



# Full wwPDB X-ray Structure Validation Report ⓘ

Nov 2, 2023 – 04:10 PM EDT

PDB ID : 3VJK  
Title : Crystal structure of human deipeptidyl peptidase IV (DPP-4) in complex with MP-513  
Authors : Akahoshi, F.; Kishida, H.; Miyaguchi, I.; Yoshida, T.; Ishii, S.  
Deposited on : 2011-10-24  
Resolution : 2.49 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  
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

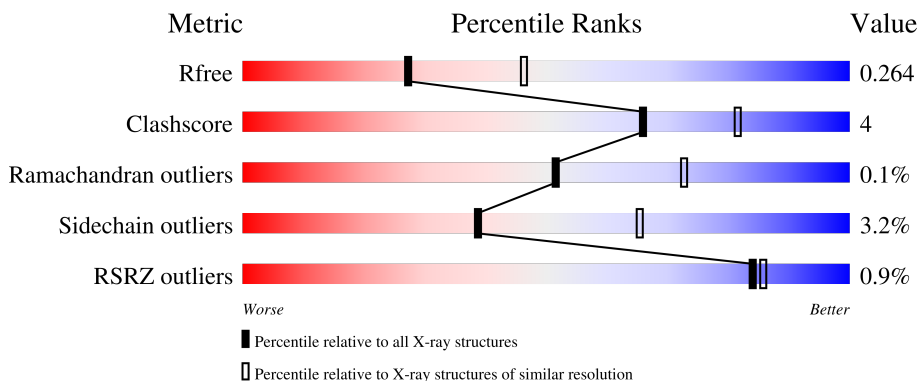
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.49 Å.

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



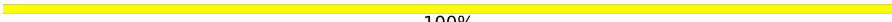
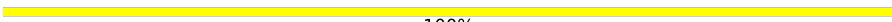
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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	740	87% 11% ..
1	B	740	86% 12% ..
2	C	2	100%
2	D	2	100%
2	E	2	100%

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Mol	Chain	Length	Quality of chain
2	F	2	 100%
2	G	2	 100%

## 2 Entry composition i

There are 5 unique types of molecules in this entry. The entry contains 12696 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 Dipeptidyl peptidase 4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	729	5971	3831	983	1131	26	0	0	0
1	B	729	5971	3831	983	1131	26	0	0	0

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	767	HIS	-	expression tag	UNP P27487
A	768	HIS	-	expression tag	UNP P27487
A	769	HIS	-	expression tag	UNP P27487
A	770	HIS	-	expression tag	UNP P27487
A	771	HIS	-	expression tag	UNP P27487
A	772	HIS	-	expression tag	UNP P27487
B	767	HIS	-	expression tag	UNP P27487
B	768	HIS	-	expression tag	UNP P27487
B	769	HIS	-	expression tag	UNP P27487
B	770	HIS	-	expression tag	UNP P27487
B	771	HIS	-	expression tag	UNP P27487
B	772	HIS	-	expression tag	UNP P27487

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



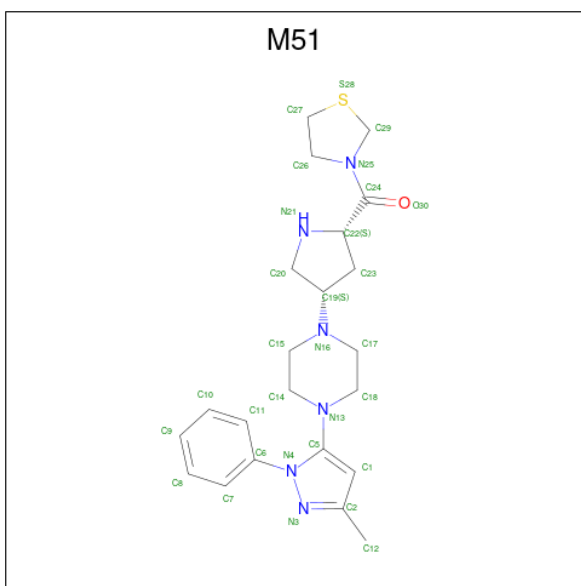
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
2	C	2	28	16	2	10	0	0	0

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

- Molecule 3 is {(2S,4S)-4-[4-(3-methyl-1-phenyl-1H-pyrazol-5-yl)piperazin-1-yl]pyrrolidin-2-yl}(1,3-thiazolidin-3-yl)methanone (three-letter code: M51) (formula: C<sub>22</sub>H<sub>30</sub>N<sub>6</sub>OS).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	S	0	0
			30	22	6	1	1		
3	B	1	Total	C	N	O	S	0	0
			30	22	6	1	1		

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C<sub>8</sub>H<sub>15</sub>NO<sub>6</sub>).



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

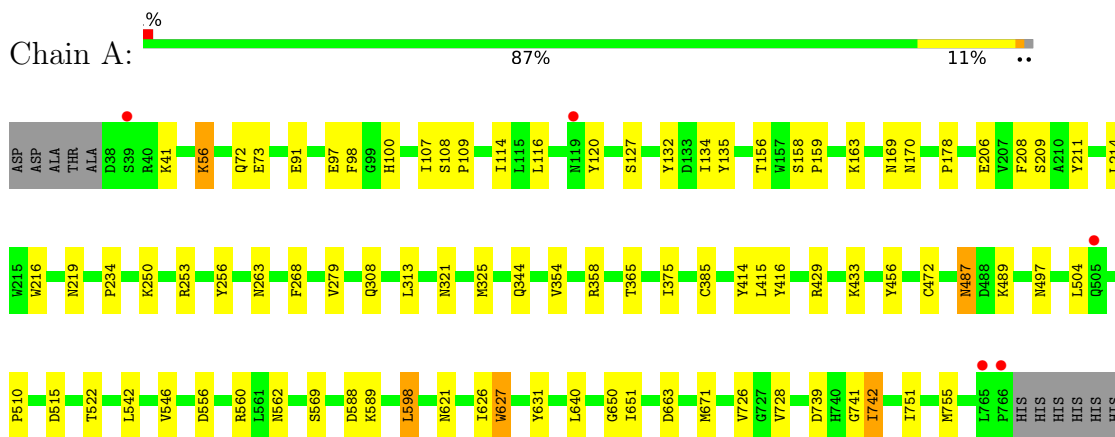
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
5	A	212	212	212	0	0
5	B	244	244	244	0	0

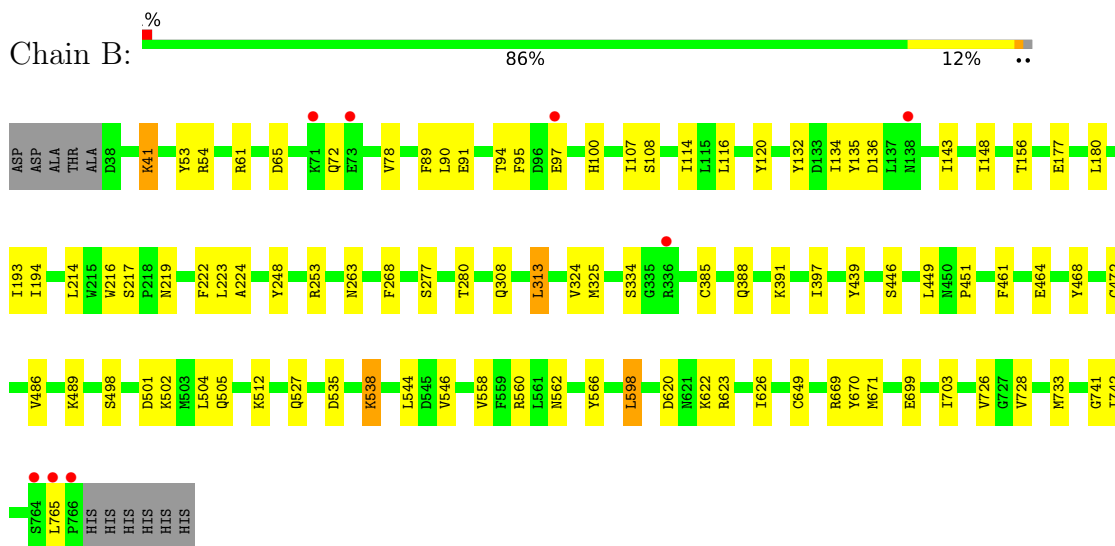
### 3 Residue-property plots [i](#)

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: Dipeptidyl peptidase 4



- Molecule 1: Dipeptidyl peptidase 4




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



MAG1  
MAG2

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

Chain D:  100%MAG1  
MAG2

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

Chain E:  100%MAG1  
MAG2

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

Chain F:  100%MAG1  
MAG2

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

Chain G:  100%MAG1  
MAG2



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	117.95Å 126.41Å 138.01Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.49 31.46 – 2.49	Depositor EDS
% Data completeness (in resolution range)	88.7 (30.00-2.49) 88.7 (31.46-2.49)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.95 (at 2.48Å)	Xtrriage
Refinement program	REFMAC 5.5.0110	Depositor
R, $R_{free}$	0.225 , 0.279 0.213 , 0.264	Depositor DCC
$R_{free}$ test set	3214 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	39.7	Xtrriage
Anisotropy	0.562	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 34.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.54$ , $\langle L^2 \rangle = 0.39$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	12696	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	37.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.29% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: M51, NAG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	0.54	0/6143	0.64	0/8355
1	B	0.58	0/6143	0.64	0/8355
All	All	0.56	0/12286	0.64	0/16710

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5971	0	5683	49	0
1	B	5971	0	5683	49	0
2	C	28	0	25	0	0
2	D	28	0	25	0	0
2	E	28	0	25	0	0
2	F	28	0	25	0	0
2	G	28	0	25	0	0
3	A	30	0	30	0	0
3	B	30	0	30	0	0
4	A	42	0	39	0	0
4	B	56	0	52	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	A	212	0	0	2	0
5	B	244	0	0	1	0
All	All	12696	0	11642	95	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 4.

All (95) 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:B:277:SER:HB3	1:B:280:THR:HG22	1.57	0.83
1:A:726:VAL:HG23	1:A:728:VAL:HG23	1.65	0.76
1:A:253:ARG:HH12	1:B:253:ARG:HH21	1.36	0.74
1:B:78:VAL:HG23	1:B:89:PHE:HB2	1.71	0.73
1:A:640:LEU:HD11	1:A:650:GLY:HA3	1.71	0.71
1:B:91:GLU:O	1:B:94:THR:HG22	1.91	0.71
1:B:219:ASN:H	1:B:308:GLN:HE22	1.40	0.69
1:A:414:TYR:CE1	1:A:433:LYS:HE2	2.29	0.67
1:B:546:VAL:HG21	1:B:626:ILE:HD11	1.77	0.67
1:A:253:ARG:NH1	1:B:253:ARG:HH21	1.94	0.65
1:A:219:ASN:H	1:A:308:GLN:HE22	1.45	0.64
1:A:751:ILE:O	1:A:755:MET:HG3	2.01	0.61
1:B:620:ASP:OD2	1:B:622:LYS:HE3	2.01	0.60
1:B:219:ASN:N	1:B:308:GLN:HE22	2.00	0.59
1:B:90:LEU:HD21	1:B:95:PHE:HE1	1.68	0.58
1:B:544:LEU:HD23	1:B:626:ILE:HD12	1.88	0.55
1:A:72:GLN:HG3	1:A:73:GLU:HG2	1.88	0.55
1:A:127:SER:HB3	1:A:211:TYR:CD1	2.42	0.54
1:A:510:PRO:HD3	1:A:569:SER:HB2	1.90	0.54
1:B:65:ASP:OD2	1:B:464:GLU:HB3	2.07	0.53
1:A:219:ASN:N	1:A:308:GLN:HE22	2.06	0.53
1:A:114:ILE:HG23	1:A:135:TYR:HB3	1.91	0.53
1:A:156:THR:HG21	1:A:214:LEU:CD1	2.39	0.52
1:A:546:VAL:HG21	1:A:626:ILE:HD11	1.94	0.50
1:A:159:PRO:HD3	1:A:216:TRP:CB	2.42	0.50
1:A:114:ILE:CG2	1:A:135:TYR:HB3	2.42	0.49
1:A:556:ASP:OD1	1:A:560:ARG:NH2	2.46	0.48
1:B:703:ILE:HA	1:B:733:MET:O	2.13	0.48
1:A:159:PRO:HD3	1:A:216:TRP:HB3	1.96	0.48
1:A:414:TYR:CD1	1:A:433:LYS:HE2	2.48	0.48
1:A:741:GLY:O	1:A:742:ILE:C	2.52	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:219:ASN:OD1	1:A:219:ASN:C	2.52	0.47
1:B:41:LYS:HE3	1:B:53:TYR:OH	2.14	0.47
1:B:41:LYS:HG2	5:B:2413:HOH:O	2.14	0.47
1:B:193:ILE:HG22	1:B:194:ILE:HG12	1.95	0.47
1:A:134:ILE:HD13	1:A:178:PRO:HB3	1.97	0.47
1:B:598:LEU:HB2	1:B:671:MET:SD	2.54	0.47
1:B:669:ARG:HD2	1:B:670:TYR:CZ	2.49	0.47
1:B:277:SER:CB	1:B:280:THR:HG22	2.35	0.47
1:B:741:GLY:O	1:B:742:ILE:C	2.53	0.46
1:A:56:LYS:HB2	1:A:497:ASN:OD1	2.15	0.46
1:B:461:PHE:CD2	1:B:468:TYR:HB3	2.51	0.46
1:A:158:SER:HB3	1:A:163:LYS:HB2	1.96	0.46
1:A:598:LEU:HD22	1:A:671:MET:HG2	1.97	0.46
1:B:156:THR:HG23	1:B:216:TRP:HE1	1.81	0.46
1:B:489:LYS:HB2	1:B:489:LYS:HE3	1.63	0.46
1:B:558:VAL:HB	1:B:560:ARG:NH1	2.32	0.45
1:B:116:LEU:O	1:B:132:TYR:HA	2.17	0.45
1:A:321:ASN:HA	1:A:354:VAL:HG23	1.98	0.45
1:B:120:TYR:C	1:B:120:TYR:CD2	2.89	0.45
1:A:268:PHE:CE2	1:A:313:LEU:HD21	2.52	0.45
1:A:487:ASN:ND2	1:A:489:LYS:H	2.14	0.45
1:A:116:LEU:O	1:A:132:TYR:HA	2.17	0.45
1:A:208:PHE:O	1:A:209:SER:C	2.54	0.44
1:A:621:ASN:HD22	1:A:621:ASN:N	2.16	0.44
1:B:388:GLN:HB2	1:B:391:LYS:HB2	1.98	0.44
1:B:446:SER:HA	1:B:449:LEU:HD12	2.00	0.44
1:B:94:THR:HG23	1:B:95:PHE:CD1	2.53	0.44
1:B:308:GLN:NE2	1:B:308:GLN:HA	2.33	0.44
1:A:107:ILE:HG22	1:A:108:SER:O	2.18	0.43
1:B:620:ASP:OD1	1:B:623:ARG:HD3	2.18	0.43
1:B:726:VAL:HG23	1:B:728:VAL:HG23	1.99	0.43
1:A:234:PRO:HB2	1:B:248:TYR:CZ	2.54	0.43
1:B:107:ILE:HG22	1:B:108:SER:O	2.18	0.43
1:B:598:LEU:HD22	1:B:671:MET:HG2	2.00	0.43
1:B:214:LEU:HD22	1:B:223:LEU:HD11	1.99	0.43
1:B:313:LEU:O	1:B:325:MET:HA	2.19	0.43
1:A:127:SER:HB3	1:A:211:TYR:CG	2.54	0.43
1:A:415:LEU:HD23	1:A:416:TYR:N	2.33	0.43
1:A:206:GLU:OE1	1:A:663:ASP:OD1	2.37	0.43
1:A:98:PHE:CE2	1:A:100:HIS:HB2	2.53	0.43
1:B:134:ILE:HD11	1:B:148:ILE:HD11	1.99	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:217:SER:HB3	1:B:222:PHE:HB2	2.01	0.42
1:A:627:TRP:HB2	1:A:651:ILE:HB	2.02	0.42
1:B:114:ILE:CG2	1:B:135:TYR:HB3	2.49	0.42
1:B:535:ASP:HB3	1:B:538:LYS:HB2	2.01	0.42
1:A:556:ASP:CG	1:A:560:ARG:HH22	2.23	0.42
1:A:598:LEU:HG	1:A:631:TYR:OH	2.19	0.42
1:B:512:LYS:HE3	1:B:527:GLN:CD	2.40	0.42
1:B:649:CYS:HA	1:B:699:GLU:O	2.19	0.42
1:A:109:PRO:HG2	1:A:158:SER:O	2.19	0.42
1:A:739:ASP:HB2	5:A:2042:HOH:O	2.19	0.42
1:B:501:ASP:O	1:B:505:GLN:HG2	2.20	0.42
1:A:169:ASN:O	1:A:170:ASN:HB2	2.20	0.42
1:A:742:ILE:HG22	1:A:742:ILE:O	2.20	0.42
1:A:325:MET:O	1:A:344:GLN:HA	2.20	0.41
1:B:397:ILE:HG22	1:B:439:TYR:CE2	2.56	0.41
1:A:120:TYR:CD1	1:A:120:TYR:C	2.94	0.41
1:A:588:ASP:O	1:A:589:LYS:C	2.59	0.41
1:B:224:ALA:HB1	1:B:268:PHE:CZ	2.56	0.41
1:B:277:SER:HB3	1:B:280:THR:CG2	2.41	0.41
1:A:429:ARG:HG3	1:A:456:TYR:CE2	2.56	0.40
1:A:279:VAL:HG22	5:A:2169:HOH:O	2.20	0.40
1:B:136:ASP:HB2	1:B:143:ILE:HD11	2.02	0.40
1:B:177:GLU:HB2	1:B:180:LEU:HG	2.04	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	727/740 (98%)	690 (95%)	36 (5%)	1 (0%)	51 73
1	B	727/740 (98%)	685 (94%)	42 (6%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	1454/1480 (98%)	1375 (95%)	78 (5%)	1 (0%)	51 73

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	742	ILE

### 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	654/663 (99%)	634 (97%)	20 (3%)	40 67
1	B	654/663 (99%)	632 (97%)	22 (3%)	37 63
All	All	1308/1326 (99%)	1266 (97%)	42 (3%)	39 65

All (42) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	41	LYS
1	A	56	LYS
1	A	91	GLU
1	A	97	GLU
1	A	250	LYS
1	A	256	TYR
1	A	263	ASN
1	A	358	ARG
1	A	365	THR
1	A	375	ILE
1	A	385	CYS
1	A	472	CYS
1	A	487	ASN
1	A	504	LEU
1	A	515	ASP
1	A	522	THR
1	A	542	LEU

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	562	ASN
1	A	598	LEU
1	A	627	TRP
1	B	41	LYS
1	B	54	ARG
1	B	61	ARG
1	B	72	GLN
1	B	97	GLU
1	B	100	HIS
1	B	263	ASN
1	B	313	LEU
1	B	324	VAL
1	B	334	SER
1	B	385	CYS
1	B	451	PRO
1	B	472	CYS
1	B	486	VAL
1	B	498	SER
1	B	502	LYS
1	B	504	LEU
1	B	538	LYS
1	B	562	ASN
1	B	566	TYR
1	B	598	LEU
1	B	765	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	112	GLN
1	A	141	GLN
1	A	169	ASN
1	A	263	ASN
1	A	286	GLN
1	A	308	GLN
1	A	345	HIS
1	A	455	GLN
1	A	487	ASN
1	A	506	ASN
1	A	520	ASN
1	A	562	ASN
1	A	621	ASN

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Mol	Chain	Res	Type
1	A	679	ASN
1	A	694	ASN
1	A	697	GLN
1	B	100	HIS
1	B	112	GLN
1	B	138	ASN
1	B	169	ASN
1	B	263	ASN
1	B	286	GLN
1	B	308	GLN
1	B	505	GLN
1	B	562	ASN
1	B	679	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](#)

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

### 5.5 Carbohydrates [i](#)

10 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
2	NAG	C	1	1,2	14,14,15	0.59	0	17,19,21	1.11	1 (5%)
2	NAG	C	2	2	14,14,15	0.58	0	17,19,21	1.05	1 (5%)
2	NAG	D	1	1,2	14,14,15	0.57	0	17,19,21	1.50	2 (11%)
2	NAG	D	2	2	14,14,15	0.50	0	17,19,21	1.49	1 (5%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	NAG	E	1	1,2	14,14,15	0.61	0	17,19,21	1.35	3 (17%)
2	NAG	E	2	2	14,14,15	0.46	0	17,19,21	1.23	3 (17%)
2	NAG	F	1	1,2	14,14,15	0.55	0	17,19,21	1.22	2 (11%)
2	NAG	F	2	2	14,14,15	0.55	0	17,19,21	1.31	2 (11%)
2	NAG	G	1	1,2	14,14,15	0.62	0	17,19,21	1.78	2 (11%)
2	NAG	G	2	2	14,14,15	0.66	0	17,19,21	1.03	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
2	NAG	C	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	C	2	2	-	2/6/23/26	0/1/1/1
2	NAG	D	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	D	2	2	-	0/6/23/26	0/1/1/1
2	NAG	E	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	E	2	2	-	2/6/23/26	0/1/1/1
2	NAG	F	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	F	2	2	-	0/6/23/26	0/1/1/1
2	NAG	G	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	G	2	2	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	1	NAG	C1-O5-C5	5.46	119.58	112.19
2	D	2	NAG	C1-O5-C5	4.72	118.59	112.19
2	D	1	NAG	C1-O5-C5	3.73	117.24	112.19
2	E	1	NAG	C1-O5-C5	3.47	116.89	112.19
2	G	1	NAG	O5-C1-C2	-3.12	106.36	111.29
2	E	2	NAG	C1-O5-C5	2.97	116.22	112.19
2	D	1	NAG	O5-C1-C2	-2.86	106.77	111.29
2	F	1	NAG	O5-C1-C2	2.54	115.30	111.29
2	E	1	NAG	O5-C1-C2	-2.40	107.50	111.29
2	F	2	NAG	O7-C7-N2	2.31	126.20	121.95
2	E	2	NAG	O4-C4-C5	2.27	114.93	109.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	1	NAG	O5-C5-C6	2.25	110.73	107.20
2	E	1	NAG	O7-C7-C8	-2.20	117.97	122.06
2	G	2	NAG	C4-C3-C2	2.19	114.22	111.02
2	F	2	NAG	C1-O5-C5	2.18	115.15	112.19
2	E	2	NAG	C3-C4-C5	-2.11	106.48	110.24
2	C	2	NAG	O5-C1-C2	-2.09	107.99	111.29
2	C	1	NAG	C1-O5-C5	-2.02	109.46	112.19

There are no chirality outliers.

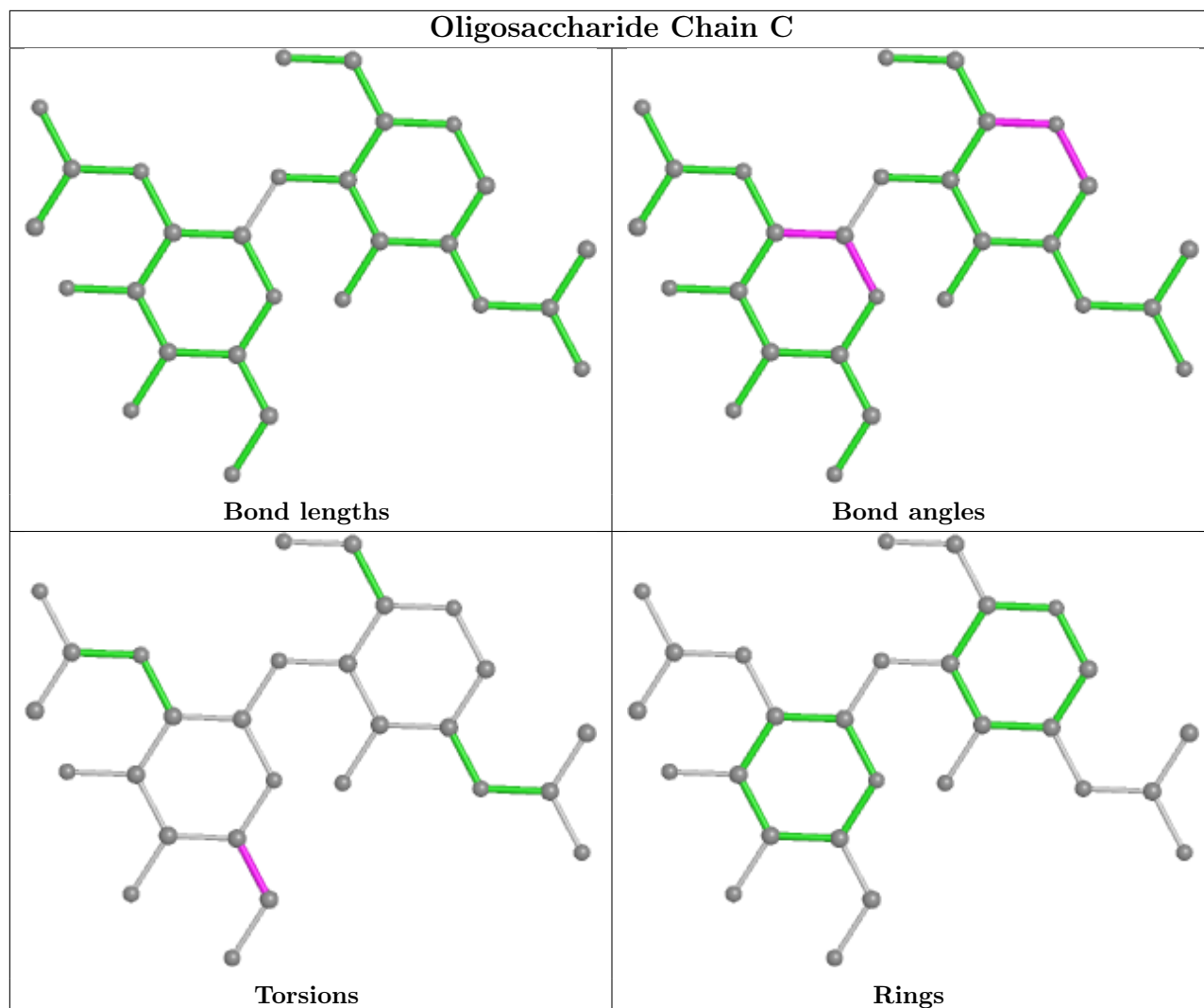
All (10) torsion outliers are listed below:

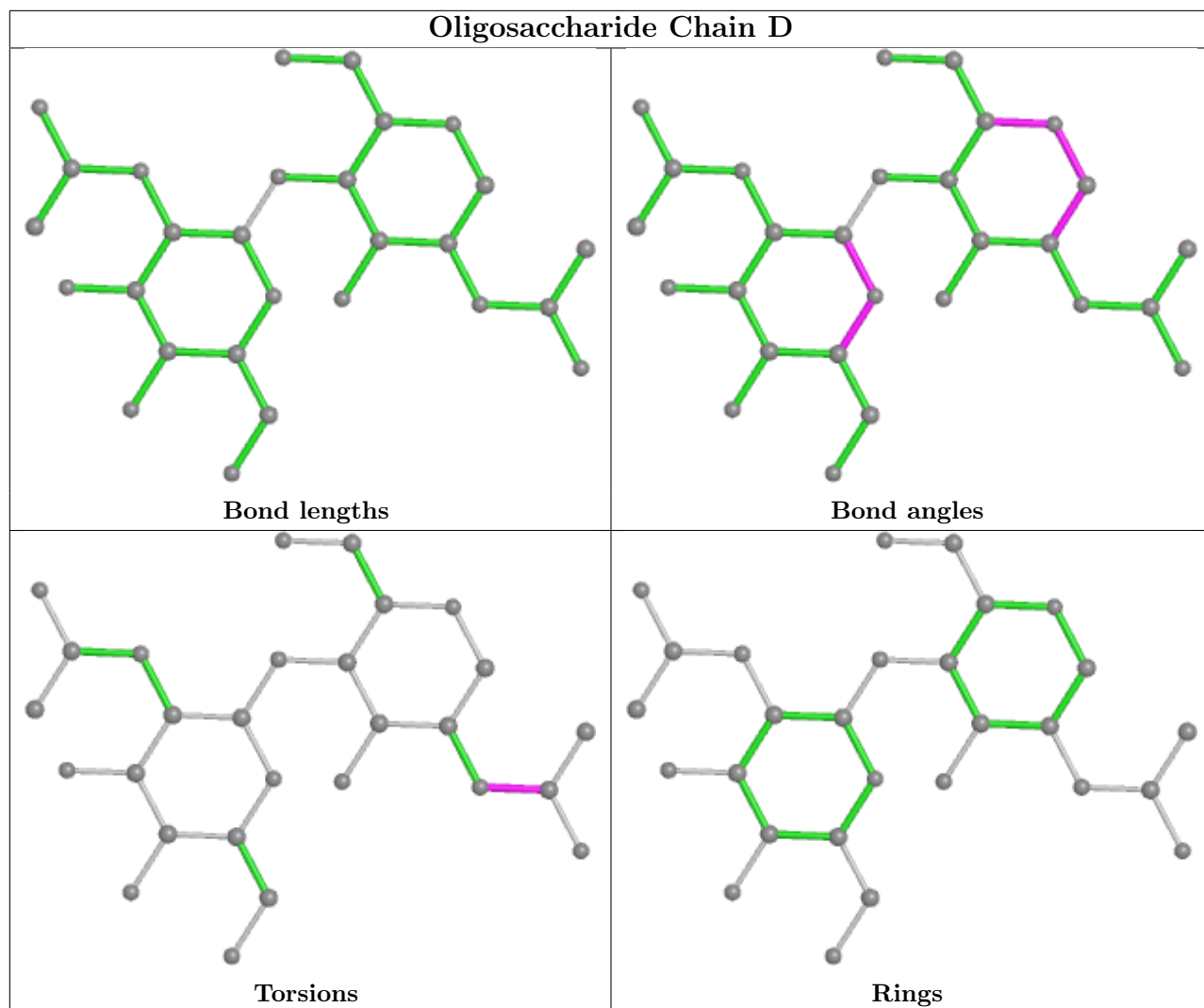
Mol	Chain	Res	Type	Atoms
2	C	2	NAG	O5-C5-C6-O6
2	E	2	NAG	O5-C5-C6-O6
2	C	2	NAG	C4-C5-C6-O6
2	E	2	NAG	C4-C5-C6-O6
2	D	1	NAG	C8-C7-N2-C2
2	D	1	NAG	O7-C7-N2-C2
2	G	2	NAG	O5-C5-C6-O6
2	G	2	NAG	C4-C5-C6-O6
2	E	1	NAG	C4-C5-C6-O6
2	E	1	NAG	O5-C5-C6-O6

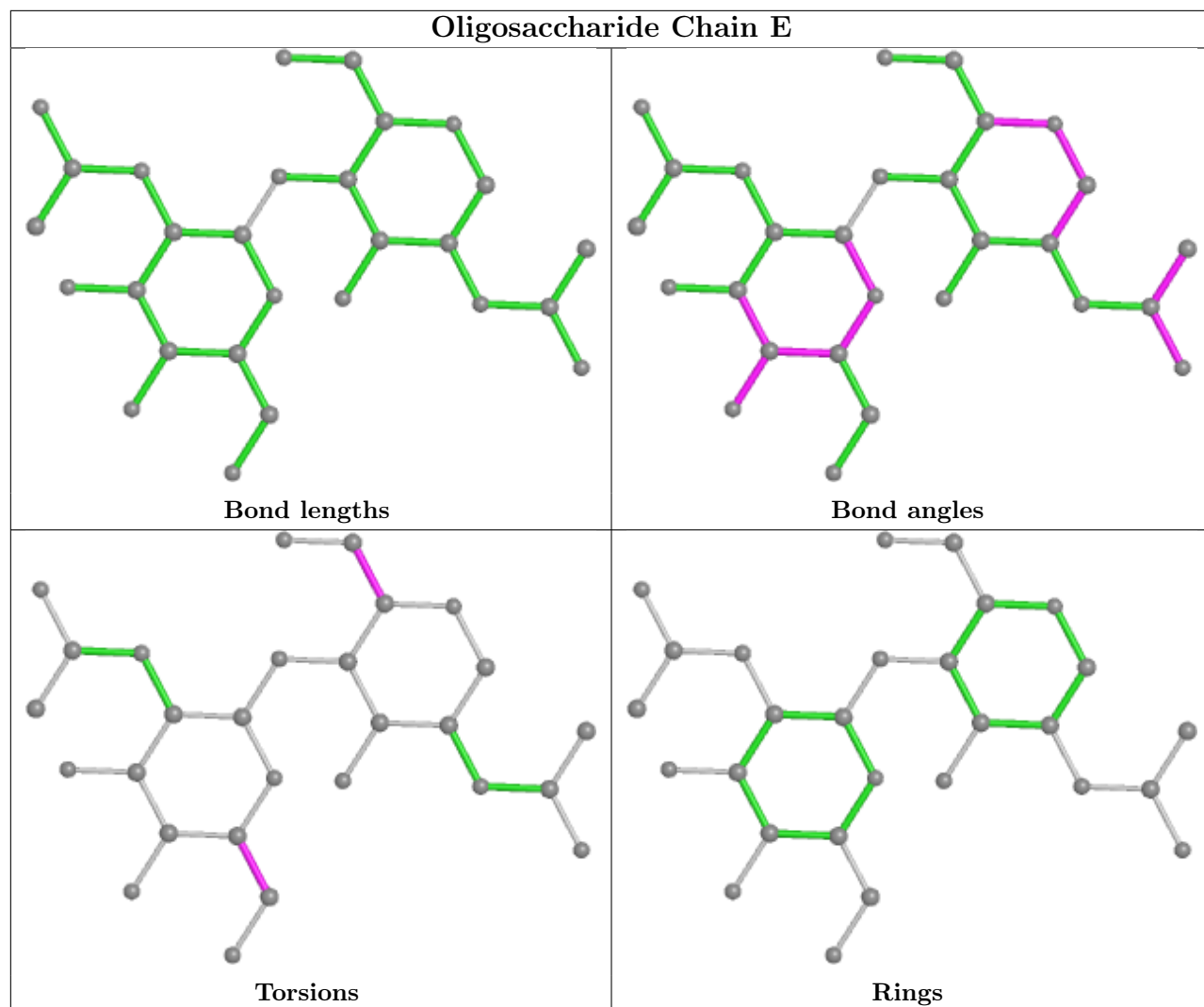
There are no ring outliers.

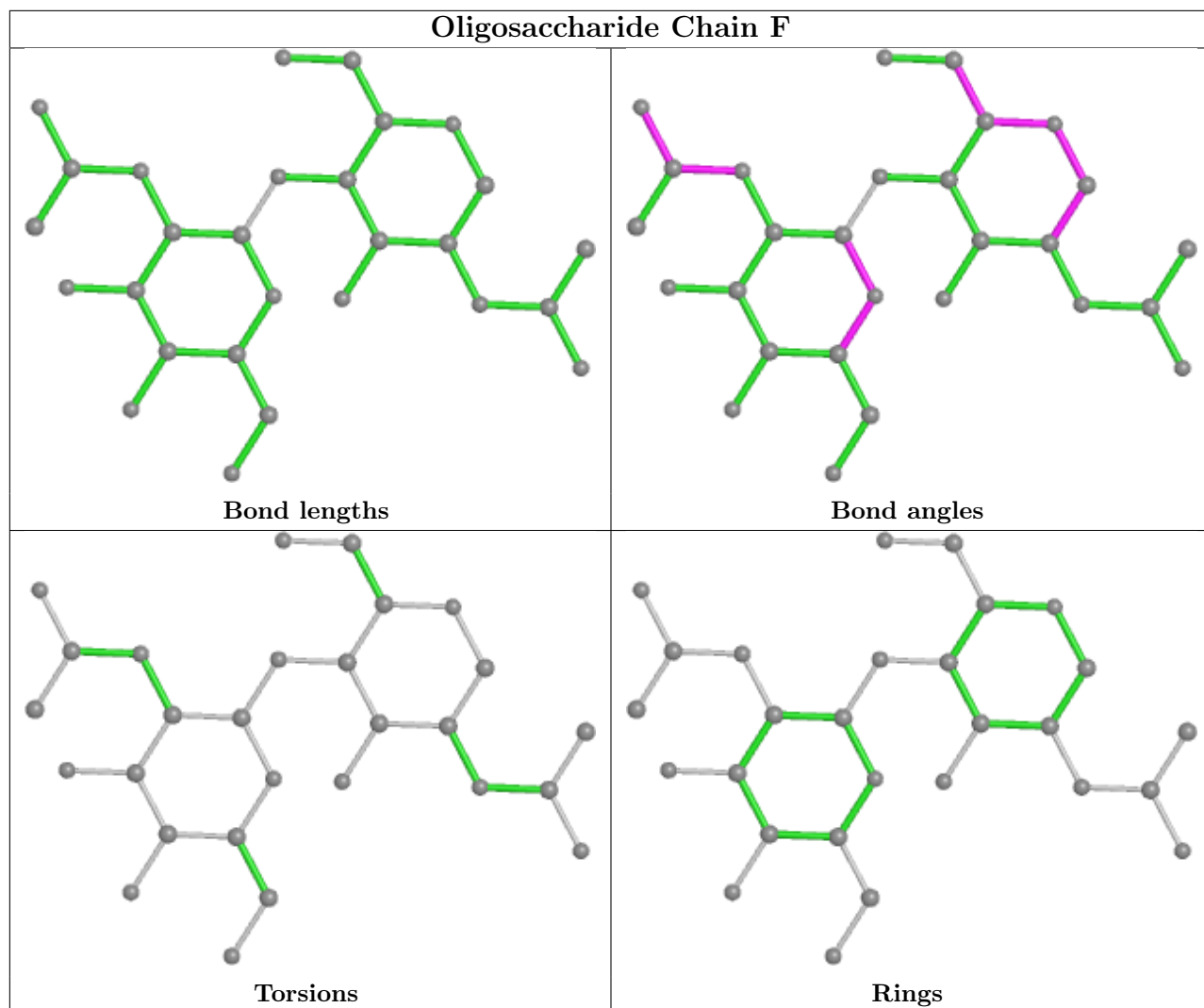
No monomer is involved in short contacts.

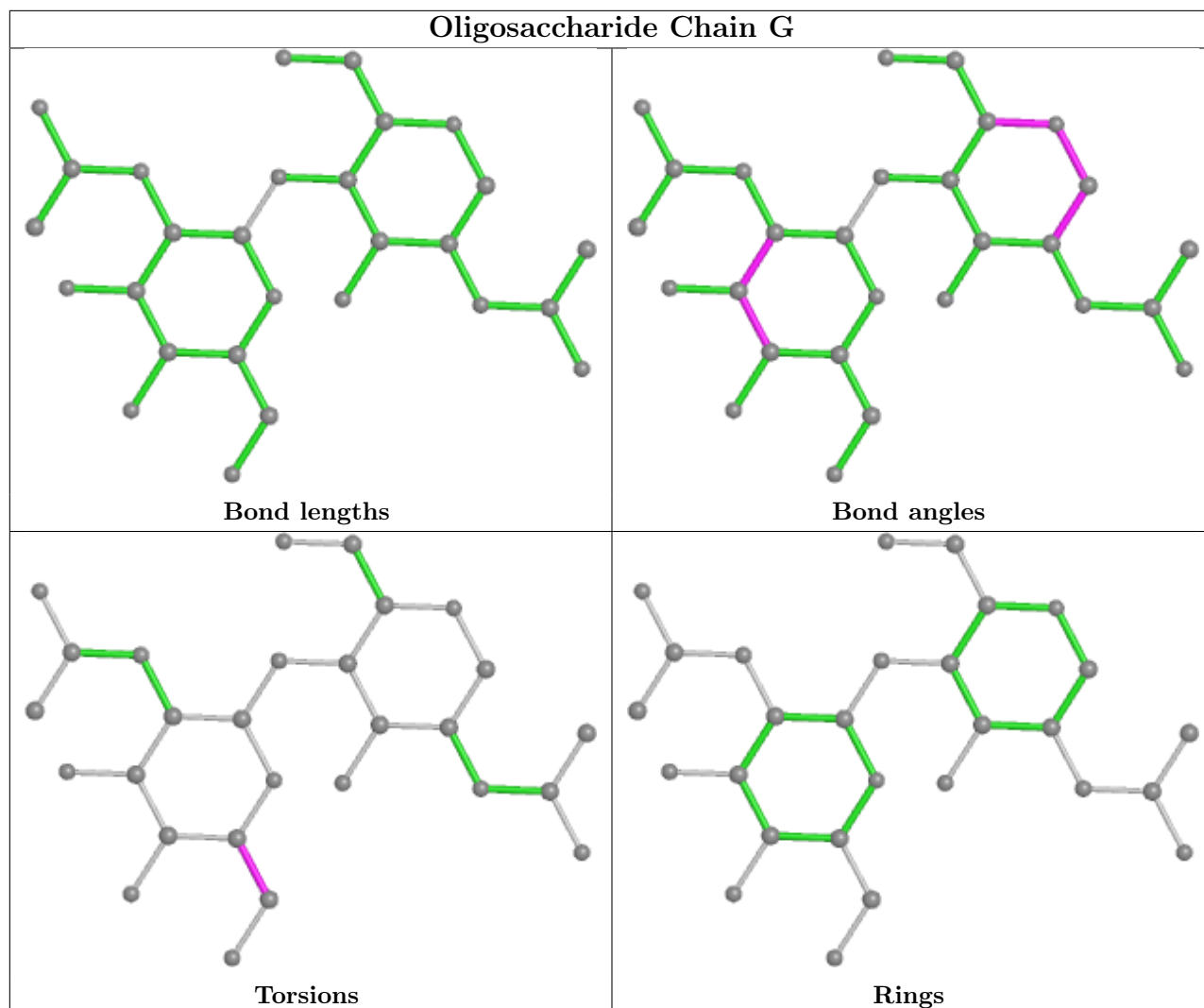
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.











## 5.6 Ligand geometry [i](#)

9 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	$\# Z  > 2$
4	NAG	B	1281	1	14,14,15	0.60	0	17,19,21	1.78	4 (23%)
4	NAG	A	1085	1	14,14,15	0.51	0	17,19,21	1.62	1 (5%)
3	M51	B	1000	-	32,34,34	1.16	4 (12%)	36,48,48	2.09	10 (27%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	NAG	B	1321	1	14,14,15	0.61	0	17,19,21	1.03	1 (5%)
4	NAG	B	1085	1	14,14,15	0.50	0	17,19,21	1.80	3 (17%)
4	NAG	A	1092	1	14,14,15	0.64	0	17,19,21	2.98	6 (35%)
3	M51	A	1000	-	32,34,34	1.00	2 (6%)	36,48,48	1.99	12 (33%)
4	NAG	B	1150	1	14,14,15	0.42	0	17,19,21	1.43	1 (5%)
4	NAG	A	1321	1	14,14,15	0.60	0	17,19,21	1.80	3 (17%)

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
4	NAG	B	1281	1	-	2/6/23/26	0/1/1/1
4	NAG	A	1085	1	-	2/6/23/26	0/1/1/1
3	M51	B	1000	-	-	2/16/46/46	0/5/5/5
4	NAG	B	1321	1	-	0/6/23/26	0/1/1/1
4	NAG	B	1085	1	-	2/6/23/26	0/1/1/1
4	NAG	A	1092	1	-	5/6/23/26	0/1/1/1
3	M51	A	1000	-	-	0/16/46/46	0/5/5/5
4	NAG	B	1150	1	-	2/6/23/26	0/1/1/1
4	NAG	A	1321	1	-	2/6/23/26	0/1/1/1

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1000	M51	C6-N4	-3.24	1.34	1.44
3	B	1000	M51	C29-S28	-3.09	1.75	1.82
3	B	1000	M51	C6-N4	-3.00	1.35	1.44
3	B	1000	M51	C5-N4	-2.29	1.34	1.37
3	A	1000	M51	C29-S28	-2.24	1.77	1.82
3	B	1000	M51	C7-C6	2.09	1.42	1.38

All (41) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1092	NAG	C2-N2-C7	7.10	133.01	122.90
4	A	1092	NAG	C1-O5-C5	6.34	120.78	112.19
4	A	1085	NAG	C1-O5-C5	5.42	119.54	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	1085	NAG	C1-O5-C5	5.39	119.50	112.19
3	B	1000	M51	C17-N16-C15	5.23	118.63	109.08
3	B	1000	M51	C12-C2-N3	5.00	130.02	120.07
4	B	1281	NAG	C1-O5-C5	4.74	118.62	112.19
3	A	1000	M51	C12-C2-N3	4.57	129.17	120.07
4	B	1150	NAG	O5-C5-C6	4.27	113.89	107.20
4	A	1321	NAG	C1-O5-C5	4.23	117.93	112.19
3	B	1000	M51	C12-C2-C1	-4.15	118.06	129.06
3	A	1000	M51	C12-C2-C1	-4.09	118.24	129.06
3	A	1000	M51	C17-N16-C15	4.07	116.52	109.08
3	A	1000	M51	C11-C6-C7	-4.04	115.35	121.33
4	A	1092	NAG	C3-C4-C5	3.83	117.07	110.24
3	B	1000	M51	C11-C6-C7	-3.79	115.71	121.33
4	B	1281	NAG	O5-C5-C6	3.75	113.08	107.20
3	A	1000	M51	C10-C11-C6	3.64	123.35	118.63
4	A	1092	NAG	C1-C2-N2	3.58	116.60	110.49
3	B	1000	M51	C27-S28-C29	3.56	100.30	91.48
4	A	1092	NAG	C8-C7-N2	3.39	121.84	116.10
3	B	1000	M51	C8-C7-C6	3.30	122.92	118.63
3	A	1000	M51	C8-C7-C6	3.08	122.62	118.63
4	A	1092	NAG	O5-C5-C4	3.05	118.25	110.83
3	B	1000	M51	C10-C11-C6	2.99	122.51	118.63
3	A	1000	M51	C7-C6-N4	2.92	125.03	119.50
4	B	1085	NAG	C2-N2-C7	2.91	127.04	122.90
4	A	1321	NAG	C4-C3-C2	-2.80	106.91	111.02
3	B	1000	M51	C11-C6-N4	2.74	124.69	119.50
4	B	1281	NAG	O5-C1-C2	-2.66	107.08	111.29
3	B	1000	M51	C18-N13-C14	2.63	117.33	111.52
4	B	1085	NAG	O7-C7-N2	2.61	126.75	121.95
3	A	1000	M51	C27-S28-C29	2.61	97.95	91.48
3	A	1000	M51	C6-N4-C5	2.55	132.00	129.04
3	A	1000	M51	C18-N13-C14	2.41	116.84	111.52
4	B	1321	NAG	C4-C3-C2	2.31	114.40	111.02
4	A	1321	NAG	O5-C1-C2	-2.29	107.67	111.29
3	A	1000	M51	C23-C22-N21	-2.18	101.98	106.22
3	A	1000	M51	C27-C26-N25	2.17	111.64	106.85
3	B	1000	M51	C15-N16-C19	-2.11	106.71	112.64
4	B	1281	NAG	C1-C2-N2	2.02	113.94	110.49

There are no chirality outliers.

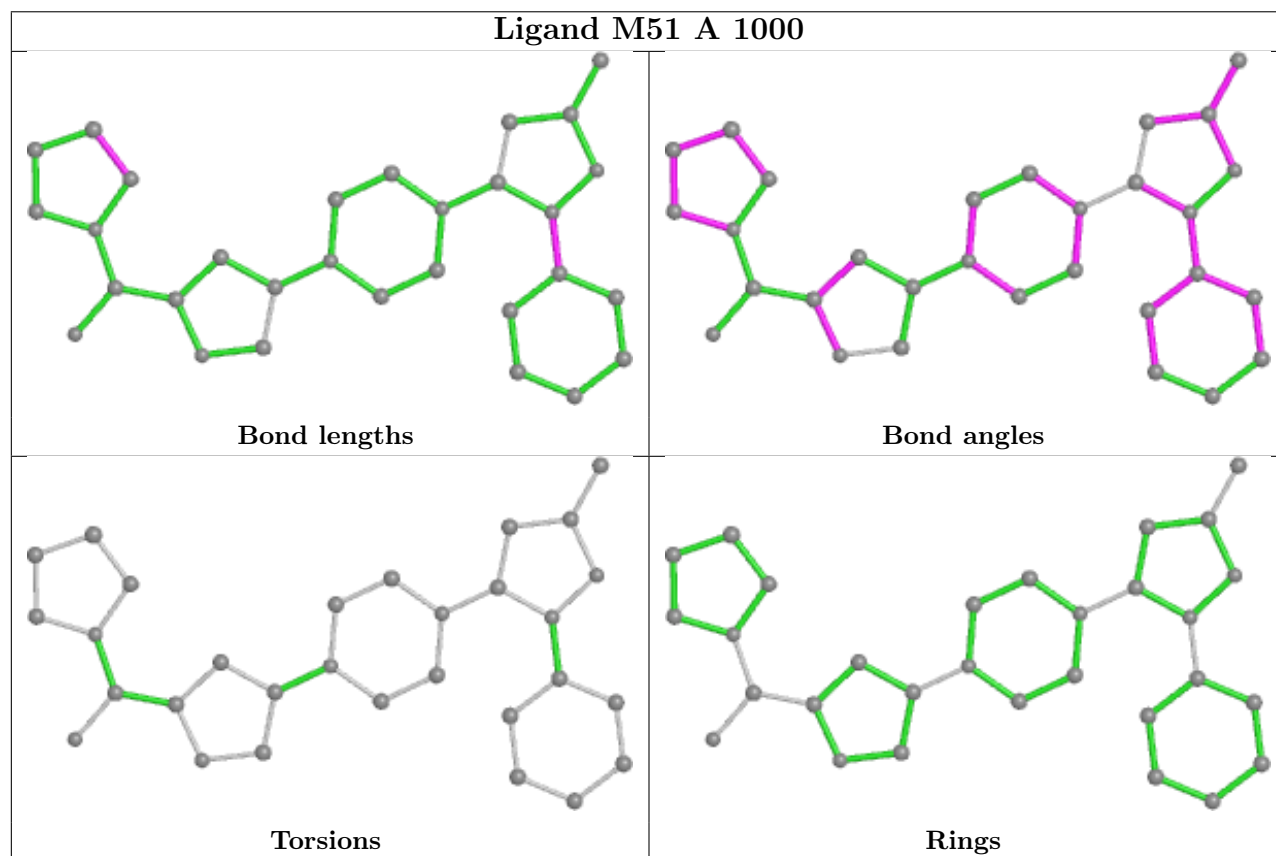
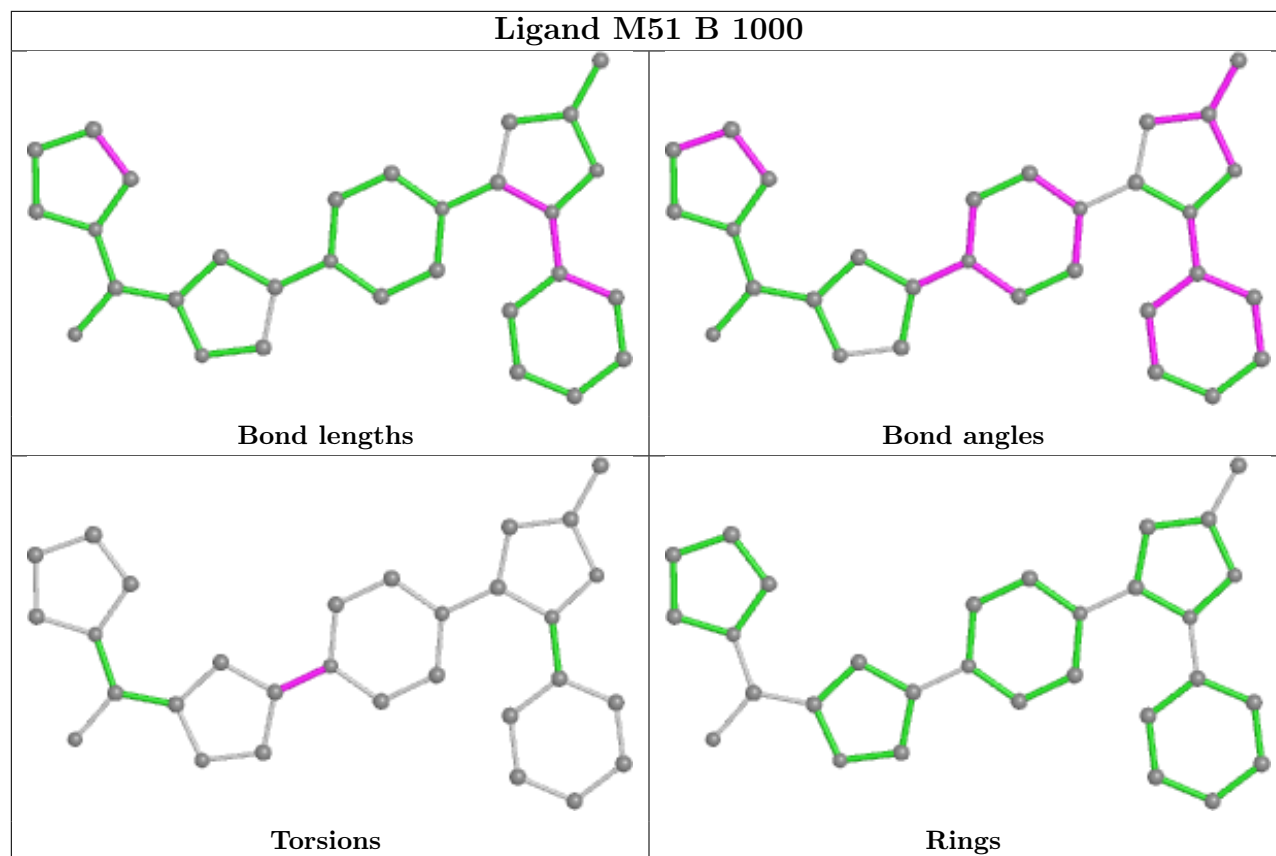
All (17) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	1092	NAG	O5-C5-C6-O6
4	A	1092	NAG	C4-C5-C6-O6
4	A	1321	NAG	C4-C5-C6-O6
4	A	1321	NAG	O5-C5-C6-O6
4	B	1281	NAG	O5-C5-C6-O6
4	B	1281	NAG	C4-C5-C6-O6
4	A	1092	NAG	C8-C7-N2-C2
4	A	1092	NAG	O7-C7-N2-C2
4	B	1150	NAG	C4-C5-C6-O6
4	A	1085	NAG	C4-C5-C6-O6
4	B	1150	NAG	O5-C5-C6-O6
4	B	1085	NAG	C4-C5-C6-O6
4	A	1092	NAG	C1-C2-N2-C7
4	A	1085	NAG	O5-C5-C6-O6
3	B	1000	M51	C20-C19-N16-C17
3	B	1000	M51	C23-C19-N16-C17
4	B	1085	NAG	O5-C5-C6-O6

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 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 [i](#)

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

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	729/740 (98%)	-0.19	5 (0%) 87 89	24, 36, 57, 75	0
1	B	729/740 (98%)	-0.24	8 (1%) 80 82	23, 35, 54, 68	0
All	All	1458/1480 (98%)	-0.21	13 (0%) 84 86	23, 35, 56, 75	0

All (13) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	766	PRO	8.3
1	B	766	PRO	7.5
1	A	765	LEU	6.1
1	B	765	LEU	5.6
1	B	336	ARG	3.2
1	B	71	LYS	2.9
1	A	505	GLN	2.6
1	A	39	SER	2.6
1	B	138	ASN	2.5
1	B	73	GLU	2.5
1	B	97	GLU	2.4
1	B	764	SER	2.1
1	A	119	ASN	2.0

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

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

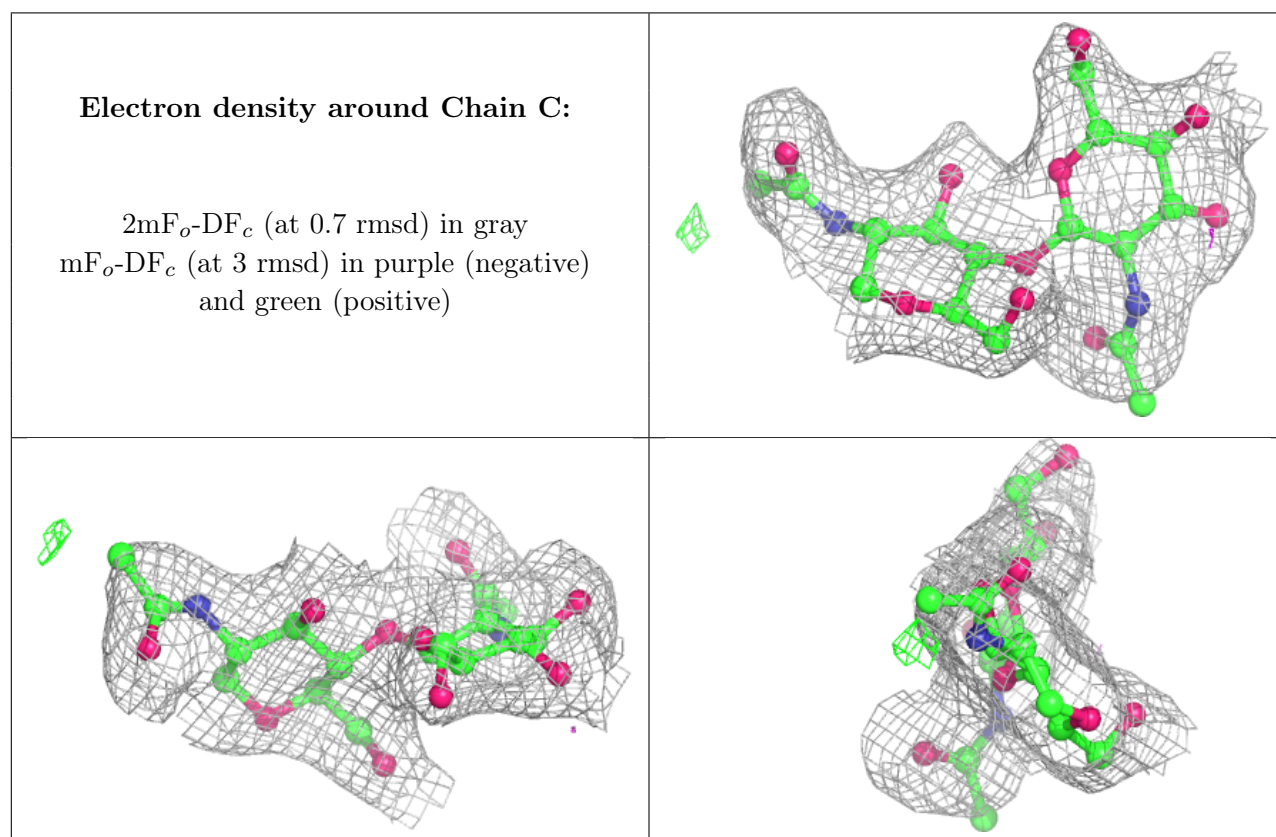
### 6.3 Carbohydrates [i](#)

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

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

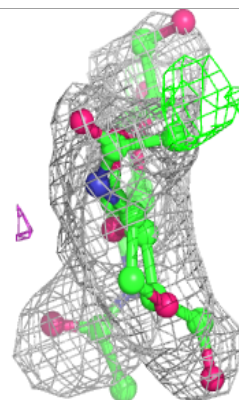
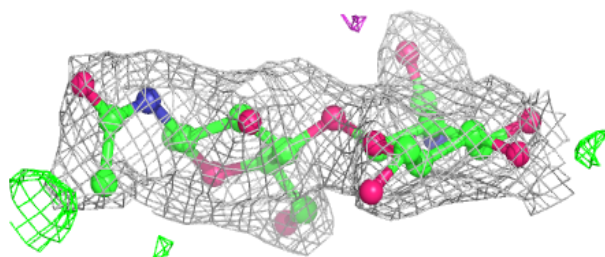
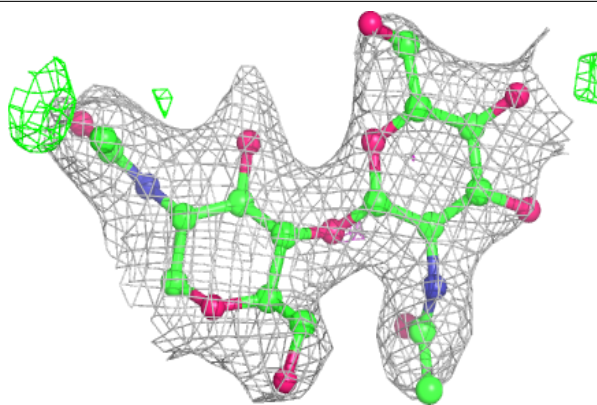
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
2	NAG	D	2	14/15	0.80	0.40	62,65,67,68	0
2	NAG	F	2	14/15	0.80	0.28	61,63,66,67	0
2	NAG	G	2	14/15	0.82	0.24	58,61,62,63	0
2	NAG	C	2	14/15	0.86	0.29	55,57,59,60	0
2	NAG	D	1	14/15	0.90	0.16	45,48,54,58	0
2	NAG	E	2	14/15	0.91	0.13	40,46,48,49	0
2	NAG	F	1	14/15	0.92	0.17	51,55,56,59	0
2	NAG	C	1	14/15	0.94	0.21	41,47,51,52	0
2	NAG	G	1	14/15	0.96	0.13	43,47,51,54	0
2	NAG	E	1	14/15	0.97	0.12	31,39,43,44	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.

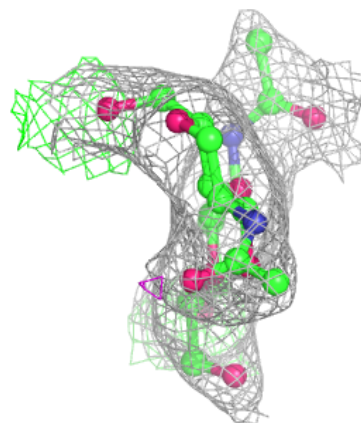
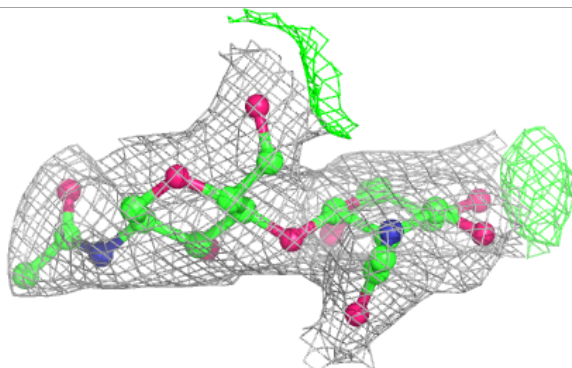
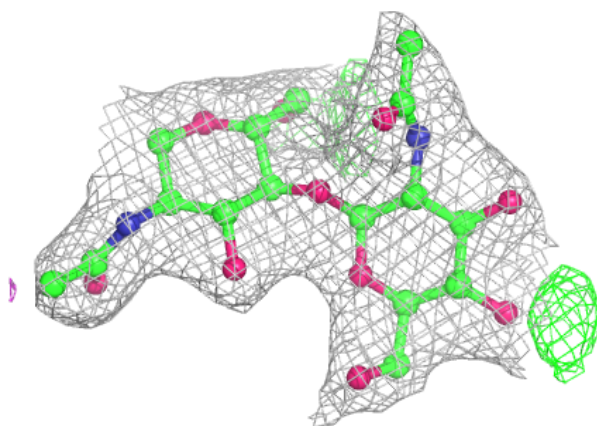


**Electron density around Chain D:**

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

**Electron density around Chain E:**

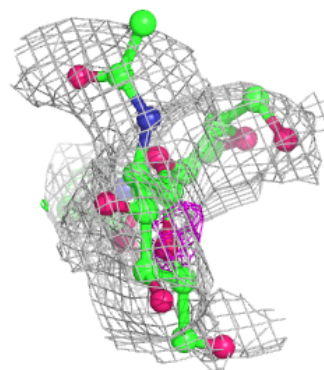
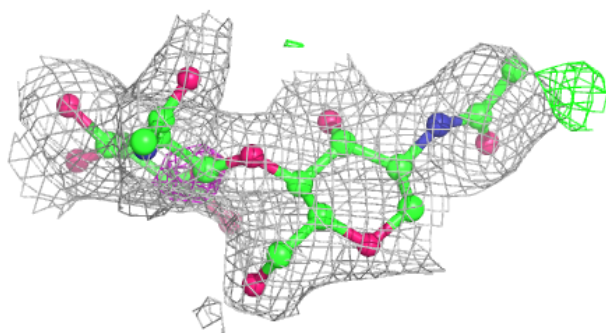
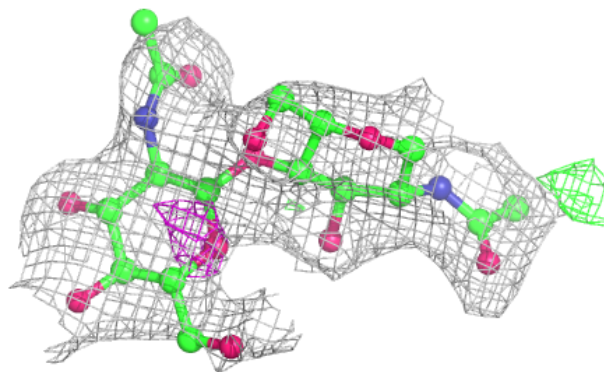
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



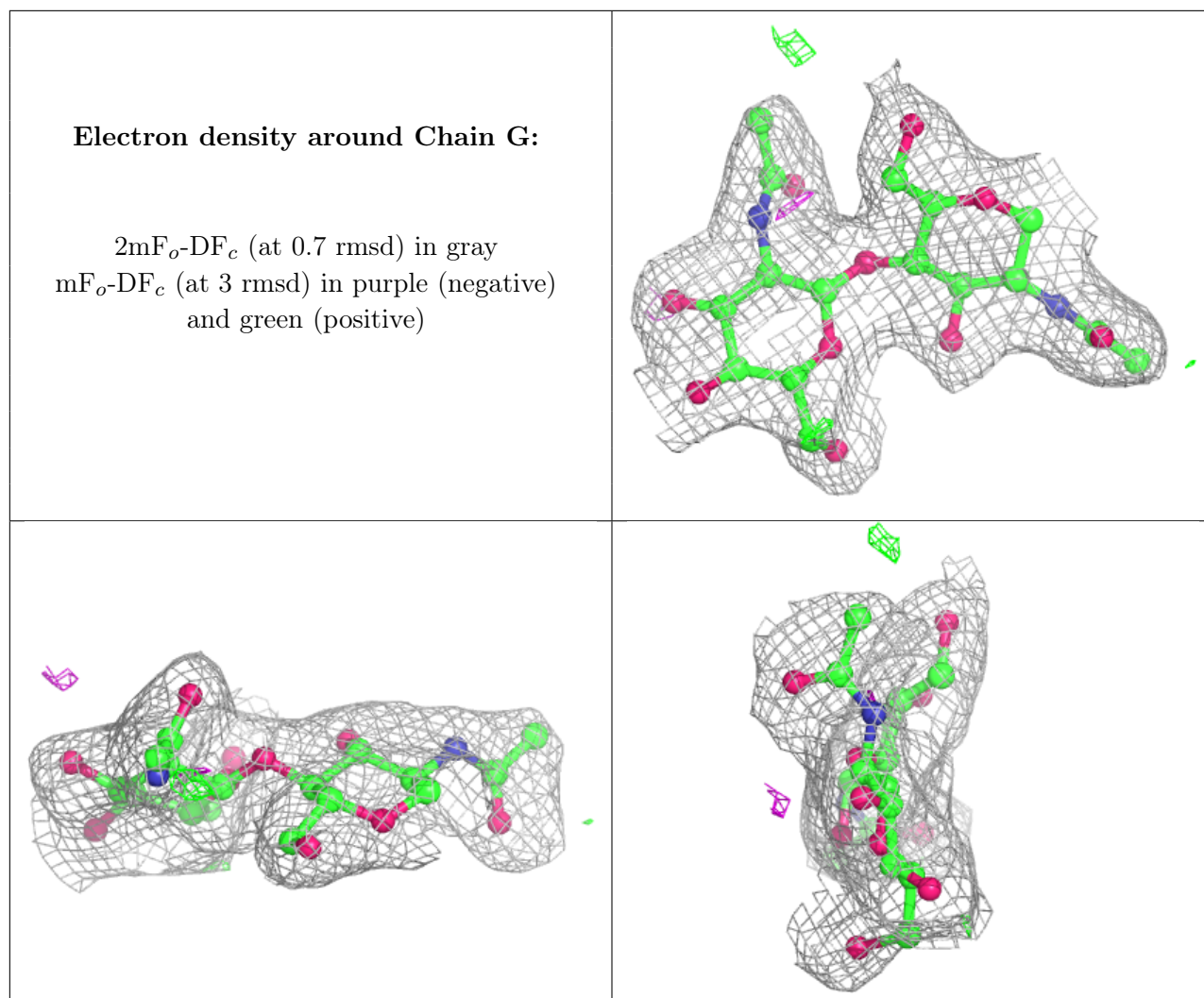


**Electron density around Chain F:**

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





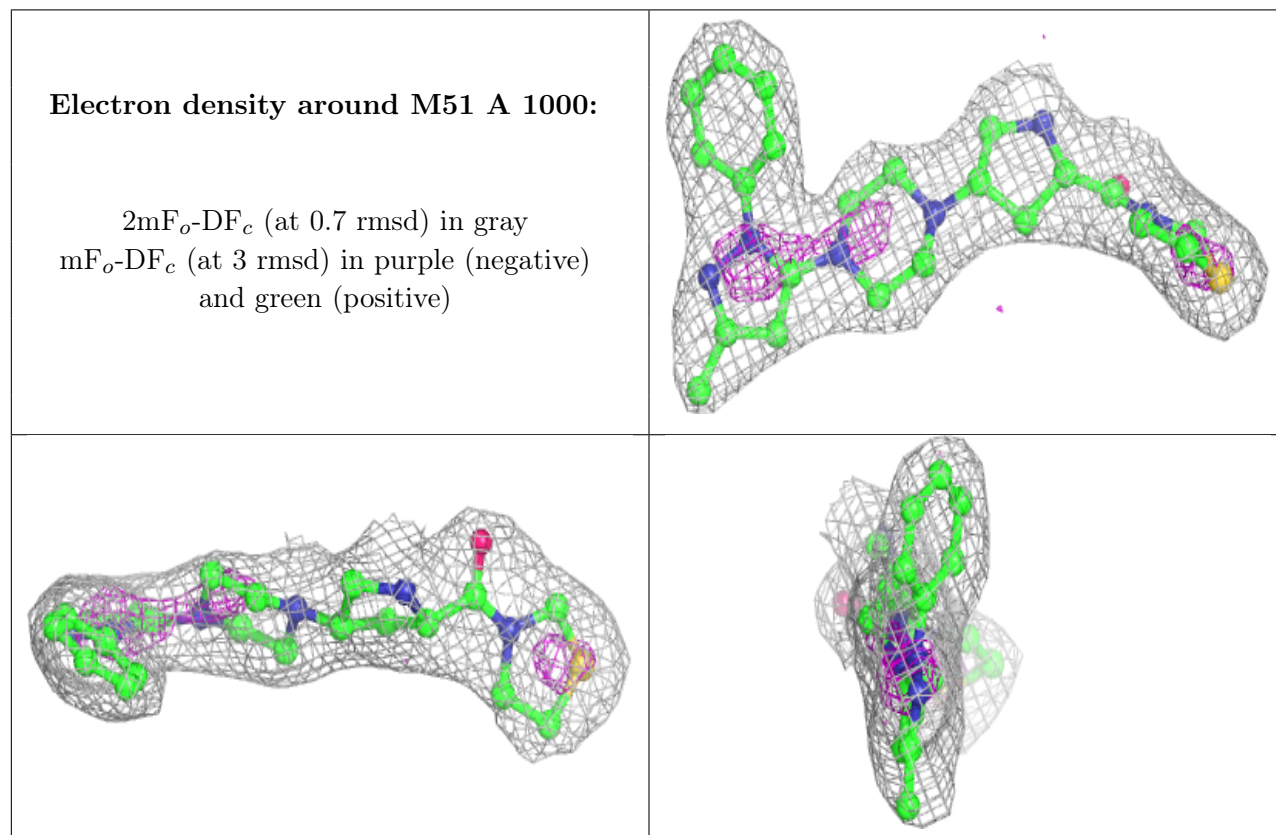


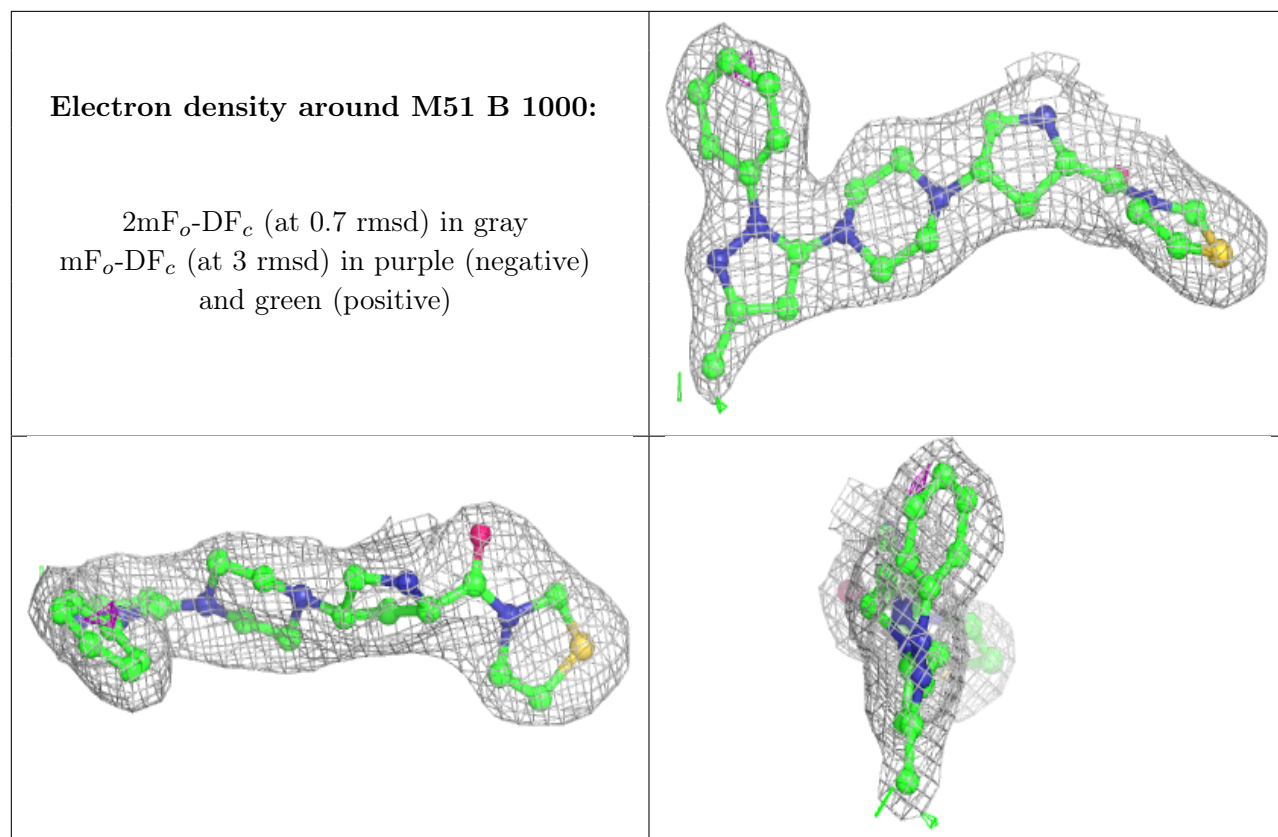
## 6.4 Ligands [i](#)

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	1092	14/15	0.76	0.24	81,82,83,84	0
4	NAG	B	1321	14/15	0.77	0.28	57,61,64,64	0
4	NAG	B	1281	14/15	0.78	0.13	59,61,62,62	0
4	NAG	A	1321	14/15	0.79	0.26	59,63,66,67	0
4	NAG	B	1150	14/15	0.83	0.20	59,61,64,65	0
4	NAG	A	1085	14/15	0.86	0.12	54,59,60,61	0
4	NAG	B	1085	14/15	0.87	0.10	53,54,58,59	0
3	M51	A	1000	30/30	0.94	0.14	26,31,35,36	0
3	M51	B	1000	30/30	0.95	0.14	30,33,35,36	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.





## 6.5 Other polymers [i](#)

There are no such residues in this entry.