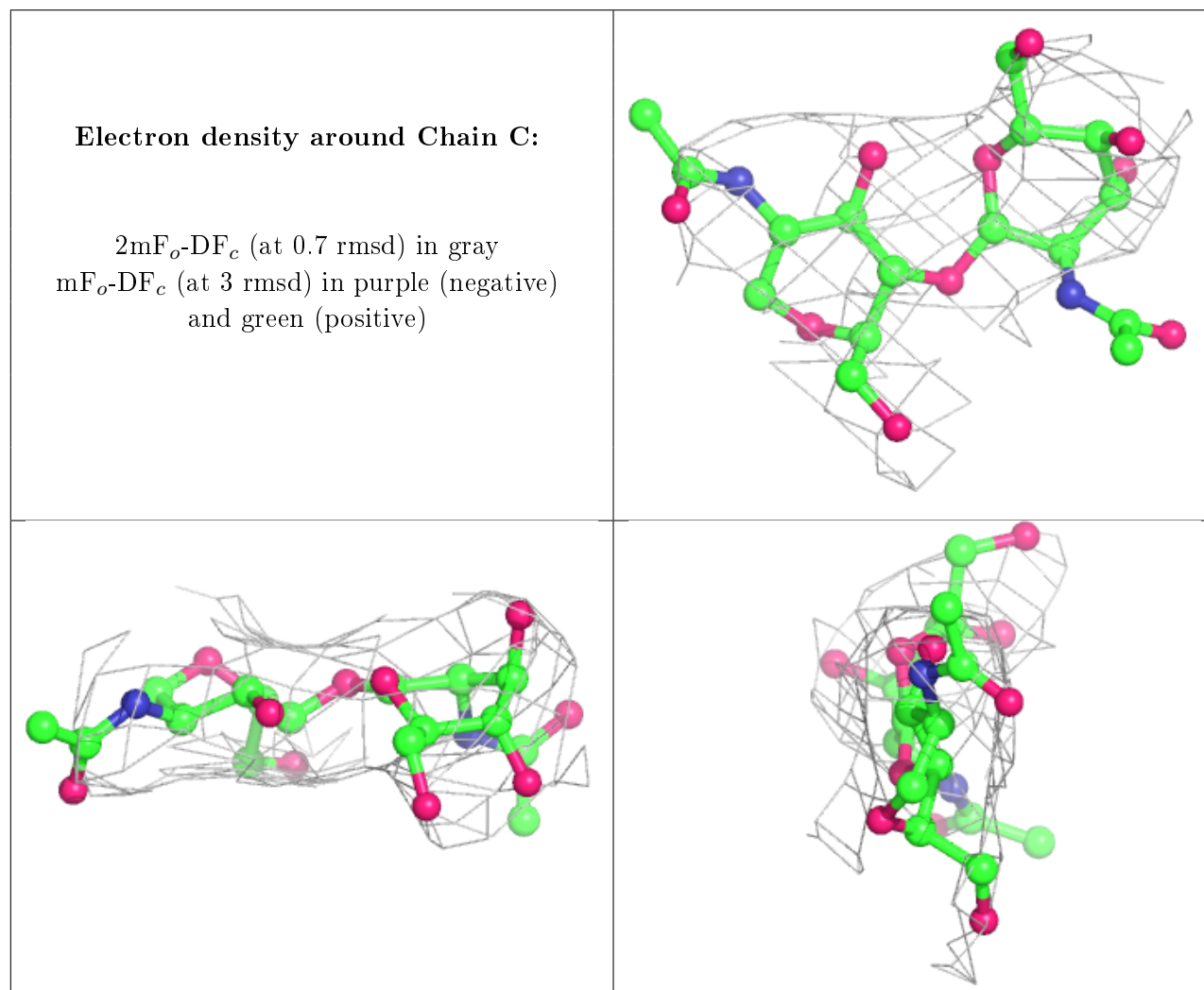
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
4	BMA	D	3	11/12	0.64	0.34	142,146,147,147	0
3	NAG	E	2	14/15	0.76	0.57	147,151,155,157	0
3	NAG	E	1	14/15	0.78	0.57	116,130,141,142	0
3	NAG	C	2	14/15	0.78	0.43	136,141,151,152	0
4	NAG	D	2	14/15	0.86	0.35	109,123,132,133	0
3	NAG	C	1	14/15	0.89	0.21	99,114,119,127	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
4	NAG	D	1	14/15	0.94	0.25	65,70,79,91	0

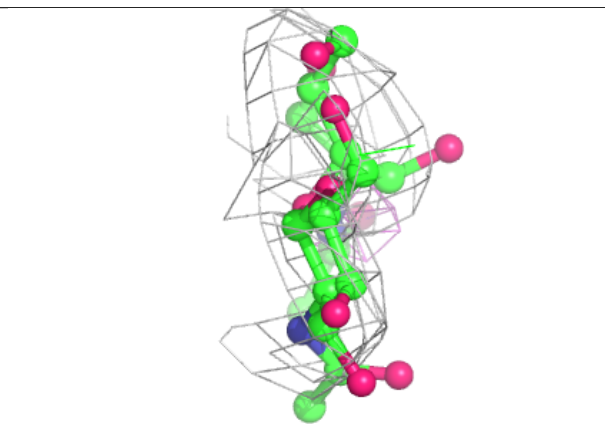
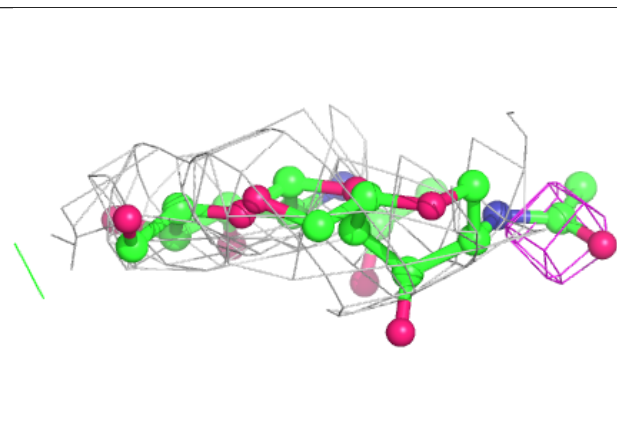
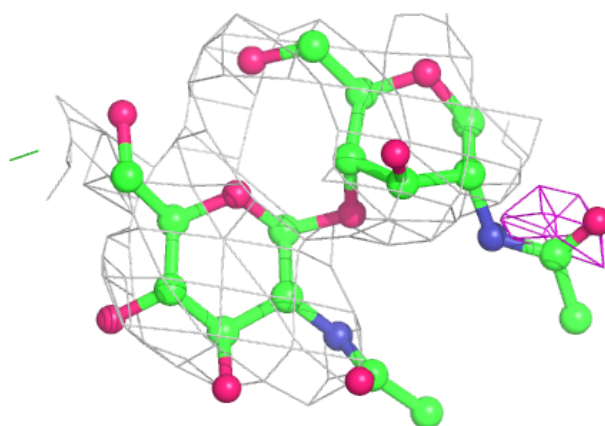
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.



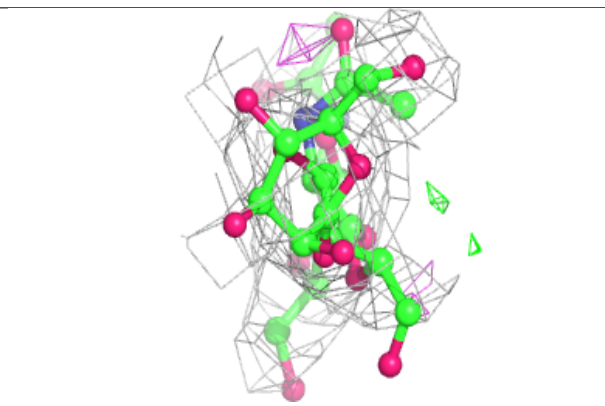
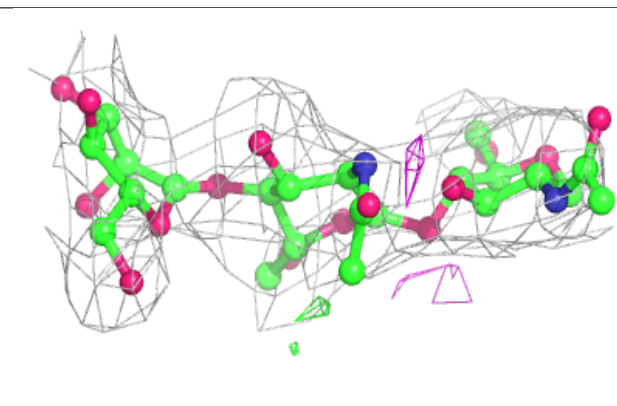
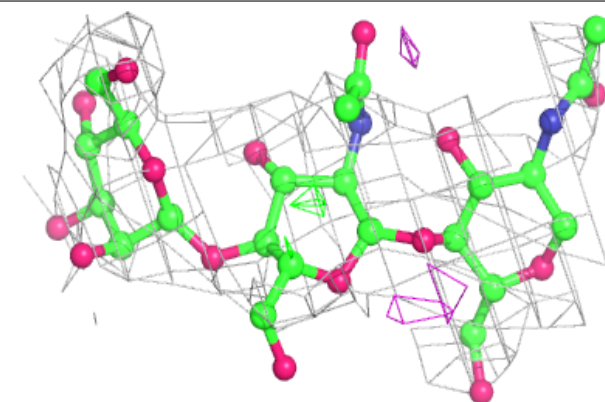


**Electron density around Chain E:**

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

**Electron density around Chain D:**

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



## 6.4 Ligands

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
5	NAG	A	1002	14/15	0.84	0.38	123,130,134,134	0

## 6.5 Other polymers

There are no such residues in this entry.