



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 8, 2026 – 05:31 AM UTC

PDB ID : 8QHL / pdb_00008qhl
Title : Human Angiotensin-1 converting enzyme N-domain in complex with the lactotripeptide VPP
Authors : Gregory, K.S.; Cozier, G.E.; Acharya, K.R.
Deposited on : 2023-09-08
Resolution : 1.90 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
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

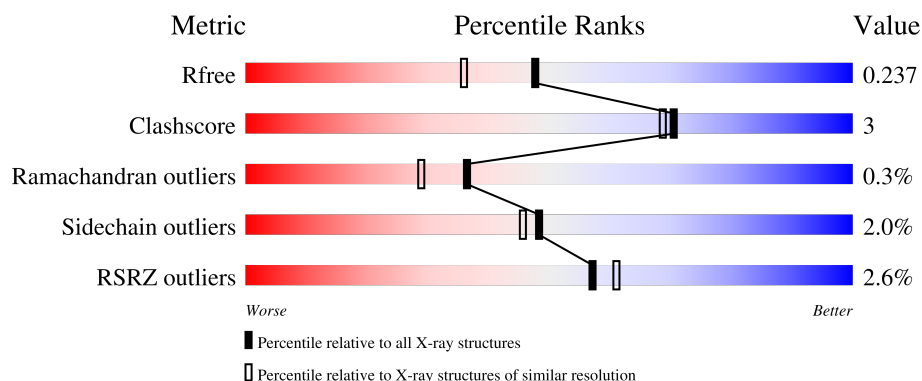
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

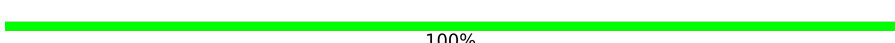
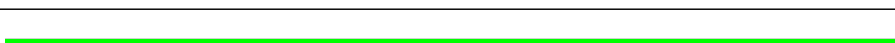
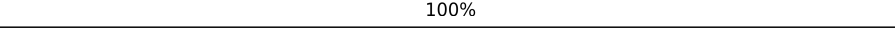
The reported resolution of this entry is 1.90 Å.

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.



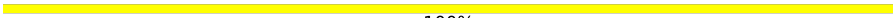
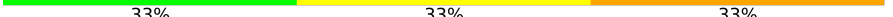
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	7789 (1.90-1.90)
Clashscore	190562	8410 (1.90-1.90)
Ramachandran outliers	187476	8333 (1.90-1.90)
Sidechain outliers	187428	8333 (1.90-1.90)
RSRZ outliers	180081	7790 (1.90-1.90)

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	
1	B	628	
2	C	3	
2	D	3	
3	E	2	

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Mol	Chain	Length	Quality of chain
3	F	2	 100%
4	G	4	 50% 50%
5	H	3	 33% 33% 33%
6	I	2	 50% 50%
6	J	2	 50% 50%

2 Entry composition

There are 16 unique types of molecules in this entry. The entry contains 10738 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Angiotensin-converting enzyme.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	603	Total	C	N	O	S	0	4	0
			4960	3184	850	907	19			
1	A	605	Total	C	N	O	S	0	4	0
			4964	3187	850	908	19			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
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
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

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

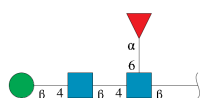
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	D	3	Total	C	N	O	0	0	0
			22	15	3	4			
2	C	3	Total	C	N	O	0	0	0
			22	15	3	4			

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



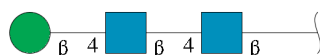
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	E	2	Total	C	N	O	0	0	0
			28	16	2	10			
3	F	2	Total	C	N	O	0	0	0
			28	16	2	10			

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



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

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



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

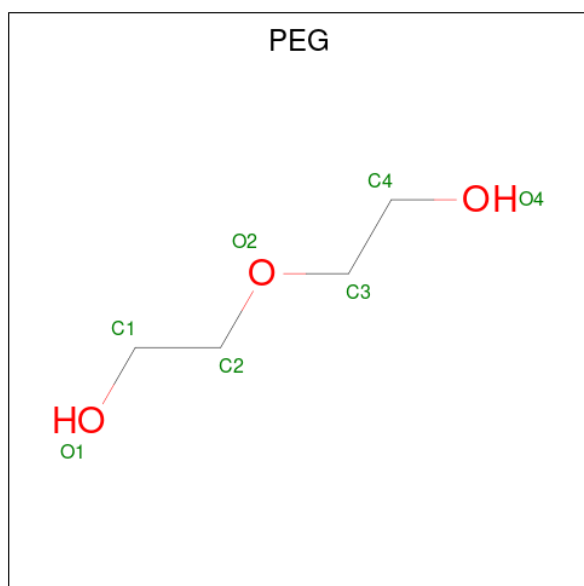
- Molecule 7 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

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

- Molecule 8 is CHLORIDE ION (CCD ID: CL) (formula: Cl) (labeled as "Ligand of Interest" by depositor).

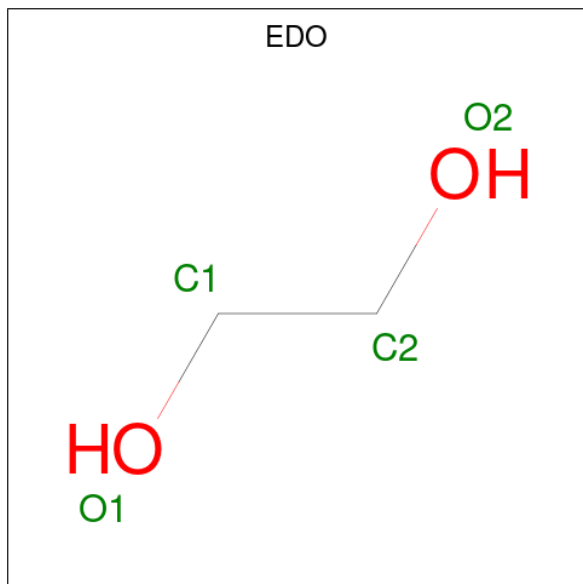
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	B	1	Total	Cl	0	0
			1	1		
8	A	1	Total	Cl	0	0
			1	1		

- Molecule 9 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: C₄H₁₀O₃).



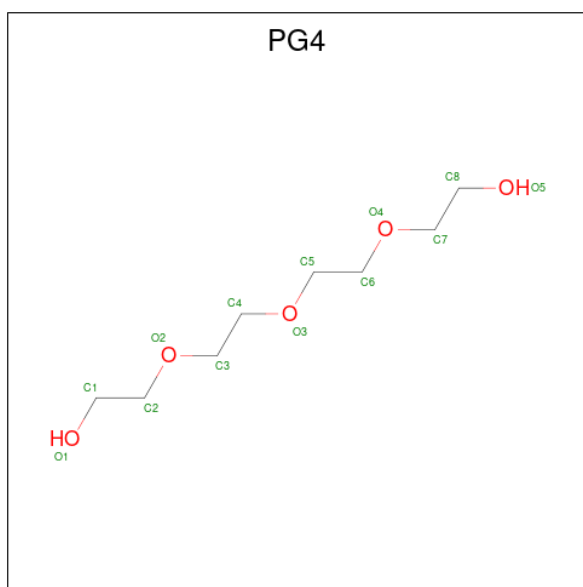
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	B	1	Total C O 7 4 3	0	0
9	B	1	Total C O 7 4 3	0	0
9	B	1	Total C O 7 4 3	0	0
9	A	1	Total C O 7 4 3	0	0
9	A	1	Total C O 7 4 3	0	0
9	A	1	Total C O 7 4 3	0	0

- Molecule 10 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: $C_2H_6O_2$).



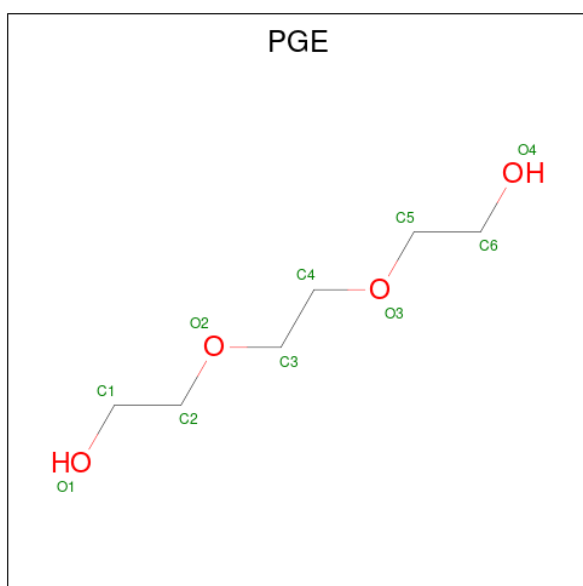
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	B	1	Total C O 4 2 2	0	0
10	B	1	Total C O 4 2 2	0	0

- Molecule 11 is TETRAETHYLENE GLYCOL (CCD ID: PG4) (formula: $C_8H_{18}O_5$).



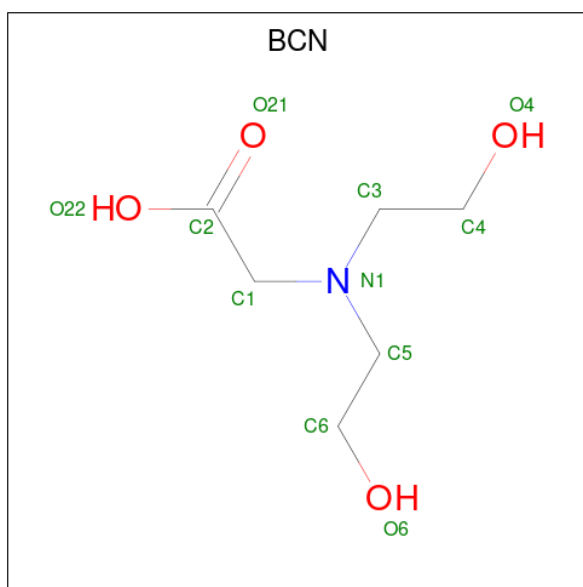
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
11	B	1	Total	C	O	0	0
			13	8	5		
11	A	1	Total	C	O	0	0
			13	8	5		

- Molecule 12 is TRIETHYLENE GLYCOL (CCD ID: PGE) (formula: $C_6H_{14}O_4$).



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

- Molecule 13 is BICINE (CCD ID: BCN) (formula: $C_6H_{13}NO_4$).

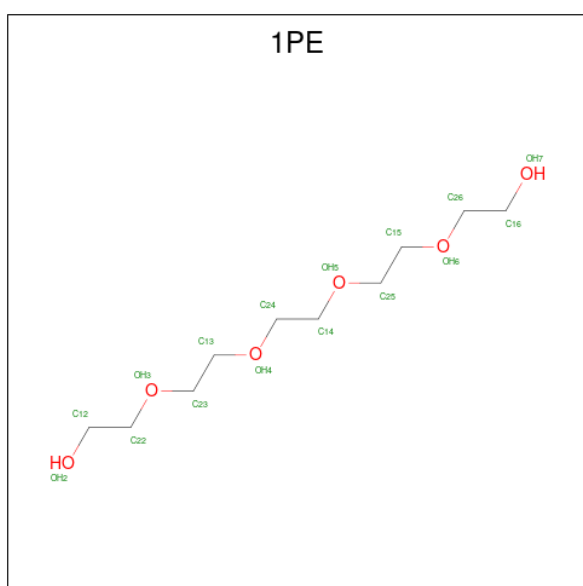


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
13	A	1	Total	C	N	O	0	0
			11	6	1	4		

- Molecule 14 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

- Molecule 15 is PENTAETHYLENE GLYCOL (CCD ID: 1PE) (formula: C₁₀H₂₂O₆).



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

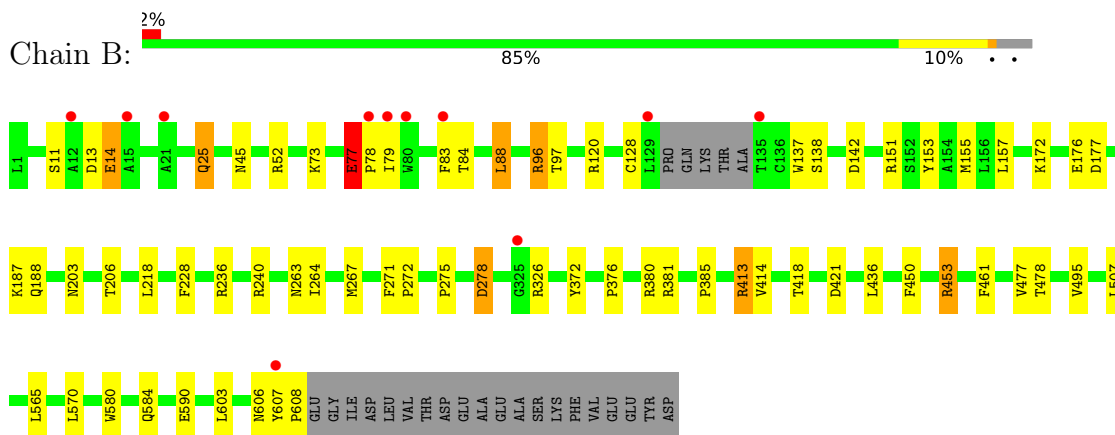
- Molecule 16 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
16	B	252	Total	O	0	0
			252	252		
16	D	3	Total	O	0	0
			3	3		
16	A	187	Total	O	0	0
			187	187		
16	C	2	Total	O	0	0
			2	2		

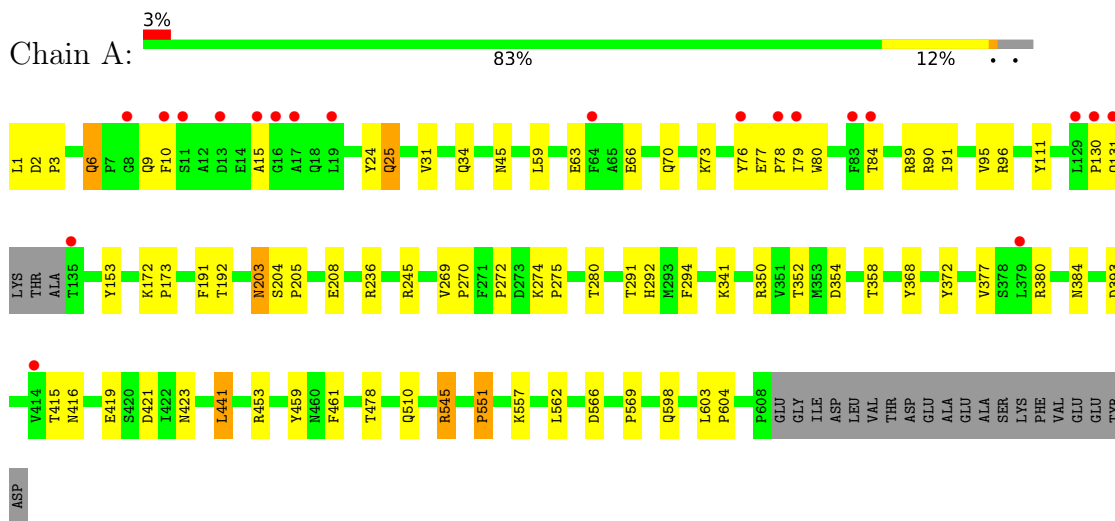
3 Residue-property plots

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

- Molecule 1: Angiotensin-converting enzyme



- Molecule 1: Angiotensin-converting enzyme



- Molecule 2: VAL-PRO-PRO

Chain D: 

There are no outlier residues recorded for this chain.

- Molecule 2: VAL-PRO-PRO

Chain C:  100%

There are no outlier residues recorded for this chain.

- Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain E:  100%

MAG1
MAG2

- Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain F:  100%

MAG1
MAG2

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

Chain G:  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 H:  33% 33% 33%

MAG1
MAG2
BMA3

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

Chain I:  50% 50%

MAG1
FUC2

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

Chain J:  50% 50%

MAG1
FUC2

4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	73.34Å 78.22Å 83.01Å 88.75° 64.70° 75.25°	Depositor
Resolution (Å)	75.27 – 1.90 75.27 – 1.90	Depositor EDS
% Data completeness (in resolution range)	97.9 (75.27-1.90) 95.9 (75.27-1.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.13 (at 1.90Å)	Xtriage
Refinement program	REFMAC 5.8.0419	Depositor
R, R_{free}	0.188 , 0.233 0.190 , 0.237	Depositor DCC
R_{free} test set	6246 reflections (2.43%)	wwPDB-VP
Wilson B-factor (Å ²)	32.4	Xtriage
Anisotropy	0.187	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 43.4	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	0.97	EDS
Total number of atoms	10738	wwPDB-VP
Average B, all atoms (Å ²)	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.69% 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: BMA, NAG, EDO, FUC, CL, ZN, PEG, BCN, PG4, MG, 1PE, PGE

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	0.84	1/5120 (0.0%)	1.32	25/6975 (0.4%)
1	B	0.93	0/5115	1.36	28/6966 (0.4%)
2	C	1.39	0/23	1.36	0/31
2	D	1.81	0/23	1.80	0/31
All	All	0.89	1/10281 (0.0%)	1.34	53/14003 (0.4%)

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	5
1	B	0	5
All	All	0	10

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	15	ALA	C-O	10.45	1.36	1.24

The worst 5 of 53 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	203	ASN	CB-CA-C	-10.63	95.38	112.06
1	B	453	ARG	CB-CG-CD	7.86	129.37	111.30
1	B	418	THR	CA-CB-OG1	-7.46	98.42	109.60
1	B	97	THR	CA-CB-OG1	-7.24	98.74	109.60
1	B	84	THR	CA-CB-OG1	-7.13	98.90	109.60

There are no chirality outliers.

5 of 10 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	120	ARG	Sidechain
1	B	151	ARG	Sidechain
1	B	380	ARG	Sidechain
1	B	453	ARG	Sidechain
1	B	96	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	4964	0	4732	29	0
1	B	4960	0	4730	30	0
2	C	22	0	22	0	0
2	D	22	0	22	0	0
3	E	28	0	25	0	0
3	F	28	0	25	0	0
4	G	49	0	44	1	0
5	H	39	0	34	1	0
6	I	24	0	22	1	0
6	J	24	0	22	1	0
7	A	1	0	0	0	0
7	B	1	0	0	0	0
8	A	1	0	0	0	0
8	B	1	0	0	0	0
9	A	21	0	30	1	0
9	B	21	0	30	2	0
10	B	8	0	12	2	0
11	A	13	0	18	2	0
11	B	13	0	18	1	0
12	B	10	0	14	0	0
13	A	11	0	12	1	0
14	A	1	0	0	0	0
15	A	32	0	44	5	0
16	A	187	0	0	4	0
16	B	252	0	0	1	0
16	C	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
16	D	3	0	0	0	0
All	All	10738	0	9856	68	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 3.

The worst 5 of 68 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)
5:H:1:NAG:H62	5:H:2:NAG:H82	1.52	0.90
1:A:292:HIS:NE2	15:A:708:1PE:H121	1.90	0.86
1:A:66:GLU:O	1:A:70:GLN:HG3	1.90	0.72
1:B:381:ARG:HH11	10:B:705:EDO:H12	1.57	0.70
1:B:88:LEU:O	1:B:88:LEU:HD23	1.93	0.68

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	605/628 (96%)	588 (97%)	14 (2%)	3 (0%)	24	16
1	B	603/628 (96%)	589 (98%)	13 (2%)	1 (0%)	43	36
2	C	1/3 (33%)	1 (100%)	0	0	100	100
2	D	1/3 (33%)	1 (100%)	0	0	100	100
All	All	1210/1262 (96%)	1179 (97%)	27 (2%)	4 (0%)	36	29

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	45	ASN

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Mol	Chain	Res	Type
1	A	416	ASN
1	B	45	ASN
1	A	78	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	524/540 (97%)	513 (98%)	11 (2%)	47	44
1	B	523/540 (97%)	513 (98%)	10 (2%)	50	47
2	C	3/3 (100%)	3 (100%)	0	100	100
2	D	3/3 (100%)	3 (100%)	0	100	100
All	All	1053/1086 (97%)	1032 (98%)	21 (2%)	48	46

5 of 21 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	368	TYR
1	A	415	THR
1	A	598	GLN
1	A	419	GLU
1	A	377	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	87	GLN
1	A	25	GLN
1	A	87	GLN
1	A	600	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

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	E	1	1,3	14,14,15	0.53	0	17,19,21	1.45	2 (11%)
3	NAG	E	2	3	14,14,15	0.60	0	17,19,21	1.64	3 (17%)
3	NAG	F	1	1,3	14,14,15	0.50	0	17,19,21	1.28	3 (17%)
3	NAG	F	2	3	14,14,15	0.59	0	17,19,21	1.56	2 (11%)
4	NAG	G	1	1,4	14,14,15	0.51	0	17,19,21	1.35	2 (11%)
4	NAG	G	2	4	14,14,15	0.44	0	17,19,21	1.77	3 (17%)
4	BMA	G	3	4	11,11,12	0.95	1 (9%)	15,15,17	1.08	1 (6%)
4	FUC	G	4	4	10,10,11	0.61	0	14,14,16	1.47	2 (14%)
5	NAG	H	1	1,5	14,14,15	0.47	0	17,19,21	1.88	2 (11%)
5	NAG	H	2	5	14,14,15	0.53	0	17,19,21	0.77	0
5	BMA	H	3	5	11,11,12	0.85	0	15,15,17	0.80	0
6	NAG	I	1	1,6	14,14,15	0.62	0	17,19,21	1.31	2 (11%)
6	FUC	I	2	6	10,10,11	0.96	1 (10%)	14,14,16	1.79	3 (21%)
6	NAG	J	1	1,6	14,14,15	0.43	0	17,19,21	1.25	2 (11%)
6	FUC	J	2	6	10,10,11	0.81	1 (10%)	14,14,16	1.73	3 (21%)

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	E	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	E	2	3	-	4/6/23/26	0/1/1/1
3	NAG	F	1	1,3	-	5/6/23/26	0/1/1/1
3	NAG	F	2	3	-	4/6/23/26	0/1/1/1
4	NAG	G	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	G	2	4	-	2/6/23/26	0/1/1/1
4	BMA	G	3	4	-	0/2/19/22	0/1/1/1
4	FUC	G	4	4	-	-	0/1/1/1
5	NAG	H	1	1,5	-	2/6/23/26	0/1/1/1
5	NAG	H	2	5	-	5/6/23/26	0/1/1/1
5	BMA	H	3	5	-	2/2/19/22	0/1/1/1
6	NAG	I	1	1,6	-	1/6/23/26	0/1/1/1
6	FUC	I	2	6	-	-	0/1/1/1
6	NAG	J	1	1,6	-	3/6/23/26	0/1/1/1
6	FUC	J	2	6	-	-	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	G	3	BMA	C2-C3	2.21	1.55	1.52
6	I	2	FUC	C4-C3	2.10	1.57	1.52
6	J	2	FUC	C2-C3	2.10	1.55	1.52

The worst 5 of 30 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	H	1	NAG	C1-C2-N2	6.19	120.19	110.43
4	G	2	NAG	C1-C2-N2	5.08	118.45	110.43
3	E	2	NAG	C2-N2-C7	4.71	129.21	122.90
3	F	2	NAG	O5-C1-C2	4.62	118.44	111.29
6	J	2	FUC	C3-C4-C5	-4.43	103.08	109.81

There are no chirality outliers.

5 of 30 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	F	1	NAG	C3-C2-N2-C7
4	G	2	NAG	C8-C7-N2-C2
4	G	2	NAG	O7-C7-N2-C2

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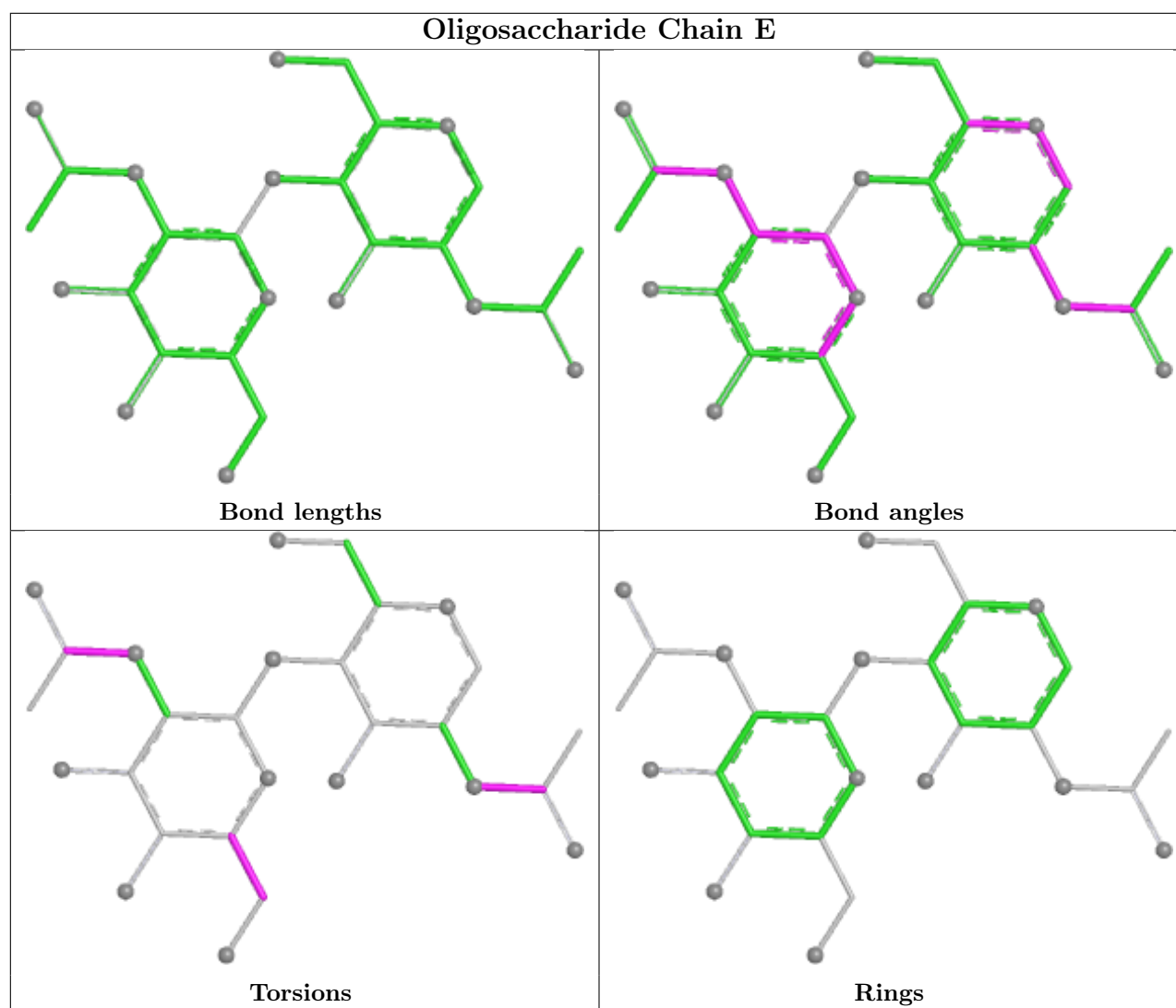
Mol	Chain	Res	Type	Atoms
5	H	1	NAG	C8-C7-N2-C2
5	H	1	NAG	O7-C7-N2-C2

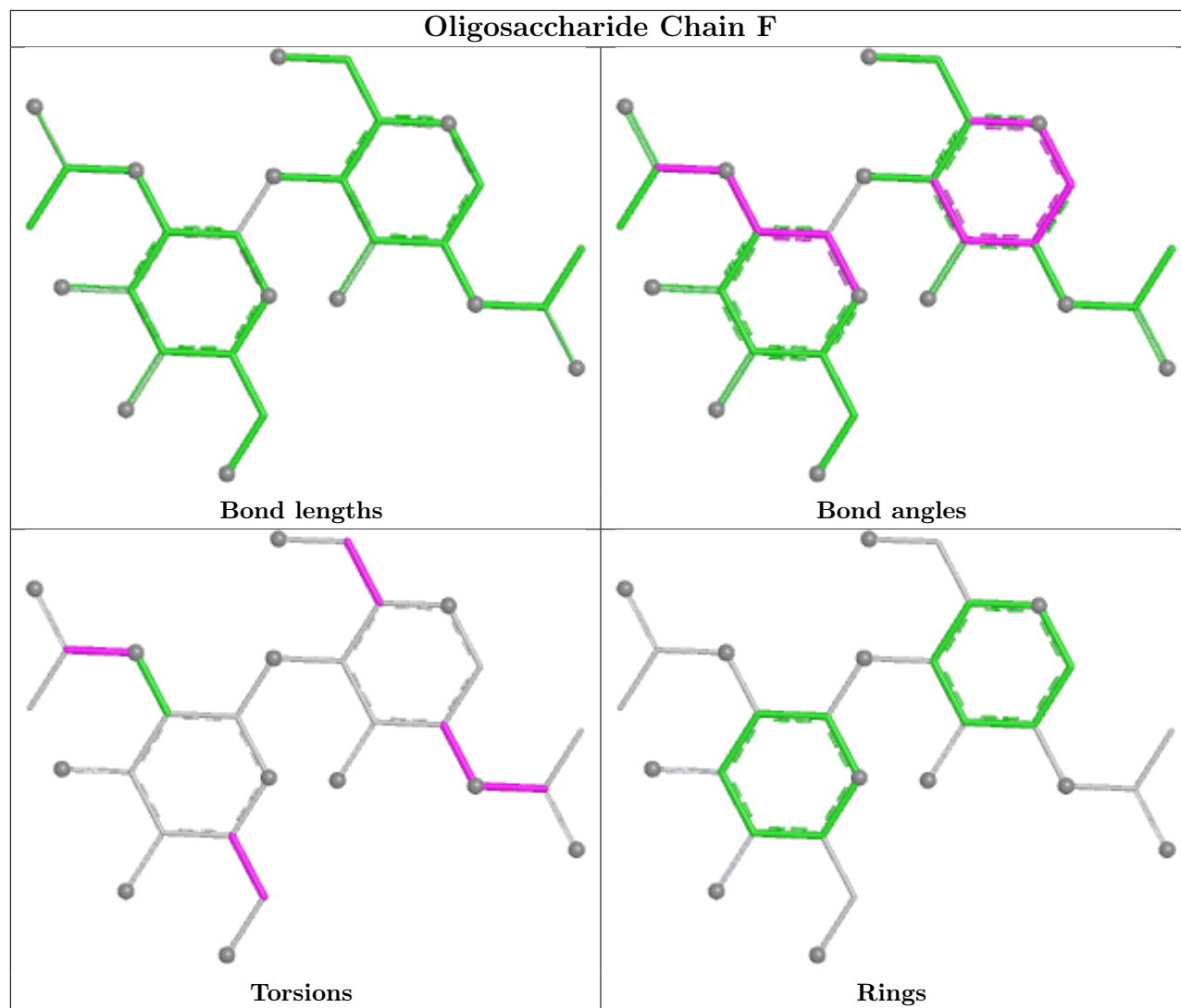
There are no ring outliers.

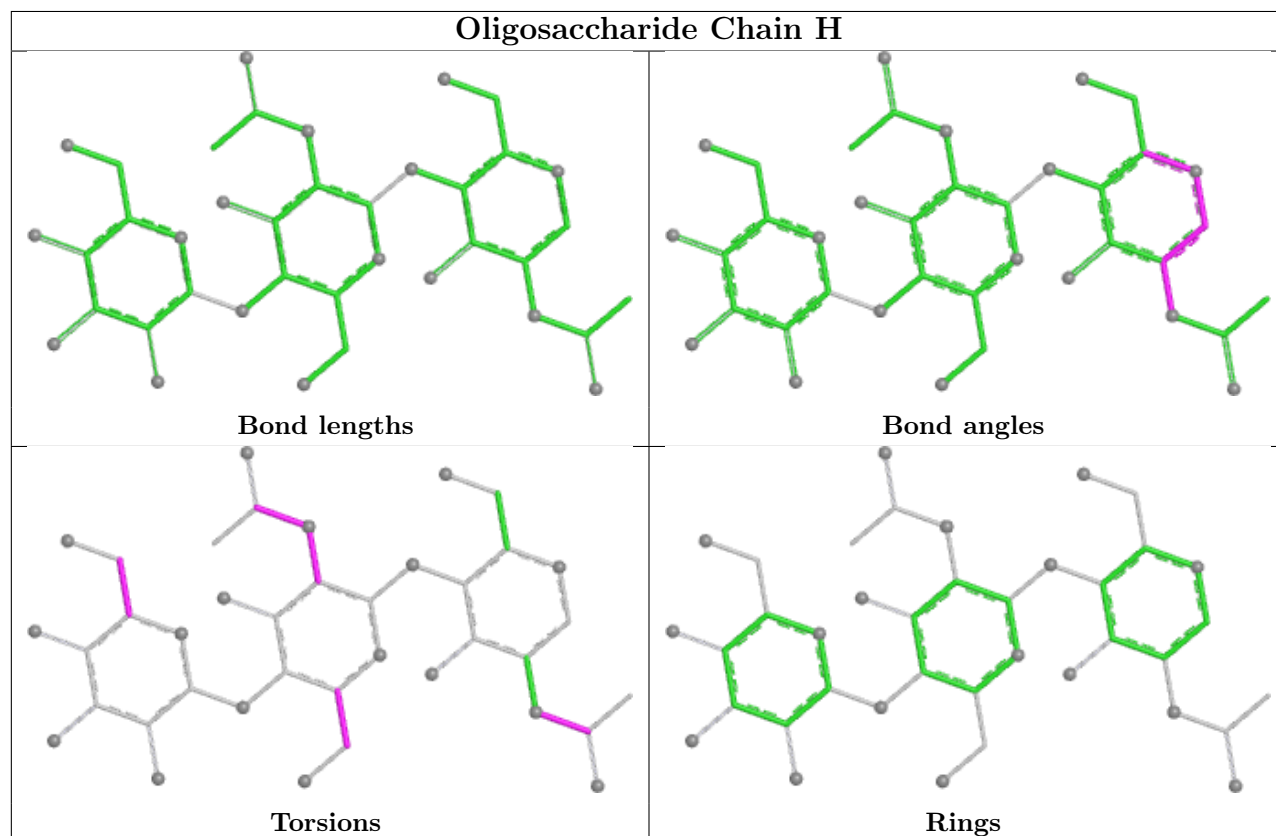
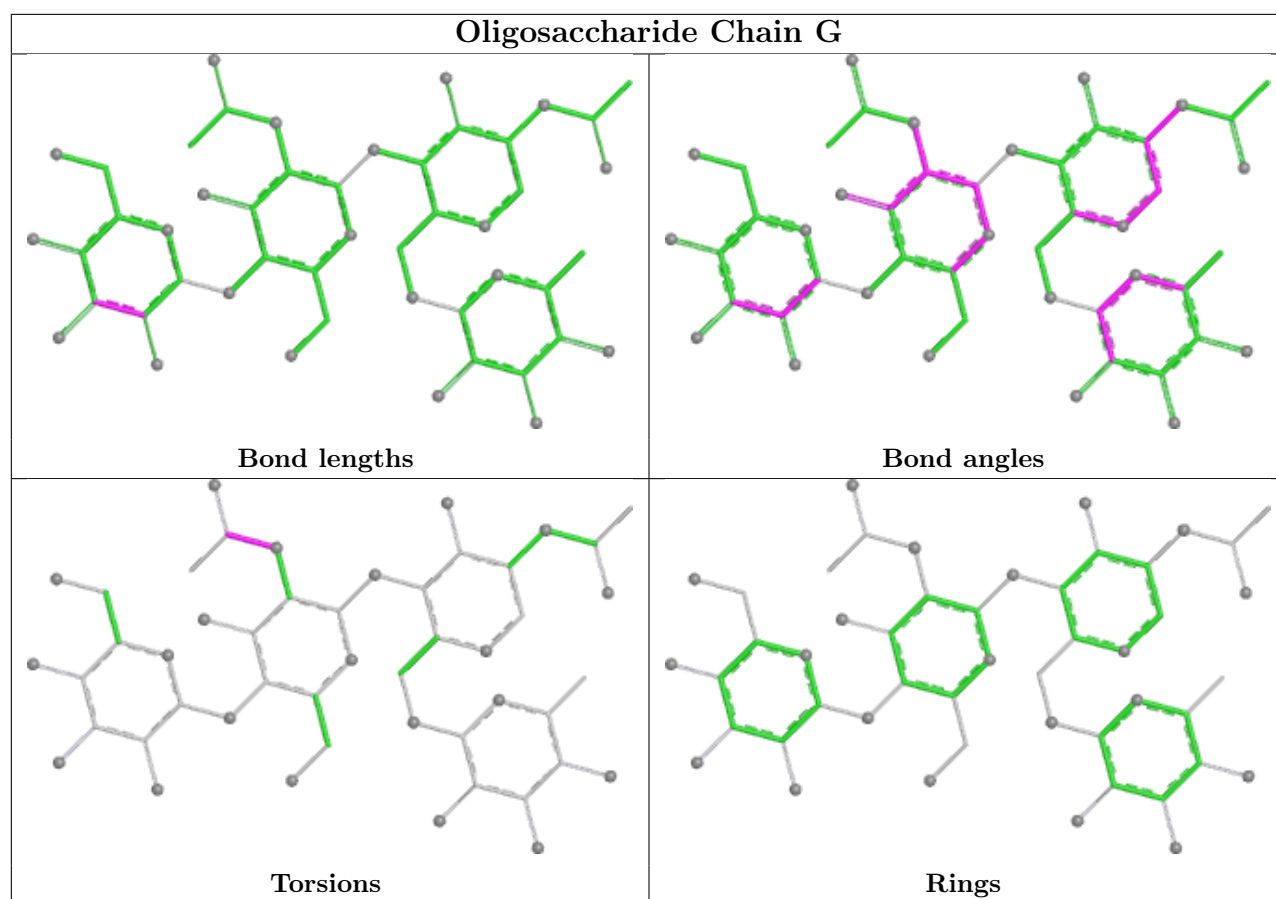
6 monomers are involved in 4 short contacts:

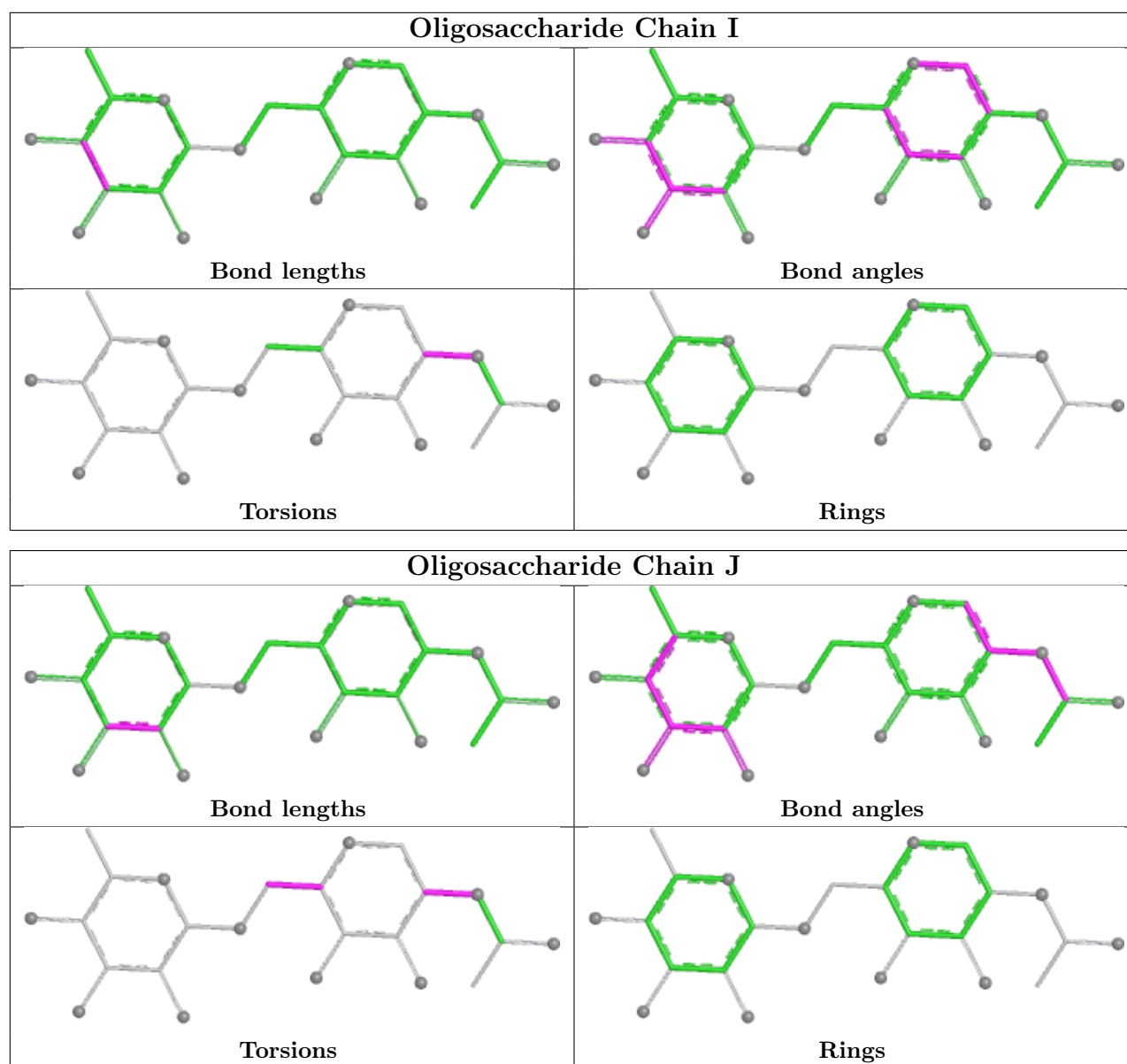
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	G	4	FUC	1	0
5	H	2	NAG	1	0
6	J	2	FUC	1	0
5	H	1	NAG	1	0
4	G	1	NAG	1	0
6	I	1	NAG	1	0

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









5.6 Ligand geometry [i](#)

Of 19 ligands modelled in this entry, 5 are monoatomic - leaving 14 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
9	PEG	A	710	-	6,6,6	0.16	0	5,5,5	0.16	0
12	PGE	B	709	-	9,9,9	0.32	0	8,8,8	0.29	0
9	PEG	B	708	-	6,6,6	0.41	0	5,5,5	0.37	0
11	PG4	B	707	-	12,12,12	0.30	0	11,11,11	0.26	0
9	PEG	B	703	-	6,6,6	0.34	0	5,5,5	0.41	0
15	1PE	A	708	-	15,15,15	0.51	0	14,14,14	0.39	0
9	PEG	A	705	-	6,6,6	0.20	0	5,5,5	0.27	0
11	PG4	A	707	-	12,12,12	0.61	0	11,11,11	0.46	0
13	BCN	A	704	-	10,10,10	1.13	1 (10%)	11,11,11	1.12	1 (9%)
10	EDO	B	705	-	3,3,3	0.26	0	2,2,2	0.44	0
15	1PE	A	709	-	15,15,15	0.58	0	14,14,14	0.41	0
9	PEG	A	703	-	6,6,6	0.26	0	5,5,5	0.16	0
10	EDO	B	704	-	3,3,3	0.18	0	2,2,2	0.14	0
9	PEG	B	706	-	6,6,6	0.60	0	5,5,5	0.76	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
9	PEG	A	710	-	-	3/4/4/4	-
12	PGE	B	709	-	-	3/7/7/7	-
9	PEG	B	708	-	-	2/4/4/4	-
11	PG4	B	707	-	-	6/10/10/10	-
9	PEG	B	703	-	-	2/4/4/4	-
15	1PE	A	708	-	-	6/13/13/13	-
9	PEG	A	705	-	-	4/4/4/4	-
11	PG4	A	707	-	-	7/10/10/10	-
13	BCN	A	704	-	-	5/10/10/10	-
10	EDO	B	705	-	-	1/1/1/1	-
15	1PE	A	709	-	-	6/13/13/13	-
9	PEG	A	703	-	-	4/4/4/4	-
10	EDO	B	704	-	-	0/1/1/1	-
9	PEG	B	706	-	-	1/4/4/4	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	A	704	BCN	C1-N1	2.35	1.52	1.47

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	A	704	BCN	C2-C1-N1	2.57	121.90	113.77

There are no chirality outliers.

5 of 50 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
13	A	704	BCN	C6-C5-N1-C1
13	A	704	BCN	N1-C1-C2-O21
9	A	705	PEG	C1-C2-O2-C3
11	B	707	PG4	C4-C3-O2-C2
13	A	704	BCN	N1-C1-C2-O22

There are no ring outliers.

9 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	B	708	PEG	1	0
11	B	707	PG4	1	0
15	A	708	1PE	5	0
11	A	707	PG4	2	0
13	A	704	BCN	1	0
10	B	705	EDO	1	0
9	A	703	PEG	1	0
10	B	704	EDO	1	0
9	B	706	PEG	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [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	605/628 (96%)	-0.07	20 (3%) 49 52	14, 41, 72, 107	4 (0%)
1	B	603/628 (96%)	-0.34	11 (1%) 67 71	12, 34, 59, 83	4 (0%)
2	C	3/3 (100%)	-0.73	0 100 100	26, 26, 28, 28	0
2	D	3/3 (100%)	-0.48	0 100 100	26, 26, 27, 28	0
All	All	1214/1262 (96%)	-0.21	31 (2%) 57 61	12, 37, 68, 107	8 (0%)

The worst 5 of 31 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	129	LEU	4.8
1	B	79	ILE	3.8
1	A	15	ALA	3.7
1	B	135	THR	3.6
1	A	135	THR	3.5

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.

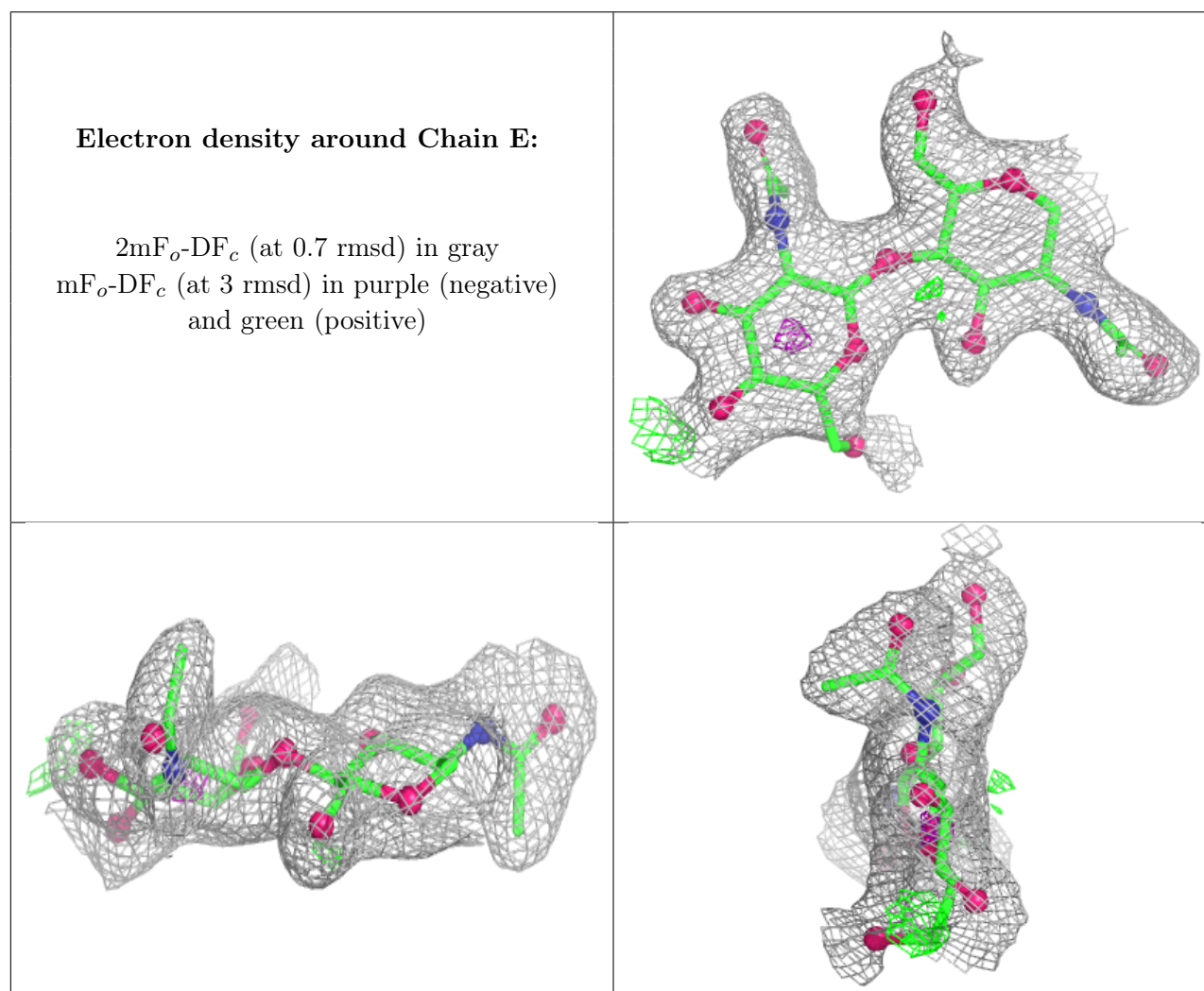
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	NAG	F	2	14/15	0.68	0.14	71,98,108,119	0
5	BMA	H	3	11/12	0.70	0.12	76,94,103,103	0

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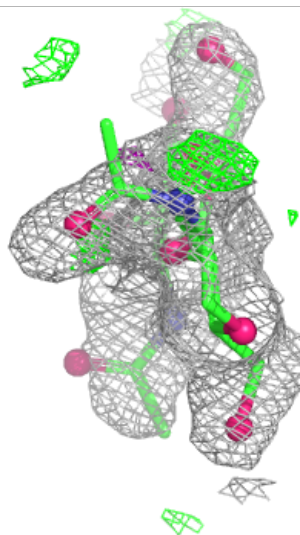
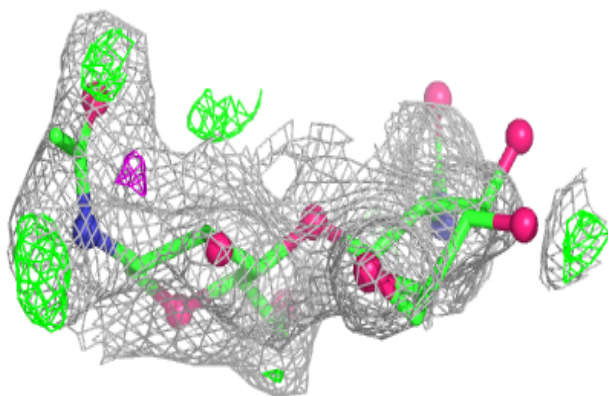
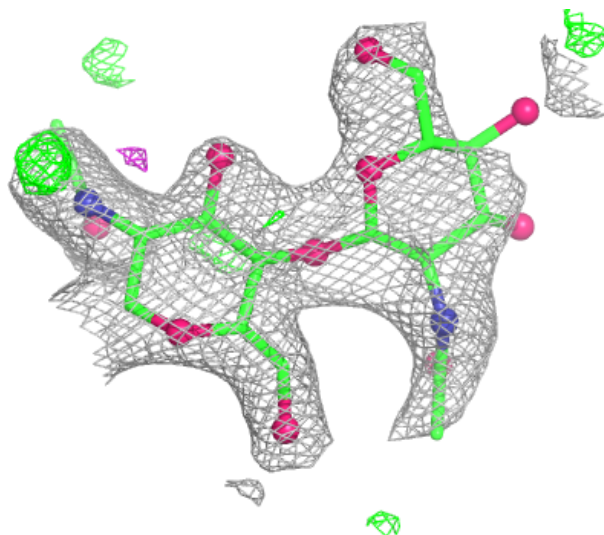
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
6	FUC	I	2	10/11	0.71	0.18	66,76,95,99	0
4	BMA	G	3	11/12	0.77	0.13	72,78,83,85	0
6	FUC	J	2	10/11	0.78	0.14	64,75,82,91	0
3	NAG	F	1	14/15	0.82	0.12	56,70,84,99	0
5	NAG	H	1	14/15	0.86	0.10	52,63,72,77	0
3	NAG	E	2	14/15	0.87	0.10	48,62,78,83	0
5	NAG	H	2	14/15	0.88	0.10	54,72,82,87	0
6	NAG	J	1	14/15	0.89	0.10	36,51,69,73	0
4	FUC	G	4	10/11	0.89	0.11	56,61,65,73	0
3	NAG	E	1	14/15	0.90	0.09	40,53,60,60	0
6	NAG	I	1	14/15	0.91	0.09	34,47,61,66	0
4	NAG	G	2	14/15	0.93	0.08	46,57,71,77	0
4	NAG	G	1	14/15	0.94	0.07	33,44,63,73	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.



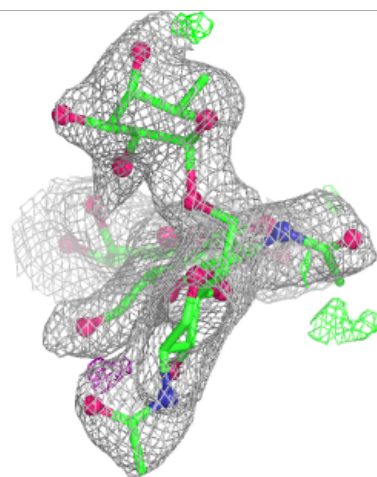
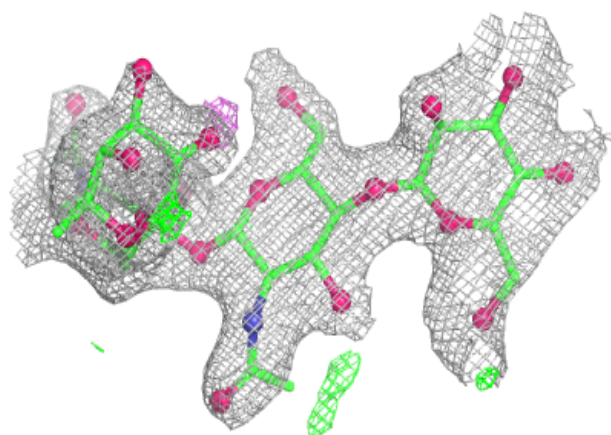
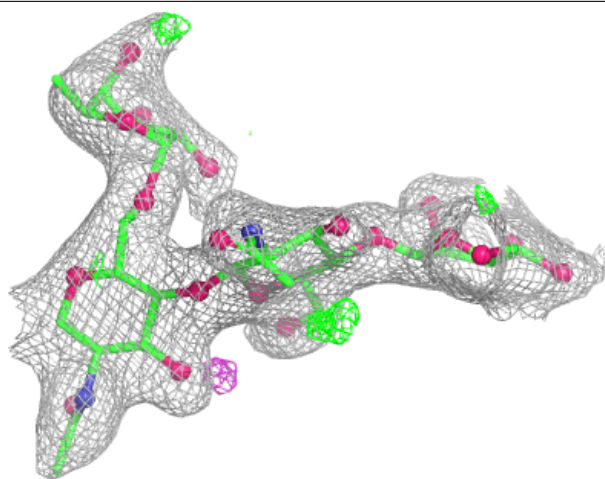
Electron density around Chain F:

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



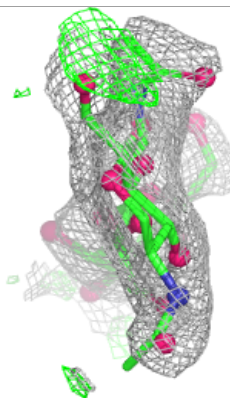
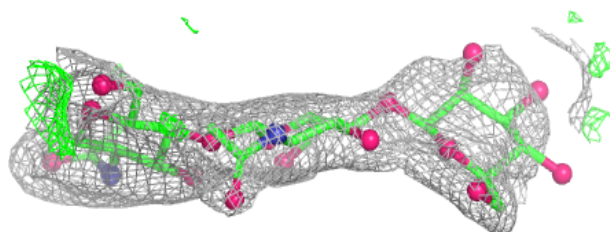
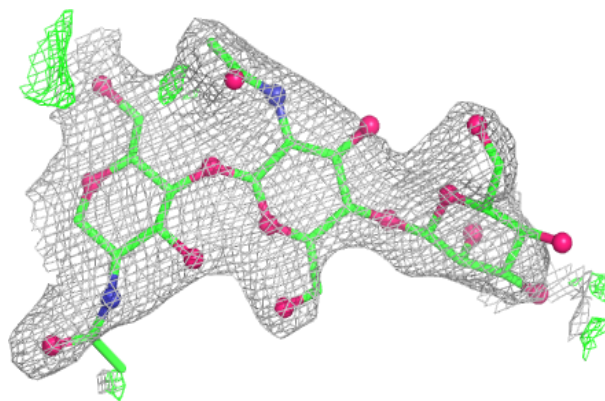
Electron density around Chain G:

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

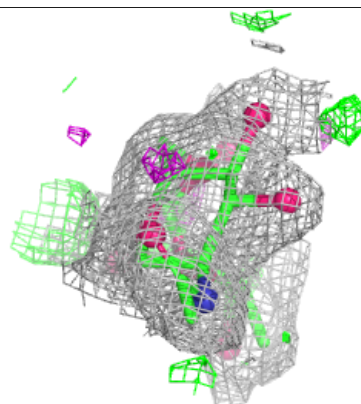
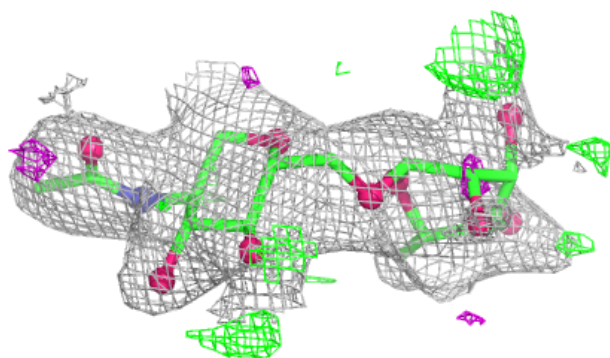
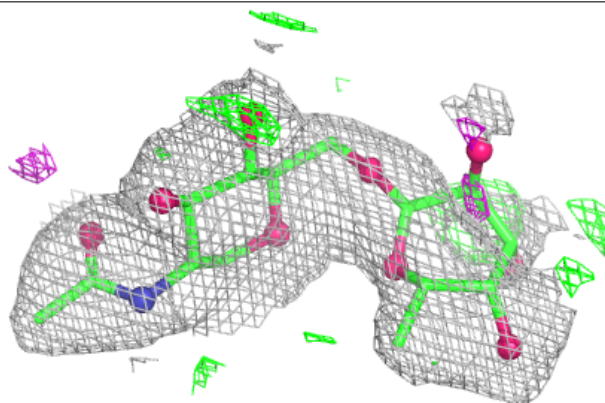


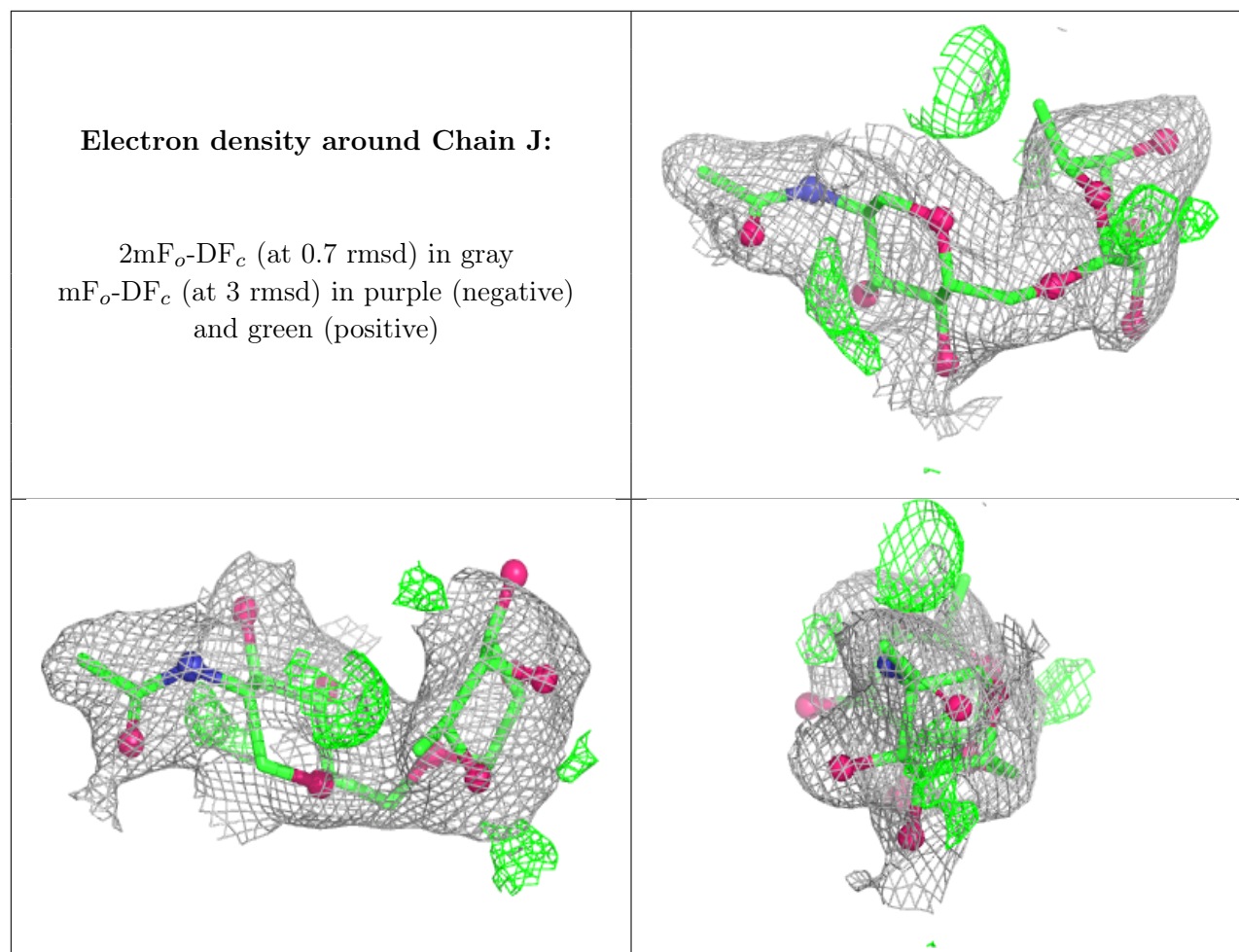
Electron density around Chain H:

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

**Electron density around Chain I:**

$2mF_o-DF_c$ (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
9	PEG	B	708	7/7	0.82	0.14	56,61,68,70	0
9	PEG	B	706	7/7	0.83	0.14	46,50,62,62	0
13	BCN	A	704	11/11	0.84	0.13	67,75,89,93	0
11	PG4	B	707	13/13	0.87	0.13	62,68,78,79	0
9	PEG	B	703	7/7	0.89	0.10	50,55,63,63	0
9	PEG	A	710	7/7	0.89	0.11	60,65,72,75	0
11	PG4	A	707	13/13	0.90	0.11	43,53,56,58	0
10	EDO	B	704	4/4	0.91	0.12	68,70,74,75	0
12	PGE	B	709	10/10	0.91	0.11	45,57,66,67	0
9	PEG	A	705	7/7	0.91	0.10	47,63,71,72	0
15	1PE	A	708	16/16	0.91	0.11	41,51,68,78	0

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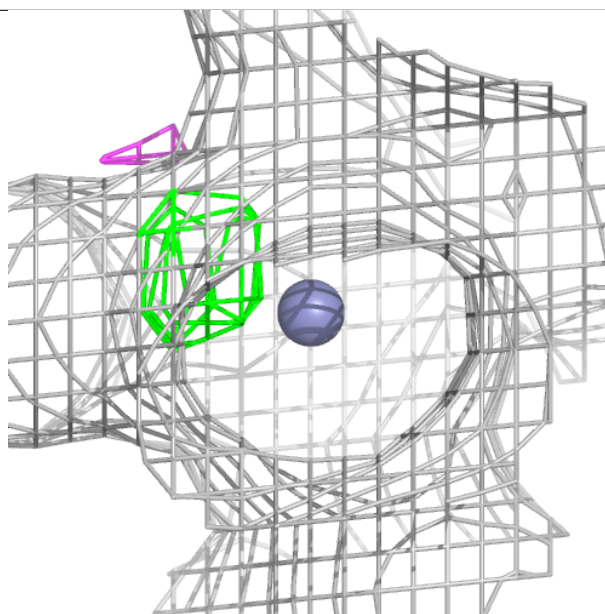
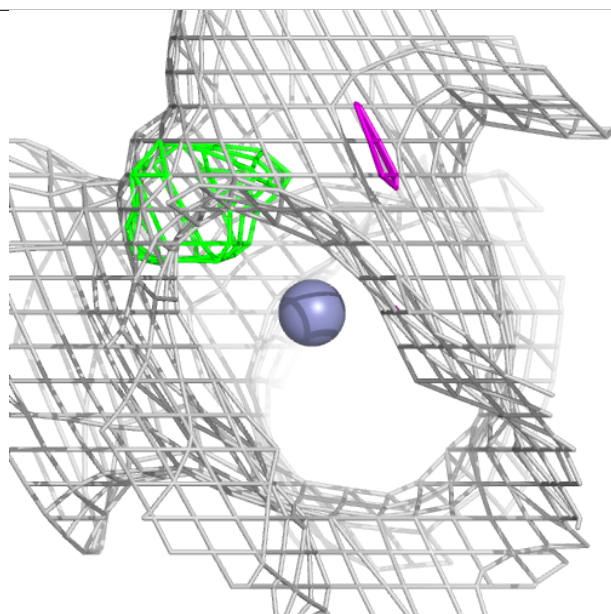
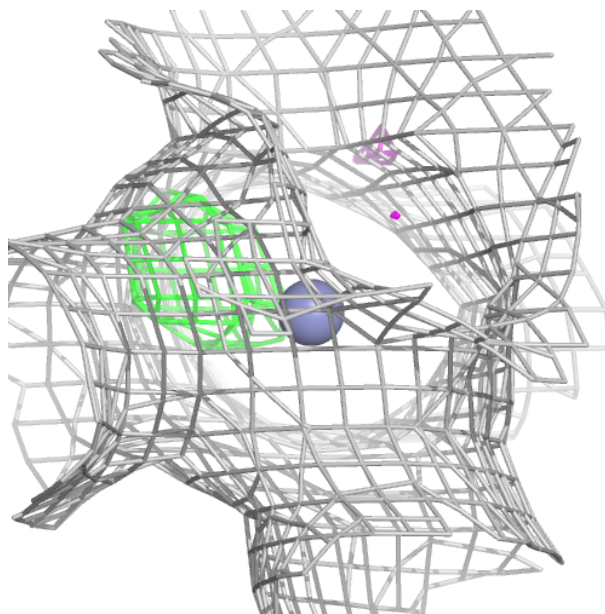
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
15	1PE	A	709	16/16	0.91	0.11	41,54,71,71	0
10	EDO	B	705	4/4	0.92	0.16	51,58,59,65	0
9	PEG	A	703	7/7	0.94	0.09	57,59,63,66	0
14	MG	A	706	1/1	0.97	0.08	49,49,49,49	0
7	ZN	B	701	1/1	0.99	0.02	25,25,25,25	0
7	ZN	A	701	1/1	0.99	0.03	27,27,27,27	0
8	CL	A	702	1/1	0.99	0.04	31,31,31,31	0
8	CL	B	702	1/1	1.00	0.05	24,24,24,24	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.

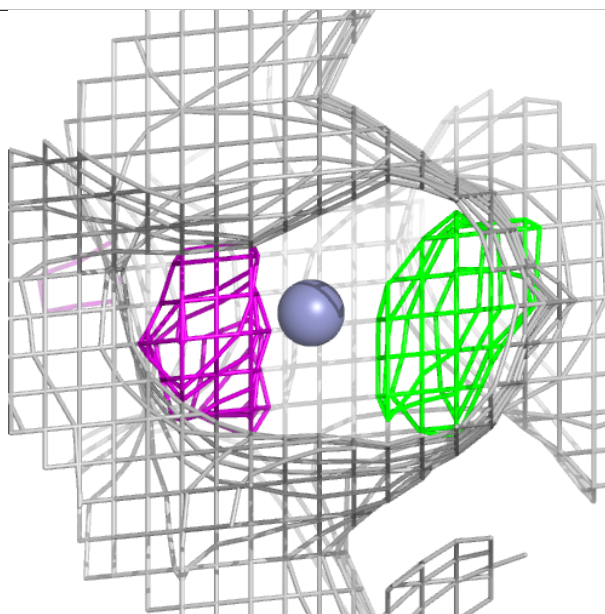
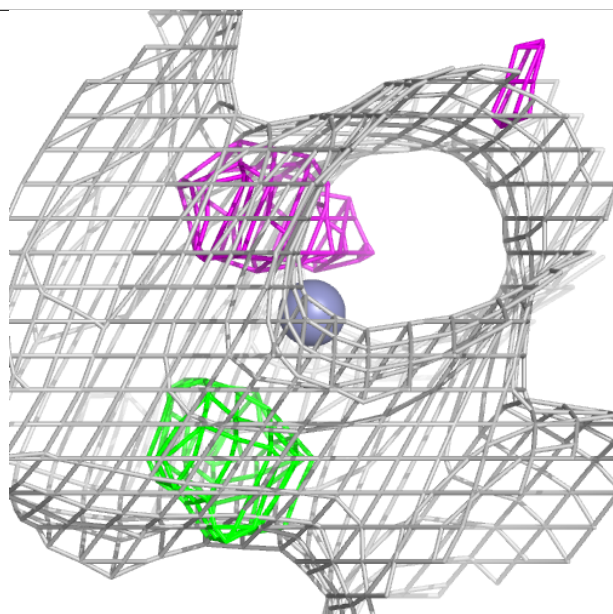
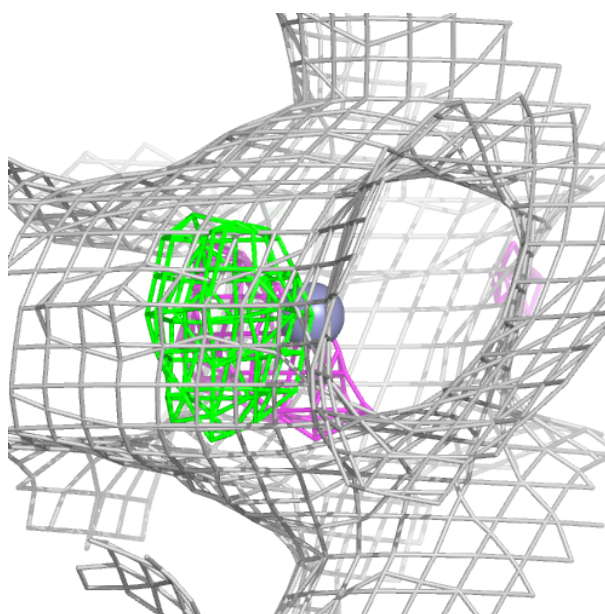
Electron density around ZN B 701:

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



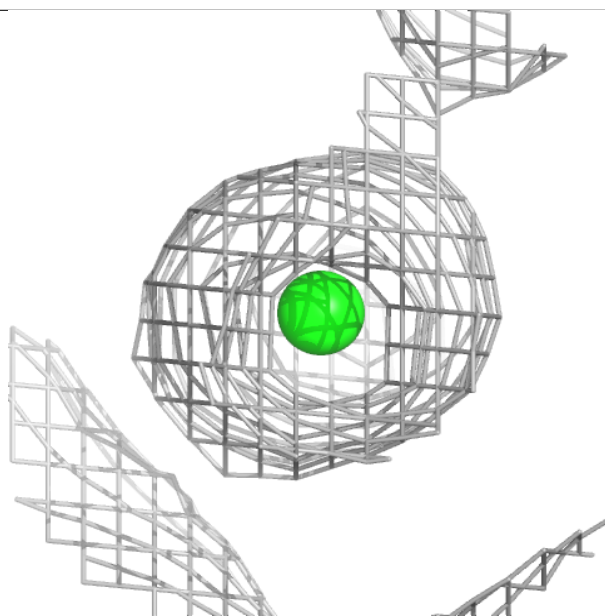
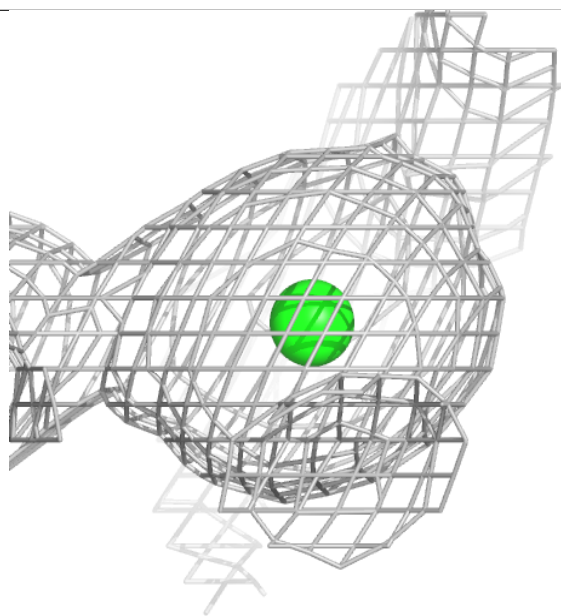
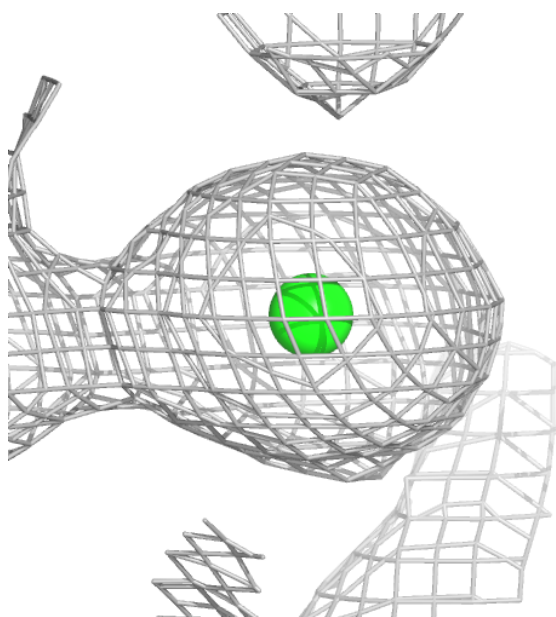
Electron density around ZN A 701:

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



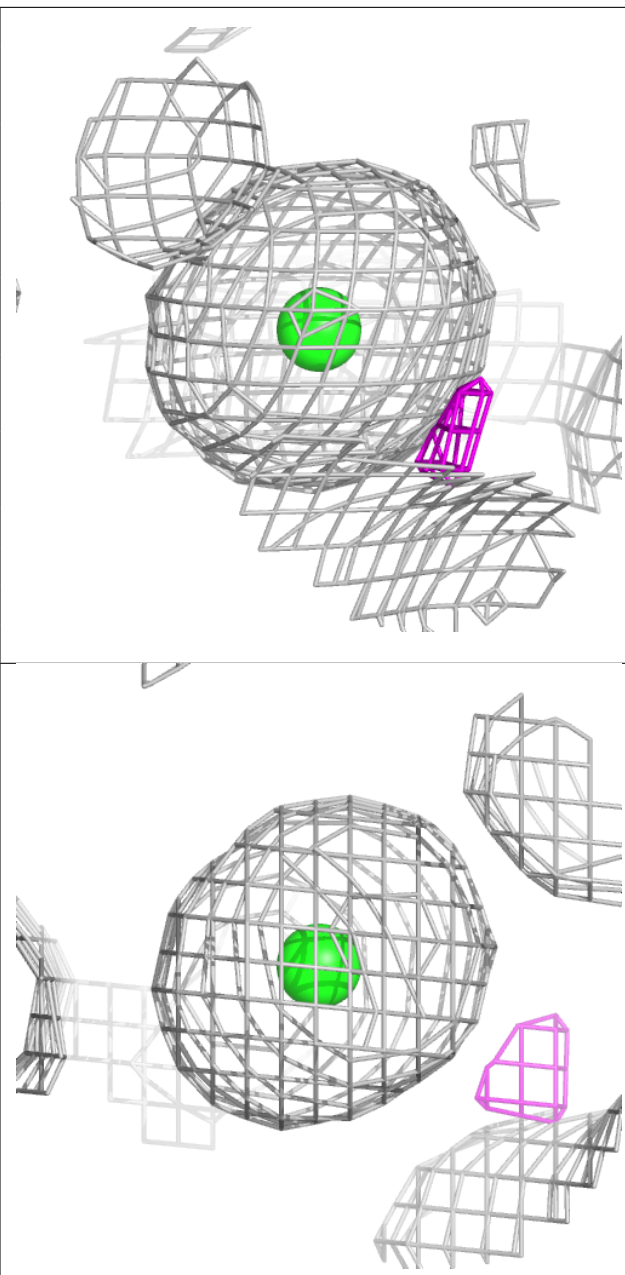
Electron density around CL A 702:

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



Electron density around CL 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)



6.5 Other polymers ⓘ

There are no such residues in this entry.