



# Full wwPDB X-ray Structure Validation Report ⓘ

May 26, 2025 – 05:03 PM EDT

PDB ID : 9CPF / pdb\_00009cpf  
Title : Structural basis of BAK sequestration by MCL-1 and consequences for apoptosis initiation  
Authors : Aggarwal, A.; Jayaraman, S.; Dey, R.; Moldoveanu, T.  
Deposited on : 2024-07-18  
Resolution : 1.70 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0rc1  
Mogul : 2022.3.0, CSD as543be (2022)  
Xtriage (Phenix) : 2.0rc1  
EDS : 3.0  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
CCP4 : 9.0.006 (Gargrove)  
Density-Fitness : 1.0.12  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.43.1

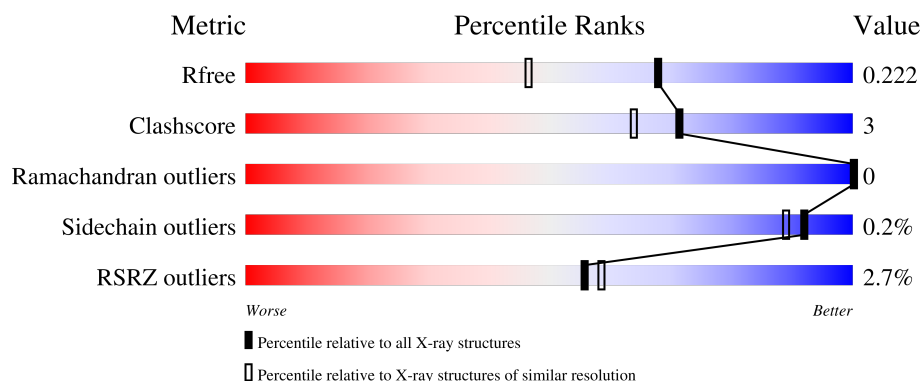
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.70 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))
$R_{free}$	164625	5161 (1.70-1.70)
Clashscore	180529	5671 (1.70-1.70)
Ramachandran outliers	177936	5594 (1.70-1.70)
Sidechain outliers	177891	5594 (1.70-1.70)
RSRZ outliers	164620	5159 (1.70-1.70)

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

Mol	Chain	Length	Quality of chain
1	A	517	<div> <div>2%</div> <div>91%</div> <div>8%</div> <div>.</div> </div>
1	B	517	<div> <div>3%</div> <div>88%</div> <div>6%</div> <div>6%</div> </div>
1	C	517	<div> <div>3%</div> <div>91%</div> <div>7%</div> <div>.</div> </div>
1	D	517	<div> <div>2%</div> <div>92%</div> <div>6%</div> <div>.</div> </div>
2	E	22	<div> <div>100%</div> </div>

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Mol	Chain	Length	Quality of chain
2	F	22	<div><div></div><div>91%</div><div>5%5%</div></div>
2	G	22	<div><div>5%</div><div></div><div>95%</div><div>5%</div></div>
2	H	22	<div><div></div><div>91%</div><div>5%5%</div></div>
3	I	2	<div><div></div><div>100%</div><div></div></div>
3	J	2	<div><div></div><div>100%</div><div></div></div>
3	K	2	<div><div></div><div>100%</div><div></div></div>
3	L	2	<div><div></div><div>100%</div><div></div></div>

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 34511 atoms, of which 16037 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 Induced myeloid leukemia cell differentiation protein Mcl-1.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	509	Total	C	H	N	O	S	0	4	0
			7823	2532	3866	661	755	9			
1	B	488	Total	C	H	N	O	S	0	6	0
			7522	2432	3719	638	724	9			
1	C	508	Total	C	H	N	O	S	0	8	0
			7820	2534	3862	659	755	10			
1	D	510	Total	C	H	N	O	S	0	7	0
			7824	2538	3859	658	759	10			

- Molecule 2 is a protein called Bcl-2 homologous antagonist/killer.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	E	22	Total	C	H	N	O	S	0	0	0
			334	100	166	34	33	1			
2	F	21	Total	C	H	N	O	S	0	0	0
			323	97	161	33	31	1			
2	G	21	Total	C	H	N	O	S	0	0	0
			323	97	161	33	31	1			
2	H	21	Total	C	H	N	O	S	0	0	0
			313	95	155	32	30	1			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	74	ALA	VAL	conflict	UNP Q16611
F	74	ALA	VAL	conflict	UNP Q16611
G	74	ALA	VAL	conflict	UNP Q16611
H	74	ALA	VAL	conflict	UNP Q16611

- Molecule 3 is an oligosaccharide called alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	I	2	Total	C	H	O	0	0	0
			45	12	22	11			
3	J	2	Total	C	H	O	0	0	0
			45	12	22	11			
3	K	2	Total	C	H	O	0	0	0
			45	12	22	11			
3	L	2	Total	C	H	O	0	0	0
			45	12	22	11			

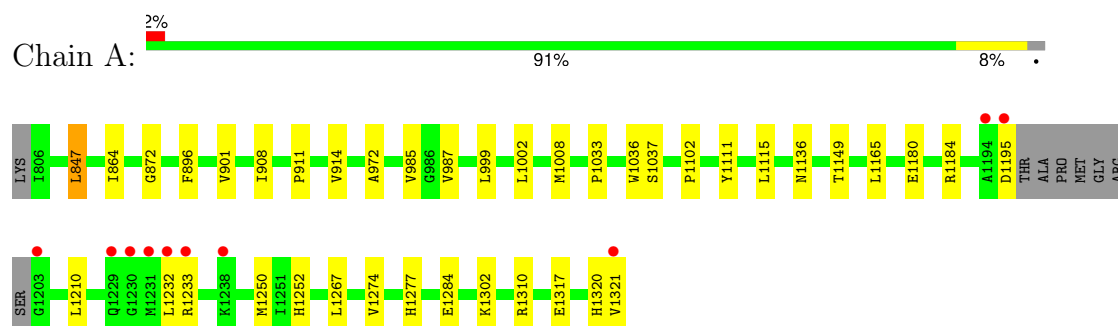
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	550	Total	O	0	0
			550	550		
4	B	478	Total	O	0	0
			478	478		
4	C	455	Total	O	0	0
			455	455		
4	D	456	Total	O	0	0
			456	456		
4	E	27	Total	O	0	0
			27	27		
4	F	22	Total	O	0	0
			22	22		
4	G	30	Total	O	0	0
			30	30		
4	H	31	Total	O	0	0
			31	31		

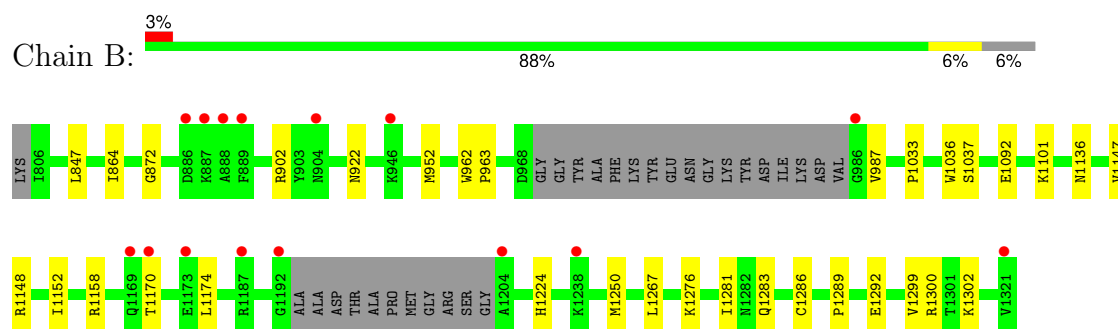
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

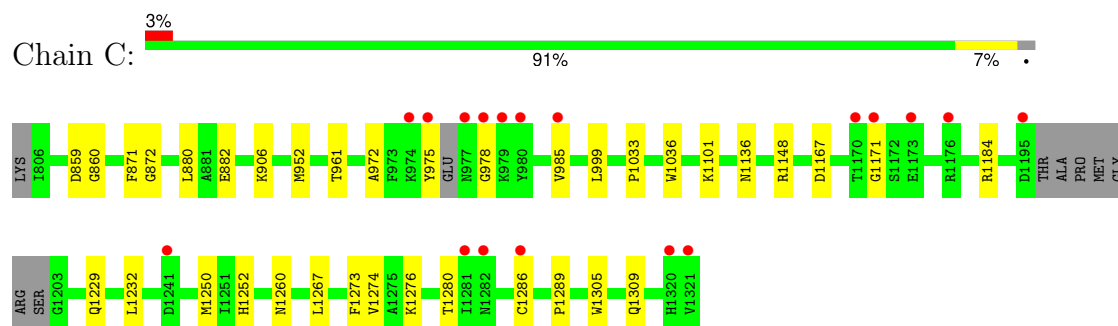
- Molecule 1: Induced myeloid leukemia cell differentiation protein Mcl-1



- Molecule 1: Induced myeloid leukemia cell differentiation protein Mcl-1

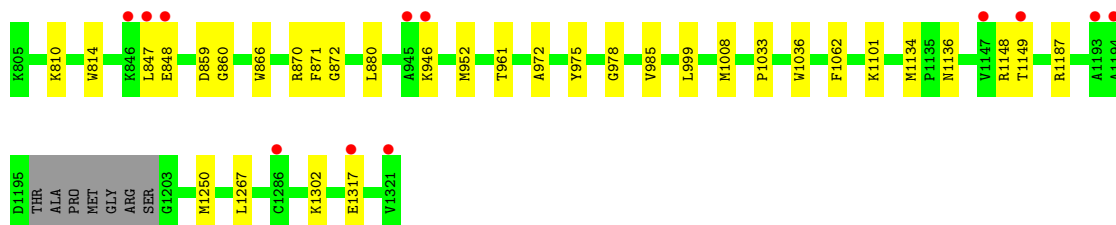


- Molecule 1: Induced myeloid leukemia cell differentiation protein Mcl-1



- Molecule 1: Induced myeloid leukemia cell differentiation protein Mcl-1





- Molecule 2: Bcl-2 homologous antagonist/killer

Chain E: 100%

There are no outlier residues recorded for this chain.

- Molecule 2: Bcl-2 homologous antagonist/killer

Chain F: 91% 5% 5%



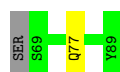
- Molecule 2: Bcl-2 homologous antagonist/killer

Chain G: 5% 95% 5%



- Molecule 2: Bcl-2 homologous antagonist/killer

Chain H: 91% 5% 5%



- Molecule 3: alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose

Chain I: 100%



- Molecule 3: alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose

Chain J: 100%



- Molecule 3: alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose

Chain K:  100%

GLC1  
GLC2

- Molecule 3: alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose

Chain L:  100%

GLC1  
GLC2

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	88.76Å 110.52Å 126.02Å 90.00° 101.17° 90.00°	Depositor
Resolution (Å)	46.35 – 1.70 46.35 – 1.70	Depositor EDS
% Data completeness (in resolution range)	97.6 (46.35-1.70) 97.7 (46.35-1.70)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.03 (at 1.70Å)	Xtriage
Refinement program	PHENIX (1.21_5207: ???)	Depositor
R, $R_{free}$	0.185 , 0.224 0.193 , 0.222	Depositor DCC
$R_{free}$ test set	259830 reflections (0.63%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	32.6	Xtriage
Anisotropy	0.204	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.42 , 47.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	34511	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 46.52 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.1312e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<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: GLC

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	0.56	0/4061	0.69	0/5514
1	B	0.55	0/3909	0.71	2/5310 (0.0%)
1	C	0.53	0/4074	0.66	0/5532
1	D	0.54	3/4082 (0.1%)	0.69	1/5545 (0.0%)
2	E	0.61	0/168	0.75	0/223
2	F	0.53	0/162	0.70	0/215
2	G	0.51	0/162	0.66	0/215
2	H	0.56	0/158	0.65	0/210
All	All	0.54	3/16776 (0.0%)	0.69	3/22764 (0.0%)

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

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

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	1148	ARG	C-N	6.45	1.42	1.33
1	D	1149[A]	THR	N-CA	5.91	1.54	1.46
1	D	1149[B]	THR	N-CA	5.91	1.54	1.46

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	1170	THR	CA-C-N	7.54	128.35	119.98
1	B	1170	THR	C-N-CA	7.54	128.35	119.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	1148	ARG	O-C-N	5.25	127.49	122.03

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1233	ARG	Sidechain

## 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	3957	3866	3867	30	0
1	B	3803	3719	3713	23	0
1	C	3958	3862	3858	28	0
1	D	3965	3859	3860	22	0
2	E	168	166	166	0	0
2	F	162	161	161	1	0
2	G	162	161	161	0	0
2	H	158	155	155	1	0
3	I	23	22	21	0	0
3	J	23	22	21	0	0
3	K	23	22	21	0	0
3	L	23	22	21	0	0
4	A	550	0	0	4	0
4	B	478	0	0	7	0
4	C	455	0	0	9	0
4	D	456	0	0	7	0
4	E	27	0	0	1	0
4	F	22	0	0	1	0
4	G	30	0	0	1	0
4	H	31	0	0	1	0
All	All	18474	16037	16025	105	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 3.

All (105) 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:952:MET:SD	4:C:1751:HOH:O	2.28	0.91
1:C:975:TYR:CZ	1:C:978:GLY:HA2	2.14	0.81
1:A:1277:HIS:ND1	4:A:1401:HOH:O	2.22	0.73
1:D:1317:GLU:HG3	4:D:1481:HOH:O	1.90	0.70
1:D:1101:LYS:NZ	4:D:1401:HOH:O	2.28	0.67
1:A:1180:GLU:OE2	1:A:1184:ARG:NH1	2.29	0.65
1:C:1276:LYS:O	1:C:1280:THR:HG23	1.97	0.64
1:D:1250:MET:HG2	1:D:1267:LEU:HD11	1.79	0.64
1:B:1174:LEU:HD22	1:B:1299:VAL:HG22	1.80	0.63
1:A:999:LEU:CD1	1:A:1008:MET:HE1	2.30	0.61
1:D:872:GLY:HA3	1:D:1136:ASN:O	2.01	0.61
1:A:1250:MET:HG2	1:A:1267:LEU:HD11	1.82	0.60
1:A:847:LEU:CD1	1:A:864:ILE:HD11	2.31	0.60
1:D:1302:LYS:NZ	4:D:1406:HOH:O	2.34	0.59
1:C:978:GLY:N	4:C:1401:HOH:O	2.26	0.59
1:C:961[A]:THR:HG23	1:C:999:LEU:HD22	1.85	0.58
1:C:1229:GLN:NE2	4:C:1403:HOH:O	2.37	0.58
1:B:1250:MET:HG2	1:B:1267:LEU:HD11	1.85	0.57
1:D:1302:LYS:NZ	4:D:1408:HOH:O	2.37	0.57
1:D:999:LEU:CD1	1:D:1008:MET:HE1	2.34	0.57
1:A:872:GLY:HA3	1:A:1136:ASN:O	2.04	0.56
1:C:1229:GLN:HG3	4:C:1747:HOH:O	2.05	0.56
1:C:1229:GLN:HG3	4:C:1790:HOH:O	2.06	0.55
1:A:1284:GLU:HG2	4:A:1741:HOH:O	2.07	0.55
1:B:902:ARG:NE	4:B:1406:HOH:O	2.35	0.55
1:C:1286:CYS:C	1:C:1289:PRO:HD2	2.32	0.55
1:D:859:ASP:CG	1:D:860:GLY:H	2.15	0.55
1:A:1232:LEU:HD13	1:A:1274:VAL:HG22	1.88	0.54
1:B:1286:CYS:C	1:B:1289:PRO:HD2	2.32	0.54
1:B:1302:LYS:NZ	4:B:1410:HOH:O	2.38	0.54
1:A:896:PHE:CZ	1:A:914:VAL:HG21	2.43	0.54
2:H:77:GLN:HG3	4:H:110:HOH:O	2.07	0.54
1:B:1174:LEU:HD23	1:B:1174:LEU:O	2.08	0.54
1:B:1276:LYS:NZ	4:B:1412:HOH:O	2.40	0.54
1:C:1250:MET:HG2	1:C:1267:LEU:HD11	1.90	0.54
1:D:1187:ARG:NH2	4:D:1405:HOH:O	2.33	0.53
1:B:847:LEU:HD11	1:B:864:ILE:CD1	2.39	0.53
1:A:1252:HIS:HD2	4:E:104:HOH:O	1.92	0.52
1:B:962:TRP:CZ3	1:B:1147:VAL:HG13	2.45	0.52
1:C:872:GLY:HA3	1:C:1136:ASN:O	2.10	0.52
1:A:1037:SER:OG	1:A:1102:PRO:HD3	2.09	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:810:LYS:NZ	4:D:1410:HOH:O	2.38	0.50
1:A:1310:ARG:NH2	1:A:1317:GLU:OE1	2.44	0.50
1:A:1149:THR:HG21	4:A:1607:HOH:O	2.11	0.50
1:C:975:TYR:CE2	1:C:978:GLY:HA2	2.47	0.50
1:B:872:GLY:HA3	1:B:1136:ASN:O	2.12	0.49
1:D:1062:PHE:CD1	1:D:1134:MET:HG2	2.47	0.49
1:C:1252:HIS:HD2	4:G:101:HOH:O	1.95	0.49
1:D:1033:PRO:HA	1:D:1036:TRP:CE2	2.47	0.49
1:D:975:TYR:OH	1:D:978:GLY:HA2	2.12	0.49
1:B:1292:GLU:OE2	4:B:1401:HOH:O	2.20	0.49
1:B:1300:ARG:NH2	4:B:1414:HOH:O	2.42	0.49
1:A:1002:LEU:HD13	1:A:1008:MET:HE2	1.95	0.49
1:B:1281:ILE:HG13	1:B:1283:GLN:HG3	1.95	0.48
1:C:972:ALA:O	1:C:985:VAL:HA	2.14	0.48
1:D:859:ASP:OD1	1:D:860:GLY:N	2.44	0.48
1:C:961[A]:THR:CG2	1:C:999:LEU:HD22	2.44	0.47
2:F:73:GLN:NE2	4:F:101:HOH:O	2.36	0.47
1:B:962:TRP:CZ2	1:B:987:VAL:HG12	2.49	0.47
1:A:896:PHE:HZ	1:A:914:VAL:HG21	1.78	0.47
1:B:962:TRP:N	1:B:963:PRO:CD	2.78	0.47
1:C:1033:PRO:HA	1:C:1036:TRP:CE2	2.50	0.47
1:A:1302:LYS:NZ	4:A:1411:HOH:O	2.46	0.46
1:A:972:ALA:O	1:A:985:VAL:HA	2.16	0.45
1:C:1167:ASP:O	1:C:1171:GLY:N	2.44	0.45
1:A:847:LEU:C	1:A:847:LEU:HD12	2.42	0.45
1:A:1033:PRO:HA	1:A:1036:TRP:CE2	2.51	0.45
1:C:1309:GLN:NE2	4:C:1418:HOH:O	2.49	0.45
1:B:1037:SER:OG	1:B:1101:LYS:HD3	2.17	0.45
1:D:999:LEU:HD11	1:D:1008:MET:HE1	1.97	0.45
1:A:1111:TYR:CE2	1:A:1115:LEU:HD11	2.52	0.44
1:A:1184:ARG:HE	1:A:1210:LEU:HD22	1.82	0.44
1:C:1229:GLN:HG2	1:C:1273:PHE:HZ	1.82	0.44
1:B:1148[B]:ARG:NH2	4:B:1429:HOH:O	2.50	0.44
1:D:999:LEU:CD1	1:D:1008:MET:CE	2.96	0.43
1:A:999:LEU:HD11	1:A:1008:MET:HE1	1.97	0.43
1:B:1033:PRO:HA	1:B:1036:TRP:CE2	2.53	0.43
1:B:1092:GLU:H	1:B:1092:GLU:CD	2.27	0.42
1:C:871[B]:PHE:HD2	1:C:880:LEU:HD11	1.84	0.42
1:D:866:TRP:CD1	1:D:870:ARG:HG3	2.54	0.42
1:A:1180:GLU:OE2	1:A:1184:ARG:CZ	2.67	0.42
1:D:814:TRP:HB3	1:D:847:LEU:HD11	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:882:GLU:OE1	1:C:906:LYS:HE2	2.18	0.42
1:B:1224:HIS:HD2	4:B:1814:HOH:O	2.01	0.42
1:C:871[B]:PHE:HD2	1:C:880:LEU:CD1	2.33	0.42
1:D:972:ALA:O	1:D:985:VAL:HA	2.19	0.42
1:A:987:VAL:HB	1:A:1165:LEU:HD22	2.02	0.42
1:C:1232:LEU:HD13	1:C:1274:VAL:HG22	2.02	0.42
1:A:901:VAL:HG21	1:A:911:PRO:HD3	2.02	0.41
1:C:1148[A]:ARG:NH1	4:C:1420:HOH:O	2.50	0.41
1:C:1101:LYS:NZ	4:C:1430:HOH:O	2.53	0.41
1:A:1195:ASP:OD1	1:A:1195:ASP:C	2.64	0.41
1:B:952:MET:HE2	1:B:952:MET:HB3	1.91	0.41
1:A:1320:HIS:O	1:A:1321:VAL:CB	2.68	0.41
1:B:1152:ILE:HG22	1:B:1158:ARG:HH21	1.85	0.41
1:C:859:ASP:OD1	1:C:860:GLY:N	2.40	0.41
1:B:922:ASN:OD1	1:B:922:ASN:C	2.64	0.41
1:A:1002:LEU:CD1	1:A:1008:MET:HE2	2.51	0.41
1:C:1260:ASN:HA	1:C:1305:TRP:CZ2	2.56	0.41
1:A:908:ILE:C	1:A:908:ILE:HD12	2.46	0.40
1:D:952:MET:HG2	4:D:1623:HOH:O	2.21	0.40
1:C:1184:ARG:NH1	4:C:1429:HOH:O	2.53	0.40
1:A:999:LEU:HD12	1:A:1008:MET:CE	2.51	0.40
1:D:871[A]:PHE:HD2	1:D:880:LEU:HD11	1.85	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	510/517 (99%)	503 (99%)	7 (1%)	0	100	100
1	B	489/517 (95%)	487 (100%)	2 (0%)	0	100	100
1	C	511/517 (99%)	505 (99%)	6 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	514/517 (99%)	507 (99%)	7 (1%)	0	100	100
2	E	20/22 (91%)	20 (100%)	0	0	100	100
2	F	19/22 (86%)	19 (100%)	0	0	100	100
2	G	19/22 (86%)	19 (100%)	0	0	100	100
2	H	19/22 (86%)	19 (100%)	0	0	100	100
All	All	2101/2156 (97%)	2079 (99%)	22 (1%)	0	100	100

There are no Ramachandran outliers to report.

### 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	408/422 (97%)	407 (100%)	1 (0%)	92	89
1	B	395/422 (94%)	395 (100%)	0	100	100
1	C	409/422 (97%)	409 (100%)	0	100	100
1	D	410/422 (97%)	408 (100%)	2 (0%)	86	82
2	E	17/17 (100%)	17 (100%)	0	100	100
2	F	16/17 (94%)	16 (100%)	0	100	100
2	G	16/17 (94%)	16 (100%)	0	100	100
2	H	15/17 (88%)	15 (100%)	0	100	100
All	All	1686/1756 (96%)	1683 (100%)	3 (0%)	92	89

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	847	LEU
1	D	848	GLU
1	D	946	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14)

such sidechains are listed below:

Mol	Chain	Res	Type
1	A	822	ASN
1	A	843	HIS
1	A	1057	GLN
1	A	1252	HIS
1	B	956	GLN
1	B	1224	HIS
1	B	1229	GLN
1	C	1221	GLN
1	C	1283	GLN
1	C	1320	HIS
1	D	1086	ASN
1	D	1221	GLN
1	D	1229	GLN
2	G	77	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

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	$\# Z  > 2$
3	GLC	I	1	3	12,12,12	0.82	1 (8%)	17,17,17	1.31	2 (11%)
3	GLC	I	2	3	11,11,12	0.74	0	15,15,17	1.28	2 (13%)
3	GLC	J	1	3	12,12,12	0.85	0	17,17,17	1.28	3 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	GLC	J	2	3	11,11,12	0.88	0	15,15,17	1.25	1 (6%)
3	GLC	K	1	3	12,12,12	0.58	0	17,17,17	1.23	1 (5%)
3	GLC	K	2	3	11,11,12	0.80	0	15,15,17	1.15	2 (13%)
3	GLC	L	1	3	12,12,12	0.68	0	17,17,17	1.05	1 (5%)
3	GLC	L	2	3	11,11,12	0.59	0	15,15,17	1.10	1 (6%)

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	GLC	I	1	3	-	0/2/22/22	0/1/1/1
3	GLC	I	2	3	-	0/2/19/22	0/1/1/1
3	GLC	J	1	3	-	0/2/22/22	0/1/1/1
3	GLC	J	2	3	-	0/2/19/22	0/1/1/1
3	GLC	K	1	3	-	0/2/22/22	0/1/1/1
3	GLC	K	2	3	-	0/2/19/22	0/1/1/1
3	GLC	L	1	3	-	0/2/22/22	0/1/1/1
3	GLC	L	2	3	-	0/2/19/22	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	I	1	GLC	O5-C5	-2.16	1.39	1.44

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	J	1	GLC	O5-C1-C2	3.60	116.63	110.30
3	I	1	GLC	O5-C1-C2	3.37	116.22	110.30
3	K	1	GLC	O5-C1-C2	2.96	115.50	110.30
3	J	2	GLC	C1-O5-C5	2.92	116.09	112.19
3	L	1	GLC	O5-C1-C2	2.83	115.27	110.30
3	I	1	GLC	O1-C1-O5	-2.66	102.51	110.41
3	J	1	GLC	C1-O5-C5	2.50	118.49	113.65
3	I	2	GLC	C1-C2-C3	2.47	113.23	109.64
3	L	2	GLC	C2-C3-C4	-2.46	106.53	110.86
3	I	2	GLC	C2-C3-C4	-2.27	106.88	110.86
3	K	2	GLC	C6-C5-C4	-2.24	107.52	113.02
3	J	1	GLC	O1-C1-O5	-2.13	104.08	110.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	K	2	GLC	C2-C3-C4	-2.10	107.17	110.86

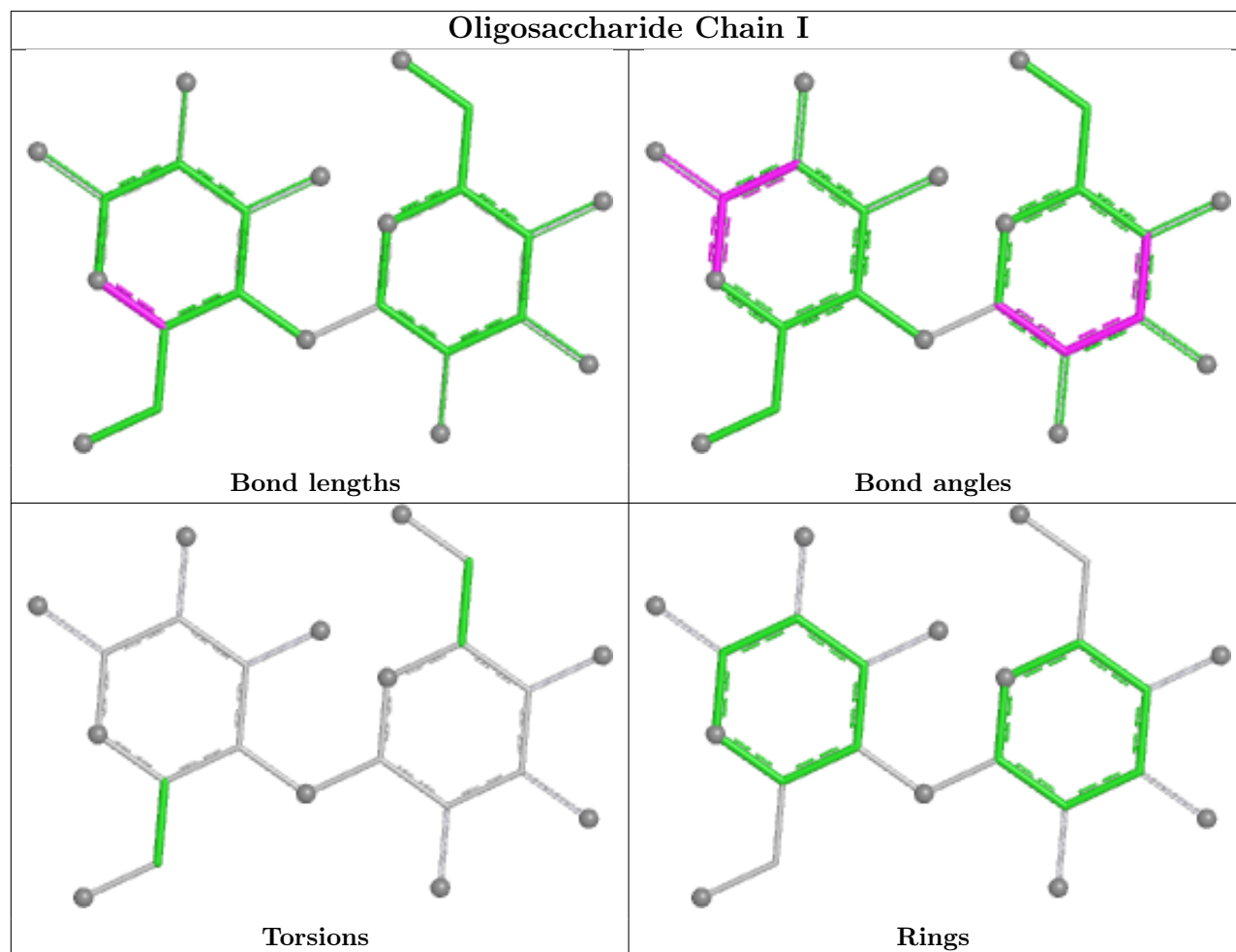
There are no chirality outliers.

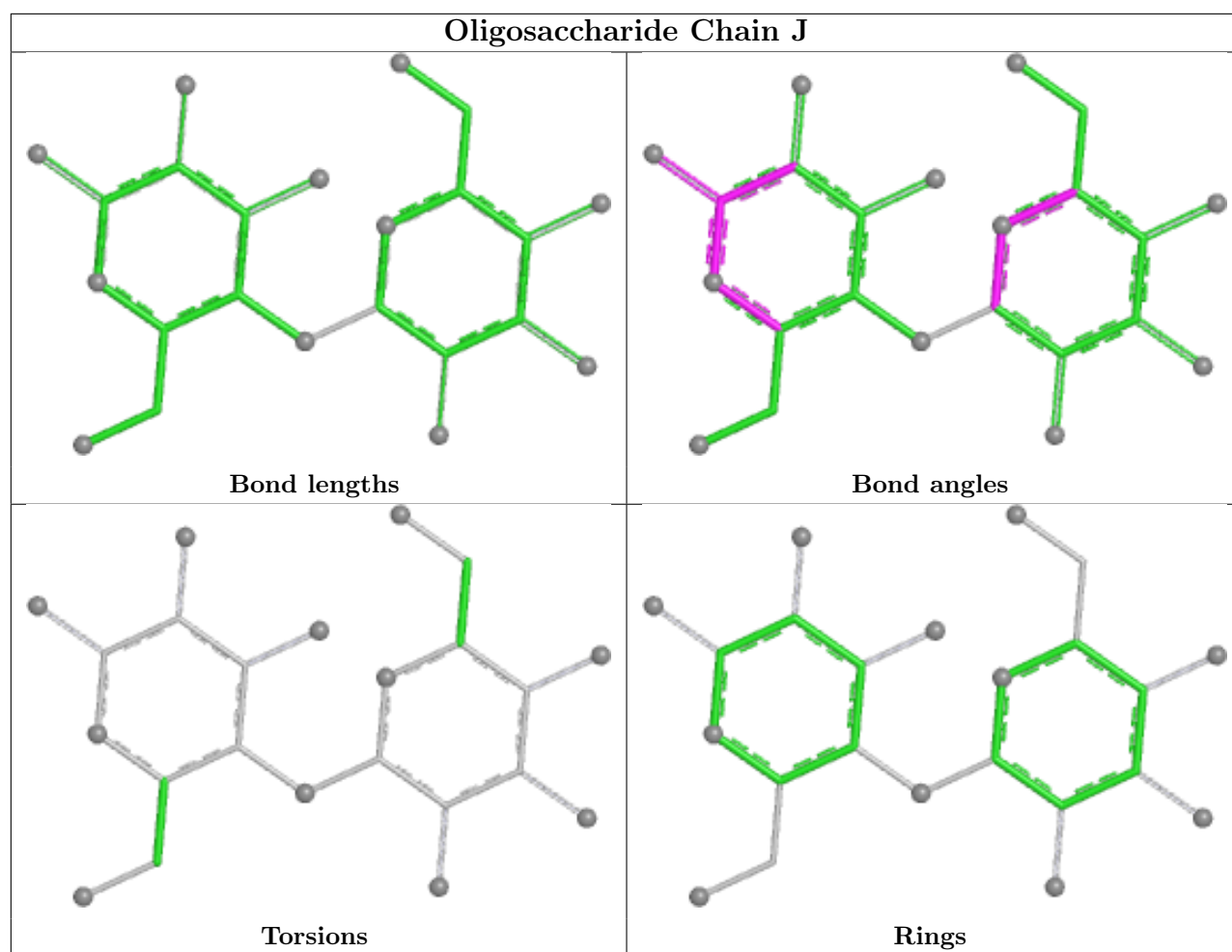
There are no torsion outliers.

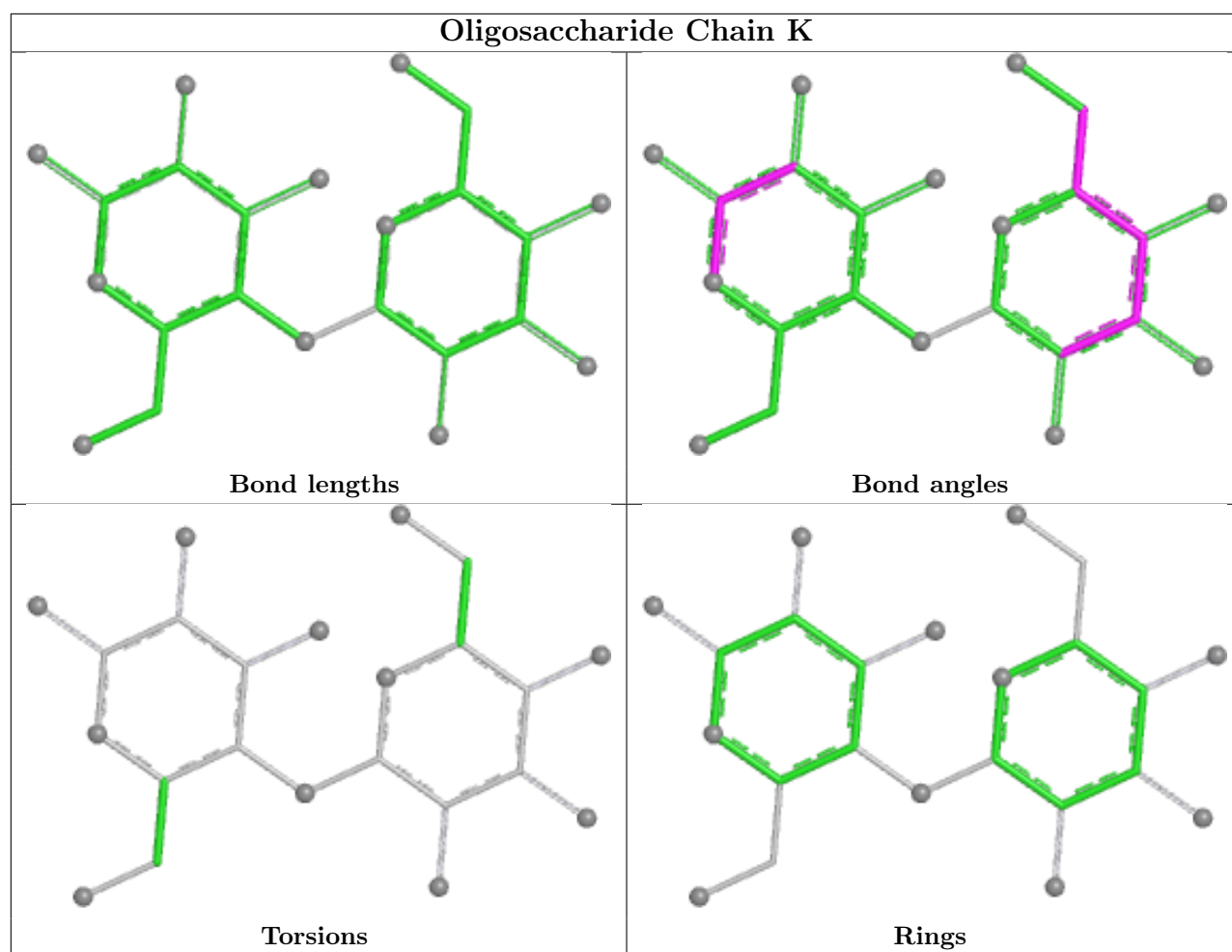
There are no ring outliers.

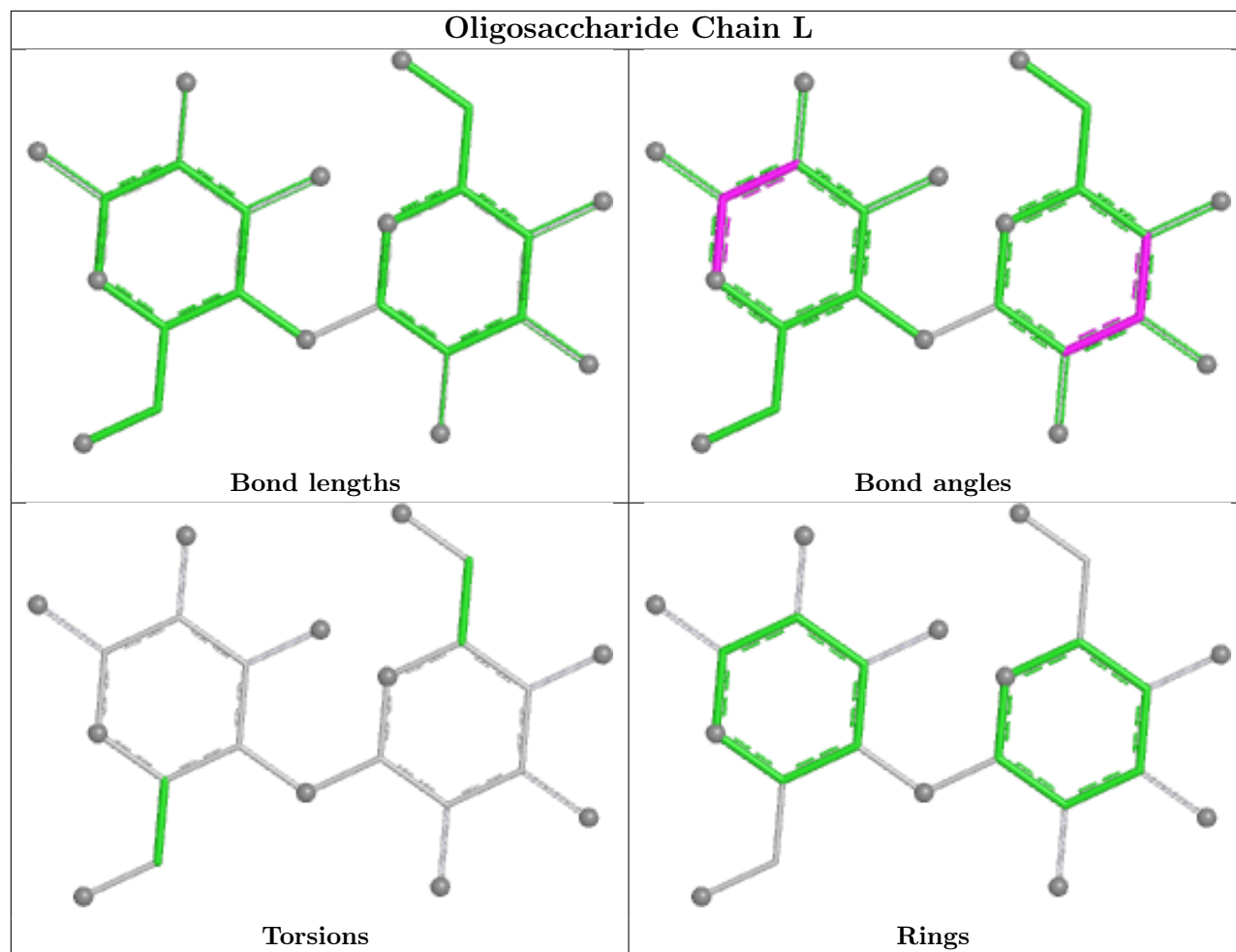
No monomer is involved in short contacts.

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









## 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	509/517 (98%)	-0.09	10 (1%) 64 68	13, 34, 51, 70	4 (0%)
1	B	488/517 (94%)	0.09	15 (3%) 51 54	15, 36, 57, 71	5 (1%)
1	C	508/517 (98%)	0.16	18 (3%) 47 50	14, 38, 62, 89	7 (1%)
1	D	510/517 (98%)	0.16	12 (2%) 59 62	15, 39, 61, 77	6 (1%)
2	E	22/22 (100%)	-0.22	0 100 100	24, 30, 43, 64	0
2	F	21/22 (95%)	-0.22	0 100 100	26, 31, 47, 55	0
2	G	21/22 (95%)	0.10	1 (4%) 36 39	27, 34, 67, 74	0
2	H	21/22 (95%)	0.19	0 100 100	27, 34, 61, 69	0
All	All	2100/2156 (97%)	0.07	56 (2%) 56 58	13, 37, 59, 89	22 (1%)

All (56) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1232	LEU	10.0
1	C	975	TYR	5.0
1	A	1231	MET	4.8
1	D	1321	VAL	4.7
1	C	978	GLY	4.7
1	B	887	LYS	4.6
1	A	1321	VAL	4.2
1	C	977	ASN	4.1
1	D	848	GLU	4.1
1	B	1321	VAL	4.1
1	B	946	LYS	4.0
1	B	888	ALA	3.9
1	B	1192	GLY	3.9
1	A	1229	GLN	3.8
1	B	1169	GLN	3.8
1	D	1149[A]	THR	3.7

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Mol	Chain	Res	Type	RSRZ
1	D	847	LEU	3.6
1	C	1241	ASP	3.6
1	A	1233	ARG	3.5
1	A	1203	GLY	3.4
1	B	1170	THR	3.4
1	C	1170	THR	3.4
1	C	1171	GLY	3.4
1	C	1173	GLU	3.3
1	D	946	LYS	3.3
1	C	1321	VAL	3.3
1	C	979	LYS	3.2
1	D	945	ALA	2.9
1	C	1320	HIS	2.8
1	A	1194	ALA	2.8
1	B	1204	ALA	2.7
1	C	1286	CYS	2.6
1	C	974	LYS	2.5
1	B	986	GLY	2.5
1	D	1317	GLU	2.5
1	A	1195	ASP	2.5
1	A	1230	GLY	2.4
1	C	985	VAL	2.4
1	C	1282	ASN	2.3
1	D	1286	CYS	2.3
1	B	889	PHE	2.3
1	C	1195	ASP	2.3
1	A	1238	LYS	2.3
1	C	1176	ARG	2.3
1	B	886	ASP	2.3
1	D	1194	ALA	2.3
1	C	980	TYR	2.3
1	B	1173	GLU	2.2
1	D	846	LYS	2.2
2	G	69	SER	2.1
1	B	904	ASN	2.1
1	C	1281	ILE	2.1
1	B	1187	ARG	2.1
1	B	1238	LYS	2.1
1	D	1147	VAL	2.0
1	D	1193	ALA	2.0

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

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

## 6.3 Carbohydrates ⓘ

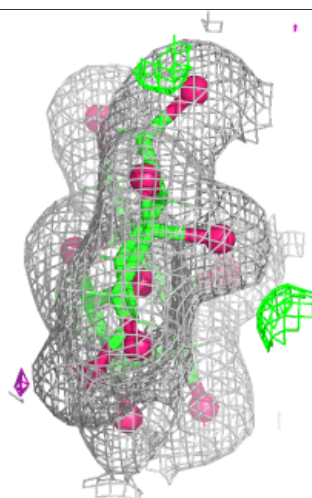
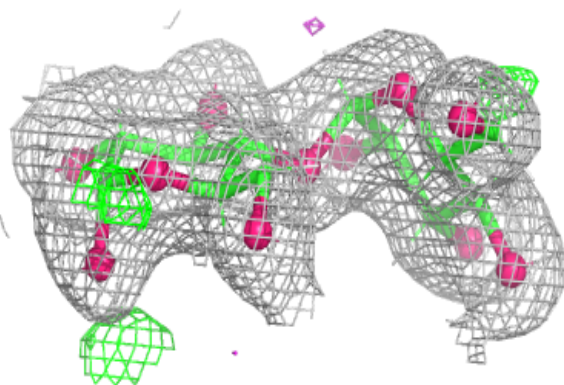
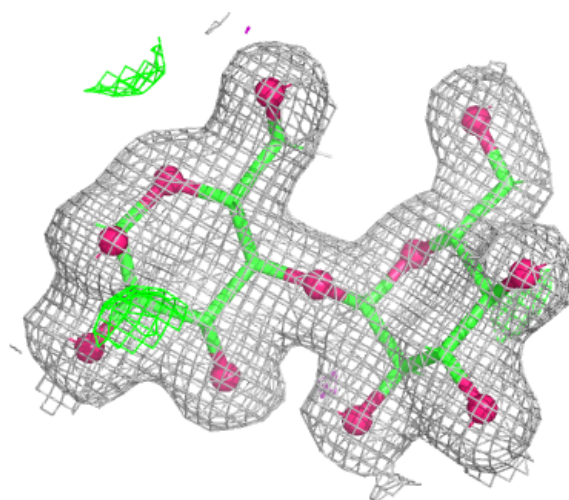
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 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
3	GLC	J	1	12/12	0.96	0.06	22,30,40,48	0
3	GLC	I	1	12/12	0.97	0.05	22,29,40,47	0
3	GLC	K	1	12/12	0.97	0.05	22,33,44,48	0
3	GLC	L	1	12/12	0.97	0.06	24,34,44,48	0
3	GLC	I	2	11/12	0.98	0.05	20,25,29,32	0
3	GLC	K	2	11/12	0.98	0.04	23,26,32,32	0
3	GLC	J	2	11/12	0.98	0.05	21,26,30,32	0
3	GLC	L	2	11/12	0.98	0.04	21,26,31,34	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.

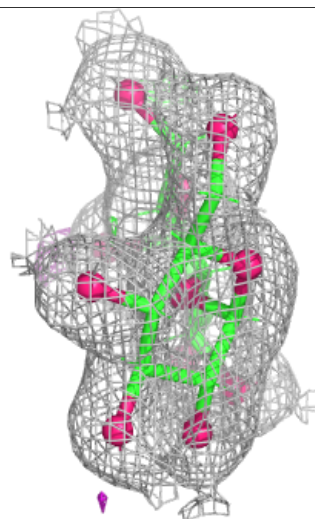
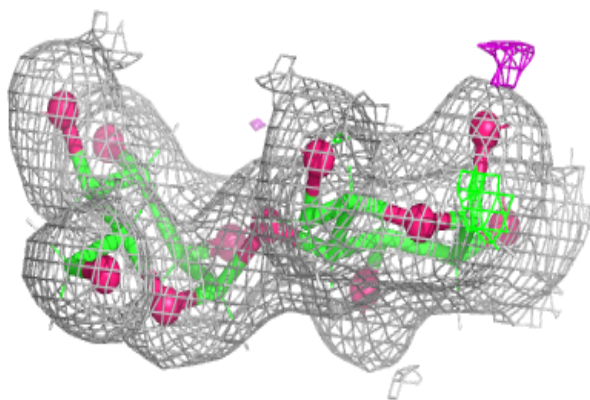
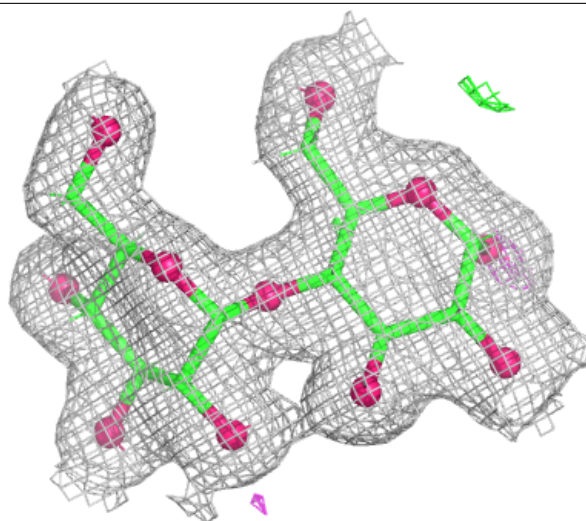
**Electron density around Chain I:**

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



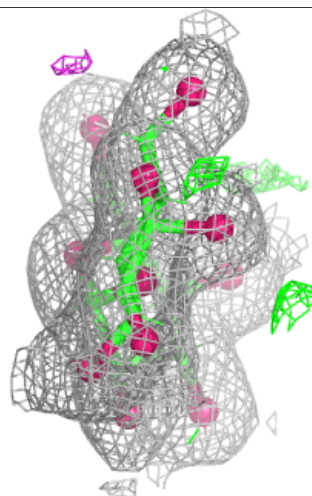
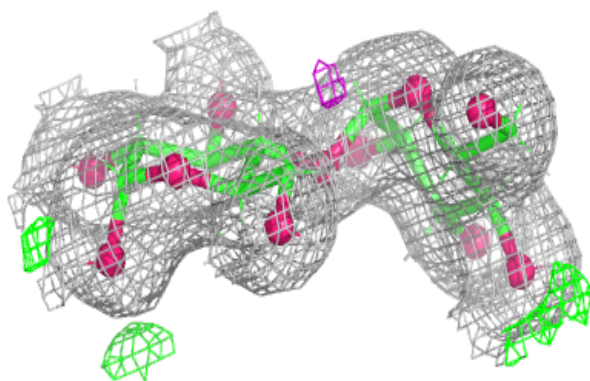
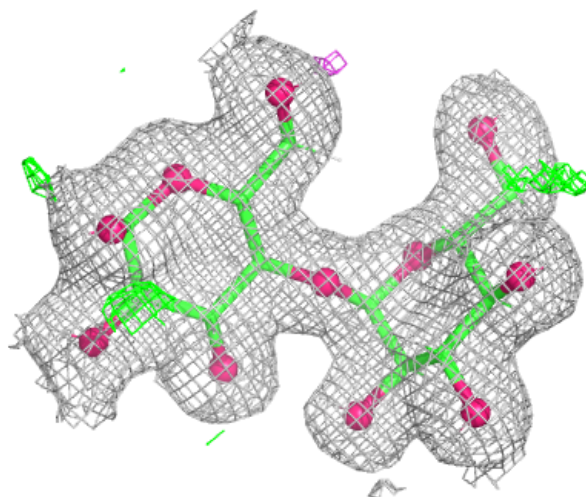
**Electron density around Chain J:**

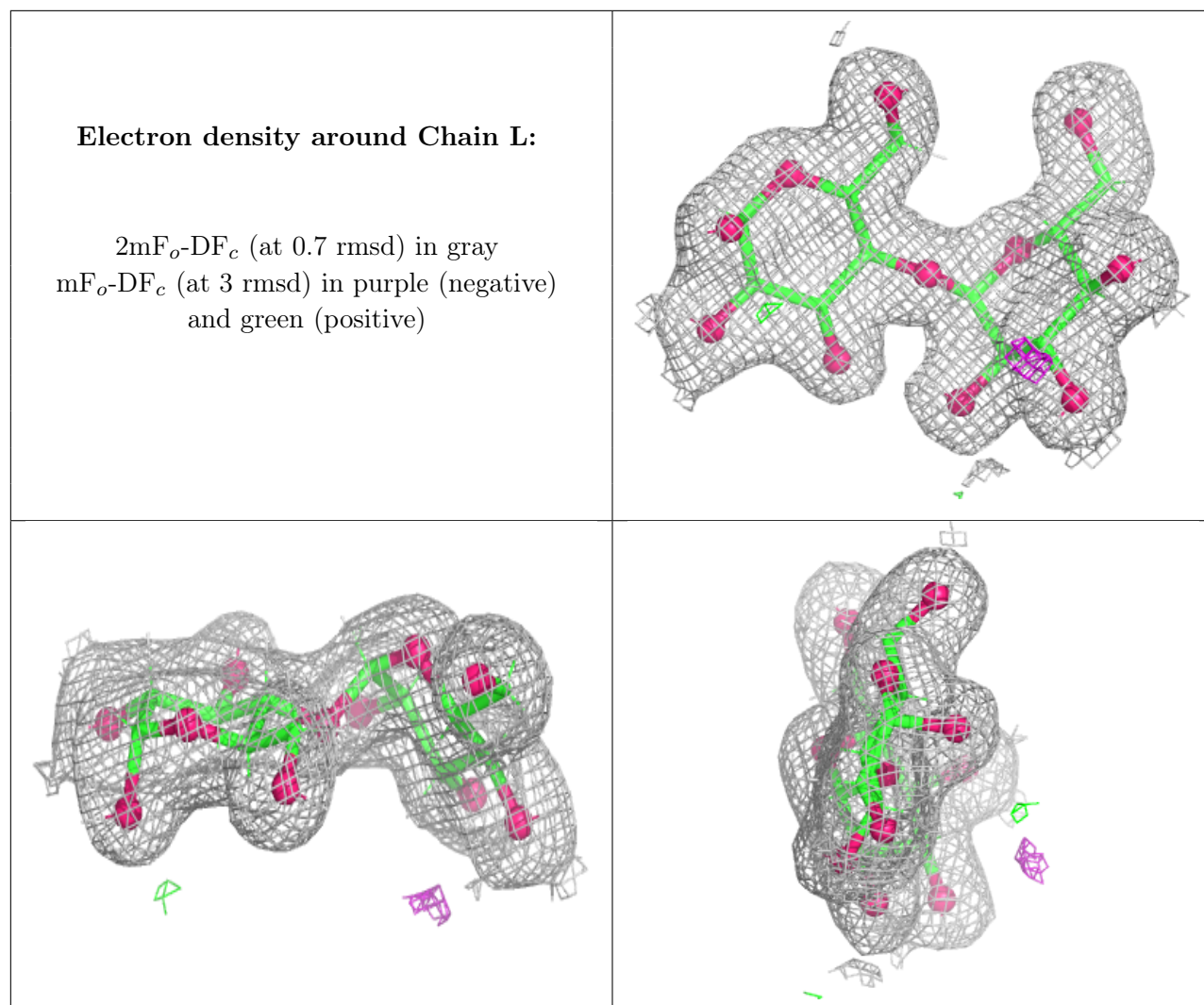
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around Chain K:**

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





## 6.4 Ligands [i](#)

There are no ligands in this entry.

## 6.5 Other polymers [i](#)

There are no such residues in this entry.