



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 15, 2024 – 08:02 AM JST

PDB ID : 5EGH  
Title : Structure of ENPP6, a choline-specific glycerophosphodiester-phosphodiesterase in complex with phosphocholine  
Authors : Morita, J.; Kano, K.; Kato, K.; Takita, H.; Ishitani, R.; Nishimasu, H.; Nureki, O.; Aoki, J.  
Deposited on : 2015-10-27  
Resolution : 1.80 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

---

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	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

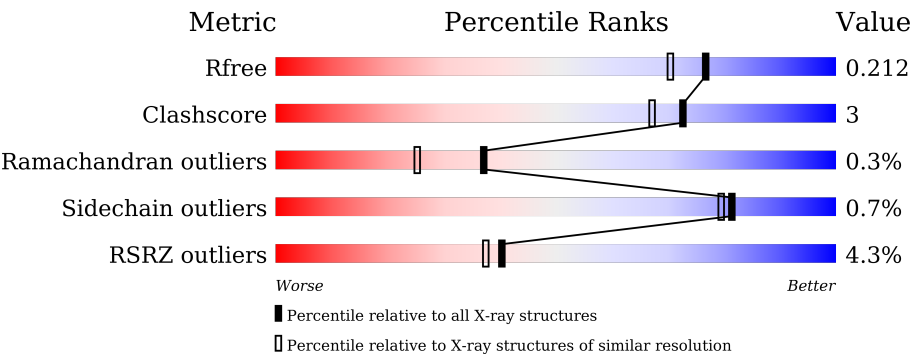
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.80 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	164625	7108 (1.80-1.80)
Clashscore	180529	8162 (1.80-1.80)
Ramachandran outliers	177936	8077 (1.80-1.80)
Sidechain outliers	177891	8076 (1.80-1.80)
RSRZ outliers	164620	7108 (1.80-1.80)

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	429	<div><div></div><div></div><div></div><div></div><div></div></div> <div>85%7%9%</div>
1	B	429	<div><div></div><div></div><div></div><div></div><div></div></div> <div>7%83%8%8%</div>
2	C	2	<div><div></div><div></div><div></div><div></div><div></div></div> <div>100%</div>
2	E	2	<div><div></div><div></div><div></div><div></div><div></div></div> <div>50%50%</div>
2	G	2	<div><div></div><div></div><div></div><div></div><div></div></div> <div>100%</div>
3	D	3	<div><div></div><div></div><div></div><div></div><div></div></div> <div>67%33%</div>

Continued on next page...

*Continued from previous page...*

Mol	Chain	Length	Quality of chain
3	F	3	 33% 33% 33%

## 2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 7187 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 Ectonucleotide pyrophosphatase/phosphodiesterase family member 6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	392	Total	C	N	O	S	0	6	0
			3220	2069	550	582	19			
1	B	393	Total	C	N	O	S	0	4	0
			3219	2068	551	581	19			

There are 20 discrepancies between the modelled and reference sequences:

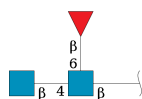
Chain	Residue	Modelled	Actual	Comment	Reference
A	393	ALA	CYS	engineered mutation	UNP Q8BGN3
A	412	SER	CYS	engineered mutation	UNP Q8BGN3
A	422	SER	-	expression tag	UNP Q8BGN3
A	423	ARG	-	expression tag	UNP Q8BGN3
A	424	GLU	-	expression tag	UNP Q8BGN3
A	425	ASN	-	expression tag	UNP Q8BGN3
A	426	LEU	-	expression tag	UNP Q8BGN3
A	427	TYR	-	expression tag	UNP Q8BGN3
A	428	PHE	-	expression tag	UNP Q8BGN3
A	429	GLN	-	expression tag	UNP Q8BGN3
B	393	ALA	CYS	engineered mutation	UNP Q8BGN3
B	412	SER	CYS	engineered mutation	UNP Q8BGN3
B	422	SER	-	expression tag	UNP Q8BGN3
B	423	ARG	-	expression tag	UNP Q8BGN3
B	424	GLU	-	expression tag	UNP Q8BGN3
B	425	ASN	-	expression tag	UNP Q8BGN3
B	426	LEU	-	expression tag	UNP Q8BGN3
B	427	TYR	-	expression tag	UNP Q8BGN3
B	428	PHE	-	expression tag	UNP Q8BGN3
B	429	GLN	-	expression tag	UNP Q8BGN3

- 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
2	C	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	G	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 3 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[beta-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose.

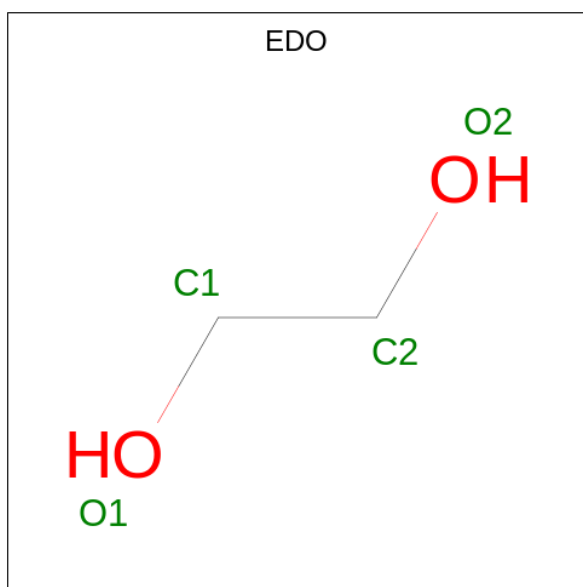


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	D	3	Total	C	N	O	0	0	0
			38	22	2	14			
3	F	3	Total	C	N	O	0	0	0
			38	22	2	14			

- Molecule 4 is ZINC ION (three-letter code: ZN) (formula: Zn).

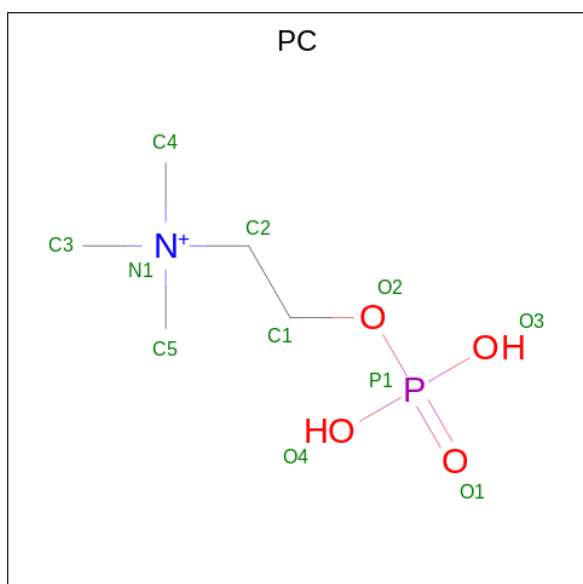
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	2	Total	Zn	0	0
			2	2		
4	B	2	Total	Zn	0	0
			2	2		

- Molecule 5 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C<sub>2</sub>H<sub>6</sub>O<sub>2</sub>).



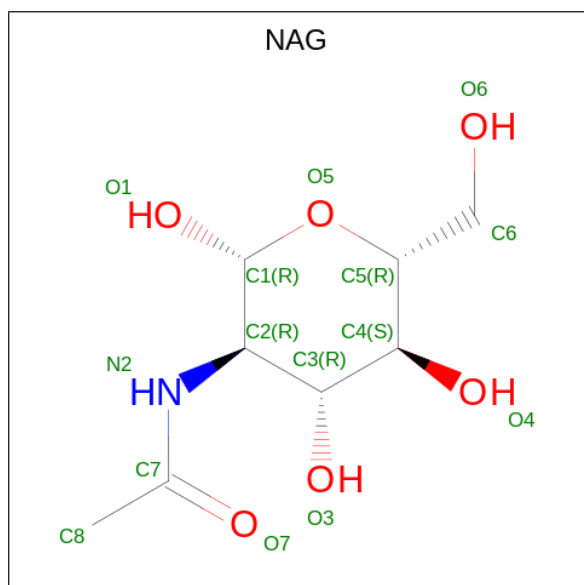
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			4	2	2		
5	A	1	Total	C	O	0	0
			4	2	2		
5	A	1	Total	C	O	0	0
			4	2	2		
5	B	1	Total	C	O	0	0
			4	2	2		
5	B	1	Total	C	O	0	0
			4	2	2		

- Molecule 6 is PHOSPHOCHOLINE (three-letter code: PC) (formula:  $C_5H_{15}NO_4P$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	A	1	Total	C	N	O	P	0	0
			11	5	1	4	1		
6	B	1	Total	C	N	O	P	0	0
			11	5	1	4	1		

- Molecule 7 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula:  $C_8H_{15}NO_6$ ).



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

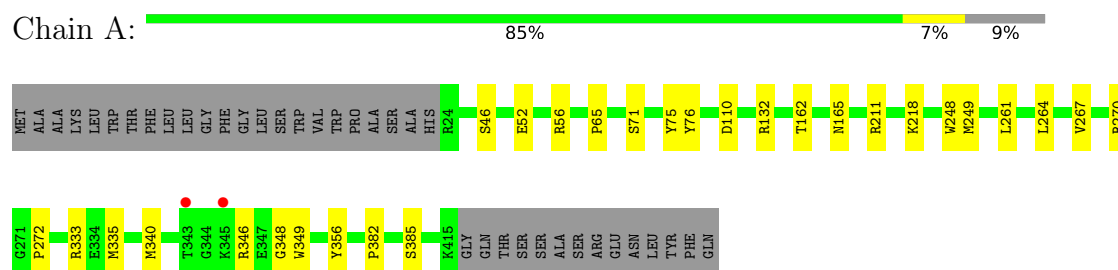
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	295	Total	O	0	0
			295	295		
8	B	233	Total	O	0	0
			233	233		

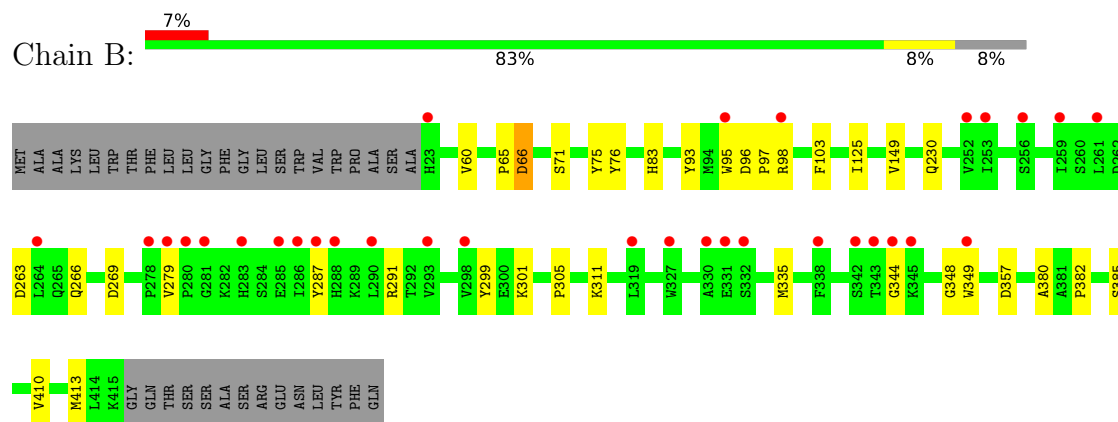
### 3 Residue-property plots

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: Ectonucleotide pyrophosphatase/phosphodiesterase family member 6



- Molecule 1: Ectonucleotide pyrophosphatase/phosphodiesterase family member 6



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



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







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

Chain G:  100%



- Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[beta-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain D:  67% 33%



- Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[beta-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain F:  33% 33% 33%



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	63.62Å 68.85Å 69.76Å 60.59° 86.99° 68.10°	Depositor
Resolution (Å)	45.63 – 1.80 45.63 – 1.80	Depositor EDS
% Data completeness (in resolution range)	93.9 (45.63-1.80) 93.9 (45.63-1.80)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.52 (at 1.81Å)	Xtriage
Refinement program	PHENIX (1.10_2155: ???)	Depositor
R, $R_{free}$	0.175 , 0.211 0.175 , 0.212	Depositor DCC
$R_{free}$ test set	4091 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	26.5	Xtriage
Anisotropy	0.073	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 39.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	7187	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.28% 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: ZN, FUL, NAG, EDO, PC

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	0.38	0/3322	0.56	0/4512
1	B	0.34	0/3315	0.53	0/4503
All	All	0.36	0/6637	0.54	0/9015

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	3220	0	3144	20	0
1	B	3219	0	3135	20	0
2	C	28	0	25	0	0
2	E	28	0	25	0	0
2	G	28	0	25	0	0
3	D	38	0	34	2	0
3	F	38	0	34	2	0
4	A	2	0	0	0	0
4	B	2	0	0	0	0
5	A	12	0	18	0	0
5	B	8	0	12	1	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	A	11	0	13	2	0
6	B	11	0	13	0	0
7	B	14	0	13	1	0
8	A	295	0	0	4	1
8	B	233	0	0	4	1
All	All	7187	0	6491	41	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 3.

All (41) 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:382:PRO:HG2	1:B:382:PRO:HG2	1.61	0.81
5:B:509:EDO:O2	8:B:601:HOH:O	2.11	0.67
1:B:348:GLY:HA2	3:F:3:FUL:O2	2.00	0.61
1:A:270:ARG:NH2	1:A:335:MET:O	2.34	0.60
1:B:230:GLN:NE2	8:B:606:HOH:O	2.36	0.58
1:A:248:TRP:O	8:A:601:HOH:O	2.17	0.58
7:B:501:NAG:O4	8:B:602:HOH:O	2.16	0.57
1:A:162:THR:H	1:A:165:ASN:HD22	1.53	0.55
1:A:348:GLY:HA2	3:D:3:FUL:O2	2.07	0.54
1:B:287:TYR:O	1:B:291:ARG:HG2	2.07	0.54
1:A:110:ASP:OD1	8:A:602:HOH:O	2.19	0.53
1:A:218:LYS:HD2	8:A:646:HOH:O	2.08	0.53
1:B:349:TRP:HB2	3:F:3:FUL:H3	1.91	0.52
1:B:287:TYR:CZ	1:B:291:ARG:HD3	2.47	0.50
1:A:132:ARG:NH2	8:A:610:HOH:O	2.43	0.50
1:B:301:LYS:HE3	1:B:311:LYS:O	2.10	0.49
1:B:95:TRP:CZ3	1:B:97:PRO:HB3	2.48	0.49
1:A:162:THR:H	1:A:165:ASN:ND2	2.11	0.49
1:A:249:MET:O	1:A:333:ARG:NH2	2.45	0.48
1:B:96:ASP:OD2	1:B:98:ARG:NH2	2.47	0.47
1:B:410:VAL:O	1:B:413:MET:HG2	2.15	0.46
1:A:52:GLU:OE2	1:A:56:ARG:NH1	2.47	0.46
1:B:269:ASP:OD2	8:B:603:HOH:O	2.20	0.46
1:B:299:TYR:CE1	1:B:305:PRO:HD3	2.51	0.45
1:A:46:SER:O	1:A:211:ARG:NH1	2.49	0.45
1:B:263:ASP:O	1:B:279:VAL:HG22	2.17	0.44
1:A:349:TRP:HB2	3:D:3:FUL:H3	2.00	0.44
1:A:71:SER:OG	6:A:512:PC:P1	2.77	0.43

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:125:ILE:HD12	1:B:149:VAL:HB	2.01	0.43
1:A:71:SER:HB3	1:A:75:TYR:CZ	2.53	0.43
1:B:95:TRP:CD2	1:B:266:GLN:HG2	2.54	0.43
1:B:60:VAL:HG12	1:B:380:ALA:HB3	2.01	0.42
1:A:272:PRO:HB3	1:A:356:TYR:CE1	2.54	0.42
1:B:65:PRO:HA	1:B:385[B]:SER:OG	2.20	0.42
1:B:71:SER:HB3	1:B:75:TYR:CZ	2.55	0.41
1:A:71:SER:OG	6:A:512:PC:O3	2.39	0.41
1:B:66:ASP:OD2	1:B:83:HIS:HA	2.21	0.41
1:A:264:LEU:HD13	1:A:267:VAL:CG2	2.50	0.41
1:B:93:TYR:HA	1:B:103:PHE:O	2.21	0.40
1:A:340:MET:HB2	1:A:346:ARG:HG2	2.02	0.40
1:A:65:PRO:HA	1:A:385[B]:SER:OG	2.20	0.40

All (1) 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)
8:A:656:HOH:O	8:B:762:HOH:O[1_464]	2.14	0.06

## 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	396/429 (92%)	379 (96%)	17 (4%)	0	100	100
1	B	395/429 (92%)	380 (96%)	13 (3%)	2 (0%)	25	14
All	All	791/858 (92%)	759 (96%)	30 (4%)	2 (0%)	37	25

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	357	ASP
1	B	344	GLY

### 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	352/377 (93%)	350 (99%)	2 (1%)	84	82
1	B	350/377 (93%)	347 (99%)	3 (1%)	75	72
All	All	702/754 (93%)	697 (99%)	5 (1%)	81	79

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	76	TYR
1	A	261	LEU
1	B	66	ASP
1	B	76	TYR
1	B	335	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	165	ASN
1	A	283	HIS
1	A	295	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 ⓘ

12 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	0.43	0	17,19,21	0.88	1 (5%)
2	NAG	C	2	2	14,14,15	0.64	1 (7%)	17,19,21	1.31	1 (5%)
3	NAG	D	1	3,1	14,14,15	0.44	0	17,19,21	0.64	0
3	NAG	D	2	3	14,14,15	0.40	0	17,19,21	0.35	0
3	FUL	D	3	3	10,10,11	1.52	3 (30%)	14,14,16	2.33	6 (42%)
2	NAG	E	1	2,1	14,14,15	0.46	0	17,19,21	0.44	0
2	NAG	E	2	2	14,14,15	0.16	0	17,19,21	0.64	1 (5%)
3	NAG	F	1	3,1	14,14,15	0.24	0	17,19,21	0.66	1 (5%)
3	NAG	F	2	3	14,14,15	0.47	0	17,19,21	0.56	0
3	FUL	F	3	3	10,10,11	1.21	1 (10%)	14,14,16	2.03	3 (21%)
2	NAG	G	1	2,1	14,14,15	0.44	0	17,19,21	0.49	0
2	NAG	G	2	2	14,14,15	0.31	0	17,19,21	0.39	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	-	0/6/23/26	0/1/1/1
2	NAG	C	2	2	-	3/6/23/26	0/1/1/1
3	NAG	D	1	3,1	-	1/6/23/26	0/1/1/1
3	NAG	D	2	3	-	0/6/23/26	0/1/1/1
3	FUL	D	3	3	-	-	0/1/1/1
2	NAG	E	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	E	2	2	-	0/6/23/26	0/1/1/1
3	NAG	F	1	3,1	-	1/6/23/26	0/1/1/1
3	NAG	F	2	3	-	2/6/23/26	0/1/1/1
3	FUL	F	3	3	-	-	0/1/1/1
2	NAG	G	1	2,1	-	0/6/23/26	0/1/1/1

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	G	2	2	-	2/6/23/26	0/1/1/1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	3	FUL	C2-C3	-2.80	1.48	1.52
3	F	3	FUL	C2-C3	-2.47	1.48	1.52
3	D	3	FUL	O5-C1	-2.42	1.39	1.43
3	D	3	FUL	C4-C5	2.29	1.57	1.52
2	C	2	NAG	O5-C1	2.27	1.47	1.43

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	2	NAG	C1-O5-C5	5.13	119.14	112.19
3	D	3	FUL	O5-C5-C4	4.61	117.79	109.52
3	F	3	FUL	C1-O5-C5	4.23	122.37	112.78
3	D	3	FUL	C3-C4-C5	3.99	115.98	109.77
3	F	3	FUL	O5-C5-C4	3.75	116.25	109.52
3	D	3	FUL	C1-O5-C5	3.26	120.17	112.78
3	F	3	FUL	C1-C2-C3	2.99	113.35	109.67
2	C	1	NAG	C1-O5-C5	2.43	115.49	112.19
3	D	3	FUL	O2-C2-C3	-2.41	105.31	110.14
3	D	3	FUL	C2-C3-C4	2.38	115.01	110.89
3	F	1	NAG	C1-O5-C5	2.33	115.34	112.19
3	D	3	FUL	C1-C2-C3	2.32	112.52	109.67
2	E	2	NAG	C1-O5-C5	2.07	115.00	112.19

There are no chirality outliers.

All (9) torsion outliers are listed below:

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

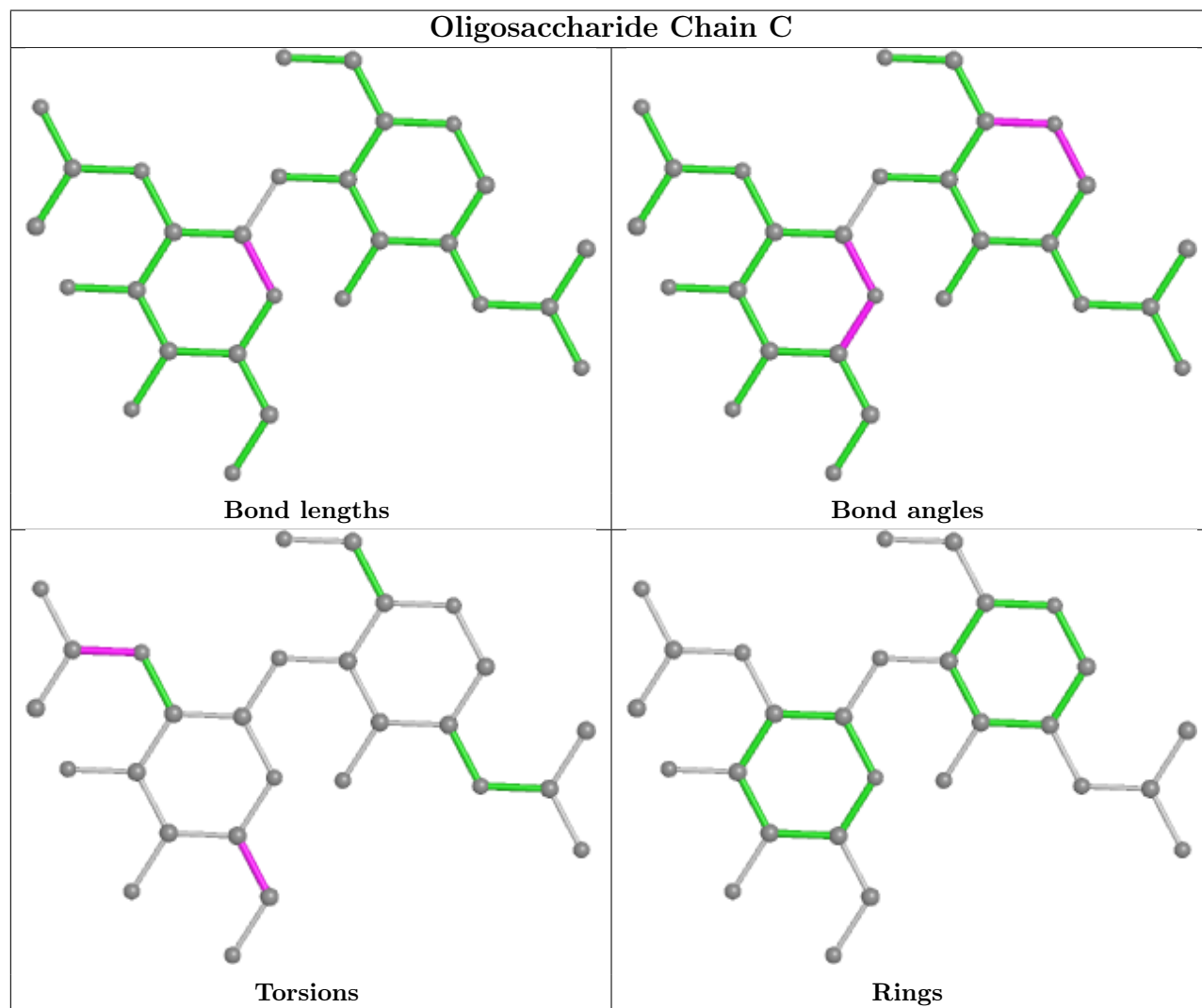


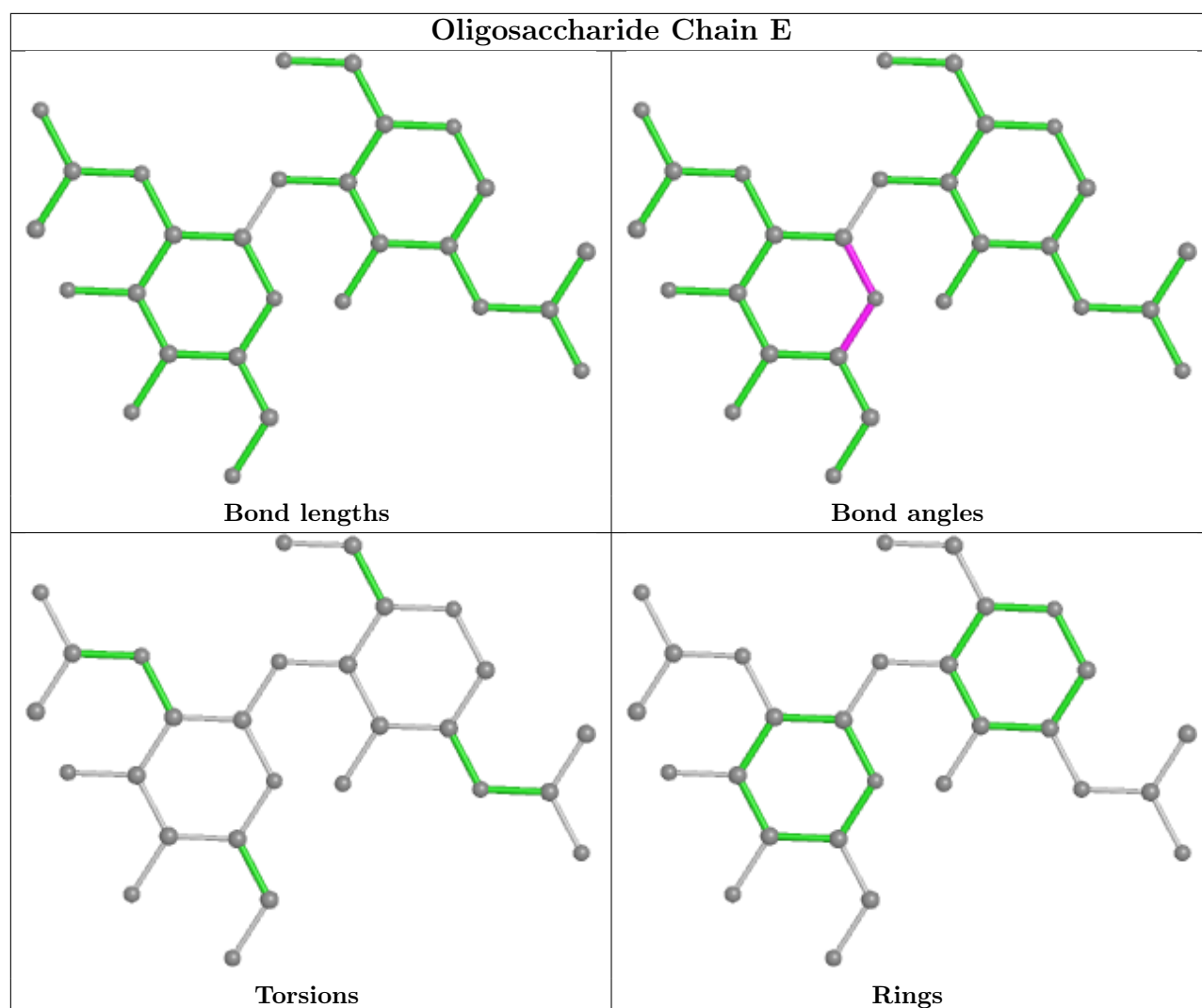
There are no ring outliers.

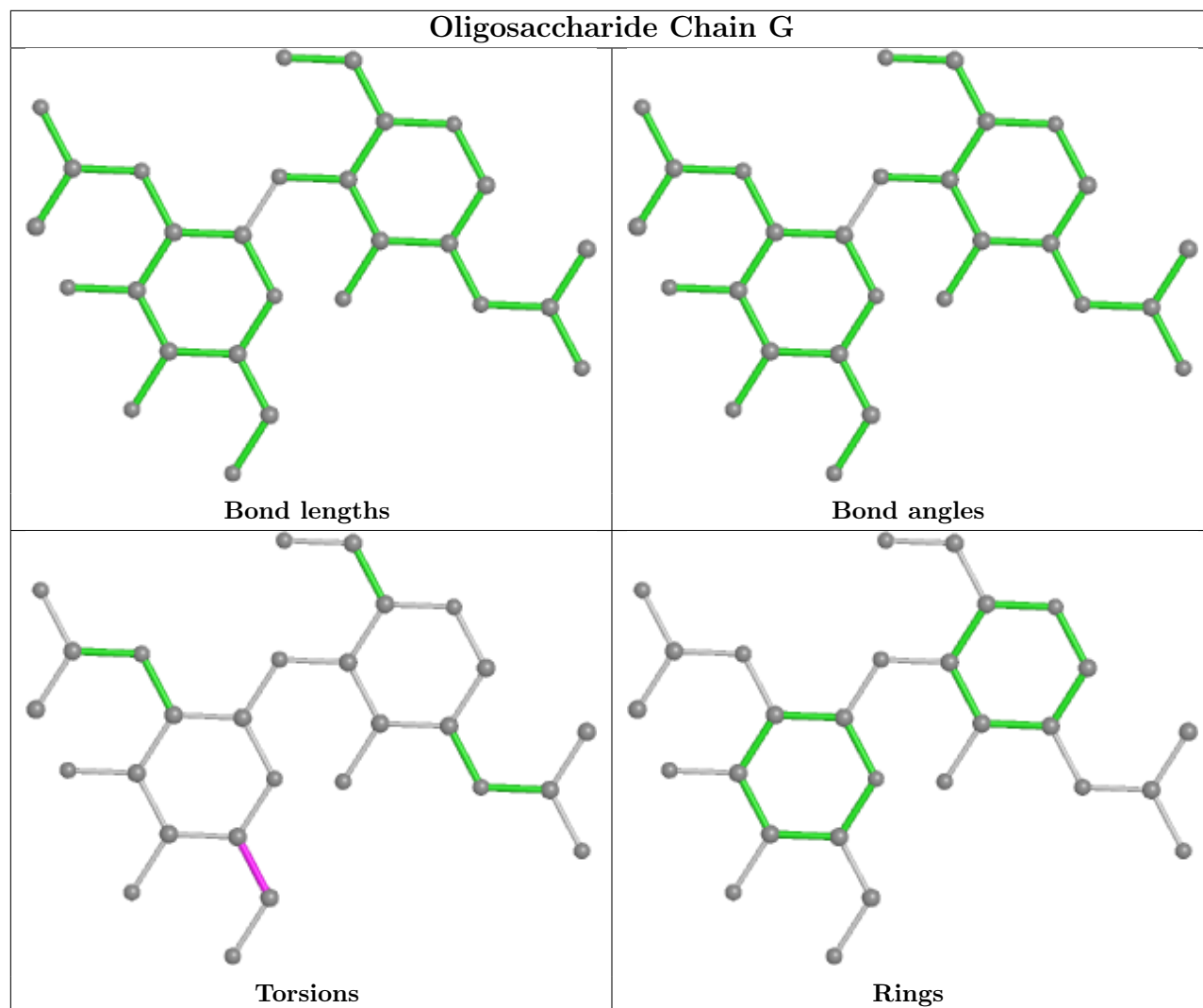
2 monomers are involved in 4 short contacts:

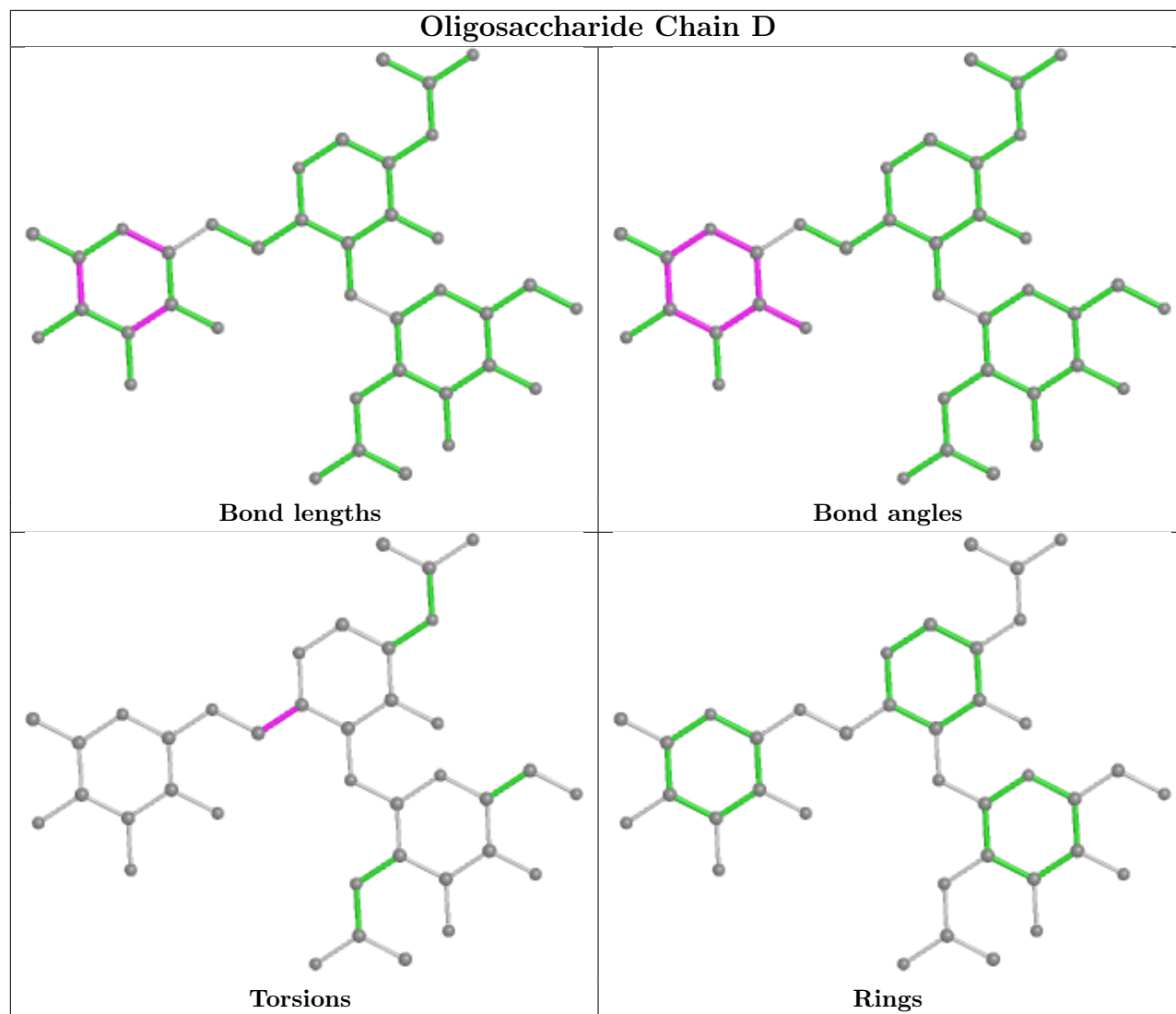
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	3	FUL	2	0
3	F	3	FUL	2	0

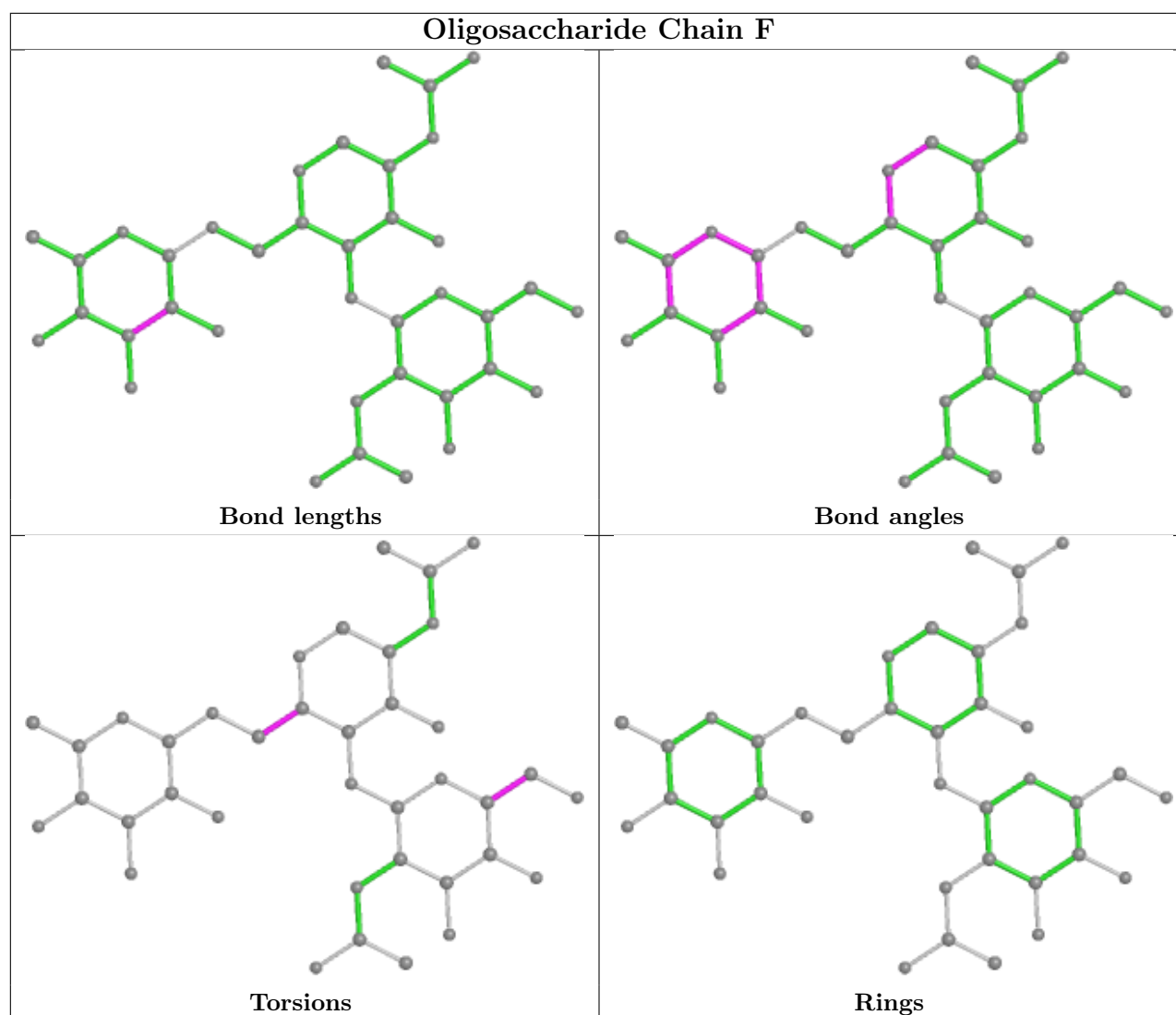
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.











## 5.6 Ligand geometry [i](#)

Of 12 ligands modelled in this entry, 4 are monoatomic - leaving 8 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	NAG	B	501	1	14,14,15	0.29	0	17,19,21	0.73	1 (5%)
5	EDO	B	511	-	3,3,3	0.48	0	2,2,2	0.35	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
6	PC	B	510	4	10,10,10	0.95	0	15,15,15	1.20	2 (13%)
5	EDO	B	509	-	3,3,3	0.47	0	2,2,2	0.24	0
6	PC	A	512	4	10,10,10	1.00	0	15,15,15	1.24	1 (6%)
5	EDO	A	510	-	3,3,3	0.47	0	2,2,2	0.45	0
5	EDO	A	511	-	3,3,3	0.40	0	2,2,2	0.46	0
5	EDO	A	513	-	3,3,3	0.50	0	2,2,2	0.14	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	NAG	B	501	1	-	0/6/23/26	0/1/1/1
5	EDO	B	511	-	-	0/1/1/1	-
6	PC	B	510	4	-	0/8/8/8	-
5	EDO	B	509	-	-	1/1/1/1	-
6	PC	A	512	4	-	0/8/8/8	-
5	EDO	A	510	-	-	1/1/1/1	-
5	EDO	A	511	-	-	0/1/1/1	-
5	EDO	A	513	-	-	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(°)
6	A	512	PC	O3-P1-O2	2.71	113.96	106.73
6	B	510	PC	C5-N1-C2	2.43	119.84	109.92
6	B	510	PC	C1-C2-N1	2.31	123.48	115.78
7	B	501	NAG	C1-O5-C5	2.30	115.31	112.19

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	510	EDO	O1-C1-C2-O2
5	B	509	EDO	O1-C1-C2-O2

There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	B	501	NAG	1	0
5	B	509	EDO	1	0
6	A	512	PC	2	0

## 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	392/429 (91%)	-0.32	2 (0%) 87 87	10, 26, 44, 73	6 (1%)
1	B	393/429 (91%)	0.24	32 (8%) 19 17	12, 31, 64, 86	4 (1%)
All	All	785/858 (91%)	-0.04	34 (4%) 40 37	10, 28, 61, 86	10 (1%)

All (34) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	279	VAL	3.7
1	B	253	ILE	3.5
1	B	343	THR	3.4
1	B	281	GLY	3.3
1	B	280	PRO	3.2
1	A	343	THR	3.1
1	B	345	LYS	3.0
1	B	286	ILE	2.9
1	B	23	HIS	2.9
1	B	349	TRP	2.6
1	B	290	LEU	2.5
1	B	344	GLY	2.5
1	B	252	VAL	2.5
1	B	342	SER	2.4
1	B	278	PRO	2.4
1	B	331	GLU	2.4
1	B	95	TRP	2.4
1	B	298	VAL	2.4
1	B	261	LEU	2.3
1	B	264	LEU	2.3
1	B	259	ILE	2.3
1	B	330	ALA	2.2
1	B	332	SER	2.2
1	A	345	LYS	2.2

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	B	327	TRP	2.2
1	B	287	TYR	2.2
1	B	256	SER	2.1
1	B	293	VAL	2.1
1	B	288	HIS	2.0
1	B	285	GLU	2.0
1	B	283	HIS	2.0
1	B	319	LEU	2.0
1	B	98	ARG	2.0
1	B	338	PHE	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](#)

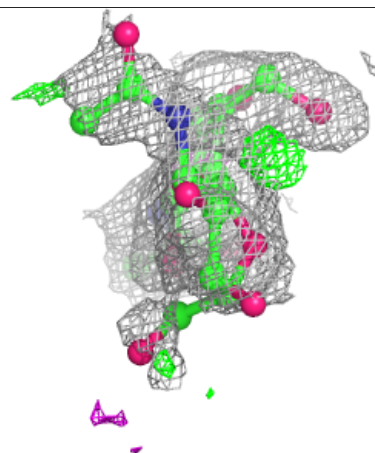
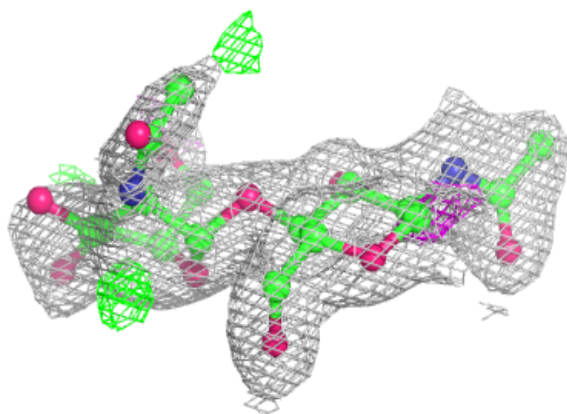
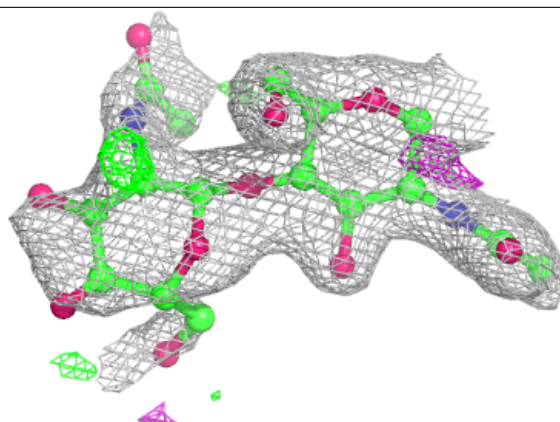
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<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	C	2	14/15	0.69	0.16	56,67,73,77	0
3	NAG	F	2	14/15	0.70	0.13	64,75,81,84	0
3	FUL	D	3	10/11	0.71	0.19	37,49,51,57	0
3	FUL	F	3	10/11	0.72	0.18	59,64,70,75	0
3	NAG	D	2	14/15	0.78	0.14	64,71,80,80	0
3	NAG	F	1	14/15	0.80	0.13	61,67,72,74	0
2	NAG	E	2	14/15	0.82	0.13	42,48,63,65	0
2	NAG	G	2	14/15	0.85	0.12	42,51,64,71	0
3	NAG	D	1	14/15	0.86	0.12	48,53,60,65	0
2	NAG	G	1	14/15	0.91	0.10	34,40,48,50	0
2	NAG	C	1	14/15	0.92	0.09	29,37,45,48	0
2	NAG	E	1	14/15	0.96	0.07	28,32,42,44	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.

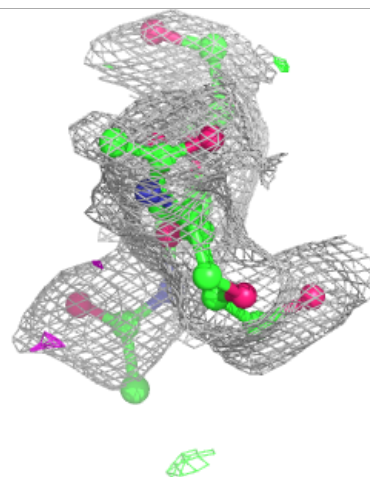
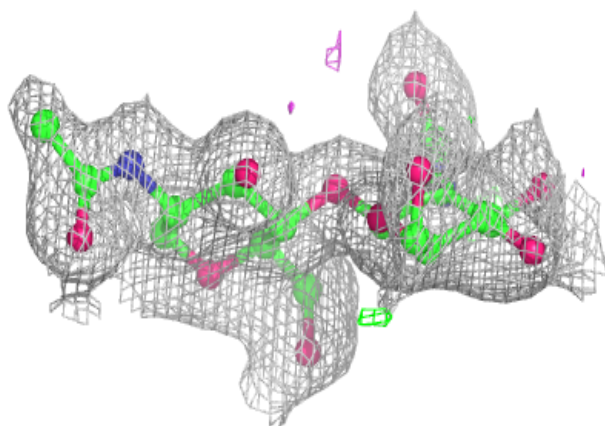
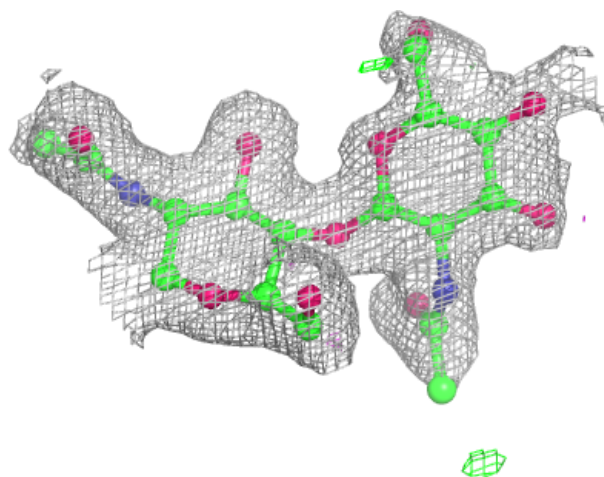
**Electron density around Chain C:**

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



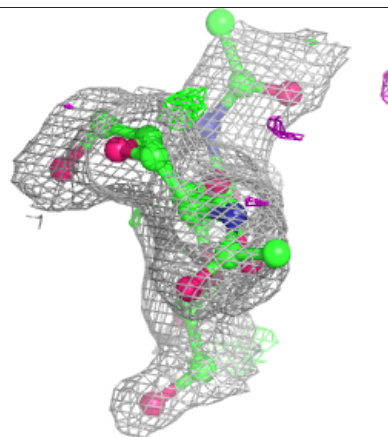
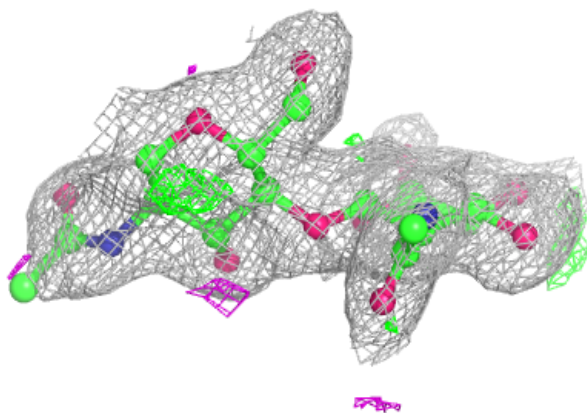
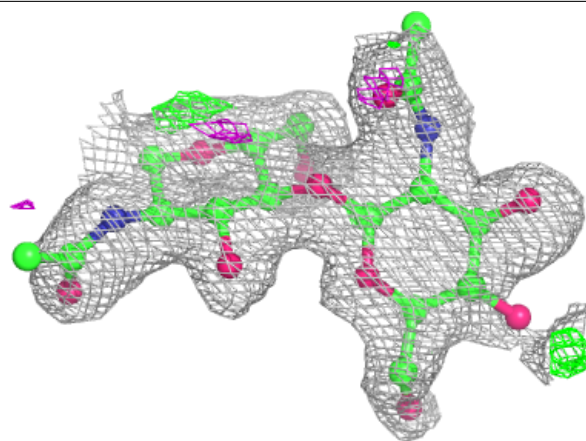
**Electron density around Chain E:**

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



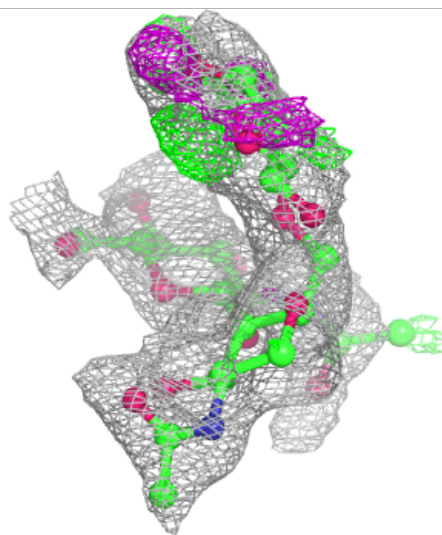
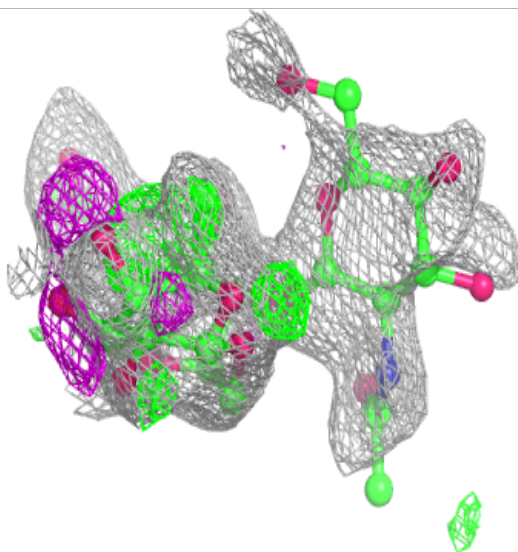
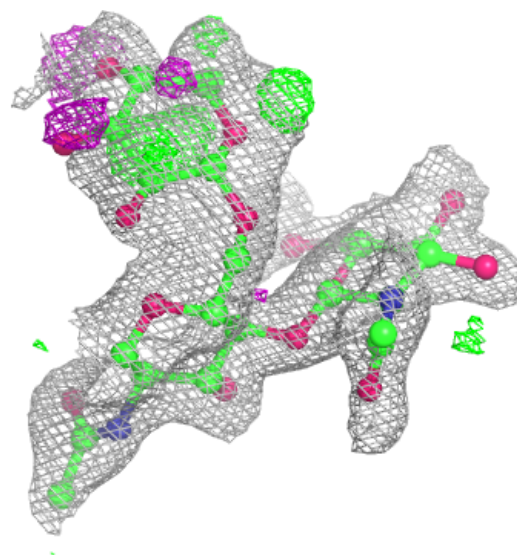
**Electron density around Chain G:**

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

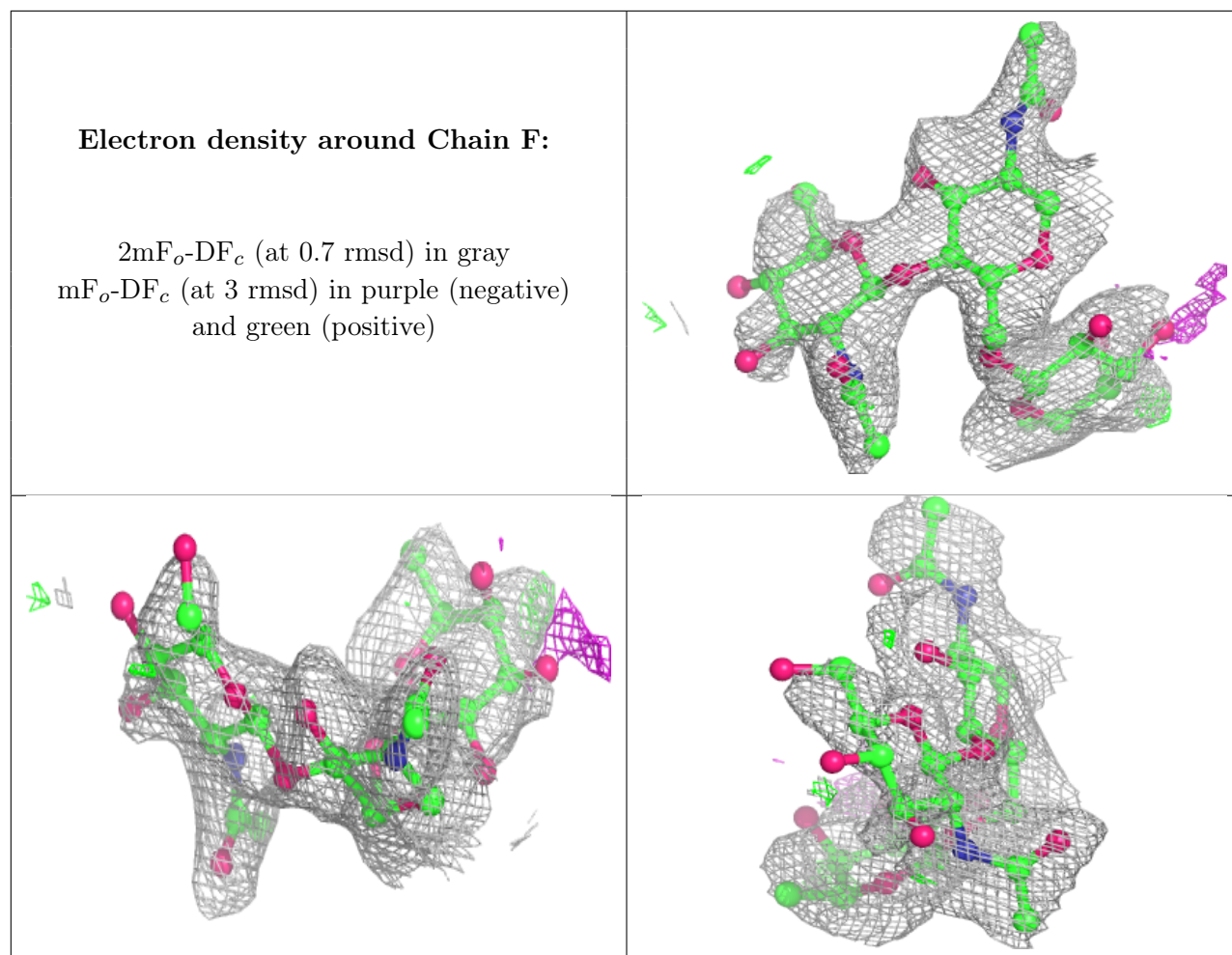


**Electron density around Chain D:**

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







## 6.4 Ligands [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
7	NAG	B	501	14/15	0.87	0.11	37,45,50,55	0
5	EDO	A	513	4/4	0.90	0.15	27,30,38,43	0
5	EDO	B	511	4/4	0.92	0.16	28,35,39,43	0
5	EDO	B	509	4/4	0.92	0.11	33,35,38,38	0
6	PC	B	510	11/11	0.94	0.10	27,34,38,42	0
6	PC	A	512	11/11	0.95	0.11	24,33,38,38	0
5	EDO	A	511	4/4	0.97	0.08	20,22,24,31	0
5	EDO	A	510	4/4	0.98	0.05	25,26,26,27	0
4	ZN	B	507	1/1	0.99	0.04	31,31,31,31	0
4	ZN	B	508	1/1	0.99	0.08	33,33,33,33	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
4	ZN	A	508	1/1	1.00	0.08	26,26,26,26	0
4	ZN	A	509	1/1	1.00	0.05	27,27,27,27	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.