



wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 25, 2025 – 01:51 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 wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at 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 : 4-5-2 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

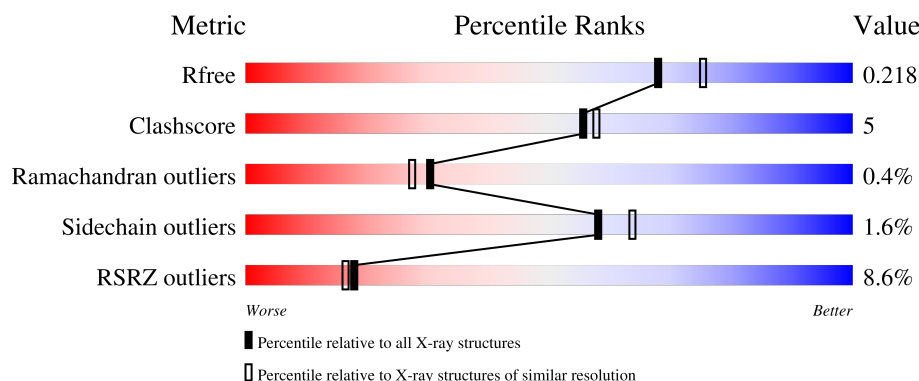
1 Overall quality at a glance

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 ≥ 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 [i](#)

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.



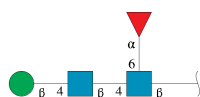
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	C	2	Total	C	N	O	0	0	0
			28	16	2	10			

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



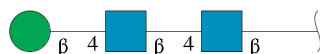
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	D	2	Total	C	N	O	0	0	0
			24	14	1	9			
3	E	2	Total	C	N	O	0	0	0
			24	14	1	9			

- 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.

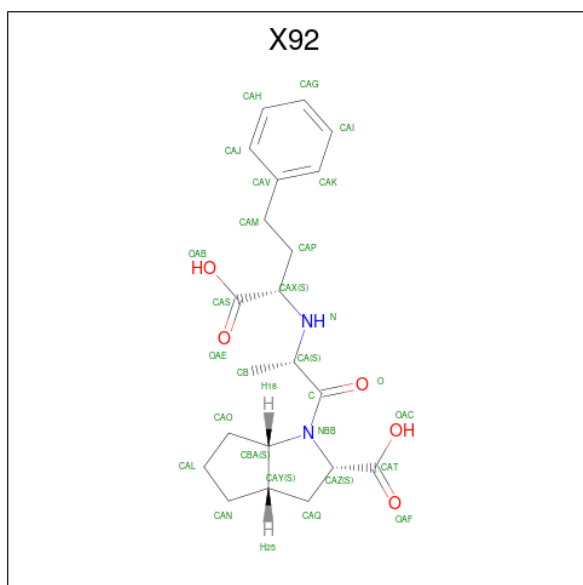


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	G	3	Total	C	N	O	0	0	0
			39	22	2	15			

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

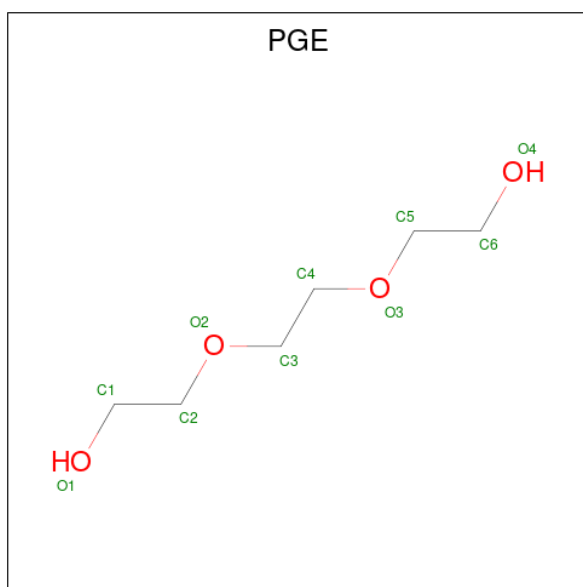
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	1	Total	Zn	0	0
			1	1		
6	B	1	Total	Zn	0	0
			1	1		

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



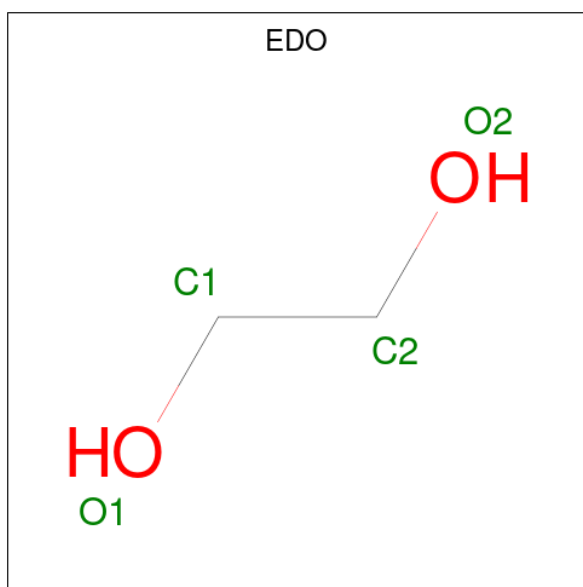
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	A	1	Total	C	N	O	0	0
			28	21	2	5		
7	B	1	Total	C	N	O	0	0
			28	21	2	5		

- 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: $C_2H_6O_2$).



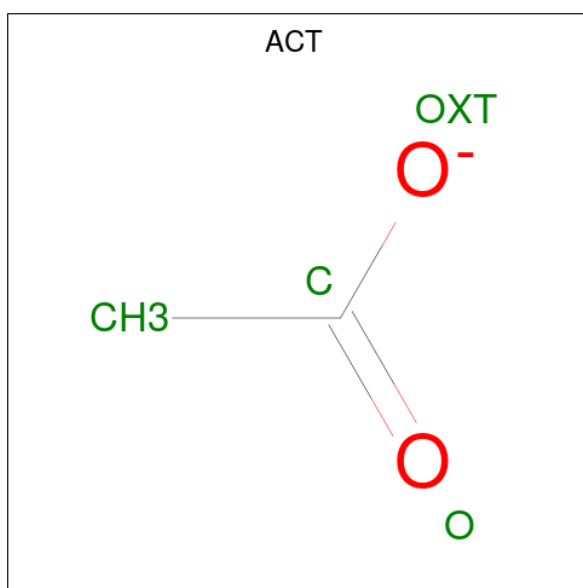
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	A	1	Total	C	O	0	0
			4	2	2		

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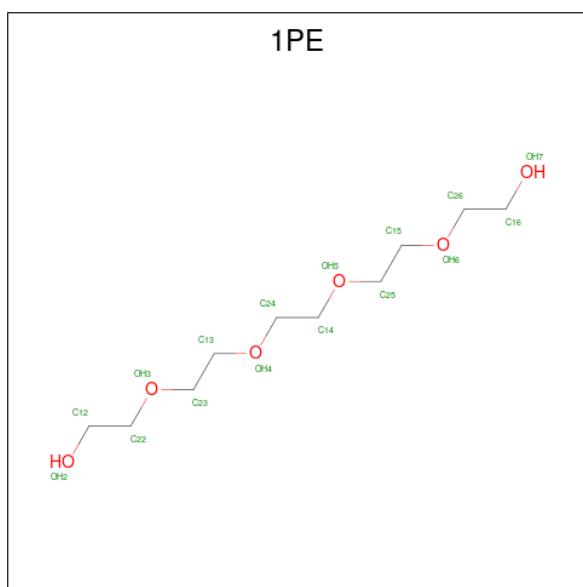
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	A	1	Total	C	O	0	0
			4	2	2		
9	A	1	Total	C	O	0	0
			4	2	2		
9	A	1	Total	C	O	0	0
			4	2	2		
9	A	1	Total	C	O	0	0
			4	2	2		
9	B	1	Total	C	O	0	0
			4	2	2		

- 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		

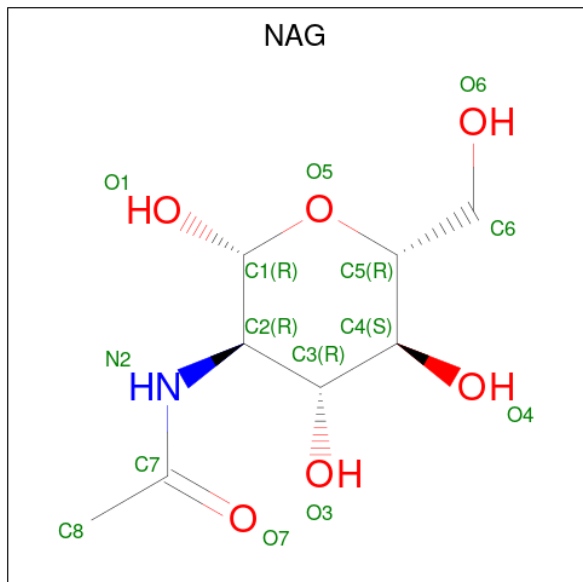
- Molecule 13 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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).

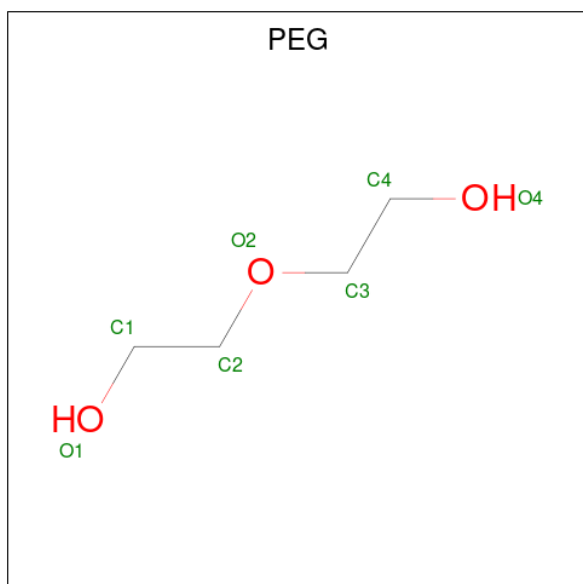
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
14	A	1	Total	Ca	0	0
			1	1		

- 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		

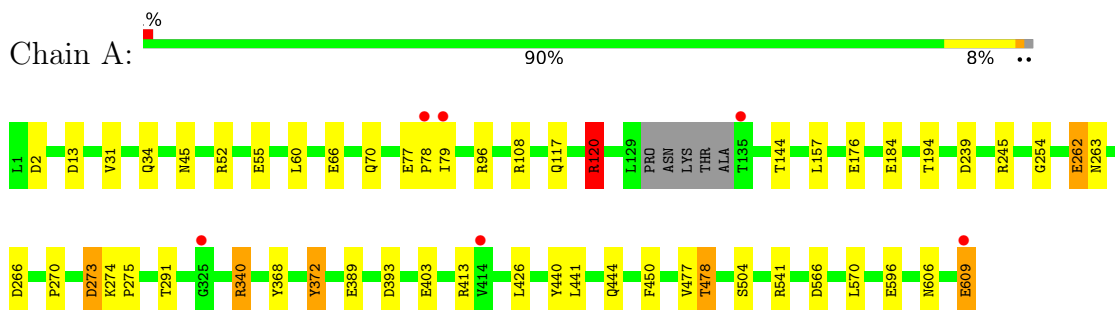
- Molecule 17 is water.

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

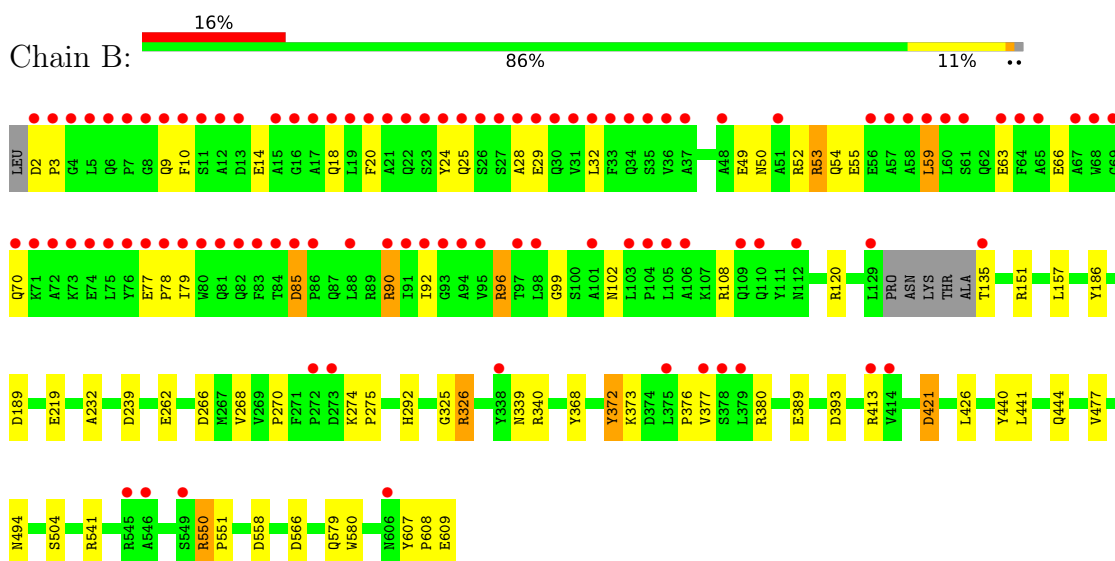
3 Residue-property plots

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.

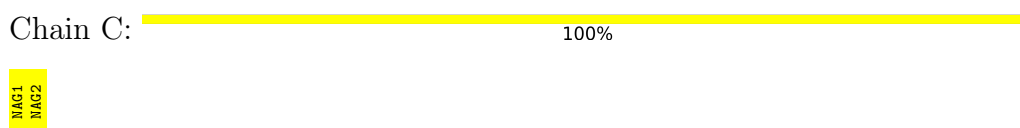
- Molecule 1: Angiotensin-converting enzyme, soluble form



- 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: α -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)-[α -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, α , β , γ	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
$\langle I/\sigma(I) \rangle$ ¹	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 ²)	26.7	Xtriage
Anisotropy	0.181	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 44.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	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 ²)	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.*

¹Intensities estimated from amplitudes.

²Theoretical 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.

The worst 5 of 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

There are no chirality outliers.

5 of 8 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	120	ARG	Sidechain

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

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	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
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.

The worst 5 of 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

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	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 [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	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

5 of 17 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	550	ARG
1	B	609	GLU
1	A	609	GLU
1	B	52	ARG
1	B	59	LEU

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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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

The worst 5 of 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

There are no chirality outliers.

5 of 17 torsion outliers are listed below:

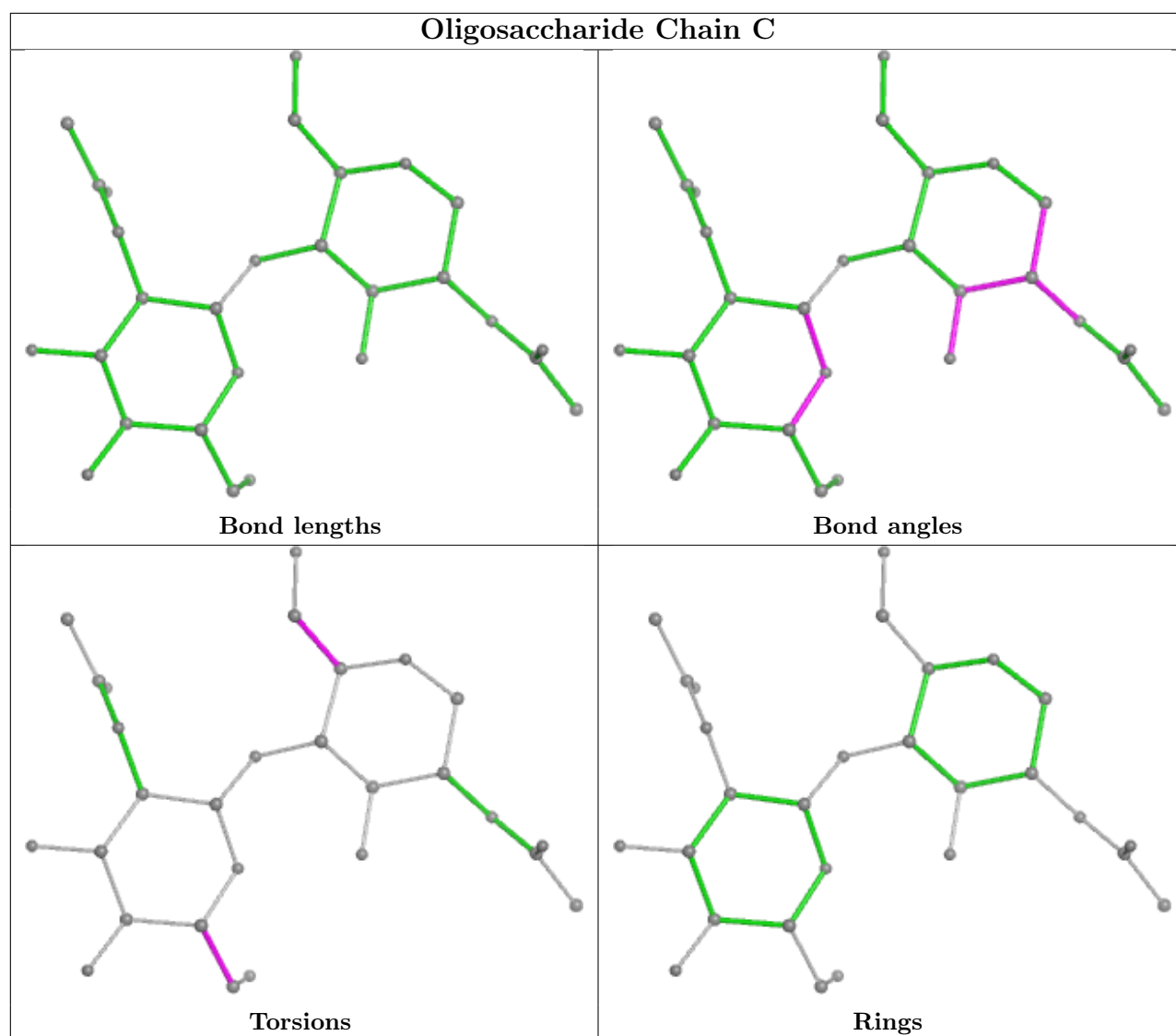
Mol	Chain	Res	Type	Atoms
4	F	2	NAG	C3-C2-N2-C7
4	F	2	NAG	C8-C7-N2-C2
4	F	2	NAG	O7-C7-N2-C2
5	G	1	NAG	C3-C2-N2-C7
3	D	1	NAG	O5-C5-C6-O6

There are no ring outliers.

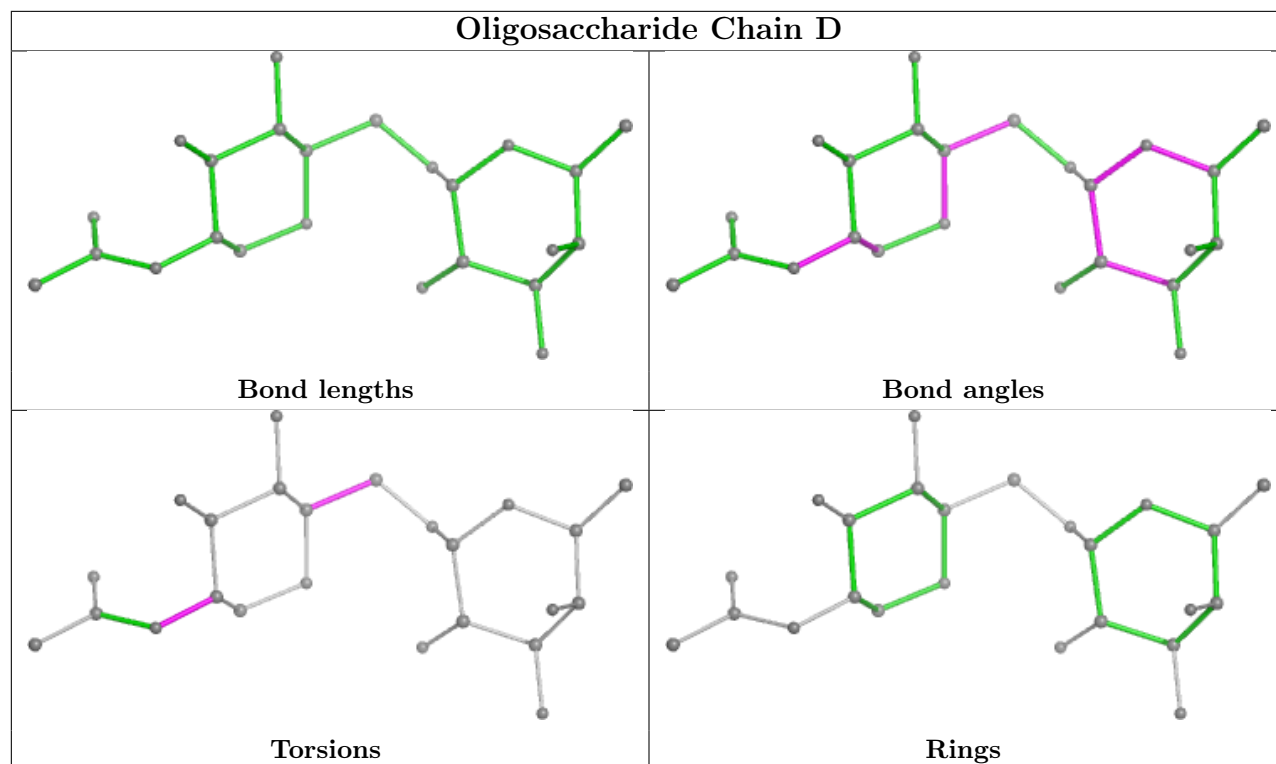
6 monomers are involved in 5 short contacts:

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

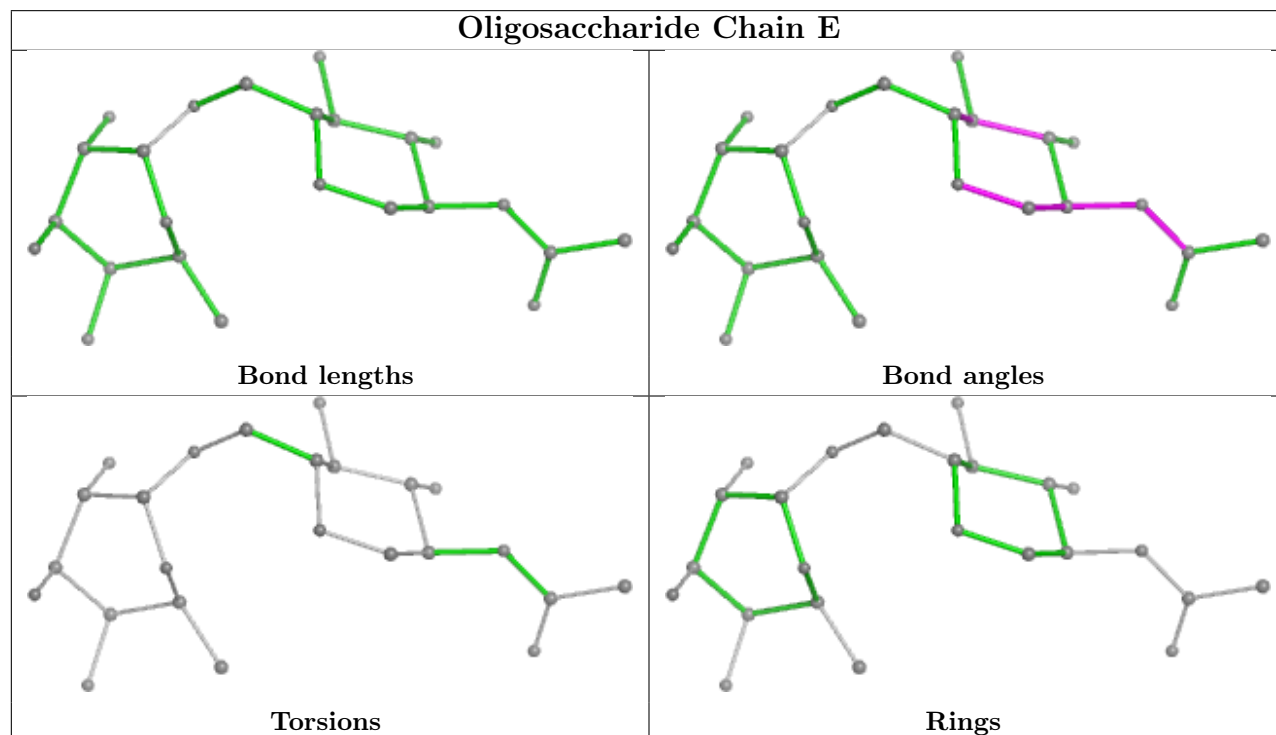
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

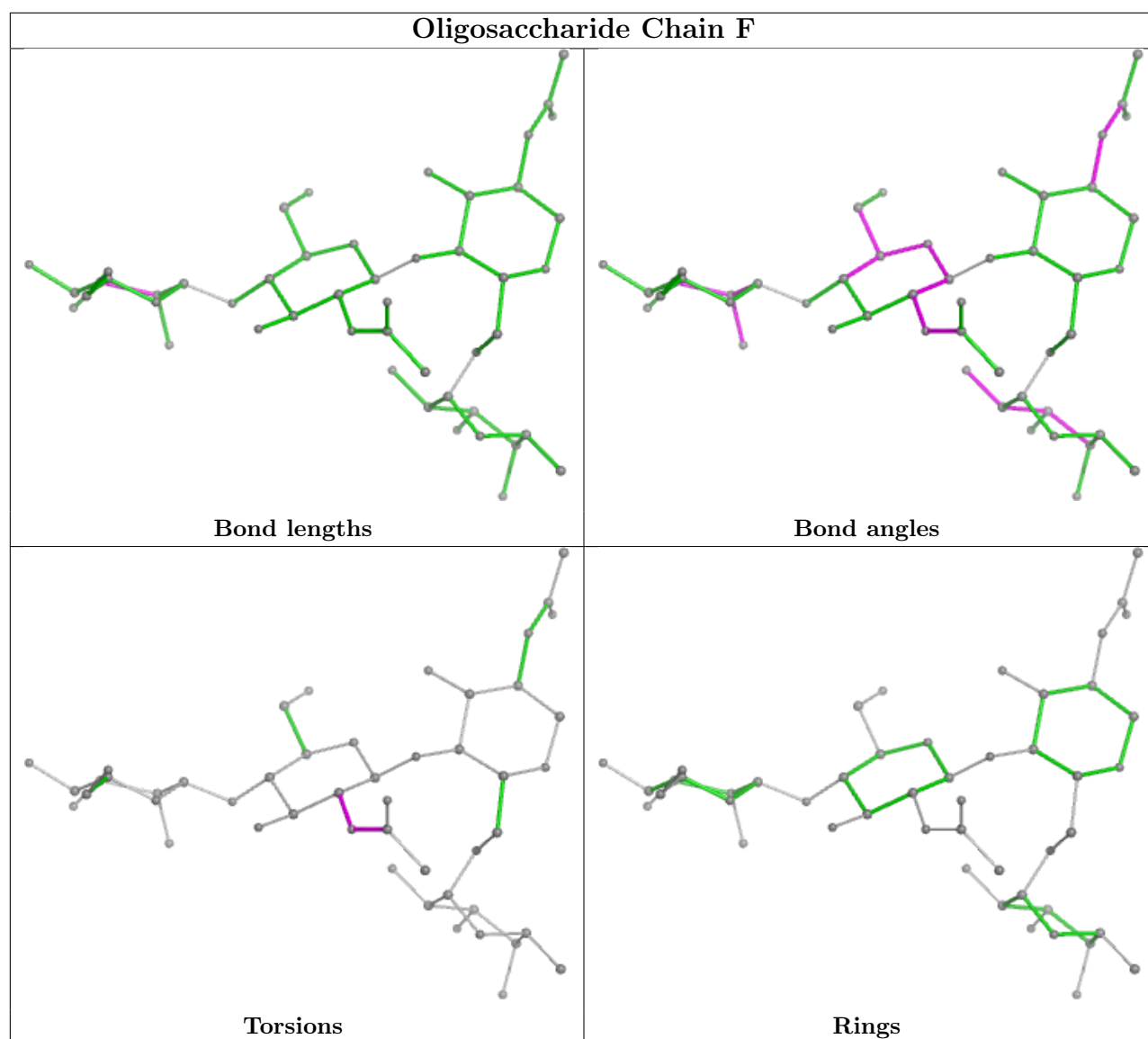


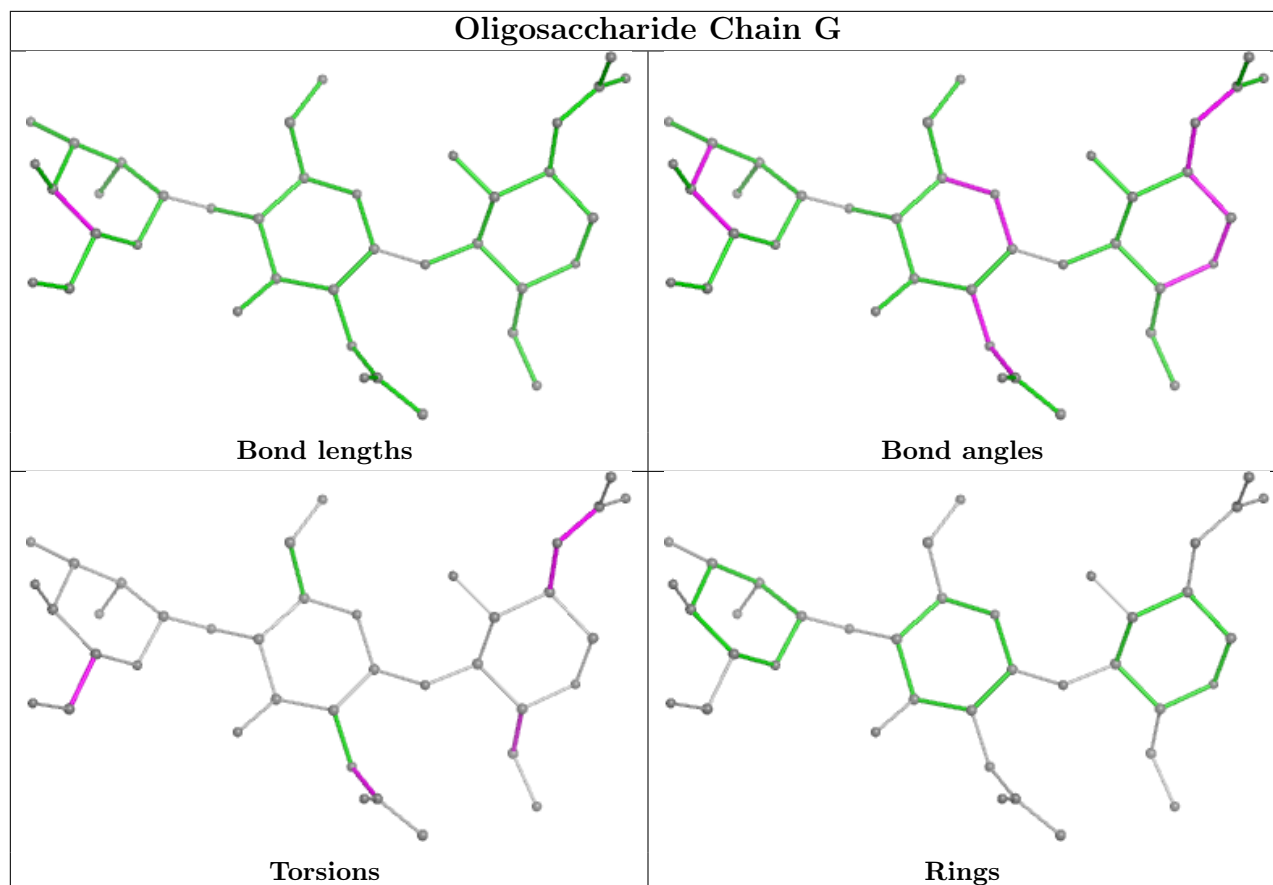
Oligosaccharide Chain D



Oligosaccharide Chain E







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

The worst 5 of 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

There are no chirality outliers.

5 of 39 torsion outliers are listed below:

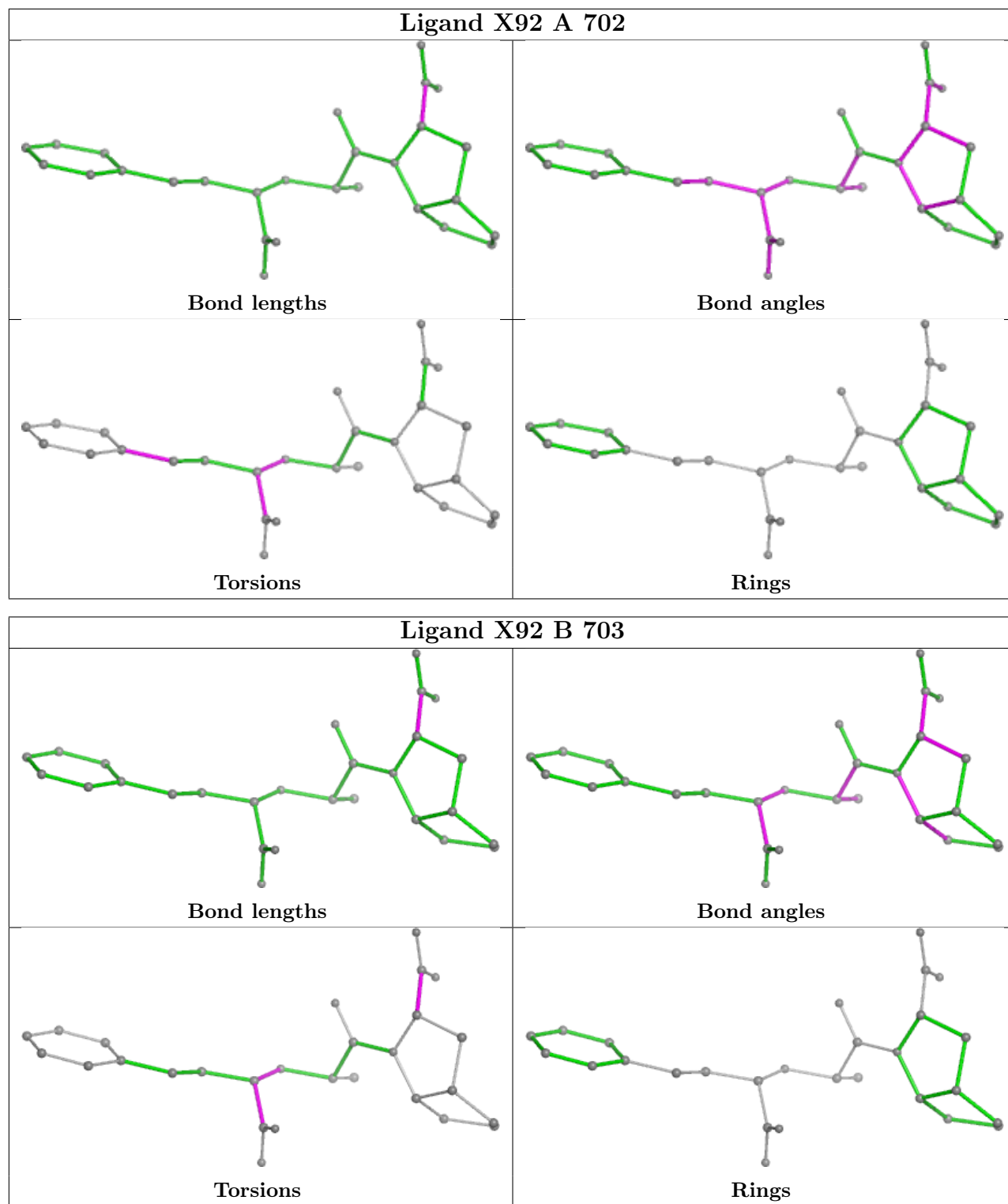
Mol	Chain	Res	Type	Atoms
7	B	703	X92	CAS-CAX-N-CA
11	B	704	1PE	C16-C26-OH6-C15
8	A	703	PGE	O3-C5-C6-O4
8	B	707	PGE	O2-C3-C4-O3
11	A	708	1PE	OH5-C14-C24-OH4

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 [i](#)

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

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th 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 ²)	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%)

The worst 5 of 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

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, 95th 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.

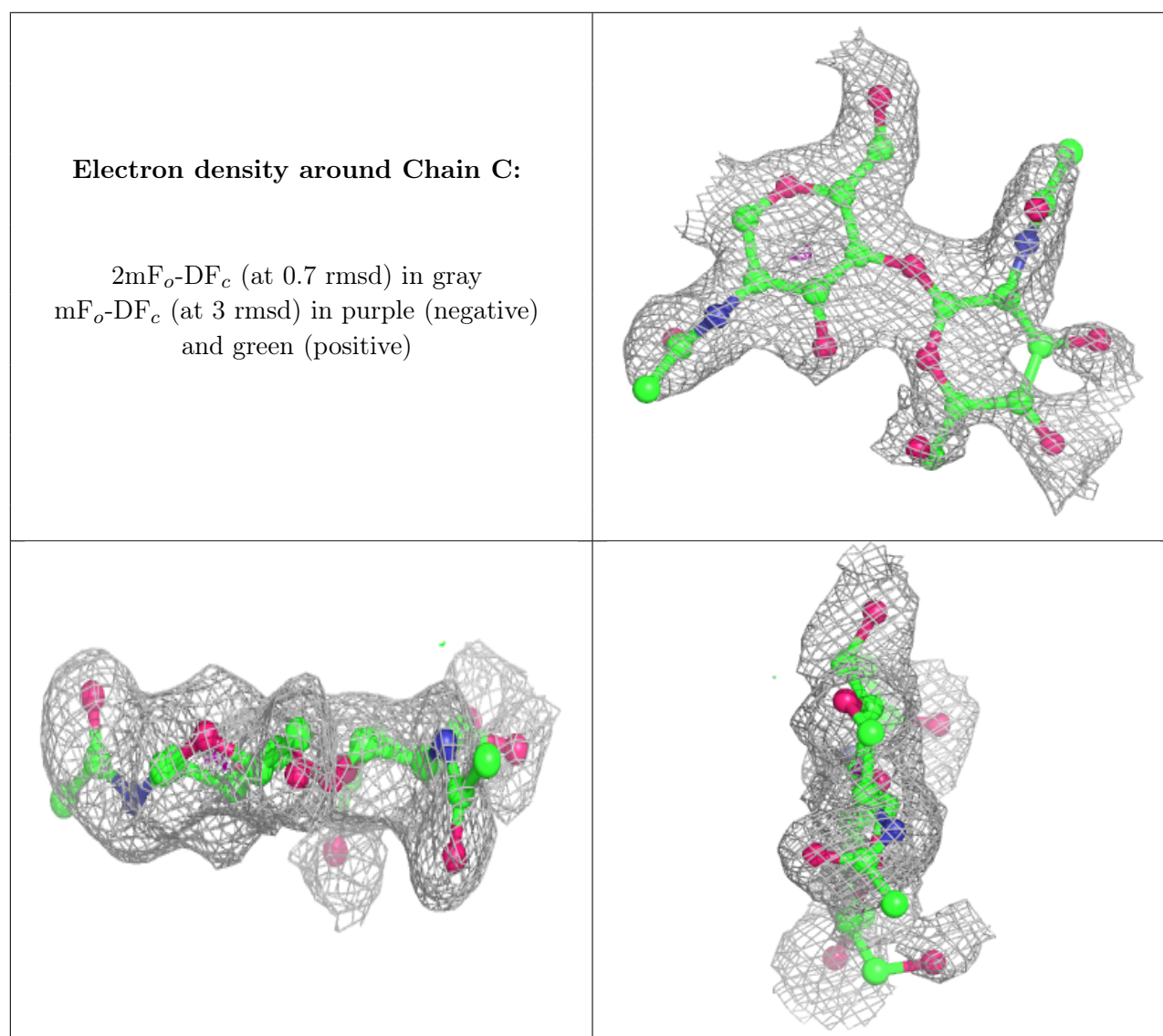
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	FUC	D	2	10/11	0.70	0.17	54,68,80,81	0
4	BMA	F	3	11/12	0.73	0.14	53,64,68,72	0
5	BMA	G	3	11/12	0.74	0.12	56,69,79,80	0
5	NAG	G	2	14/15	0.79	0.12	44,55,64,68	0
3	FUC	E	2	10/11	0.80	0.16	56,70,81,88	0

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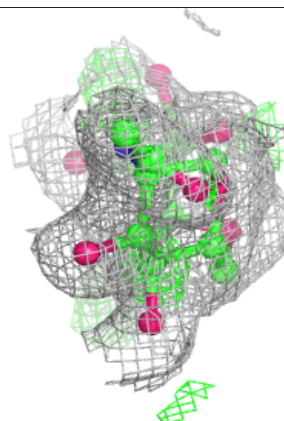
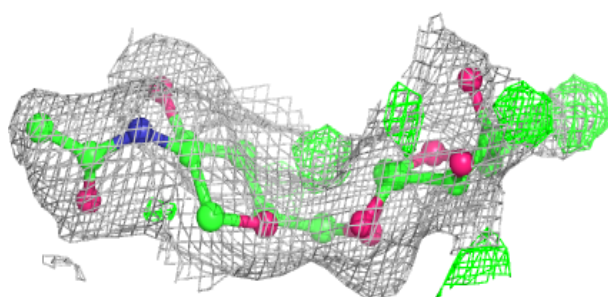
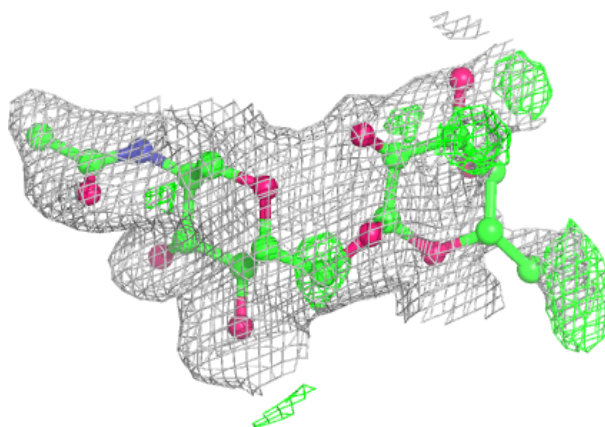
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	NAG	C	2	14/15	0.80	0.14	49,66,80,80	0
5	NAG	G	1	14/15	0.82	0.10	48,54,61,65	0
4	FUC	F	4	10/11	0.84	0.13	36,46,51,59	0
2	NAG	C	1	14/15	0.87	0.11	38,43,52,58	0
3	NAG	E	1	14/15	0.88	0.11	30,40,52,63	0
4	NAG	F	2	14/15	0.92	0.09	36,44,51,57	0
4	NAG	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.

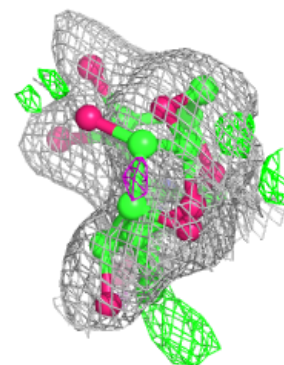
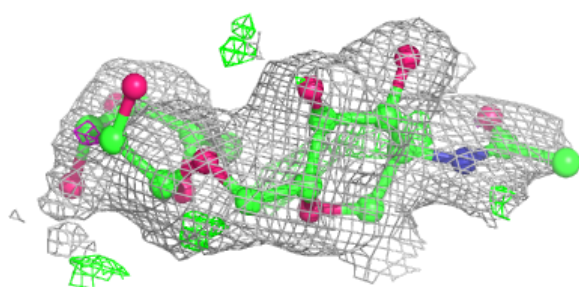
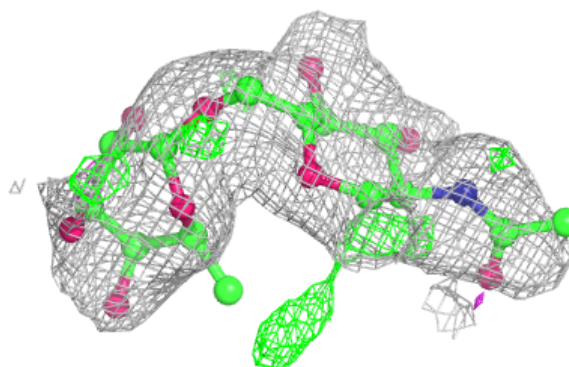


Electron density around Chain D:

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

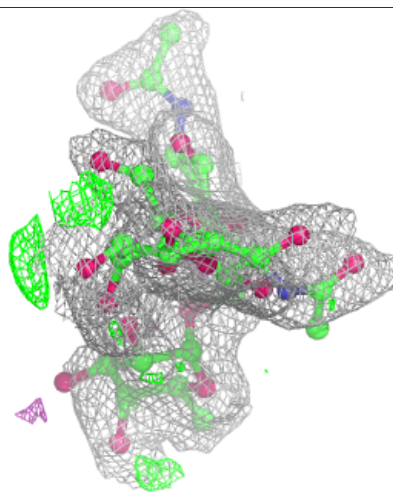
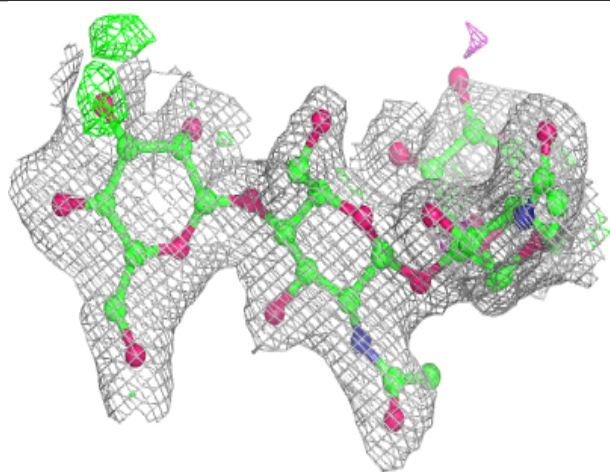
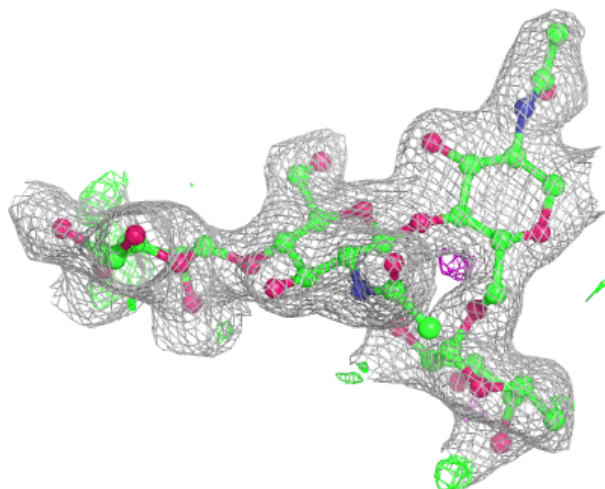
**Electron density around Chain E:**

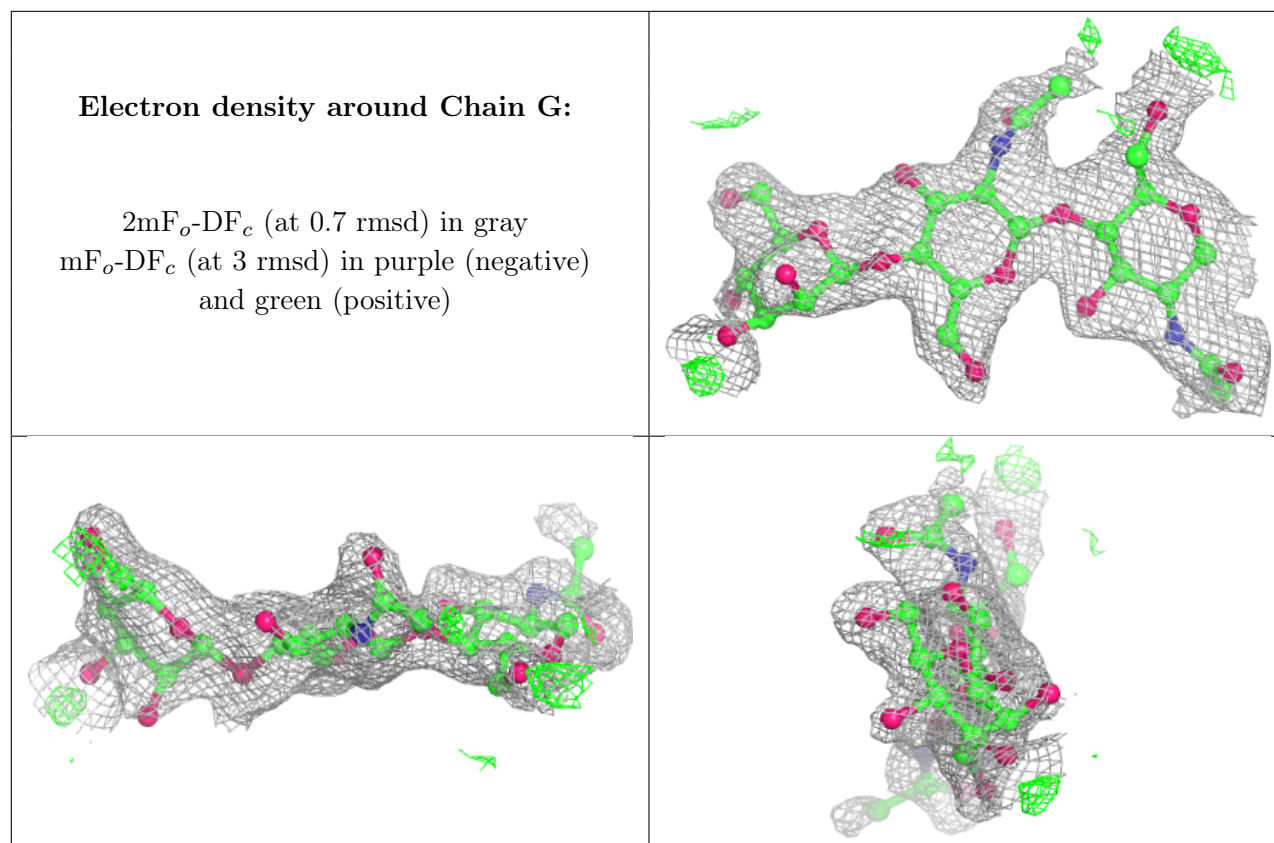
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



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, 95th 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 ²)	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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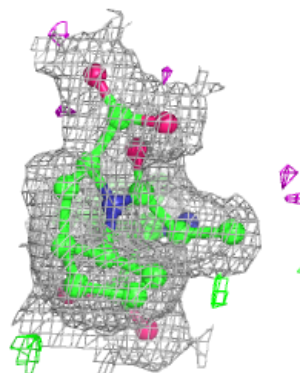
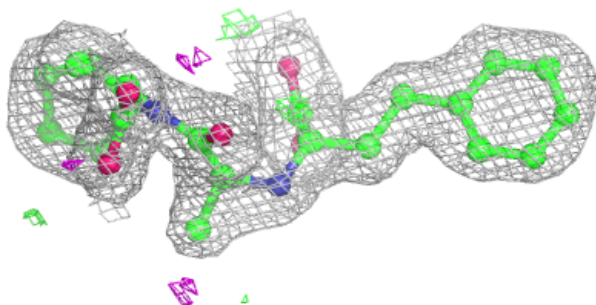
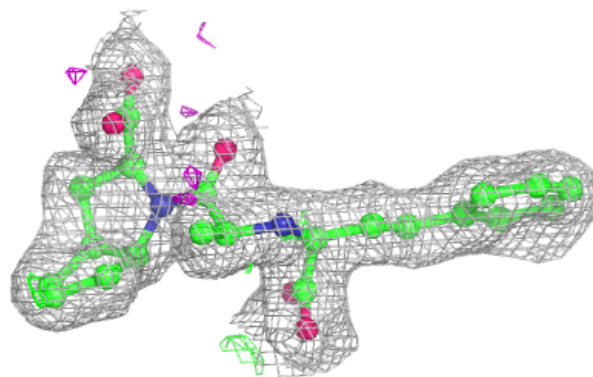
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
11	1PE	A	708	16/16	0.95	0.08	20,26,43,44	0
9	EDO	A	705	4/4	0.95	0.17	25,26,28,29	0
13	MG	B	711	1/1	0.96	0.08	29,29,29,29	0
14	CA	A	713	1/1	0.97	0.06	21,21,21,21	1
7	X92	A	702	28/28	0.97	0.05	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.

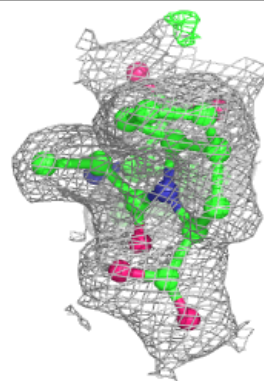
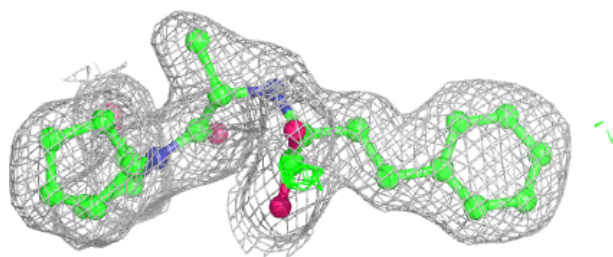
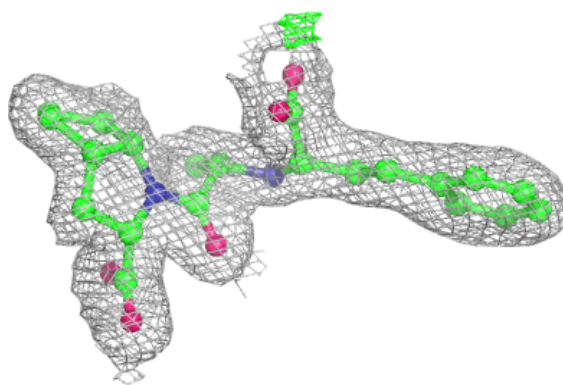
Electron density around X92 A 702:

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



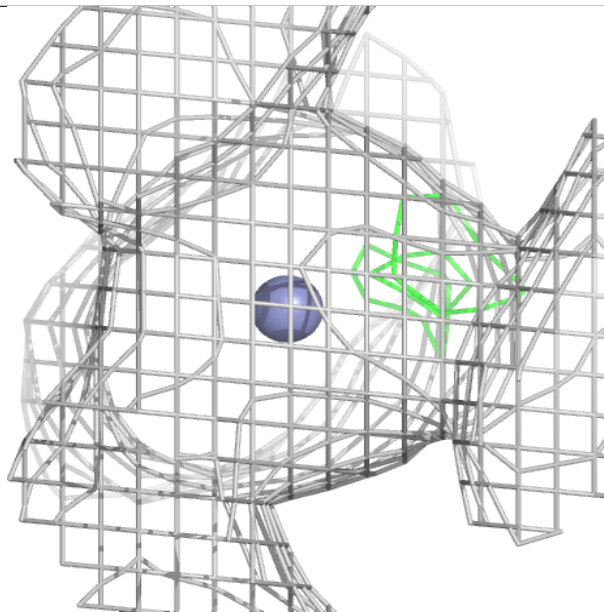
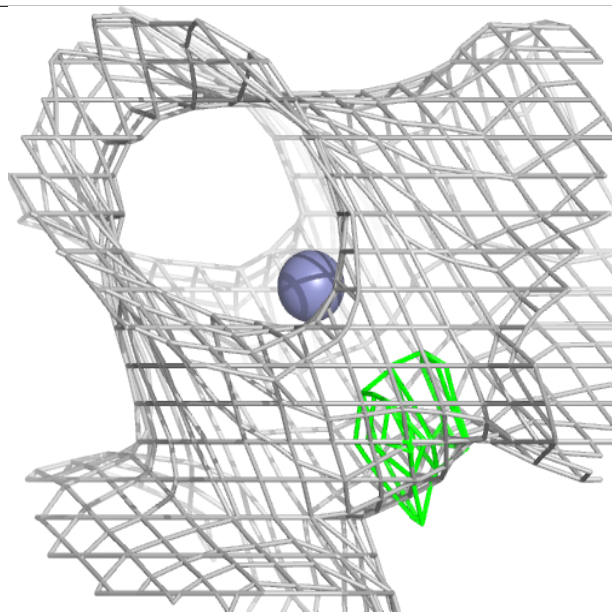
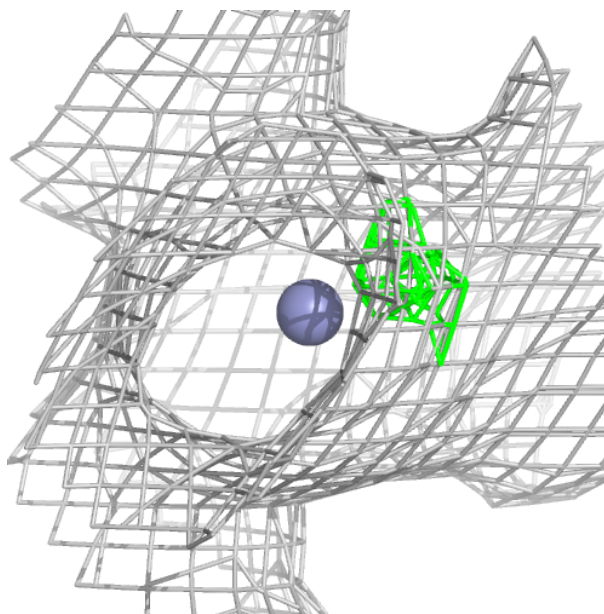
Electron density around X92 B 703:

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



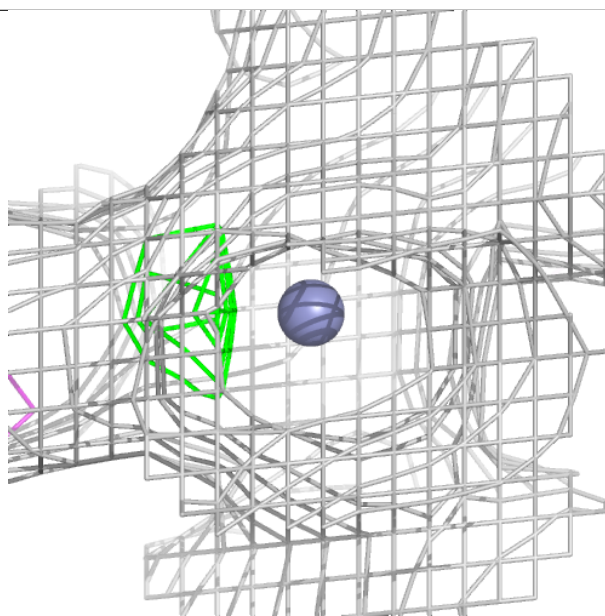
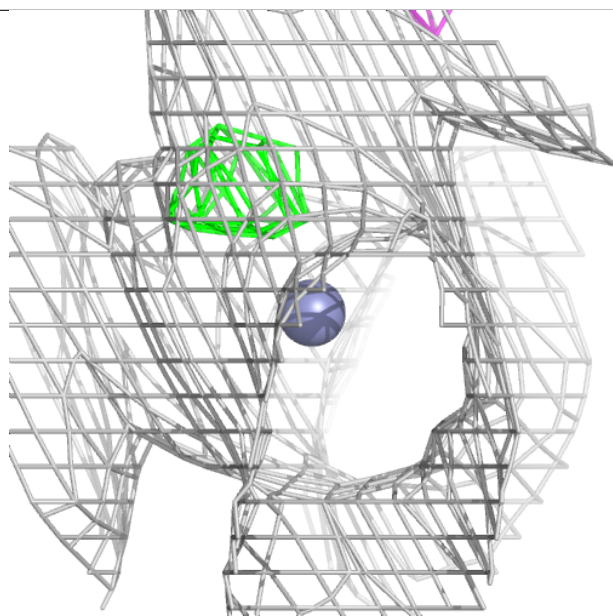
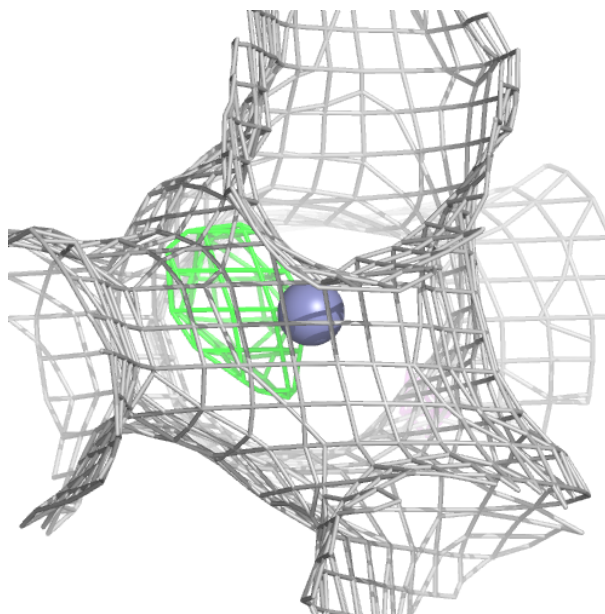
Electron density around ZN B 702:

$2mF_o-DF_c$ (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.