



# Full wwPDB X-ray Structure Validation Report ⓘ

Jun 19, 2024 – 02:34 PM EDT

PDB ID : 4BZS  
Title : Human angiotensin converting enzyme N-domain in complex with K-26  
Authors : Kramer, G.J.; Mohd, A.; Schwager, S.L.U.; Masuyer, G.; Acharya, K.R.; Sturrock, E.D.; Bachmann, B.O.  
Deposited on : 2013-07-29  
Resolution : 2.10 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	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
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)	:	2.37.1

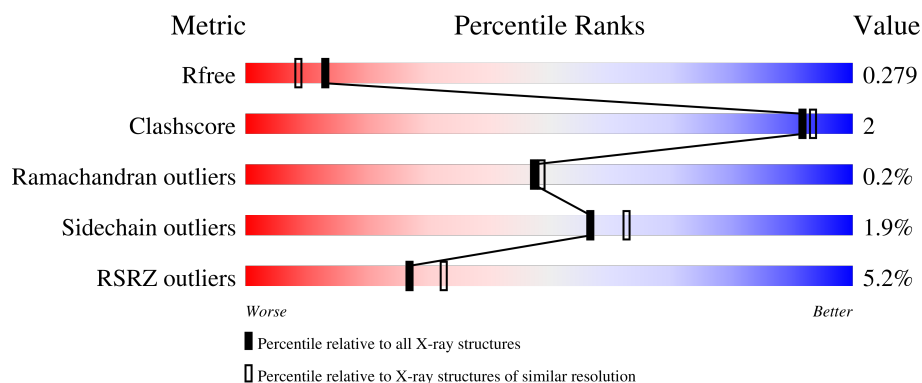
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.10 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.




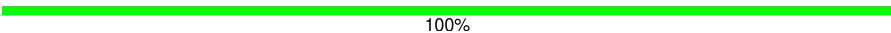
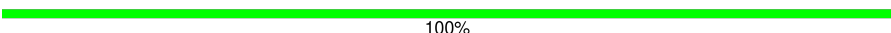
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (2.10-2.10)

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	629	<div> <div>6%</div> <div> <div></div> <div>92%</div> <div>5%</div> <div></div> </div> </div>
1	B	629	<div> <div>4%</div> <div> <div></div> <div>90%</div> <div>7%</div> <div></div> </div> </div>
2	C	2	<div> <div></div> <div>100%</div> </div>
2	F	2	<div> <div></div> <div>100%</div> </div>
3	D	2	<div> <div></div> <div> <div>50%</div> <div>50%</div> </div> </div>

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Mol	Chain	Length	Quality of chain
3	G	2	
4	E	3	
4	H	3	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	FUC	C	2	-	-	-	X

## 2 Entry composition

There are 13 unique types of molecules in this entry. The entry contains 10447 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 ANGIOTENSIN-CONVERTING ENZYME.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	612	Total	C	N	O	S	4	0	0
			4980	3197	855	909	19			
1	B	610	Total	C	N	O	S	1	0	0
			4961	3186	853	903	19			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	629	LEU	-	expression tag	UNP P12821
A	576	LEU	PRO	engineered mutation	UNP P12821
B	629	LEU	-	expression tag	UNP P12821
B	576	LEU	PRO	engineered mutation	UNP P12821

- Molecule 2 is an oligosaccharide called alpha-L-fucopyranose-(1-6)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	C	2	Total	C	N	O	0	0	0
			24	14	1	9			
2	F	2	Total	C	N	O	0	0	0
			24	14	1	9			

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	D	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			

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



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

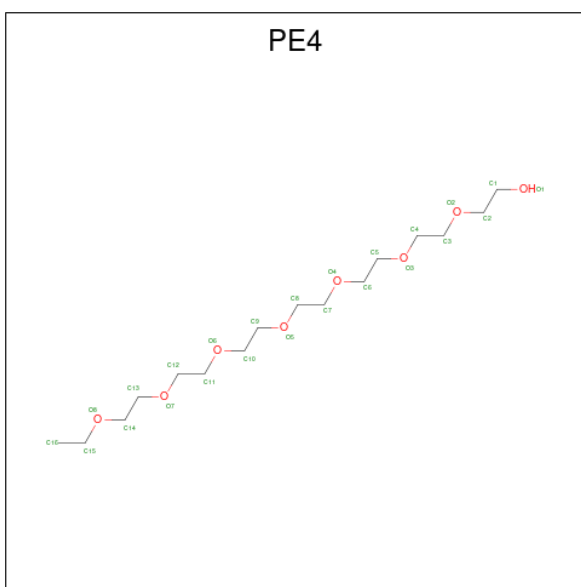
- Molecule 5 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	Zn	0	0
			1	1		
5	B	1	Total	Zn	0	0
			1	1		

- Molecule 6 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

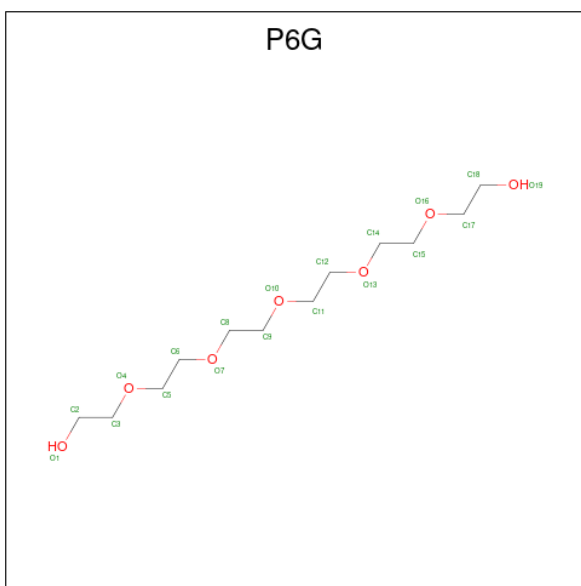
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	1	Total	Cl	0	0
			1	1		
6	B	1	Total	Cl	0	0
			1	1		

- Molecule 7 is 2-{2-[2-(2-{2-[2-(2-ETHOXY-ETHOXY)-ETHOXY]-ETHOXY}-ETHOXY)-ETHOXY]-ETHOXY}-ETHANOL (three-letter code: PE4) (formula: C<sub>16</sub>H<sub>34</sub>O<sub>8</sub>).



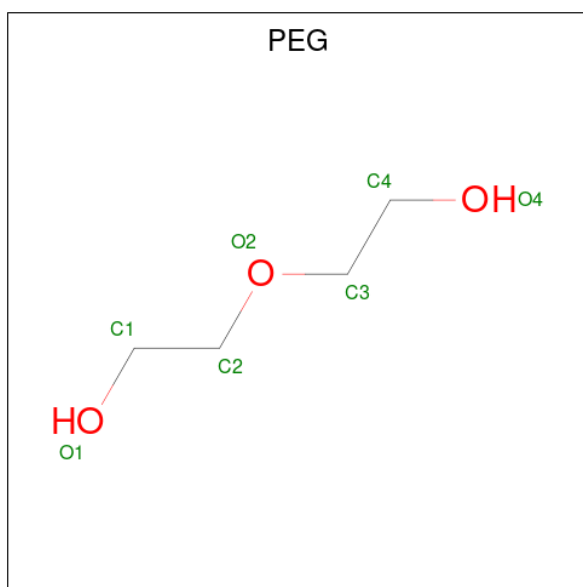
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	C	O	0	0
			13	8	5		

- Molecule 8 is HEXAETHYLENE GLYCOL (three-letter code: P6G) (formula:  $C_{12}H_{26}O_7$ ).



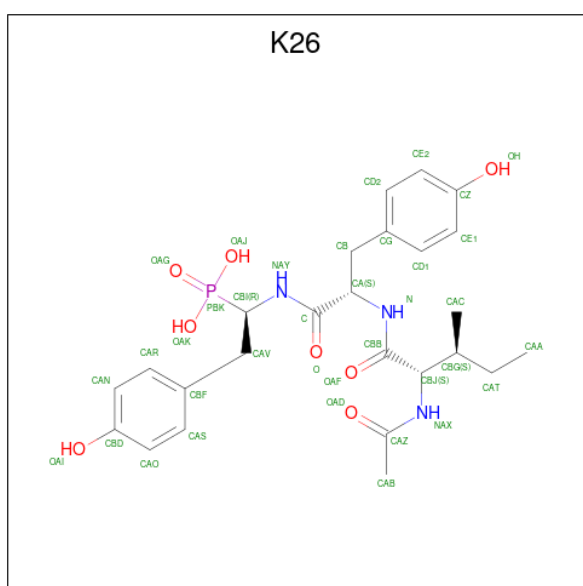
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	A	1	Total	C	O	0	0
			19	12	7		

- Molecule 9 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula:  $C_4H_{10}O_3$ ).



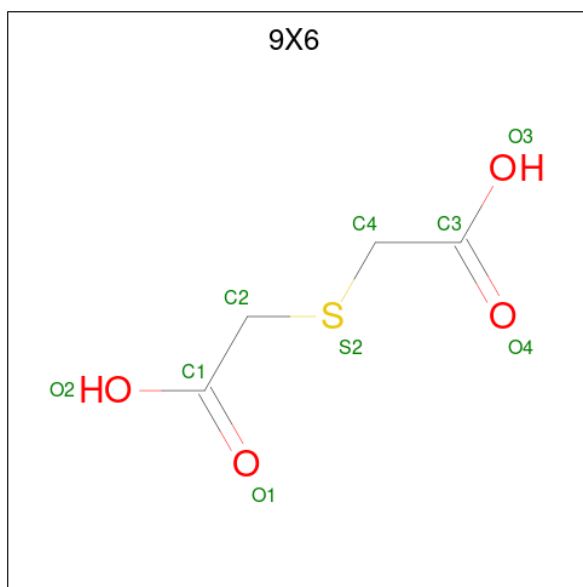
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	A	1	Total C O 7 4 3	0	0
9	B	1	Total C O 7 4 3	0	0
9	B	1	Total C O 7 4 3	0	0
9	B	1	Total C O 7 4 3	0	0

- Molecule 10 is N-ACETYL-L-ILE-L-TYR-(R)-1-AMINO-2-(4-HYDROXYPHENYL)ETHYLPHOSPHONIC ACID (three-letter code: K26) (formula:  $C_{25}H_{34}N_3O_8P$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
10	A	1	Total	C	N	O	P	0	0
			37	25	3	8	1		
10	B	1	Total	C	N	O	P	0	0
			37	25	3	8	1		

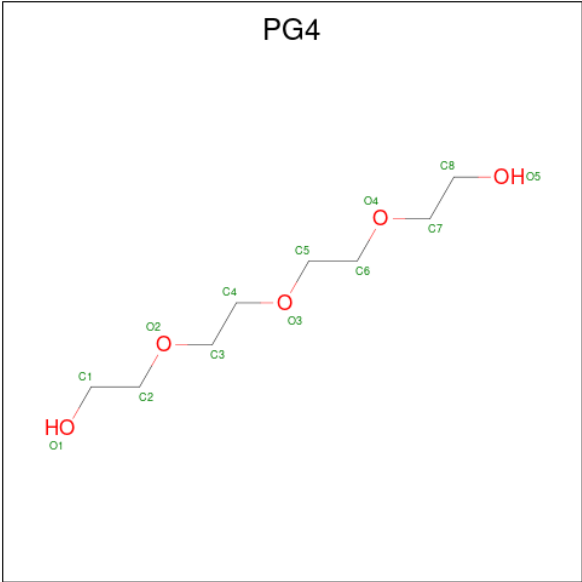
- Molecule 11 is thiodiglycolic acid (three-letter code: 9X6) (formula:  $C_4H_6O_4S$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
11	A	1	Total	C	O	S	0	0
			9	4	4	1		
11	B	1	Total	C	O	S	0	0
			9	4	4	1		

- Molecule 12 is TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula:  $C_8H_{18}O_5$ ).





Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
12	B	1	Total	C	O	0	0
			7	4	3		

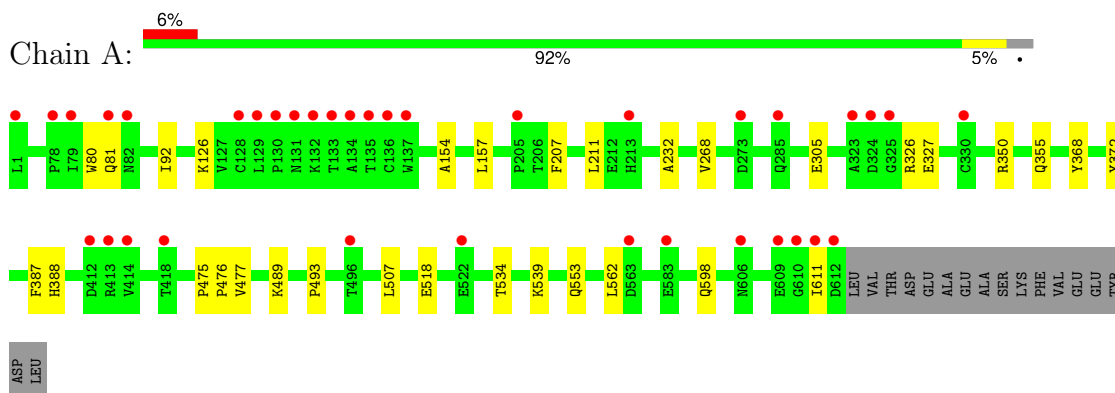
- Molecule 13 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
13	A	65	Total	O	0	0
			65	65		
13	B	96	Total	O	0	0
			96	96		

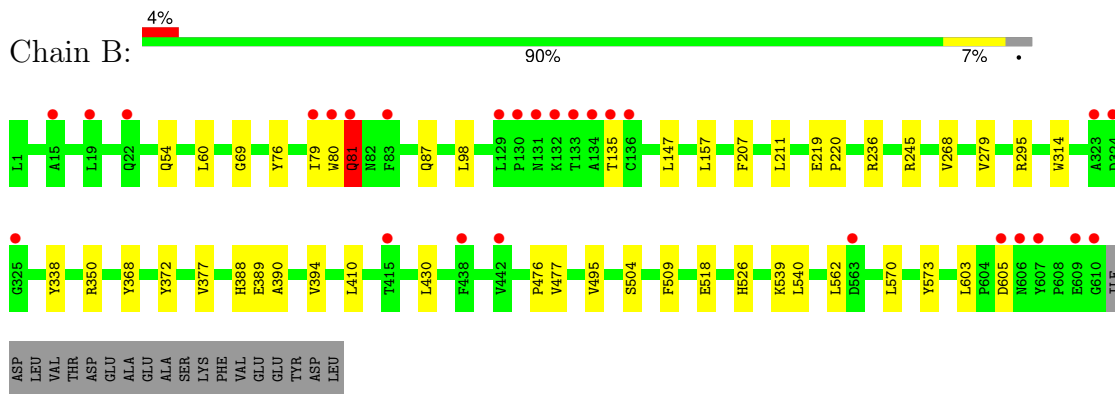
### 3 Residue-property plots

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

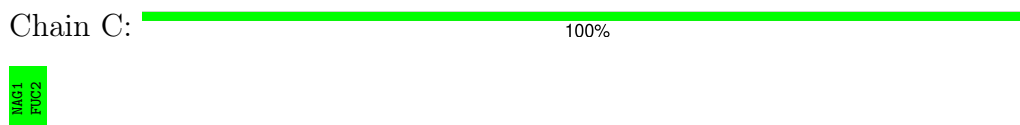
- Molecule 1: ANGIOTENSIN-CONVERTING ENZYME



- Molecule 1: ANGIOTENSIN-CONVERTING ENZYME



- Molecule 2: alpha-L-fucopyranose-(1-6)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 2: alpha-L-fucopyranose-(1-6)-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 4: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



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



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	73.00Å 77.32Å 82.07Å 88.69° 64.53° 75.29°	Depositor
Resolution (Å)	36.61 – 2.10 36.58 – 2.10	Depositor EDS
% Data completeness (in resolution range)	83.5 (36.61-2.10) 83.5 (36.58-2.10)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.62 (at 2.10Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, $R_{free}$	0.233 , 0.277 0.235 , 0.279	Depositor DCC
$R_{free}$ test set	3841 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	37.1	Xtriage
Anisotropy	0.240	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 41.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	10447	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.43% 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: PG4, PE4, K26, 9X6, NAG, ZN, BMA, P6G, CL, FUC, PEG

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	0.29	1/5137 (0.0%)	0.45	1/7002 (0.0%)
1	B	0.28	0/5118	0.46	0/6976
All	All	0.29	1/10255 (0.0%)	0.46	1/13978 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	126	LYS	CG-CD	-6.45	1.30	1.52

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	92	ILE	CB-CG1-CD1	-5.70	97.95	113.90

There are no chirality outliers.

There are no planarity outliers.

### 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	4980	0	4752	13	0
1	B	4961	0	4735	18	0
2	C	24	0	22	0	0
2	F	24	0	22	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	D	28	0	25	1	0
3	G	28	0	25	0	0
4	E	39	0	34	0	0
4	H	39	0	33	0	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
6	A	1	0	0	0	0
6	B	1	0	0	0	0
7	A	13	0	17	0	0
8	A	19	0	26	0	0
9	A	7	0	10	0	0
9	B	21	0	30	0	0
10	A	37	0	31	0	0
10	B	37	0	30	0	0
11	A	9	0	4	0	0
11	B	9	0	4	1	0
12	B	7	0	9	0	0
13	A	65	0	0	1	0
13	B	96	0	0	0	0
All	All	10447	0	9809	32	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 2.

All (32) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:598:GLN:NE2	13:A:2064:HOH:O	2.19	0.65
1:A:326:ARG:HD3	3:D:1:NAG:H82	1.86	0.56
1:B:76:TYR:HD1	1:B:79:ILE:HD11	1.76	0.51
1:B:477:VAL:HG12	1:B:603:LEU:HD21	1.93	0.51
1:A:305:GLU:HG3	1:A:534:THR:HG22	1.93	0.50
1:B:69:GLY:HA3	1:B:98:LEU:HD21	1.94	0.50
1:A:157:LEU:HD11	1:A:477:VAL:HG13	1.93	0.49
1:B:509:PHE:CE2	1:B:570:LEU:HD13	2.48	0.49
1:B:279:VAL:HG11	1:B:410:LEU:HD13	1.95	0.49
1:B:495:VAL:HG12	1:B:495:VAL:O	2.13	0.49
1:B:157:LEU:HD13	1:B:476:PRO:HB2	1.96	0.48
1:A:207:PHE:CE2	1:A:211:LEU:HD11	2.49	0.48
1:A:518:GLU:HG3	1:A:539:LYS:HD2	1.95	0.47
1:A:350:ARG:H	1:A:355:GLN:HE21	1.62	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:80:TRP:O	1:B:81:GLN:CG	2.65	0.44
1:A:489:LYS:O	1:A:493:PRO:HD2	2.18	0.44
1:B:518:GLU:HG3	1:B:539:LYS:HD2	1.98	0.44
1:B:389:GLU:HB2	1:B:504:SER:HB2	2.00	0.43
1:A:154:ALA:HB1	1:A:611:ILE:HG21	2.00	0.43
1:A:80:TRP:O	1:A:81:GLN:HB2	2.19	0.43
1:B:390:ALA:O	1:B:394:VAL:HG23	2.19	0.43
1:A:232:ALA:CB	1:A:268:VAL:HG12	2.49	0.42
1:B:207:PHE:CE2	1:B:211:LEU:HD11	2.54	0.42
1:B:80:TRP:O	1:B:81:GLN:CB	2.68	0.42
1:A:387:PHE:CE1	1:A:507:LEU:HD21	2.56	0.41
1:B:268:VAL:HG21	1:B:430:LEU:HD11	2.03	0.41
1:A:475:PRO:HA	1:A:476:PRO:HD3	1.93	0.41
1:B:526:HIS:HA	1:B:573:TYR:CE2	2.56	0.41
1:B:338:TYR:CD1	1:B:377:VAL:HG23	2.56	0.41
1:B:219:GLU:HB3	1:B:220:PRO:HD3	2.03	0.40
1:B:295:ARG:HD2	1:B:314:TRP:CH2	2.56	0.40
11:B:1612:9X6:C3	11:B:1612:9X6:O1	2.69	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	610/629 (97%)	589 (97%)	21 (3%)	0	100	100
1	B	608/629 (97%)	592 (97%)	14 (2%)	2 (0%)	41	41
All	All	1218/1258 (97%)	1181 (97%)	35 (3%)	2 (0%)	47	49

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	135	THR
1	B	81	GLN

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	524/541 (97%)	518 (99%)	6 (1%)	73	79
1	B	521/541 (96%)	507 (97%)	14 (3%)	44	48
All	All	1045/1082 (97%)	1025 (98%)	20 (2%)	57	63

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	327	GLU
1	A	368	TYR
1	A	372	TYR
1	A	388	HIS
1	A	553	GLN
1	A	562	LEU
1	B	54	GLN
1	B	60	LEU
1	B	81	GLN
1	B	87	GLN
1	B	147	LEU
1	B	236	ARG
1	B	245	ARG
1	B	350	ARG
1	B	368	TYR
1	B	372	TYR
1	B	388	HIS
1	B	540	LEU
1	B	562	LEU
1	B	605	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:



Mol	Chain	Res	Type
1	A	216	GLN
1	A	355	GLN
1	A	553	GLN
1	A	568	GLN
1	A	582	GLN
1	B	81	GLN
1	B	367	GLN
1	B	526	HIS

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates ⓘ

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	$\# Z  > 2$
2	NAG	C	1	2,1	14,14,15	0.49	0	17,19,21	0.77	0
2	FUC	C	2	2	10,10,11	0.63	0	14,14,16	0.48	0
3	NAG	D	1	3,1	14,14,15	0.52	0	17,19,21	1.04	2 (11%)
3	NAG	D	2	3	14,14,15	0.50	0	17,19,21	0.72	0
4	NAG	E	1	4,1	14,14,15	0.48	0	17,19,21	0.76	0
4	NAG	E	2	4	14,14,15	0.54	0	17,19,21	0.67	0
4	BMA	E	3	4	11,11,12	0.30	0	15,15,17	0.49	0
2	NAG	F	1	2,1	14,14,15	0.50	0	17,19,21	0.79	0
2	FUC	F	2	2	10,10,11	0.62	0	14,14,16	0.51	0
3	NAG	G	1	3,1	14,14,15	0.53	0	17,19,21	1.10	2 (11%)
3	NAG	G	2	3	14,14,15	0.47	0	17,19,21	0.75	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	NAG	H	1	4,1	14,14,15	0.49	0	17,19,21	0.66	0
4	NAG	H	2	4	14,14,15	0.45	0	17,19,21	0.76	0
4	BMA	H	3	4	11,11,12	0.33	0	15,15,17	0.59	0

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	2,1	-	2/6/23/26	0/1/1/1
2	FUC	C	2	2	-	-	0/1/1/1
3	NAG	D	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	D	2	3	-	0/6/23/26	0/1/1/1
4	NAG	E	1	4,1	-	0/6/23/26	0/1/1/1
4	NAG	E	2	4	-	0/6/23/26	0/1/1/1
4	BMA	E	3	4	-	2/2/19/22	0/1/1/1
2	NAG	F	1	2,1	-	0/6/23/26	0/1/1/1
2	FUC	F	2	2	-	-	0/1/1/1
3	NAG	G	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	G	2	3	-	0/6/23/26	0/1/1/1
4	NAG	H	1	4,1	-	0/6/23/26	0/1/1/1
4	NAG	H	2	4	-	2/6/23/26	0/1/1/1
4	BMA	H	3	4	-	2/2/19/22	0/1/1/1

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	G	1	NAG	C1-O5-C5	2.61	115.68	112.19
3	G	1	NAG	O5-C1-C2	-2.53	107.38	111.29
3	D	1	NAG	O5-C1-C2	-2.32	107.70	111.29
3	D	1	NAG	C1-O5-C5	2.04	114.92	112.19

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	1	NAG	O5-C5-C6-O6
4	H	2	NAG	O5-C5-C6-O6

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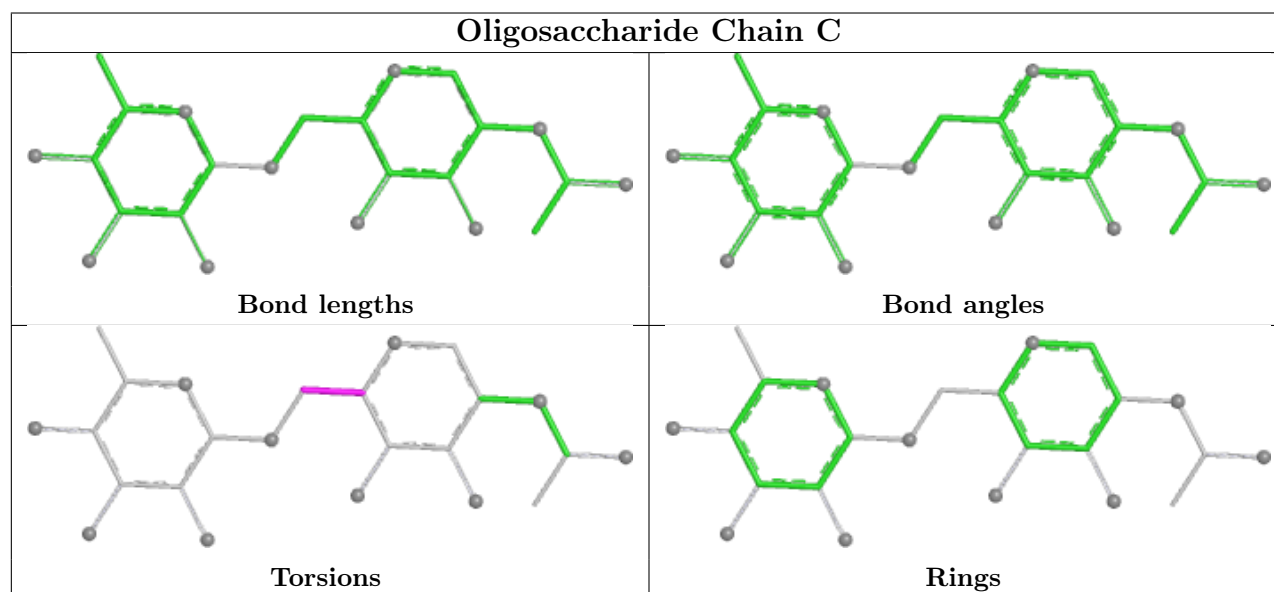
Mol	Chain	Res	Type	Atoms
4	E	3	BMA	C4-C5-C6-O6
4	E	3	BMA	O5-C5-C6-O6
4	H	3	BMA	O5-C5-C6-O6
4	H	2	NAG	C4-C5-C6-O6
2	C	1	NAG	C4-C5-C6-O6
4	H	3	BMA	C4-C5-C6-O6

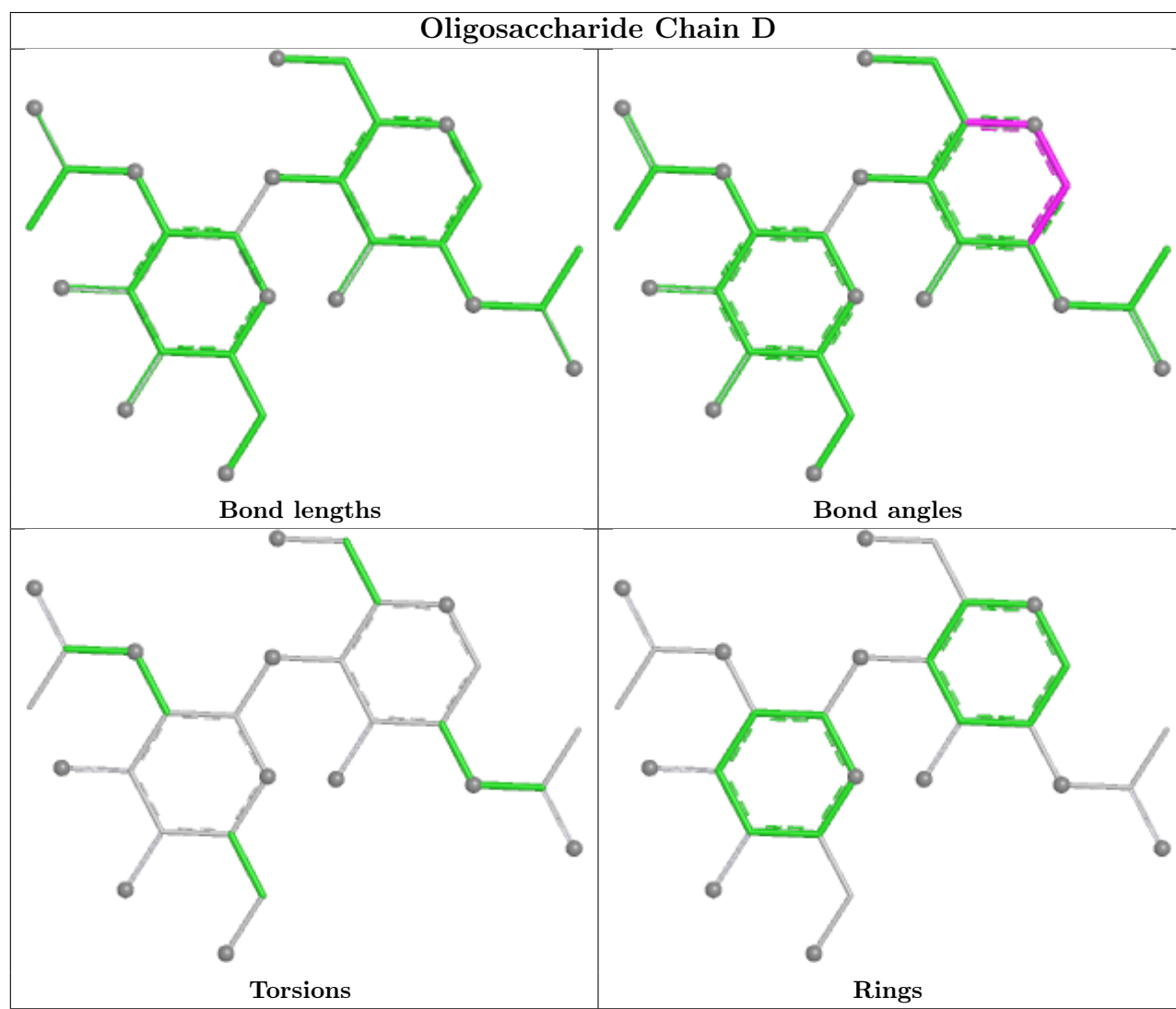
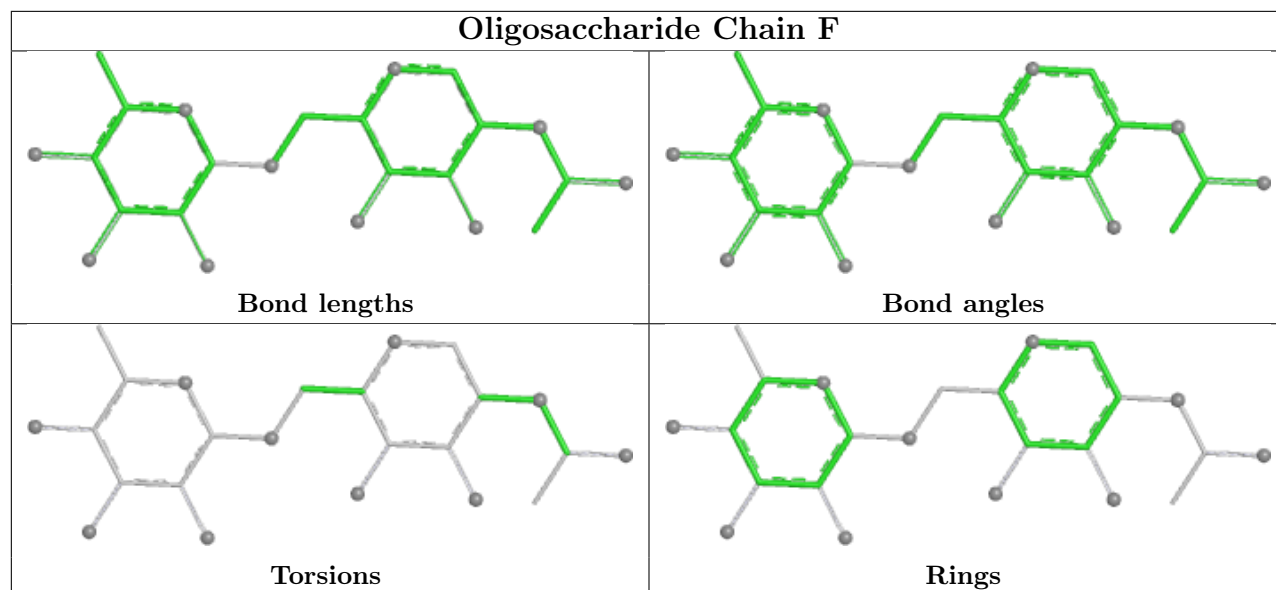
There are no ring outliers.

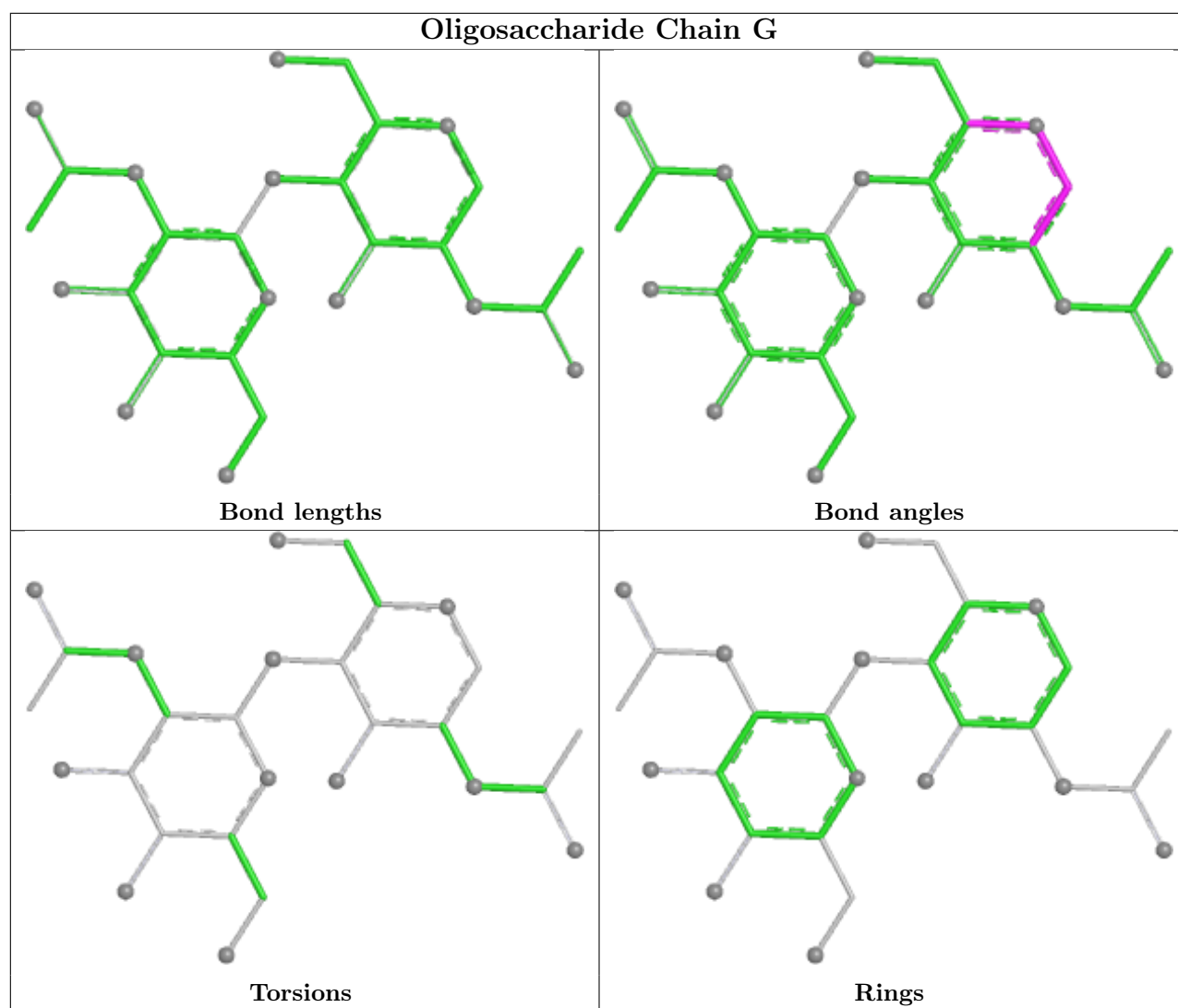
1 monomer is involved in 1 short contact:

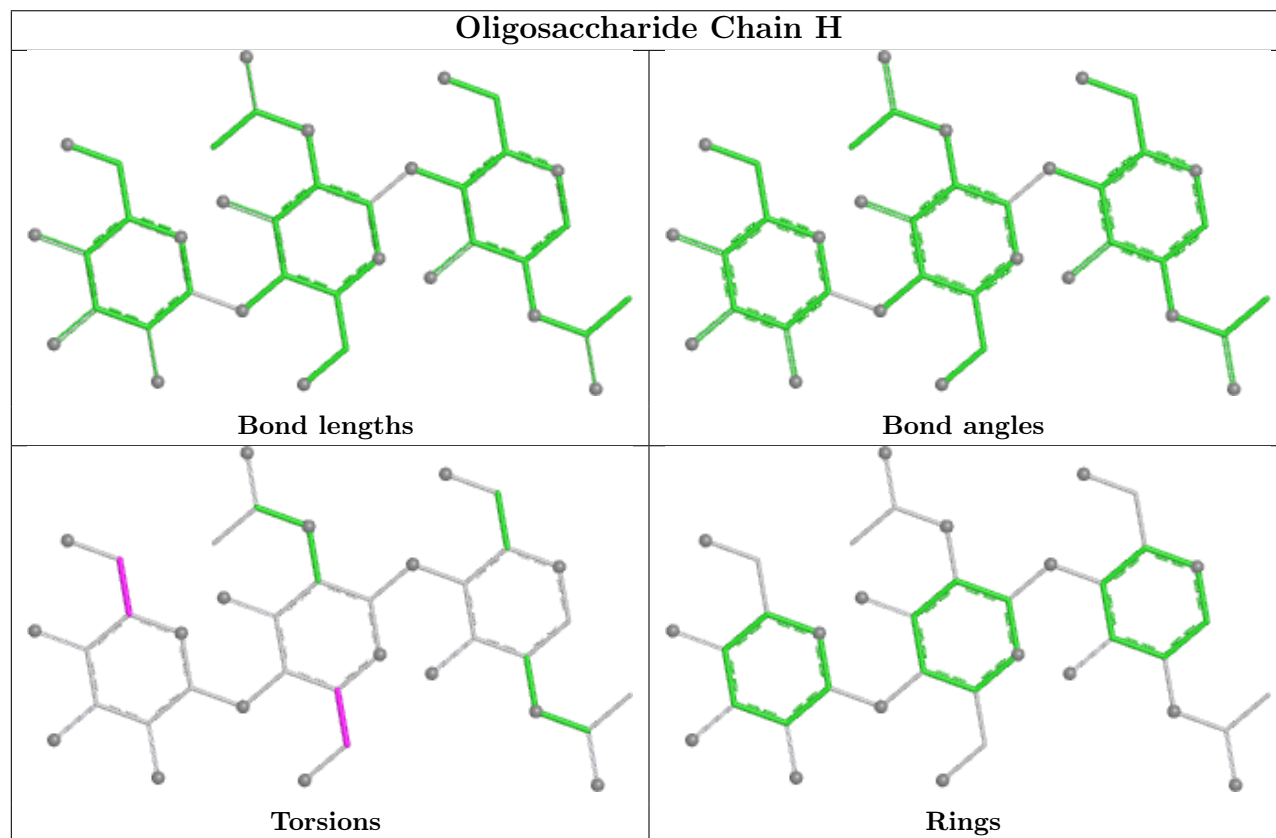
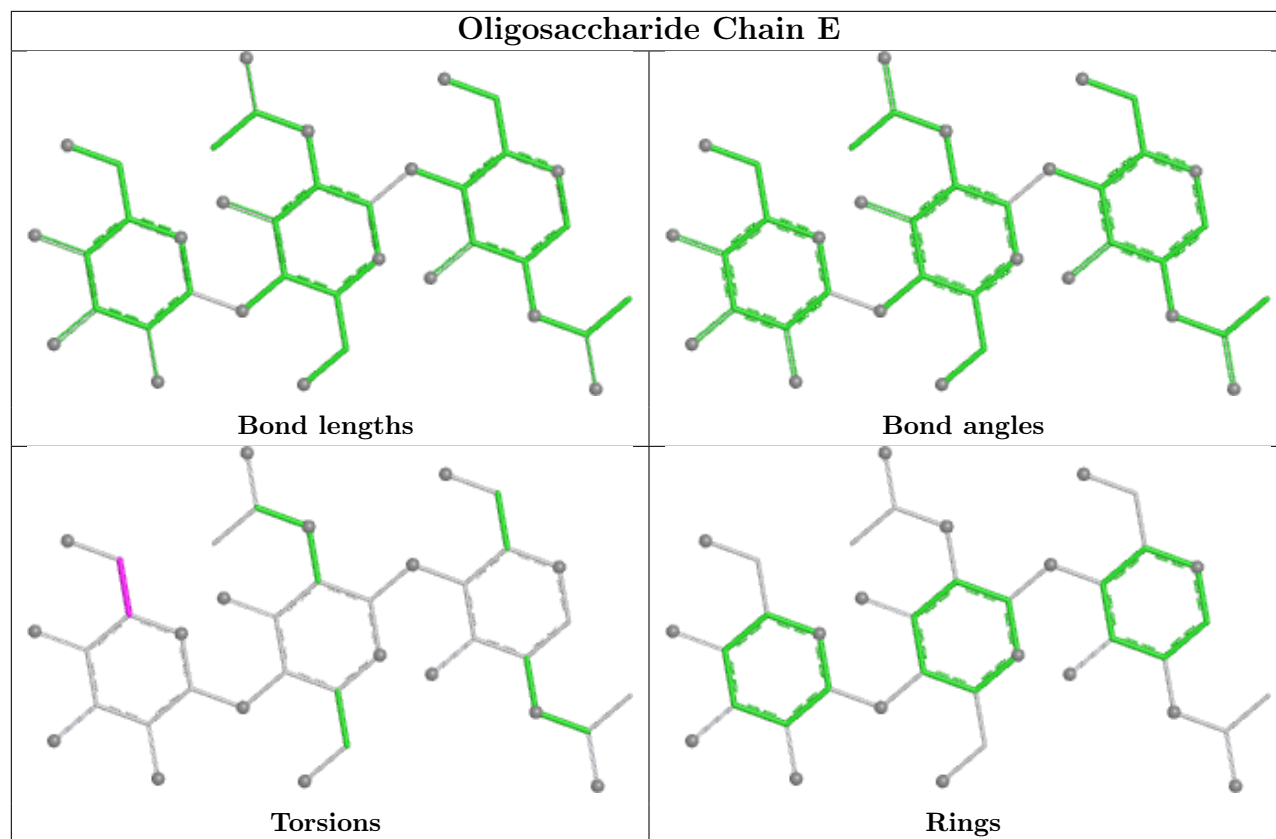
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	1	NAG	1	0

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









## 5.6 Ligand geometry

Of 15 ligands modelled in this entry, 4 are monoatomic - leaving 11 for Mogul analysis.

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
7	PE4	A	703	-	12,12,23	0.47	0	11,11,22	0.16	0
8	P6G	A	704	-	18,18,18	0.49	0	17,17,17	0.17	0
11	9X6	B	1612	-	8,8,8	1.28	0	9,9,9	2.35	2 (22%)
10	K26	B	1001	5	38,38,38	1.68	4 (10%)	49,53,53	1.31	5 (10%)
11	9X6	A	1613	-	8,8,8	1.36	0	9,9,9	1.74	2 (22%)
9	PEG	B	704	-	6,6,6	0.43	0	5,5,5	0.25	0
9	PEG	A	705	-	6,6,6	0.48	0	5,5,5	0.22	0
10	K26	A	1001	5	38,38,38	1.65	4 (10%)	49,53,53	1.26	5 (10%)
9	PEG	B	705	-	6,6,6	0.46	0	5,5,5	0.25	0
9	PEG	B	703	-	6,6,6	0.51	0	5,5,5	0.26	0
12	PG4	B	1611	-	6,6,12	0.45	0	5,5,11	0.19	0

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
7	PE4	A	703	-	-	5/10/10/21	-
8	P6G	A	704	-	-	3/16/16/16	-
11	9X6	B	1612	-	-	5/6/6/6	-
10	K26	B	1001	5	-	3/40/40/40	0/2/2/2
11	9X6	A	1613	-	-	4/6/6/6	-
9	PEG	B	704	-	-	2/4/4/4	-
9	PEG	A	705	-	-	1/4/4/4	-
10	K26	A	1001	5	-	3/40/40/40	0/2/2/2
9	PEG	B	705	-	-	2/4/4/4	-
9	PEG	B	703	-	-	2/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
12	PG4	B	1611	-	-	3/4/4/10	-

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	B	1001	K26	PBK-OAJ	-5.45	1.46	1.54
10	A	1001	K26	PBK-OAJ	-5.36	1.46	1.54
10	B	1001	K26	PBK-OAK	-5.28	1.46	1.54
10	A	1001	K26	PBK-OAK	-5.19	1.46	1.54
10	B	1001	K26	CAV-CBF	-4.30	1.41	1.51
10	A	1001	K26	CAV-CBF	-4.27	1.41	1.51
10	A	1001	K26	CB-CG	-4.16	1.41	1.51
10	B	1001	K26	CB-CG	-4.11	1.41	1.51

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	B	1001	K26	OAG-PBK-CBI	-6.51	101.13	113.80
11	B	1612	9X6	C2-S2-C4	6.00	114.51	100.69
10	A	1001	K26	OAG-PBK-CBI	-5.90	102.32	113.80
10	B	1001	K26	OAK-PBK-OAJ	3.20	116.28	107.58
11	A	1613	9X6	C2-S2-C4	3.14	107.93	100.69
10	A	1001	K26	OAK-PBK-OAJ	3.04	115.83	107.58
10	A	1001	K26	C-CA-N	-2.69	103.84	111.11
10	A	1001	K26	CG-CB-CA	-2.25	107.38	113.36
10	B	1001	K26	C-CA-N	-2.23	105.06	111.11
11	A	1613	9X6	C1-C2-S2	-2.14	107.62	113.18
10	B	1001	K26	CAV-CBI-NAY	-2.09	108.92	111.36
10	A	1001	K26	CAV-CBI-NAY	-2.09	108.92	111.36
11	B	1612	9X6	O3-C3-C4	2.02	119.93	113.38
10	B	1001	K26	CG-CB-CA	-2.00	108.03	113.36

There are no chirality outliers.

All (33) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
11	B	1612	9X6	C3-C4-S2-C2
7	A	703	PE4	O1-C1-C2-O2
9	B	703	PEG	O2-C3-C4-O4
10	A	1001	K26	CAC-CBG-CBJ-CBB
9	B	704	PEG	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
7	A	703	PE4	O2-C3-C4-O3
8	A	704	P6G	O10-C11-C12-O13
10	A	1001	K26	CAT-CBG-CBJ-NAX
12	B	1611	PG4	O1-C1-C2-O2
10	B	1001	K26	CAA-CAT-CBG-CAC
10	A	1001	K26	CAV-CBI-PBK-OAG
10	B	1001	K26	CAV-CBI-PBK-OAG
11	A	1613	9X6	O1-C1-C2-S2
11	B	1612	9X6	O4-C3-C4-S2
11	B	1612	9X6	O3-C3-C4-S2
11	B	1612	9X6	O1-C1-C2-S2
9	B	704	PEG	O2-C3-C4-O4
12	B	1611	PG4	O2-C3-C4-O3
9	A	705	PEG	C1-C2-O2-C3
9	B	705	PEG	O2-C3-C4-O4
7	A	703	PE4	O4-C7-C8-O5
7	A	703	PE4	O3-C5-C6-O4
10	B	1001	K26	CAA-CAT-CBG-CBJ
7	A	703	PE4	C4-C3-O2-C2
11	A	1613	9X6	O2-C1-C2-S2
11	B	1612	9X6	O2-C1-C2-S2
8	A	704	P6G	C5-C6-O7-C8
9	B	705	PEG	C1-C2-O2-C3
8	A	704	P6G	O7-C8-C9-O10
9	B	703	PEG	C4-C3-O2-C2
11	A	1613	9X6	O4-C3-C4-S2
11	A	1613	9X6	O3-C3-C4-S2
12	B	1611	PG4	C1-C2-O2-C3

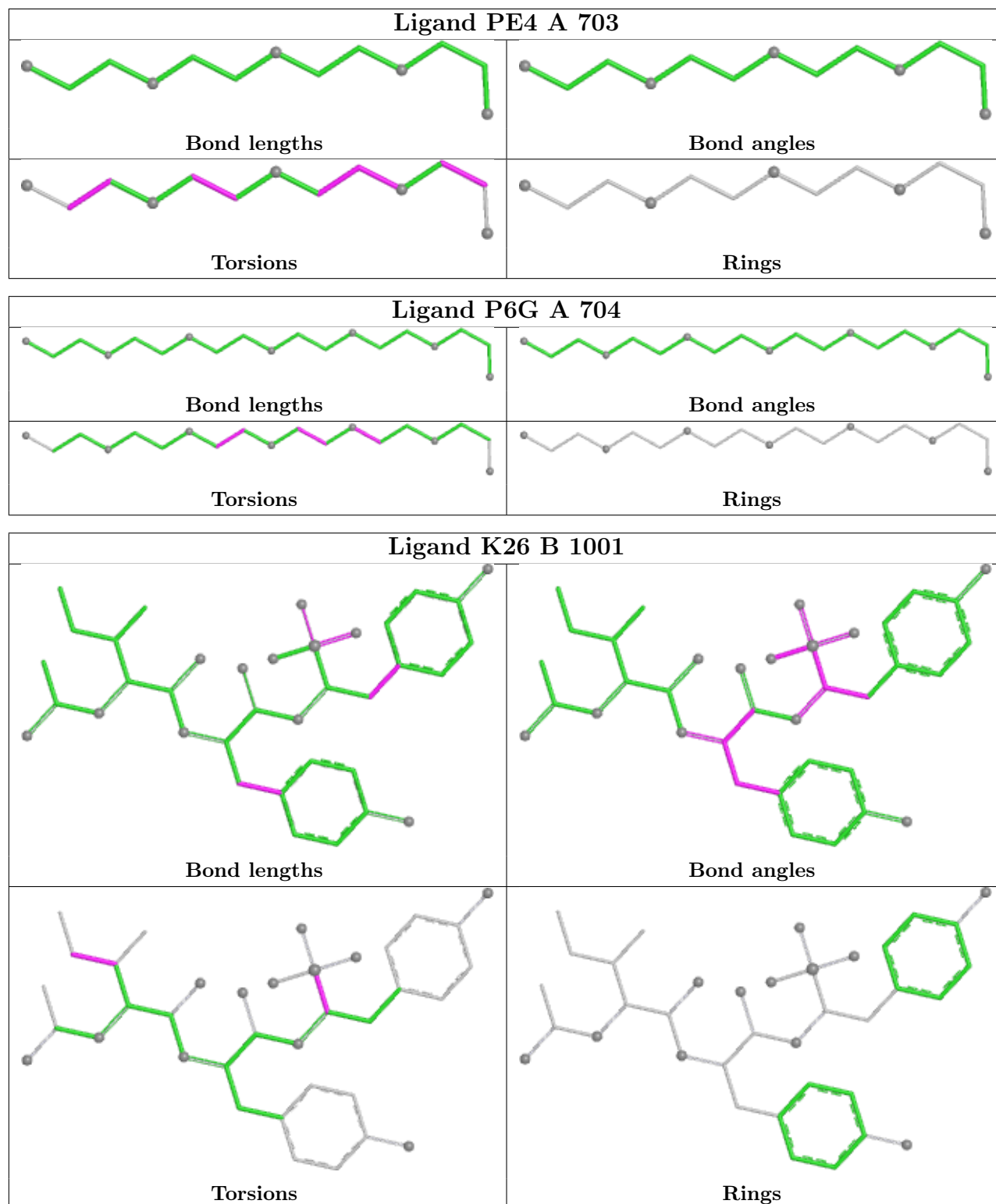
There are no ring outliers.

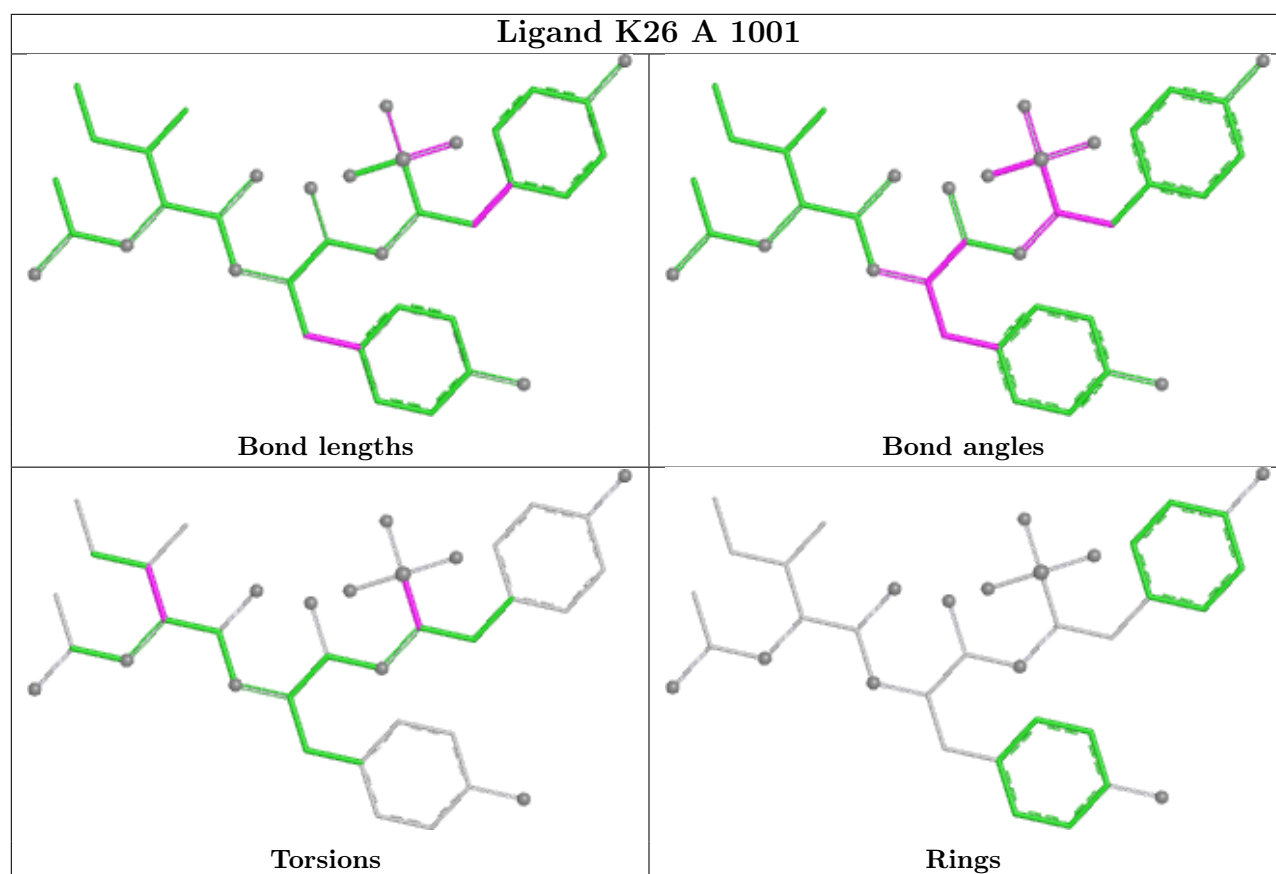
1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	B	1612	9X6	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	612/629 (97%)	0.38	36 (5%) 22 27	22, 40, 70, 102	2 (0%)
1	B	610/629 (96%)	0.14	27 (4%) 34 40	22, 36, 61, 89	1 (0%)
All	All	1222/1258 (97%)	0.26	63 (5%) 27 32	22, 38, 65, 102	3 (0%)

All (63) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	610	GLY	8.1
1	B	610	GLY	7.7
1	A	133	THR	7.3
1	A	134	ALA	6.4
1	A	132	LYS	6.4
1	A	131	ASN	6.1
1	A	413	ARG	5.8
1	B	130	PRO	5.6
1	A	325	GLY	5.2
1	A	130	PRO	5.0
1	A	129	LEU	4.9
1	B	135	THR	4.7
1	B	79	ILE	4.6
1	A	609	GLU	4.6
1	B	134	ALA	4.5
1	A	418	THR	4.3
1	B	325	GLY	4.1
1	A	82	ASN	4.0
1	A	136	CYS	4.0
1	A	412	ASP	3.9
1	A	135	THR	3.7
1	A	273	ASP	3.7
1	B	131	ASN	3.7
1	A	612	ASP	3.6

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Mol	Chain	Res	Type	RSRZ
1	B	133	THR	3.5
1	B	605	ASP	3.4
1	A	81	GLN	3.4
1	A	1	LEU	3.3
1	B	324	ASP	3.2
1	B	129	LEU	3.2
1	A	330	CYS	3.1
1	B	609	GLU	3.1
1	A	606	ASN	3.0
1	A	128	CYS	3.0
1	A	324	ASP	3.0
1	B	80	TRP	2.9
1	B	22	GLN	2.9
1	A	78	PRO	2.9
1	B	132	LYS	2.9
1	A	79	ILE	2.7
1	B	415	THR	2.6
1	A	323	ALA	2.6
1	A	285	GLN	2.6
1	B	19	LEU	2.6
1	B	606	ASN	2.5
1	A	563	ASP	2.5
1	B	136	CYS	2.4
1	A	414	VAL	2.4
1	B	81	GLN	2.4
1	B	607	TYR	2.3
1	B	438	PHE	2.3
1	B	83	PHE	2.3
1	A	522	GLU	2.3
1	A	611	ILE	2.2
1	A	496	THR	2.2
1	A	205	PRO	2.2
1	B	323	ALA	2.1
1	A	583	GLU	2.1
1	B	15	ALA	2.1
1	A	213	HIS	2.1
1	A	137	TRP	2.0
1	B	442	VAL	2.0
1	B	563	ASP	2.0

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

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

## 6.3 Carbohydrates ⓘ

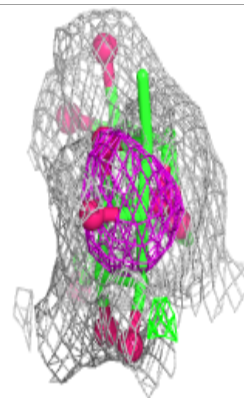
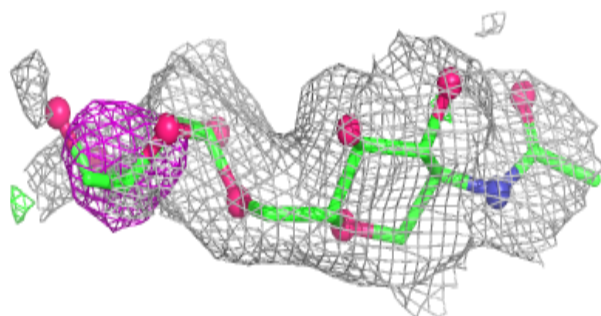
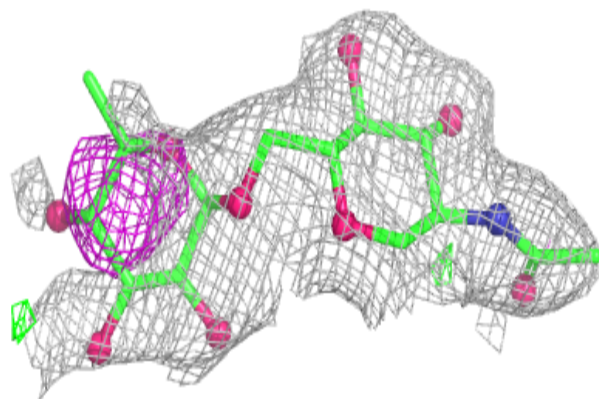
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
2	FUC	C	2	10/11	0.58	0.44	68,70,71,71	0
4	BMA	H	3	11/12	0.66	0.31	72,74,74,74	0
4	BMA	E	3	11/12	0.72	0.40	89,91,92,93	0
2	FUC	F	2	10/11	0.75	0.36	63,64,65,66	0
4	NAG	E	2	14/15	0.83	0.27	81,82,85,87	0
2	NAG	F	1	14/15	0.84	0.15	47,50,55,60	0
4	NAG	E	1	14/15	0.85	0.17	74,75,76,78	0
3	NAG	D	2	14/15	0.85	0.48	73,76,78,79	0
4	NAG	H	1	14/15	0.86	0.14	56,58,62,62	0
2	NAG	C	1	14/15	0.88	0.14	50,53,59,64	0
3	NAG	G	2	14/15	0.90	0.26	54,55,57,58	0
3	NAG	D	1	14/15	0.90	0.28	56,61,63,68	0
3	NAG	G	1	14/15	0.90	0.13	49,50,51,52	0
4	NAG	H	2	14/15	0.91	0.17	65,67,69,70	0

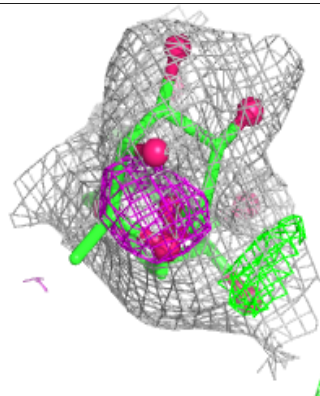
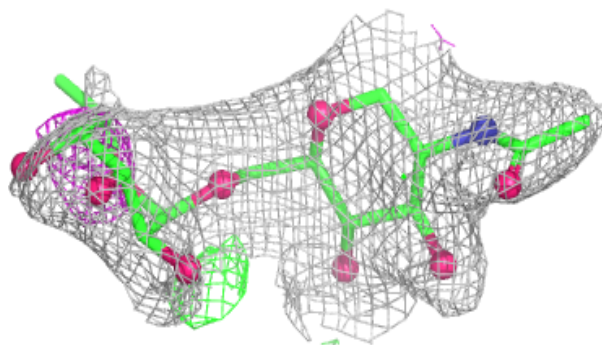
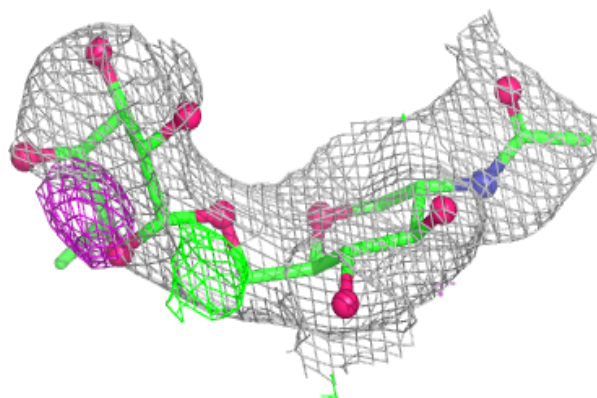
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

**Electron density around Chain C:**

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

**Electron density around Chain F:**

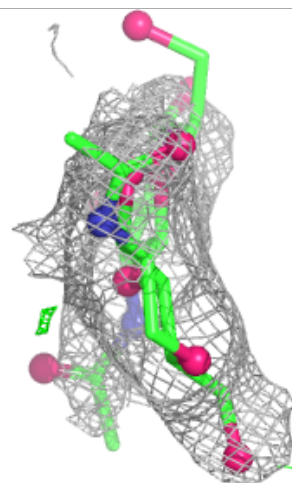
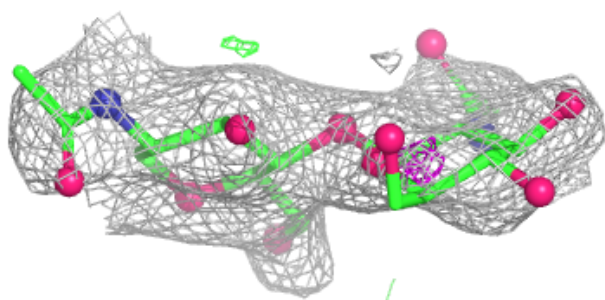
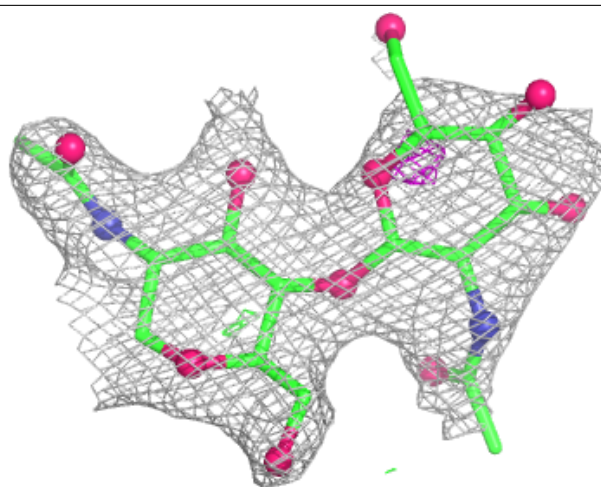
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





**Electron density around Chain D:**

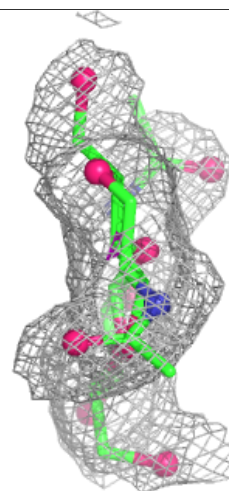
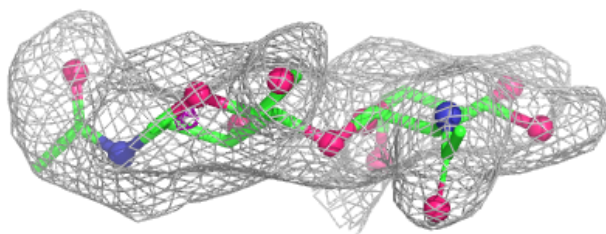
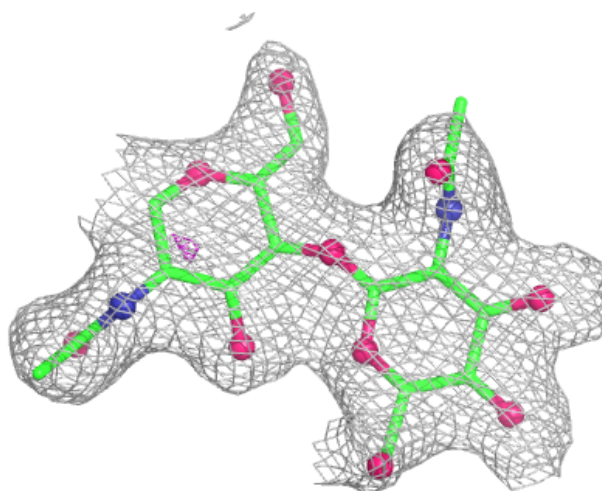
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





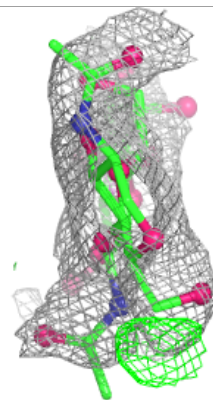
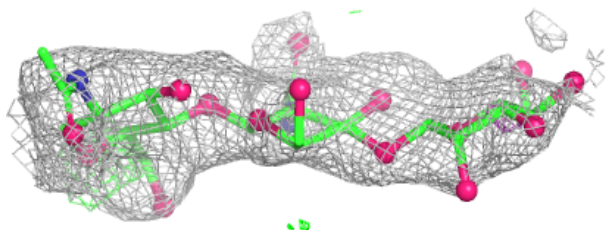
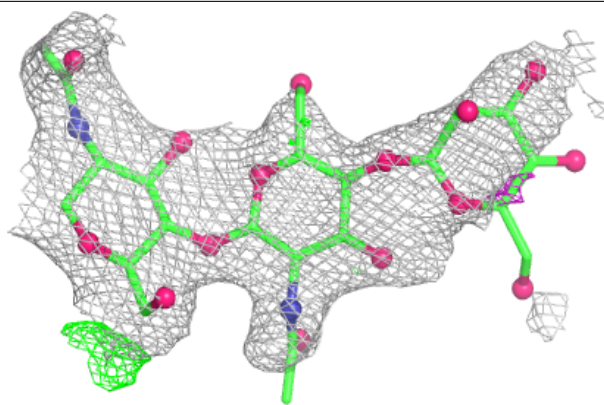
**Electron density around Chain G:**

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

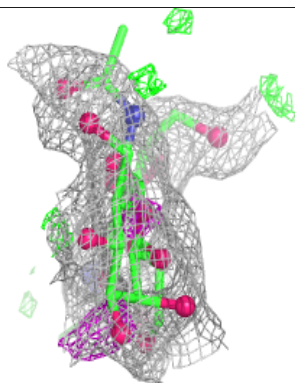
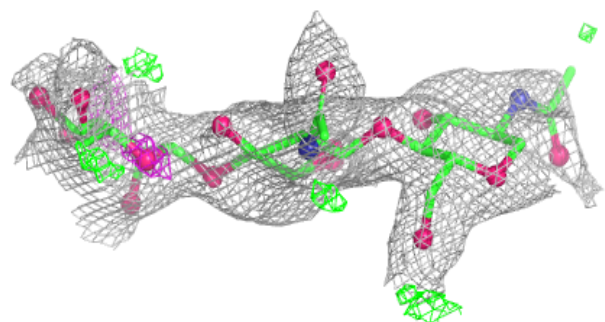
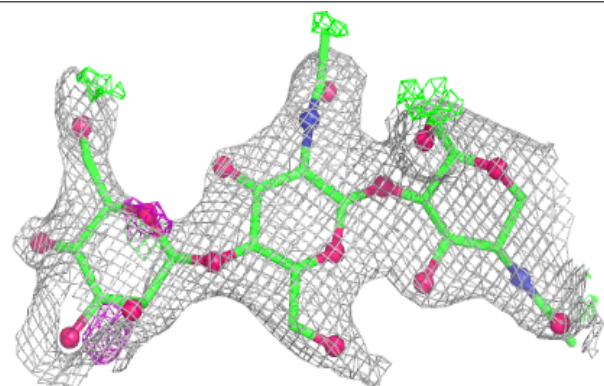


**Electron density around Chain E:**

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

**Electron density around Chain H:**

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



## 6.4 Ligands

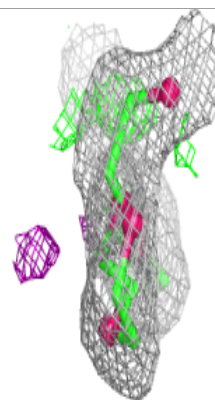
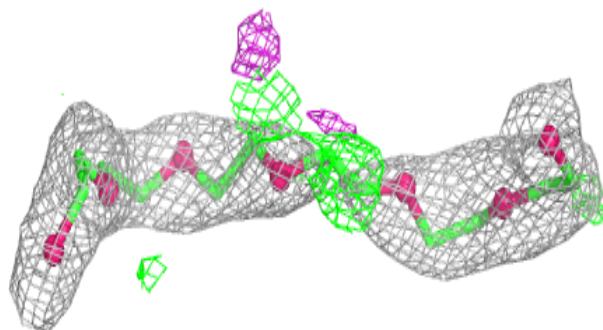
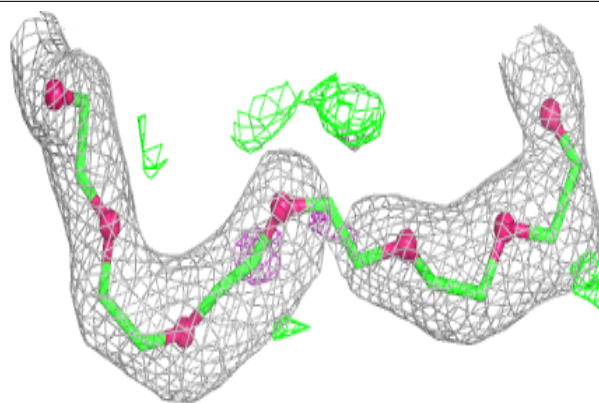
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
9	PEG	B	705	7/7	0.74	0.18	52,53,53,53	0
9	PEG	A	705	7/7	0.78	0.17	54,55,55,56	0
8	P6G	A	704	19/19	0.80	0.17	53,56,57,57	0
9	PEG	B	703	7/7	0.81	0.18	44,46,47,47	0
9	PEG	B	704	7/7	0.84	0.18	58,59,61,62	0
7	PE4	A	703	13/24	0.86	0.13	43,45,51,51	0
11	9X6	A	1613	9/9	0.86	0.20	37,39,40,42	0
11	9X6	B	1612	9/9	0.87	0.21	41,43,44,47	0
12	PG4	B	1611	7/13	0.90	0.13	48,49,49,49	0
10	K26	B	1001	37/37	0.94	0.16	26,31,36,37	0
10	K26	A	1001	37/37	0.94	0.17	25,30,33,34	0
5	ZN	B	701	1/1	0.98	0.10	37,37,37,37	0
6	CL	B	702	1/1	0.99	0.10	27,27,27,27	0
5	ZN	A	701	1/1	0.99	0.06	35,35,35,35	0
6	CL	A	702	1/1	0.99	0.05	29,29,29,29	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.

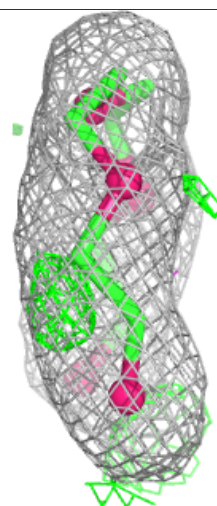
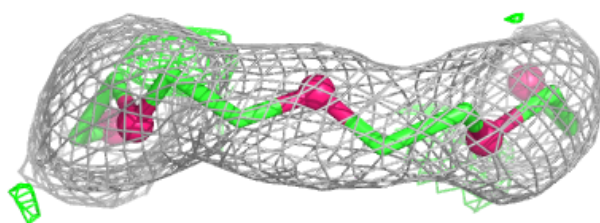
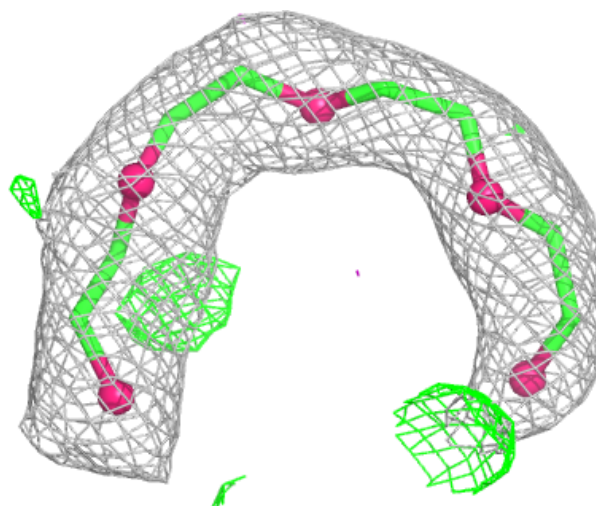
**Electron density around P6G A 704:**

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



**Electron density around PE4 A 703:**

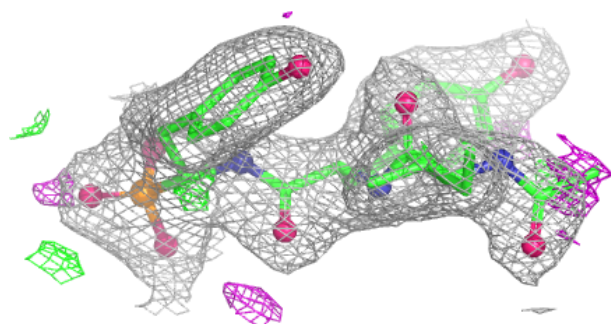
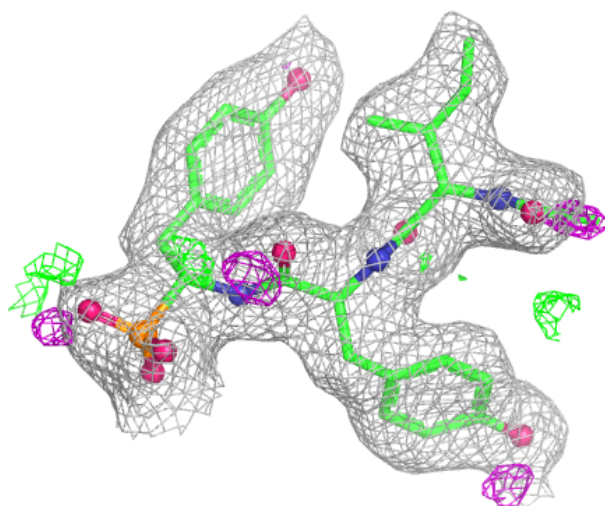
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





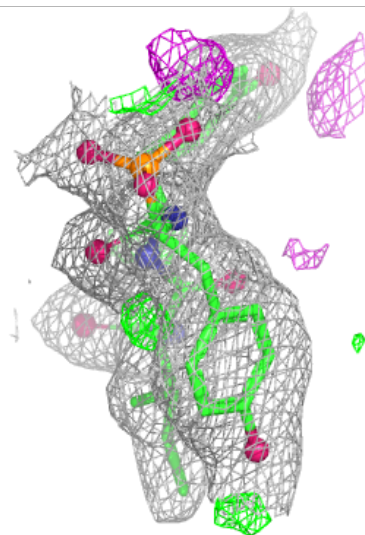
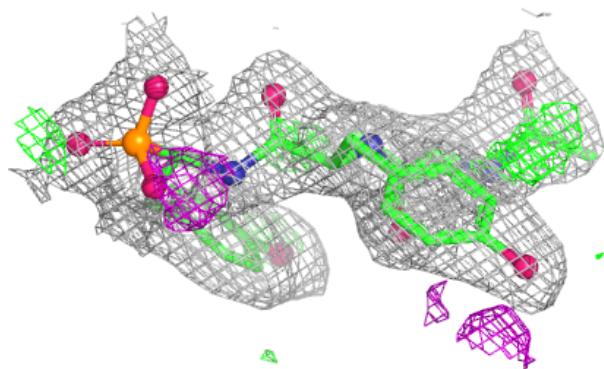
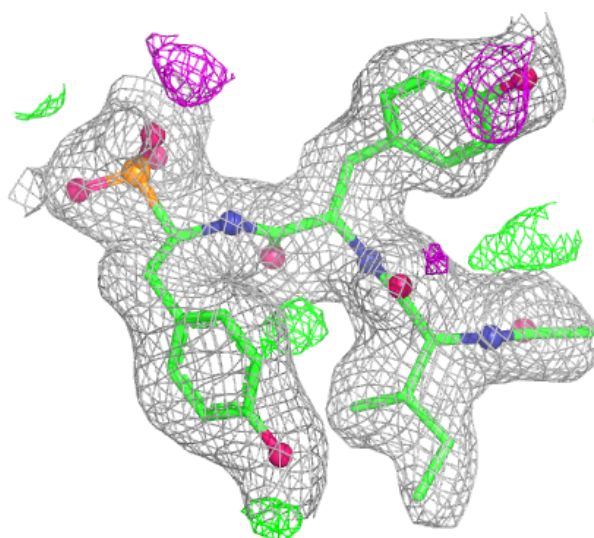
**Electron density around K26 B 1001:**

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



**Electron density around K26 A 1001:**

$2mF_o-DF_c$  (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.