



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 20, 2026 – 06:17 AM UTC

PDB ID : 8QFX / pdb_00008qfx
Title : Human Angiotensin-1 converting enzyme N-domain in complex with the lactotripeptide IPP
Authors : Gregory, K.S.; Acharya, K.R.; Cozier, G.E.
Deposited on : 2023-09-05
Resolution : 1.60 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 Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

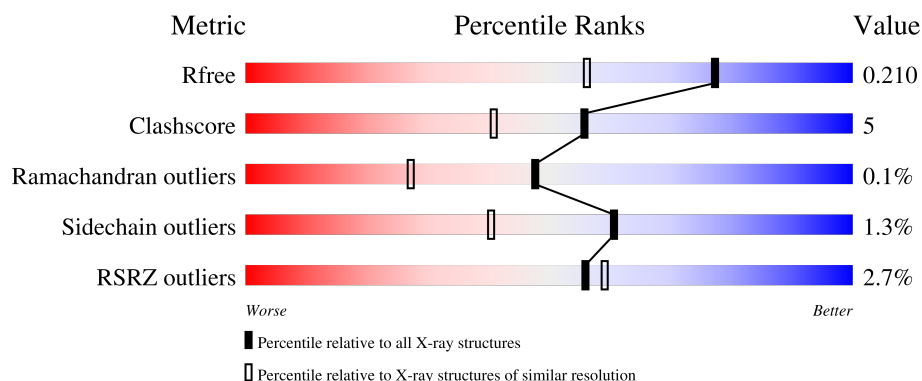
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.60 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.



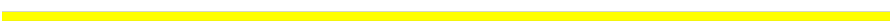
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	4673 (1.60-1.60)
Clashscore	190562	4931 (1.60-1.60)
Ramachandran outliers	187476	4831 (1.60-1.60)
Sidechain outliers	187428	4830 (1.60-1.60)
RSRZ outliers	180081	4672 (1.60-1.60)

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	628	5% 87% 9% ..
1	B	628	% 92% 5% .
1	C	628	2% 87% 9% .
1	D	628	2% 88% 7% ..
2	E	3	100%

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Mol	Chain	Length	Quality of chain
2	F	3	 100%
2	G	3	 67% 33%
2	H	3	 100%
3	I	2	 100%
3	J	2	 50% 50%
3	L	2	 100%
3	N	2	 100%
4	K	3	 33% 33% 33%
5	P	2	 50% 50%
5	R	2	 100%

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
16	ACT	D	712	-	-	X	-
18	PG4	C	706	-	-	X	-

2 Entry composition

There are 20 unique types of molecules in this entry. The entry contains 23659 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	609	Total	C	N	O	S	0	20	0
			5129	3284	882	944	19			
1	B	613	Total	C	N	O	S	0	18	0
			5138	3292	880	946	20			
1	C	606	Total	C	N	O	S	0	15	0
			5075	3250	875	931	19			
1	D	605	Total	C	N	O	S	0	18	0
			5069	3250	867	931	21			

There are 32 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	131	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	131	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
C	9	GLN	ASN	engineered mutation	UNP P12821
C	25	GLN	ASN	engineered mutation	UNP P12821
C	82	GLN	ASN	engineered mutation	UNP P12821
C	117	GLN	ASN	engineered mutation	UNP P12821
C	131	GLN	ASN	engineered mutation	UNP P12821

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Chain	Residue	Modelled	Actual	Comment	Reference
C	289	GLN	ASN	engineered mutation	UNP P12821
C	545	ARG	GLN	engineered mutation	UNP P12821
C	576	LEU	PRO	engineered mutation	UNP P12821
D	9	GLN	ASN	engineered mutation	UNP P12821
D	25	GLN	ASN	engineered mutation	UNP P12821
D	82	GLN	ASN	engineered mutation	UNP P12821
D	117	GLN	ASN	engineered mutation	UNP P12821
D	131	GLN	ASN	engineered mutation	UNP P12821
D	289	GLN	ASN	engineered mutation	UNP P12821
D	545	ARG	GLN	engineered mutation	UNP P12821
D	576	LEU	PRO	engineered mutation	UNP P12821

- Molecule 2 is a protein called ILE-PRO-PRO.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	E	3	Total	C	N	O	0	0	0
			23	16	3	4			
2	F	3	Total	C	N	O	0	0	0
			23	16	3	4			
2	G	3	Total	C	N	O	0	0	0
			23	16	3	4			
2	H	3	Total	C	N	O	0	0	0
			23	16	3	4			

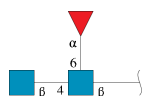
- Molecule 3 is an oligosaccharide called alpha-L-fucopyranose-(1-6)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	I	2	Total	C	N	O	0	0	0
			24	14	1	9			
3	J	2	Total	C	N	O	0	0	0
			24	14	1	9			
3	L	2	Total	C	N	O	0	0	0
			24	14	1	9			
3	N	2	Total	C	N	O	0	0	0
			24	14	1	9			

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

pha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose.



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

- Molecule 5 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
5	P	2	Total	C	N	O	0	0	0
			28	16	2	10			
5	R	2	Total	C	N	O	0	0	0
			28	16	2	10			

- 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		
6	C	1	Total	Zn	0	0
			1	1		
6	D	1	Total	Zn	0	0
			1	1		

- Molecule 7 is CHLORIDE ION (CCD ID: CL) (formula: Cl) (labeled as "Ligand of Interest" by depositor).

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

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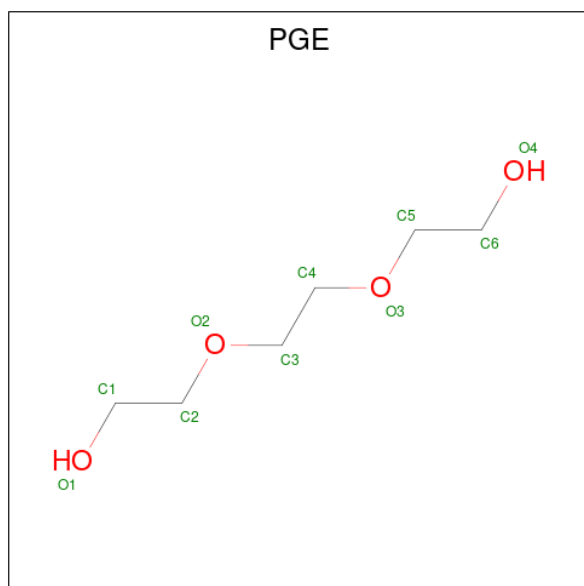
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	C	1	Total	Cl	0	0
			1	1		
7	D	1	Total	Cl	0	0
			1	1		

- Molecule 8 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	1	Total	Mg	0	0
			1	1		
8	B	1	Total	Mg	0	0
			1	1		
8	C	1	Total	Mg	0	0
			1	1		
8	D	1	Total	Mg	0	0
			1	1		

- Molecule 9 is TRIETHYLENE GLYCOL (CCD ID: PGE) (formula: C₆H₁₄O₄).



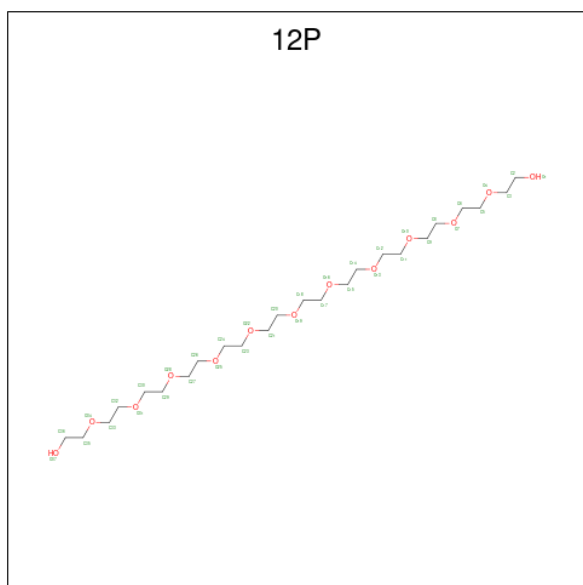
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	A	1	Total	C	O	0	0
			10	6	4		
9	A	1	Total	C	O	0	0
			10	6	4		
9	B	1	Total	C	O	0	0
			10	6	4		

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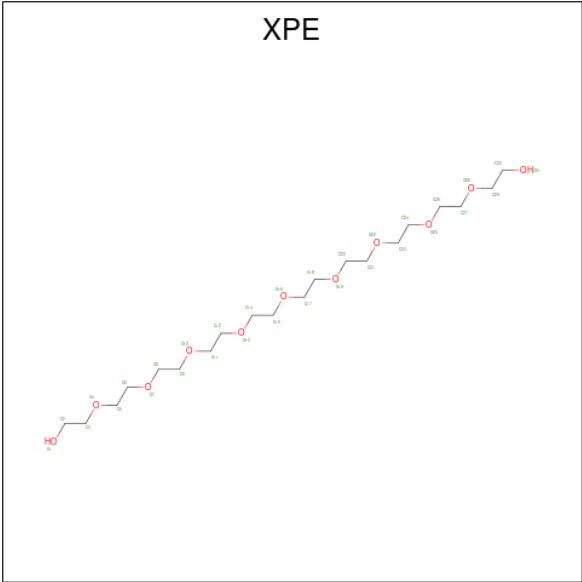
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	C	1	Total	C	O	0	0
			10	6	4		
9	D	1	Total	C	O	0	0
			10	6	4		

- Molecule 10 is DODECAETHYLENE GLYCOL (CCD ID: 12P) (formula: $C_{24}H_{50}O_{13}$).



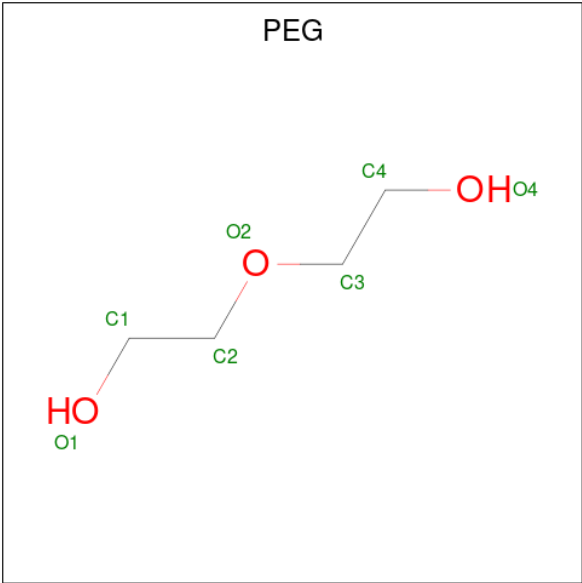
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	A	1	Total	C	O	0	0
			37	24	13		

- Molecule 11 is 3,6,9,12,15,18,21,24,27-NONAOXANONACOSANE-1,29-DIOL (CCD ID: XPE) (formula: $C_{20}H_{42}O_{11}$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
11	A	1	Total	C	O	0	0
			31	20	11		
11	D	1	Total	C	O	0	1
			62	40	22		

- Molecule 12 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: C₄H₁₀O₃).



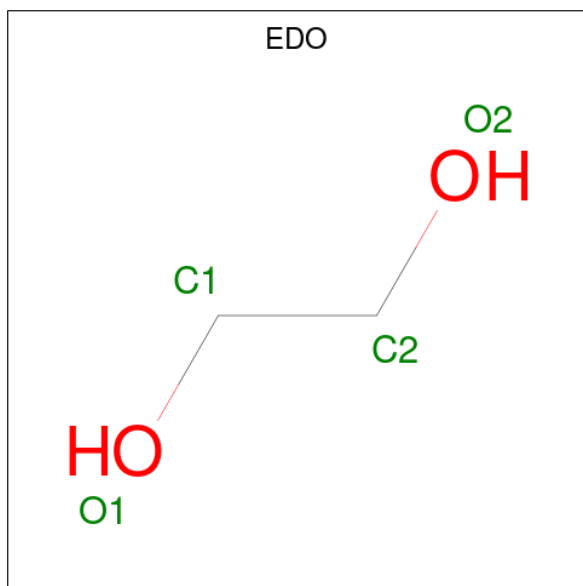
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
12	A	1	Total	C	O	0	0
			7	4	3		
12	A	1	Total	C	O	0	0
			7	4	3		

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

- Molecule 13 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



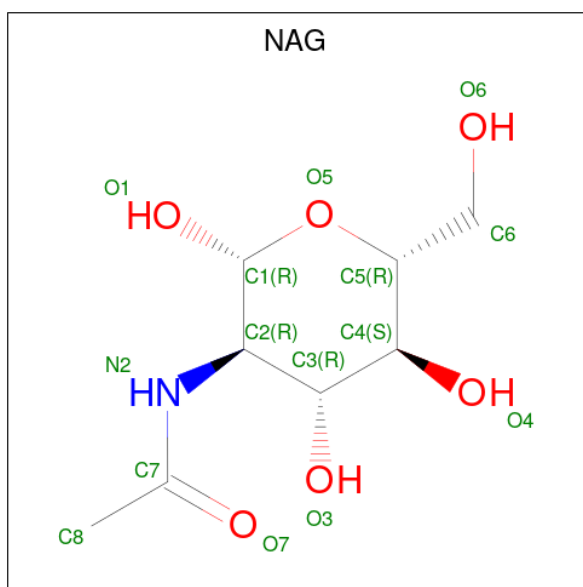
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
13	A	1	Total	C	O	0	0
			4	2	2		
13	A	1	Total	C	O	0	0
			4	2	2		

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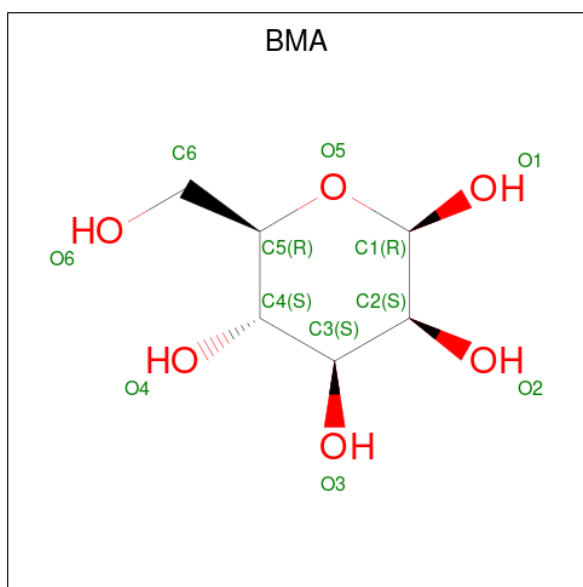
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
13	A	1	Total 4	C 2	O 2	0	0
13	A	1	Total 4	C 2	O 2	0	0
13	A	1	Total 4	C 2	O 2	0	0
13	B	1	Total 4	C 2	O 2	0	0
13	B	1	Total 4	C 2	O 2	0	0
13	B	1	Total 4	C 2	O 2	0	0
13	B	1	Total 4	C 2	O 2	0	0
13	C	1	Total 4	C 2	O 2	0	0
13	C	1	Total 4	C 2	O 2	0	0
13	C	1	Total 4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

- Molecule 14 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).



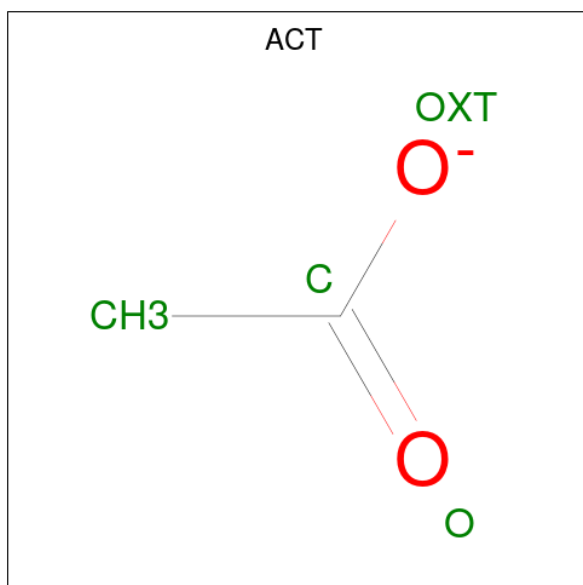
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
14	A	1	Total	C	N	O	0	0
			14	8	1	5		
14	A	1	Total	C	N	O	0	0
			14	8	1	5		
14	A	1	Total	C	N	O	0	0
			14	8	1	5		
14	A	1	Total	C	N	O	0	0
			14	8	1	5		
14	B	1	Total	C	N	O	0	0
			14	8	1	5		
14	B	1	Total	C	N	O	0	0
			14	8	1	5		
14	C	1	Total	C	N	O	0	0
			14	8	1	5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

- Molecule 15 is beta-D-mannopyranose (CCD ID: BMA) (formula: $C_6H_{12}O_6$).



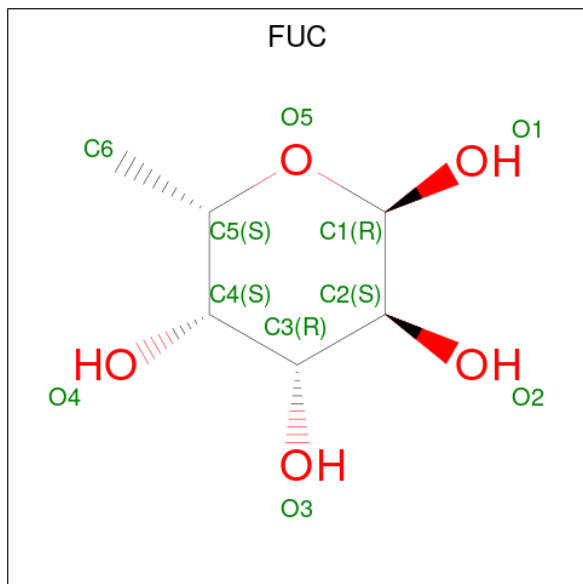
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
15	A	1	Total	C	O	0	0
			11	6	5		
15	B	1	Total	C	O	0	0
			11	6	5		
15	C	1	Total	C	O	0	0
			11	6	5		
15	D	1	Total	C	O	0	0
			11	6	5		

- Molecule 16 is ACETATE ION (CCD ID: ACT) (formula: $C_2H_3O_2$).



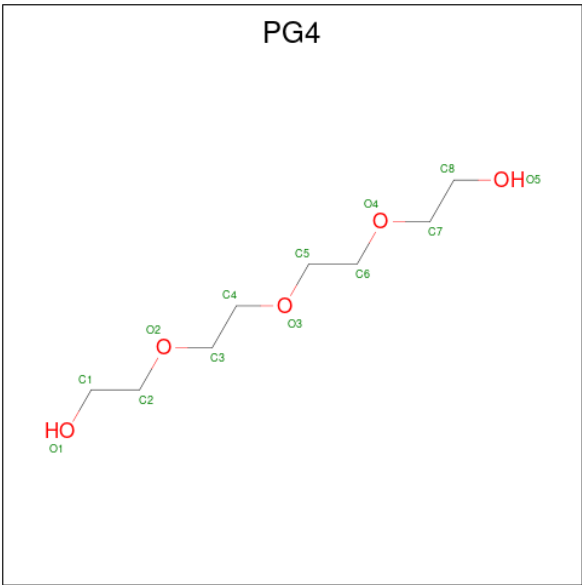
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
16	B	1	Total	C	O	0	0
			4	2	2		
16	C	1	Total	C	O	0	0
			4	2	2		
16	D	1	Total	C	O	0	0
			4	2	2		

- Molecule 17 is alpha-L-fucopyranose (CCD ID: FUC) (formula: $C_6H_{12}O_5$).



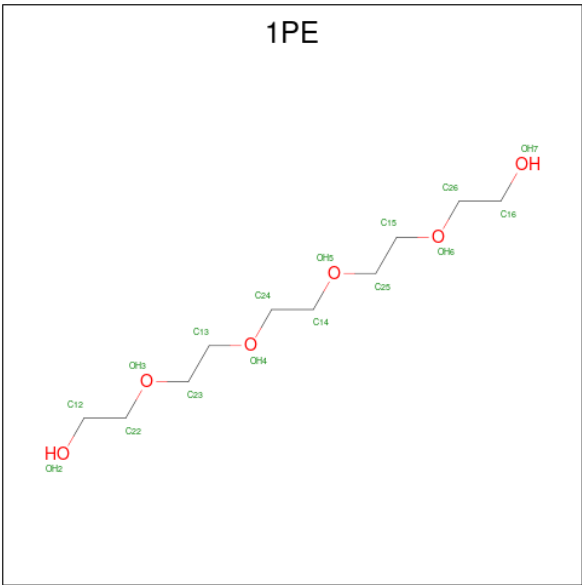
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
17	B	1	Total	C	O	0	0
			10	6	4		
17	D	1	Total	C	O	0	0
			10	6	4		

- Molecule 18 is TETRAETHYLENE GLYCOL (CCD ID: PG4) (formula: $C_8H_{18}O_5$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
18	C	1	Total	C	O	0	0
			13	8	5		
18	D	1	Total	C	O	0	0
			13	8	5		

- Molecule 19 is PENTAETHYLENE GLYCOL (CCD ID: 1PE) (formula: C₁₀H₂₂O₆).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
19	C	1	Total	C	O	0	0
			16	10	6		

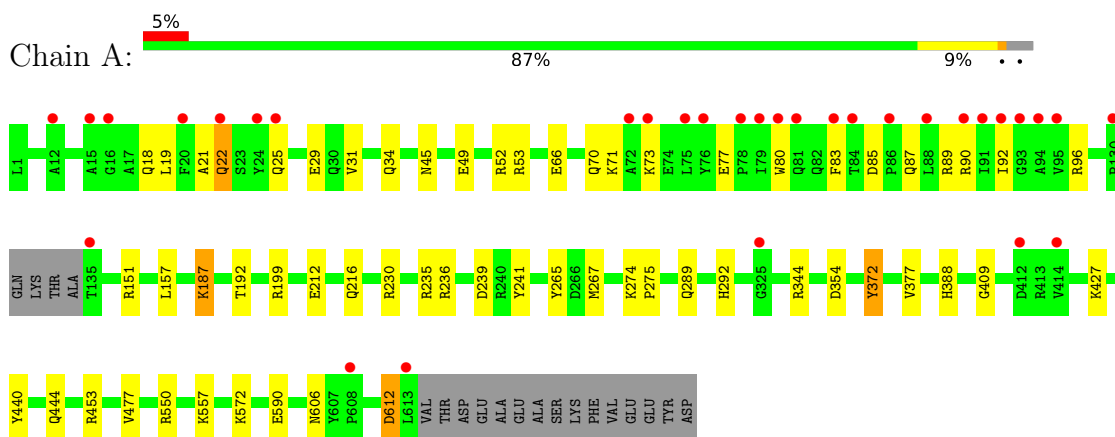
- Molecule 20 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
20	A	576	Total 576	O 576	0	0
20	B	622	Total 622	O 622	0	0
20	C	572	Total 572	O 572	0	0
20	D	547	Total 547	O 547	0	0
20	E	2	Total 2	O 2	0	0
20	F	2	Total 2	O 2	0	0
20	G	2	Total 2	O 2	0	0
20	H	2	Total 2	O 2	0	0

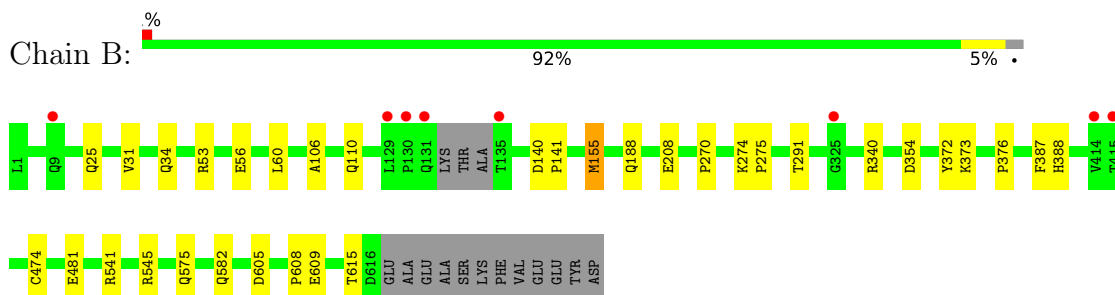
3 Residue-property plots [i](#)

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

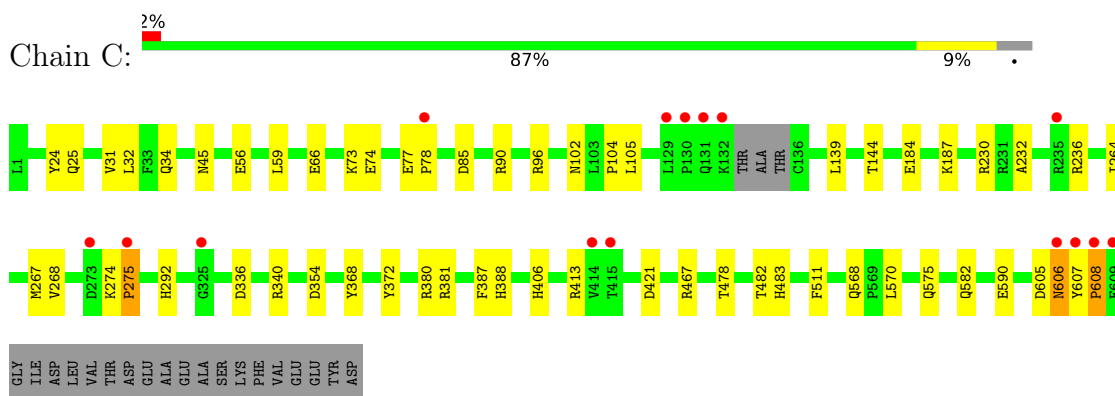
- Molecule 1: Angiotensin-converting enzyme, soluble form



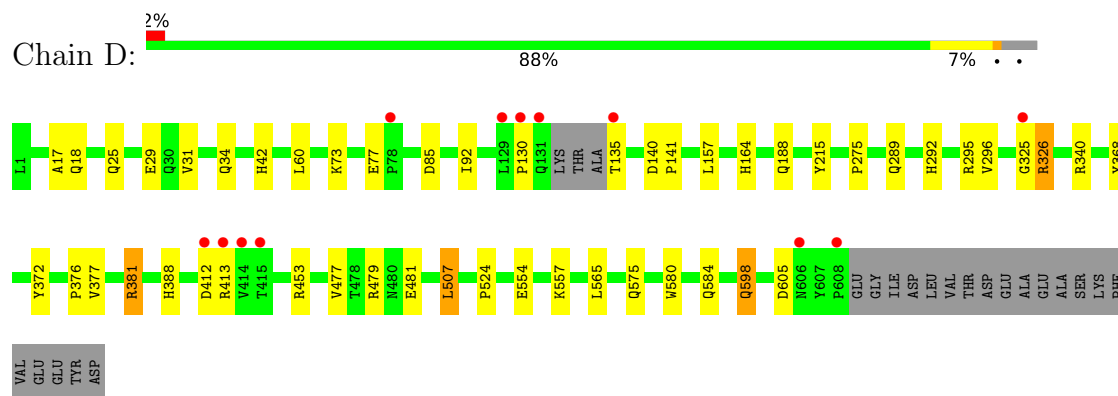
- Molecule 1: Angiotensin-converting enzyme, soluble form



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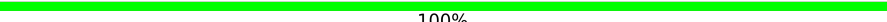


- Molecule 2: ILE-PRO-PRO

Chain E:  100%

There are no outlier residues recorded for this chain.

- Molecule 2: ILE-PRO-PRO

Chain F:  100%

There are no outlier residues recorded for this chain.

- Molecule 2: ILE-PRO-PRO

Chain G:  67% 33%

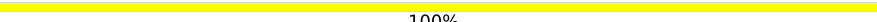


- Molecule 2: ILE-PRO-PRO

Chain H:  100%

There are no outlier residues recorded for this chain.

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

Chain I:  100%



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

Chain J:  50% 50%



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

Chain L:  100%

NAG1
FUC2

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

Chain N:  100%

NAG1
FUC2

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

Chain K:  33% 33% 33%

NAG1
NAG2
FUC3

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

Chain P:  50% 50%

NAG1
NAG2

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

Chain R:  100%

NAG1
NAG2

4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	74.23Å 103.39Å 115.42Å 84.95° 85.49° 81.55°	Depositor
Resolution (Å)	79.45 – 1.60 79.45 – 1.60	Depositor EDS
% Data completeness (in resolution range)	97.1 (79.45-1.60) 95.2 (79.45-1.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.37 (at 1.60Å)	Xtriage
Refinement program	REFMAC 5.8.0419	Depositor
R, R_{free}	0.181 , 0.211 0.179 , 0.210	Depositor DCC
R_{free} test set	21617 reflections (4.00%)	wwPDB-VP
Wilson B-factor (Å ²)	16.4	Xtriage
Anisotropy	0.253	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 41.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	23659	wwPDB-VP
Average B, all atoms (Å ²)	24.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 35.30 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 5.9563e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: CL, PG4, FUC, PGE, NAG, EDO, XPE, MG, ACT, 1PE, BMA, ZN, 12P, PEG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	0.97	0/5288	1.17	19/7199 (0.3%)
1	B	1.00	0/5297	1.17	7/7212 (0.1%)
1	C	0.97	1/5231 (0.0%)	1.14	15/7120 (0.2%)
1	D	0.90	2/5234 (0.0%)	1.13	8/7126 (0.1%)
2	E	1.49	0/24	1.30	0/32
2	F	1.21	0/24	1.16	0/32
2	G	1.25	0/24	1.09	0/32
2	H	1.42	0/24	1.05	0/32
All	All	0.97	3/21146 (0.0%)	1.15	49/28785 (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	1
1	B	0	1
1	C	0	6
1	D	0	2
All	All	0	10

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	164	HIS	CE1-NE2	6.68	1.39	1.32
1	C	483	HIS	CE1-NE2	5.39	1.38	1.32
1	D	42	HIS	CG-CD2	5.22	1.41	1.35

The worst 5 of 49 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	188	GLN	CB-CG-CD	-10.50	94.75	112.60
1	A	85	ASP	CB-CA-C	8.76	120.15	110.08
1	A	354	ASP	CA-CB-CG	8.06	120.66	112.60
1	C	354	ASP	CA-CB-CG	7.80	120.40	112.60
1	B	582	GLN	CB-CA-C	-7.37	98.56	110.79

There are no chirality outliers.

5 of 10 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	550	ARG	Sidechain
1	B	53	ARG	Sidechain
1	C	230	ARG	Sidechain
1	C	236	ARG	Sidechain
1	C	340	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	5129	0	4887	39	0
1	B	5138	0	4902	23	0
1	C	5075	0	4834	40	0
1	D	5069	0	4835	30	0
2	E	23	0	27	0	0
2	F	23	0	27	0	0
2	G	23	0	27	1	0
2	H	23	0	27	0	0
3	I	24	0	21	0	0
3	J	24	0	21	0	0
3	L	24	0	22	3	0
3	N	24	0	22	3	0
4	K	38	0	34	4	0
5	P	28	0	25	3	0
5	R	28	0	25	0	0
6	A	1	0	0	0	0
6	B	1	0	0	0	0
6	C	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	D	1	0	0	0	0
7	A	1	0	0	0	0
7	B	1	0	0	0	0
7	C	1	0	0	0	0
7	D	1	0	0	0	0
8	A	1	0	0	0	0
8	B	1	0	0	0	0
8	C	1	0	0	0	0
8	D	1	0	0	0	0
9	A	20	0	28	3	0
9	B	10	0	14	0	0
9	C	10	0	14	2	0
9	D	10	0	14	1	0
10	A	37	0	50	9	0
11	A	31	0	42	4	0
11	D	62	0	84	12	0
12	A	28	0	40	2	0
12	B	28	0	40	3	0
12	C	7	0	10	2	0
12	D	14	0	20	0	0
13	A	20	0	30	1	0
13	B	16	0	24	3	0
13	C	20	0	30	8	0
13	D	16	0	24	3	0
14	A	56	0	51	7	0
14	B	28	0	26	8	0
14	C	42	0	39	6	0
14	D	56	0	52	9	0
15	A	11	0	10	2	0
15	B	11	0	10	4	0
15	C	11	0	10	4	0
15	D	11	0	10	2	0
16	B	4	0	3	1	0
16	C	4	0	3	1	0
16	D	4	0	3	2	0
17	B	10	0	10	4	0
17	D	10	0	10	3	0
18	C	13	0	18	12	0
18	D	13	0	18	1	0
19	C	16	0	22	2	0
20	A	576	0	0	4	0
20	B	622	0	0	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
20	C	572	0	0	12	0
20	D	547	0	0	15	0
20	E	2	0	0	0	0
20	F	2	0	0	0	0
20	G	2	0	0	0	0
20	H	2	0	0	0	0
All	All	23659	0	20495	198	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 198 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)
14:A:717:NAG:O4	15:A:718:BMA:C1	1.68	1.42
14:C:716:NAG:O4	14:C:717:NAG:C1	1.69	1.39
15:C:714:BMA:C1	4:K:2:NAG:O4	1.75	1.32
14:B:714:NAG:O4	15:B:715:BMA:C1	1.77	1.32
14:A:720:NAG:O4	14:A:721:NAG:C1	1.88	1.19

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	625/628 (100%)	616 (99%)	9 (1%)	0	100	100
1	B	627/628 (100%)	617 (98%)	10 (2%)	0	100	100
1	C	617/628 (98%)	608 (98%)	9 (2%)	0	100	100
1	D	619/628 (99%)	610 (98%)	7 (1%)	2 (0%)	36	20
2	E	1/3 (33%)	1 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	F	1/3 (33%)	1 (100%)	0	0	100	100
2	G	1/3 (33%)	1 (100%)	0	0	100	100
2	H	1/3 (33%)	1 (100%)	0	0	100	100
All	All	2492/2524 (99%)	2455 (98%)	35 (1%)	2 (0%)	48	27

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	326	ARG
1	D	130	PRO

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	544/540 (101%)	536 (98%)	8 (2%)	57	35
1	B	546/540 (101%)	538 (98%)	8 (2%)	57	35
1	C	537/540 (99%)	532 (99%)	5 (1%)	70	55
1	D	539/540 (100%)	532 (99%)	7 (1%)	61	40
2	E	3/3 (100%)	3 (100%)	0	100	100
2	F	3/3 (100%)	3 (100%)	0	100	100
2	G	3/3 (100%)	3 (100%)	0	100	100
2	H	3/3 (100%)	3 (100%)	0	100	100
All	All	2178/2172 (100%)	2150 (99%)	28 (1%)	61	40

5 of 28 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	608	PRO
1	D	557	LYS
1	C	372	TYR
1	D	372	TYR

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Mol	Chain	Res	Type
1	C	368	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 29 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	109	GLN
1	D	588	ASN
1	C	588	ASN
1	D	371	GLN
1	C	582	GLN

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 ⓘ

15 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	$\# Z > 2$
3	NAG	I	1	3,1	14,14,15	0.67	0	17,19,21	1.54	3 (17%)
3	FUC	I	2	3	10,10,11	0.50	0	14,14,16	1.57	2 (14%)
3	NAG	J	1	3,1	14,14,15	0.51	0	17,19,21	1.53	3 (17%)
3	FUC	J	2	3	10,10,11	0.60	0	14,14,16	0.79	0
4	NAG	K	1	4,1	14,14,15	0.33	0	17,19,21	1.75	4 (23%)
4	NAG	K	2	4	14,14,15	0.34	0	17,19,21	1.73	3 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	FUC	K	3	4	10,10,11	0.66	0	14,14,16	0.75	0
3	NAG	L	1	3,1	14,14,15	0.76	0	17,19,21	2.29	5 (29%)
3	FUC	L	2	3	10,10,11	0.80	0	14,14,16	1.31	2 (14%)
3	NAG	N	1	3,1	14,14,15	0.71	0	17,19,21	1.90	5 (29%)
3	FUC	N	2	3	10,10,11	0.50	0	14,14,16	1.17	1 (7%)
5	NAG	P	1	5,1	14,14,15	0.34	0	17,19,21	1.66	3 (17%)
5	NAG	P	2	5	14,14,15	0.47	0	17,19,21	1.00	2 (11%)
5	NAG	R	1	5,1	14,14,15	0.57	0	17,19,21	1.51	4 (23%)
5	NAG	R	2	5	14,14,15	0.58	0	17,19,21	1.25	3 (17%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	I	1	3,1	-	0/6/23/26	0/1/1/1
3	FUC	I	2	3	-	-	0/1/1/1
3	NAG	J	1	3,1	-	0/6/23/26	0/1/1/1
3	FUC	J	2	3	-	-	0/1/1/1
4	NAG	K	1	4,1	-	0/6/23/26	0/1/1/1
4	NAG	K	2	4	-	2/6/23/26	0/1/1/1
4	FUC	K	3	4	-	-	0/1/1/1
3	NAG	L	1	3,1	-	2/6/23/26	0/1/1/1
3	FUC	L	2	3	-	-	0/1/1/1
3	NAG	N	1	3,1	-	2/6/23/26	0/1/1/1
3	FUC	N	2	3	-	-	0/1/1/1
5	NAG	P	1	5,1	-	2/6/23/26	0/1/1/1
5	NAG	P	2	5	-	3/6/23/26	0/1/1/1
5	NAG	R	1	5,1	-	0/6/23/26	0/1/1/1
5	NAG	R	2	5	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

The worst 5 of 40 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L	1	NAG	O3-C3-C2	6.11	122.09	109.40
4	K	1	NAG	C2-N2-C7	4.92	129.49	122.90
3	I	2	FUC	O2-C2-C3	4.46	119.39	110.15

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	K	2	NAG	C2-N2-C7	4.45	128.87	122.90
3	I	1	NAG	C1-O5-C5	4.20	117.82	112.19

There are no chirality outliers.

5 of 13 torsion outliers are listed below:

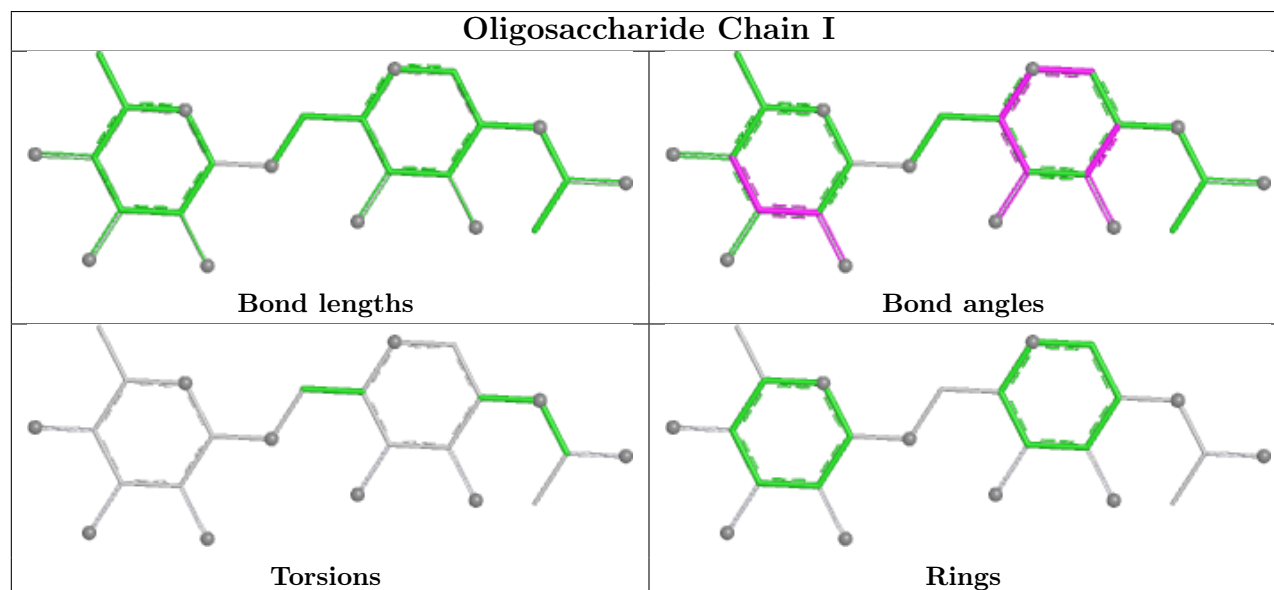
Mol	Chain	Res	Type	Atoms
3	L	1	NAG	C1-C2-N2-C7
5	P	2	NAG	C8-C7-N2-C2
5	P	2	NAG	O7-C7-N2-C2
5	P	1	NAG	O5-C5-C6-O6
5	P	1	NAG	C4-C5-C6-O6

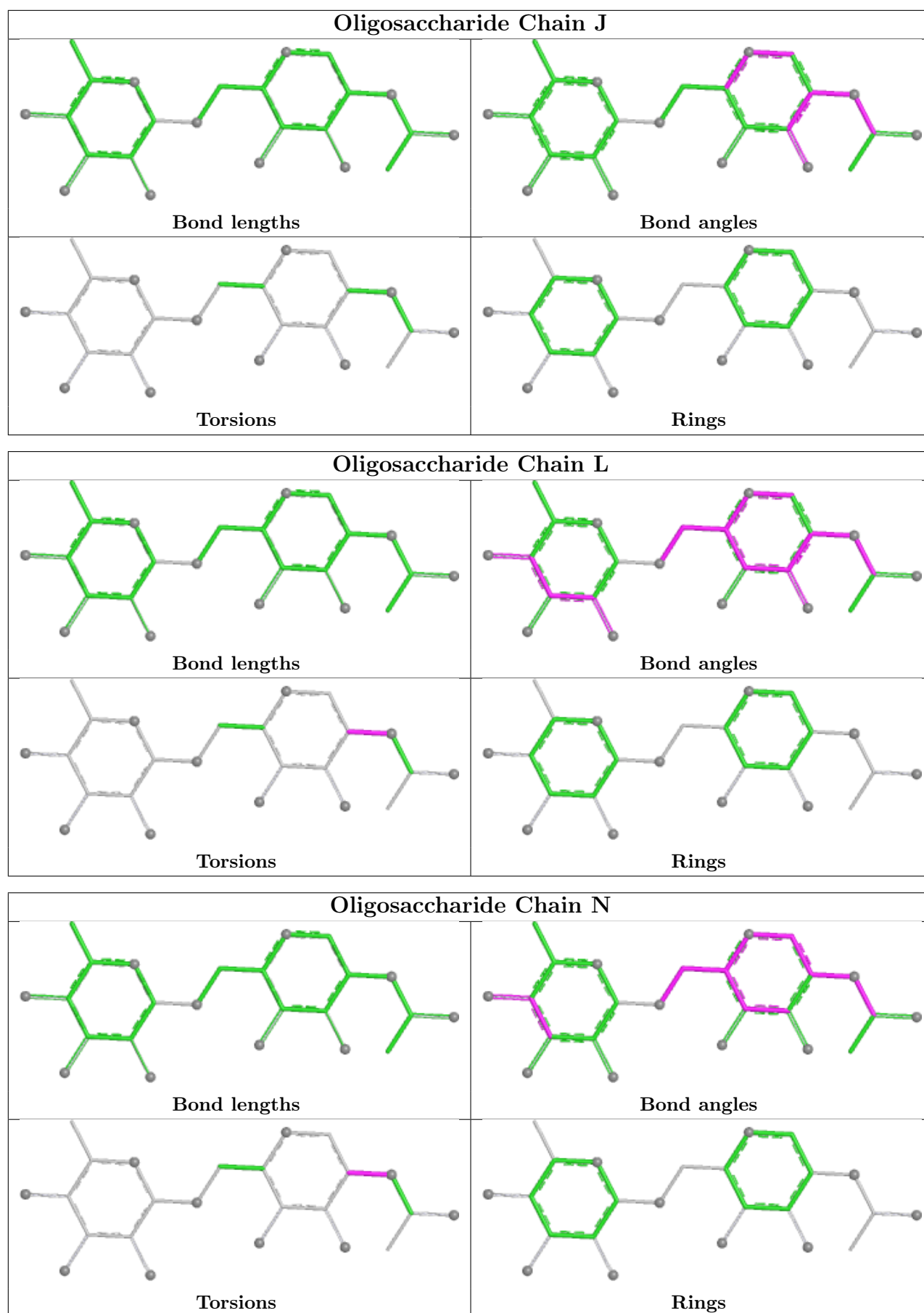
There are no ring outliers.

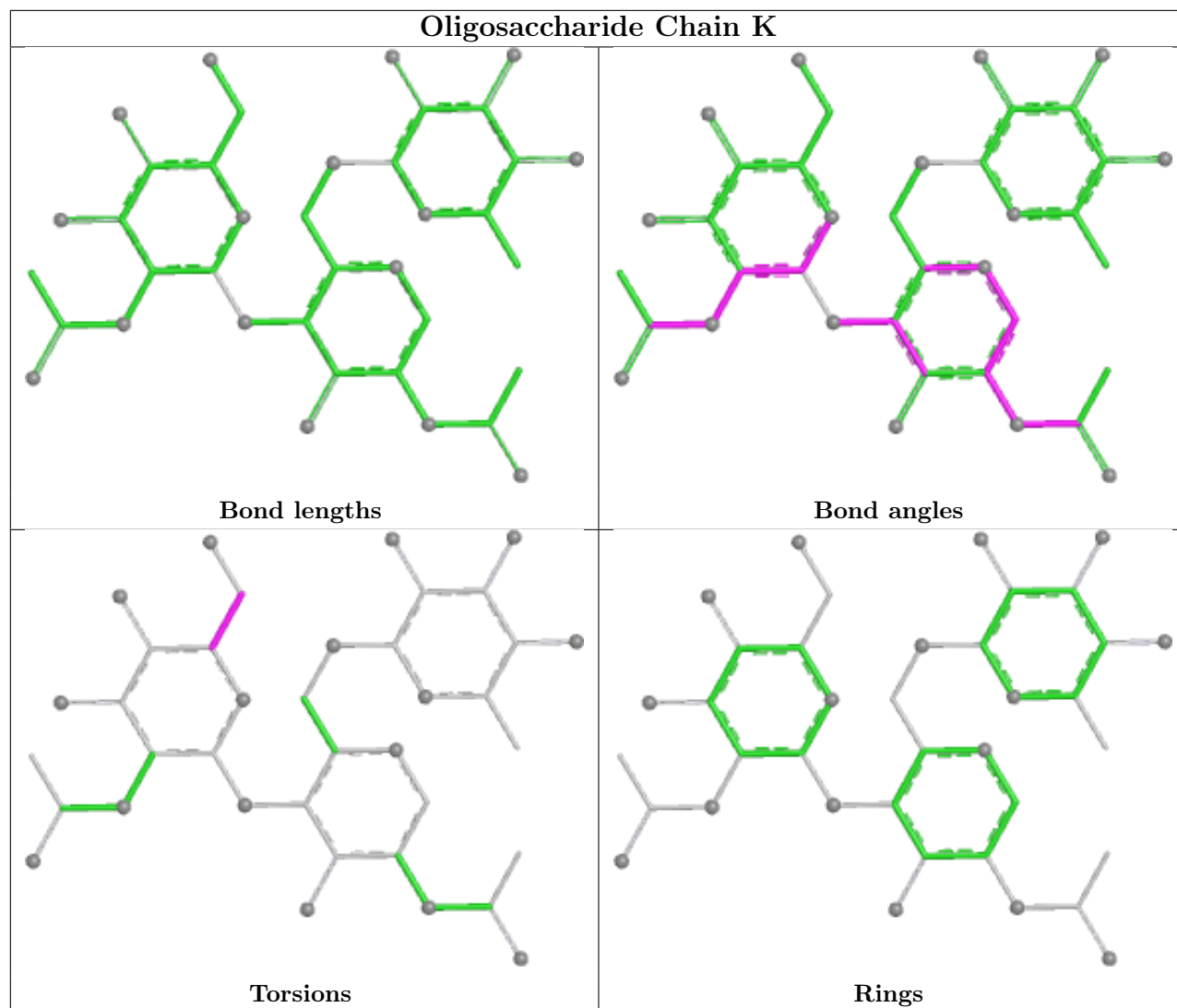
6 monomers are involved in 13 short contacts:

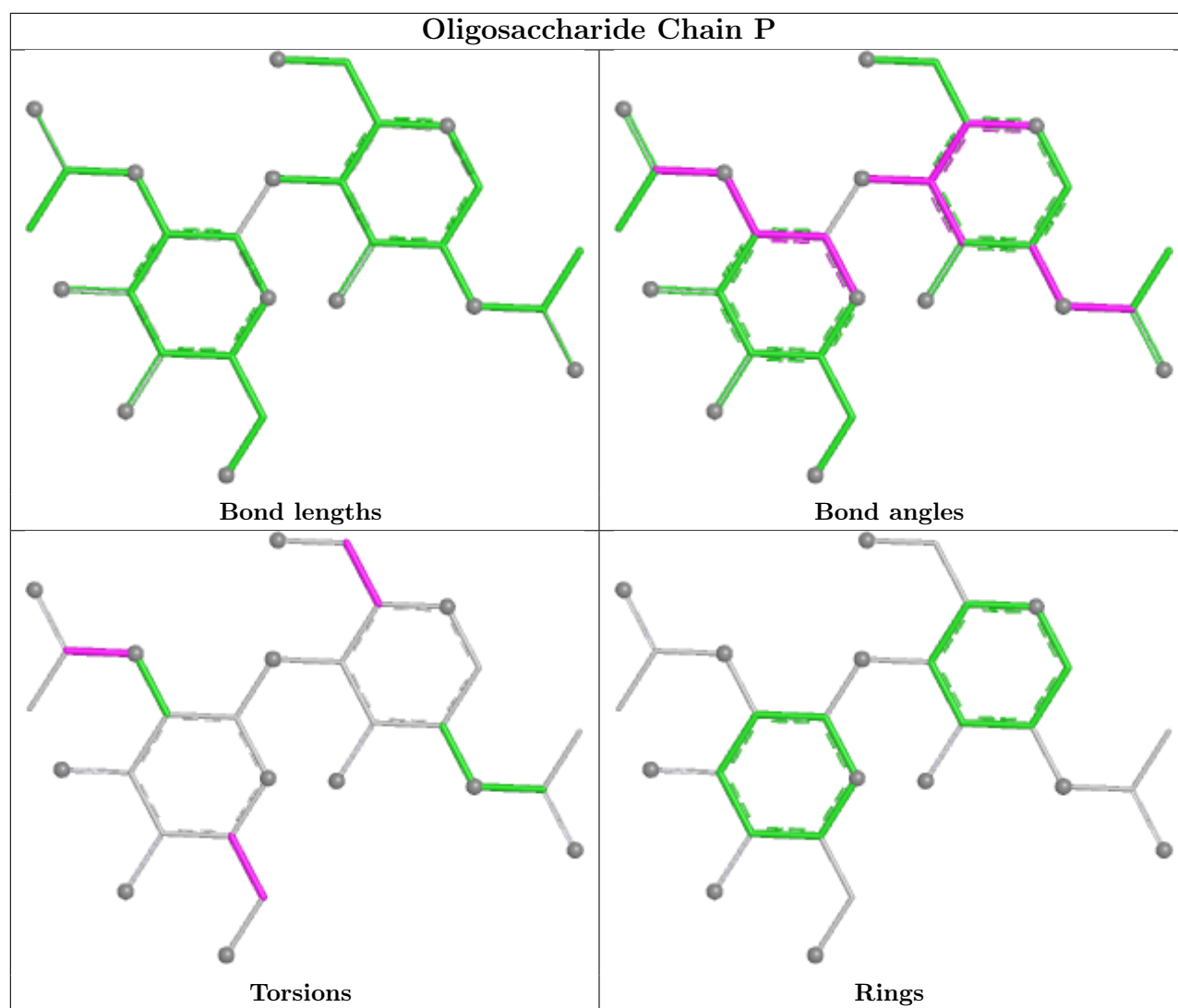
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	N	1	NAG	3	0
3	L	1	NAG	3	0
4	K	2	NAG	4	0
5	P	2	NAG	3	0
3	N	2	FUC	1	0
3	L	2	FUC	1	0

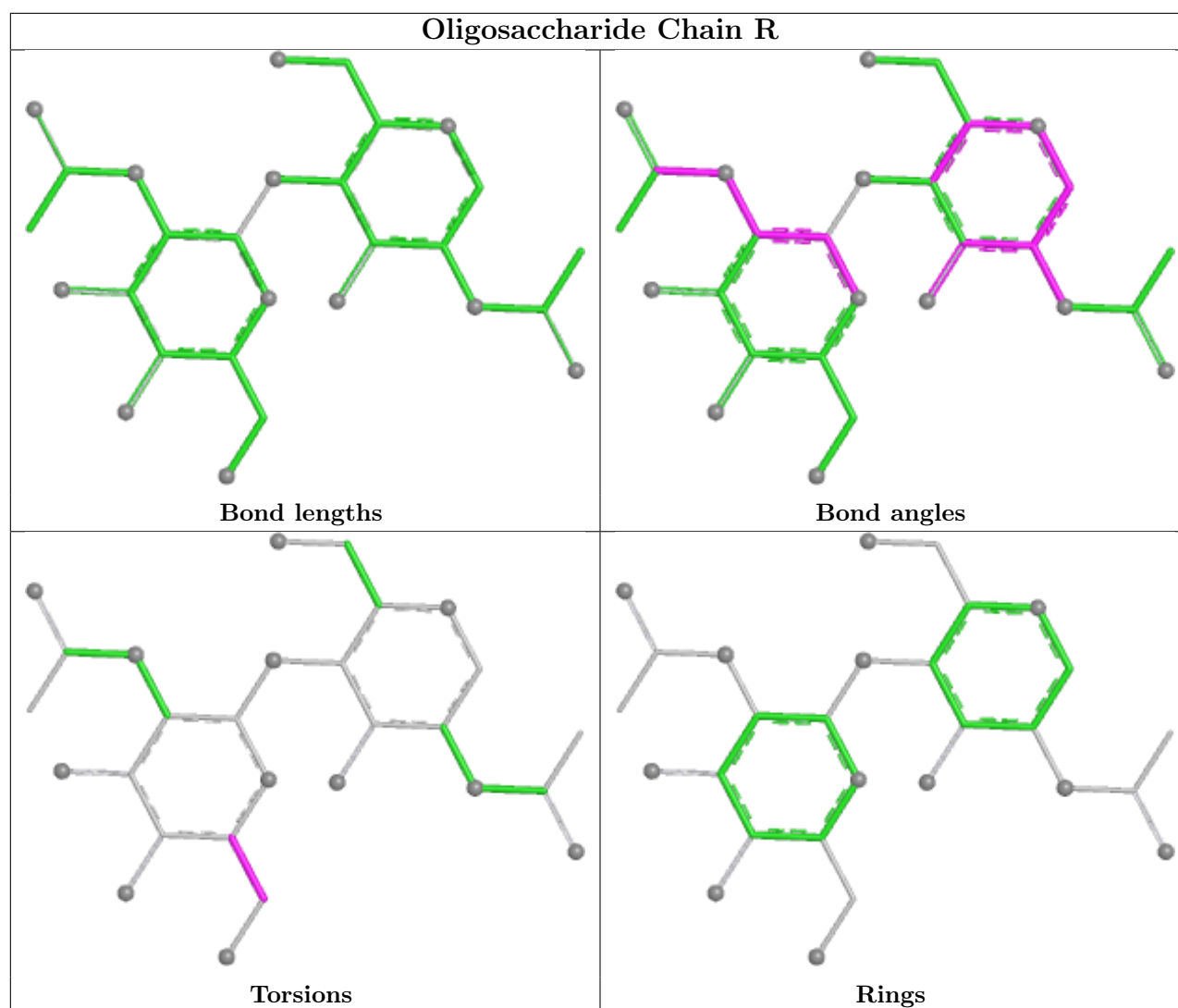
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.











5.6 Ligand geometry [i](#)

Of 75 ligands modelled in this entry, 12 are monoatomic - leaving 63 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	$\# Z > 2$
13	EDO	A	710	-	3,3,3	0.86	0	2,2,2	0.79	0
12	PEG	B	707	-	6,6,6	0.42	0	5,5,5	0.28	0
9	PGE	A	704	-	9,9,9	0.29	0	8,8,8	0.33	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
12	PEG	A	707	-	6,6,6	0.54	0	5,5,5	0.32	0
12	PEG	A	709	-	6,6,6	0.19	0	5,5,5	0.11	0
12	PEG	D	707	-	6,6,6	0.16	0	5,5,5	0.42	0
12	PEG	A	714	-	6,6,6	0.28	0	5,5,5	0.18	0
13	EDO	C	709	-	3,3,3	0.22	0	2,2,2	0.87	0
11	XPE	D	705[A]	-	30,30,30	0.27	0	29,29,29	0.21	0
12	PEG	B	704	-	6,6,6	0.24	0	5,5,5	0.17	0
10	12P	A	705	-	36,36,36	0.41	0	35,35,35	0.40	0
14	NAG	A	719	-	14,14,15	0.51	0	17,19,21	2.70	4 (23%)
14	NAG	D	716	-	14,14,15	0.51	0	17,19,21	2.23	5 (29%)
13	EDO	B	705	-	3,3,3	0.35	0	2,2,2	0.27	0
17	FUC	B	717	-	10,10,11	0.48	0	14,14,16	1.14	2 (14%)
13	EDO	D	710	-	3,3,3	0.25	0	2,2,2	0.39	0
13	EDO	B	712	-	3,3,3	1.44	0	2,2,2	1.87	0
9	PGE	C	708	-	9,9,9	0.45	0	8,8,8	0.40	0
12	PEG	A	712	-	6,6,6	0.36	0	5,5,5	0.40	0
13	EDO	A	715	-	3,3,3	0.34	0	2,2,2	0.54	0
14	NAG	C	716	1	14,14,15	0.58	0	17,19,21	0.92	1 (5%)
15	BMA	D	713	-	11,11,12	0.67	0	15,15,17	0.68	0
17	FUC	D	717	-	10,10,11	0.78	0	14,14,16	1.10	0
13	EDO	D	709	-	3,3,3	0.22	0	2,2,2	0.47	0
14	NAG	D	718	1	14,14,15	0.51	0	17,19,21	1.46	2 (11%)
11	XPE	A	706	-	30,30,30	0.52	0	29,29,29	0.52	0
14	NAG	B	714	-	14,14,15	0.44	0	17,19,21	2.04	3 (17%)
13	EDO	C	710	-	3,3,3	0.24	0	2,2,2	0.36	0
14	NAG	A	717	-	14,14,15	0.43	0	17,19,21	1.63	3 (17%)
13	EDO	A	716	-	3,3,3	0.56	0	2,2,2	1.10	0
11	XPE	D	705[C]	-	30,30,30	0.44	0	29,29,29	0.36	0
16	ACT	C	713	-	3,3,3	1.23	0	3,3,3	1.27	0
13	EDO	A	711	-	3,3,3	0.55	0	2,2,2	1.12	0
14	NAG	B	716	1	14,14,15	0.59	0	17,19,21	1.44	3 (17%)
13	EDO	B	710	-	3,3,3	0.28	0	2,2,2	0.67	0
14	NAG	A	721	-	14,14,15	0.47	0	17,19,21	1.31	1 (5%)
13	EDO	A	713	-	3,3,3	0.36	0	2,2,2	0.45	0
19	1PE	C	707	-	15,15,15	0.39	0	14,14,14	0.19	0
9	PGE	B	709	-	9,9,9	0.42	0	8,8,8	0.26	0
13	EDO	D	711	-	3,3,3	0.37	0	2,2,2	0.85	0
12	PEG	B	706	-	6,6,6	0.48	0	5,5,5	0.36	0
18	PG4	C	706	-	12,12,12	0.58	0	11,11,11	0.51	0
14	NAG	C	715	-	14,14,15	0.47	0	17,19,21	1.30	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
15	BMA	C	714	-	11,11,12	0.74	0	15,15,17	1.10	1 (6%)
14	NAG	A	720	1	14,14,15	0.50	0	17,19,21	1.12	1 (5%)
15	BMA	B	715	-	11,11,12	0.79	0	15,15,17	0.93	0
14	NAG	D	719	-	14,14,15	0.54	0	17,19,21	1.16	1 (5%)
15	BMA	A	718	-	11,11,12	0.54	0	15,15,17	1.08	1 (6%)
9	PGE	D	701	-	9,9,9	0.36	0	8,8,8	0.37	0
9	PGE	A	708	-	9,9,9	0.33	0	8,8,8	0.18	0
13	EDO	C	701	-	3,3,3	0.39	0	2,2,2	1.07	0
12	PEG	C	705	-	6,6,6	0.42	0	5,5,5	0.31	0
13	EDO	C	711	-	3,3,3	0.29	0	2,2,2	0.10	0
13	EDO	D	714	-	3,3,3	0.18	0	2,2,2	0.07	0
14	NAG	C	717	-	14,14,15	0.41	0	17,19,21	1.13	3 (17%)
14	NAG	D	715	1	14,14,15	0.47	0	17,19,21	1.67	3 (17%)
16	ACT	B	713	-	3,3,3	1.72	2 (66%)	3,3,3	0.54	0
16	ACT	D	712	-	3,3,3	1.25	0	3,3,3	0.91	0
13	EDO	B	711	-	3,3,3	0.22	0	2,2,2	0.10	0
12	PEG	B	708	-	6,6,6	0.48	0	5,5,5	0.33	0
13	EDO	C	712	-	3,3,3	0.28	0	2,2,2	0.47	0
12	PEG	D	708	-	6,6,6	0.17	0	5,5,5	0.13	0
18	PG4	D	706	-	12,12,12	0.44	0	11,11,11	0.37	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
13	EDO	A	710	-	-	1/1/1/1	-
12	PEG	B	707	-	-	2/4/4/4	-
9	PGE	A	704	-	-	3/7/7/7	-
12	PEG	A	707	-	-	2/4/4/4	-
12	PEG	A	709	-	-	1/4/4/4	-
12	PEG	D	707	-	-	1/4/4/4	-
12	PEG	A	714	-	-	4/4/4/4	-
13	EDO	C	709	-	-	1/1/1/1	-
11	XPE	D	705[A]	-	-	15/28/28/28	-
12	PEG	B	704	-	-	2/4/4/4	-
10	12P	A	705	-	-	21/34/34/34	-
14	NAG	A	719	-	-	3/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	NAG	D	716	-	-	3/6/23/26	0/1/1/1
13	EDO	B	705	-	-	1/1/1/1	-
17	FUC	B	717	-	-	-	0/1/1/1
13	EDO	D	710	-	-	1/1/1/1	-
13	EDO	B	712	-	-	1/1/1/1	-
9	PGE	C	708	-	-	4/7/7/7	-
12	PEG	A	712	-	-	3/4/4/4	-
13	EDO	A	715	-	-	1/1/1/1	-
14	NAG	C	716	1	-	1/6/23/26	0/1/1/1
15	BMA	D	713	-	-	2/2/19/22	0/1/1/1
17	FUC	D	717	-	-	-	0/1/1/1
13	EDO	D	709	-	-	1/1/1/1	-
14	NAG	D	718	1	-	0/6/23/26	0/1/1/1
11	XPE	A	706	-	-	7/28/28/28	-
14	NAG	B	714	-	-	0/6/23/26	0/1/1/1
13	EDO	C	710	-	-	1/1/1/1	-
14	NAG	A	717	-	-	2/6/23/26	0/1/1/1
13	EDO	A	716	-	-	1/1/1/1	-
11	XPE	D	705[C]	-	-	17/28/28/28	-
13	EDO	A	711	-	-	1/1/1/1	-
14	NAG	B	716	1	-	4/6/23/26	0/1/1/1
13	EDO	B	710	-	-	1/1/1/1	-
14	NAG	A	721	-	-	0/6/23/26	0/1/1/1
13	EDO	A	713	-	-	0/1/1/1	-
19	1PE	C	707	-	-	9/13/13/13	-
9	PGE	B	709	-	-	3/7/7/7	-
13	EDO	D	711	-	-	1/1/1/1	-
12	PEG	B	706	-	-	3/4/4/4	-
18	PG4	C	706	-	-	3/10/10/10	-
14	NAG	C	715	-	-	3/6/23/26	0/1/1/1
15	BMA	C	714	-	-	0/2/19/22	0/1/1/1
14	NAG	A	720	1	-	2/6/23/26	0/1/1/1
15	BMA	B	715	-	-	0/2/19/22	0/1/1/1
14	NAG	D	719	-	-	2/6/23/26	0/1/1/1
15	BMA	A	718	-	-	0/2/19/22	0/1/1/1
9	PGE	D	701	-	-	6/7/7/7	-
9	PGE	A	708	-	-	3/7/7/7	-
13	EDO	C	701	-	-	1/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
12	PEG	C	705	-	-	2/4/4/4	-
13	EDO	C	711	-	-	1/1/1/1	-
13	EDO	D	714	-	-	1/1/1/1	-
14	NAG	C	717	-	-	3/6/23/26	0/1/1/1
14	NAG	D	715	1	-	1/6/23/26	0/1/1/1
13	EDO	B	711	-	-	1/1/1/1	-
12	PEG	B	708	-	-	1/4/4/4	-
13	EDO	C	712	-	-	1/1/1/1	-
12	PEG	D	708	-	-	2/4/4/4	-
18	PG4	D	706	-	-	8/10/10/10	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	B	713	ACT	O-C	2.08	1.31	1.22
16	B	713	ACT	CH3-C	2.05	1.57	1.49

The worst 5 of 35 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	A	719	NAG	O5-C1-C2	8.26	124.06	111.29
14	B	714	NAG	O5-C1-C2	6.39	121.17	111.29
14	A	719	NAG	C2-N2-C7	5.85	130.75	122.90
14	D	716	NAG	O5-C1-C2	-5.51	102.77	111.29
14	D	716	NAG	C2-N2-C7	5.21	129.89	122.90

There are no chirality outliers.

5 of 165 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
14	A	719	NAG	C3-C2-N2-C7
14	C	715	NAG	C1-C2-N2-C7
14	D	715	NAG	C1-C2-N2-C7
14	D	716	NAG	C8-C7-N2-C2
14	D	716	NAG	O7-C7-N2-C2

There are no ring outliers.

44 monomers are involved in 107 short contacts:

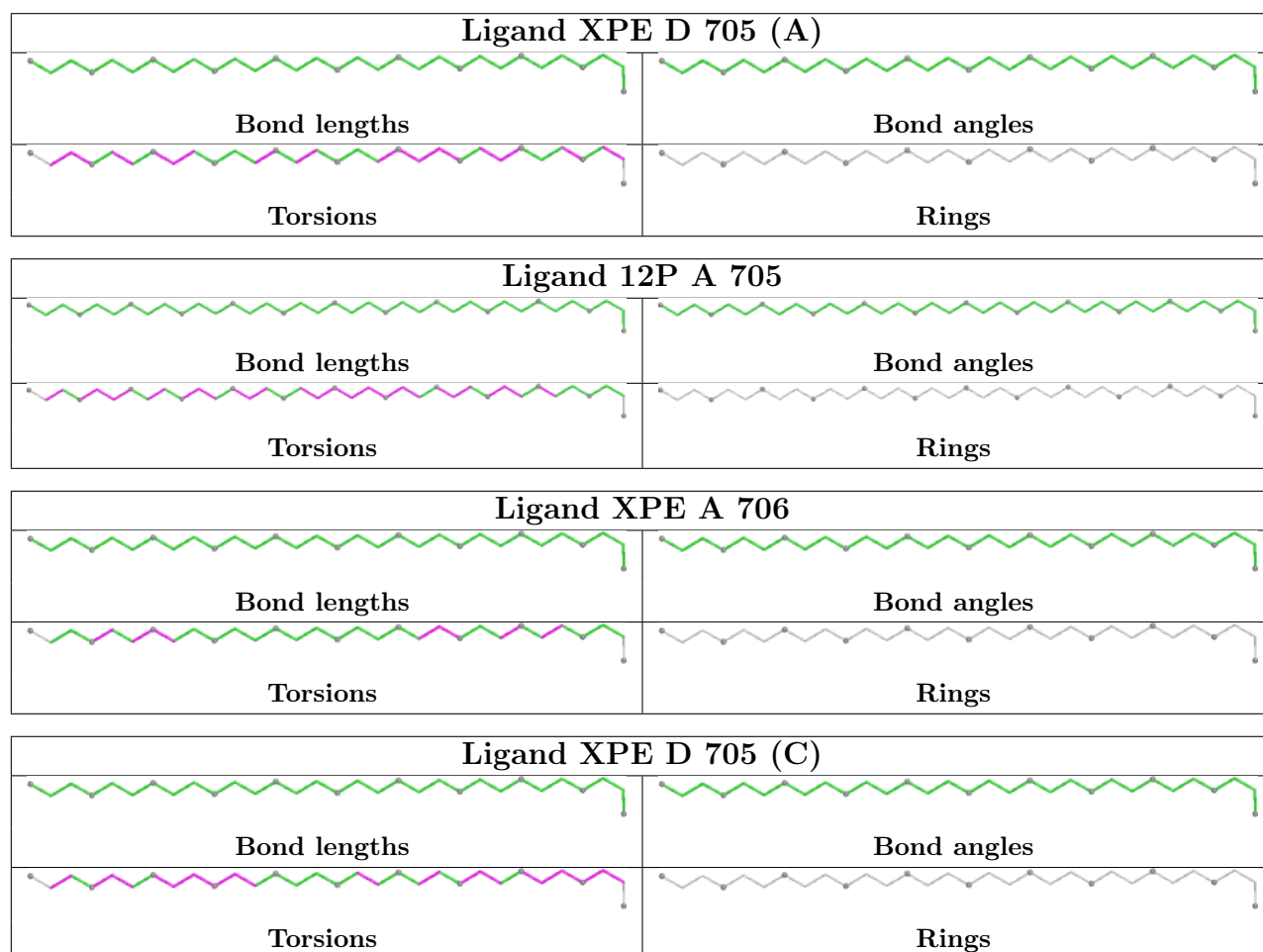
Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	A	704	PGE	3	0
13	C	709	EDO	2	0
11	D	705[A]	XPE	9	0
10	A	705	12P	9	0
14	A	719	NAG	2	0
14	D	716	NAG	3	0
17	B	717	FUC	4	0
13	B	712	EDO	3	0
9	C	708	PGE	2	0
12	A	712	PEG	2	0
14	C	716	NAG	3	0
15	D	713	BMA	2	0
17	D	717	FUC	3	0
13	D	709	EDO	2	0
14	D	718	NAG	4	0
11	A	706	XPE	4	0
14	B	714	NAG	4	0
14	A	717	NAG	2	0
11	D	705[C]	XPE	3	0
16	C	713	ACT	1	0
13	A	711	EDO	1	0
14	B	716	NAG	4	0
14	A	721	NAG	3	0
19	C	707	1PE	2	0
13	D	711	EDO	1	0
12	B	706	PEG	1	0
18	C	706	PG4	12	0
14	C	715	NAG	3	0
15	C	714	BMA	4	0
14	A	720	NAG	3	0
15	B	715	BMA	4	0
14	D	719	NAG	2	0
15	A	718	BMA	2	0
9	D	701	PGE	1	0
13	C	701	EDO	2	0
12	C	705	PEG	2	0
13	C	711	EDO	2	0
14	C	717	NAG	3	0
14	D	715	NAG	5	0
16	B	713	ACT	1	0
16	D	712	ACT	2	0
12	B	708	PEG	2	0
13	C	712	EDO	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
18	D	706	PG4	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers ⓘ

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	609/628 (96%)	-0.10	32 (5%) 32 33	7, 19, 42, 70	20 (3%)
1	B	613/628 (97%)	-0.35	8 (1%) 75 79	6, 18, 35, 78	18 (2%)
1	C	606/628 (96%)	-0.26	15 (2%) 58 61	7, 19, 38, 90	15 (2%)
1	D	605/628 (96%)	-0.13	12 (1%) 65 69	8, 22, 41, 87	18 (2%)
2	E	3/3 (100%)	-0.85	0 100 100	13, 13, 14, 15	0
2	F	3/3 (100%)	-0.63	0 100 100	13, 13, 14, 15	0
2	G	3/3 (100%)	-0.57	0 100 100	14, 14, 14, 15	0
2	H	3/3 (100%)	-0.43	0 100 100	16, 16, 16, 17	0
All	All	2445/2524 (96%)	-0.21	67 (2%) 56 59	6, 20, 40, 90	71 (2%)

The worst 5 of 67 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	613	LEU	7.0
1	A	130	PRO	5.1
1	D	414	VAL	4.9
1	B	135	THR	4.7
1	A	91	ILE	4.6

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

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

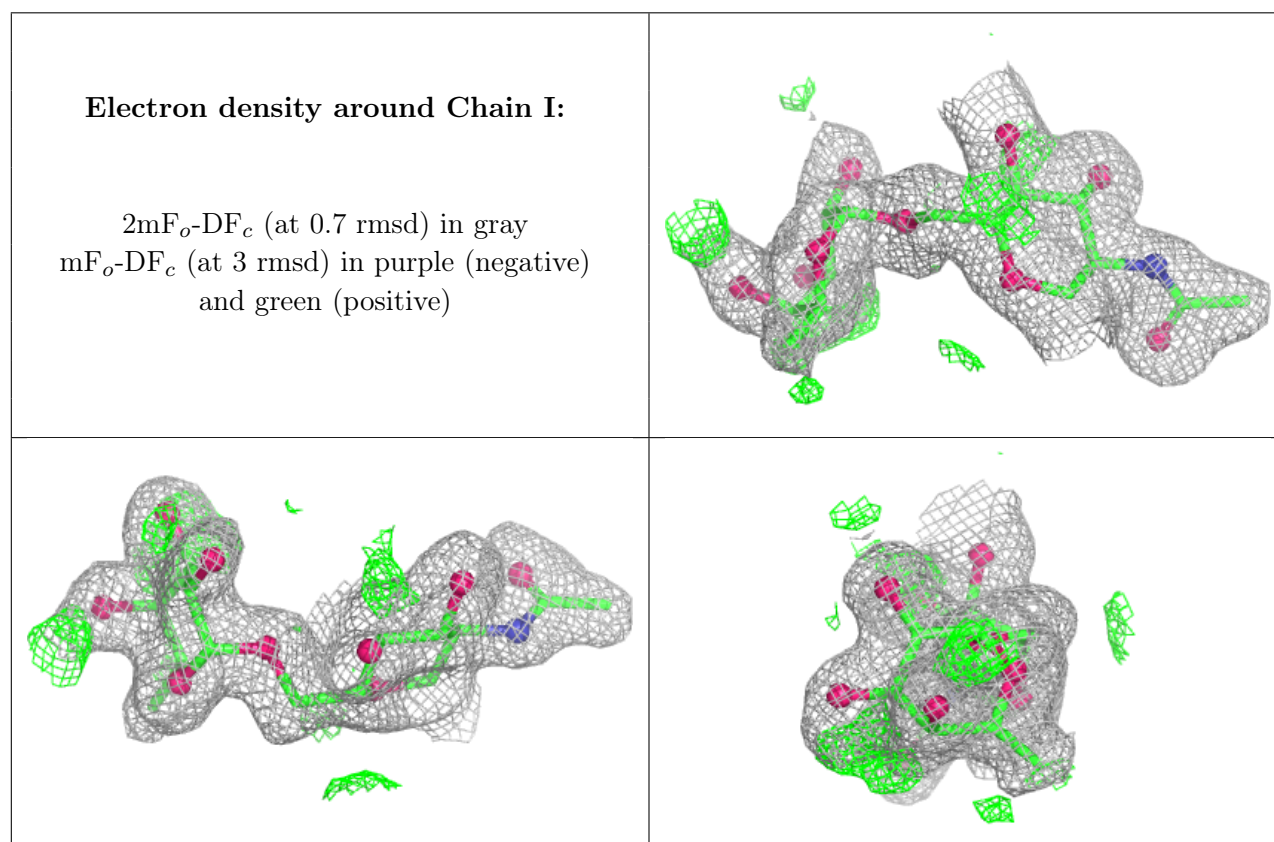
6.3 Carbohydrates [i](#)

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.

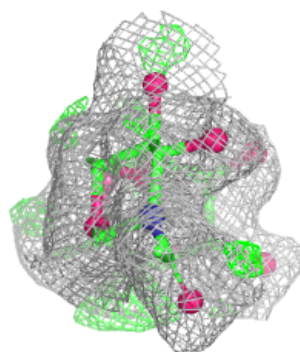
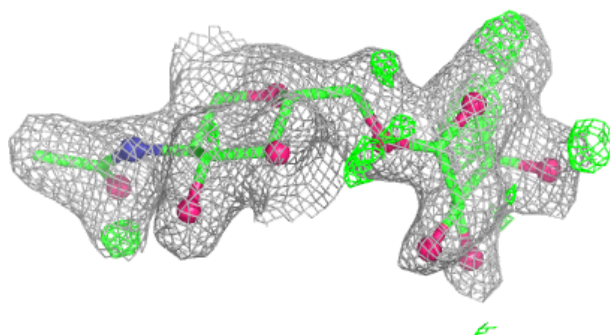
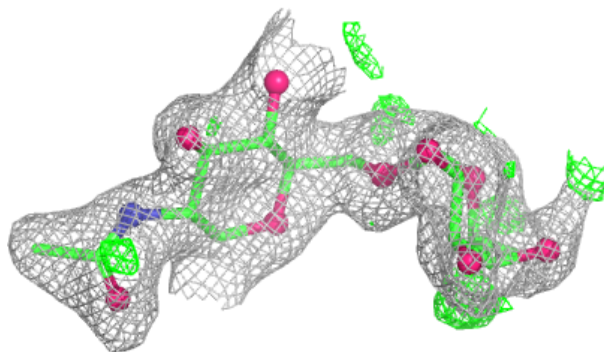
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	NAG	N	1	14/15	0.83	0.14	23,30,38,39	0
3	FUC	J	2	10/11	0.84	0.15	25,33,43,45	10
3	FUC	L	2	10/11	0.85	0.14	39,43,48,48	0
4	FUC	K	3	10/11	0.86	0.14	45,49,55,60	0
3	FUC	I	2	10/11	0.87	0.13	27,30,32,34	10
4	NAG	K	2	14/15	0.88	0.12	40,46,58,60	0
3	NAG	L	1	14/15	0.90	0.10	27,34,42,43	0
3	FUC	N	2	10/11	-	-	42,49,56,63	0
3	NAG	J	1	14/15	0.93	0.10	24,31,37,43	0
4	NAG	K	1	14/15	0.93	0.08	34,41,47,53	0
3	NAG	I	1	14/15	0.95	0.08	23,27,34,35	0
5	NAG	P	1	14/15	-	-	42,51,68,72	0
5	NAG	P	2	14/15	-	-	41,54,67,68	0
5	NAG	R	1	14/15	-	-	19,25,31,31	14
5	NAG	R	2	14/15	-	-	34,42,63,64	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.

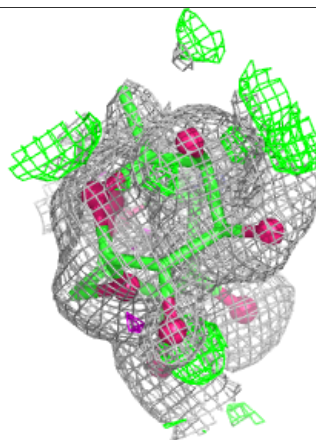
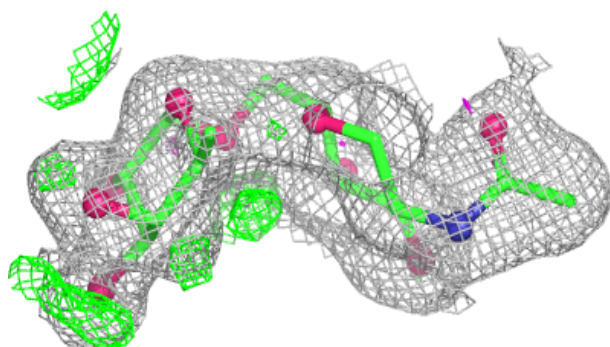
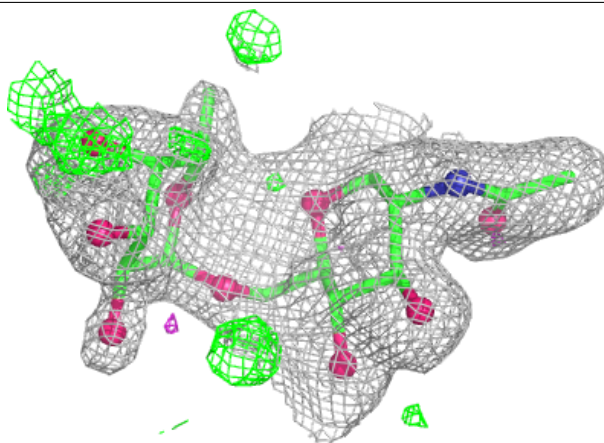


Electron density around Chain J:

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

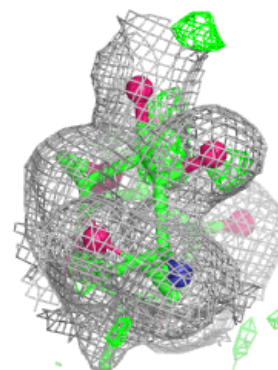
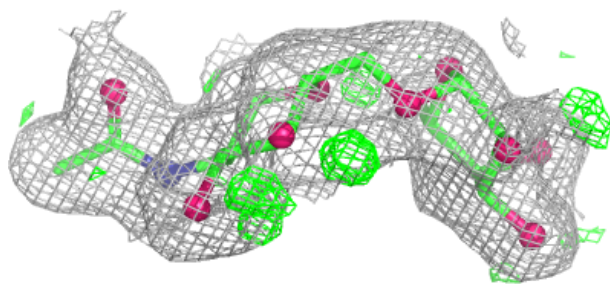
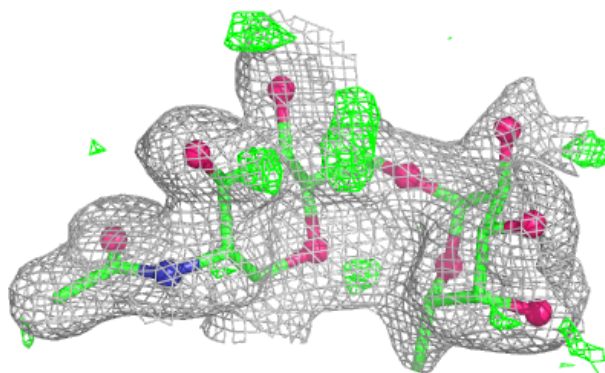
**Electron density around Chain L:**

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



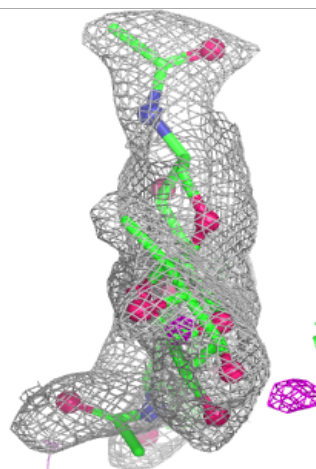
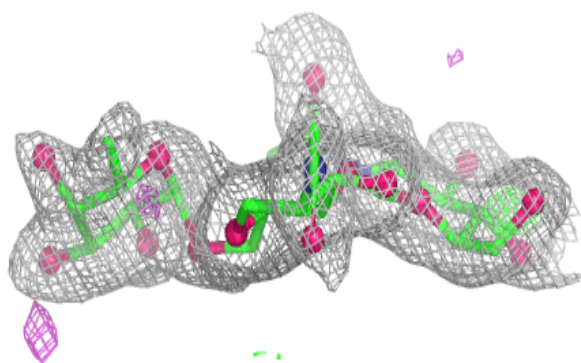
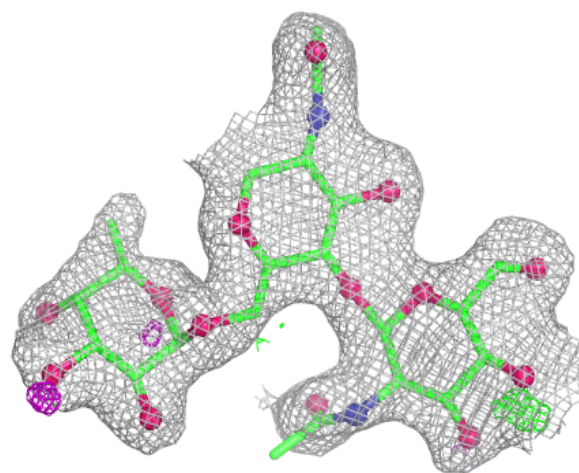
Electron density around Chain N:

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



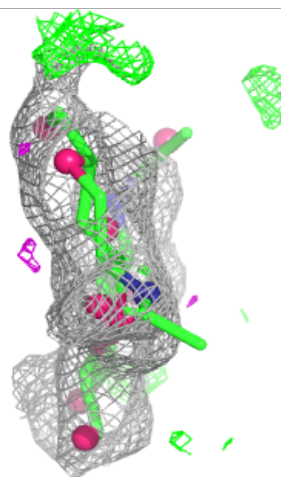
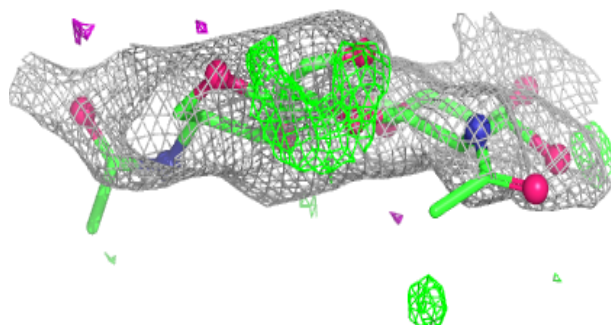
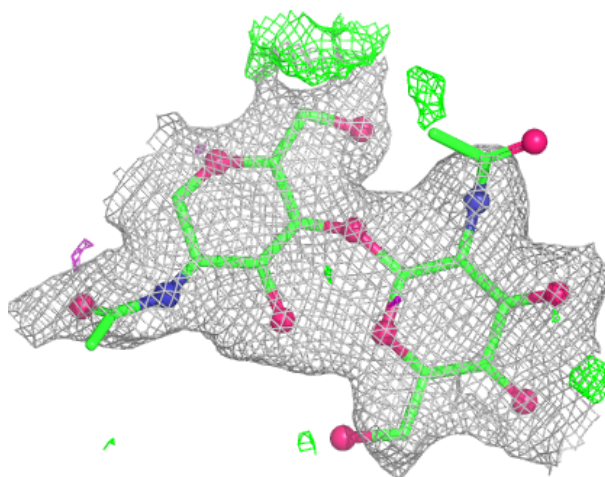
Electron density around Chain K:

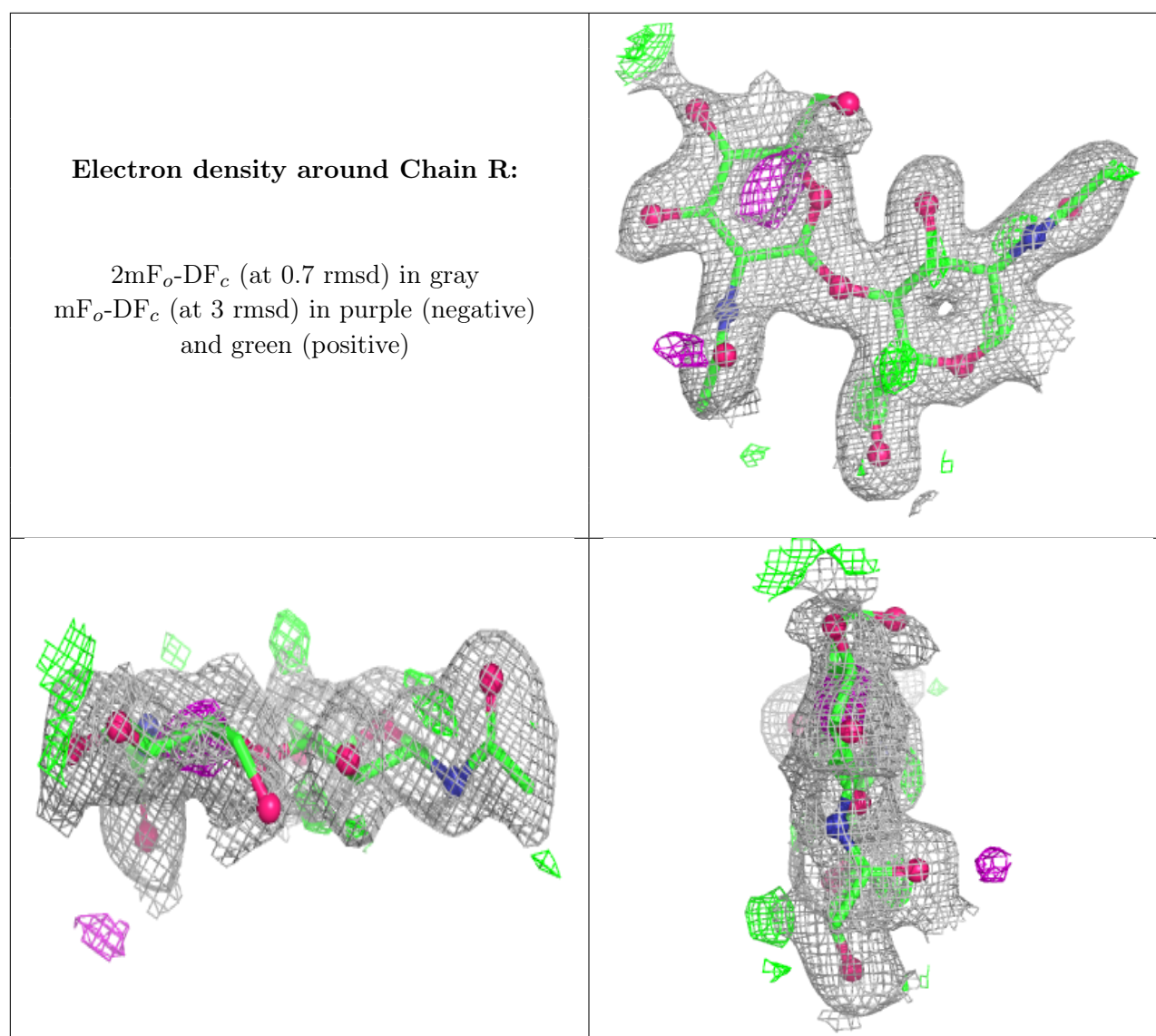
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around Chain P:

$2mF_o-DF_c$ (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
14	NAG	D	716	14/15	0.59	0.20	45,73,94,106	0
14	NAG	A	719	14/15	0.64	0.18	51,63,75,78	0
14	NAG	C	717	14/15	0.69	0.16	57,74,92,96	0
15	BMA	C	714	11/12	0.70	0.15	47,55,66,80	0
14	NAG	D	719	14/15	0.72	0.17	49,65,74,74	0
12	PEG	B	707	7/7	0.74	0.20	57,60,64,72	0
15	BMA	D	713	11/12	0.74	0.14	58,69,74,79	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
14	NAG	A	721	14/15	0.75	0.15	50,55,67,77	0
13	EDO	A	713	4/4	0.75	0.18	49,55,56,60	0
15	BMA	A	718	11/12	0.76	0.15	54,63,69,75	0
13	EDO	C	709	4/4	0.77	0.17	31,41,46,47	0
15	BMA	B	715	11/12	0.77	0.14	36,37,47,48	0
14	NAG	C	715	14/15	0.79	0.14	45,60,73,78	0
12	PEG	A	714	7/7	0.80	0.17	47,53,58,59	0
9	PGE	A	708	10/10	0.80	0.18	44,49,57,58	0
13	EDO	D	709	4/4	0.80	0.15	45,47,48,59	0
13	EDO	D	711	4/4	0.80	0.15	45,46,46,46	0
13	EDO	D	714	4/4	0.80	0.17	49,57,61,68	0
13	EDO	B	711	4/4	0.81	0.16	46,47,48,50	0
12	PEG	C	705	7/7	0.81	0.14	36,46,49,50	0
13	EDO	C	711	4/4	0.81	0.17	42,49,49,57	0
12	PEG	A	709	7/7	0.81	0.17	47,51,57,62	0
18	PG4	D	706	13/13	0.81	0.17	42,47,54,55	0
13	EDO	A	715	4/4	0.82	0.16	40,46,48,48	0
18	PG4	C	706	13/13	0.82	0.19	32,57,71,73	0
12	PEG	B	708	7/7	0.82	0.17	40,41,52,55	0
12	PEG	A	707	7/7	0.83	0.17	36,44,53,62	0
19	1PE	C	707	16/16	0.83	0.16	37,49,59,68	0
17	FUC	B	717	10/11	0.84	0.13	33,45,51,60	0
12	PEG	D	707	7/7	0.84	0.17	42,52,56,58	0
13	EDO	B	705	4/4	0.84	0.17	44,45,46,51	0
9	PGE	A	704	10/10	0.84	0.19	46,56,63,67	0
9	PGE	B	709	10/10	0.85	0.14	44,51,57,59	0
13	EDO	B	712	4/4	0.85	0.23	29,33,34,37	0
9	PGE	C	708	10/10	0.85	0.14	30,44,53,60	0
12	PEG	A	712	7/7	0.86	0.16	49,56,72,76	0
14	NAG	A	717	14/15	0.86	0.13	38,43,52,53	0
13	EDO	C	701	4/4	0.86	0.14	40,43,45,49	0
13	EDO	A	710	4/4	0.86	0.14	38,38,42,44	0
16	ACT	D	712	4/4	0.87	0.14	24,33,33,34	0
13	EDO	B	710	4/4	0.87	0.15	40,41,46,53	0
17	FUC	D	717	10/11	0.87	0.11	37,47,52,52	0
13	EDO	C	710	4/4	0.87	0.12	42,44,46,54	0
14	NAG	A	720	14/15	0.87	0.11	27,31,37,39	0
13	EDO	A	716	4/4	0.87	0.14	26,37,38,43	0
12	PEG	B	706	7/7	0.88	0.14	46,47,49,58	0
9	PGE	D	701	10/10	0.88	0.14	38,44,47,48	0
14	NAG	B	716	14/15	0.88	0.11	29,36,44,46	0
13	EDO	C	712	4/4	0.88	0.13	41,42,46,53	0

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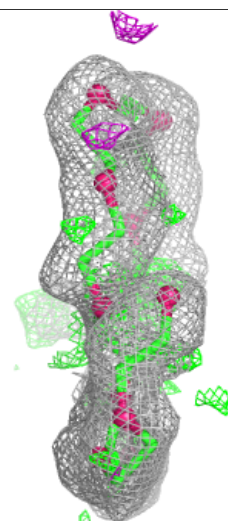
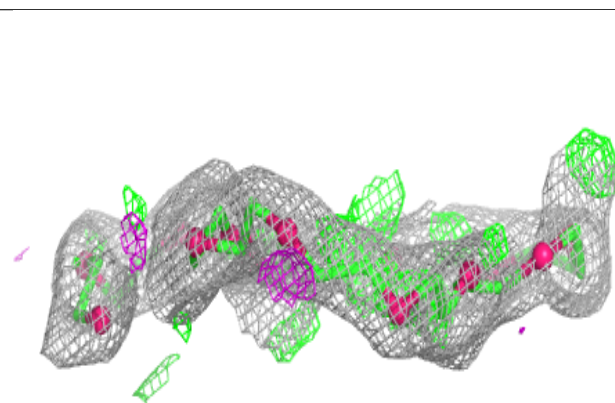
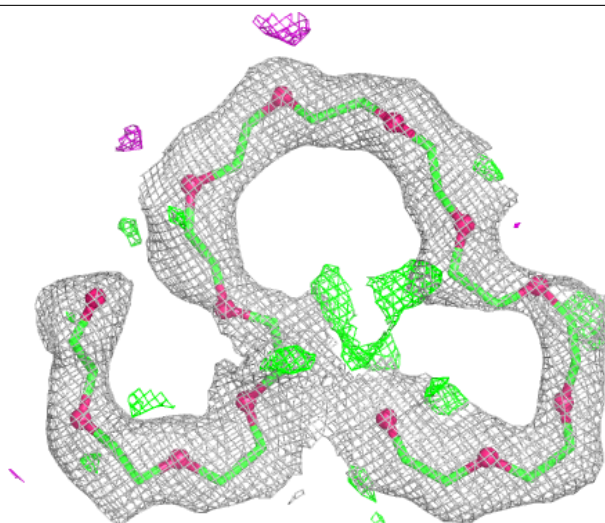
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
14	NAG	C	716	14/15	0.88	0.12	25,31,41,42	14
10	12P	A	705	37/37	0.88	0.14	32,43,59,63	0
11	XPE	D	705[A]	31/31	0.89	0.16	26,34,37,37	31
13	EDO	D	710	4/4	0.89	0.13	31,31,40,43	0
11	XPE	D	705[C]	31/31	0.89	0.16	33,39,54,57	31
14	NAG	D	715	14/15	0.89	0.10	28,31,42,48	0
14	NAG	D	718	14/15	0.90	0.10	26,30,35,39	14
13	EDO	A	711	4/4	0.90	0.13	34,36,37,39	0
12	PEG	D	708	7/7	0.91	0.11	48,49,54,56	0
14	NAG	B	714	14/15	0.91	0.12	27,31,40,41	0
16	ACT	B	713	4/4	0.91	0.17	28,28,34,38	0
12	PEG	B	704	7/7	0.92	0.10	34,40,47,48	0
11	XPE	A	706	31/31	0.93	0.11	19,34,47,48	0
16	ACT	C	713	4/4	0.93	0.11	22,28,29,32	0
8	MG	D	704	1/1	0.97	0.14	29,29,29,29	0
8	MG	A	703	1/1	0.99	0.05	20,20,20,20	0
8	MG	C	704	1/1	0.99	0.07	23,23,23,23	0
6	ZN	A	701	1/1	0.99	0.02	14,14,14,14	0
6	ZN	B	701	1/1	0.99	0.03	12,12,12,12	0
6	ZN	C	702	1/1	0.99	0.02	13,13,13,13	0
6	ZN	D	702	1/1	0.99	0.02	16,16,16,16	0
7	CL	B	702	1/1	1.00	0.02	14,14,14,14	0
7	CL	C	703	1/1	1.00	0.02	14,14,14,14	0
7	CL	D	703	1/1	1.00	0.02	16,16,16,16	0
7	CL	A	702	1/1	1.00	0.02	15,15,15,15	0
8	MG	B	703	1/1	1.00	0.05	11,11,11,11	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.

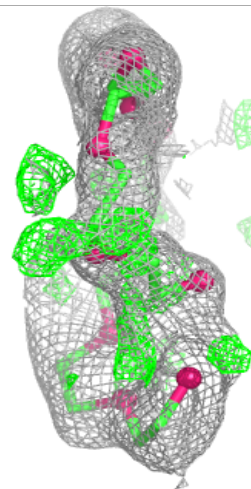
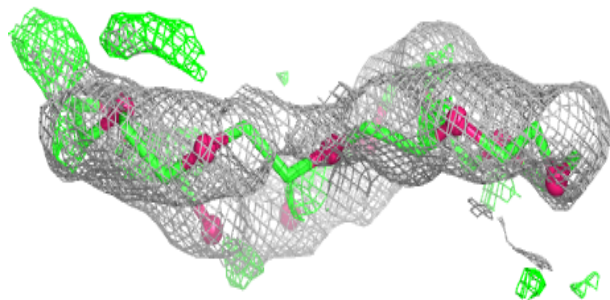
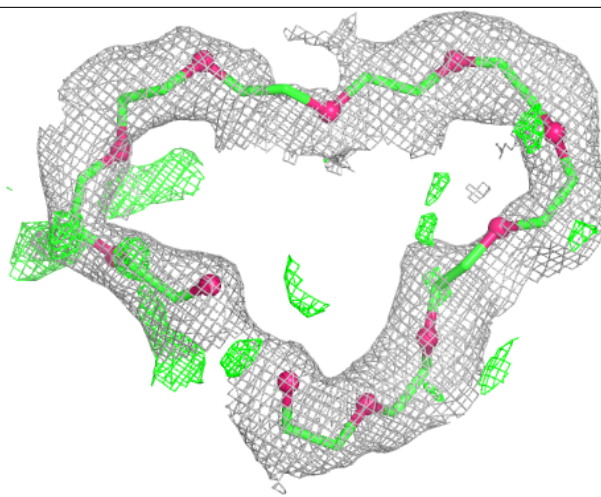
Electron density around 12P A 705:

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



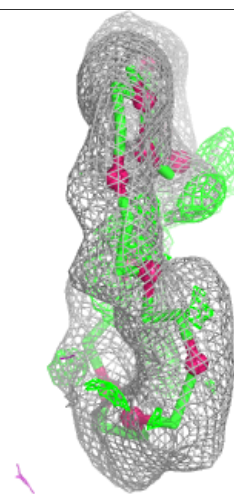
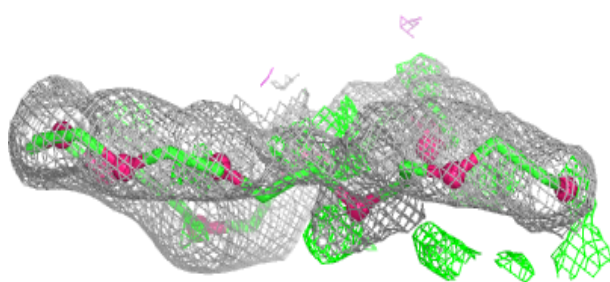
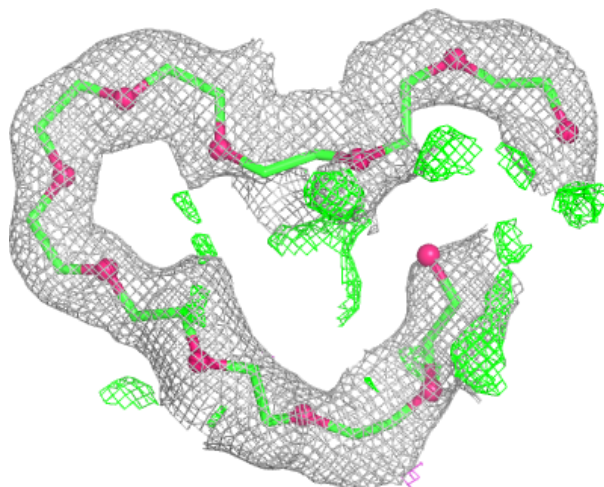
Electron density around XPE D 705 (A):

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



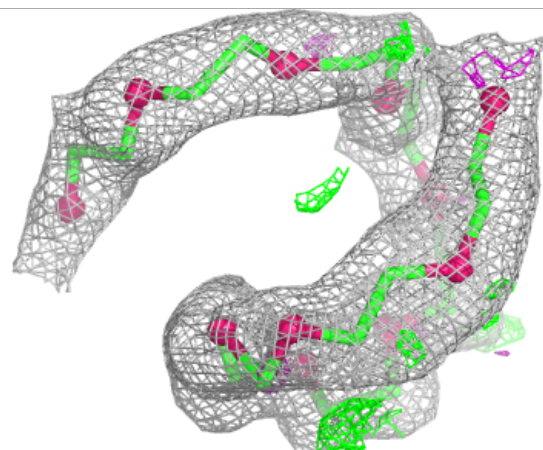
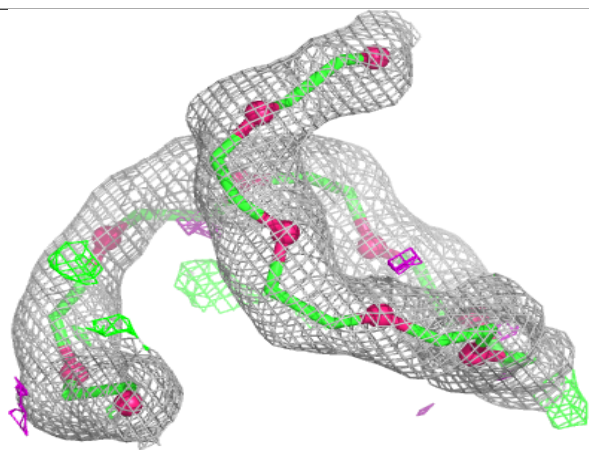
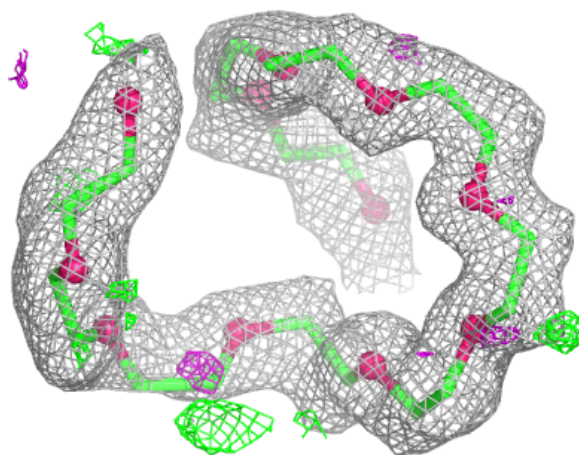
Electron density around XPE D 705 (C):

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



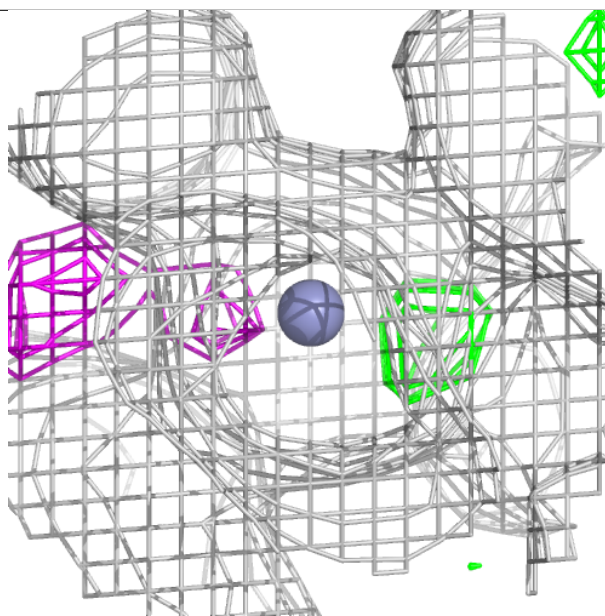
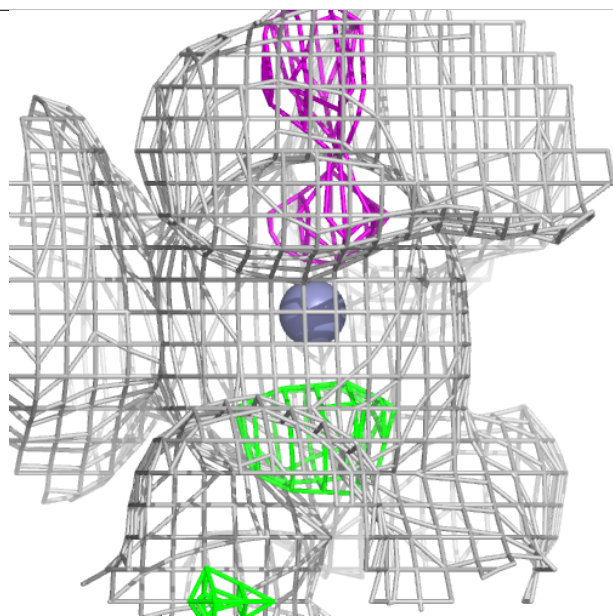
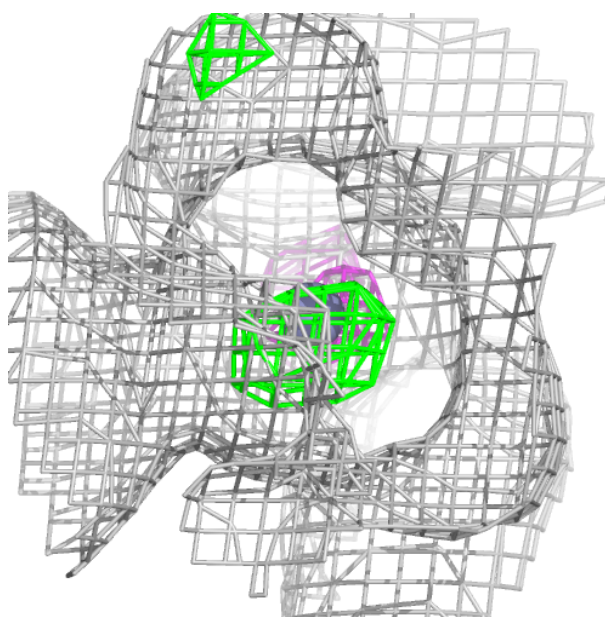
Electron density around XPE A 706:

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



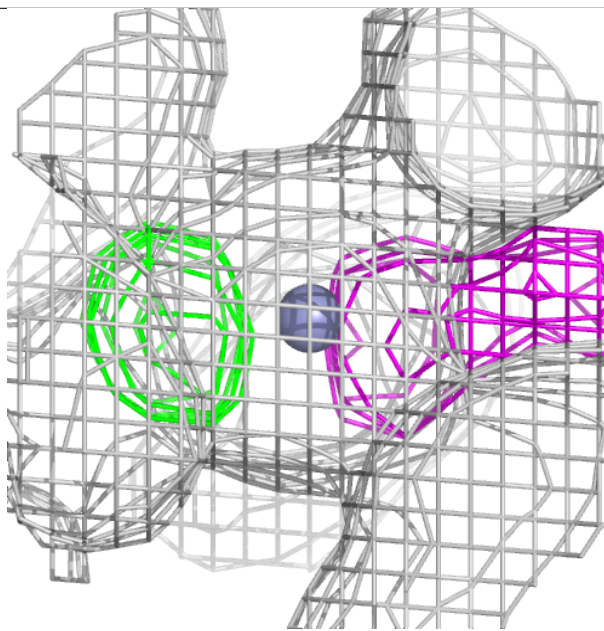
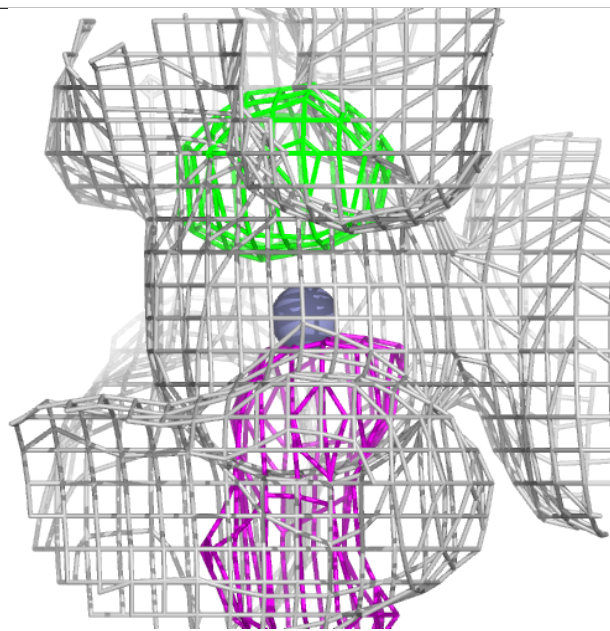
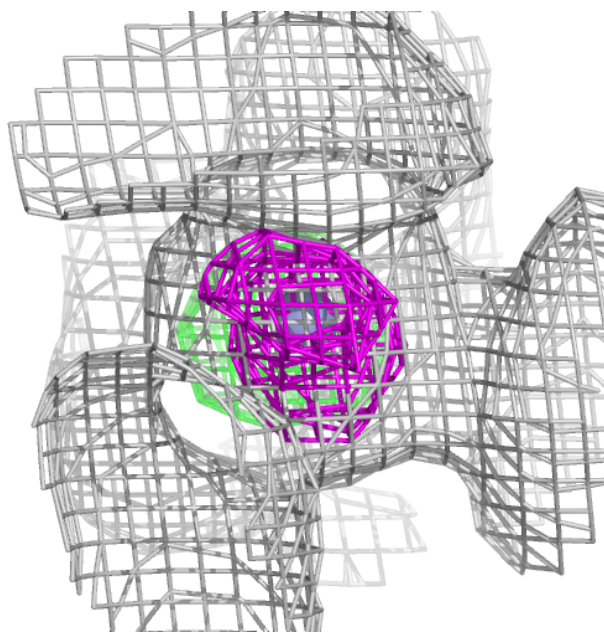
Electron density around ZN A 701:

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



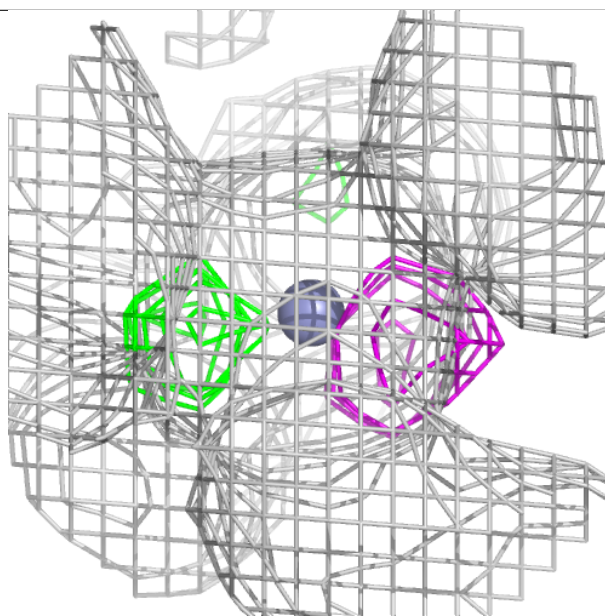
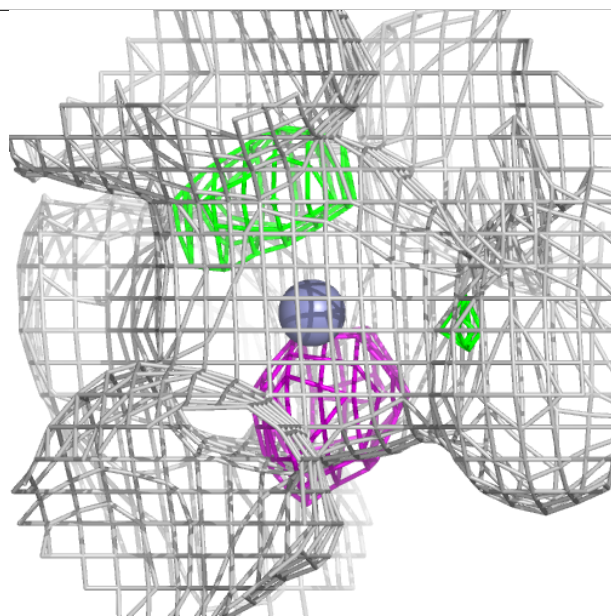
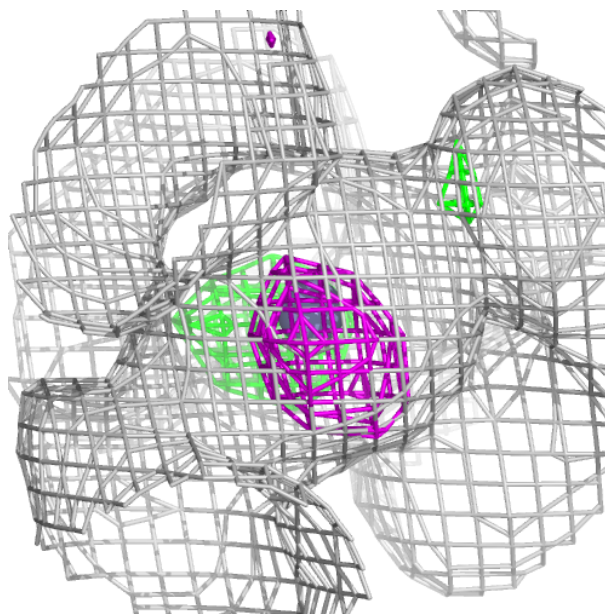
Electron density around ZN B 701:

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



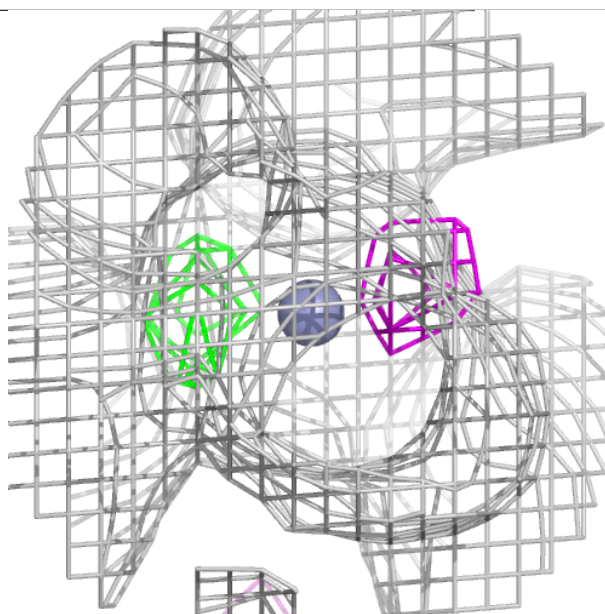
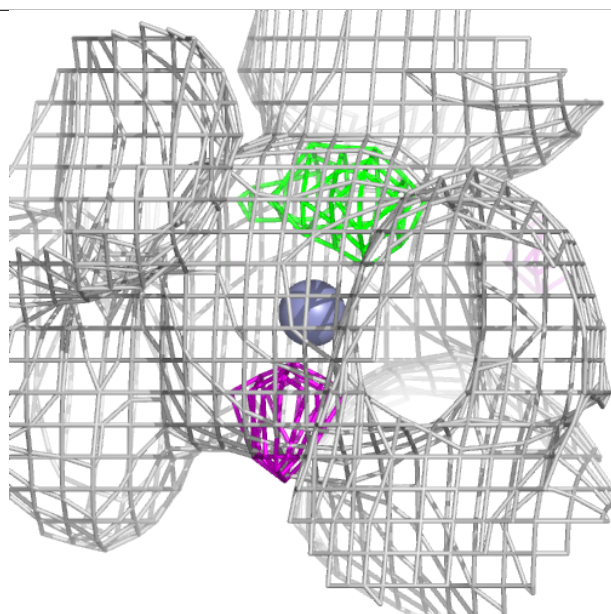
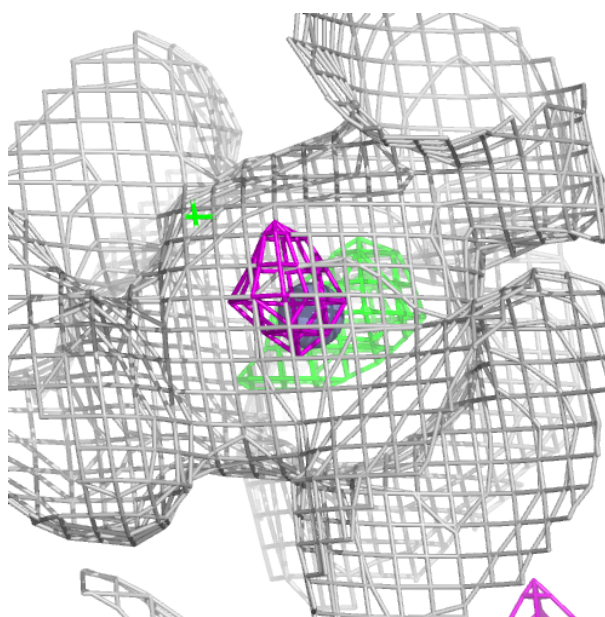
Electron density around ZN C 702:

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



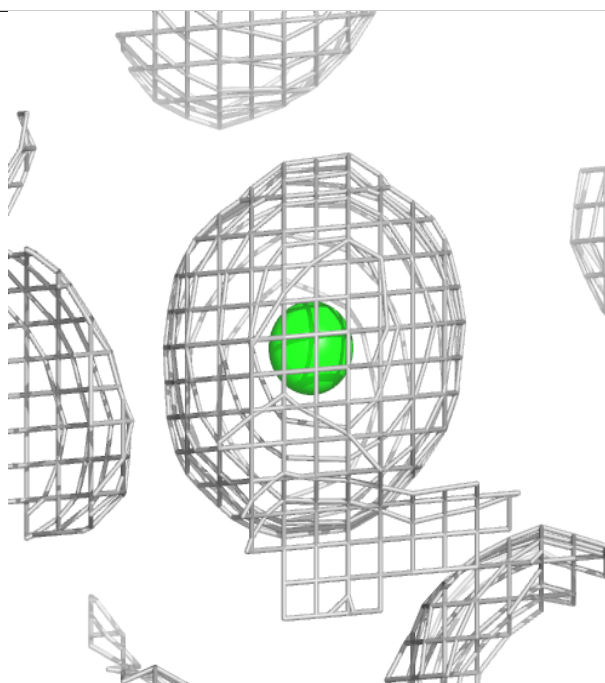
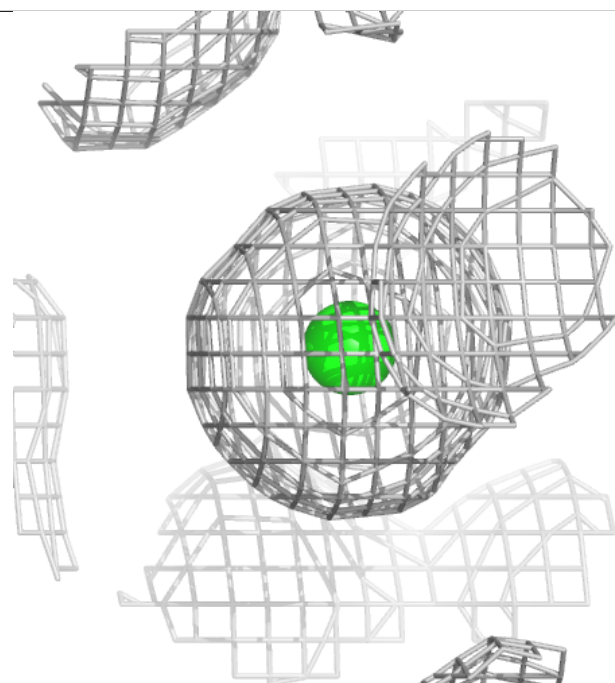
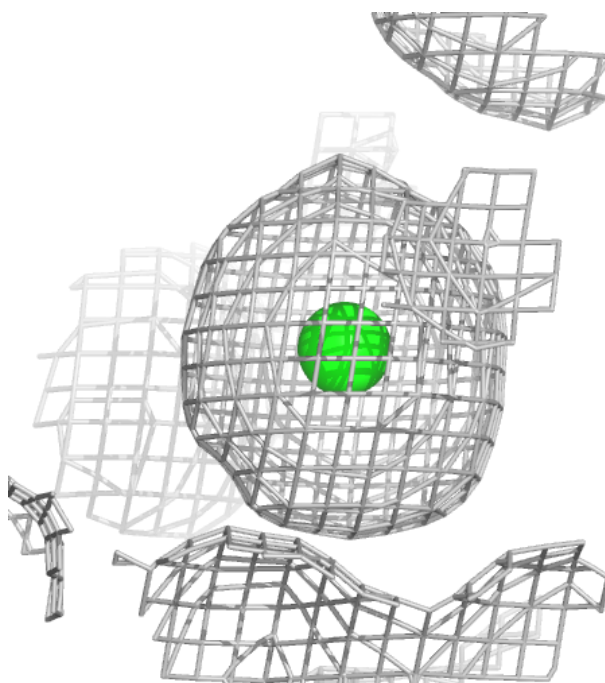
Electron density around ZN D 702:

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



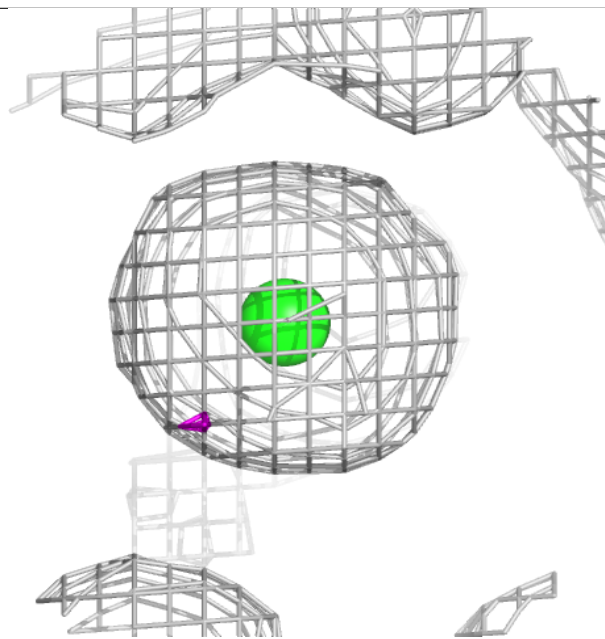
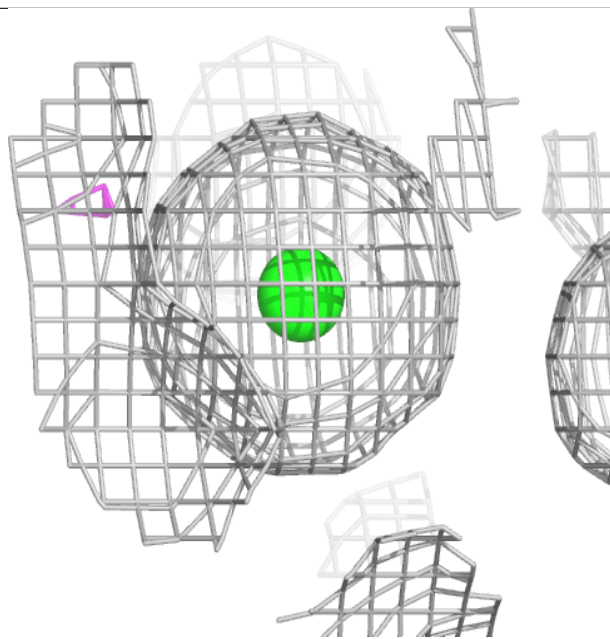
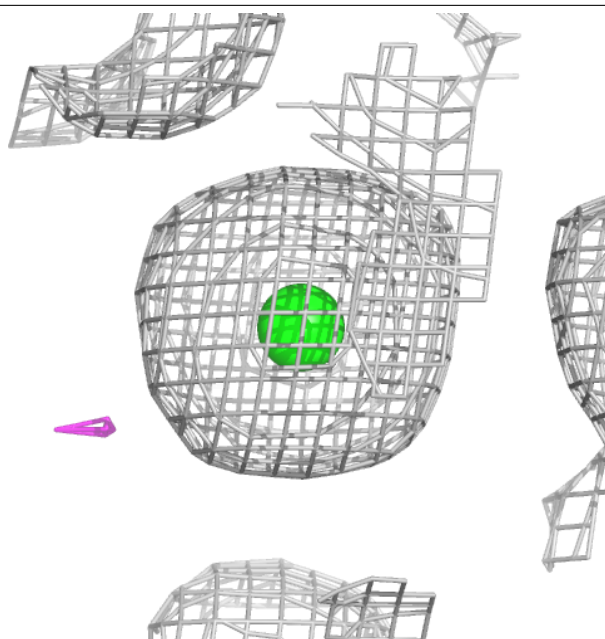
Electron density around CL B 702:

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



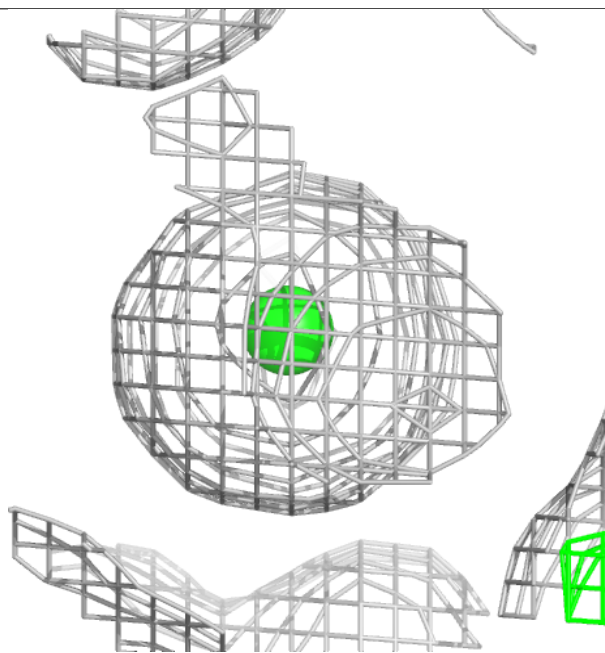
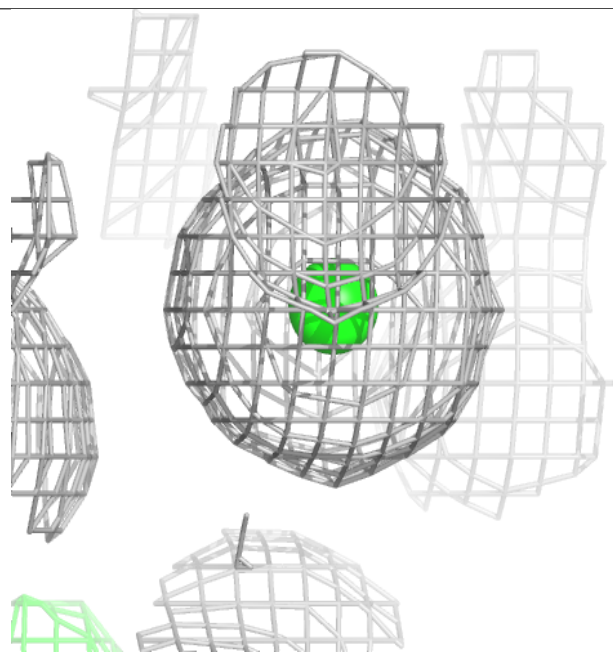
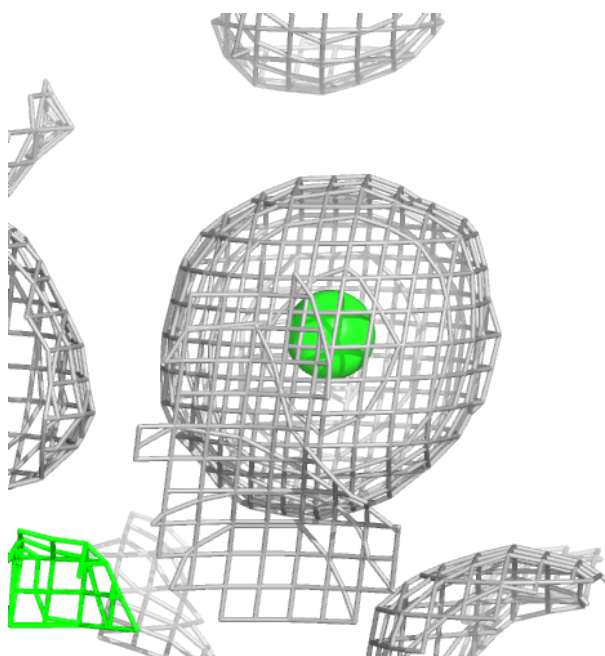
Electron density around CL C 703:

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



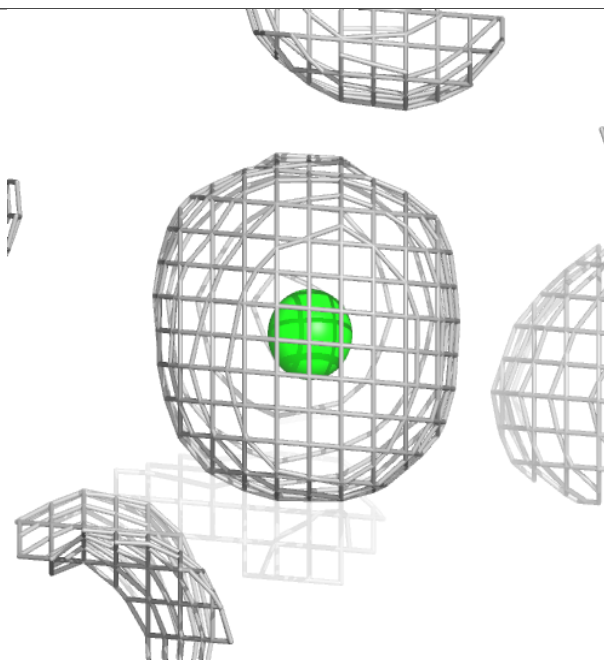
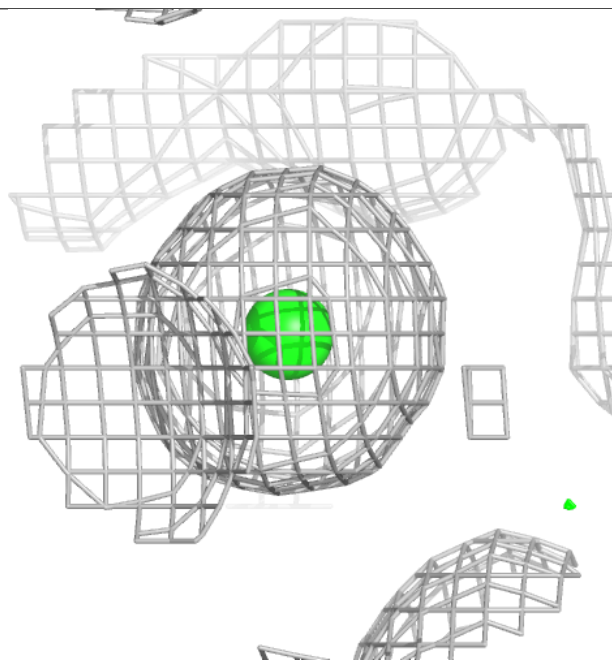
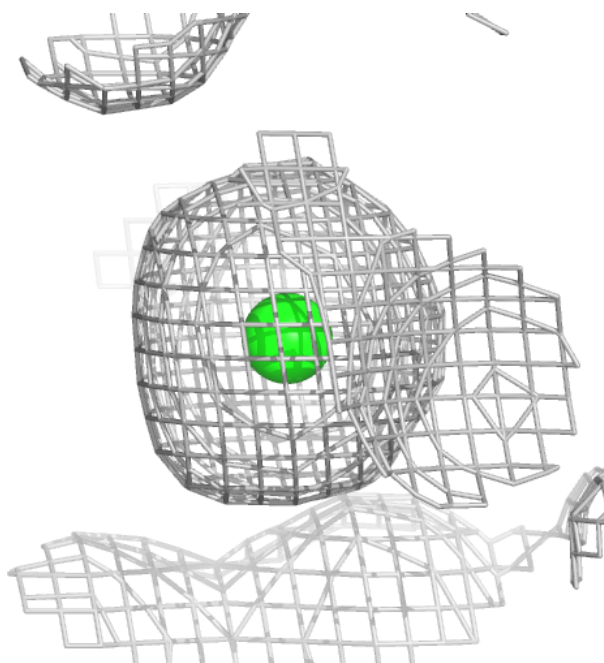
Electron density around CL D 703:

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



Electron density around CL 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)



6.5 Other polymers [i](#)

There are no such residues in this entry.