



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 25, 2025 – 01:55 am BST

PDB ID : 9QAR / pdb\_00009qar  
Title : Human angiotensin-1 converting enzyme N-domain in complex with ramiprilat  
Authors : Gregory, K.S.; Acharya, K.R.  
Deposited on : 2025-02-28  
Resolution : 2.00 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4-5-2 with Phenix2.0rc1  
Mogul : 1.8.4, CSD as541be (2020)  
Xtriage (Phenix) : 2.0rc1  
EDS : 3.0  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
CCP4 : 9.0.006 (Gargrove)  
Density-Fitness : 1.0.12  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.45.1

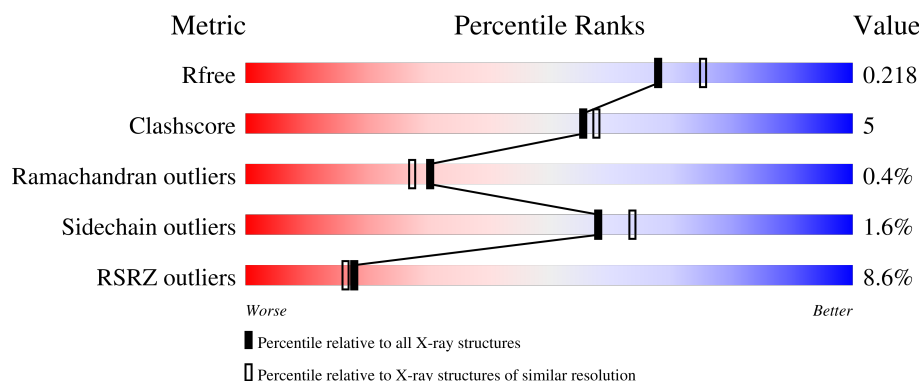
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.00 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	9409 (2.00-2.00)
Clashscore	180529	10737 (2.00-2.00)
Ramachandran outliers	177936	10628 (2.00-2.00)
Sidechain outliers	177891	10627 (2.00-2.00)
RSRZ outliers	164620	9409 (2.00-2.00)

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	609	<div> <div>16%</div> <div>90%</div> <div>8%</div> <div>..</div> </div>
1	B	609	<div> <div>16%</div> <div>86%</div> <div>11%</div> <div>..</div> </div>
2	C	2	<div> <div>100%</div> </div>
3	D	2	<div> <div>50%</div> <div>50%</div> </div>
3	E	2	<div> <div>50%</div> <div>50%</div> </div>

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Mol	Chain	Length	Quality of chain
4	F	4	
5	G	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
10	ACT	A	706	-	-	X	-
9	EDO	A	705	-	-	X	-

## 2 Entry composition

There are 17 unique types of molecules in this entry. The entry contains 11096 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.

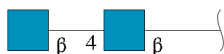
- Molecule 1 is a protein called Angiotensin-converting enzyme, soluble form.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	604	Total	C	N	O	S	0	7	0
			5002	3209	862	912	19			
1	B	603	Total	C	N	O	S	0	5	0
			4971	3188	856	908	19			

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	9	GLN	ASN	engineered mutation	UNP P12821
A	25	GLN	ASN	engineered mutation	UNP P12821
A	82	GLN	ASN	engineered mutation	UNP P12821
A	117	GLN	ASN	engineered mutation	UNP P12821
A	289	GLN	ASN	engineered mutation	UNP P12821
A	545	ARG	GLN	engineered mutation	UNP P12821
A	576	LEU	PRO	engineered mutation	UNP P12821
B	9	GLN	ASN	engineered mutation	UNP P12821
B	25	GLN	ASN	engineered mutation	UNP P12821
B	82	GLN	ASN	engineered mutation	UNP P12821
B	117	GLN	ASN	engineered mutation	UNP P12821
B	289	GLN	ASN	engineered mutation	UNP P12821
B	545	ARG	GLN	engineered mutation	UNP P12821
B	576	LEU	PRO	engineered mutation	UNP P12821

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



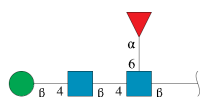
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	C	2	Total	C	N	O	0	0	0
			28	16	2	10			

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



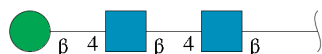
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	D	2	Total	C	N	O	0	0	0
			24	14	1	9			
3	E	2	Total	C	N	O	0	0	0
			24	14	1	9			

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	F	4	Total	C	N	O	0	0	0
			49	28	2	19			

- Molecule 5 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.

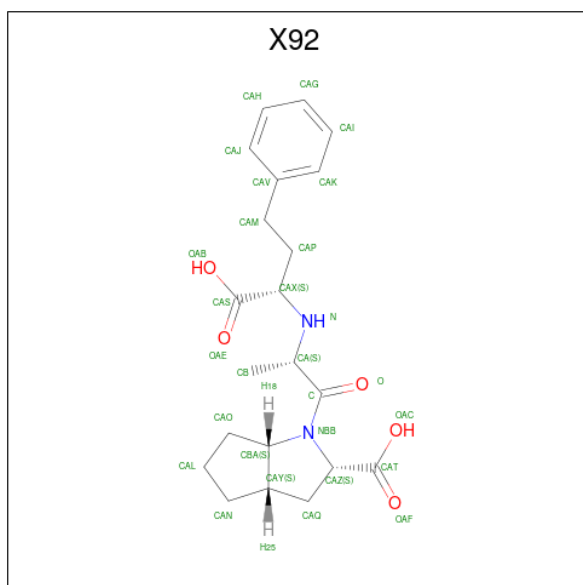


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	G	3	Total	C	N	O	0	0	0
			39	22	2	15			

- Molecule 6 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

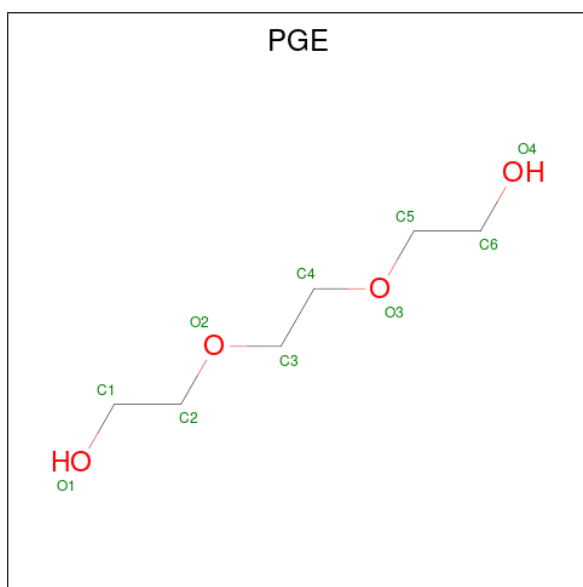
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	1	Total	Zn	0	0
			1	1		
6	B	1	Total	Zn	0	0
			1	1		

- Molecule 7 is Ramiprilat (CCD ID: X92) (formula:  $C_{21}H_{28}N_2O_5$ ) (labeled as "Ligand of Interest" by depositor).



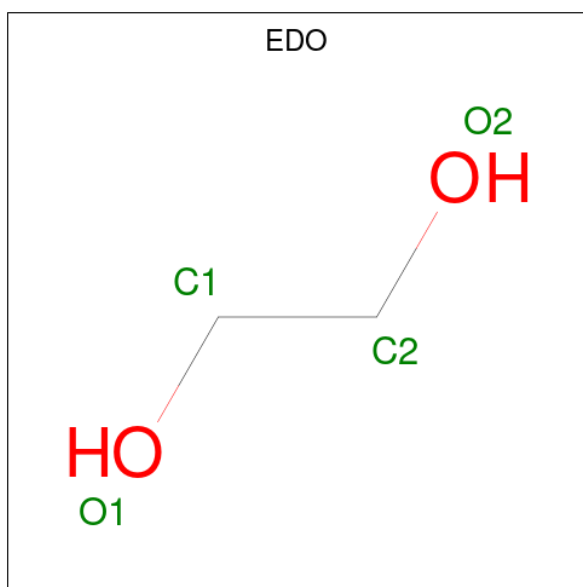
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	A	1	Total	C	N	O	0	0
			28	21	2	5		
7	B	1	Total	C	N	O	0	0
			28	21	2	5		

- Molecule 8 is TRIETHYLENE GLYCOL (CCD ID: PGE) (formula:  $C_6H_{14}O_4$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	A	1	Total	C	O	0	0
			10	6	4		
8	B	1	Total	C	O	0	0
			10	6	4		
8	B	1	Total	C	O	0	0
			10	6	4		

- Molecule 9 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula:  $C_2H_6O_2$ ).



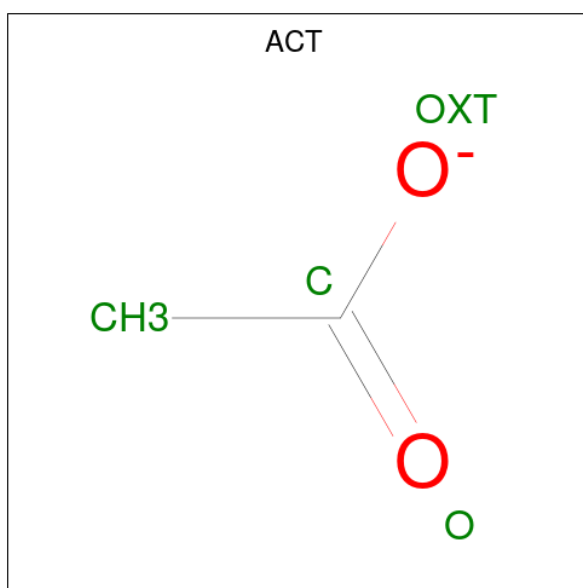
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	A	1	Total	C	O	0	0
			4	2	2		

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

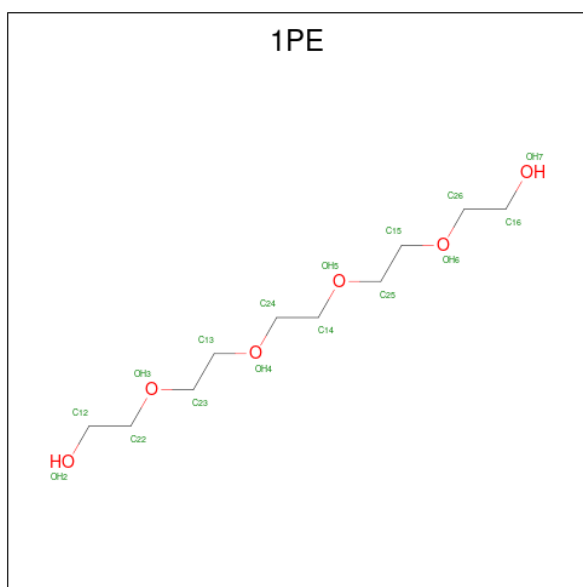
- Molecule 10 is ACETATE ION (CCD ID: ACT) (formula:  $C_2H_3O_2$ ).



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

- Molecule 11 is PENTAETHYLENE GLYCOL (CCD ID: 1PE) (formula:  $C_{10}H_{22}O_6$ ).





Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
11	A	1	Total	C	O	0	0
			16	10	6		
11	B	1	Total	C	O	0	0
			16	10	6		

- Molecule 12 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

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

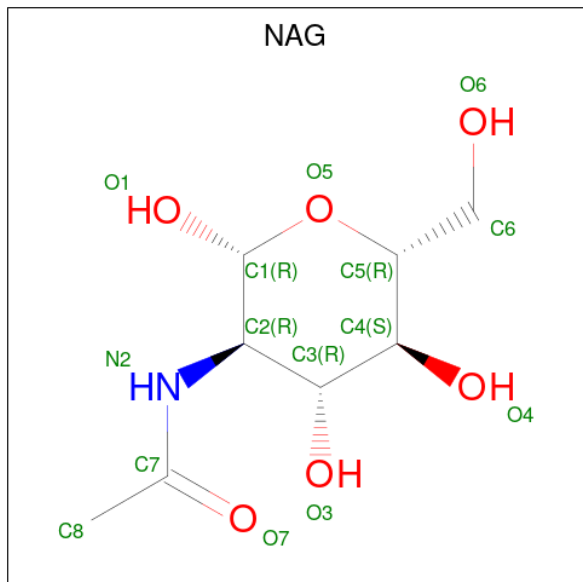
- Molecule 13 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
13	A	1	Total	Mg	0	0
			1	1		
13	B	1	Total	Mg	0	0
			1	1		

- Molecule 14 is CALCIUM ION (CCD ID: CA) (formula: Ca).

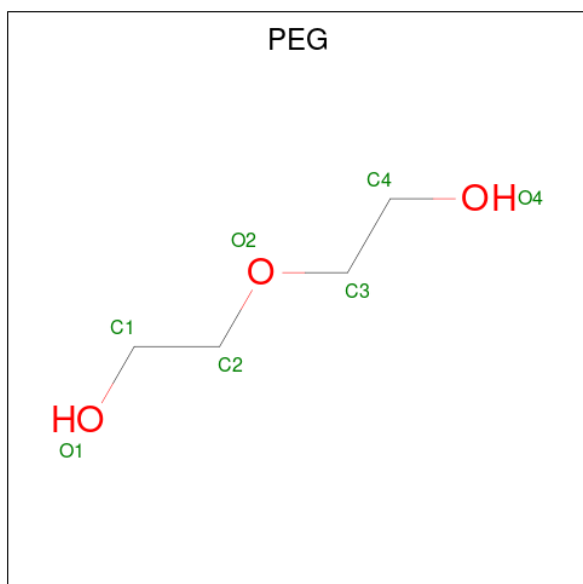
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
14	A	1	Total	Ca	0	0
			1	1		

- Molecule 15 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula:  $C_8H_{15}NO_6$ ).



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

- Molecule 16 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula:  $C_4H_{10}O_3$ ).



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

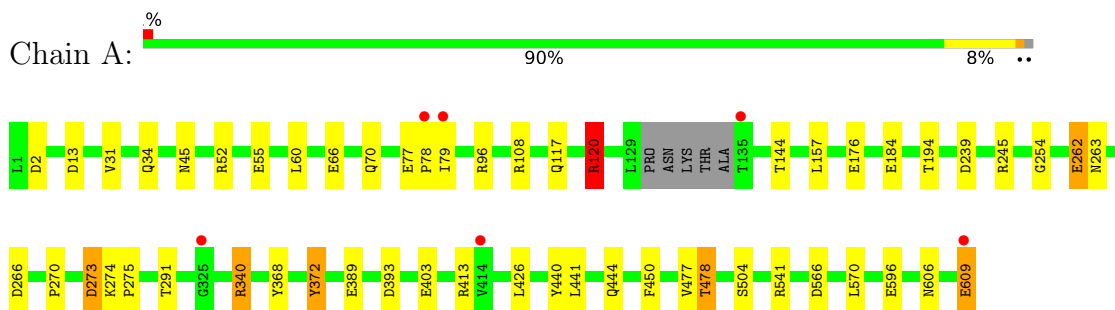
- Molecule 17 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
17	A	483	Total 483	O 483	0	0
17	B	298	Total 298	O 298	0	0

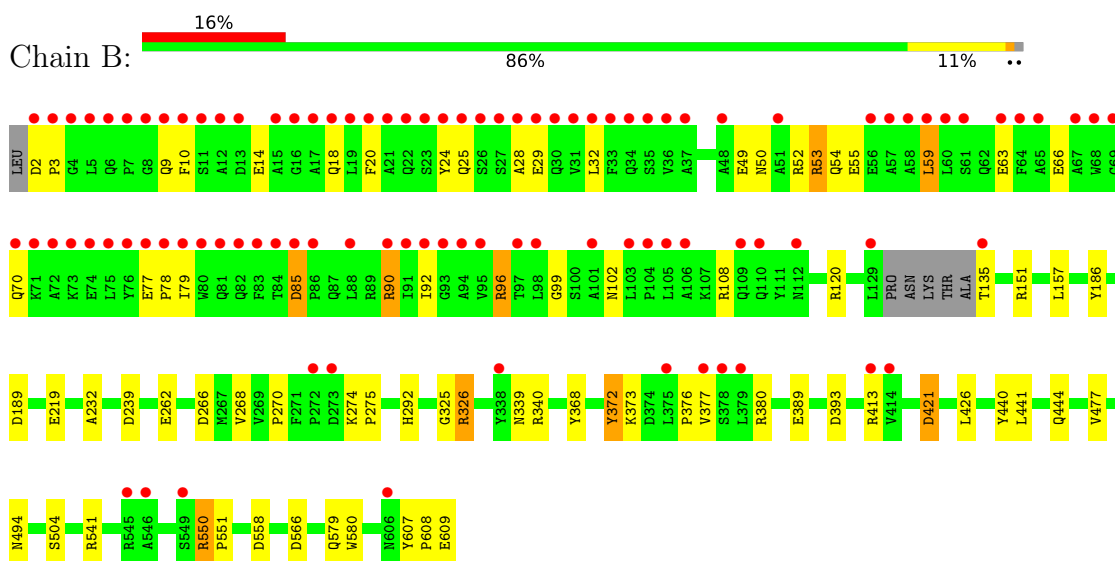
### 3 Residue-property plots

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.

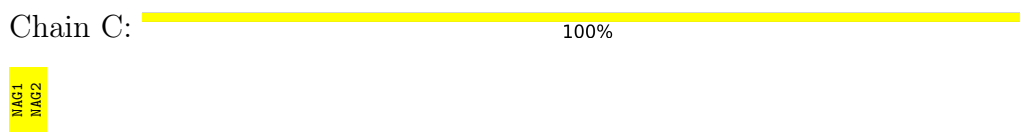
- Molecule 1: Angiotensin-converting enzyme, soluble form



- Molecule 1: Angiotensin-converting enzyme, soluble form



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



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

Chain D:  50% 50%


MAG1  
FUC2

- Molecule 3:  $\alpha$ -L-fucopyranose-(1-6)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain E:  50% 50%

MAG1  
FUC2

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

Chain F:  50% 50%

MAG1  
MAG2  
BMA3  
FUC4

- Molecule 5: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain G:  33% 67%

MAG1  
MAG2  
BMA3

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	73.28Å 77.81Å 83.43Å 88.38° 63.98° 74.55°	Depositor
Resolution (Å)	74.61 – 2.00 74.61 – 2.00	Depositor EDS
% Data completeness (in resolution range)	98.1 (74.61-2.00) 97.1 (74.61-2.00)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.54 (at 2.00Å)	Xtriage
Refinement program	REFMAC 5.8.0430 (refmacat 0.4.100)	Depositor
R, $R_{free}$	0.177 , 0.212 0.184 , 0.218	Depositor DCC
$R_{free}$ test set	5267 reflections (4.91%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	26.7	Xtriage
Anisotropy	0.181	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 44.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	11096	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.02% 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, PEG, PGE, CL, NAG, 1PE, CA, FUC, X92, BMA, ACT, MG, EDO

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	0.78	0/5157	1.19	8/7022 (0.1%)
1	B	0.71	0/5126	1.17	15/6980 (0.2%)
All	All	0.75	0/10283	1.18	23/14002 (0.2%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	4
1	B	0	4
All	All	0	8

There are no bond length outliers.

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	54	GLN	CB-CA-C	8.58	124.35	110.88
1	B	54	GLN	N-CA-CB	-8.31	97.96	110.01
1	B	266	ASP	CA-CB-CG	7.57	120.17	112.60
1	A	541	ARG	CD-NE-CZ	6.52	133.53	124.40
1	B	50	ASN	CB-CA-C	6.18	121.36	110.85
1	B	135	THR	CA-CB-OG1	-6.12	100.42	109.60
1	A	262	GLU	CB-CG-CD	6.08	122.93	112.60
1	B	262	GLU	CB-CG-CD	5.87	122.57	112.60
1	A	372	TYR	CA-CB-CG	5.77	124.29	113.90
1	B	90	ARG	CB-CA-C	-5.69	101.17	110.85
1	B	566	ASP	CA-CB-CG	5.68	118.28	112.60
1	B	421	ASP	CA-CB-CG	5.54	118.14	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	478	THR	CA-CB-OG1	-5.52	101.32	109.60
1	A	393	ASP	CA-CB-CG	5.51	118.11	112.60
1	B	239	ASP	CA-CB-CG	5.47	118.07	112.60
1	A	566	ASP	CA-CB-CG	5.46	118.06	112.60
1	B	393	ASP	CA-CB-CG	5.42	118.03	112.60
1	B	372	TYR	CA-CB-CG	5.32	123.47	113.90
1	B	494	ASN	CA-CB-CG	-5.27	107.33	112.60
1	B	219	GLU	CB-CG-CD	5.26	121.55	112.60
1	A	13	ASP	CA-CB-CG	5.09	117.69	112.60
1	B	85	ASP	CA-CB-CG	5.07	117.67	112.60
1	A	2	ASP	CA-CB-CG	5.01	117.61	112.60

There are no chirality outliers.

All (8) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	120	ARG	Sidechain
1	A	245	ARG	Sidechain
1	A	340	ARG	Sidechain
1	A	413	ARG	Sidechain
1	B	120	ARG	Sidechain
1	B	53	ARG	Sidechain
1	B	541	ARG	Sidechain
1	B	90	ARG	Sidechain

## 5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5002	0	4773	36	0
1	B	4971	0	4736	44	0
2	C	28	0	25	0	0
3	D	24	0	22	1	0
3	E	24	0	22	1	0
4	F	49	0	43	2	0
5	G	39	0	34	1	0
6	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	B	1	0	0	0	0
7	A	28	0	26	1	0
7	B	28	0	26	2	0
8	A	10	0	14	0	0
8	B	20	0	28	1	0
9	A	20	0	30	6	0
9	B	4	0	6	0	0
10	A	4	0	3	2	0
10	B	4	0	3	0	0
11	A	16	0	22	1	0
11	B	16	0	22	3	0
12	A	1	0	0	0	0
12	B	1	0	0	0	0
13	A	1	0	0	0	0
13	B	1	0	0	0	0
14	A	1	0	0	0	0
15	B	14	0	13	0	0
16	B	7	0	10	1	0
17	A	483	0	0	9	0
17	B	298	0	0	3	0
All	All	11096	0	9858	92	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 5.

All (92) 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)
4:F:1:NAG:H61	4:F:2:NAG:H82	1.39	1.01
1:A:96:ARG:HH11	1:A:96:ARG:HG3	1.38	0.88
11:B:704:1PE:H141	17:B:1048:HOH:O	1.86	0.74
1:B:59:LEU:O	1:B:63:GLU:HG3	1.88	0.72
7:B:703:X92:CAJ	11:B:704:1PE:H242	2.23	0.69
1:B:49:GLU:HG3	1:B:53:ARG:NH2	2.09	0.68
1:B:55:GLU:OE2	17:B:801:HOH:O	2.12	0.68
1:A:117[A]:GLN:OE1	1:A:120:ARG:NH2	2.28	0.66
1:A:478:THR:HB	3:D:2:FUC:O3	1.97	0.64
1:B:325:GLY:O	1:B:326:ARG:C	2.42	0.62
1:B:340:ARG:HG2	1:B:373:LYS:O	2.02	0.58
1:B:32:LEU:HD12	1:B:377:VAL:HG22	1.85	0.58
1:A:96:ARG:HG3	1:A:96:ARG:NH1	2.16	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:25:GLN:CD	1:B:376:PRO:HB3	2.29	0.57
1:A:291:THR:HG23	17:A:1107:HOH:O	2.05	0.57
1:A:157:LEU:HD11	1:A:477:VAL:HG13	1.86	0.56
1:A:340:ARG:NE	17:A:817:HOH:O	2.39	0.55
1:A:60:LEU:HD23	1:A:60:LEU:O	2.07	0.55
1:B:426:LEU:C	1:B:426:LEU:HD13	2.32	0.54
4:F:1:NAG:H61	4:F:2:NAG:C8	2.27	0.54
1:A:184:GLU:OE1	17:A:801:HOH:O	2.19	0.54
1:A:66:GLU:O	1:A:70:GLN:HG3	2.08	0.54
1:B:92:ILE:O	1:B:96:ARG:HG3	2.07	0.53
1:B:550:ARG:NH1	1:B:558:ASP:OD2	2.42	0.53
1:B:32:LEU:HD12	1:B:377:VAL:CG2	2.39	0.53
1:B:325:GLY:O	1:B:326:ARG:O	2.26	0.53
1:B:29:GLU:CD	1:B:380:ARG:HH22	2.18	0.52
1:B:66:GLU:HG2	1:B:70:GLN:NE2	2.24	0.52
1:B:157:LEU:HD11	1:B:477:VAL:HG13	1.91	0.52
1:A:254:GLY:O	9:A:705:EDO:H12	2.09	0.52
1:B:28:ALA:HB3	1:B:377:VAL:HG11	1.92	0.51
1:A:263:ASN:HD21	9:A:705:EDO:H21	1.75	0.51
1:B:274:LYS:HB3	1:B:275:PRO:HD2	1.92	0.51
1:B:440:TYR:O	1:B:444[B]:GLN:HG2	2.11	0.51
1:B:28:ALA:HB3	1:B:377:VAL:CG1	2.40	0.50
1:B:66:GLU:CD	1:B:108:ARG:HH22	2.19	0.50
1:B:14:GLU:OE2	1:B:85:ASP:HB3	2.12	0.50
1:B:29:GLU:HA	1:B:377:VAL:HG21	1.94	0.50
1:A:31:VAL:O	1:A:34:GLN:HG3	2.11	0.50
1:A:60:LEU:HD23	1:A:60:LEU:C	2.37	0.50
1:A:440:TYR:CE1	1:A:444[B]:GLN:NE2	2.79	0.50
1:B:24:TYR:HD2	1:B:25:GLN:HG3	1.76	0.50
1:B:274:LYS:HB3	1:B:275:PRO:CD	2.42	0.49
1:B:270:PRO:HB3	1:B:580:TRP:CH2	2.48	0.49
1:A:273:ASP:HB2	17:A:935:HOH:O	2.12	0.48
1:B:28:ALA:CB	1:B:377:VAL:HG11	2.44	0.48
1:B:102:ASN:HD21	1:B:189:ASP:CG	2.21	0.48
1:A:270:PRO:HD3	1:A:426:LEU:HD23	1.96	0.48
1:B:25:GLN:CG	1:B:376:PRO:HB3	2.44	0.48
10:A:706:ACT:H3	17:A:934:HOH:O	2.12	0.48
11:A:708:1PE:H131	11:A:708:1PE:H251	1.96	0.47
1:B:441:LEU:C	1:B:441:LEU:HD12	2.39	0.47
1:A:609:GLU:H	1:A:609:GLU:CD	2.21	0.47
1:B:14:GLU:O	1:B:18:GLN:HG2	2.13	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:49:GLU:HG3	1:B:53:ARG:HH22	1.76	0.47
1:B:10:PHE:CE2	1:B:20:PHE:HA	2.49	0.47
1:A:270:PRO:HD3	1:A:426:LEU:CD2	2.44	0.46
1:A:31:VAL:HG13	1:A:60:LEU:HD22	1.98	0.46
1:B:2:ASP:OD1	1:B:3:PRO:HD2	2.16	0.46
1:A:144:THR:HG23	9:A:705:EDO:H22	1.96	0.46
1:B:77:GLU:N	1:B:78:PRO:CD	2.79	0.46
1:A:176:GLU:OE1	17:A:802:HOH:O	2.21	0.45
1:A:66:GLU:CD	1:A:108:ARG:HH22	2.24	0.45
1:A:274:LYS:HB3	1:A:275:PRO:HD2	1.99	0.45
1:A:144:THR:CG2	9:A:705:EDO:H22	2.47	0.44
1:A:77:GLU:N	1:A:78:PRO:CD	2.79	0.44
5:G:1:NAG:C6	5:G:2:NAG:H82	2.47	0.44
1:A:262:GLU:OE2	1:A:263:ASN:ND2	2.49	0.44
1:A:274:LYS:HB3	1:A:275:PRO:CD	2.47	0.44
1:B:151[A]:ARG:HH11	1:B:151[A]:ARG:HG3	1.83	0.44
1:A:239:ASP:H	9:A:709:EDO:H11	1.83	0.43
1:A:55:GLU:OE2	17:A:803:HOH:O	2.21	0.43
1:A:441:LEU:HD12	1:A:441:LEU:C	2.44	0.42
1:B:232:ALA:CB	1:B:268:VAL:HG12	2.48	0.42
1:B:292:HIS:HE2	16:B:706:PEG:H22	1.83	0.42
7:B:703:X92:CAH	11:B:704:1PE:H242	2.49	0.42
1:A:570:LEU:C	1:A:570:LEU:HD23	2.44	0.42
9:A:705:EDO:H11	17:A:1024:HOH:O	2.18	0.42
1:B:389:GLU:HB2	1:B:504[A]:SER:HB2	2.01	0.42
8:B:707:PGE:H5	17:B:1042:HOH:O	2.19	0.42
1:B:151[A]:ARG:HA	1:B:151[A]:ARG:HD3	1.88	0.42
1:B:9:GLN:C	1:B:10:PHE:CD1	2.98	0.42
1:B:339:ASN:O	1:B:340:ARG:HB2	2.20	0.42
1:A:389:GLU:HB2	1:A:504:SER:HB2	2.02	0.41
1:A:52:ARG:NH1	1:A:52:ARG:HG2	2.36	0.41
7:A:702:X92:O	7:A:702:X92:CAT	2.69	0.41
1:A:194:THR:HB	1:A:450:PHE:CD1	2.56	0.41
1:B:607:TYR:HA	1:B:608:PRO:HA	1.85	0.40
1:A:596:GLU:OE2	3:E:1:NAG:O7	2.39	0.40
1:B:99:GLY:HA2	1:B:186:TYR:CE1	2.56	0.40
1:B:550:ARG:HG3	1:B:551:PRO:HD2	2.02	0.40
10:A:706:ACT:H1	17:A:893:HOH:O	2.20	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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	607/609 (100%)	594 (98%)	11 (2%)	2 (0%)	37	35
1	B	604/609 (99%)	587 (97%)	14 (2%)	3 (0%)	25	21
All	All	1211/1218 (99%)	1181 (98%)	25 (2%)	5 (0%)	30	27

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	326	ARG
1	B	413	ARG
1	A	45	ASN
1	A	79	ILE
1	B	79	ILE

### 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	527/524 (101%)	519 (98%)	8 (2%)	60	66
1	B	524/524 (100%)	515 (98%)	9 (2%)	56	61
All	All	1051/1048 (100%)	1034 (98%)	17 (2%)	58	64

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	120	ARG

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Mol	Chain	Res	Type
1	A	266	ASP
1	A	273	ASP
1	A	368	TYR
1	A	372	TYR
1	A	403	GLU
1	A	606	ASN
1	A	609	GLU
1	B	52	ARG
1	B	59	LEU
1	B	96	ARG
1	B	368	TYR
1	B	372	TYR
1	B	421	ASP
1	B	550	ARG
1	B	579	GLN
1	B	609	GLU

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	110	GLN
1	B	6	GLN
1	B	70	GLN

### 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](#)

13 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	0.60	0	17,19,21	1.37	2 (11%)
2	NAG	C	2	2	14,14,15	0.53	0	17,19,21	1.13	1 (5%)
3	NAG	D	1	3,1	14,14,15	0.64	0	17,19,21	1.80	2 (11%)
3	FUC	D	2	3	10,10,11	0.60	0	14,14,16	1.99	3 (21%)
3	NAG	E	1	3,1	14,14,15	0.45	0	17,19,21	1.60	3 (17%)
3	FUC	E	2	3	10,10,11	0.31	0	14,14,16	0.78	0
4	NAG	F	1	4,1	14,14,15	0.64	0	17,19,21	0.97	1 (5%)
4	NAG	F	2	4	14,14,15	0.39	0	17,19,21	2.53	4 (23%)
4	BMA	F	3	4	11,11,12	1.33	1 (9%)	15,15,17	1.28	2 (13%)
4	FUC	F	4	4	10,10,11	0.79	0	14,14,16	1.14	2 (14%)
5	NAG	G	1	5,1	14,14,15	0.62	0	17,19,21	1.98	3 (17%)
5	NAG	G	2	5	14,14,15	0.38	0	17,19,21	1.15	2 (11%)
5	BMA	G	3	5	11,11,12	0.98	1 (9%)	15,15,17	1.30	1 (6%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	C	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	C	2	2	-	2/6/23/26	0/1/1/1
3	NAG	D	1	3,1	-	3/6/23/26	0/1/1/1
3	FUC	D	2	3	-	-	0/1/1/1
3	NAG	E	1	3,1	-	0/6/23/26	0/1/1/1
3	FUC	E	2	3	-	-	0/1/1/1
4	NAG	F	1	4,1	-	0/6/23/26	0/1/1/1
4	NAG	F	2	4	-	3/6/23/26	0/1/1/1
4	BMA	F	3	4	-	0/2/19/22	0/1/1/1
4	FUC	F	4	4	-	-	0/1/1/1
5	NAG	G	1	5,1	-	4/6/23/26	0/1/1/1
5	NAG	G	2	5	-	2/6/23/26	0/1/1/1
5	BMA	G	3	5	-	1/2/19/22	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	F	3	BMA	C2-C3	3.93	1.58	1.52
5	G	3	BMA	C4-C5	2.06	1.57	1.53

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	F	2	NAG	C1-C2-N2	6.70	121.92	110.49
4	F	2	NAG	C2-N2-C7	5.74	131.07	122.90
5	G	1	NAG	C1-C2-N2	5.43	119.77	110.49
3	D	1	NAG	C1-C2-N2	5.19	119.36	110.49
3	D	2	FUC	C1-C2-C3	5.09	115.93	109.67
5	G	1	NAG	C1-O5-C5	4.46	118.23	112.19
4	F	2	NAG	C1-O5-C5	4.46	118.23	112.19
3	D	2	FUC	O5-C1-C2	3.81	116.65	110.77
3	E	1	NAG	O5-C1-C2	3.56	116.91	111.29
2	C	2	NAG	C1-O5-C5	3.56	117.01	112.19
5	G	1	NAG	C2-N2-C7	3.55	127.95	122.90
5	G	3	BMA	C3-C4-C5	3.48	116.44	110.24
2	C	1	NAG	C1-C2-N2	3.11	115.80	110.49
3	E	1	NAG	C2-N2-C7	2.88	127.01	122.90
2	C	1	NAG	O3-C3-C2	-2.79	103.70	109.47
3	D	1	NAG	O5-C5-C6	2.76	111.53	107.20
4	F	3	BMA	O2-C2-C3	2.67	115.48	110.14
4	F	3	BMA	C1-C2-C3	2.59	112.85	109.67
3	E	1	NAG	C3-C4-C5	-2.50	105.77	110.24
4	F	1	NAG	C2-N2-C7	2.45	126.40	122.90
3	D	2	FUC	C1-O5-C5	2.38	118.18	112.78
5	G	2	NAG	C1-O5-C5	2.36	115.38	112.19
5	G	2	NAG	C2-N2-C7	2.24	126.09	122.90
4	F	4	FUC	O2-C2-C3	2.12	114.39	110.14
4	F	2	NAG	C6-C5-C4	-2.03	108.26	113.00
4	F	4	FUC	C2-C3-C4	2.01	114.38	110.89

There are no chirality outliers.

All (17) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	F	2	NAG	C3-C2-N2-C7
4	F	2	NAG	C8-C7-N2-C2
4	F	2	NAG	O7-C7-N2-C2
5	G	1	NAG	C3-C2-N2-C7
3	D	1	NAG	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
5	G	2	NAG	C8-C7-N2-C2
5	G	2	NAG	O7-C7-N2-C2
3	D	1	NAG	C4-C5-C6-O6
5	G	1	NAG	C8-C7-N2-C2
5	G	1	NAG	O7-C7-N2-C2
5	G	3	BMA	O5-C5-C6-O6
2	C	2	NAG	C4-C5-C6-O6
5	G	1	NAG	C4-C5-C6-O6
2	C	2	NAG	O5-C5-C6-O6
2	C	1	NAG	C4-C5-C6-O6
2	C	1	NAG	O5-C5-C6-O6
3	D	1	NAG	C3-C2-N2-C7

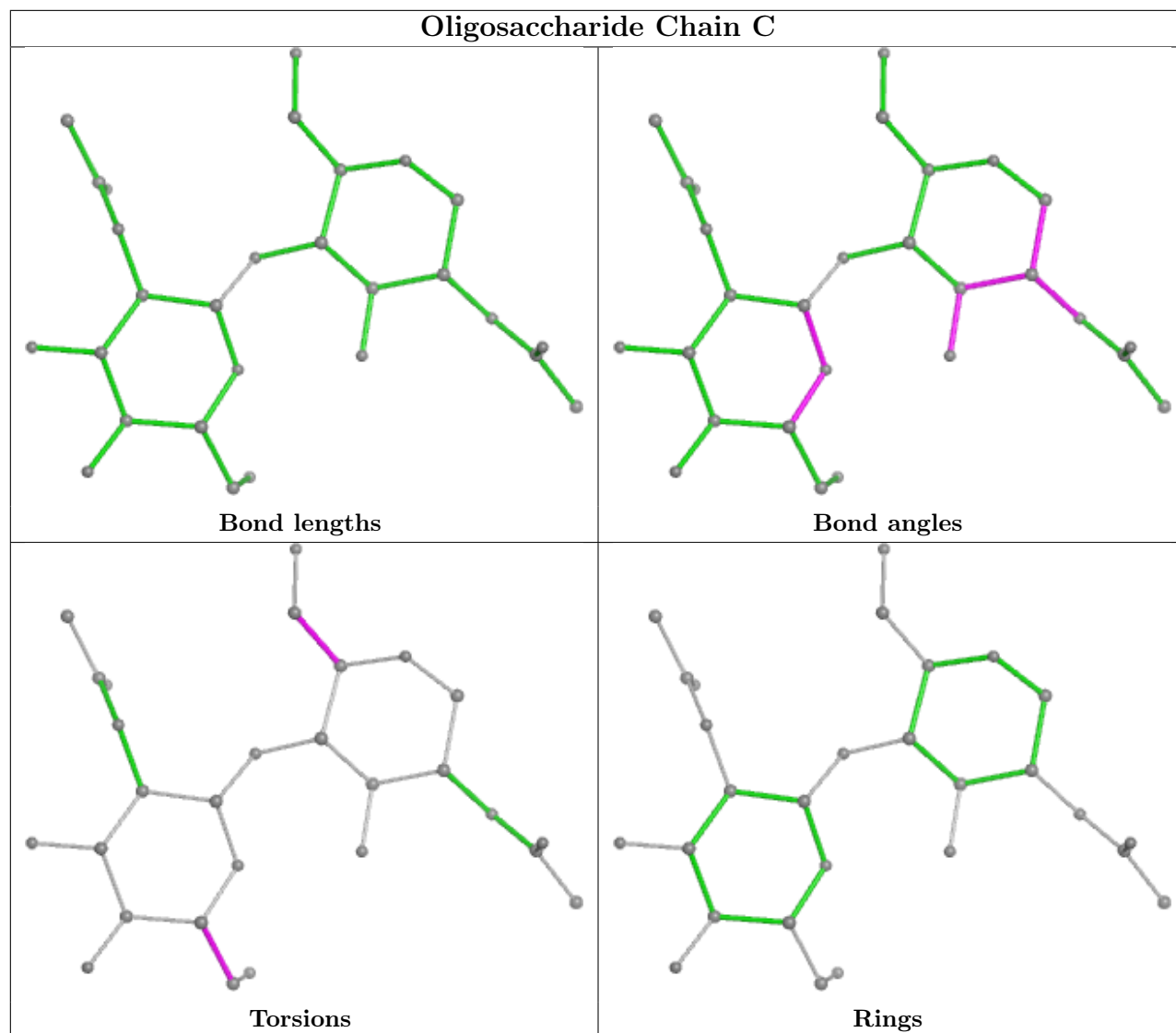
There are no ring outliers.

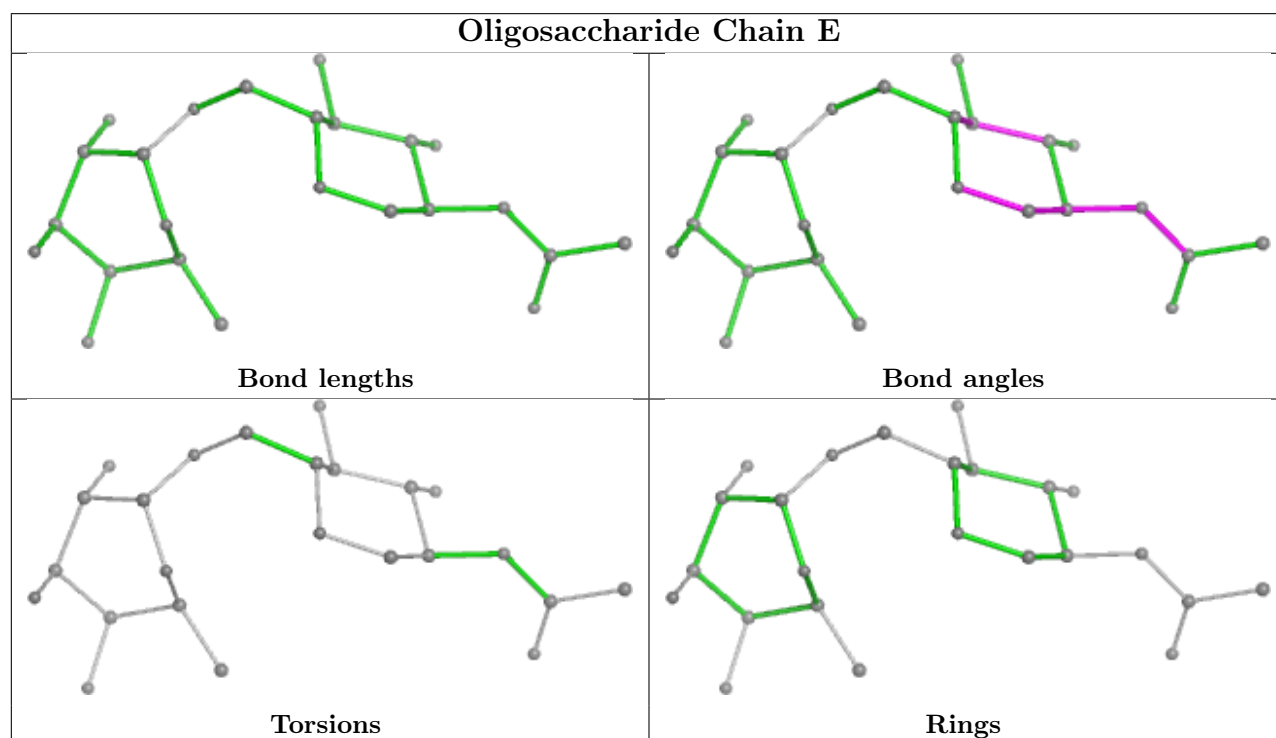
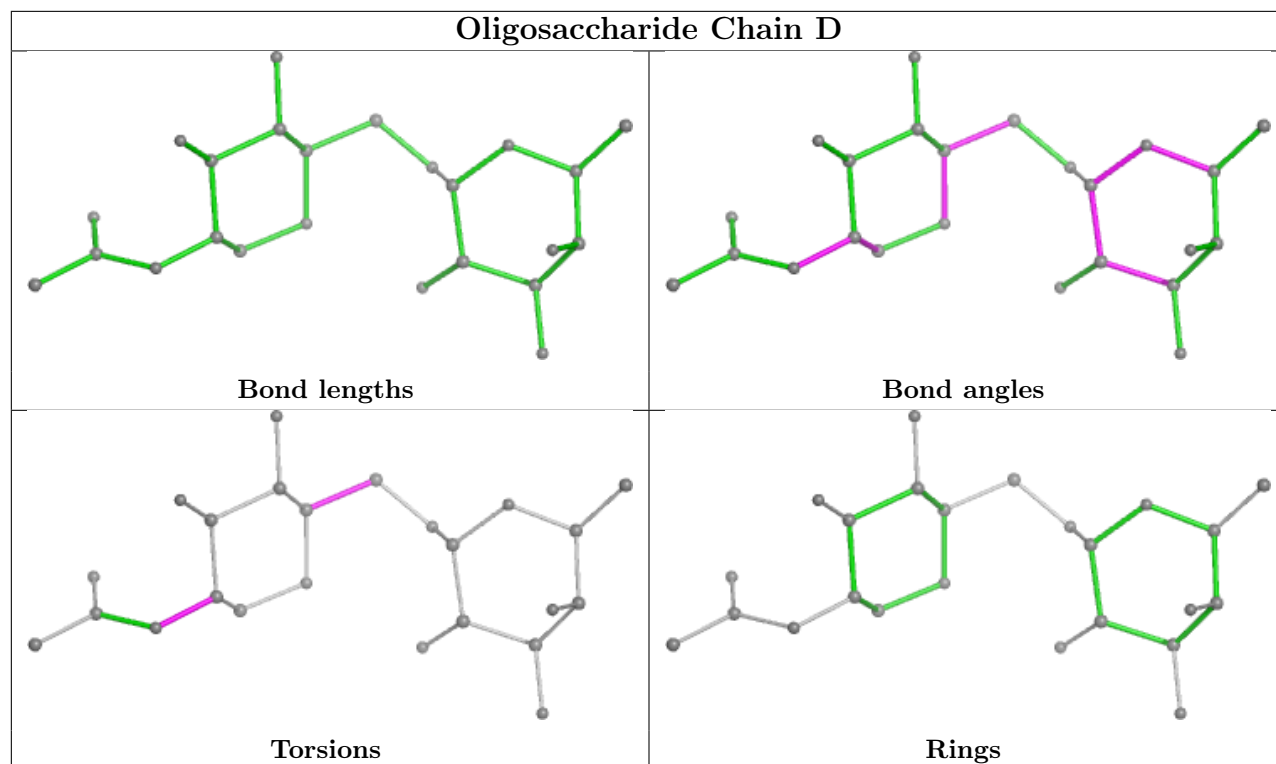
6 monomers are involved in 5 short contacts:

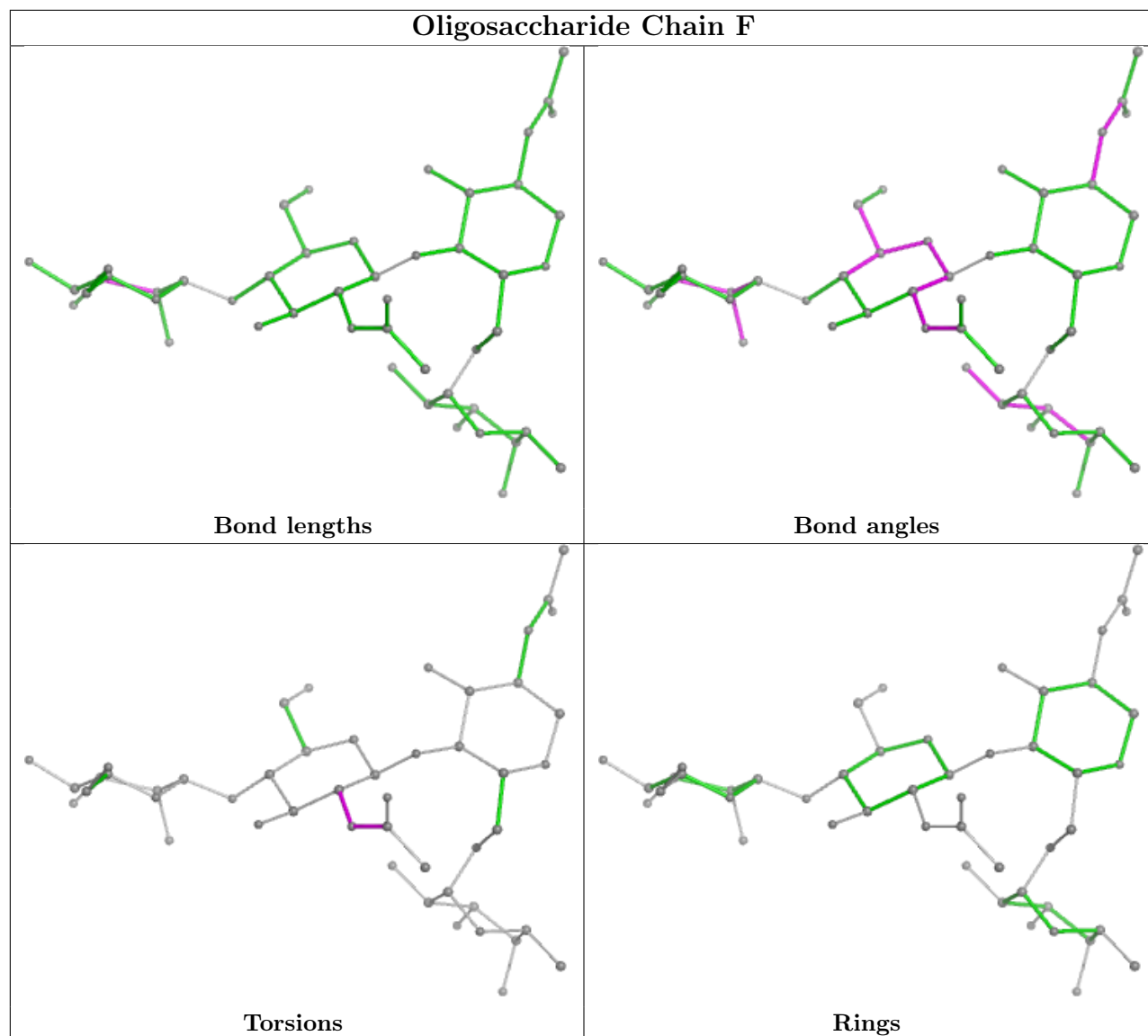
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	2	FUC	1	0
3	E	1	NAG	1	0
4	F	1	NAG	2	0
5	G	2	NAG	1	0
5	G	1	NAG	1	0
4	F	2	NAG	2	0

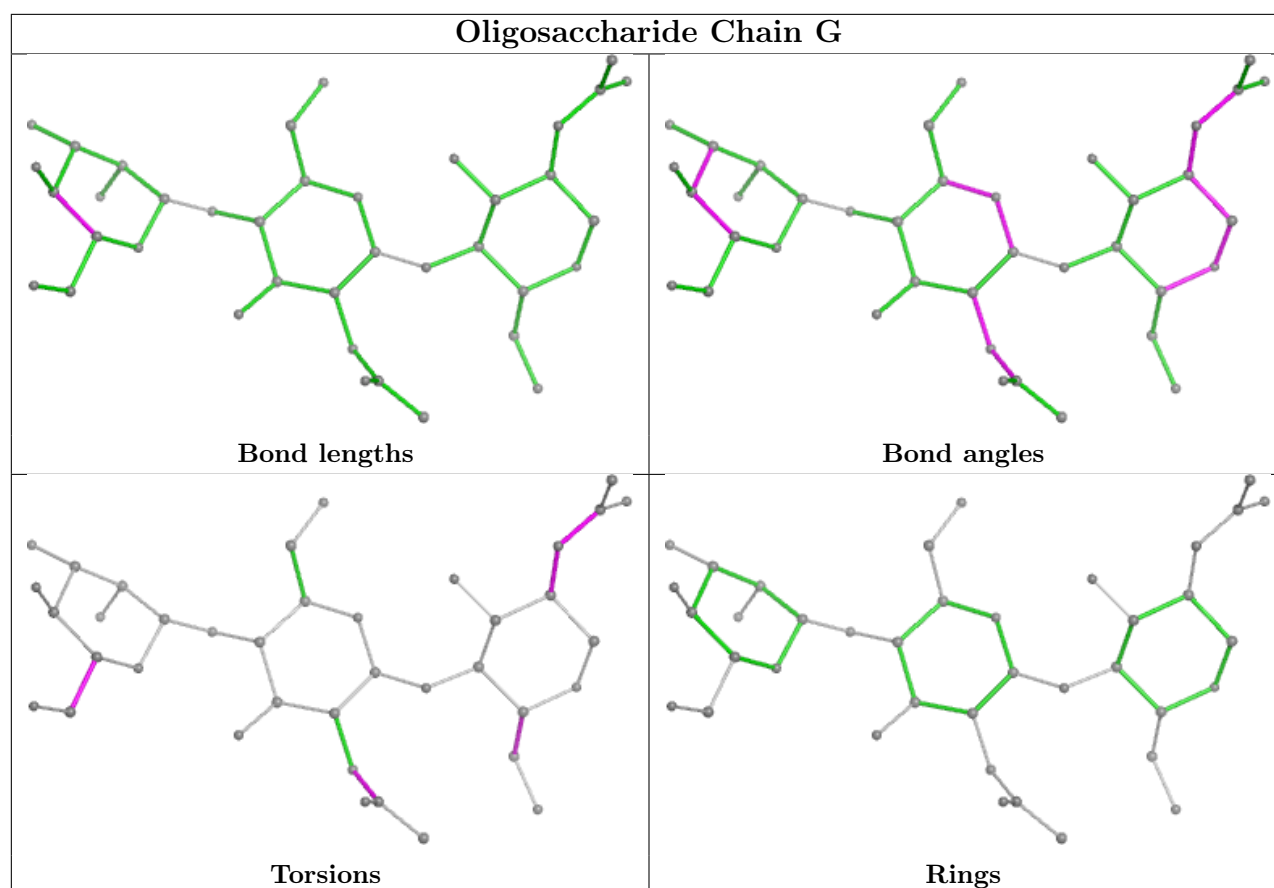
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.











## 5.6 Ligand geometry [i](#)

Of 24 ligands modelled in this entry, 7 are monoatomic - leaving 17 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	$\# Z  > 2$
8	PGE	B	707	-	9,9,9	0.19	0	8,8,8	0.19	0
9	EDO	A	707	-	3,3,3	0.50	0	2,2,2	0.73	0
7	X92	A	702	6	30,30,30	1.04	1 (3%)	39,42,42	1.74	9 (23%)
15	NAG	B	701	1	14,14,15	0.52	0	17,19,21	1.33	3 (17%)
9	EDO	A	709	-	3,3,3	0.22	0	2,2,2	0.40	0
7	X92	B	703	6	30,30,30	0.87	1 (3%)	39,42,42	1.30	4 (10%)
9	EDO	A	711	-	3,3,3	0.38	0	2,2,2	0.32	0
11	1PE	A	708	-	15,15,15	0.57	0	14,14,14	0.63	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
10	ACT	A	706	-	3,3,3	1.18	0	3,3,3	1.11	0
10	ACT	B	708	-	3,3,3	1.26	0	3,3,3	1.23	0
8	PGE	A	703	-	9,9,9	0.52	0	8,8,8	0.29	0
8	PGE	B	705	-	9,9,9	0.49	0	8,8,8	0.50	0
9	EDO	A	704	-	3,3,3	0.10	0	2,2,2	0.28	0
9	EDO	B	709	-	3,3,3	0.31	0	2,2,2	0.31	0
11	1PE	B	704	-	15,15,15	0.53	0	14,14,14	0.56	0
16	PEG	B	706	-	6,6,6	0.50	0	5,5,5	0.41	0
9	EDO	A	705	13	3,3,3	0.29	0	2,2,2	0.63	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
8	PGE	B	707	-	-	3/7/7/7	-
9	EDO	A	707	-	-	1/1/1/1	-
7	X92	A	702	6	-	4/25/47/47	0/3/3/3
15	NAG	B	701	1	-	1/6/23/26	0/1/1/1
9	EDO	A	709	-	-	0/1/1/1	-
7	X92	B	703	6	-	3/25/47/47	0/3/3/3
9	EDO	A	711	-	-	1/1/1/1	-
11	1PE	A	708	-	-	6/13/13/13	-
8	PGE	A	703	-	-	5/7/7/7	-
8	PGE	B	705	-	-	3/7/7/7	-
9	EDO	A	704	-	-	1/1/1/1	-
9	EDO	B	709	-	-	1/1/1/1	-
11	1PE	B	704	-	-	7/13/13/13	-
16	PEG	B	706	-	-	3/4/4/4	-
9	EDO	A	705	13	-	0/1/1/1	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	A	702	X92	CAZ-CAT	-3.08	1.47	1.52
7	B	703	X92	CAZ-CAT	-2.71	1.47	1.52

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	702	X92	CAQ-CAZ-NBB	4.87	109.65	103.47
7	A	702	X92	CAQ-CAZ-CAT	4.65	117.44	110.92
7	B	703	X92	CAQ-CAZ-CAT	4.65	117.44	110.92
15	B	701	NAG	C4-C3-C2	3.98	116.86	111.02
7	B	703	X92	CAS-CAX-N	3.13	119.48	109.21
7	A	702	X92	CAM-CAP-CAX	2.94	119.00	113.21
7	A	702	X92	CAS-CAX-N	2.91	118.76	109.21
7	B	703	X92	CB-CA-C	2.75	114.73	109.73
7	A	702	X92	OAE-CAS-CAX	-2.54	113.91	122.26
7	A	702	X92	CB-CA-C	2.47	114.21	109.73
7	A	702	X92	CAY-CBA-NBB	2.44	105.85	102.24
7	A	702	X92	OAF-CAT-CAZ	-2.40	114.91	122.48
7	A	702	X92	OAB-CAS-CAX	2.39	121.34	113.40
15	B	701	NAG	O3-C3-C2	-2.21	104.89	109.47
15	B	701	NAG	O5-C1-C2	-2.20	107.81	111.29
7	B	703	X92	CAO-CBA-NBB	2.18	117.97	114.79

There are no chirality outliers.

All (39) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	B	703	X92	CAS-CAX-N-CA
11	B	704	1PE	C16-C26-OH6-C15
8	A	703	PGE	O3-C5-C6-O4
8	B	707	PGE	O2-C3-C4-O3
11	A	708	1PE	OH5-C14-C24-OH4
8	B	705	PGE	O3-C5-C6-O4
11	B	704	1PE	OH2-C12-C22-OH3
11	A	708	1PE	OH6-C15-C25-OH5
11	B	704	1PE	OH5-C14-C24-OH4
16	B	706	PEG	O2-C3-C4-O4
9	A	704	EDO	O1-C1-C2-O2
9	A	711	EDO	O1-C1-C2-O2
8	B	705	PGE	O1-C1-C2-O2
9	B	709	EDO	O1-C1-C2-O2
7	A	702	X92	CAS-CAX-N-CA
9	A	707	EDO	O1-C1-C2-O2
11	A	708	1PE	C14-C24-OH4-C13
7	A	702	X92	OAB-CAS-CAX-N
8	B	707	PGE	C1-C2-O2-C3
7	A	702	X92	OAE-CAS-CAX-N
8	A	703	PGE	C6-C5-O3-C4
15	B	701	NAG	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
8	A	703	PGE	O1-C1-C2-O2
8	A	703	PGE	O2-C3-C4-O3
11	B	704	1PE	C12-C22-OH3-C23
8	A	703	PGE	C4-C3-O2-C2
11	A	708	1PE	C24-C14-OH5-C25
11	B	704	1PE	OH7-C16-C26-OH6
11	B	704	1PE	OH6-C15-C25-OH5
7	B	703	X92	OAE-CAS-CAX-N
16	B	706	PEG	C4-C3-O2-C2
11	A	708	1PE	C25-C15-OH6-C26
8	B	707	PGE	C6-C5-O3-C4
16	B	706	PEG	C1-C2-O2-C3
11	B	704	1PE	C15-C25-OH5-C14
8	B	705	PGE	O2-C3-C4-O3
7	B	703	X92	OAC-CAT-CAZ-NBB
7	A	702	X92	CAP-CAM-CAV-CAK
11	A	708	1PE	OH4-C13-C23-OH3

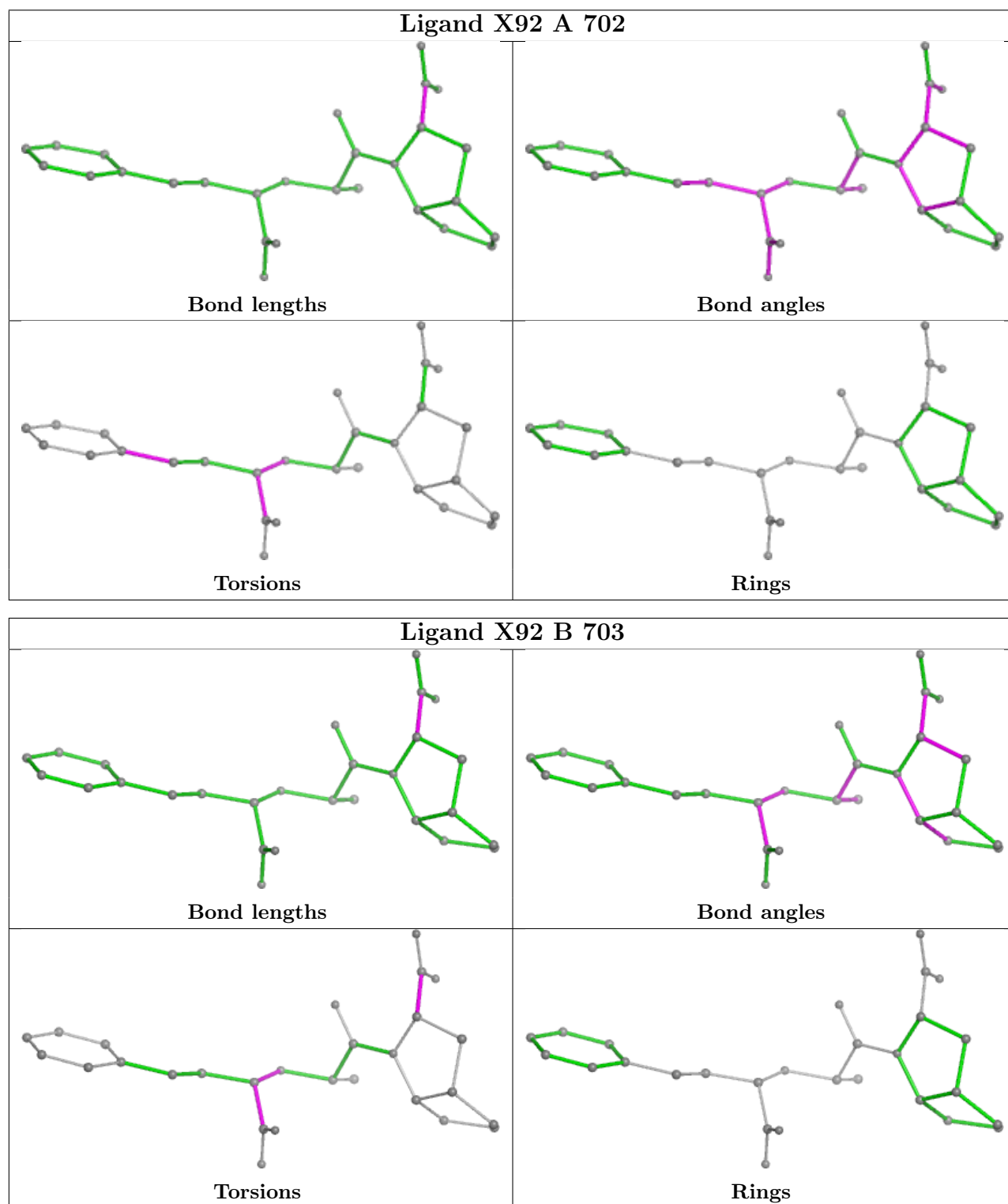
There are no ring outliers.

9 monomers are involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	B	707	PGE	1	0
7	A	702	X92	1	0
9	A	709	EDO	1	0
7	B	703	X92	2	0
11	A	708	1PE	1	0
10	A	706	ACT	2	0
11	B	704	1PE	3	0
16	B	706	PEG	1	0
9	A	705	EDO	5	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 ⓘ

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	604/609 (99%)	-0.49	6 (0%) 79 78	8, 24, 44, 69	7 (1%)
1	B	603/609 (99%)	0.51	98 (16%) 5 5	9, 35, 80, 125	5 (0%)
All	All	1207/1218 (99%)	0.01	104 (8%) 18 16	8, 28, 68, 125	12 (0%)

All (104) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	5	LEU	7.3
1	B	19	LEU	7.1
1	B	24	TYR	6.6
1	B	31	VAL	6.3
1	B	8	GLY	6.1
1	B	75	LEU	5.9
1	B	84	THR	5.8
1	B	4	GLY	5.7
1	B	88	LEU	5.6
1	B	377	VAL	5.5
1	B	11	SER	5.5
1	B	129	LEU	5.5
1	B	10	PHE	5.3
1	B	17	ALA	5.1
1	B	67	ALA	5.1
1	B	91	ILE	5.1
1	B	64	PHE	5.1
1	B	28	ALA	5.0
1	B	15	ALA	5.0
1	B	20	PHE	4.9
1	B	92	ILE	4.7
1	B	93	GLY	4.6
1	B	83	PHE	4.6
1	B	56	GLU	4.5

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Mol	Chain	Res	Type	RSRZ
1	B	79	ILE	4.5
1	B	378	SER	4.5
1	B	80	TRP	4.4
1	B	95	VAL	4.4
1	B	9	GLN	4.3
1	B	27	SER	4.2
1	B	78	PRO	4.2
1	B	25	GLN	4.2
1	B	6	GLN	4.1
1	B	68	TRP	4.1
1	B	94	ALA	4.1
1	B	18	GLN	4.0
1	B	60	LEU	4.0
1	B	135	THR	3.9
1	B	71	LYS	3.9
1	B	21	ALA	3.9
1	B	59	LEU	3.8
1	B	57	ALA	3.8
1	B	13	ASP	3.8
1	B	16	GLY	3.7
1	B	76	TYR	3.7
1	B	7	PRO	3.6
1	B	379	LEU	3.6
1	B	101	ALA	3.6
1	B	414	VAL	3.4
1	A	135	THR	3.4
1	B	338	TYR	3.4
1	B	69	GLY	3.4
1	B	22	GLN	3.4
1	B	12	ALA	3.3
1	B	23	SER	3.3
1	B	35	SER	3.2
1	B	26	SER	3.1
1	B	70	GLN	3.1
1	B	61	SER	3.0
1	B	90	ARG	3.0
1	B	58	ALA	3.0
1	B	81	GLN	2.9
1	B	72	ALA	2.9
1	B	82	GLN	2.9
1	B	2	ASP	2.9
1	B	3	PRO	2.8

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Mol	Chain	Res	Type	RSRZ
1	B	98	LEU	2.8
1	B	85	ASP	2.8
1	B	106	ALA	2.7
1	B	546	ALA	2.7
1	B	48	ALA	2.7
1	B	73	LYS	2.7
1	B	549	SER	2.7
1	B	29	GLU	2.6
1	A	79	ILE	2.6
1	B	104	PRO	2.6
1	B	65	ALA	2.6
1	B	63	GLU	2.6
1	B	34	GLN	2.6
1	B	86	PRO	2.6
1	B	105	LEU	2.6
1	B	74	GLU	2.5
1	B	103	LEU	2.5
1	B	33	PHE	2.5
1	B	273	ASP	2.5
1	B	36	VAL	2.5
1	A	609	GLU	2.5
1	A	414	VAL	2.4
1	B	413	ARG	2.4
1	B	606	ASN	2.3
1	B	51	ALA	2.3
1	A	78	PRO	2.3
1	B	112	ASN	2.3
1	B	30	GLN	2.3
1	B	37	ALA	2.3
1	B	97	THR	2.2
1	B	545	ARG	2.2
1	A	325	GLY	2.1
1	B	110	GLN	2.1
1	B	32	LEU	2.1
1	B	109	GLN	2.1
1	B	272	PRO	2.1
1	B	375	LEU	2.1
1	B	77	GLU	2.0

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

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

### 6.3 Carbohydrates

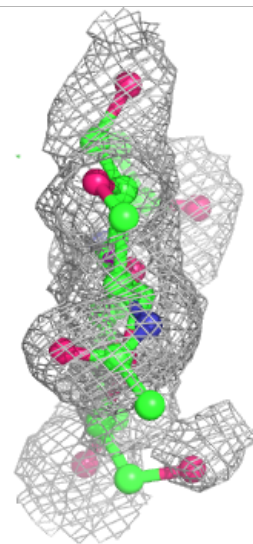
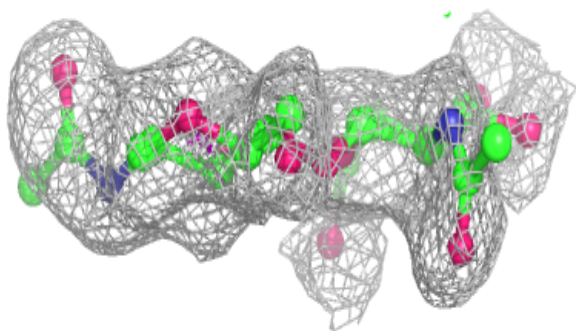
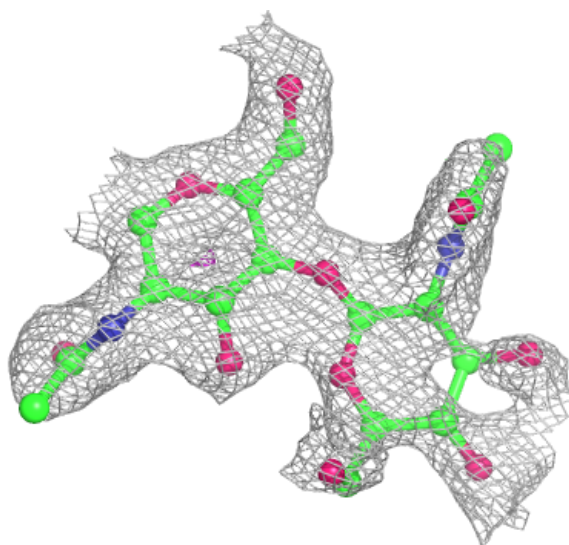
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
3	FUC	D	2	10/11	0.70	0.17	54,68,80,81	0
4	BMA	F	3	11/12	0.73	0.14	53,64,68,72	0
5	BMA	G	3	11/12	0.74	0.12	56,69,79,80	0
5	NAG	G	2	14/15	0.79	0.12	44,55,64,68	0
3	FUC	E	2	10/11	0.80	0.16	56,70,81,88	0
2	NAG	C	2	14/15	0.80	0.14	49,66,80,80	0
5	NAG	G	1	14/15	0.82	0.10	48,54,61,65	0
4	FUC	F	4	10/11	0.84	0.13	36,46,51,59	0
2	NAG	C	1	14/15	0.87	0.11	38,43,52,58	0
3	NAG	E	1	14/15	0.88	0.11	30,40,52,63	0
4	NAG	F	2	14/15	0.92	0.09	36,44,51,57	0
4	NAG	F	1	14/15	0.92	0.08	26,34,38,41	0
3	NAG	D	1	14/15	0.93	0.08	25,34,41,44	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.

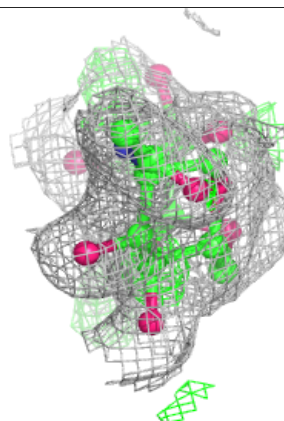
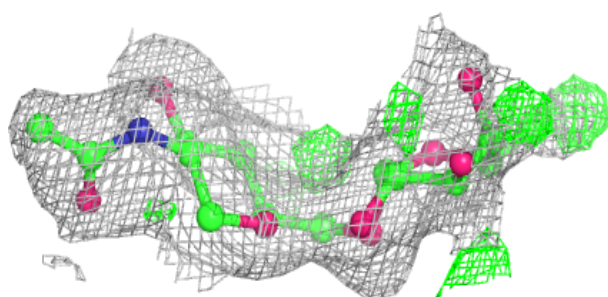
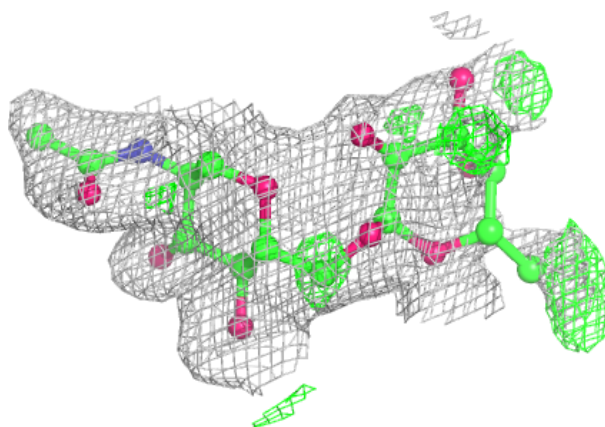
**Electron density around Chain C:**

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

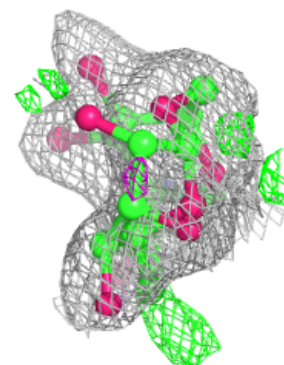
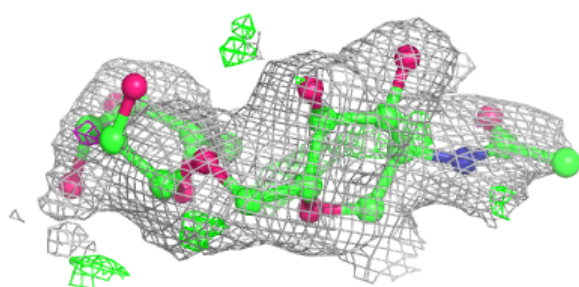
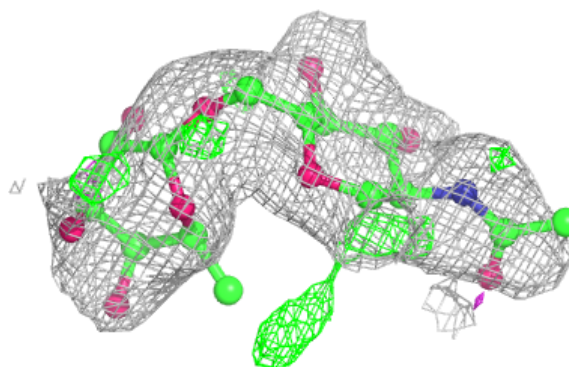


**Electron density around Chain D:**

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

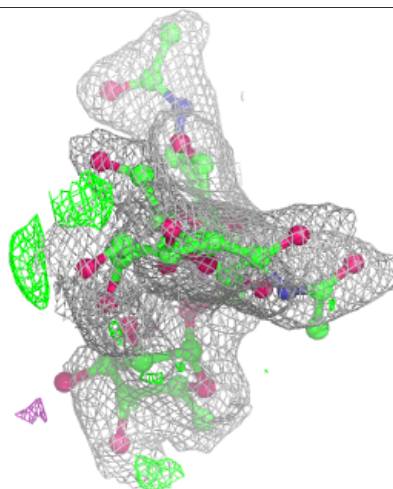
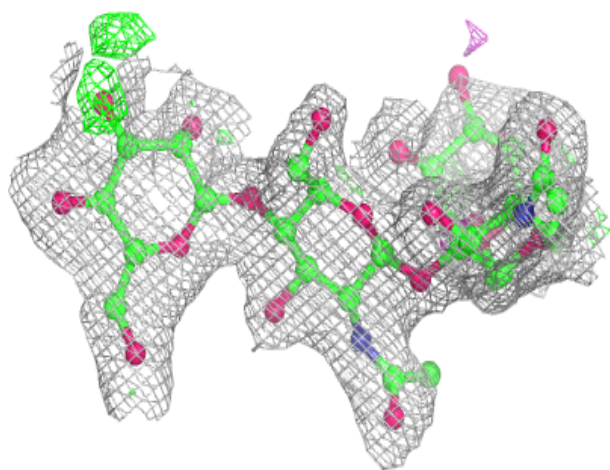
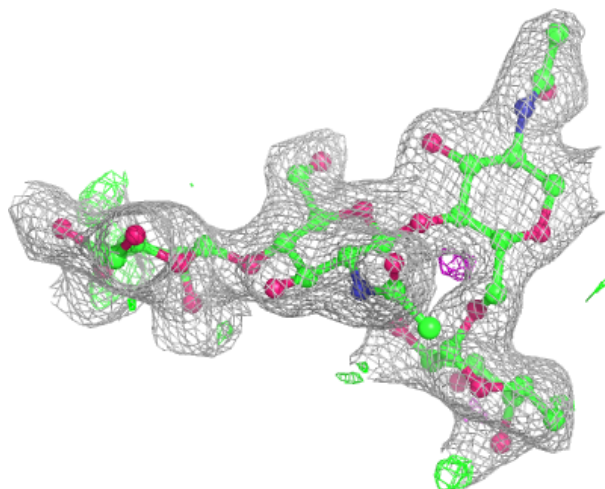
**Electron density around Chain E:**

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

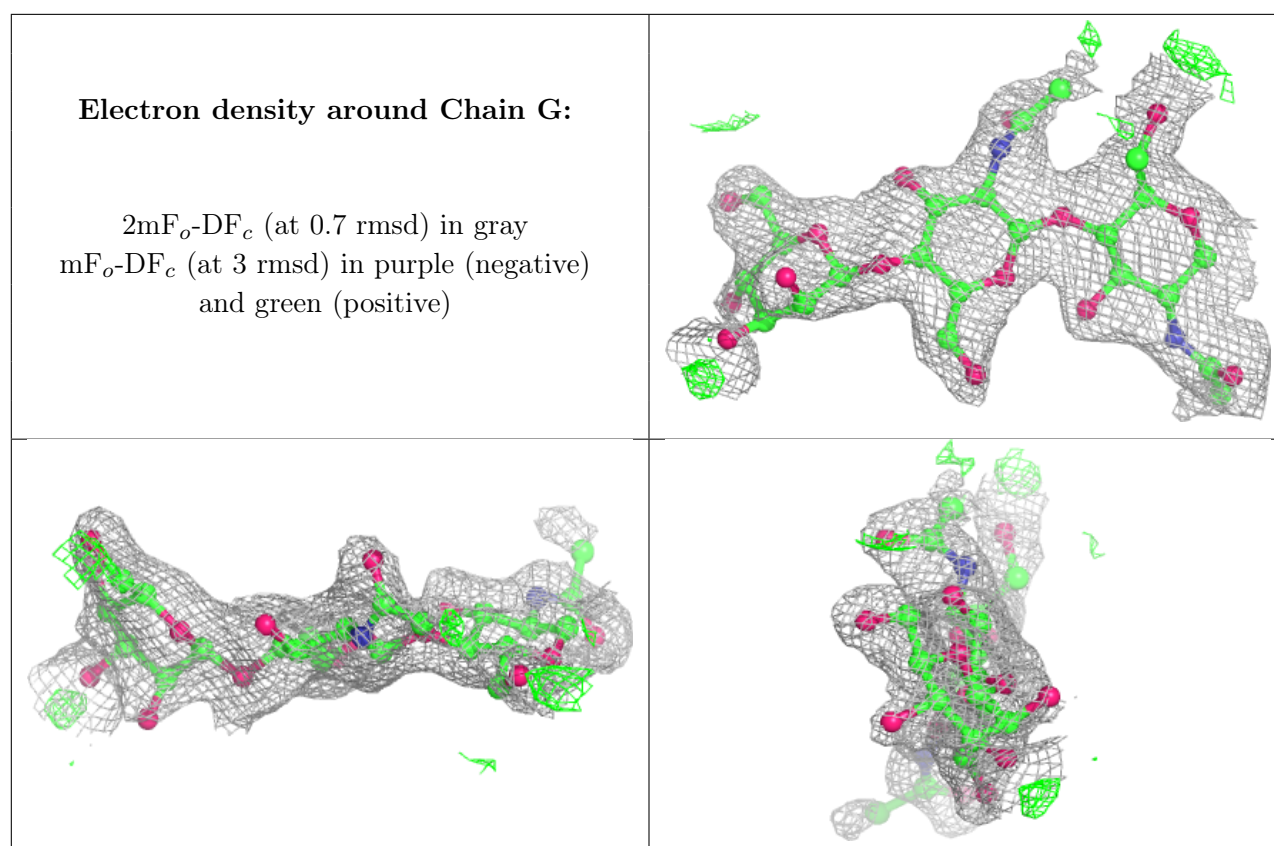


**Electron density around Chain F:**

$2mF_o-DF_c$  (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
10	ACT	B	708	4/4	0.74	0.20	34,37,45,45	0
9	EDO	A	709	4/4	0.80	0.16	62,62,63,65	0
15	NAG	B	701	14/15	0.80	0.14	65,69,78,78	0
8	PGE	B	705	10/10	0.82	0.18	44,54,63,65	0
8	PGE	A	703	10/10	0.82	0.16	44,51,57,63	0
10	ACT	A	706	4/4	0.86	0.14	24,32,36,39	0
9	EDO	B	709	4/4	0.87	0.11	50,51,51,52	0
9	EDO	A	711	4/4	0.88	0.18	43,45,46,47	0
9	EDO	A	707	4/4	0.89	0.12	43,45,49,49	0
9	EDO	A	704	4/4	0.90	0.10	42,44,47,48	0
16	PEG	B	706	7/7	0.90	0.12	48,55,58,60	0
11	1PE	B	704	16/16	0.91	0.12	32,40,57,57	0
8	PGE	B	707	10/10	0.93	0.11	53,55,58,58	0
13	MG	A	712	1/1	0.95	0.07	32,32,32,32	0

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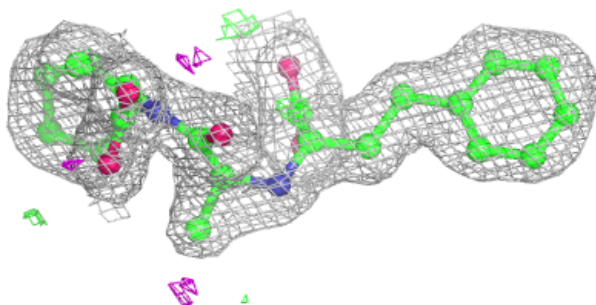
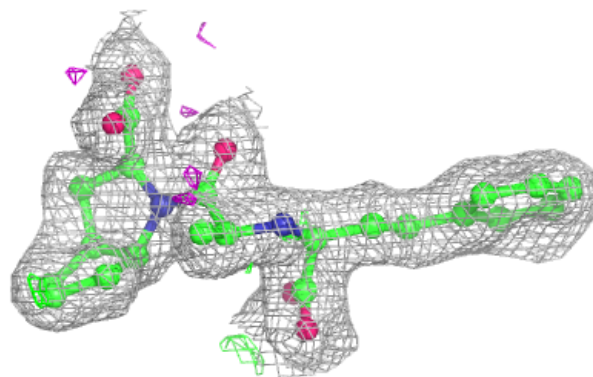
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
11	1PE	A	708	16/16	0.95	0.08	20,26,43,44	0
9	EDO	A	705	4/4	0.95	0.17	25,26,28,29	0
13	MG	B	711	1/1	0.96	0.08	29,29,29,29	0
14	CA	A	713	1/1	0.97	0.06	21,21,21,21	1
7	X92	A	702	28/28	0.97	0.05	13,16,18,19	0
12	CL	B	710	1/1	0.97	0.05	25,25,25,25	0
7	X92	B	703	28/28	0.98	0.04	16,19,26,27	0
6	ZN	B	702	1/1	0.99	0.02	21,21,21,21	0
6	ZN	A	701	1/1	0.99	0.02	16,16,16,16	0
12	CL	A	710	1/1	1.00	0.04	16,16,16,16	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.

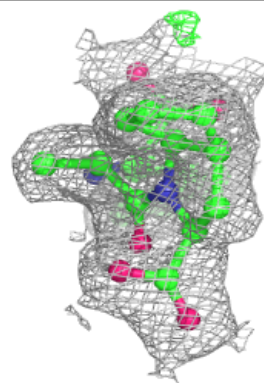
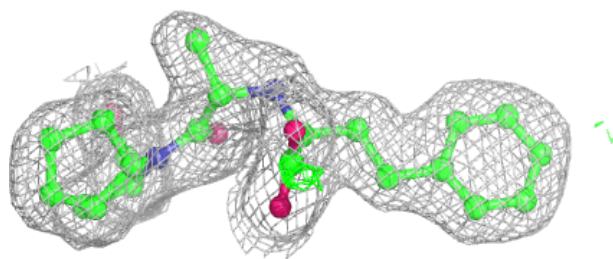
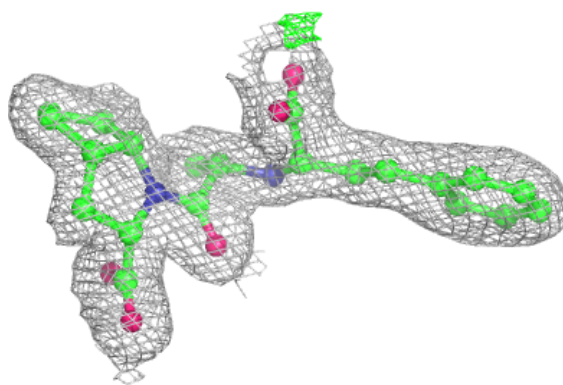
#### Electron density around X92 A 702:

2mF<sub>o</sub>-DF<sub>c</sub> (at 0.7 rmsd) in gray  
mF<sub>o</sub>-DF<sub>c</sub> (at 3 rmsd) in purple (negative)  
and green (positive)



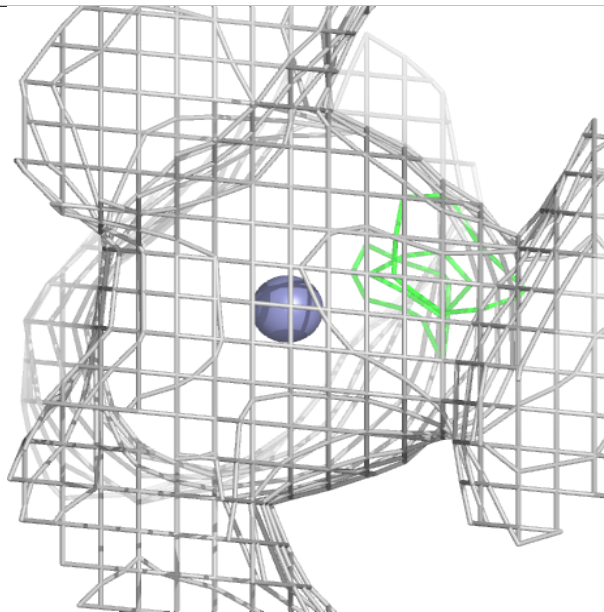
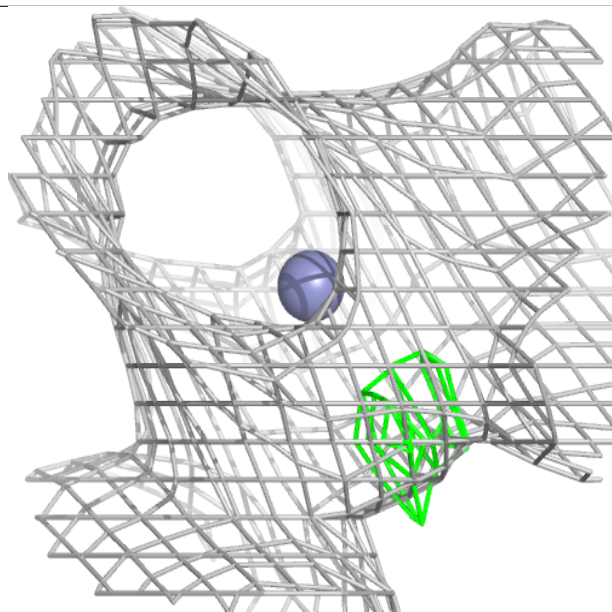
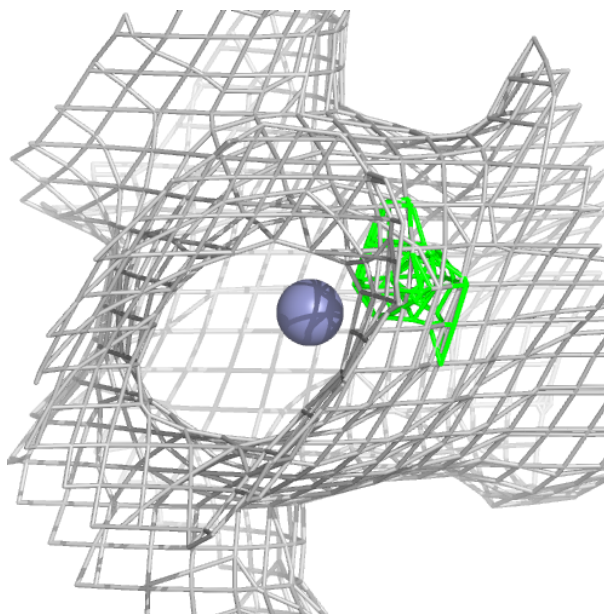
**Electron density around X92 B 703:**

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



**Electron density around ZN B 702:**

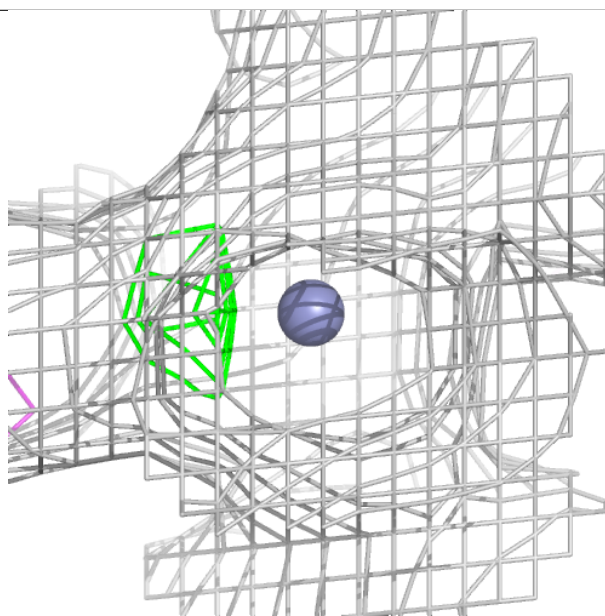
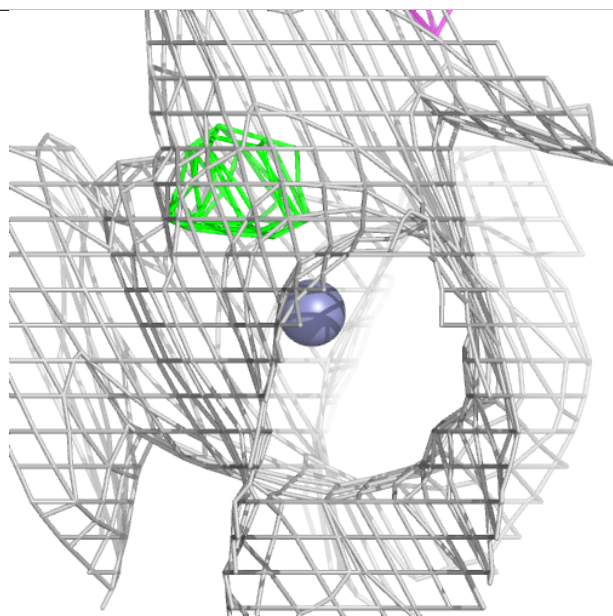
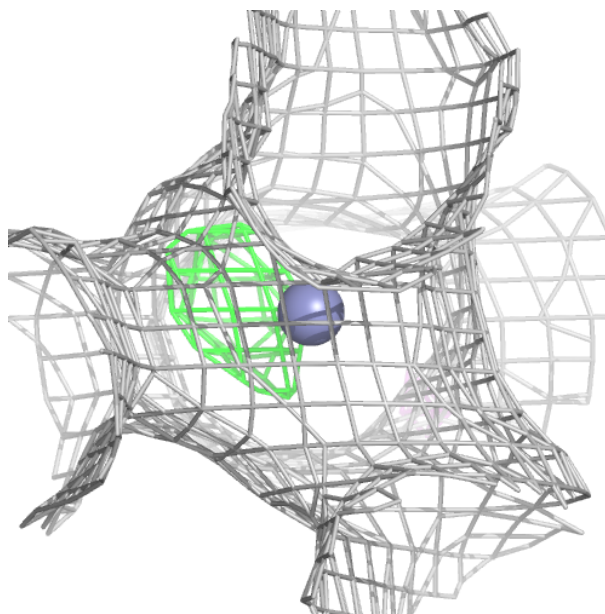
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





**Electron density around ZN A 701:**

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



## 6.5 Other polymers ⓘ

There are no such residues in this entry.