



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 23, 2024 – 10:30 AM EDT

PDB ID : 5IJD  
Title : The crystal structure of mouse TLR4/MD-2/lipid A complex  
Authors : Wang, Y.; Su, L.; Morin, M.D.; Jones, B.T.; Whitby, L.R.; Surakattula, M.; Huang, H.; Shi, H.; Choi, J.H.; Wang, K.; Moresco, E.M.; Berger, M.; Zhan, X.; Zhang, H.; Boger, D.L.; Beutler, B.  
Deposited on : 2016-03-01  
Resolution : 2.70 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 : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.36.1  
buster-report : 1.1.7 (2018)  
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) : 2.36.1

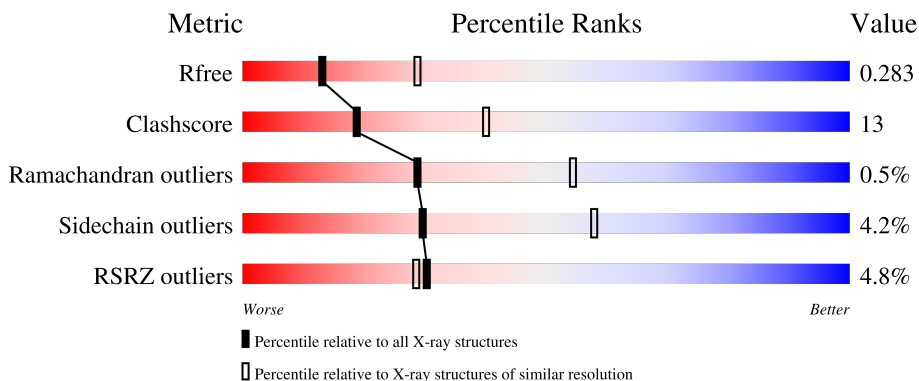
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.70 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))
$R_{free}$	130704	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)

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	594	
1	B	594	
2	C	150	
2	D	150	

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Mol	Chain	Length	Quality of chain
3	E	2	 100%
3	F	2	 100%
3	G	2	 50% 50%
3	H	2	 100%
3	I	2	 100%
3	J	2	 100%
3	K	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
3	NAG	E	2	X	-	-	-
3	NAG	G	1	X	-	-	-
3	NAG	H	2	X	-	-	-
3	NAG	J	1	X	-	-	-
3	NAG	J	2	X	-	-	-
3	NAG	K	2	X	-	-	-
4	NAG	B	705	X	-	-	-

## 2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 12385 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 Toll-like receptor 4, Variable lymphocyte receptor B chimera.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	590	4708	3011	784	889	24	0	1	0
1	B	592	4713	3014	783	891	25	0	0	0

- Molecule 2 is a protein called Lymphocyte antigen 96.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	C	137	1112	718	188	199	7	0	0	0
2	D	137	1112	718	188	199	7	0	0	0

There are 16 discrepancies between the modelled and reference sequences:

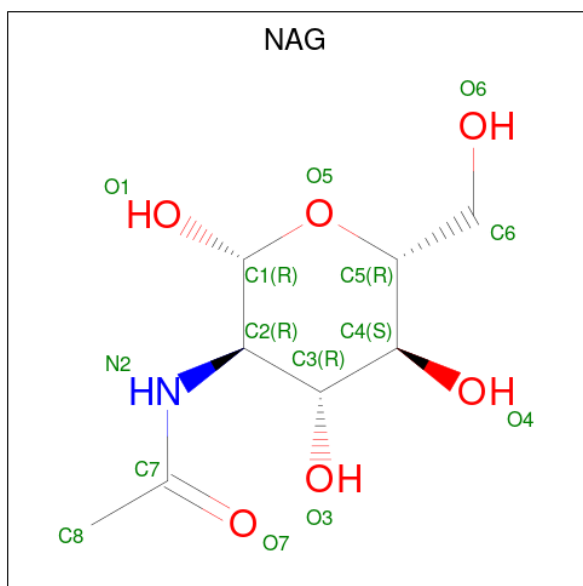
Chain	Residue	Modelled	Actual	Comment	Reference
C	161	LYS	-	cloning artifact	UNP Q9JHF9
C	162	GLY	-	cloning artifact	UNP Q9JHF9
C	163	GLU	-	cloning artifact	UNP Q9JHF9
C	164	ASN	-	cloning artifact	UNP Q9JHF9
C	165	LEU	-	cloning artifact	UNP Q9JHF9
C	166	TYR	-	cloning artifact	UNP Q9JHF9
C	167	PHE	-	cloning artifact	UNP Q9JHF9
C	168	GLN	-	cloning artifact	UNP Q9JHF9
D	161	LYS	-	cloning artifact	UNP Q9JHF9
D	162	GLY	-	cloning artifact	UNP Q9JHF9
D	163	GLU	-	cloning artifact	UNP Q9JHF9
D	164	ASN	-	cloning artifact	UNP Q9JHF9
D	165	LEU	-	cloning artifact	UNP Q9JHF9
D	166	TYR	-	cloning artifact	UNP Q9JHF9
D	167	PHE	-	cloning artifact	UNP Q9JHF9
D	168	GLN	-	cloning artifact	UNP Q9JHF9

- 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
			Total	C	N	O			
3	E	2	Total	C	N	O	0	0	0
			28	16	2	10			
3	F	2	Total	C	N	O	0	0	0
			28	16	2	10			
3	G	2	Total	C	N	O	0	0	0
			28	16	2	10			
3	H	2	Total	C	N	O	0	0	0
			28	16	2	10			
3	I	2	Total	C	N	O	0	0	0
			28	16	2	10			
3	J	2	Total	C	N	O	0	0	0
			28	16	2	10			
3	K	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula:  $C_8H_{15}NO_6$ ).



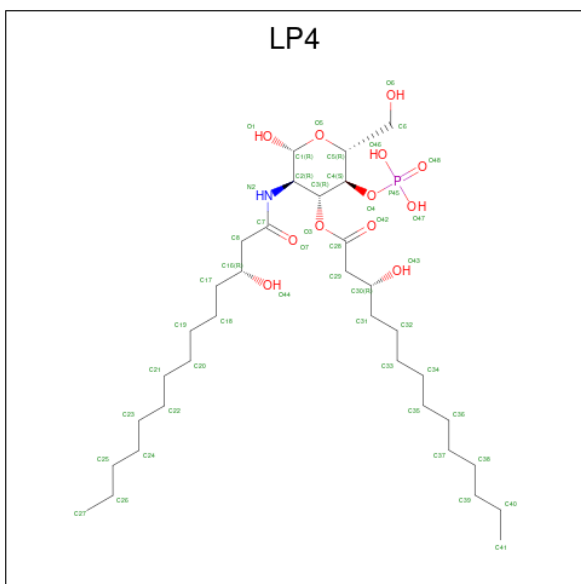
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
4	A	1	Total	C	N	O	0	0
			14	8	1	5		

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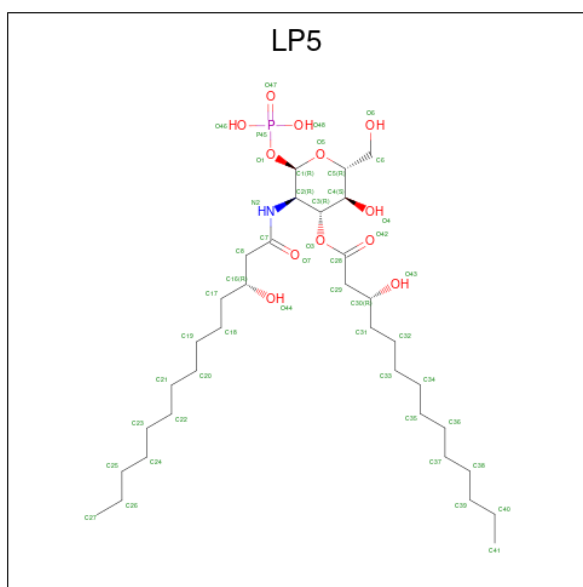
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			14	8	1	5		
4	C	1	Total	C	N	O	0	0
			14	8	1	5		
4	D	1	Total	C	N	O	0	0
			14	8	1	5		
4	B	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 5 is 2-deoxy-3-O-[(3R)-3-hydroxytetradecanoyl]-2-{[(3R)-3-hydroxytetradecanoylamino]-4-O-phosphono-beta-D-glucopyranose (three-letter code: LP4) (formula:  $C_{34}H_{66}NO_{12}P$ ).



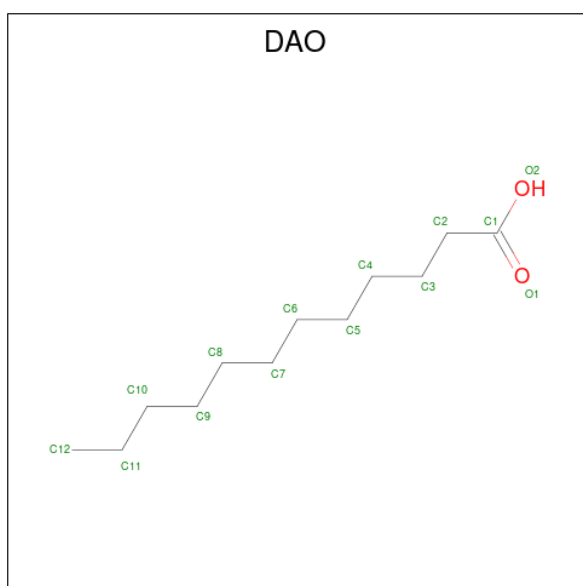
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	C	1	Total	C	N	O	P	0	0
			45	32	1	11	1		
5	D	1	Total	C	N	O	P	0	0
			45	32	1	11	1		

- Molecule 6 is (R)-((2R,3S,4R,5R,6R)-3-HYDROXY-2-(HYDROXYMETHYL)-5-((R)-3-HYDROXYTETRADECANAMIDO)-6-(PHOSPHONOOXY)Tetrahydro-2H-pyran-4-yl) 3-hydroxytetradecanoate (three-letter code: LP5) (formula:  $C_{34}H_{66}NO_{12}P$ ).



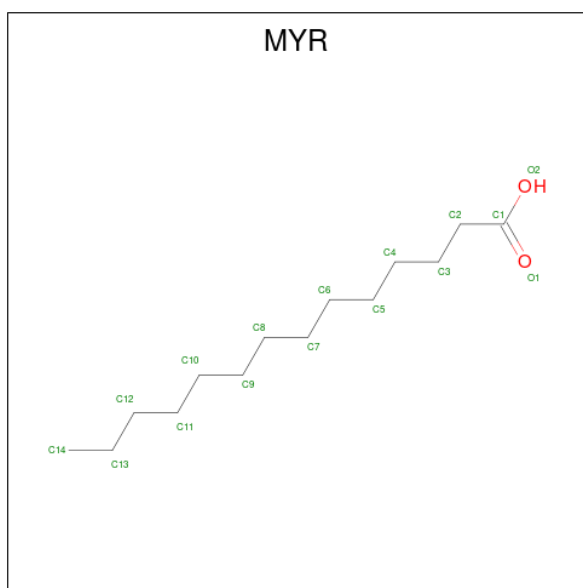
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
6	C	1	Total	C	N	O	P	0	0
			48	34	1	12	1		
6	D	1	Total	C	N	O	P	0	0
			48	34	1	12	1		

- Molecule 7 is LAURIC ACID (three-letter code: DAO) (formula:  $C_{12}H_{24}O_2$ ).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	
7	C	1	Total	C	O	0	0
			13	12	1		
7	D	1	Total	C	O	0	0
			13	12	1		

- Molecule 8 is MYRISTIC ACID (three-letter code: MYR) (formula: C<sub>14</sub>H<sub>28</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	C	1	Total C O 15 14 1	0	0
8	D	1	Total C O 15 14 1	0	0

- Molecule 9 is water.

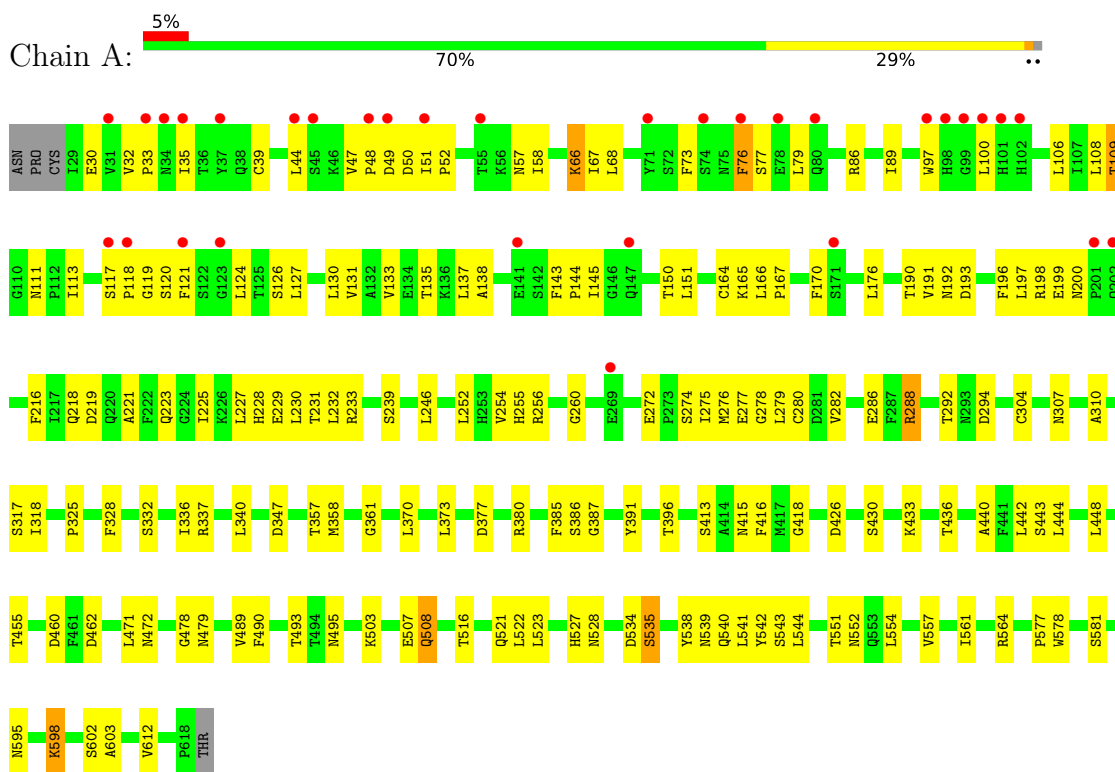
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	A	92	Total O 92 92	0	0
9	C	29	Total O 29 29	0	0
9	D	22	Total O 22 22	0	0
9	B	89	Total O 89 89	0	0



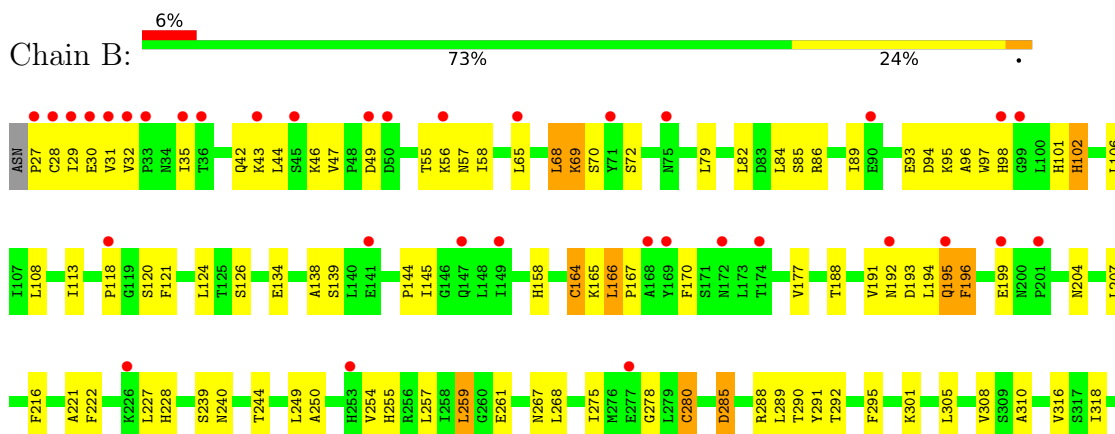
### 3 Residue-property plots [i](#)

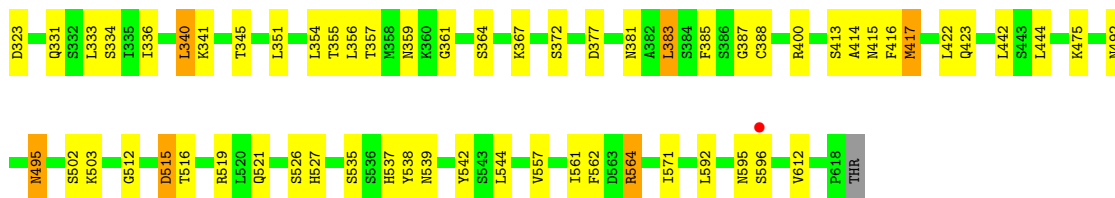
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Toll-like receptor 4, Variable lymphocyte receptor B chimera

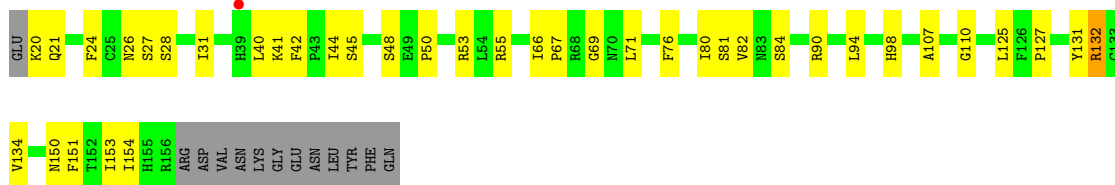


- Molecule 1: Toll-like receptor 4, Variable lymphocyte receptor B chimera

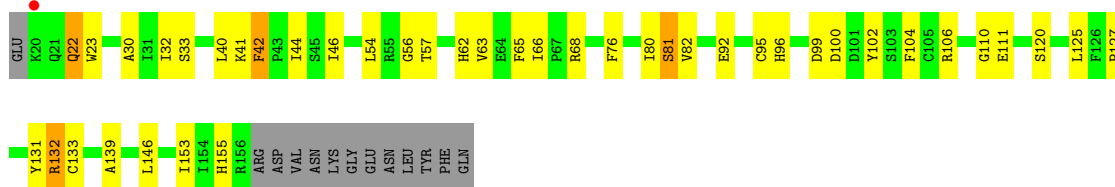




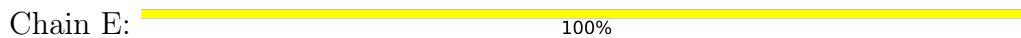
• Molecule 2: Lymphocyte antigen 96



• Molecule 2: Lymphocyte antigen 96



• 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



• 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 H:  100%

MAG1  
MAG2

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

Chain I:  100%


MAG1  
MAG2

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

Chain J:  100%

MAG1  
MAG2

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

Chain K:  50%

MAG1  
MAG2

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	66.84Å 145.74Å 136.19Å 90.00° 100.67° 90.00°	Depositor
Resolution (Å)	39.34 – 2.70 39.31 – 2.69	Depositor EDS
% Data completeness (in resolution range)	77.2 (39.34-2.70) 77.2 (39.31-2.69)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.39 (at 2.69Å)	Xtrriage
Refinement program	REFMAC 5.8.0049	Depositor
R, $R_{free}$	0.215 , 0.285 0.217 , 0.283	Depositor DCC
$R_{free}$ test set	1978 reflections (3.61%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	38.3	Xtrriage
Anisotropy	0.269	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 43.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.34$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	12385	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	44.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.08% of the height of the origin peak. No significant pseudotranslation is detected.*

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

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality [i](#)

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

Bond lengths and bond angles in the following residue types are not validated in this section: DAO, LP5, NAG, MYR, LP4

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	0.67	0/4811	0.81	3/6519 (0.0%)
1	B	0.63	0/4814	0.81	3/6524 (0.0%)
2	C	0.69	0/1143	0.85	0/1544
2	D	0.69	0/1143	0.83	0/1544
All	All	0.66	0/11911	0.82	6/16131 (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	2
1	B	0	1
2	C	0	1
All	All	0	4

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	32	VAL	N-CA-C	-8.56	87.90	111.00
1	A	288	ARG	NE-CZ-NH1	6.11	123.36	120.30
1	A	426	ASP	CB-CG-OD2	5.49	123.24	118.30
1	B	383	LEU	CA-CB-CG	5.40	127.72	115.30
1	B	31	VAL	N-CA-C	5.36	125.47	111.00
1	A	460	ASP	CB-CA-C	-5.35	99.70	110.40

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	278	GLY	Peptide
1	A	361	GLY	Peptide
1	B	361	GLY	Peptide
2	C	132	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	4708	0	4698	136	2
1	B	4713	0	4694	115	2
2	C	1112	0	1075	28	0
2	D	1112	0	1075	34	0
3	E	28	0	25	0	0
3	F	28	0	25	0	0
3	G	28	0	25	3	0
3	H	28	0	25	0	0
3	I	28	0	25	0	0
3	J	28	0	25	0	0
3	K	28	0	25	1	0
4	A	28	0	26	4	0
4	B	14	0	13	1	0
4	C	14	0	13	0	0
4	D	14	0	13	0	0
5	C	45	0	53	0	0
5	D	45	0	53	1	0
6	C	48	0	63	2	0
6	D	48	0	63	1	0
7	C	13	0	23	0	0
7	D	13	0	23	0	0
8	C	15	0	27	1	0
8	D	15	0	27	2	0
9	A	92	0	0	5	0
9	B	89	0	0	5	0
9	C	29	0	0	0	0
9	D	22	0	0	3	0
All	All	12385	0	12114	316	2

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 13.

All (316) 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)
5:D:804:LP4:C1	6:D:805:LP5:O6	1.64	1.44
1:A:117:SER:O	1:A:119:GLY:N	2.04	0.90
1:A:191:VAL:HG12	1:A:221:ALA:HA	1.55	0.85
1:B:261:GLU:OE2	1:B:267:ASN:HB3	1.77	0.83
1:B:255:HIS:ND1	1:B:285:ASP:OD2	2.12	0.83
2:C:21:GLN:HE21	2:C:24:PHE:HB3	1.44	0.82
1:B:29:ILE:HG22	1:B:30:GLU:N	1.92	0.82
1:A:252:LEU:HB3	1:A:282:VAL:HG23	1.65	0.78
1:B:387:GLY:HA2	1:B:413:SER:OG	1.84	0.78
1:B:170:PHE:HB2	1:B:196:PHE:CZ	2.20	0.76
1:B:29:ILE:HG22	1:B:30:GLU:H	1.51	0.74
1:B:340:LEU:HB2	1:B:359:ASN:HD21	1.53	0.72
1:B:97:TRP:HB3	1:B:124:LEU:HD21	1.71	0.72
1:A:433:LYS:HE2	9:A:872:HOH:O	1.90	0.71
1:B:170:PHE:CB	1:B:196:PHE:CZ	2.75	0.70
1:A:97:TRP:HB3	1:A:100:LEU:CD2	2.21	0.70
1:A:97:TRP:HB3	1:A:100:LEU:HD23	1.72	0.69
1:A:228:HIS:O	1:A:255:HIS:HB3	1.92	0.69
1:A:557:VAL:CG1	1:A:561:ILE:HG21	2.23	0.69
1:B:29:ILE:CG2	1:B:30:GLU:H	2.05	0.69
1:A:106:LEU:HD11	1:A:108:LEU:HD21	1.75	0.68
1:B:612:VAL:HA	9:B:872:HOH:O	1.92	0.68
1:B:29:ILE:CG2	1:B:30:GLU:N	2.57	0.68
1:A:292:THR:HG22	1:A:294:ASP:O	1.93	0.68
1:A:479:ASN:O	9:A:801:HOH:O	2.13	0.67
1:B:557:VAL:CG1	1:B:561:ILE:HG21	2.24	0.67
1:B:69:LYS:O	1:B:72:SER:HB2	1.96	0.66
1:A:51:ILE:HG23	1:A:52:PRO:HD2	1.78	0.65
1:A:66:LYS:HA	1:A:89:ILE:HA	1.77	0.65
1:B:240:ASN:O	1:B:244:THR:HG22	1.96	0.65
1:A:279:LEU:HA	1:A:282:VAL:HG12	1.79	0.65
1:B:35:ILE:HG23	1:B:56:LYS:HE2	1.80	0.64
1:A:32:VAL:CG1	1:A:35:ILE:CG2	2.76	0.64
2:D:82:VAL:HG22	2:D:131:TYR:CE2	2.33	0.64
1:A:76:PHE:CD1	1:A:76:PHE:N	2.66	0.63
3:G:1:NAG:O3	3:G:1:NAG:H82	1.99	0.62
1:A:239:SER:OG	1:A:275:ILE:HD11	1.99	0.62
2:D:99:ASP:OD1	1:B:288:ARG:NH1	2.32	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:32:VAL:HG12	1:A:35:ILE:HG22	1.82	0.62
1:B:46:LYS:HA	1:B:65:LEU:HD22	1.81	0.62
2:D:66:ILE:HG13	2:D:111:GLU:O	1.99	0.62
1:A:522:LEU:C	1:A:522:LEU:HD23	2.19	0.62
1:A:109:THR:HG22	1:A:131:VAL:HG12	1.82	0.61
2:C:82:VAL:HG21	6:C:205:LP5:H272	1.83	0.61
1:A:164:CYS:O	1:A:166:LEU:HD12	2.01	0.61
1:B:55:THR:HG21	1:B:58:ILE:CD1	2.31	0.60
1:A:337[B]:ARG:NH1	2:C:98:HIS:O	2.35	0.60
2:D:153:ILE:N	2:D:153:ILE:HD12	2.17	0.60
1:A:252:LEU:HB3	1:A:282:VAL:CG2	2.31	0.60
1:A:30:GLU:OE1	1:A:33:PRO:HA	2.02	0.60
1:B:82:LEU:HD23	1:B:106:LEU:HD13	1.84	0.60
2:C:71:LEU:HD12	2:C:107:ALA:HB3	1.83	0.59
1:B:194:LEU:HD21	1:B:222:PHE:CE1	2.38	0.59
1:A:32:VAL:HG12	1:A:35:ILE:CG2	2.33	0.58
1:B:516:THR:O	1:B:516:THR:HG22	2.03	0.58
1:B:82:LEU:HD21	1:B:84:LEU:HD11	1.86	0.57
9:B:805:HOH:O	3:K:1:NAG:H83	2.03	0.57
4:A:704:NAG:H82	4:A:704:NAG:O3	2.04	0.57
2:D:30:ALA:HB1	2:D:32:ILE:HD12	1.86	0.57
1:A:121:PHE:CZ	1:A:130:LEU:HD21	2.39	0.57
1:B:592:LEU:O	1:B:596:SER:N	2.37	0.57
1:A:239:SER:OG	1:A:275:ILE:CD1	2.52	0.57
1:A:280:CYS:HB3	1:A:304:CYS:SG	2.45	0.56
1:B:55:THR:HG21	1:B:58:ILE:HD11	1.87	0.56
1:A:307:ASN:HD22	4:A:703:NAG:H83	1.70	0.56
1:B:166:LEU:HD12	1:B:166:LEU:N	2.20	0.56
1:B:257:LEU:HD21	1:B:259:LEU:HD22	1.87	0.56
1:B:79:LEU:O	1:B:102:HIS:O	2.24	0.56
1:B:331:GLN:O	1:B:351:LEU:HD12	2.06	0.56
1:B:170:PHE:HB3	1:B:196:PHE:CZ	2.41	0.56
1:B:377:ASP:OD1	1:B:377:ASP:C	2.44	0.56
1:A:97:TRP:HA	1:A:100:LEU:HD22	1.87	0.55
2:C:82:VAL:HG22	2:C:131:TYR:CE2	2.41	0.55
1:A:49:ASP:OD1	1:A:50:ASP:N	2.39	0.55
1:A:557:VAL:HG13	1:A:561:ILE:HG21	1.88	0.55
1:A:436:THR:HG22	9:A:856:HOH:O	2.07	0.55
2:D:56:GLY:O	2:D:57:THR:OG1	2.21	0.55
4:A:704:NAG:C8	9:D:916:HOH:O	2.54	0.55
1:B:336:ILE:HG12	1:B:357:THR:HG22	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:89:ILE:HG22	1:A:113:ILE:HG22	1.89	0.55
1:A:280:CYS:CB	1:A:304:CYS:SG	2.95	0.55
1:B:537:HIS:HB2	1:B:538:TYR:CE2	2.42	0.55
1:A:325:PRO:HG2	1:A:328:PHE:CE1	2.42	0.54
1:A:73:PHE:HE1	1:A:100:LEU:HD21	1.73	0.54
2:D:96:HIS:N	2:D:100:ASP:OD2	2.37	0.54
1:A:336:ILE:HG12	1:A:357:THR:HG22	1.90	0.54
1:A:97:TRP:CA	1:A:100:LEU:HD22	2.38	0.54
1:A:256:ARG:NE	1:A:286:GLU:OE2	2.32	0.54
1:B:571:ILE:HG23	1:B:571:ILE:O	2.07	0.54
1:A:503:LYS:HA	1:A:527:HIS:O	2.08	0.54
1:B:492:ASN:HB2	9:B:883:HOH:O	2.08	0.54
2:D:42:PHE:CD2	2:D:68:ARG:HG3	2.43	0.54
2:D:95:CYS:HA	2:D:100:ASP:OD2	2.08	0.53
1:A:231:THR:HG21	9:A:864:HOH:O	2.07	0.53
1:B:27:PRO:O	1:B:28:CYS:HB2	2.08	0.53
1:A:538:TYR:HA	1:A:541:LEU:HD12	1.91	0.53
1:A:539:ASN:OD1	1:A:539:ASN:C	2.46	0.53
4:A:704:NAG:H5	9:A:871:HOH:O	2.08	0.53
1:B:165:LYS:CB	1:B:193:ASP:HA	2.39	0.53
1:A:68:LEU:HD13	1:A:97:TRP:CH2	2.44	0.53
1:A:336:ILE:HG12	1:A:357:THR:CG2	2.39	0.53
1:A:370:LEU:HD12	1:A:373:LEU:HD22	1.90	0.53
2:C:31:ILE:CG2	2:C:154:ILE:HB	2.39	0.53
1:A:280:CYS:HB3	1:A:304:CYS:CB	2.38	0.53
1:B:414:ALA:HB1	1:B:417:MET:HE1	1.92	0.52
1:B:188:THR:HA	1:B:216:PHE:O	2.09	0.52
2:C:27:SER:OG	2:C:28:SER:N	2.42	0.52
2:D:66:ILE:HD11	2:D:110:GLY:C	2.30	0.52
1:B:70:SER:HB2	1:B:95:LYS:HB3	1.91	0.52
2:D:30:ALA:HB1	2:D:32:ILE:CD1	2.40	0.52
1:B:188:THR:HG22	1:B:216:PHE:HB3	1.92	0.52
1:B:194:LEU:HD21	1:B:222:PHE:CD1	2.45	0.52
2:D:132:ARG:HG3	2:D:133:CYS:N	2.25	0.52
2:C:132:ARG:HD3	2:C:151:PHE:O	2.09	0.51
1:B:35:ILE:CG2	1:B:56:LYS:HE2	2.38	0.51
1:B:512:GLY:HA2	1:B:515:ASP:OD2	2.10	0.51
1:B:539:ASN:HA	1:B:564:ARG:HG3	1.91	0.51
2:C:127:PRO:O	2:C:131:TYR:OH	2.15	0.51
2:C:132:ARG:HD2	2:C:150:ASN:OD1	2.11	0.51
1:A:223:GLN:O	1:A:225:ILE:HD12	2.09	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:46:ILE:HD12	2:D:63:VAL:HG22	1.93	0.51
2:D:81:SER:HB3	9:D:910:HOH:O	2.11	0.51
1:A:121:PHE:CE1	1:A:130:LEU:CD2	2.94	0.50
2:C:67:PRO:HB2	2:C:69:GLY:O	2.11	0.50
1:B:170:PHE:HB3	1:B:196:PHE:HZ	1.77	0.50
1:A:121:PHE:CE1	1:A:130:LEU:HD22	2.47	0.50
2:C:132:ARG:NH1	3:G:1:NAG:H5	2.27	0.50
1:B:170:PHE:HB2	1:B:196:PHE:CE2	2.46	0.50
2:C:153:ILE:N	2:C:153:ILE:HD12	2.26	0.49
1:A:227:LEU:O	1:A:254:VAL:HA	2.13	0.49
2:C:21:GLN:NE2	2:C:24:PHE:HB3	2.21	0.49
1:A:109:THR:HB	1:A:133:VAL:HB	1.93	0.49
1:A:137:LEU:HD23	1:A:138:ALA:N	2.27	0.49
1:A:191:VAL:HG12	1:A:221:ALA:CA	2.37	0.49
1:A:416:PHE:HB3	1:A:444:LEU:HD21	1.93	0.49
1:A:430:SER:O	1:A:455:THR:HA	2.13	0.49
1:A:391:TYR:HB2	1:A:418:GLY:HA3	1.94	0.49
1:A:595:ASN:HB3	1:A:598:LYS:HG3	1.94	0.49
1:A:170:PHE:HB3	1:A:196:PHE:CZ	2.48	0.48
1:A:275:ILE:HG22	1:A:275:ILE:O	2.13	0.48
1:A:229:GLU:OE1	1:A:256:ARG:NH1	2.42	0.48
1:A:442:LEU:HD23	2:D:125:LEU:O	2.13	0.48
1:A:137:LEU:HD23	1:A:137:LEU:C	2.34	0.48
2:C:66:ILE:HG23	2:C:110:GLY:O	2.14	0.48
1:A:97:TRP:HB3	1:A:100:LEU:HD22	1.95	0.48
1:B:249:LEU:O	1:B:250:ALA:C	2.51	0.48
1:A:603:ALA:O	1:A:612:VAL:HG23	2.14	0.48
1:B:165:LYS:HB2	1:B:193:ASP:HA	1.95	0.48
1:A:252:LEU:CB	1:A:282:VAL:HG23	2.38	0.47
2:D:99:ASP:OD2	1:B:288:ARG:HD3	2.14	0.47
1:A:216:PHE:CZ	1:A:218:GLN:HA	2.49	0.47
1:A:256:ARG:HD3	1:A:288:ARG:HD2	1.95	0.47
1:B:94:ASP:O	1:B:95:LYS:CB	2.61	0.47
1:A:121:PHE:HE1	1:A:130:LEU:HD22	1.80	0.47
1:A:507:GLU:C	1:A:508:GLN:HG3	2.33	0.47
1:B:354:LEU:HD12	1:B:355:THR:N	2.29	0.47
1:B:475:LYS:HG2	9:B:821:HOH:O	2.14	0.47
2:D:41:LYS:O	2:D:42:PHE:C	2.52	0.47
1:B:495:ASN:N	1:B:495:ASN:OD1	2.47	0.47
1:A:274:SER:C	1:A:276:MET:H	2.18	0.47
1:A:387:GLY:HA2	1:A:413:SER:OG	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:44:ILE:HA	2:D:65:PHE:CB	2.45	0.47
1:B:121:PHE:CD2	1:B:145:ILE:HG22	2.49	0.47
1:B:177:VAL:HG12	1:B:177:VAL:O	2.15	0.47
1:B:502:SER:HA	1:B:526:SER:O	2.15	0.47
1:A:233:ARG:HA	1:A:260:GLY:O	2.14	0.47
2:D:127:PRO:O	2:D:131:TYR:OH	2.17	0.47
1:A:121:PHE:CZ	1:A:145:ILE:CG2	2.99	0.46
1:A:448:LEU:O	1:A:471:LEU:HD12	2.14	0.46
1:A:534:ASP:OD1	1:A:535:SER:N	2.49	0.46
2:D:102:TYR:HB3	2:D:104:PHE:CE2	2.50	0.46
1:B:134:GLU:HA	1:B:158:HIS:O	2.15	0.46
2:C:80:ILE:HG22	2:C:81:SER:N	2.30	0.46
1:B:191:VAL:HG12	1:B:221:ALA:HA	1.98	0.46
1:B:192:ASN:O	1:B:193:ASP:C	2.55	0.46
1:B:333:LEU:HD12	1:B:334:SER:H	1.81	0.46
1:A:117:SER:C	1:A:119:GLY:N	2.69	0.46
1:A:370:LEU:O	1:A:396:THR:HB	2.16	0.46
1:A:111:ASN:O	1:A:135:THR:HA	2.16	0.46
1:B:227:LEU:O	1:B:254:VAL:HA	2.16	0.46
1:A:246:LEU:HD13	1:A:279:LEU:HD11	1.98	0.45
2:C:53:ARG:HE	2:C:55:ARG:HB3	1.80	0.45
1:A:190:THR:O	1:A:193:ASP:HB2	2.16	0.45
1:A:272:GLU:O	1:A:275:ILE:HG13	2.16	0.45
1:A:377:ASP:C	1:A:377:ASP:OD1	2.54	0.45
1:B:56:LYS:HG3	1:B:57:ASN:HD22	1.80	0.45
1:A:540:GLN:HA	1:A:542:TYR:CE1	2.52	0.45
1:B:278:GLY:C	1:B:280:CYS:N	2.70	0.45
1:A:121:PHE:CE2	1:A:145:ILE:HG23	2.51	0.45
1:B:561:ILE:HG23	1:B:562:PHE:CD1	2.52	0.45
2:D:99:ASP:OD2	1:B:288:ARG:CD	2.65	0.45
1:B:192:ASN:O	1:B:195:GLN:HB3	2.17	0.45
1:B:207:LEU:HD12	1:B:227:LEU:HD11	1.97	0.45
1:A:557:VAL:CG1	1:A:561:ILE:CG2	2.94	0.45
2:C:45:SER:O	2:C:45:SER:OG	2.32	0.45
4:B:705:NAG:H5	9:B:852:HOH:O	2.16	0.45
1:A:166:LEU:HD12	1:A:166:LEU:N	2.32	0.45
1:B:503:LYS:HA	1:B:527:HIS:O	2.17	0.45
1:A:126:SER:HA	1:A:150:THR:HG21	1.99	0.44
1:A:286:GLU:HG2	1:A:310:ALA:HB3	1.99	0.44
1:A:66:LYS:O	1:A:67:ILE:HD13	2.18	0.44
1:A:462:ASP:HA	1:A:489:VAL:HG12	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:80:ILE:HG22	2:D:81:SER:N	2.30	0.44
1:B:166:LEU:HD12	1:B:166:LEU:H	1.82	0.44
1:B:289:LEU:HD21	1:B:295:PHE:HE1	1.82	0.44
1:B:308:VAL:HG12	1:B:310:ALA:H	1.83	0.44
1:A:44:LEU:HD21	1:A:48:PRO:HD3	1.99	0.44
1:A:280:CYS:HG	1:A:304:CYS:HG	1.11	0.44
1:B:519:ARG:HH11	1:B:519:ARG:HG3	1.82	0.44
1:A:137:LEU:HD12	1:A:143:PHE:CE1	2.53	0.44
1:A:276:MET:O	1:A:277:GLU:C	2.55	0.44
1:A:416:PHE:CB	1:A:444:LEU:HD21	2.48	0.44
1:A:522:LEU:HD23	1:A:523:LEU:N	2.33	0.44
1:A:554:LEU:O	1:A:577:PRO:HD2	2.17	0.44
1:B:118:PRO:HA	1:B:144:PRO:HB3	2.00	0.44
1:B:170:PHE:CB	1:B:196:PHE:CE2	2.99	0.44
1:A:415:ASN:O	1:A:443:SER:OG	2.35	0.44
2:D:100:ASP:CG	9:D:901:HOH:O	2.55	0.44
1:B:47:VAL:HG21	1:B:72:SER:OG	2.17	0.44
1:B:95:LYS:HA	1:B:98:HIS:CD2	2.53	0.44
1:B:354:LEU:HD12	1:B:355:THR:H	1.83	0.44
1:B:571:ILE:O	1:B:571:ILE:CG2	2.66	0.44
2:D:76:PHE:CZ	8:D:807:MYR:H132	2.53	0.44
2:D:139:ALA:HB2	2:D:146:LEU:HD11	2.00	0.44
1:B:415:ASN:N	1:B:417:MET:CE	2.81	0.44
1:A:97:TRP:CD1	1:A:120:SER:O	2.71	0.44
1:A:280:CYS:HB3	1:A:304:CYS:HB3	2.00	0.44
1:A:472:ASN:HA	1:A:495:ASN:O	2.18	0.44
1:B:195:GLN:O	1:B:196:PHE:HB2	2.18	0.44
1:B:557:VAL:HG13	1:B:561:ILE:HG21	1.98	0.44
1:A:124:LEU:HD12	1:A:127:LEU:HD13	1.99	0.44
1:A:478:GLY:HA2	1:A:503:LYS:O	2.17	0.44
1:A:540:GLN:HA	1:A:542:TYR:CZ	2.53	0.44
1:A:58:ILE:HD11	1:A:79:LEU:HD13	2.00	0.43
1:A:198:ARG:HG3	1:A:198:ARG:HH11	1.83	0.43
2:C:44:ILE:CG2	2:C:45:SER:N	2.81	0.43
1:B:68:LEU:HD13	1:B:89:ILE:HD13	2.00	0.43
1:B:138:ALA:O	1:B:139:SER:HB2	2.17	0.43
1:B:595:ASN:O	1:B:596:SER:C	2.56	0.43
1:B:164:CYS:SG	1:B:193:ASP:HB3	2.58	0.43
1:B:400:ARG:C	1:B:422:LEU:HD12	2.38	0.43
1:A:121:PHE:CE2	1:A:145:ILE:CG2	3.01	0.43
1:A:521:GLN:C	1:A:544:LEU:HD12	2.39	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:57:ASN:C	1:A:58:ILE:HG13	2.39	0.43
1:A:256:ARG:HA	1:A:286:GLU:O	2.18	0.43
6:C:205:LP5:O42	6:C:205:LP5:N2	2.52	0.43
2:D:22:GLN:O	2:D:23:TRP:HB2	2.18	0.43
2:D:92:GLU:HB3	8:D:807:MYR:H52	2.01	0.43
1:B:42:GLN:O	1:B:43:LYS:C	2.55	0.43
1:A:516:THR:HG22	1:A:516:THR:O	2.18	0.43
1:B:381:ASN:HB2	1:B:383:LEU:HB2	2.01	0.43
1:B:415:ASN:H	1:B:417:MET:CE	2.31	0.43
1:B:539:ASN:OD1	1:B:564:ARG:HD2	2.19	0.43
1:A:113:ILE:HG13	1:A:113:ILE:O	2.19	0.43
1:A:415:ASN:HB3	1:A:440:ALA:HA	2.00	0.43
2:C:44:ILE:HG22	2:C:45:SER:N	2.33	0.43
1:B:516:THR:O	1:B:516:THR:CG2	2.66	0.43
1:A:165:LYS:O	1:A:167:PRO:HD3	2.19	0.43
1:A:490:PHE:HA	1:A:493:THR:OG1	2.19	0.43
1:A:528:ASN:O	1:A:552:ASN:HA	2.19	0.43
2:C:20:LYS:O	2:C:21:GLN:C	2.56	0.43
2:D:82:VAL:HG22	2:D:131:TYR:CD2	2.53	0.43
1:B:416:PHE:HB3	1:B:444:LEU:HD21	2.01	0.43
1:B:255:HIS:CE1	1:B:285:ASP:OD2	2.71	0.42
1:A:68:LEU:HD13	1:A:97:TRP:HH2	1.84	0.42
1:B:70:SER:HA	1:B:96:ALA:HA	2.01	0.42
1:B:204:ASN:OD1	1:B:228:HIS:HB2	2.20	0.42
1:B:102:HIS:HA	1:B:126:SER:HB2	2.01	0.42
1:B:291:TYR:CG	1:B:292:THR:N	2.87	0.42
1:A:121:PHE:CE1	1:A:130:LEU:HD21	2.55	0.42
1:A:124:LEU:O	1:A:126:SER:N	2.52	0.42
1:A:252:LEU:HD23	1:A:282:VAL:HG21	2.01	0.42
1:A:557:VAL:HG23	1:A:578:TRP:HZ3	1.84	0.42
1:B:261:GLU:HG3	1:B:292:THR:HA	2.02	0.42
2:C:41:LYS:O	2:C:42:PHE:C	2.56	0.42
2:D:46:ILE:CD1	2:D:63:VAL:HG22	2.50	0.42
1:A:124:LEU:HB3	1:A:127:LEU:HB2	2.01	0.42
2:D:54:LEU:HD12	2:D:155:HIS:ND1	2.35	0.42
1:A:151:LEU:O	1:A:176:LEU:N	2.53	0.42
2:C:48:SER:OG	2:C:50:PRO:O	2.22	0.42
1:A:89:ILE:HG22	1:A:113:ILE:CG2	2.49	0.42
1:A:318:ILE:HG23	1:A:340:LEU:CD1	2.50	0.42
1:A:47:VAL:HG11	1:A:76:PHE:HE2	1.85	0.41
2:C:125:LEU:HG	1:B:442:LEU:HD23	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:285:ASP:OD1	1:B:285:ASP:N	2.53	0.41
3:G:1:NAG:O3	3:G:1:NAG:C8	2.68	0.41
1:A:358:MET:HA	1:A:380:ARG:O	2.20	0.41
1:B:94:ASP:O	1:B:95:LYS:HB2	2.20	0.41
1:B:521:GLN:HA	1:B:544:LEU:HA	2.01	0.41
1:B:301:LYS:HD3	1:B:323:ASP:O	2.21	0.41
1:B:535:SER:O	1:B:539:ASN:ND2	2.54	0.41
2:C:26:ASN:HB3	2:C:31:ILE:HG13	2.02	0.41
2:D:44:ILE:HA	2:D:65:PHE:HB3	2.03	0.41
1:A:143:PHE:HA	1:A:144:PRO:HD3	1.75	0.41
1:B:170:PHE:CB	1:B:196:PHE:HZ	2.30	0.41
1:B:195:GLN:O	1:B:196:PHE:CB	2.69	0.41
1:A:527:HIS:CD2	1:A:551:THR:HG21	2.56	0.41
1:B:85:SER:O	1:B:86:ARG:C	2.59	0.41
1:B:97:TRP:CD1	1:B:124:LEU:HD11	2.56	0.41
1:B:316:VAL:HG12	1:B:318:ILE:H	1.86	0.41
1:A:121:PHE:HZ	1:A:130:LEU:HD21	1.85	0.41
2:C:66:ILE:HA	2:C:67:PRO:HD2	1.95	0.41
2:C:76:PHE:CE2	8:C:207:MYR:H143	2.56	0.41
1:B:305:LEU:O	1:B:308:VAL:HG23	2.21	0.41
1:A:230:LEU:HD21	1:A:232:LEU:HD11	2.04	0.40
1:B:199:GLU:OE1	1:B:199:GLU:N	2.54	0.40
1:B:239:SER:HB3	1:B:275:ILE:HD11	2.03	0.40
1:A:106:LEU:CD1	1:A:108:LEU:HD21	2.49	0.40
2:D:32:ILE:CG2	2:D:33:SER:N	2.85	0.40
1:A:86:ARG:HG3	1:A:86:ARG:O	2.21	0.40
2:D:46:ILE:HA	2:D:62:HIS:O	2.21	0.40
1:A:199:GLU:O	1:A:200:ASN:CG	2.60	0.40
2:C:94:LEU:HD23	2:C:94:LEU:HA	1.93	0.40
2:D:92:GLU:OE2	2:D:92:GLU:HA	2.21	0.40
1:B:89:ILE:HG22	1:B:113:ILE:HD11	2.03	0.40
1:B:356:LEU:C	1:B:356:LEU:HD23	2.42	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:564:ARG:NH1	1:B:542:TYR:CD1[1_655]	2.15	0.05
1:A:540:GLN:O	1:B:519:ARG:NH2[1_655]	2.18	0.02

## 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	589/594 (99%)	516 (88%)	72 (12%)	1 (0%)	47	73
1	B	590/594 (99%)	521 (88%)	64 (11%)	5 (1%)	19	43
2	C	135/150 (90%)	119 (88%)	16 (12%)	0	100	100
2	D	135/150 (90%)	114 (84%)	20 (15%)	1 (1%)	22	46
All	All	1449/1488 (97%)	1270 (88%)	172 (12%)	7 (0%)	29	54

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	196	PHE
1	B	195	GLN
1	A	118	PRO
1	B	515	ASP
1	B	93	GLU
1	B	167	PRO
2	D	42	PHE

### 5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	548/551 (100%)	529 (96%)	19 (4%)	36	65
1	B	549/551 (100%)	522 (95%)	27 (5%)	25	52
2	C	124/136 (91%)	120 (97%)	4 (3%)	39	68

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
2	D	124/136 (91%)	118 (95%)	6 (5%)	25 53
All	All	1345/1374 (98%)	1289 (96%)	56 (4%)	30 58

All (56) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	39	CYS
1	A	66	LYS
1	A	76	PHE
1	A	77	SER
1	A	109	THR
1	A	192	ASN
1	A	197	LEU
1	A	219	ASP
1	A	317	SER
1	A	332	SER
1	A	347	ASP
1	A	385	PHE
1	A	386	SER
1	A	508	GLN
1	A	535	SER
1	A	543	SER
1	A	581	SER
1	A	598	LYS
1	A	602	SER
2	C	40	LEU
2	C	84	SER
2	C	90	ARG
2	C	134	VAL
2	D	22	GLN
2	D	40	LEU
2	D	81	SER
2	D	106	ARG
2	D	120	SER
2	D	132	ARG
1	B	44	LEU
1	B	49	ASP
1	B	68	LEU
1	B	69	LYS
1	B	101	HIS
1	B	102	HIS
1	B	108	LEU

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Mol	Chain	Res	Type
1	B	120	SER
1	B	164	CYS
1	B	166	LEU
1	B	259	LEU
1	B	268	LEU
1	B	280	CYS
1	B	285	ASP
1	B	290	THR
1	B	340	LEU
1	B	341	LYS
1	B	345	THR
1	B	364	SER
1	B	367	LYS
1	B	372	SER
1	B	385	PHE
1	B	388	CYS
1	B	417	MET
1	B	423	GLN
1	B	495	ASN
1	B	564	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
2	C	21	GLN
2	C	98	HIS
2	C	130	HIS
1	B	57	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

19 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond

length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	NAG	F	1	3,1	14,14,15	0.71	0	17,19,21	1.97	4 (23%)
3	NAG	G	1	2,3	14,14,15	0.72	0	17,19,21	2.20	7 (41%)
3	NAG	H	2	3	14,14,15	0.86	1 (7%)	17,19,21	1.54	2 (11%)
3	NAG	J	2	3	14,14,15	0.78	0	17,19,21	1.55	3 (17%)
3	NAG	E	1	3,1	14,14,15	0.57	0	17,19,21	1.36	3 (17%)
3	NAG	I	1	3,1	14,14,15	0.52	0	17,19,21	2.01	4 (23%)
3	NAG	G	2	3	14,14,15	0.57	0	17,19,21	1.88	5 (29%)
4	NAG	A	704	1	14,14,15	0.71	0	17,19,21	2.10	6 (35%)
4	NAG	A	703	1	14,14,15	0.59	0	17,19,21	2.31	6 (35%)
3	NAG	E	2	3	14,14,15	0.48	0	17,19,21	1.65	4 (23%)
3	NAG	K	1	3,1	14,14,15	0.94	1 (7%)	17,19,21	1.99	4 (23%)
3	NAG	J	1	3,1	14,14,15	0.80	0	17,19,21	2.00	5 (29%)
3	NAG	I	2	3	14,14,15	0.75	1 (7%)	17,19,21	1.60	4 (23%)
4	NAG	D	803	2	14,14,15	0.96	0	17,19,21	2.96	8 (47%)
3	NAG	K	2	3	14,14,15	0.73	0	17,19,21	1.50	2 (11%)
4	NAG	C	201	2	14,14,15	0.65	0	17,19,21	1.60	4 (23%)
3	NAG	H	1	2,3	14,14,15	0.77	1 (7%)	17,19,21	2.95	7 (41%)
4	NAG	B	705	1	14,14,15	1.30	3 (21%)	17,19,21	2.44	4 (23%)
3	NAG	F	2	3	14,14,15	0.61	0	17,19,21	1.14	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
3	NAG	F	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	G	1	2,3	1/1/5/7	4/6/23/26	0/1/1/1
3	NAG	H	2	3	1/1/5/7	4/6/23/26	0/1/1/1
3	NAG	J	2	3	1/1/5/7	2/6/23/26	0/1/1/1
3	NAG	E	1	3,1	-	2/6/23/26	0/1/1/1
3	NAG	I	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	G	2	3	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	A	704	1	-	4/6/23/26	0/1/1/1
4	NAG	A	703	1	-	3/6/23/26	0/1/1/1
3	NAG	E	2	3	1/1/5/7	2/6/23/26	0/1/1/1
3	NAG	K	1	3,1	-	2/6/23/26	0/1/1/1
3	NAG	J	1	3,1	1/1/5/7	2/6/23/26	0/1/1/1
3	NAG	I	2	3	-	4/6/23/26	0/1/1/1
4	NAG	D	803	2	-	3/6/23/26	0/1/1/1
3	NAG	K	2	3	1/1/5/7	4/6/23/26	0/1/1/1
4	NAG	C	201	2	-	2/6/23/26	0/1/1/1
3	NAG	H	1	2,3	-	4/6/23/26	0/1/1/1
4	NAG	B	705	1	1/1/5/7	4/6/23/26	0/1/1/1
3	NAG	F	2	3	-	3/6/23/26	0/1/1/1

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	705	NAG	C1-C2	2.95	1.56	1.52
3	K	1	NAG	C1-C2	2.70	1.56	1.52
4	B	705	NAG	C3-C2	2.55	1.57	1.52
4	B	705	NAG	O5-C1	-2.32	1.40	1.43
3	I	2	NAG	C1-C2	2.25	1.55	1.52
3	H	2	NAG	C1-C2	2.15	1.55	1.52
3	H	1	NAG	O5-C1	-2.04	1.40	1.43

All (83) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	H	1	NAG	C2-N2-C7	7.56	133.67	122.90
4	B	705	NAG	O5-C1-C2	-7.14	100.02	111.29
3	I	1	NAG	C1-O5-C5	6.54	121.05	112.19
4	D	803	NAG	C4-C3-C2	-5.86	102.42	111.02
3	H	1	NAG	C8-C7-N2	5.74	125.81	116.10
4	D	803	NAG	O5-C1-C2	-5.27	102.96	111.29
4	A	703	NAG	C1-O5-C5	5.03	119.01	112.19
3	F	1	NAG	C1-O5-C5	4.92	118.86	112.19
3	K	1	NAG	C8-C7-N2	4.90	124.39	116.10
3	G	1	NAG	C8-C7-N2	4.59	123.86	116.10
4	B	705	NAG	C4-C3-C2	4.58	117.73	111.02
3	J	2	NAG	C4-C3-C2	4.54	117.68	111.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	704	NAG	C4-C3-C2	-4.43	104.53	111.02
3	J	1	NAG	C4-C3-C2	4.28	117.29	111.02
4	D	803	NAG	C2-N2-C7	4.27	128.99	122.90
3	E	2	NAG	C4-C3-C2	-4.19	104.88	111.02
3	H	1	NAG	C1-C2-N2	-4.14	103.41	110.49
3	K	1	NAG	O7-C7-N2	-4.01	114.57	121.95
3	G	2	NAG	O5-C1-C2	-3.98	105.00	111.29
3	I	2	NAG	C1-O5-C5	3.93	117.51	112.19
4	A	703	NAG	C8-C7-N2	3.88	122.67	116.10
4	D	803	NAG	O3-C3-C2	3.86	117.44	109.47
4	D	803	NAG	C1-O5-C5	3.85	117.41	112.19
3	G	2	NAG	C3-C4-C5	3.75	116.92	110.24
3	K	2	NAG	C1-O5-C5	-3.71	107.17	112.19
4	D	803	NAG	C1-C2-N2	3.67	116.75	110.49
3	G	1	NAG	C2-N2-C7	3.61	128.04	122.90
4	A	704	NAG	C2-N2-C7	3.60	128.03	122.90
3	J	1	NAG	C3-C4-C5	3.57	116.61	110.24
4	B	705	NAG	O5-C5-C4	-3.56	102.17	110.83
3	H	2	NAG	C3-C4-C5	-3.45	104.08	110.24
4	A	703	NAG	C4-C3-C2	3.40	116.00	111.02
3	H	1	NAG	O7-C7-N2	-3.30	115.89	121.95
4	A	703	NAG	O7-C7-C8	-3.23	116.05	122.06
3	H	2	NAG	O5-C5-C4	-3.22	103.00	110.83
3	F	1	NAG	C4-C3-C2	-3.16	106.39	111.02
4	A	703	NAG	C2-N2-C7	3.15	127.39	122.90
4	A	704	NAG	C8-C7-N2	3.15	121.43	116.10
4	A	704	NAG	O3-C3-C2	3.14	115.97	109.47
3	G	1	NAG	O7-C7-C8	-3.10	116.31	122.06
3	F	1	NAG	O4-C4-C5	3.06	116.89	109.30
3	F	2	NAG	C1-O5-C5	3.05	116.33	112.19
4	C	201	NAG	C1-O5-C5	3.03	116.30	112.19
3	J	1	NAG	O4-C4-C5	3.02	116.79	109.30
3	G	2	NAG	C1-C2-N2	2.94	115.51	110.49
3	H	1	NAG	C1-O5-C5	2.91	116.13	112.19
3	E	2	NAG	C1-O5-C5	2.90	116.12	112.19
4	C	201	NAG	C4-C3-C2	-2.79	106.94	111.02
3	I	2	NAG	C3-C4-C5	-2.77	105.29	110.24
3	J	2	NAG	C1-O5-C5	2.76	115.93	112.19
4	A	704	NAG	O5-C5-C6	2.75	111.52	107.20
4	D	803	NAG	O5-C5-C6	2.73	111.48	107.20
3	K	1	NAG	C2-N2-C7	2.71	126.77	122.90
3	I	1	NAG	C4-C3-C2	-2.67	107.10	111.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	J	1	NAG	O5-C1-C2	-2.61	107.16	111.29
4	C	201	NAG	C1-C2-N2	2.59	114.91	110.49
3	E	2	NAG	O5-C1-C2	-2.56	107.24	111.29
3	E	1	NAG	O4-C4-C3	2.54	116.23	110.35
3	H	1	NAG	O3-C3-C2	2.54	114.72	109.47
3	G	2	NAG	C4-C3-C2	2.51	114.70	111.02
3	K	1	NAG	O4-C4-C5	2.50	115.50	109.30
4	B	705	NAG	O5-C5-C6	2.49	111.11	107.20
3	I	2	NAG	O5-C5-C6	2.48	111.09	107.20
4	A	703	NAG	O3-C3-C2	-2.44	104.42	109.47
3	G	1	NAG	O5-C5-C6	2.42	111.00	107.20
4	D	803	NAG	O5-C5-C4	2.41	116.68	110.83
3	I	1	NAG	O4-C4-C5	2.37	115.19	109.30
3	I	1	NAG	O4-C4-C3	2.34	115.77	110.35
3	G	1	NAG	O3-C3-C4	-2.33	104.95	110.35
4	C	201	NAG	O5-C1-C2	-2.31	107.64	111.29
3	E	1	NAG	C1-C2-N2	-2.29	106.58	110.49
3	I	2	NAG	O7-C7-C8	-2.28	117.81	122.06
3	E	2	NAG	C2-N2-C7	-2.22	119.74	122.90
3	G	1	NAG	O5-C1-C2	-2.21	107.79	111.29
3	E	1	NAG	O5-C5-C4	-2.18	105.52	110.83
3	J	2	NAG	C3-C4-C5	2.14	114.06	110.24
3	F	1	NAG	C2-N2-C7	-2.14	119.86	122.90
4	A	704	NAG	O4-C4-C5	2.13	114.58	109.30
3	K	2	NAG	O4-C4-C3	-2.08	105.53	110.35
3	G	1	NAG	C1-O5-C5	2.08	115.01	112.19
3	J	1	NAG	O7-C7-C8	-2.05	118.25	122.06
3	H	1	NAG	O7-C7-C8	-2.03	118.29	122.06
3	G	2	NAG	C8-C7-N2	2.02	119.52	116.10

All (7) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	E	2	NAG	C1
3	G	1	NAG	C1
3	H	2	NAG	C1
3	J	1	NAG	C1
3	J	2	NAG	C1
4	B	705	NAG	C1
3	K	2	NAG	C1

All (51) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	H	1	NAG	C3-C2-N2-C7
4	D	803	NAG	C3-C2-N2-C7
4	C	201	NAG	C4-C5-C6-O6
3	F	2	NAG	C1-C2-N2-C7
4	D	803	NAG	C4-C5-C6-O6
3	J	2	NAG	C4-C5-C6-O6
4	D	803	NAG	O5-C5-C6-O6
3	K	2	NAG	O5-C5-C6-O6
3	G	2	NAG	O5-C5-C6-O6
4	C	201	NAG	O5-C5-C6-O6
3	J	1	NAG	O5-C5-C6-O6
3	J	2	NAG	O5-C5-C6-O6
3	E	1	NAG	C1-C2-N2-C7
3	I	2	NAG	C1-C2-N2-C7
4	A	703	NAG	C8-C7-N2-C2
4	A	703	NAG	O7-C7-N2-C2
4	A	704	NAG	C8-C7-N2-C2
4	A	704	NAG	O7-C7-N2-C2
3	G	1	NAG	C8-C7-N2-C2
3	G	1	NAG	O7-C7-N2-C2
3	H	1	NAG	C8-C7-N2-C2
3	H	1	NAG	O7-C7-N2-C2
3	K	1	NAG	C8-C7-N2-C2
3	K	1	NAG	O7-C7-N2-C2
3	E	2	NAG	O5-C5-C6-O6
3	I	2	NAG	C4-C5-C6-O6
3	K	2	NAG	C4-C5-C6-O6
3	G	2	NAG	C4-C5-C6-O6
4	B	705	NAG	C1-C2-N2-C7
4	B	705	NAG	O5-C5-C6-O6
3	K	2	NAG	C1-C2-N2-C7
3	G	1	NAG	C1-C2-N2-C7
3	H	2	NAG	C1-C2-N2-C7
4	A	704	NAG	C1-C2-N2-C7
3	E	2	NAG	C4-C5-C6-O6
3	I	2	NAG	C3-C2-N2-C7
3	J	1	NAG	C4-C5-C6-O6
3	I	2	NAG	O5-C5-C6-O6
3	H	2	NAG	O5-C5-C6-O6
4	B	705	NAG	C4-C5-C6-O6
3	H	2	NAG	C4-C5-C6-O6
3	F	2	NAG	O5-C5-C6-O6
3	E	1	NAG	C3-C2-N2-C7

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Mol	Chain	Res	Type	Atoms
3	F	2	NAG	C3-C2-N2-C7
3	G	1	NAG	C3-C2-N2-C7
4	B	705	NAG	C3-C2-N2-C7
4	A	704	NAG	C4-C5-C6-O6
4	A	703	NAG	C4-C5-C6-O6
3	H	1	NAG	C1-C2-N2-C7
3	H	2	NAG	C3-C2-N2-C7
3	K	2	NAG	C3-C2-N2-C7

There are no ring outliers.

5 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	G	1	NAG	3	0
4	A	704	NAG	3	0
4	A	703	NAG	1	0
3	K	1	NAG	1	0
4	B	705	NAG	1	0

## 5.5 Carbohydrates [i](#)

14 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	E	1	3,1	14,14,15	0.57	0	17,19,21	1.36	3 (17%)
3	NAG	E	2	3	14,14,15	0.48	0	17,19,21	1.65	4 (23%)
3	NAG	F	1	3,1	14,14,15	0.71	0	17,19,21	1.97	4 (23%)
3	NAG	F	2	3	14,14,15	0.61	0	17,19,21	1.14	1 (5%)
3	NAG	G	1	2,3	14,14,15	0.72	0	17,19,21	2.20	7 (41%)
3	NAG	G	2	3	14,14,15	0.57	0	17,19,21	1.88	5 (29%)
3	NAG	H	1	2,3	14,14,15	0.77	1 (7%)	17,19,21	2.95	7 (41%)
3	NAG	H	2	3	14,14,15	0.86	1 (7%)	17,19,21	1.54	2 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	NAG	I	1	3,1	14,14,15	0.52	0	17,19,21	2.01	4 (23%)
3	NAG	I	2	3	14,14,15	0.75	1 (7%)	17,19,21	1.60	4 (23%)
3	NAG	J	1	3,1	14,14,15	0.80	0	17,19,21	2.00	5 (29%)
3	NAG	J	2	3	14,14,15	0.78	0	17,19,21	1.55	3 (17%)
3	NAG	K	1	3,1	14,14,15	0.94	1 (7%)	17,19,21	1.99	4 (23%)
3	NAG	K	2	3	14,14,15	0.73	0	17,19,21	1.50	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	E	1	3,1	-	2/6/23/26	0/1/1/1
3	NAG	E	2	3	1/1/5/7	2/6/23/26	0/1/1/1
3	NAG	F	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	F	2	3	-	3/6/23/26	0/1/1/1
3	NAG	G	1	2,3	1/1/5/7	4/6/23/26	0/1/1/1
3	NAG	G	2	3	-	2/6/23/26	0/1/1/1
3	NAG	H	1	2,3	-	4/6/23/26	0/1/1/1
3	NAG	H	2	3	1/1/5/7	4/6/23/26	0/1/1/1
3	NAG	I	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	I	2	3	-	4/6/23/26	0/1/1/1
3	NAG	J	1	3,1	1/1/5/7	2/6/23/26	0/1/1/1
3	NAG	J	2	3	1/1/5/7	2/6/23/26	0/1/1/1
3	NAG	K	1	3,1	-	2/6/23/26	0/1/1/1
3	NAG	K	2	3	1/1/5/7	4/6/23/26	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	K	1	NAG	C1-C2	2.70	1.56	1.52
3	I	2	NAG	C1-C2	2.25	1.55	1.52
3	H	2	NAG	C1-C2	2.15	1.55	1.52
3	H	1	NAG	O5-C1	-2.04	1.40	1.43

All (55) bond angle outliers are listed below:



Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	H	1	NAG	C2-N2-C7	7.56	133.67	122.90
3	I	1	NAG	C1-O5-C5	6.54	121.05	112.19
3	H	1	NAG	C8-C7-N2	5.74	125.81	116.10
3	F	1	NAG	C1-O5-C5	4.92	118.86	112.19
3	K	1	NAG	C8-C7-N2	4.90	124.39	116.10
3	G	1	NAG	C8-C7-N2	4.59	123.86	116.10
3	J	2	NAG	C4-C3-C2	4.54	117.68	111.02
3	J	1	NAG	C4-C3-C2	4.28	117.29	111.02
3	E	2	NAG	C4-C3-C2	-4.19	104.88	111.02
3	H	1	NAG	C1-C2-N2	-4.14	103.41	110.49
3	K	1	NAG	O7-C7-N2	-4.01	114.57	121.95
3	G	2	NAG	O5-C1-C2	-3.98	105.00	111.29
3	I	2	NAG	C1-O5-C5	3.93	117.51	112.19
3	G	2	NAG	C3-C4-C5	3.75	116.92	110.24
3	K	2	NAG	C1-O5-C5	-3.71	107.17	112.19
3	G	1	NAG	C2-N2-C7	3.61	128.04	122.90
3	J	1	NAG	C3-C4-C5	3.57	116.61	110.24
3	H	2	NAG	C3-C4-C5	-3.45	104.08	110.24
3	H	1	NAG	O7-C7-N2	-3.30	115.89	121.95
3	H	2	NAG	O5-C5-C4	-3.22	103.00	110.83
3	F	1	NAG	C4-C3-C2	-3.16	106.39	111.02
3	G	1	NAG	O7-C7-C8	-3.10	116.31	122.06
3	F	1	NAG	O4-C4-C5	3.06	116.89	109.30
3	F	2	NAG	C1-O5-C5	3.05	116.33	112.19
3	J	1	NAG	O4-C4-C5	3.02	116.79	109.30
3	G	2	NAG	C1-C2-N2	2.94	115.51	110.49
3	H	1	NAG	C1-O5-C5	2.91	116.13	112.19
3	E	2	NAG	C1-O5-C5	2.90	116.12	112.19
3	I	2	NAG	C3-C4-C5	-2.77	105.29	110.24
3	J	2	NAG	C1-O5-C5	2.76	115.93	112.19
3	K	1	NAG	C2-N2-C7	2.71	126.77	122.90
3	I	1	NAG	C4-C3-C2	-2.67	107.10	111.02
3	J	1	NAG	O5-C1-C2	-2.61	107.16	111.29
3	E	2	NAG	O5-C1-C2	-2.56	107.24	111.29
3	E	1	NAG	O4-C4-C3	2.54	116.23	110.35
3	H	1	NAG	O3-C3-C2	2.54	114.72	109.47
3	G	2	NAG	C4-C3-C2	2.51	114.70	111.02
3	K	1	NAG	O4-C4-C5	2.50	115.50	109.30
3	I	2	NAG	O5-C5-C6	2.48	111.09	107.20
3	G	1	NAG	O5-C5-C6	2.42	111.00	107.20
3	I	1	NAG	O4-C4-C5	2.37	115.19	109.30
3	I	1	NAG	O4-C4-C3	2.34	115.77	110.35
3	G	1	NAG	O3-C3-C4	-2.33	104.95	110.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	1	NAG	C1-C2-N2	-2.29	106.58	110.49
3	I	2	NAG	O7-C7-C8	-2.28	117.81	122.06
3	E	2	NAG	C2-N2-C7	-2.22	119.74	122.90
3	G	1	NAG	O5-C1-C2	-2.21	107.79	111.29
3	E	1	NAG	O5-C5-C4	-2.18	105.52	110.83
3	J	2	NAG	C3-C4-C5	2.14	114.06	110.24
3	F	1	NAG	C2-N2-C7	-2.14	119.86	122.90
3	K	2	NAG	O4-C4-C3	-2.08	105.53	110.35
3	G	1	NAG	C1-O5-C5	2.08	115.01	112.19
3	J	1	NAG	O7-C7-C8	-2.05	118.25	122.06
3	H	1	NAG	O7-C7-C8	-2.03	118.29	122.06
3	G	2	NAG	C8-C7-N2	2.02	119.52	116.10

All (6) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	E	2	NAG	C1
3	G	1	NAG	C1
3	H	2	NAG	C1
3	J	1	NAG	C1
3	J	2	NAG	C1
3	K	2	NAG	C1

All (35) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	H	1	NAG	C3-C2-N2-C7
3	F	2	NAG	C1-C2-N2-C7
3	J	2	NAG	C4-C5-C6-O6
3	K	2	NAG	O5-C5-C6-O6
3	G	2	NAG	O5-C5-C6-O6
3	J	1	NAG	O5-C5-C6-O6
3	J	2	NAG	O5-C5-C6-O6
3	E	1	NAG	C1-C2-N2-C7
3	I	2	NAG	C1-C2-N2-C7
3	G	1	NAG	C8-C7-N2-C2
3	G	1	NAG	O7-C7-N2-C2
3	H	1	NAG	C8-C7-N2-C2
3	H	1	NAG	O7-C7-N2-C2
3	K	1	NAG	C8-C7-N2-C2
3	K	1	NAG	O7-C7-N2-C2
3	E	2	NAG	O5-C5-C6-O6

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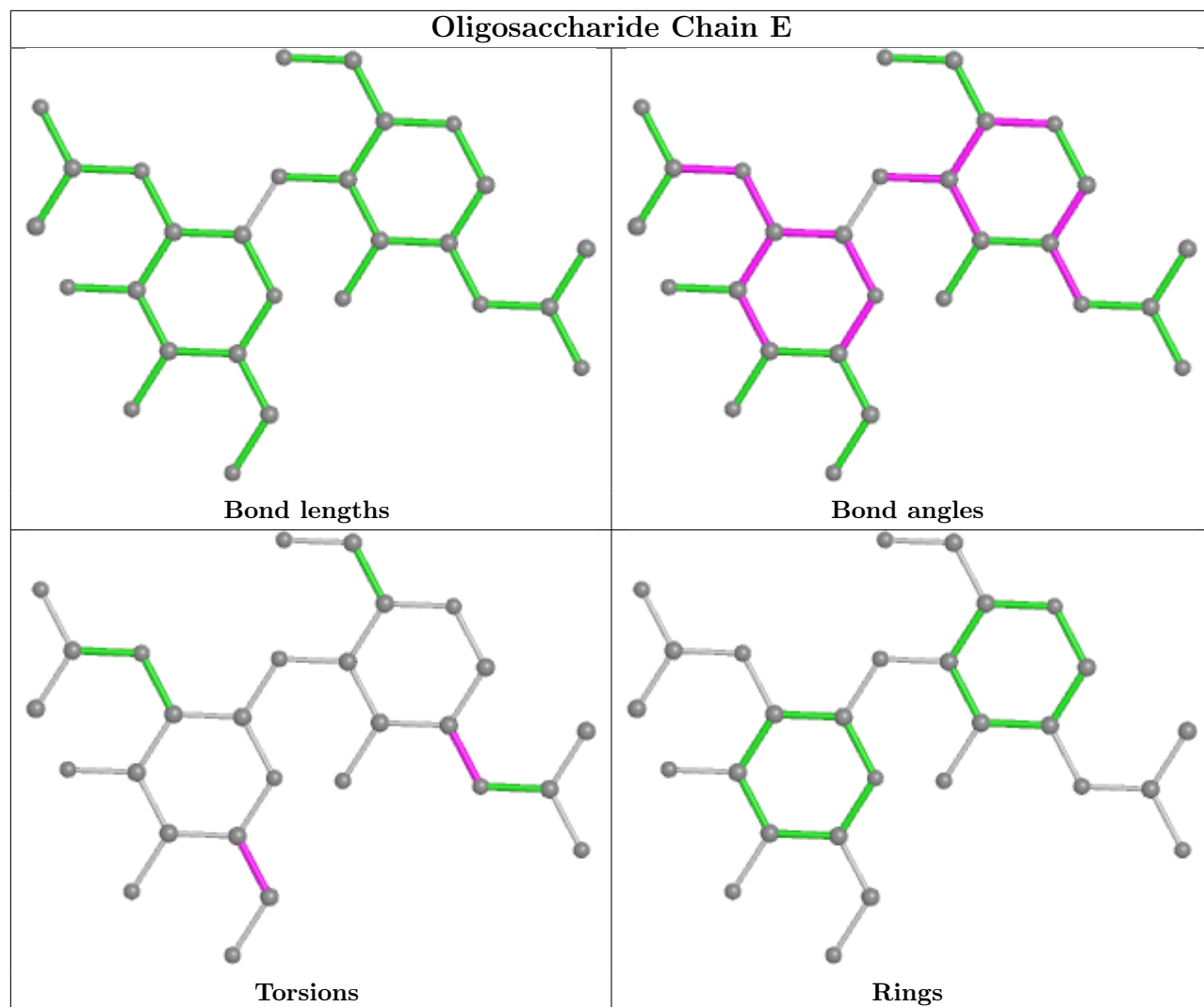
Mol	Chain	Res	Type	Atoms
3	I	2	NAG	C4-C5-C6-O6
3	K	2	NAG	C4-C5-C6-O6
3	G	2	NAG	C4-C5-C6-O6
3	K	2	NAG	C1-C2-N2-C7
3	G	1	NAG	C1-C2-N2-C7
3	H	2	NAG	C1-C2-N2-C7
3	E	2	NAG	C4-C5-C6-O6
3	I	2	NAG	C3-C2-N2-C7
3	J	1	NAG	C4-C5-C6-O6
3	I	2	NAG	O5-C5-C6-O6
3	H	2	NAG	O5-C5-C6-O6
3	H	2	NAG	C4-C5-C6-O6
3	F	2	NAG	O5-C5-C6-O6
3	E	1	NAG	C3-C2-N2-C7
3	F	2	NAG	C3-C2-N2-C7
3	G	1	NAG	C3-C2-N2-C7
3	H	1	NAG	C1-C2-N2-C7
3	H	2	NAG	C3-C2-N2-C7
3	K	2	NAG	C3-C2-N2-C7

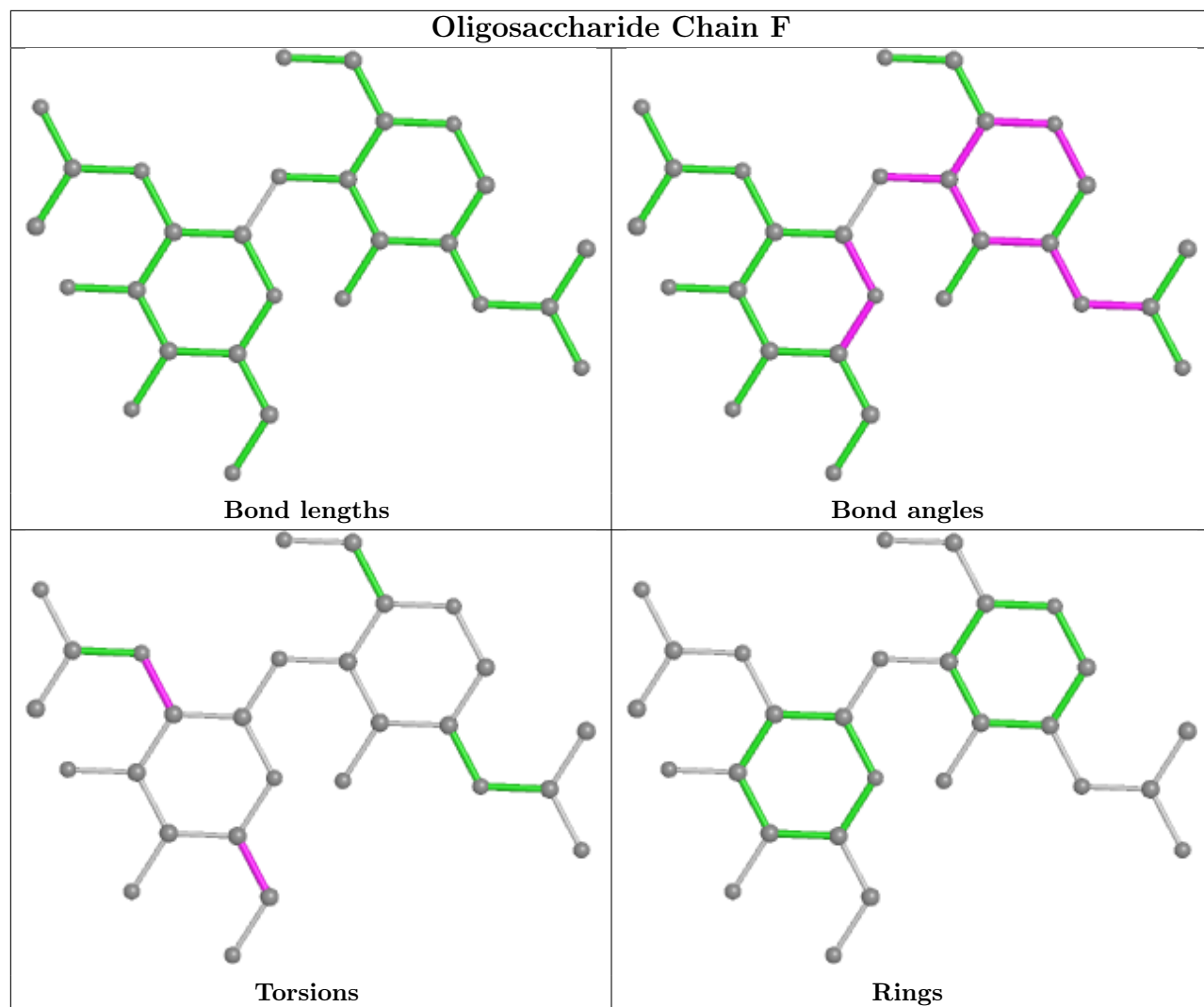
There are no ring outliers.

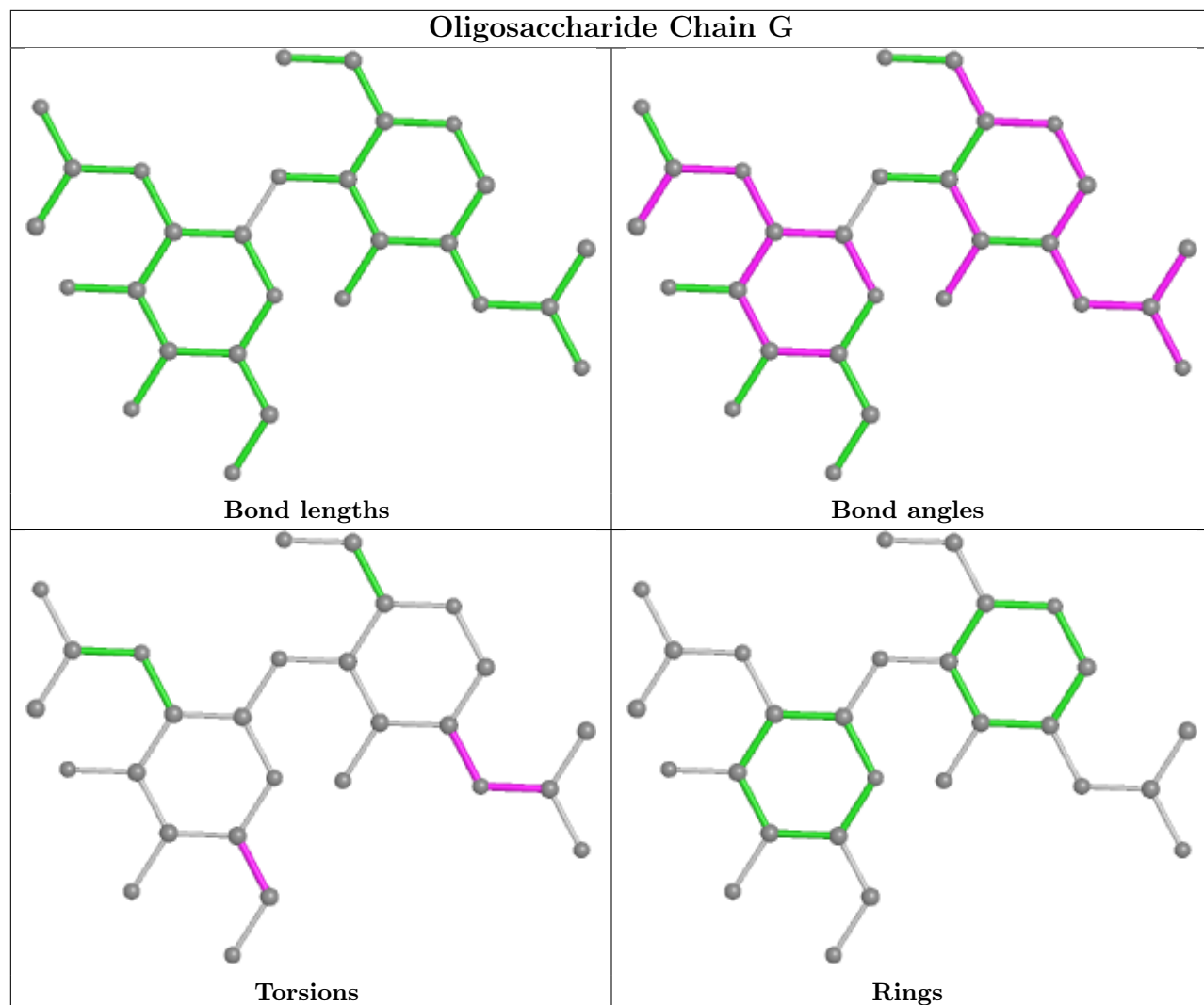
2 monomers are involved in 4 short contacts:

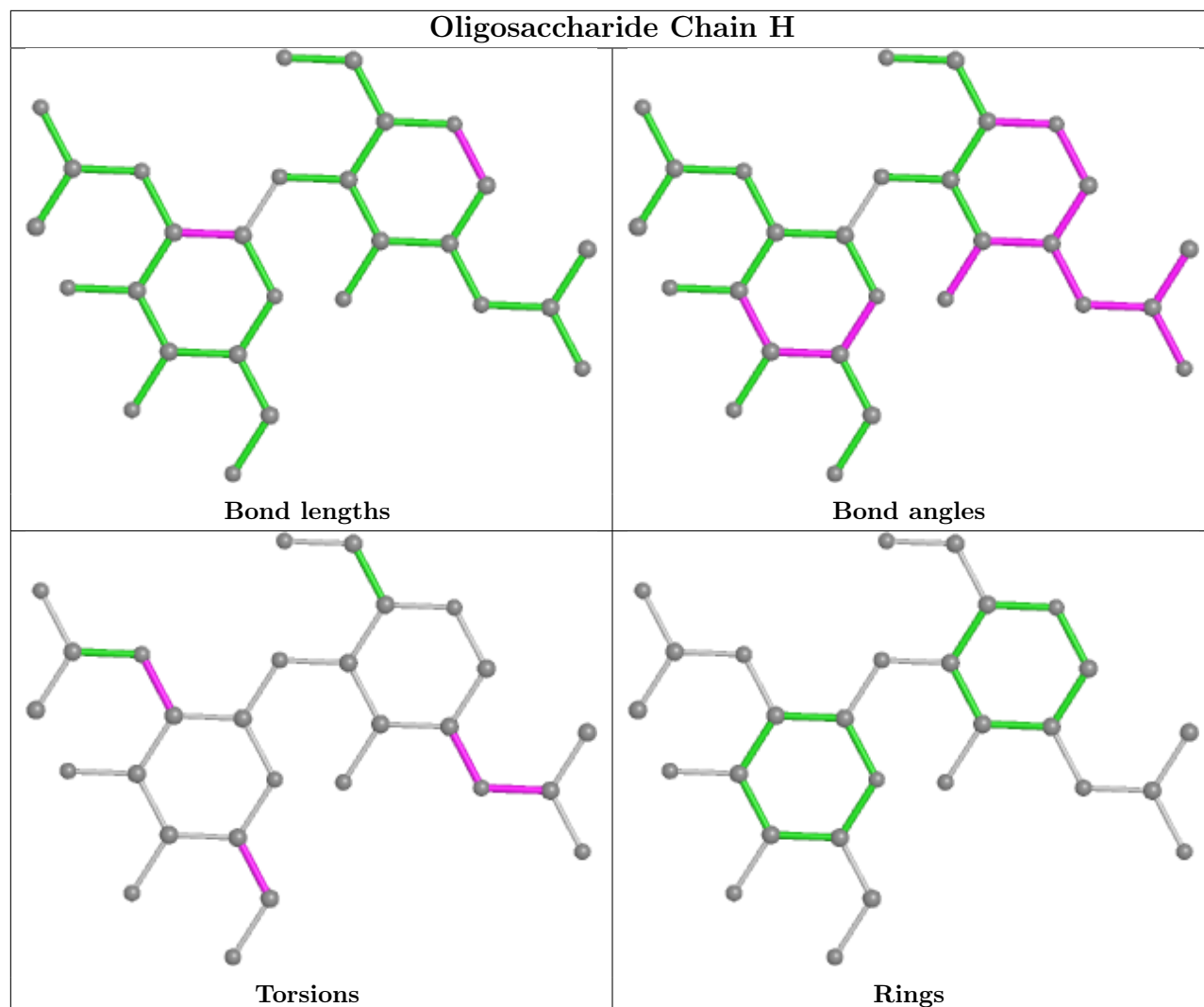
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	K	1	NAG	1	0
3	G	1	NAG	3	0

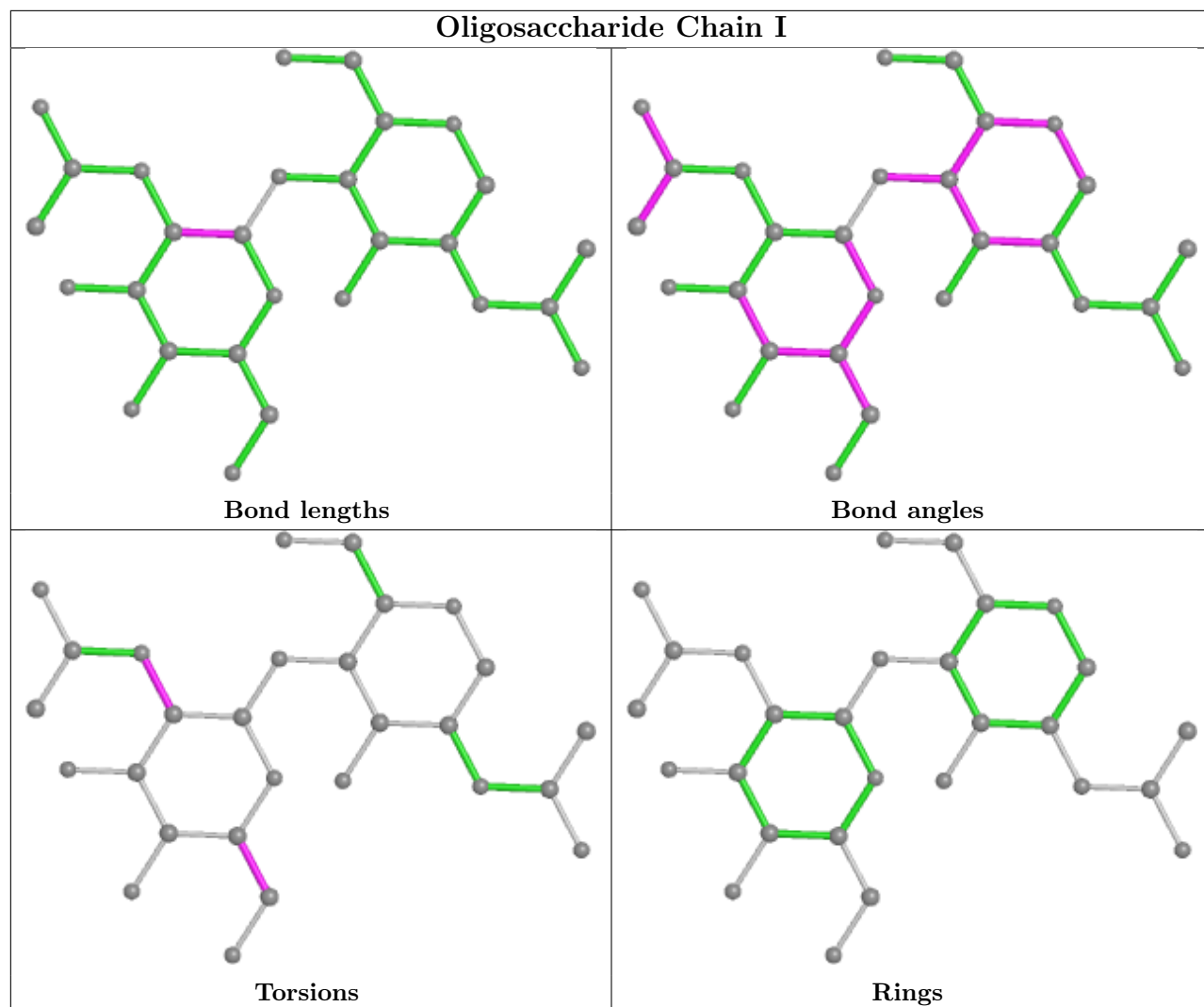
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.



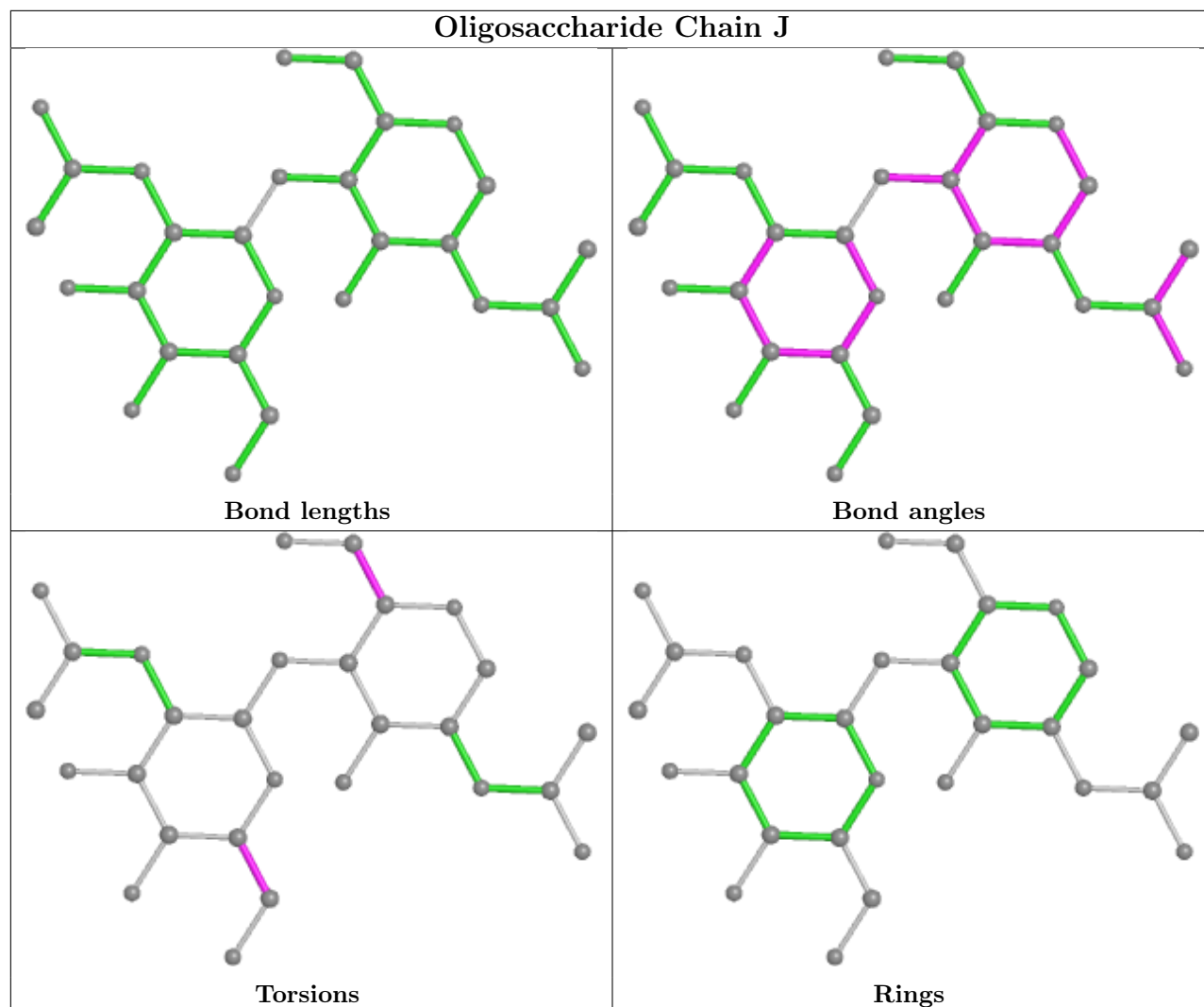


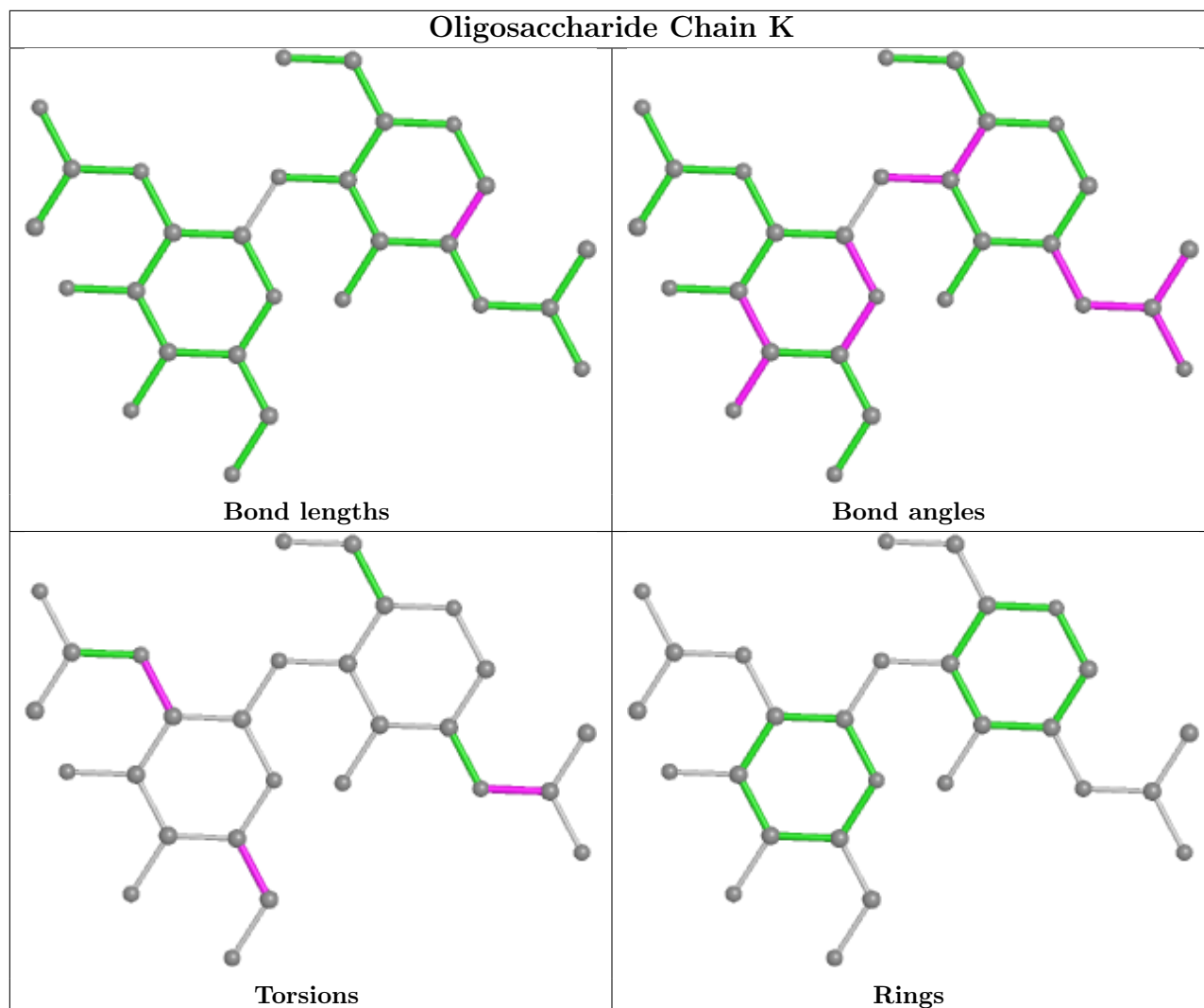












## 5.6 Ligand geometry [i](#)

13 ligands 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$
6	LP5	C	205	-	47,48,48	0.76	2 (4%)	57,60,60	1.27	4 (7%)
4	NAG	C	201	2	14,14,15	0.65	0	17,19,21	1.60	4 (23%)
4	NAG	B	705	1	14,14,15	1.30	3 (21%)	17,19,21	2.44	4 (23%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
7	DAO	C	206	-	12,12,13	0.51	0	11,11,13	0.85	1 (9%)
5	LP4	D	804	-	45,45,48	0.88	2 (4%)	54,56,60	1.59	8 (14%)
8	MYR	C	207	-	14,14,15	0.38	0	13,13,15	0.98	0
6	LP5	D	805	-	47,48,48	0.75	2 (4%)	57,60,60	1.32	6 (10%)
7	DAO	D	806	-	12,12,13	0.51	0	11,11,13	0.56	0
8	MYR	D	807	-	14,14,15	0.37	0	13,13,15	1.03	1 (7%)
4	NAG	A	704	1	14,14,15	0.71	0	17,19,21	2.10	6 (35%)
5	LP4	C	204	-	45,45,48	0.79	2 (4%)	54,56,60	1.75	13 (24%)
4	NAG	D	803	2	14,14,15	0.96	0	17,19,21	2.96	8 (47%)
4	NAG	A	703	1	14,14,15	0.59	0	17,19,21	2.31	6 (35%)

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
6	LP5	C	205	-	-	15/44/65/65	0/1/1/1
4	NAG	C	201	2	-	2/6/23/26	0/1/1/1
4	NAG	B	705	1	1/1/5/7	4/6/23/26	0/1/1/1
7	DAO	C	206	-	-	6/9/10/11	-
5	LP4	D	804	-	-	12/43/60/65	0/1/1/1
8	MYR	C	207	-	-	3/11/12/13	-
6	LP5	D	805	-	-	13/44/65/65	0/1/1/1
7	DAO	D	806	-	-	3/9/10/11	-
8	MYR	D	807	-	-	5/11/12/13	-
4	NAG	A	704	1	-	4/6/23/26	0/1/1/1
5	LP4	C	204	-	-	13/43/60/65	0/1/1/1
4	NAG	D	803	2	-	3/6/23/26	0/1/1/1
4	NAG	A	703	1	-	3/6/23/26	0/1/1/1

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	D	804	LP4	O3-C28	3.93	1.45	1.34
5	C	204	LP4	O3-C28	3.62	1.44	1.34
6	C	205	LP5	O3-C28	3.53	1.44	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	D	805	LP5	O3-C28	3.50	1.44	1.34
4	B	705	NAG	C1-C2	2.95	1.56	1.52
6	C	205	LP5	O3-C3	-2.65	1.40	1.44
4	B	705	NAG	C3-C2	2.55	1.57	1.52
5	D	804	LP4	O3-C3	-2.51	1.41	1.44
4	B	705	NAG	O5-C1	-2.32	1.40	1.43
6	D	805	LP5	O3-C3	-2.23	1.41	1.44
5	C	204	LP4	O3-C3	-2.22	1.41	1.44

All (61) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	705	NAG	O5-C1-C2	-7.14	100.02	111.29
4	D	803	NAG	C4-C3-C2	-5.86	102.42	111.02
4	D	803	NAG	O5-C1-C2	-5.27	102.96	111.29
4	A	703	NAG	C1-O5-C5	5.03	119.01	112.19
5	D	804	LP4	C1-C2-N2	-4.99	101.96	110.49
5	C	204	LP4	C1-C2-C3	-4.69	102.47	109.17
4	B	705	NAG	C4-C3-C2	4.58	117.73	111.02
4	A	704	NAG	C4-C3-C2	-4.43	104.53	111.02
6	D	805	LP5	C1-C2-N2	-4.38	103.45	111.00
5	C	204	LP4	C3-C2-N2	4.36	118.66	110.58
6	C	205	LP5	C1-C2-N2	-4.33	103.55	111.00
4	D	803	NAG	C2-N2-C7	4.27	128.99	122.90
5	D	804	LP4	C3-C2-N2	4.14	118.26	110.58
6	C	205	LP5	C3-C2-N2	3.96	117.48	110.91
4	A	703	NAG	C8-C7-N2	3.88	122.67	116.10
4	D	803	NAG	O3-C3-C2	3.86	117.44	109.47
4	D	803	NAG	C1-O5-C5	3.85	117.41	112.19
4	D	803	NAG	C1-C2-N2	3.67	116.75	110.49
4	A	704	NAG	C2-N2-C7	3.60	128.03	122.90
5	D	804	LP4	O3-C3-C4	-3.59	101.08	108.25
4	B	705	NAG	O5-C5-C4	-3.56	102.17	110.83
5	C	204	LP4	O5-C5-C6	3.51	112.71	107.20
5	C	204	LP4	C3-C4-C5	3.49	117.84	110.55
4	A	703	NAG	C4-C3-C2	3.40	116.00	111.02
5	C	204	LP4	O5-C1-C2	-3.32	106.05	111.29
4	A	703	NAG	O7-C7-C8	-3.23	116.05	122.06
4	A	703	NAG	C2-N2-C7	3.15	127.39	122.90
4	A	704	NAG	C8-C7-N2	3.15	121.43	116.10
4	A	704	NAG	O3-C3-C2	3.14	115.97	109.47
5	D	804	LP4	O7-C7-C8	-3.11	116.94	121.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	201	NAG	C1-O5-C5	3.03	116.30	112.19
6	D	805	LP5	O46-P45-O48	3.01	119.13	107.64
5	C	204	LP4	C4-C3-C2	-2.98	107.21	111.99
5	C	204	LP4	O3-C28-C29	2.88	116.75	111.46
4	C	201	NAG	C4-C3-C2	-2.79	106.94	111.02
5	C	204	LP4	C32-C31-C30	-2.77	106.87	114.85
4	A	704	NAG	O5-C5-C6	2.75	111.52	107.20
4	D	803	NAG	O5-C5-C6	2.73	111.48	107.20
5	C	204	LP4	O47-P45-O48	2.64	121.03	110.68
5	D	804	LP4	O5-C5-C6	2.61	111.29	107.20
4	C	201	NAG	C1-C2-N2	2.59	114.91	110.49
5	C	204	LP4	O3-C3-C2	2.53	112.81	108.38
4	B	705	NAG	O5-C5-C6	2.49	111.11	107.20
6	D	805	LP5	O3-C28-C29	2.49	116.03	111.46
6	C	205	LP5	O3-C28-C29	2.49	116.03	111.46
4	A	703	NAG	O3-C3-C2	-2.44	104.42	109.47
5	C	204	LP4	O3-C3-C4	-2.42	103.41	108.25
4	D	803	NAG	O5-C5-C4	2.41	116.68	110.83
5	C	204	LP4	C1-C2-N2	-2.40	106.38	110.49
6	D	805	LP5	O5-C1-C2	-2.40	105.89	110.58
5	D	804	LP4	O43-C30-C29	2.31	115.78	109.65
4	C	201	NAG	O5-C1-C2	-2.31	107.64	111.29
8	D	807	MYR	O1-C1-C2	-2.31	111.76	126.89
6	D	805	LP5	O1-C1-C2	-2.26	104.31	108.40
5	D	804	LP4	C31-C30-C29	-2.22	104.78	112.78
7	C	206	DAO	O1-C1-C2	-2.21	112.36	126.89
6	C	205	LP5	O48-P45-O47	2.21	119.35	110.68
4	A	704	NAG	O4-C4-C5	2.13	114.58	109.30
6	D	805	LP5	O43-C30-C31	2.13	115.29	109.21
5	C	204	LP4	C39-C38-C37	-2.10	103.75	114.42
5	D	804	LP4	C1-O5-C5	2.08	115.00	112.19

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	B	705	NAG	C1

All (86) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	D	803	NAG	C3-C2-N2-C7
5	C	204	LP4	C17-C16-C8-C7

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Mol	Chain	Res	Type	Atoms
5	C	204	LP4	O44-C16-C8-C7
5	C	204	LP4	C29-C30-C31-C32
5	C	204	LP4	O43-C30-C31-C32
5	D	804	LP4	C17-C16-C8-C7
5	D	804	LP4	O44-C16-C8-C7
5	D	804	LP4	C8-C16-C17-C18
5	D	804	LP4	O44-C16-C17-C18
5	D	804	LP4	C28-C29-C30-C31
5	D	804	LP4	C28-C29-C30-O43
6	D	805	LP5	C8-C16-C17-C18
8	D	807	MYR	C1-C2-C3-C4
4	C	201	NAG	C4-C5-C6-O6
4	D	803	NAG	C4-C5-C6-O6
4	D	803	NAG	O5-C5-C6-O6
4	C	201	NAG	O5-C5-C6-O6
6	C	205	LP5	C2-C3-O3-C28
4	A	703	NAG	C8-C7-N2-C2
4	A	703	NAG	O7-C7-N2-C2
4	A	704	NAG	C8-C7-N2-C2
4	A	704	NAG	O7-C7-N2-C2
6	C	205	LP5	O44-C16-C17-C18
6	D	805	LP5	O43-C30-C31-C32
6	C	205	LP5	C4-C3-O3-C28
6	C	205	LP5	C17-C18-C19-C20
8	D	807	MYR	C9-C10-C11-C12
6	D	805	LP5	C17-C18-C19-C20
7	C	206	DAO	C6-C7-C8-C9
5	D	804	LP4	C21-C22-C23-C24
4	B	705	NAG	C1-C2-N2-C7
4	B	705	NAG	O5-C5-C6-O6
6	D	805	LP5	C29-C28-O3-C3
8	C	207	MYR	C9-C10-C11-C12
6	C	205	LP5	C33-C34-C35-C36
5	C	204	LP4	C18-C19-C20-C21
5	C	204	LP4	C29-C28-O3-C3
5	C	204	LP4	O42-C28-O3-C3
6	D	805	LP5	O42-C28-O3-C3
8	D	807	MYR	C3-C4-C5-C6
4	A	704	NAG	C1-C2-N2-C7
7	D	806	DAO	C6-C7-C8-C9
6	C	205	LP5	O43-C30-C31-C32
6	D	805	LP5	C31-C32-C33-C34

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Mol	Chain	Res	Type	Atoms
6	D	805	LP5	C33-C34-C35-C36
7	C	206	DAO	C5-C6-C7-C8
5	C	204	LP4	C19-C20-C21-C22
6	C	205	LP5	C24-C25-C26-C27
6	D	805	LP5	C38-C39-C40-C41
5	C	204	LP4	C17-C18-C19-C20
8	C	207	MYR	C2-C3-C4-C5
6	D	805	LP5	O44-C16-C17-C18
6	C	205	LP5	C35-C36-C37-C38
6	D	805	LP5	C22-C23-C24-C25
7	C	206	DAO	C3-C4-C5-C6
5	D	804	LP4	C22-C23-C24-C25
5	C	204	LP4	C28-C29-C30-C31
6	C	205	LP5	C29-C28-O3-C3
5	C	204	LP4	O5-C5-C6-O6
8	C	207	MYR	C10-C11-C12-C13
8	D	807	MYR	C7-C8-C9-C10
5	D	804	LP4	C31-C32-C33-C34
4	B	705	NAG	C4-C5-C6-O6
5	D	804	LP4	C33-C34-C35-C36
6	C	205	LP5	C34-C35-C36-C37
7	C	206	DAO	C1-C2-C3-C4
6	C	205	LP5	C31-C32-C33-C34
6	D	805	LP5	C32-C33-C34-C35
7	C	206	DAO	C11-C10-C9-C8
6	C	205	LP5	O42-C28-O3-C3
7	D	806	DAO	C2-C3-C4-C5
4	B	705	NAG	C3-C2-N2-C7
6	D	805	LP5	C37-C38-C39-C40
7	C	206	DAO	C9-C10-C11-C12
5	D	804	LP4	C36-C37-C38-C39
4	A	704	NAG	C4-C5-C6-O6
6	C	205	LP5	C8-C16-C17-C18
5	D	804	LP4	C34-C35-C36-C37
6	C	205	LP5	C36-C37-C38-C39
6	D	805	LP5	C21-C22-C23-C24
4	A	703	NAG	C4-C5-C6-O6
5	C	204	LP4	C21-C22-C23-C24
6	C	205	LP5	C32-C33-C34-C35
8	D	807	MYR	C11-C12-C13-C14
5	C	204	LP4	C22-C23-C24-C25
7	D	806	DAO	C3-C4-C5-C6

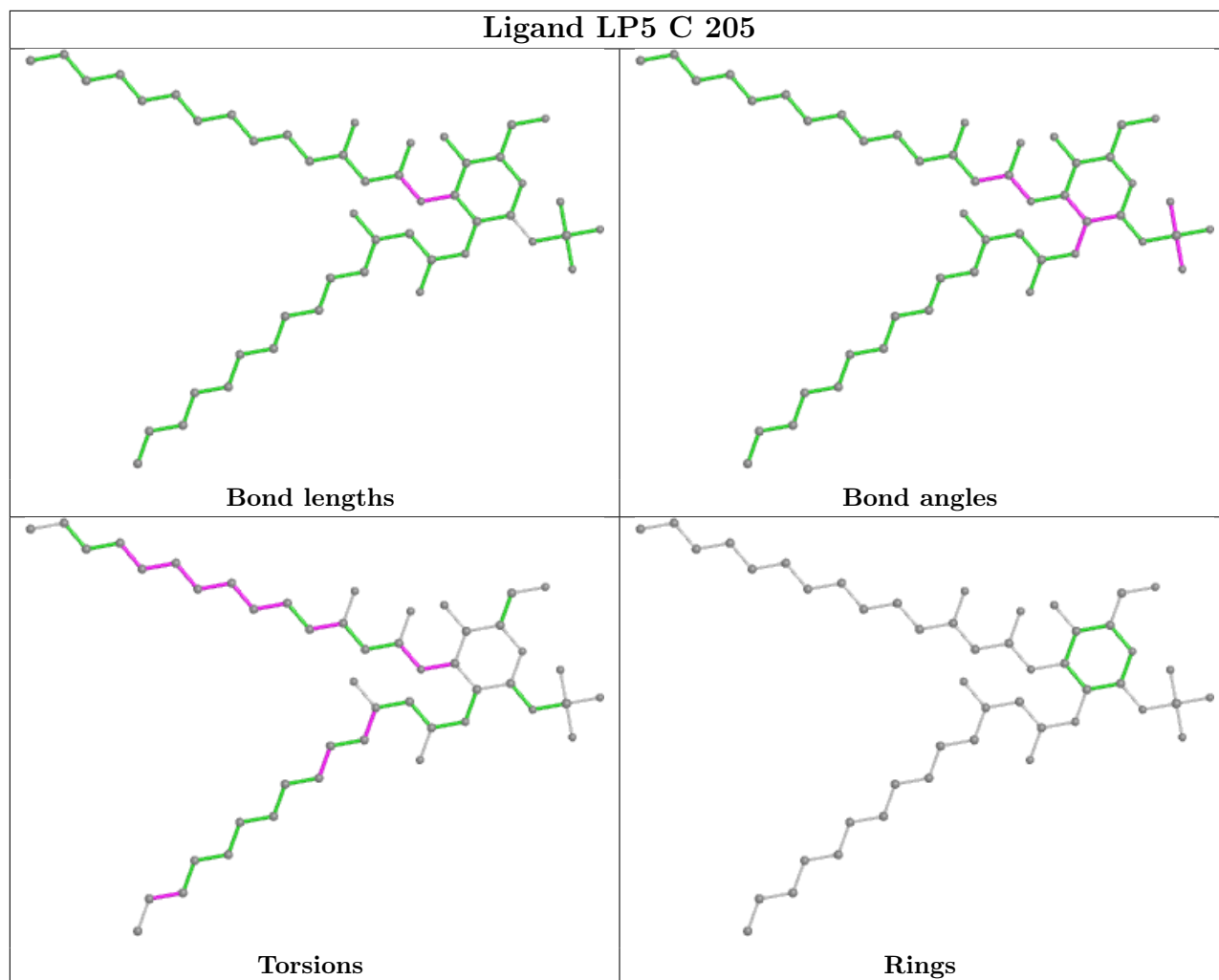
There are no ring outliers.

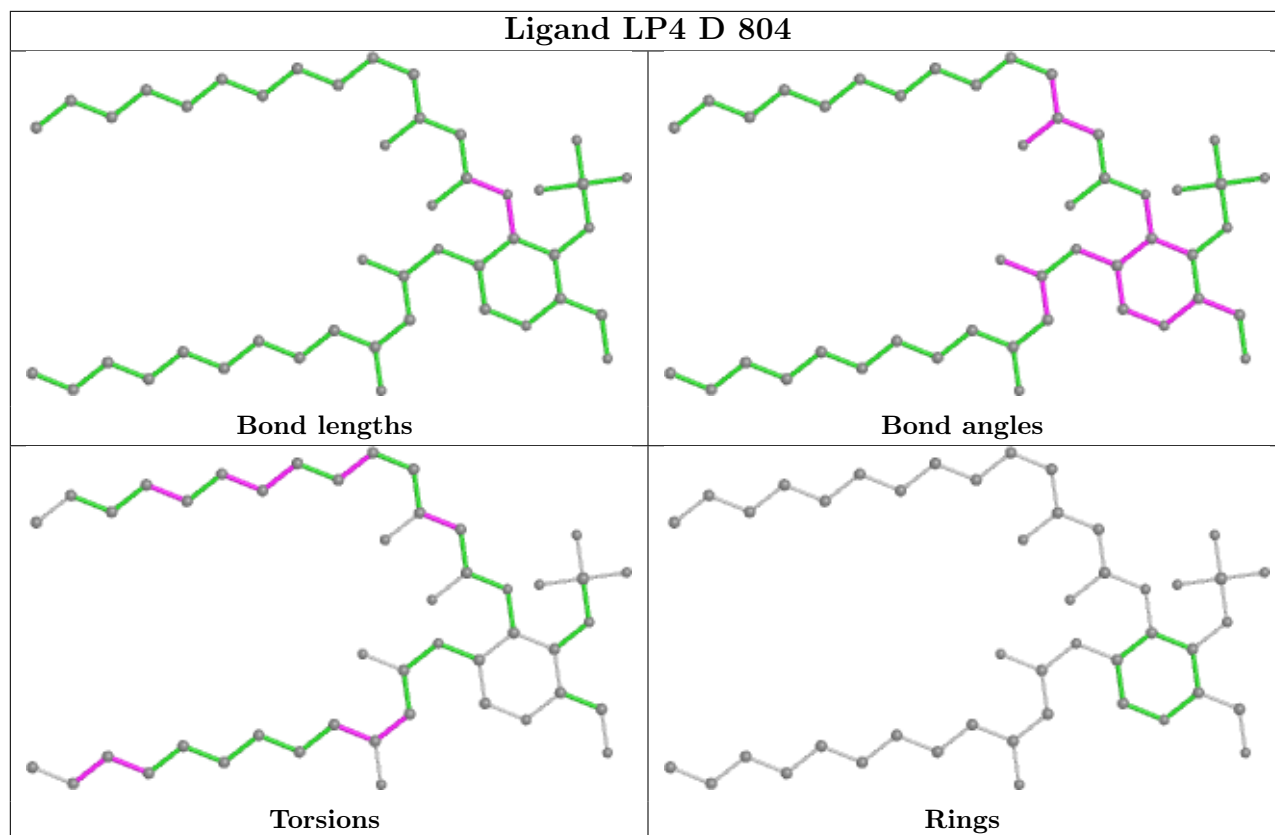
8 monomers are involved in 11 short contacts:

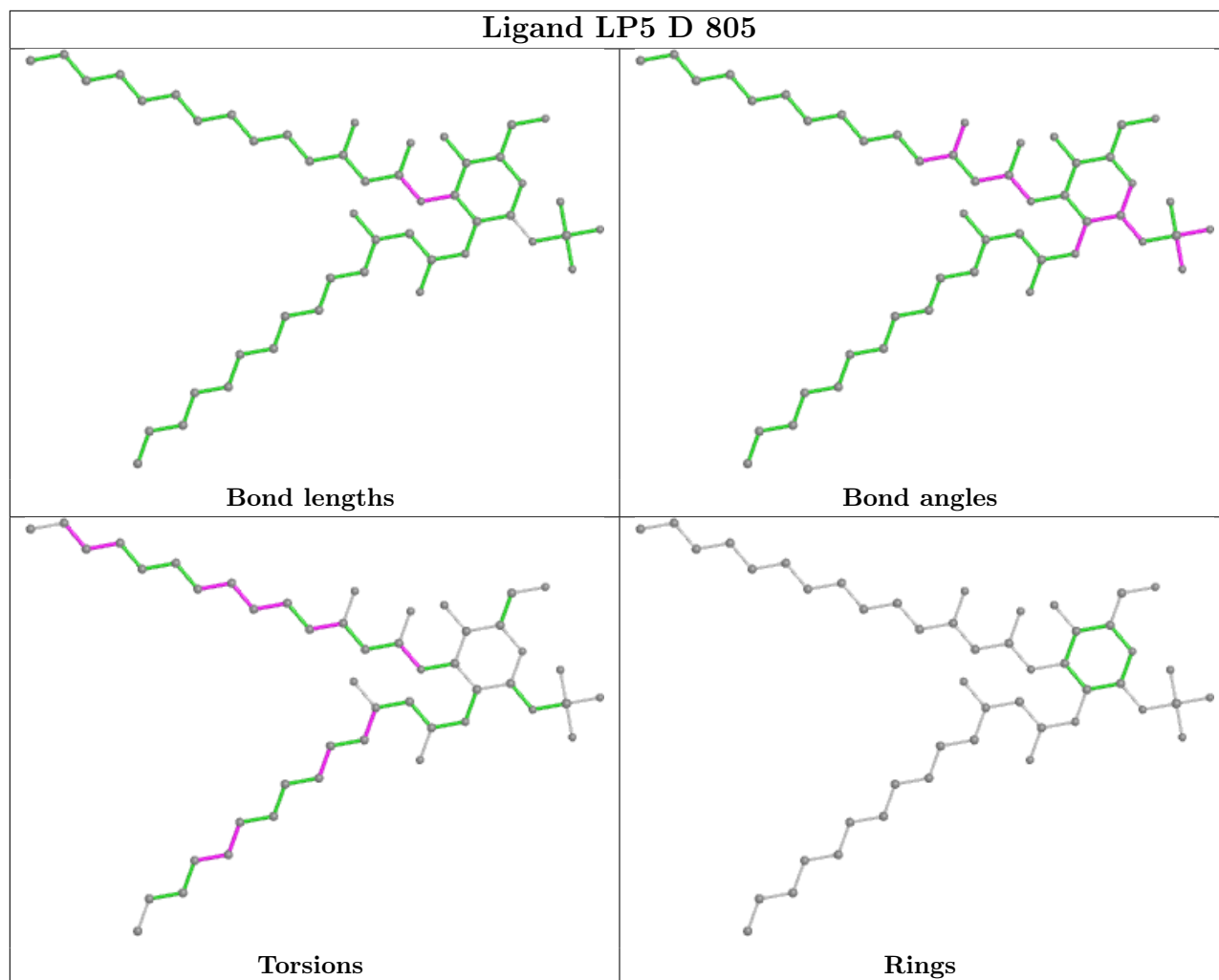
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	C	205	LP5	2	0
4	B	705	NAG	1	0
5	D	804	LP4	1	0
8	C	207	MYR	1	0
6	D	805	LP5	1	0
8	D	807	MYR	2	0
4	A	704	NAG	3	0
4	A	703	NAG	1	0

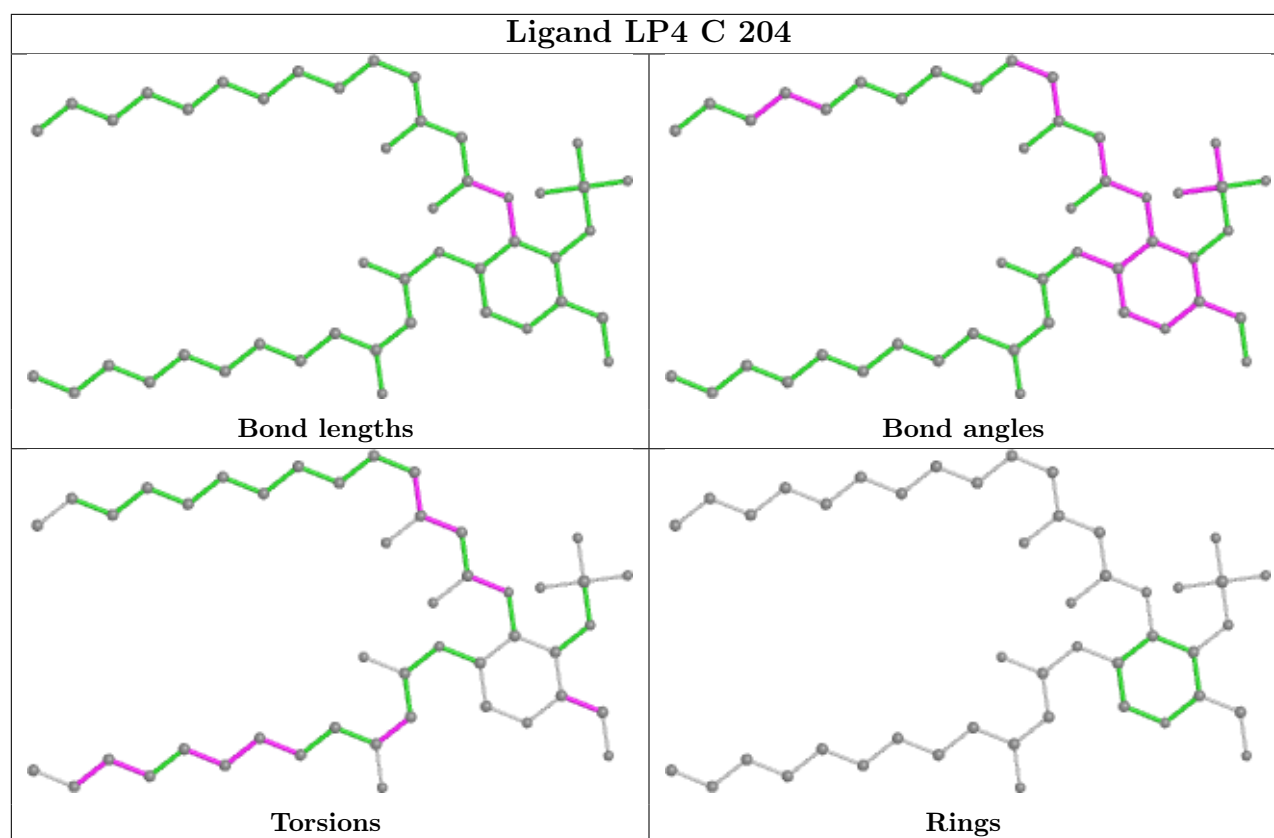
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.











## 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	590/594 (99%)	-0.05	32 (5%) 25 24	9, 33, 95, 142	0
1	B	592/594 (99%)	0.09	36 (6%) 21 20	10, 43, 99, 132	0
2	C	137/150 (91%)	-0.27	1 (0%) 87 89	20, 35, 55, 76	0
2	D	137/150 (91%)	-0.13	1 (0%) 87 89	23, 42, 65, 79	0
All	All	1456/1488 (97%)	-0.02	70 (4%) 30 28	9, 37, 95, 142	0

All (70) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	30	GLU	5.6
1	B	29	ILE	5.0
1	A	33	PRO	4.9
1	B	32	VAL	4.3
1	B	33	PRO	4.3
1	A	31	VAL	4.3
1	B	56	LYS	4.1
1	A	80	GLN	4.0
1	B	35	ILE	3.9
1	B	195	GLN	3.9
1	A	49	ASP	3.9
1	B	98	HIS	3.9
1	A	44	LEU	3.8
1	B	147	GLN	3.7
1	B	31	VAL	3.7
1	A	34	ASN	3.6
1	B	149	ILE	3.6
1	A	121	PHE	3.5
1	A	51	ILE	3.5
1	A	55	THR	3.5
1	A	76	PHE	3.4

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	A	98	HIS	3.4
1	A	45	SER	3.4
1	A	123	GLY	3.4
1	A	102	HIS	3.3
1	B	28	CYS	3.3
1	B	50	ASP	3.3
1	B	118	PRO	3.2
1	A	99	GLY	3.1
1	A	147	GLN	3.1
1	A	101	HIS	3.1
2	C	39	HIS	2.9
1	A	269	GLU	2.9
1	B	27	PRO	2.9
1	B	75	ASN	2.9
1	A	141	GLU	2.9
1	A	37	TYR	2.8
1	B	141	GLU	2.8
1	B	168	ALA	2.7
1	A	78	GLU	2.6
1	B	199	GLU	2.6
1	B	71	TYR	2.5
1	A	48	PRO	2.5
1	A	100	LEU	2.5
1	A	71	TYR	2.5
1	B	49	ASP	2.5
1	A	171	SER	2.4
1	B	226	LYS	2.4
1	B	253	HIS	2.4
1	B	192	ASN	2.4
1	B	169	TYR	2.4
1	A	117	SER	2.3
2	D	20	LYS	2.3
1	A	97	TRP	2.2
1	B	174	THR	2.2
1	A	118	PRO	2.1
1	B	65	LEU	2.1
1	B	201	PRO	2.1
1	A	74	SER	2.1
1	B	596	SER	2.1
1	A	202	GLN	2.1
1	B	36	THR	2.1
1	B	172	ASN	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	45	SER	2.1
1	A	35	ILE	2.1
1	B	43	LYS	2.1
1	A	201	PRO	2.0
1	B	99	GLY	2.0
1	B	277	GLU	2.0
1	B	90	GLU	2.0

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
3	NAG	J	2	14/15	0.65	0.34	95,108,117,122	0
4	NAG	A	703	14/15	0.73	0.28	52,76,83,84	0
4	NAG	B	705	14/15	0.76	0.20	67,75,83,85	0
3	NAG	J	1	14/15	0.79	0.39	98,106,115,118	0
3	NAG	I	2	14/15	0.83	0.31	70,82,103,104	0
4	NAG	D	803	14/15	0.84	0.21	68,74,77,77	0
3	NAG	F	2	14/15	0.86	0.25	39,52,57,60	0
4	NAG	A	704	14/15	0.86	0.27	66,72,77,78	0
4	NAG	C	201	14/15	0.87	0.34	66,74,83,92	0
3	NAG	H	2	14/15	0.87	0.44	78,86,88,90	0
3	NAG	E	1	14/15	0.87	0.20	59,65,74,75	0
3	NAG	I	1	14/15	0.87	0.30	84,88,91,94	0
3	NAG	K	2	14/15	0.88	0.26	42,48,52,56	0
3	NAG	E	2	14/15	0.89	0.22	64,76,82,86	0
3	NAG	G	1	14/15	0.89	0.16	45,48,53,62	0
3	NAG	G	2	14/15	0.91	0.36	65,74,85,87	0
3	NAG	H	1	14/15	0.92	0.20	47,52,59,70	0
3	NAG	K	1	14/15	0.96	0.14	24,27,33,37	0
3	NAG	F	1	14/15	0.96	0.14	26,30,33,38	0

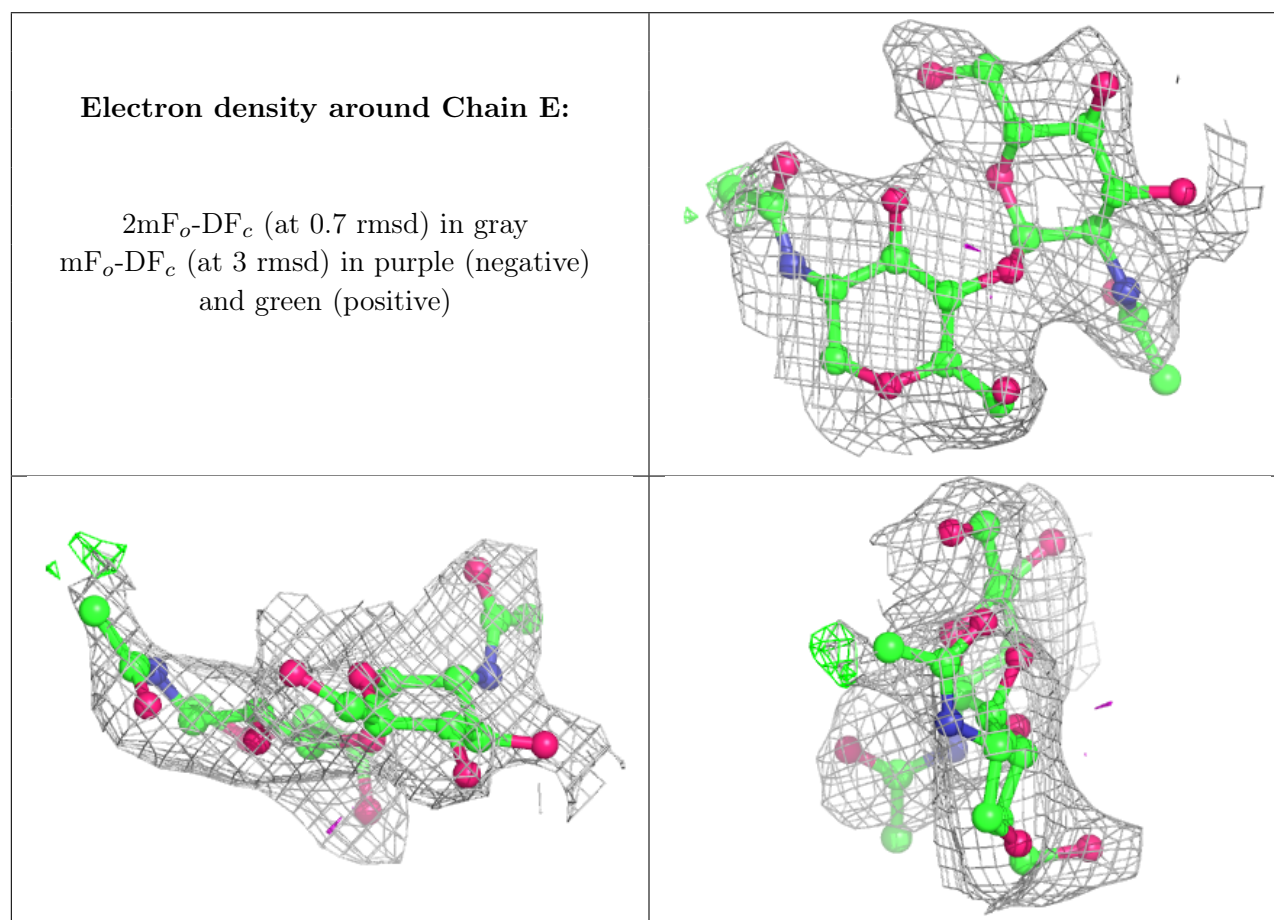
## 6.3 Carbohydrates [i](#)

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

labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	NAG	J	2	14/15	0.65	0.34	95,108,117,122	0
3	NAG	J	1	14/15	0.79	0.39	98,106,115,118	0
3	NAG	I	2	14/15	0.83	0.31	70,82,103,104	0
3	NAG	F	2	14/15	0.86	0.25	39,52,57,60	0
3	NAG	E	1	14/15	0.87	0.20	59,65,74,75	0
3	NAG	H	2	14/15	0.87	0.44	78,86,88,90	0
3	NAG	I	1	14/15	0.87	0.30	84,88,91,94	0
3	NAG	K	2	14/15	0.88	0.26	42,48,52,56	0
3	NAG	E	2	14/15	0.89	0.22	64,76,82,86	0
3	NAG	G	1	14/15	0.89	0.16	45,48,53,62	0
3	NAG	G	2	14/15	0.91	0.36	65,74,85,87	0
3	NAG	H	1	14/15	0.92	0.20	47,52,59,70	0
3	NAG	K	1	14/15	0.96	0.14	24,27,33,37	0
3	NAG	F	1	14/15	0.96	0.14	26,30,33,38	0

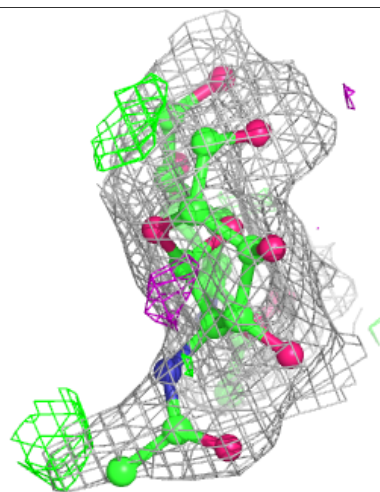
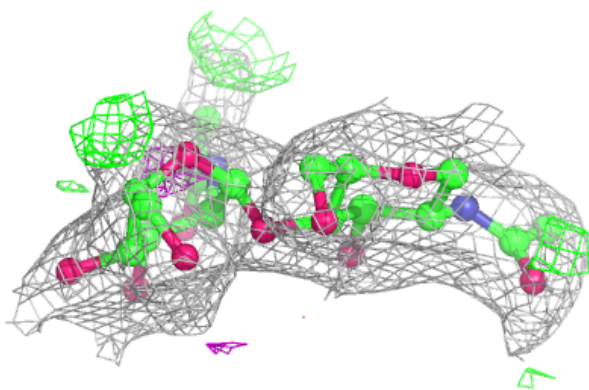
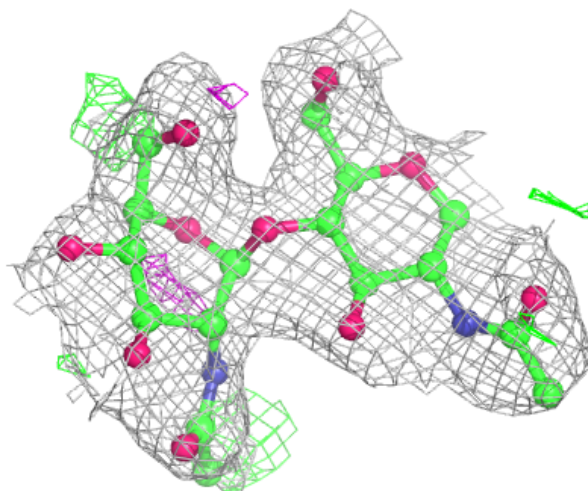
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.





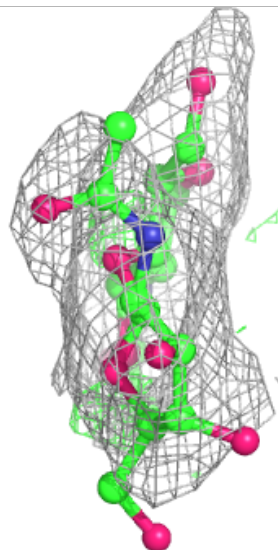
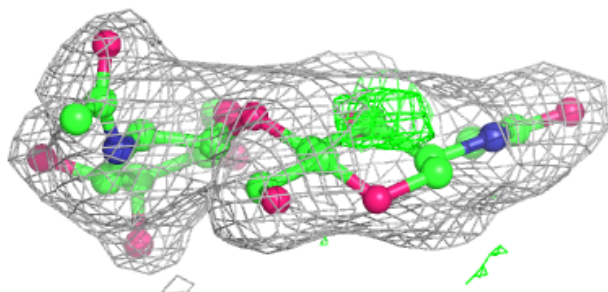
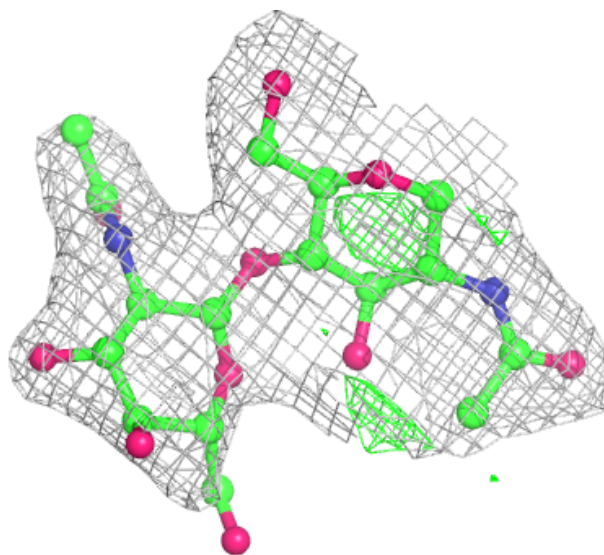
**Electron density around Chain F:**

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



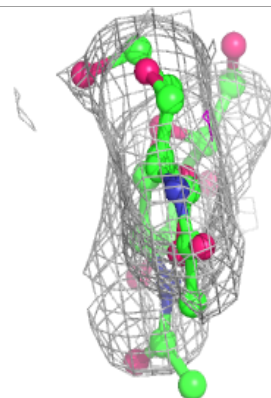
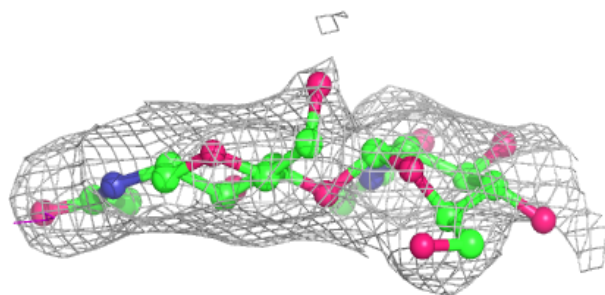
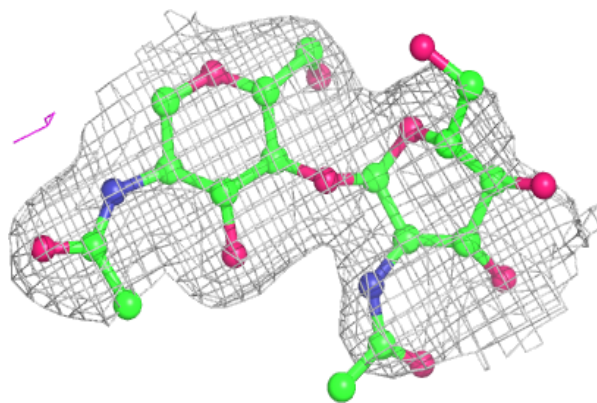
**Electron density around Chain G:**

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



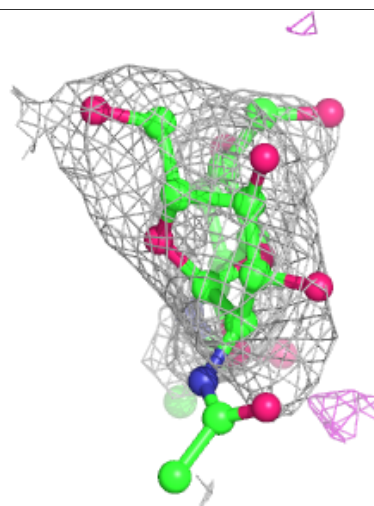
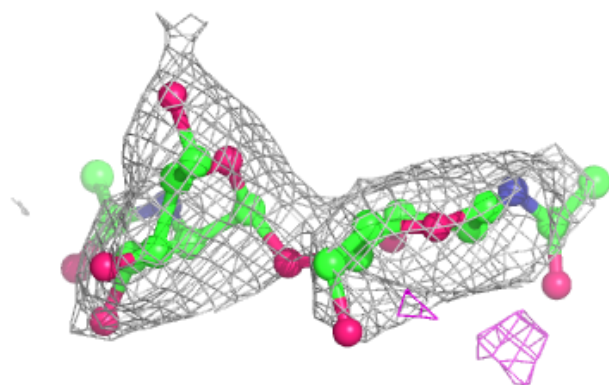
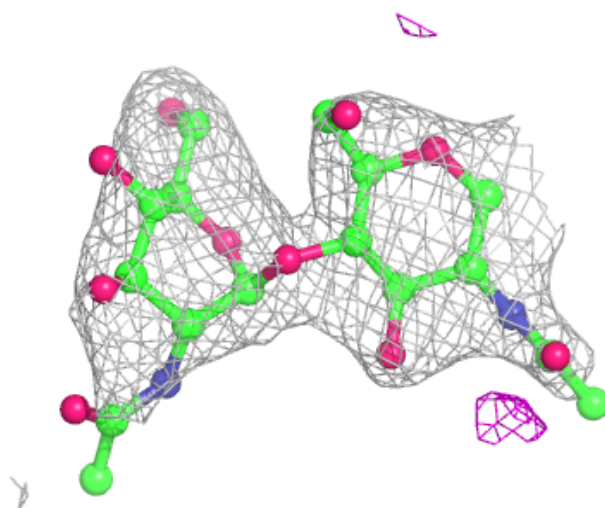
**Electron density around Chain H:**

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



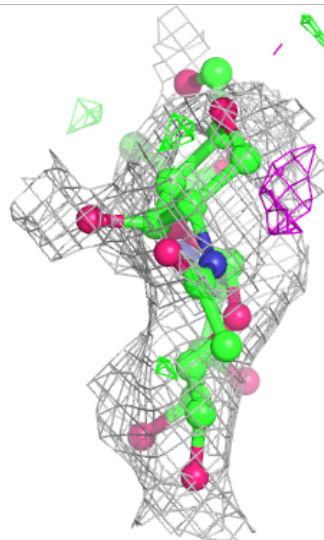
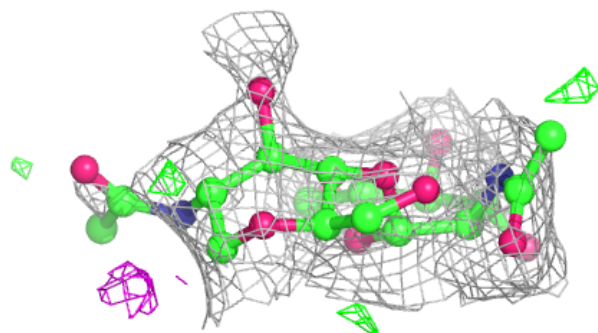
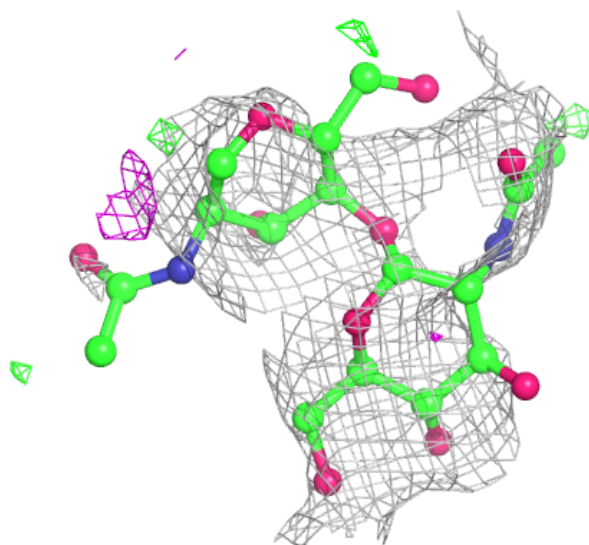
**Electron density around Chain I:**

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

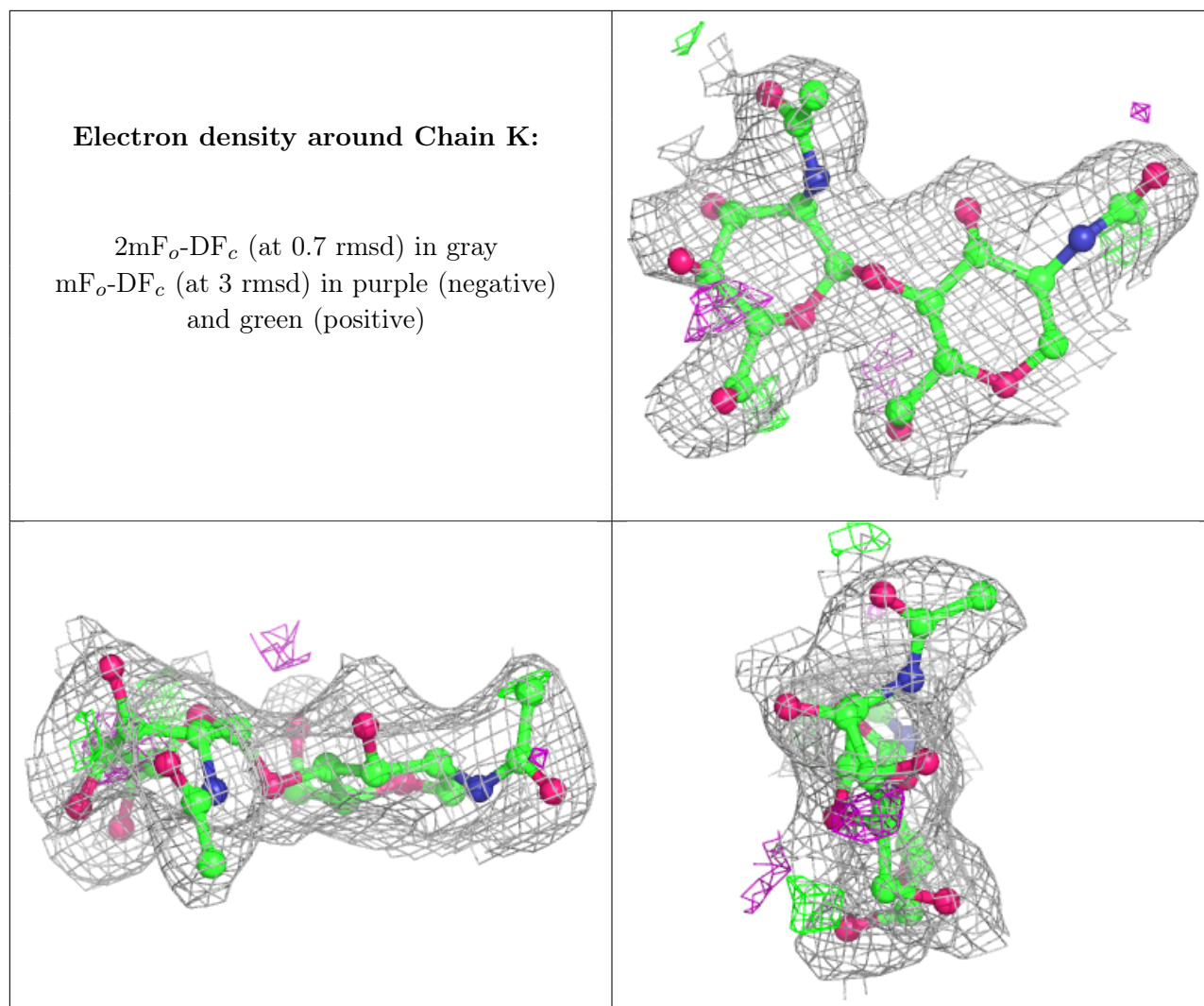


**Electron density around Chain J:**

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







## 6.4 Ligands [i](#)

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

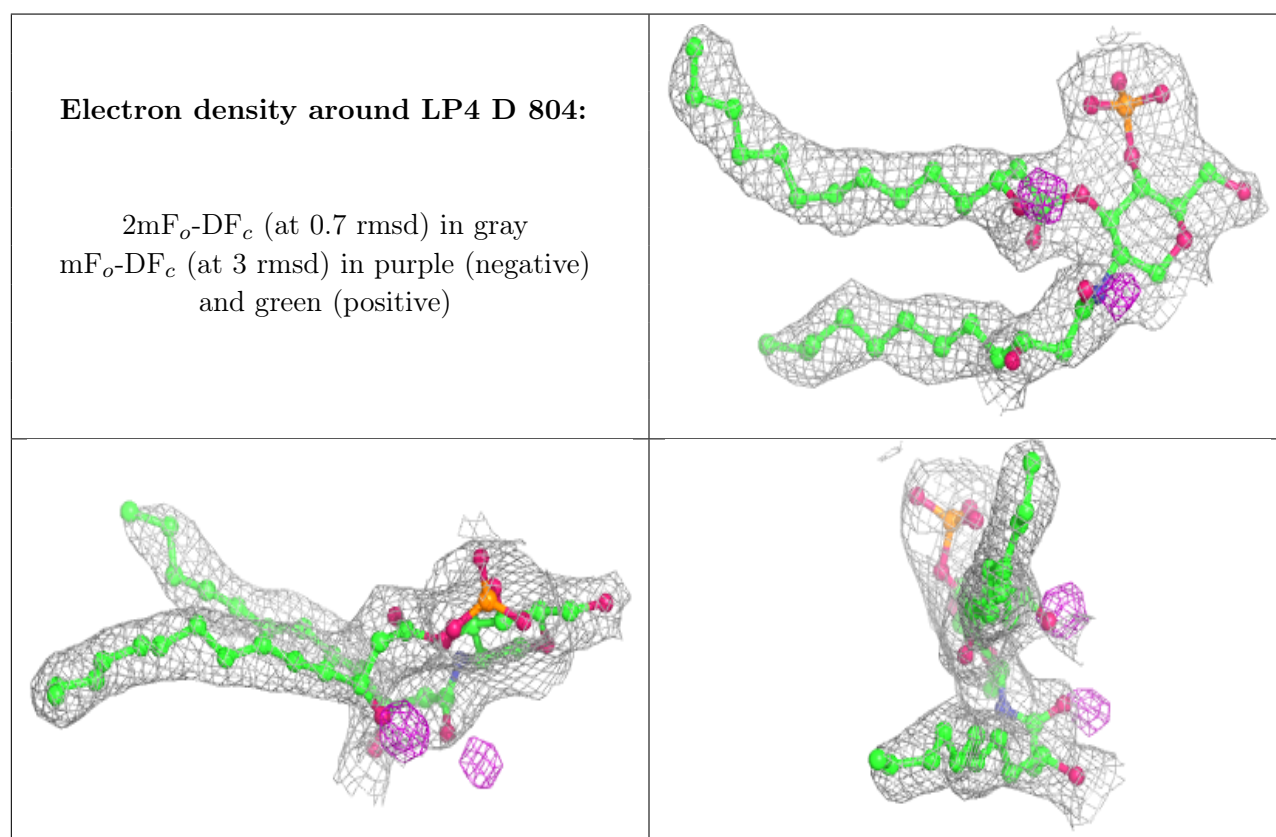
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
4	NAG	A	703	14/15	0.73	0.28	52,76,83,84	0
4	NAG	B	705	14/15	0.76	0.20	67,75,83,85	0
4	NAG	D	803	14/15	0.84	0.21	68,74,77,77	0
8	MYR	D	807	15/16	0.84	0.34	46,50,65,66	0
8	MYR	C	207	15/16	0.85	0.36	52,62,77,89	0
7	DAO	C	206	13/14	0.85	0.29	39,44,59,65	0
4	NAG	A	704	14/15	0.86	0.27	66,72,77,78	0
4	NAG	C	201	14/15	0.87	0.34	66,74,83,92	0

*Continued on next page...*

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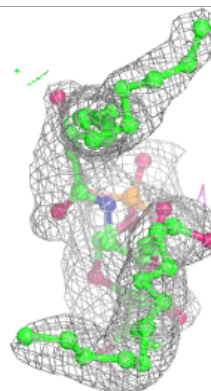
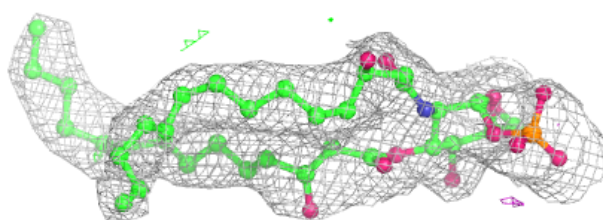
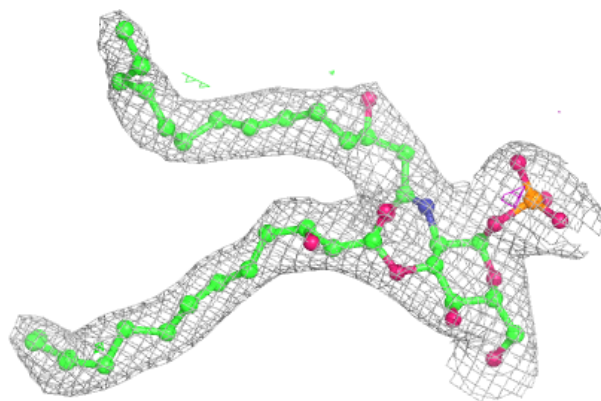
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
7	DAO	D	806	13/14	0.92	0.18	45,51,63,69	0
5	LP4	D	804	45/48	0.93	0.17	35,50,59,68	0
6	LP5	C	205	48/48	0.94	0.15	38,46,56,61	0
6	LP5	D	805	48/48	0.94	0.16	31,45,63,67	0
5	LP4	C	204	45/48	0.94	0.16	28,37,52,56	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

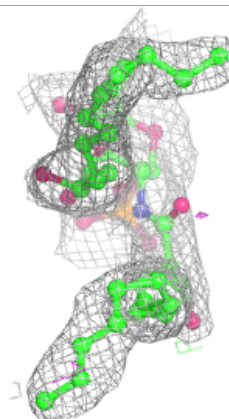
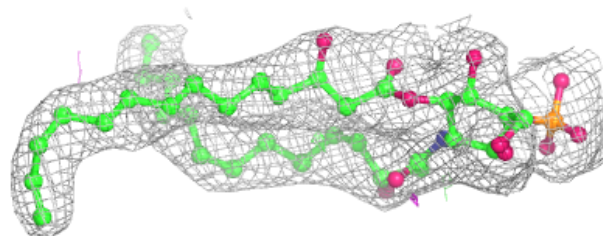
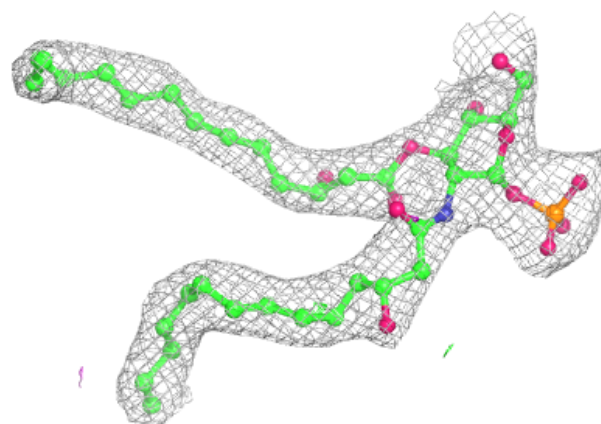


**Electron density around LP5 C 205:**

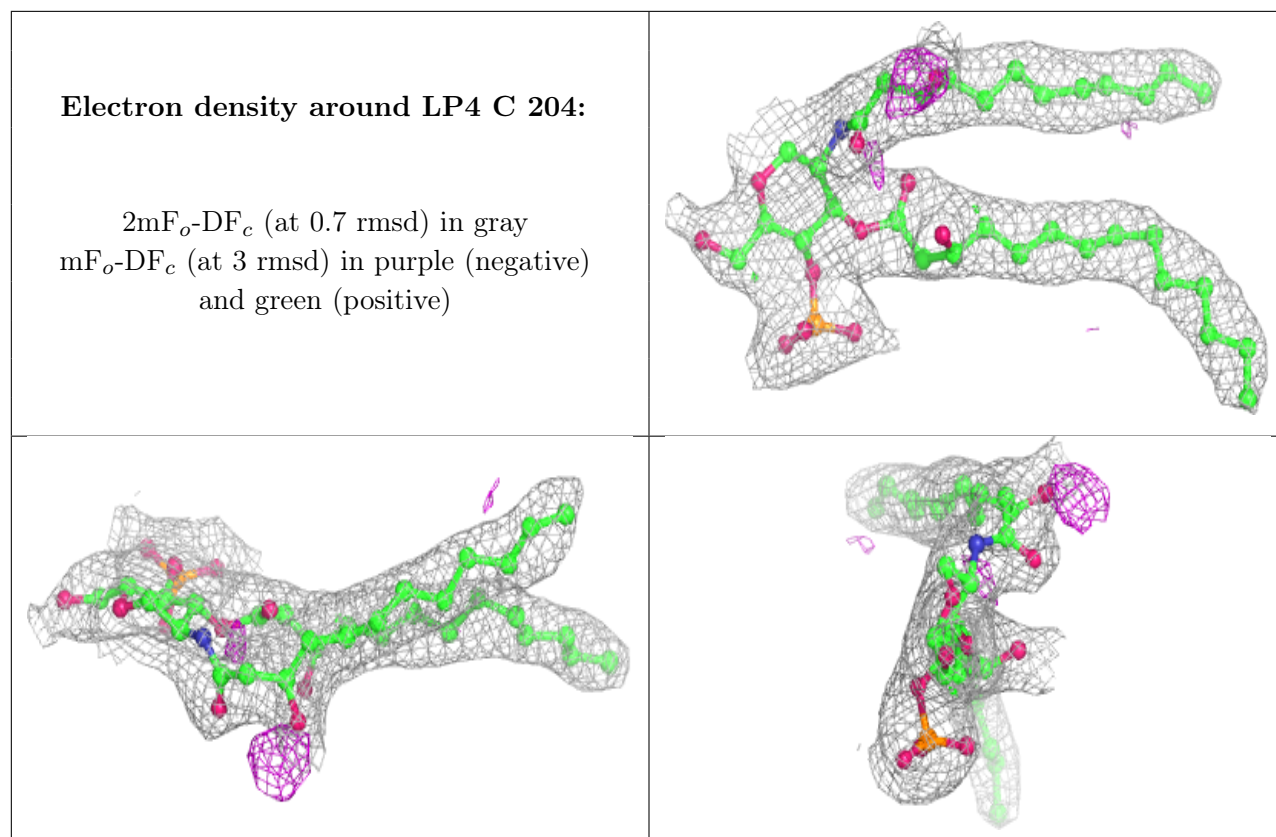
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

**Electron density around LP5 D 805:**

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







## 6.5 Other polymers [i](#)

There are no such residues in this entry.