



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 9, 2026 – 03:40 PM UTC

PDB ID : 9SSB / pdb_00009ssb
Title : Human angiotensin 1-converting enzyme N-domain in complex with zofenopri-
lat
Authors : Gregory, K.S.; Acharya, K.R.
Deposited on : 2025-09-25
Resolution : 2.00 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4-5-2 with Phenix2.0
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

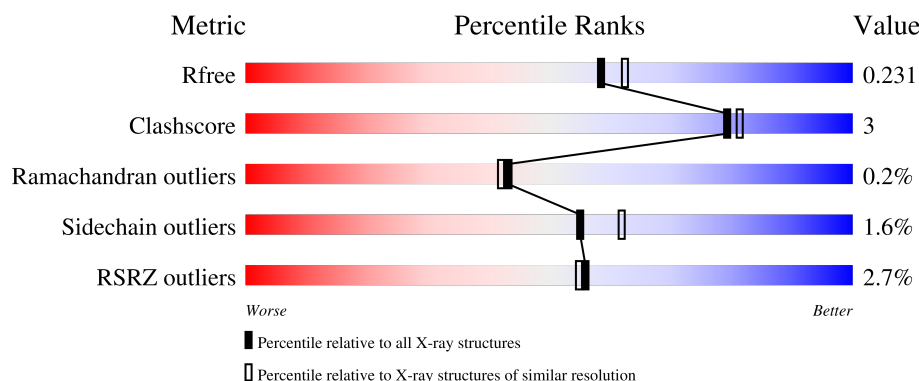
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 Å.

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




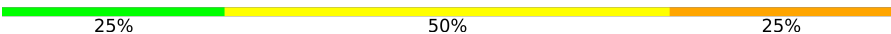
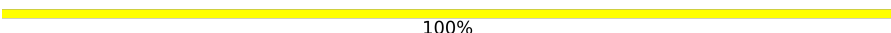
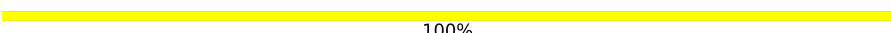
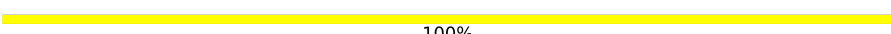
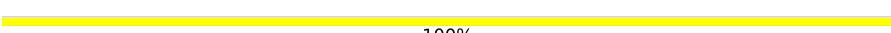
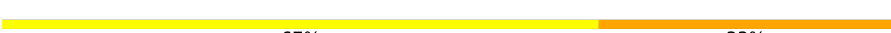



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (2.00-2.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	628	<div> <div>3%</div> <div>89%</div> <div>6%</div> <div>.</div> </div>
1	B	628	<div> <div>4%</div> <div>88%</div> <div>8%</div> <div>..</div> </div>
1	C	628	<div> <div>2%</div> <div>89%</div> <div>7%</div> <div>.</div> </div>
1	D	628	<div> <div>2%</div> <div>89%</div> <div>8%</div> <div>.</div> </div>
2	E	4	<div> <div>25%</div> <div>25%</div> <div>50%</div> </div>

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	K	4	 25% 75%
2	M	4	 25% 50% 25%
3	H	2	 100%
3	N	2	 100%
3	Q	2	 100%
4	O	3	 100%
5	P	3	 67% 33%
6	F	2	 100%
6	G	2	 100%
6	R	2	 50% 50%

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
9	PEG	A	705	-	-	X	-

2 Entry composition

There are 21 unique types of molecules in this entry. The entry contains 21759 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	603	Total	C	N	O	S	0	4	0
			4958	3186	850	902	20			
1	B	607	Total	C	N	O	S	0	7	0
			5012	3215	861	917	19			
1	C	601	Total	C	N	O	S	0	7	0
			4972	3191	856	905	20			
1	D	611	Total	C	N	O	S	0	10	0
			5060	3244	866	930	20			

There are 32 discrepancies between the modelled and reference sequences:

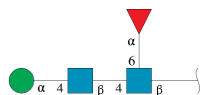
Chain	Residue	Modelled	Actual	Comment	Reference
A	9	GLN	ASN	conflict	UNP P12821
A	25	GLN	ASN	conflict	UNP P12821
A	82	GLN	ASN	conflict	UNP P12821
A	117	GLN	ASN	conflict	UNP P12821
A	131	GLN	ASN	conflict	UNP P12821
A	289	GLN	ASN	conflict	UNP P12821
A	545	ARG	GLN	conflict	UNP P12821
A	576	LEU	PRO	conflict	UNP P12821
B	9	GLN	ASN	conflict	UNP P12821
B	25	GLN	ASN	conflict	UNP P12821
B	82	GLN	ASN	conflict	UNP P12821
B	117	GLN	ASN	conflict	UNP P12821
B	131	GLN	ASN	conflict	UNP P12821
B	289	GLN	ASN	conflict	UNP P12821
B	545	ARG	GLN	conflict	UNP P12821
B	576	LEU	PRO	conflict	UNP P12821
C	9	GLN	ASN	conflict	UNP P12821
C	25	GLN	ASN	conflict	UNP P12821
C	82	GLN	ASN	conflict	UNP P12821
C	117	GLN	ASN	conflict	UNP P12821
C	131	GLN	ASN	conflict	UNP P12821

Continued on next page...

Continued from previous page...

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

- Molecule 2 is an oligosaccharide called alpha-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.



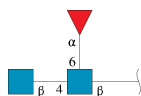
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	E	4	Total	C	N	O	0	0	0
			49	28	2	19			
2	K	4	Total	C	N	O	0	0	0
			49	28	2	19			
2	M	4	Total	C	N	O	0	0	0
			49	28	2	19			

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



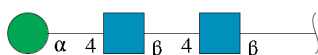
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	N	2	Total	C	N	O	0	0	0
			24	14	1	9			
3	H	2	Total	C	N	O	0	0	0
			24	14	1	9			
3	Q	2	Total	C	N	O	0	0	0
			24	14	1	9			

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



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

- Molecule 5 is an oligosaccharide called alpha-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	P	3	Total	C	N	O	0	0	0
			39	22	2	15			

- Molecule 6 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
6	F	2	Total	C	N	O	0	0	0
			28	16	2	10			
6	G	2	Total	C	N	O	0	0	0
			28	16	2	10			
6	R	2	Total	C	N	O	0	0	0
			28	16	2	10			

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

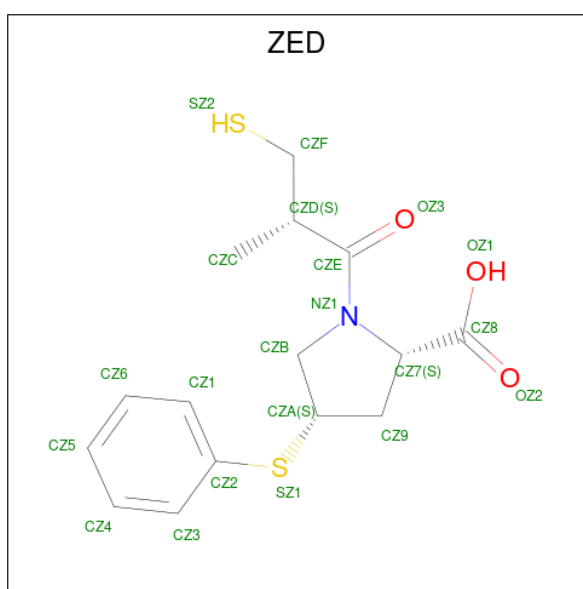
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	1	Total	Zn	0	0
			1	1		

Continued on next page...

Continued from previous page...

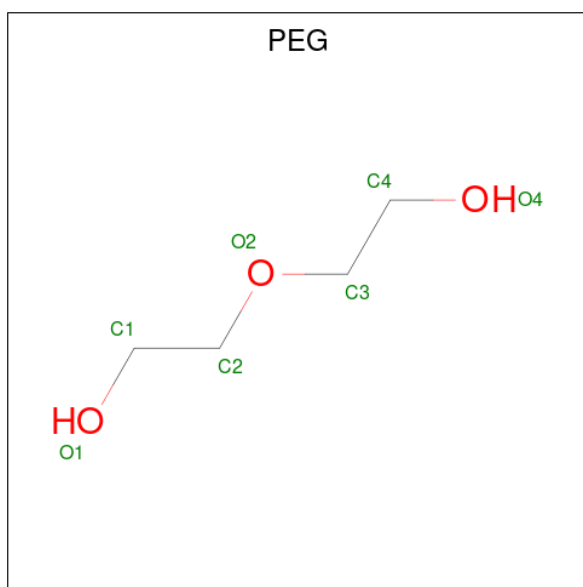
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	B	1	Total	Zn	0	0
			1	1		
7	C	1	Total	Zn	0	0
			1	1		
7	D	1	Total	Zn	0	0
			1	1		

- Molecule 8 is L-PROLINE, 1-[(2S)-3-MERCAPTO-2-METHYL-1-OXOPROPYL]-4-(PHE NYLTHIO)-, 4S (CCD ID: ZED) (formula: C₁₅H₁₉NO₃S₂) (labeled as "Ligand of Interest" by depositor).



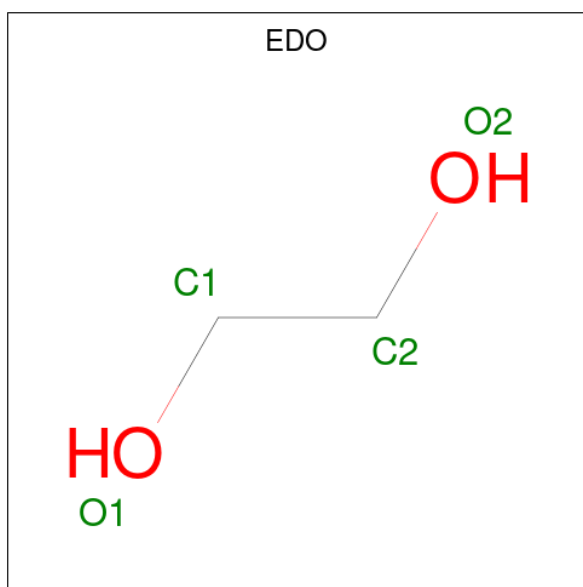
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
8	A	1	Total	C	N	O	S	0	0
			21	15	1	3	2		
8	B	1	Total	C	N	O	S	0	0
			21	15	1	3	2		
8	C	1	Total	C	N	O	S	0	0
			21	15	1	3	2		
8	D	1	Total	C	N	O	S	0	0
			21	15	1	3	2		

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



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

- Molecule 10 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



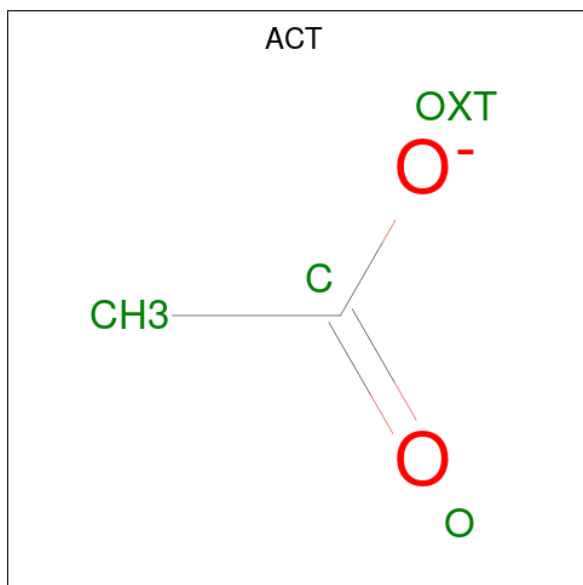
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	A	1	Total	C	O	0	0
			4	2	2		
10	A	1	Total	C	O	0	0
			4	2	2		
10	A	1	Total	C	O	0	0
			4	2	2		
10	A	1	Total	C	O	0	0
			4	2	2		
10	A	1	Total	C	O	0	0
			4	2	2		
10	B	1	Total	C	O	0	0
			4	2	2		
10	B	1	Total	C	O	0	0
			4	2	2		
10	B	1	Total	C	O	0	0
			4	2	2		
10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

Continued on next page...

Continued from previous page...

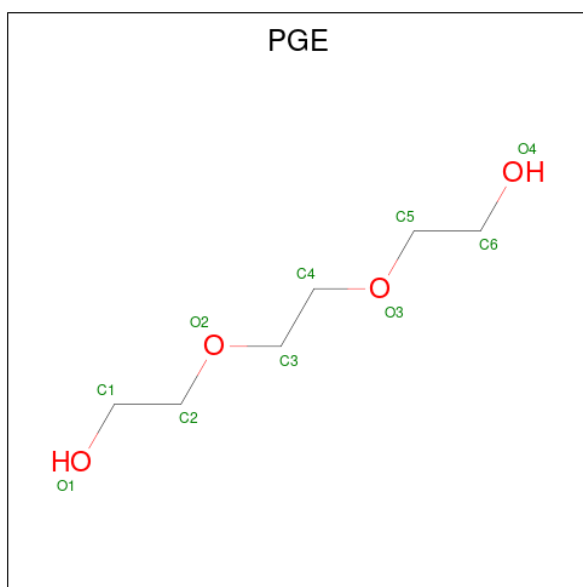
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	C	1	Total	C	O	0	0
			4	2	2		
10	D	1	Total	C	O	0	0
			4	2	2		
10	D	1	Total	C	O	0	0
			4	2	2		

- Molecule 11 is ACETATE ION (CCD ID: ACT) (formula: $C_2H_3O_2$).



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

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

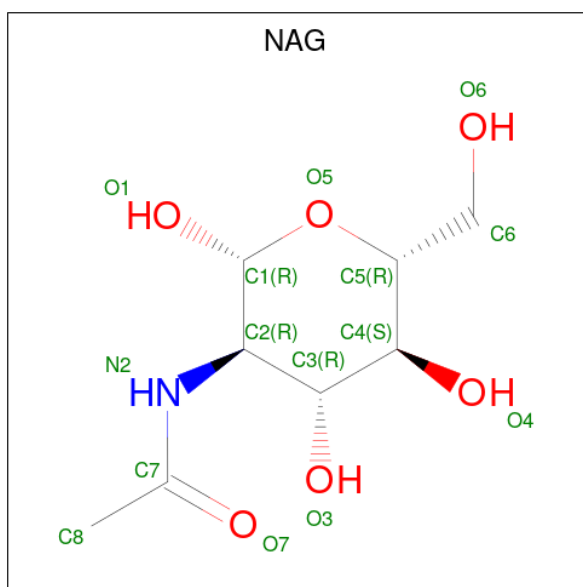


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
12	A	1	Total	C	O	0	0
			10	6	4		
12	C	1	Total	C	O	0	0
			10	6	4		
12	D	1	Total	C	O	0	0
			10	6	4		

- Molecule 13 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
13	A	1	Total	Ca	0	0
			1	1		
13	B	1	Total	Ca	0	0
			1	1		
13	C	1	Total	Ca	0	0
			1	1		
13	D	1	Total	Ca	0	0
			1	1		

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

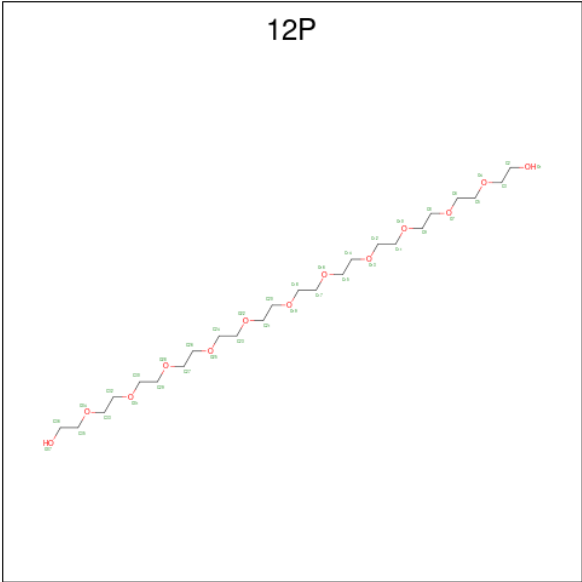


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
14	A	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 15 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

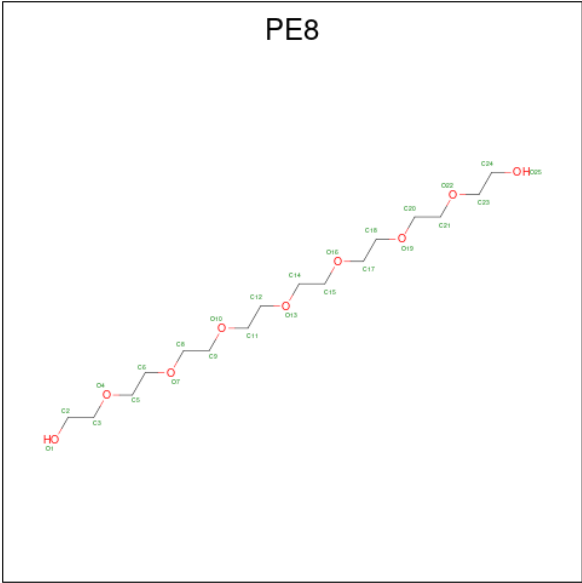
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
15	A	1	Total	Cl	0	0
			1	1		
15	B	1	Total	Cl	0	0
			1	1		
15	C	1	Total	Cl	0	0
			1	1		
15	D	1	Total	Cl	0	0
			1	1		

- Molecule 16 is DODECAETHYLENE GLYCOL (CCD ID: 12P) (formula: C₂₄H₅₀O₁₃).



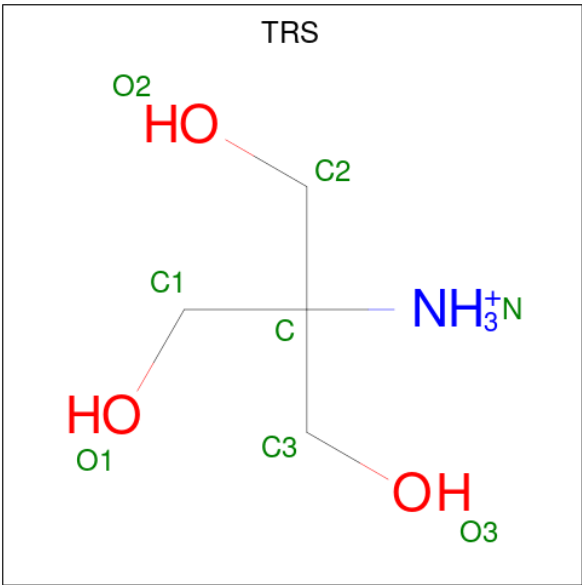
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
16	A	1	Total	C	O	0	1
			74	48	26		

- Molecule 17 is 3,6,9,12,15,18,21-HEPTAOXATRICOSANE-1,23-DIOL (CCD ID: PE8) (formula: C₁₆H₃₄O₉).



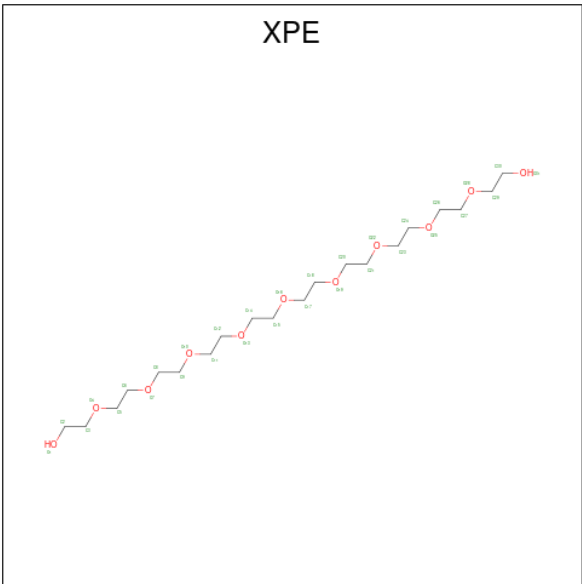
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
17	B	1	Total	C	O	0	0
			25	16	9		

- Molecule 18 is 2-AMINO-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (CCD ID: TRS) (formula: C₄H₁₂NO₃).



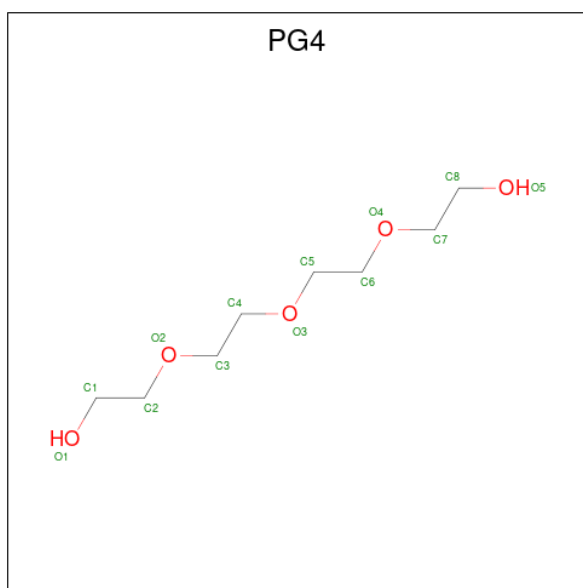
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
18	B	1	Total	C	N	O	0	0
			8	4	1	3		
18	C	1	Total	C	N	O	0	0
			8	4	1	3		

- Molecule 19 is 3,6,9,12,15,18,21,24,27-NONAOXANONACOSANE-1,29-DIOL (CCD ID: XPE) (formula: C₂₀H₄₂O₁₁).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
19	C	1	Total	C	O	0	0
			31	20	11		

- Molecule 20 is TETRAETHYLENE GLYCOL (CCD ID: PG4) (formula: $C_8H_{18}O_5$).



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

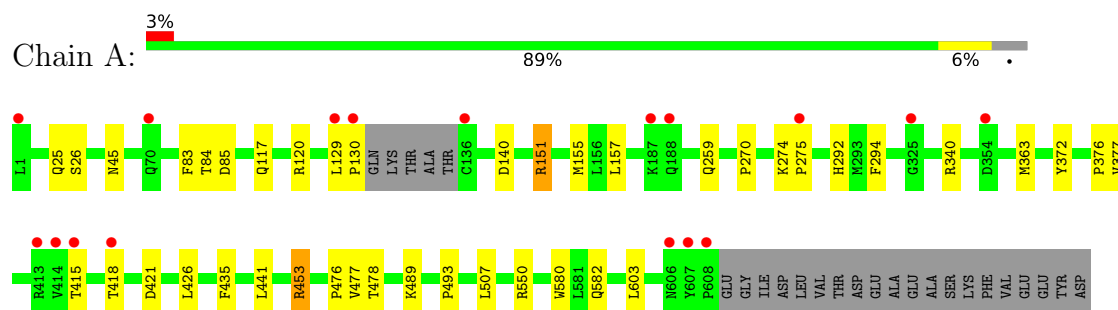
- Molecule 21 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
21	A	232	Total	O	0	0
			232	232		
21	B	259	Total	O	0	0
			259	259		
21	C	186	Total	O	0	0
			186	186		
21	D	266	Total	O	0	0
			266	266		

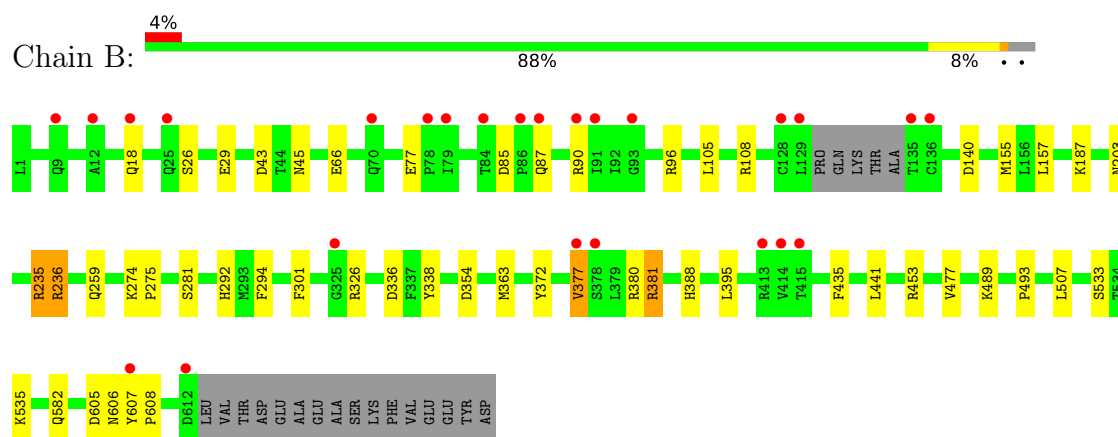
3 Residue-property plots [i](#)

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.

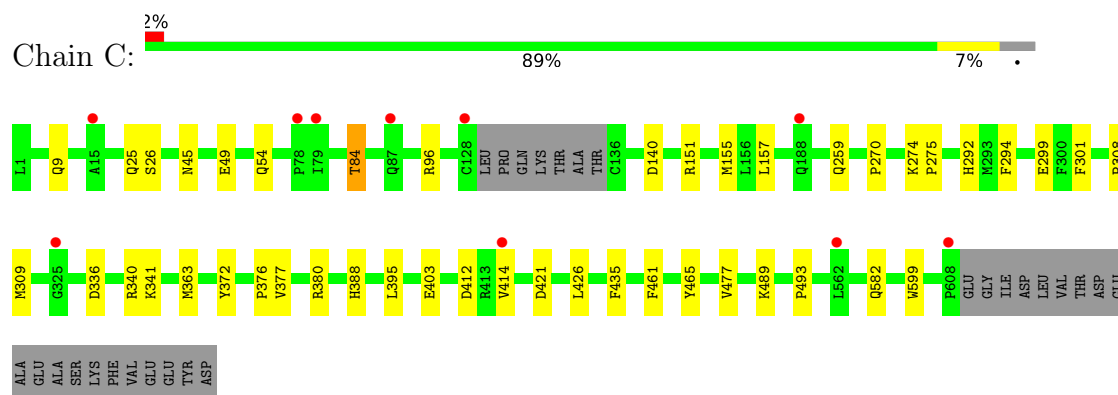
- Molecule 1: Angiotensin-converting enzyme, soluble form



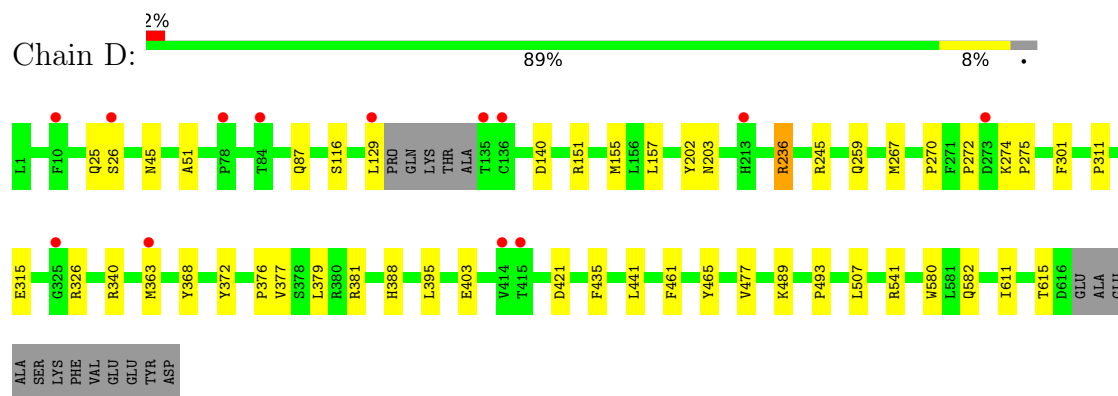
- Molecule 1: Angiotensin-converting enzyme, soluble form



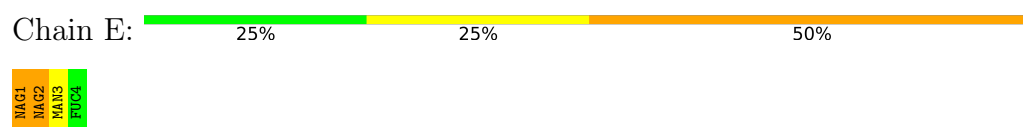
- Molecule 1: Angiotensin-converting enzyme, soluble form



- Molecule 1: Angiotensin-converting enzyme, soluble form



- Molecule 2: alpha-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



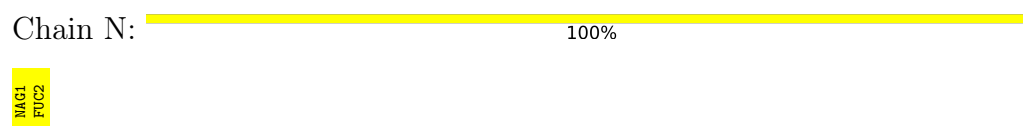
- Molecule 2: alpha-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose



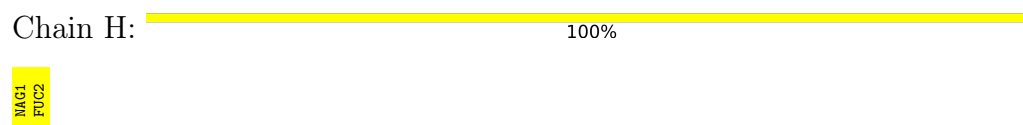
- Molecule 2: alpha-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose



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



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



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

Chain Q:  100%


MAG1
FUC2

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

Chain O:  100%

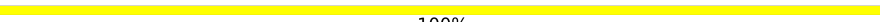
MAG1
MAG2
FUC3

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

Chain P:  67% 33%

MAG1
MAG2
MAN3

- Molecule 6: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain F:  100%

MAG1
MAG2

- Molecule 6: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain G:  100%

MAG1
MAG2

- Molecule 6: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain R:  50% 50%

MAG1
MAG2

4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	73.53Å 101.88Å 114.27Å 84.90° 85.46° 81.35°	Depositor
Resolution (Å)	72.53 – 2.00 72.53 – 2.00	Depositor EDS
% Data completeness (in resolution range)	98.1 (72.53-2.00) 98.1 (72.53-2.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.64 (at 2.00Å)	Xtriage
Refinement program	REFMAC 5.8.0431 (refmacat 0.4.105)	Depositor
R, R_{free}	0.201 , 0.226 0.207 , 0.231	Depositor DCC
R_{free} test set	10583 reflections (4.81%)	wwPDB-VP
Wilson B-factor (Å ²)	24.4	Xtriage
Anisotropy	0.458	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 30.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.52$, $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	21759	wwPDB-VP
Average B, all atoms (Å ²)	30.0	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 41.45 % 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 2.3573e-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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: FUC, PG4, MAN, 12P, CA, PE8, ZED, XPE, NAG, TRS, PGE, EDO, ACT, CL, PEG, ZN

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	0.61	0/5114	1.02	9/6966 (0.1%)
1	B	0.62	0/5167	1.04	9/7036 (0.1%)
1	C	0.61	0/5127	1.00	5/6981 (0.1%)
1	D	0.63	0/5215	1.02	5/7102 (0.1%)
All	All	0.62	0/20623	1.02	28/28085 (0.1%)

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	3
1	B	0	4
1	C	0	2
1	D	0	5
All	All	0	14

There are no bond length outliers.

The worst 5 of 28 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	236	ARG	CG-CD-NE	-7.74	94.97	112.00
1	C	582	GLN	CB-CA-C	-6.83	99.89	110.81
1	A	140	ASP	CA-CB-CG	6.41	119.01	112.60
1	A	582	GLN	CB-CA-C	-6.30	100.74	110.81
1	D	582	GLN	CB-CA-C	-6.30	100.74	110.81

There are no chirality outliers.

5 of 14 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	340	ARG	Sidechain
1	A	453	ARG	Sidechain
1	A	550	ARG	Sidechain
1	B	235	ARG	Sidechain
1	B	90	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	4958	0	4738	28	0
1	B	5012	0	4783	25	0
1	C	4972	0	4746	23	0
1	D	5060	0	4822	24	0
2	E	49	0	43	1	0
2	K	49	0	43	0	0
2	M	49	0	43	1	0
3	H	24	0	22	0	0
3	N	24	0	22	0	0
3	Q	24	0	22	0	0
4	O	38	0	34	0	0
5	P	39	0	34	1	0
6	F	28	0	25	0	0
6	G	28	0	25	2	0
6	R	28	0	25	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	21	0	17	0	0
8	B	21	0	17	0	0
8	C	21	0	17	0	0
8	D	21	0	17	0	0
9	A	21	0	30	6	0
9	B	14	0	20	1	0
9	C	21	0	30	1	0
9	D	7	0	10	0	0
10	A	20	0	30	2	0
10	B	16	0	24	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
10	C	24	0	36	0	0
10	D	8	0	12	0	0
11	A	4	0	3	1	0
12	A	10	0	14	0	0
12	C	10	0	14	5	0
12	D	10	0	14	0	0
13	A	1	0	0	0	0
13	B	1	0	0	0	0
13	C	1	0	0	0	0
13	D	1	0	0	0	0
14	A	14	0	13	0	0
15	A	1	0	0	0	0
15	B	1	0	0	0	0
15	C	1	0	0	0	0
15	D	1	0	0	0	0
16	A	74	0	98	8	0
17	B	25	0	34	2	0
18	B	8	0	12	1	0
18	C	8	0	12	1	0
19	C	31	0	42	1	0
20	D	13	0	18	0	0
21	A	232	0	0	1	1
21	B	259	0	0	5	0
21	C	186	0	0	2	0
21	D	266	0	0	1	1
All	All	21759	0	19961	109	1

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

The worst 5 of 109 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)
16:A:716[A]:12P:O19	16:A:716[A]:12P:H242	1.54	1.07
1:B:235:ARG:HB3	17:B:703:PE8:H22	1.63	0.78
1:D:236:ARG:CD	1:D:267:MET:HE3	2.19	0.71
16:A:716[A]:12P:O19	16:A:716[A]:12P:C24	2.35	0.71
1:C:599:TRP:HA	9:C:706:PEG:H32	1.74	0.70

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:A:996:HOH:O	21:D:845:HOH:O[1_454]	2.19	0.01

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	603/628 (96%)	597 (99%)	5 (1%)	1 (0%)	43	42
1	B	610/628 (97%)	602 (99%)	7 (1%)	1 (0%)	43	42
1	C	604/628 (96%)	595 (98%)	8 (1%)	1 (0%)	43	42
1	D	617/628 (98%)	607 (98%)	9 (2%)	1 (0%)	43	42
All	All	2434/2512 (97%)	2401 (99%)	29 (1%)	4 (0%)	43	42

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	45	ASN
1	D	45	ASN
1	B	45	ASN
1	C	45	ASN

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	523/540 (97%)	517 (99%)	6 (1%)	65	73
1	B	529/540 (98%)	522 (99%)	7 (1%)	61	68

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	524/540 (97%)	512 (98%)	12 (2%)	44	49
1	D	535/540 (99%)	525 (98%)	10 (2%)	50	56
All	All	2111/2160 (98%)	2076 (98%)	35 (2%)	55	60

5 of 35 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	363	MET
1	D	368	TYR
1	D	388	HIS
1	B	535	LYS
1	B	388	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 28 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	579	GLN
1	D	582	GLN
1	C	213	HIS
1	D	213	HIS
1	C	109	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 ⓘ

30 monosaccharides are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the

expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	NAG	E	1	2,1	14,14,15	0.49	0	17,19,21	1.47	2 (11%)
2	NAG	E	2	2	14,14,15	0.38	0	17,19,21	1.19	2 (11%)
2	MAN	E	3	2	11,11,12	0.58	0	15,15,17	0.99	1 (6%)
2	FUC	E	4	2	10,10,11	0.42	0	14,14,16	0.48	0
6	NAG	F	1	6,1	14,14,15	0.56	0	17,19,21	1.22	2 (11%)
6	NAG	F	2	6	14,14,15	0.41	0	17,19,21	1.18	2 (11%)
6	NAG	G	1	6,1	14,14,15	0.36	0	17,19,21	1.41	2 (11%)
6	NAG	G	2	6	14,14,15	0.40	0	17,19,21	0.95	1 (5%)
3	NAG	H	1	3,1	14,14,15	0.45	0	17,19,21	1.54	2 (11%)
3	FUC	H	2	3	10,10,11	0.49	0	14,14,16	1.11	1 (7%)
2	NAG	K	1	2,1	14,14,15	0.58	0	17,19,21	1.04	1 (5%)
2	NAG	K	2	2	14,14,15	0.37	0	17,19,21	1.44	1 (5%)
2	MAN	K	3	2	11,11,12	0.55	0	15,15,17	1.64	2 (13%)
2	FUC	K	4	2	10,10,11	0.52	0	14,14,16	0.71	0
2	NAG	M	1	2,1	14,14,15	0.37	0	17,19,21	1.20	2 (11%)
2	NAG	M	2	2	14,14,15	0.25	0	17,19,21	0.78	0
2	MAN	M	3	2	11,11,12	0.55	0	15,15,17	1.05	1 (6%)
2	FUC	M	4	2	10,10,11	0.44	0	14,14,16	1.26	1 (7%)
3	NAG	N	1	3,1	14,14,15	0.42	0	17,19,21	1.08	1 (5%)
3	FUC	N	2	3	10,10,11	0.48	0	14,14,16	1.39	1 (7%)
4	NAG	O	1	4,1	14,14,15	0.71	0	17,19,21	1.06	1 (5%)
4	NAG	O	2	4	14,14,15	0.48	0	17,19,21	1.33	2 (11%)
4	FUC	O	3	4	10,10,11	0.50	0	14,14,16	1.29	1 (7%)
5	NAG	P	1	5,1	14,14,15	0.41	0	17,19,21	1.34	1 (5%)
5	NAG	P	2	5	14,14,15	0.34	0	17,19,21	1.01	1 (5%)
5	MAN	P	3	5	11,11,12	0.68	1 (9%)	15,15,17	1.29	2 (13%)
3	NAG	Q	1	3,1	14,14,15	0.42	0	17,19,21	1.01	2 (11%)
3	FUC	Q	2	3	10,10,11	0.40	0	14,14,16	1.02	1 (7%)
6	NAG	R	1	6,1	14,14,15	0.30	0	17,19,21	0.70	0
6	NAG	R	2	6	14,14,15	0.38	0	17,19,21	0.76	1 (5%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns.

'-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	E	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	E	2	2	-	2/6/23/26	0/1/1/1
2	MAN	E	3	2	-	2/2/19/22	0/1/1/1
2	FUC	E	4	2	-	-	0/1/1/1
6	NAG	F	1	6,1	-	2/6/23/26	0/1/1/1
6	NAG	F	2	6	-	3/6/23/26	0/1/1/1
6	NAG	G	1	6,1	-	2/6/23/26	0/1/1/1
6	NAG	G	2	6	-	2/6/23/26	0/1/1/1
3	NAG	H	1	3,1	-	1/6/23/26	0/1/1/1
3	FUC	H	2	3	-	-	0/1/1/1
2	NAG	K	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	K	2	2	-	4/6/23/26	0/1/1/1
2	MAN	K	3	2	-	1/2/19/22	0/1/1/1
2	FUC	K	4	2	-	-	0/1/1/1
2	NAG	M	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	M	2	2	-	0/6/23/26	0/1/1/1
2	MAN	M	3	2	-	2/2/19/22	0/1/1/1
2	FUC	M	4	2	-	-	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
4	NAG	O	1	4,1	-	2/6/23/26	0/1/1/1
4	NAG	O	2	4	-	4/6/23/26	0/1/1/1
4	FUC	O	3	4	-	-	0/1/1/1
5	NAG	P	1	5,1	-	5/6/23/26	0/1/1/1
5	NAG	P	2	5	-	2/6/23/26	0/1/1/1
5	MAN	P	3	5	-	0/2/19/22	1/1/1/1
3	NAG	Q	1	3,1	-	2/6/23/26	0/1/1/1
3	FUC	Q	2	3	-	-	0/1/1/1
6	NAG	R	1	6,1	-	1/6/23/26	0/1/1/1
6	NAG	R	2	6	-	0/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	P	3	MAN	O5-C5	2.13	1.47	1.43

The worst 5 of 37 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	K	3	MAN	C1-O5-C5	4.57	118.32	112.19
2	K	2	NAG	C1-C2-N2	4.47	117.47	110.43
2	E	1	NAG	C2-N2-C7	4.39	128.78	122.90
5	P	1	NAG	C2-N2-C7	4.07	128.36	122.90
3	H	1	NAG	C1-C2-N2	4.07	116.84	110.43

There are no chirality outliers.

5 of 39 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	H	1	NAG	C1-C2-N2-C7
5	P	1	NAG	C8-C7-N2-C2
5	P	1	NAG	O7-C7-N2-C2
6	F	1	NAG	C8-C7-N2-C2
6	F	2	NAG	C1-C2-N2-C7

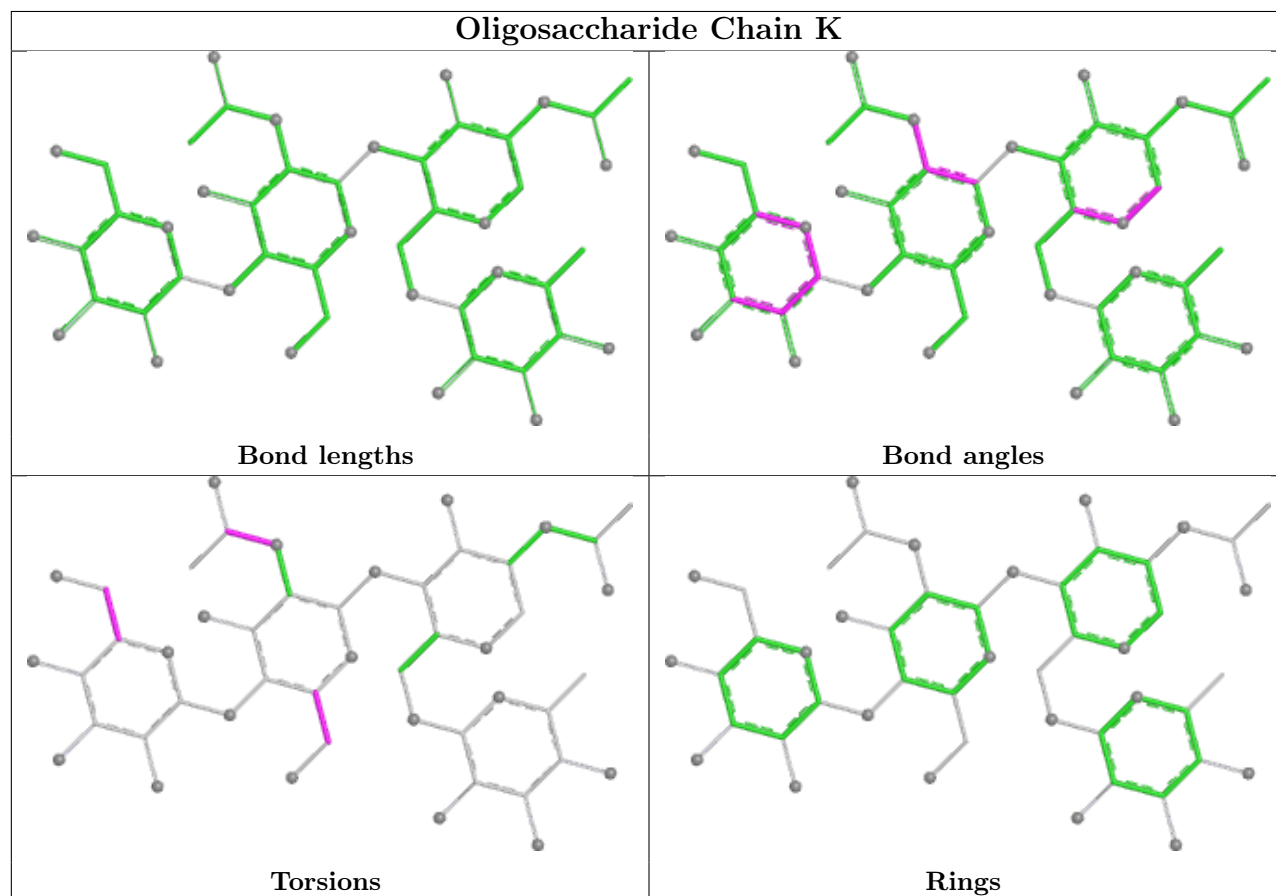
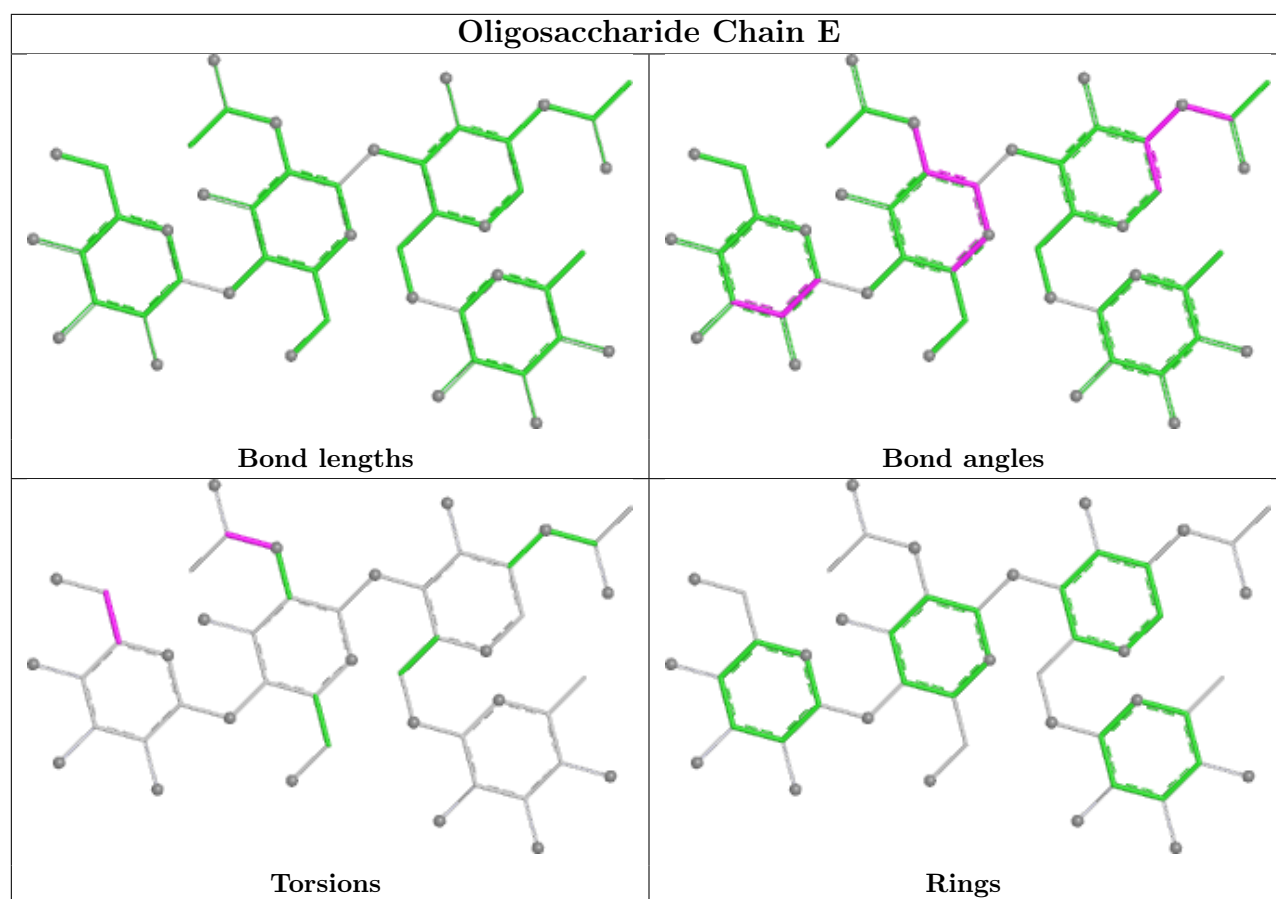
All (1) ring outliers are listed below:

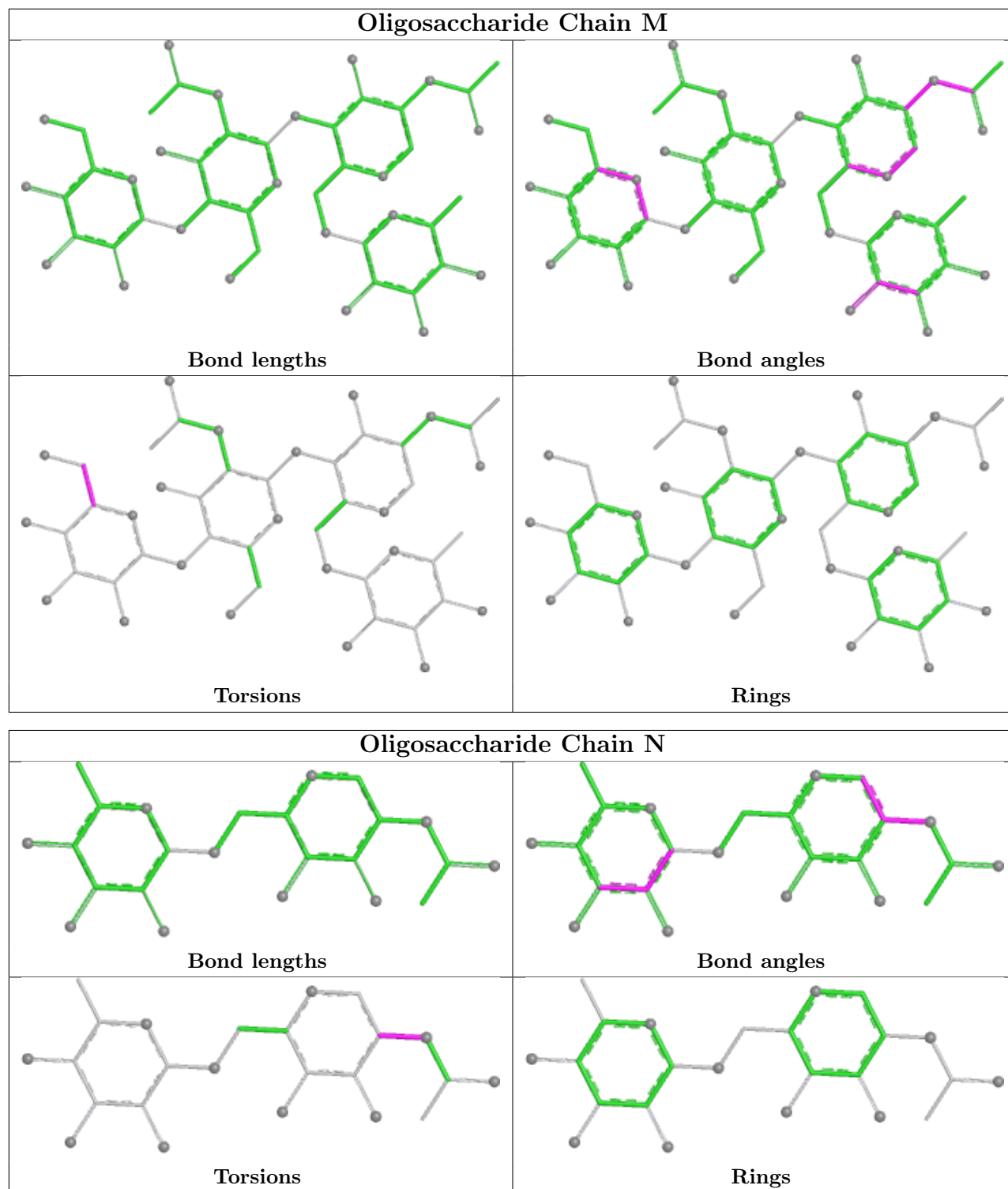
Mol	Chain	Res	Type	Atoms
5	P	3	MAN	C1-C2-C3-C4-C5-O5

6 monomers are involved in 5 short contacts:

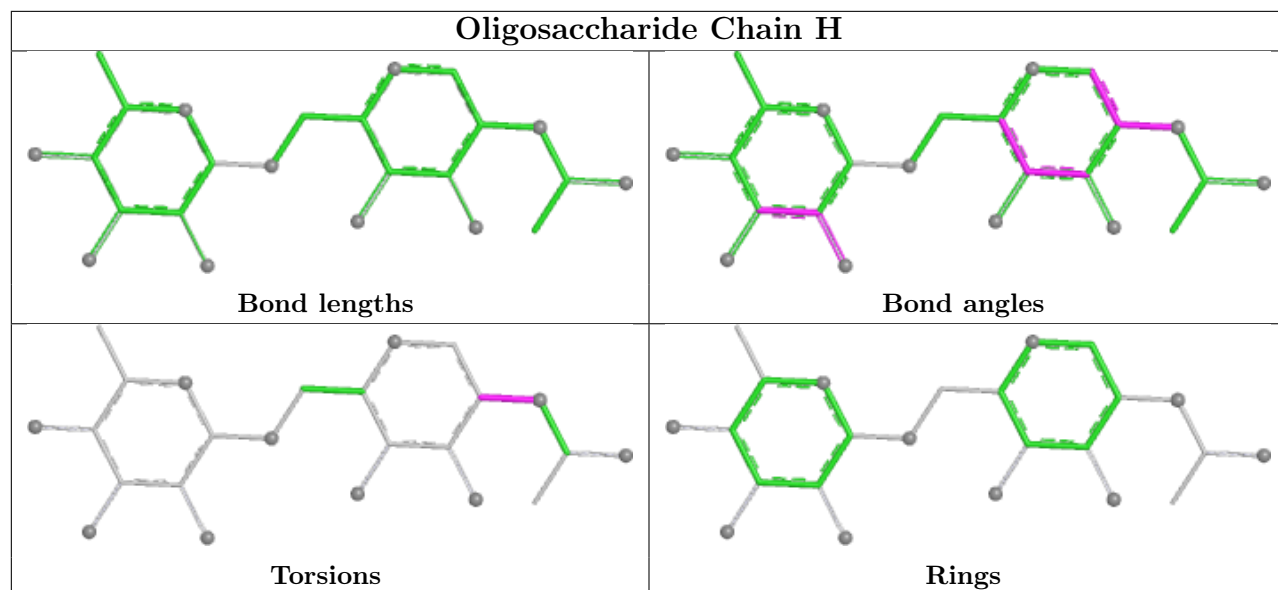
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	1	NAG	1	0
6	G	1	NAG	1	0
2	M	4	FUC	1	0
6	G	2	NAG	2	0
5	P	1	NAG	1	0
2	E	2	NAG	1	0

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

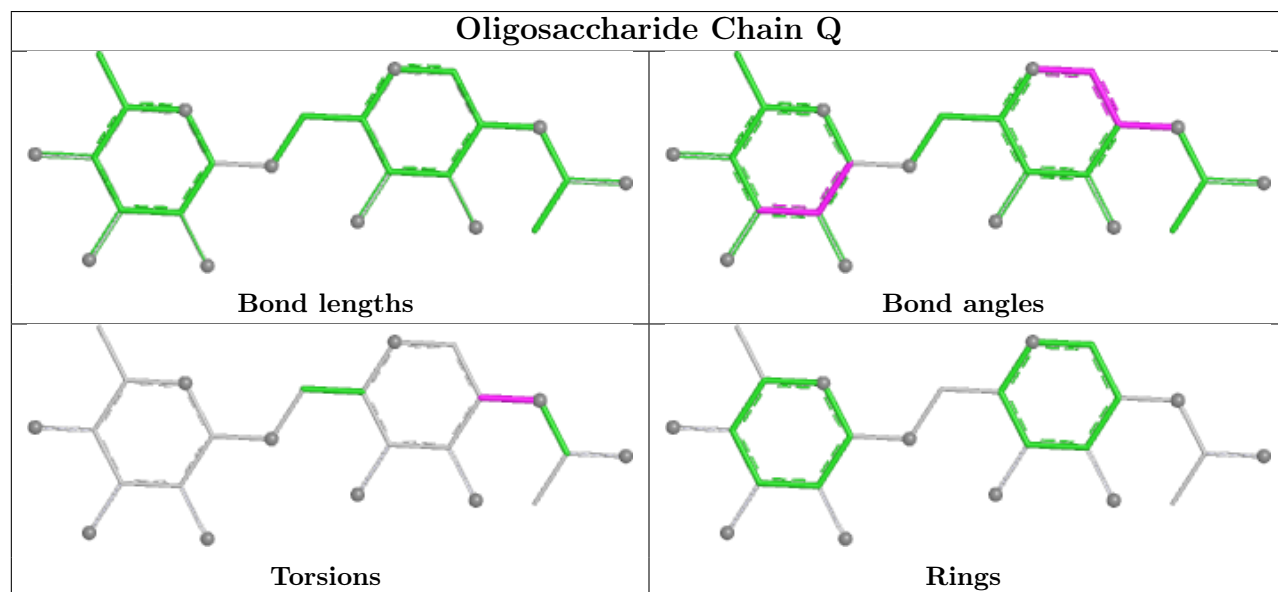


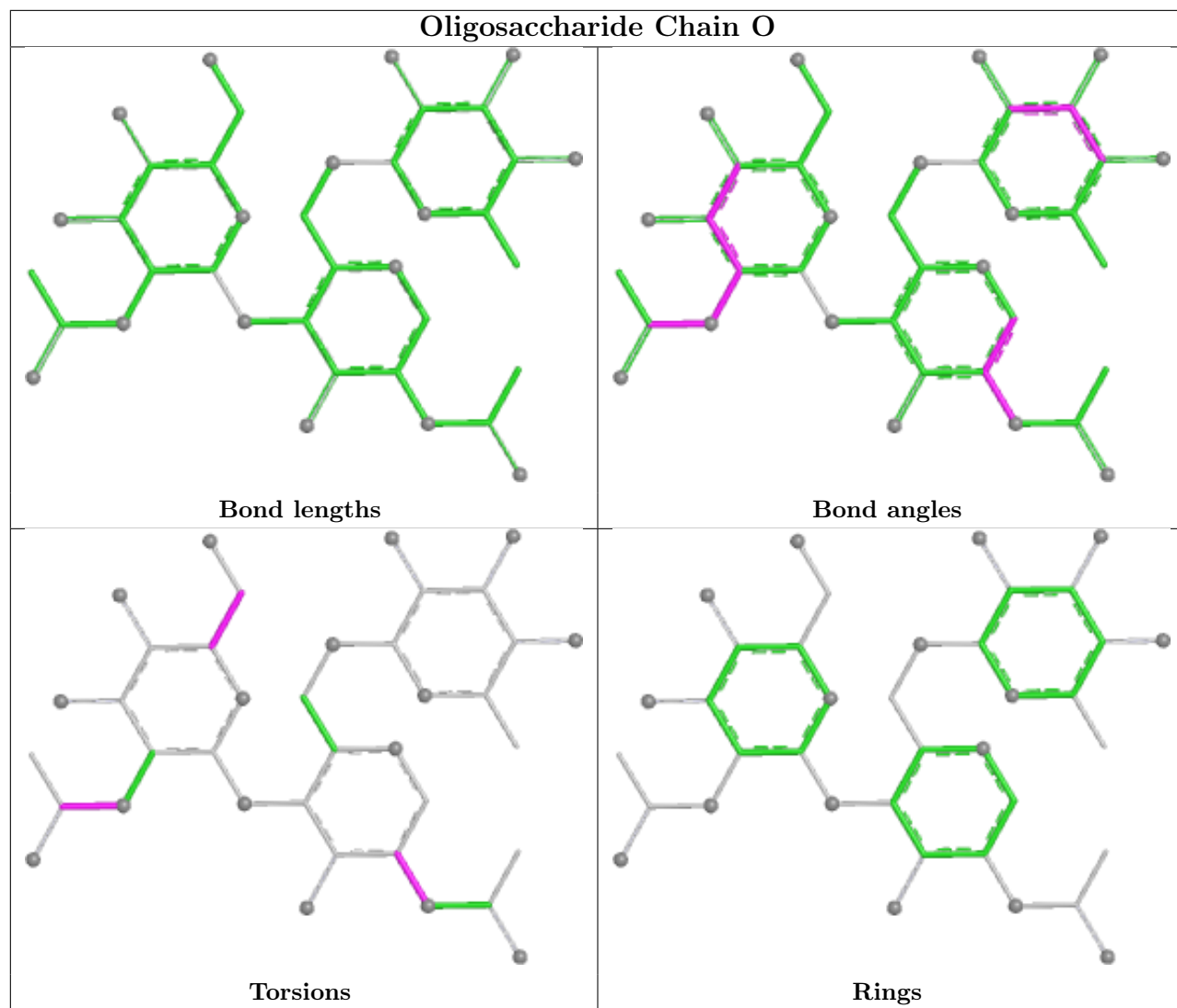


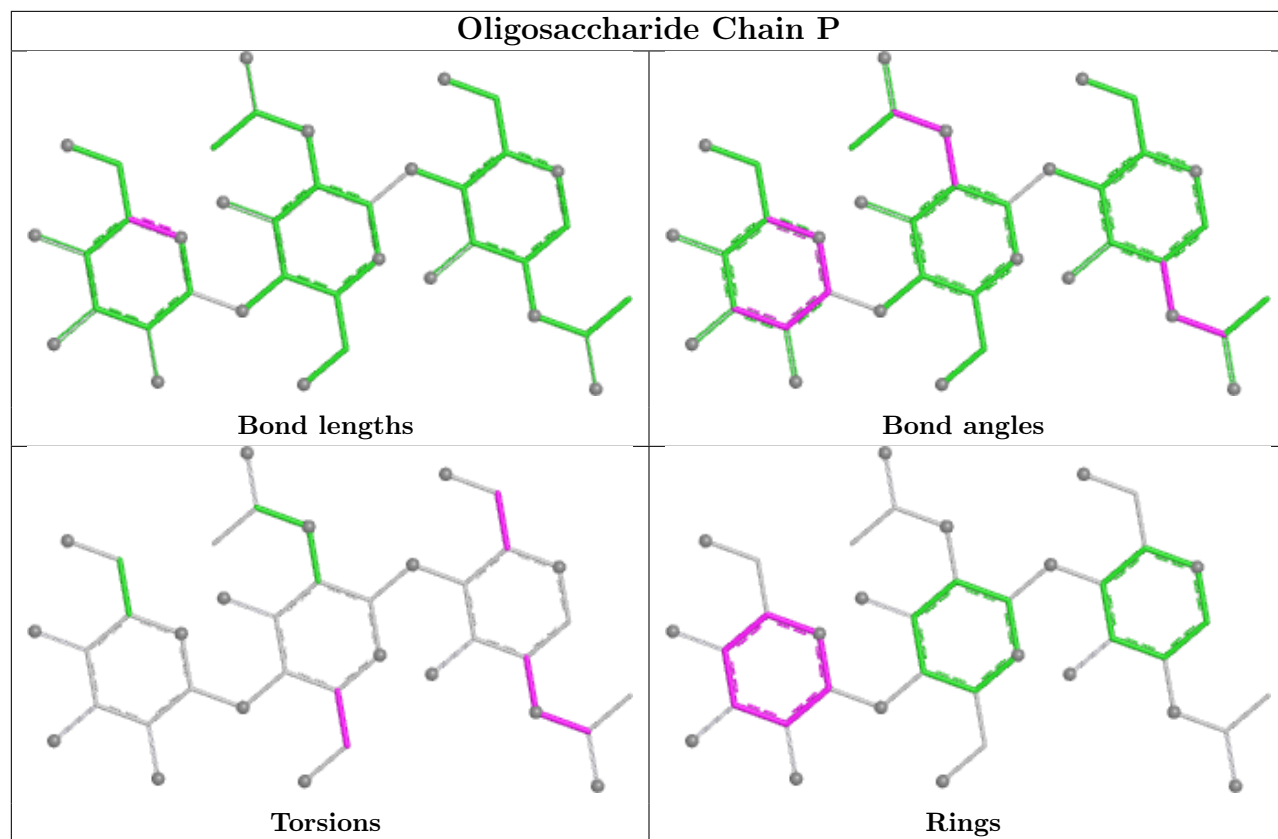
Oligosaccharide Chain H

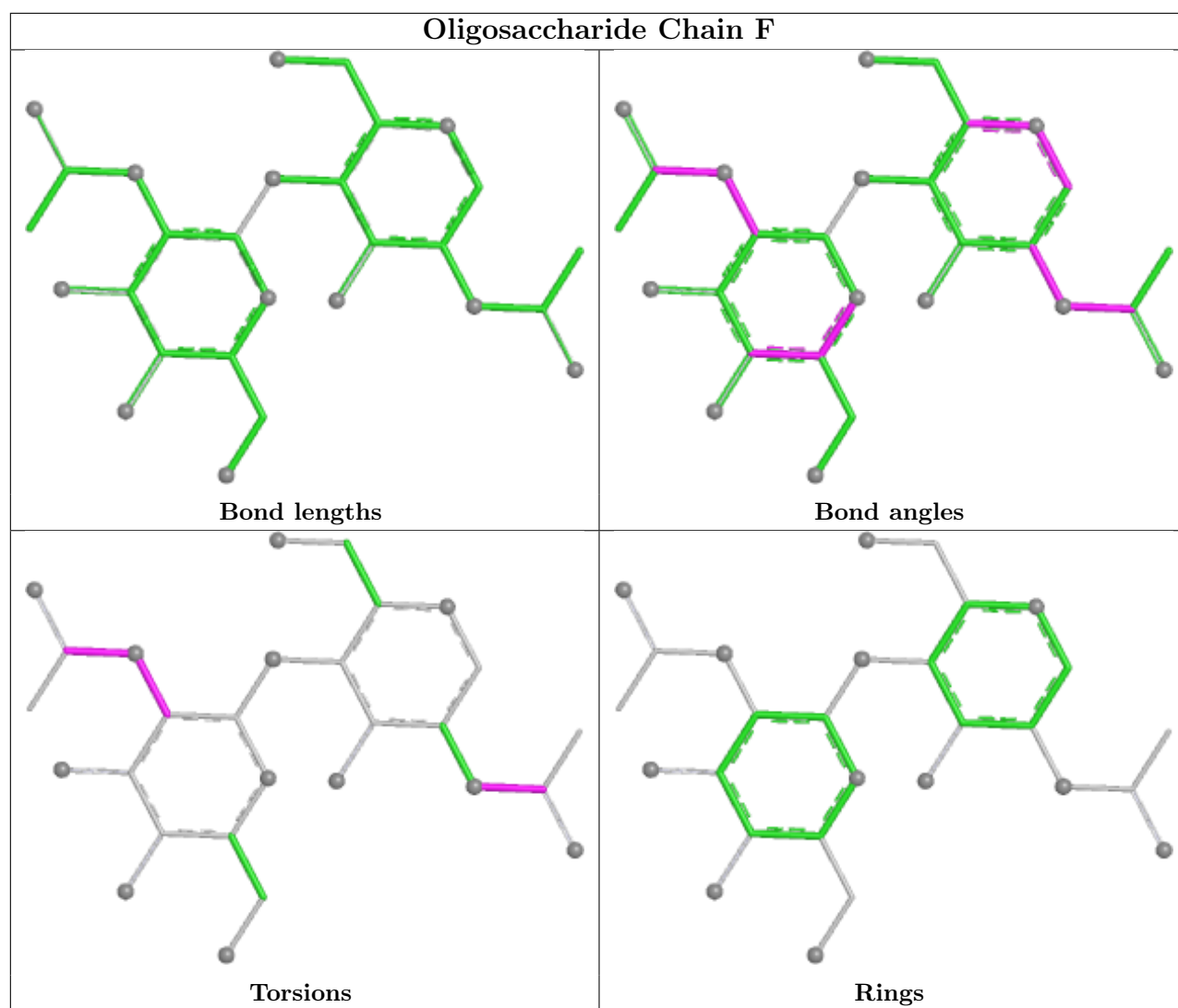


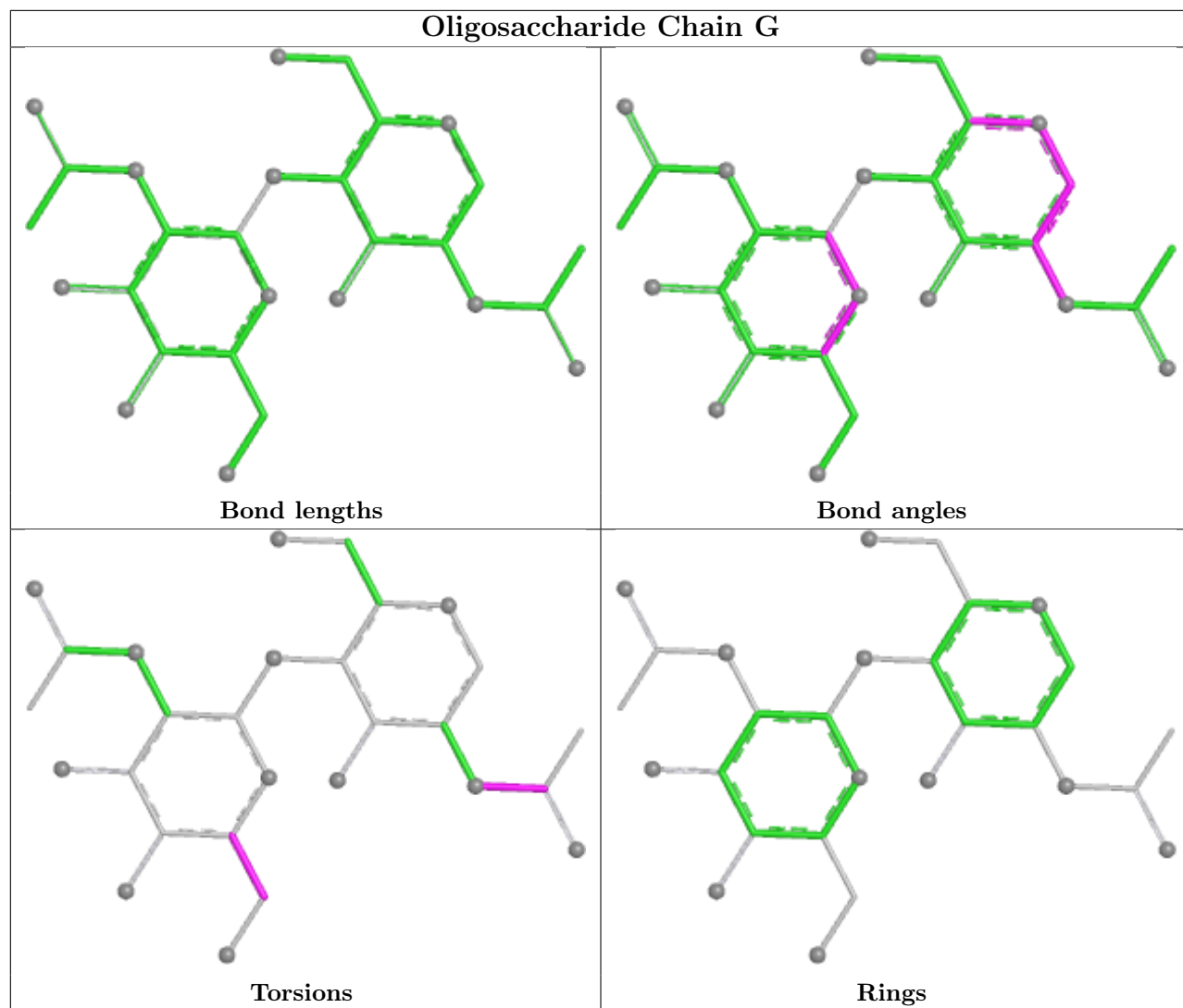
Oligosaccharide Chain Q

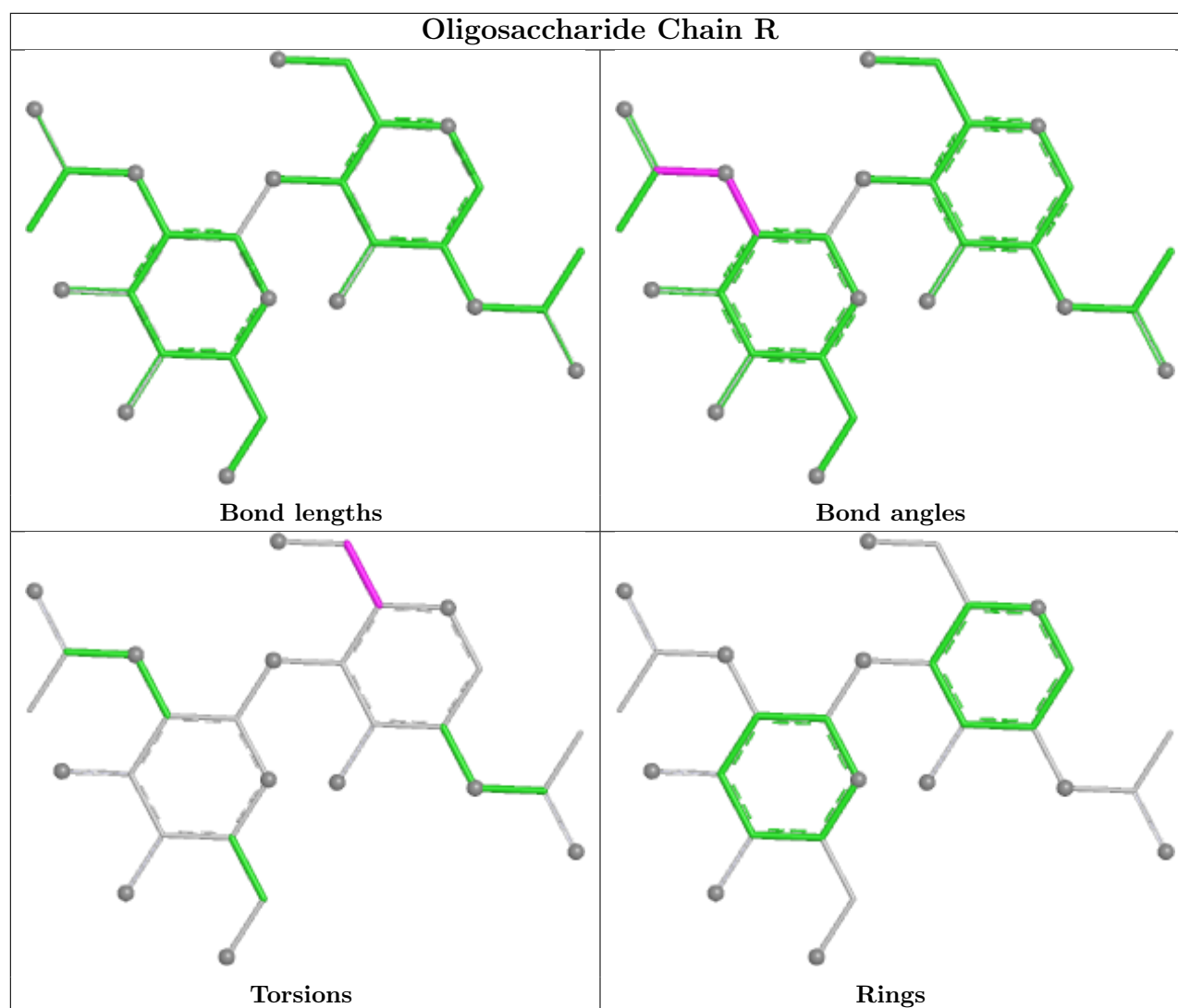












5.6 Ligand geometry [i](#)

Of 54 ligands modelled in this entry, 12 are monoatomic - leaving 42 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	$\# Z > 2$
10	EDO	B	705	-	3,3,3	0.14	0	2,2,2	0.14	0
9	PEG	B	704	-	6,6,6	0.36	0	5,5,5	0.23	0
10	EDO	C	710	-	3,3,3	0.10	0	2,2,2	0.16	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
18	TRS	B	710	-	7,7,7	0.18	0	9,9,9	0.34	0
9	PEG	D	706	-	6,6,6	0.33	0	5,5,5	0.18	0
9	PEG	C	706	-	6,6,6	0.38	0	5,5,5	0.35	0
10	EDO	C	712	-	3,3,3	0.17	0	2,2,2	0.09	0
9	PEG	B	706	-	6,6,6	0.21	0	5,5,5	0.07	0
10	EDO	A	710	-	3,3,3	0.25	0	2,2,2	0.35	0
10	EDO	A	711	-	3,3,3	0.27	0	2,2,2	0.45	0
8	ZED	D	702	7	22,22,22	0.50	0	24,30,30	0.87	1 (4%)
8	ZED	B	702	7	22,22,22	0.62	0	24,30,30	1.71	2 (8%)
16	12P	A	716[B]	-	36,36,36	0.30	0	35,35,35	0.15	0
12	PGE	C	714	-	9,9,9	0.35	0	8,8,8	0.55	0
10	EDO	C	709	-	3,3,3	0.40	0	2,2,2	0.26	0
10	EDO	B	709	-	3,3,3	0.09	0	2,2,2	0.09	0
10	EDO	A	707	-	3,3,3	0.29	0	2,2,2	0.16	0
14	NAG	A	714	1	14,14,15	0.44	0	17,19,21	1.13	2 (11%)
20	PG4	D	704	-	12,12,12	0.31	0	11,11,11	0.15	0
9	PEG	C	707	-	6,6,6	0.19	0	5,5,5	0.20	0
10	EDO	A	708	-	3,3,3	0.09	0	2,2,2	0.13	0
9	PEG	A	703	-	6,6,6	0.33	0	5,5,5	0.18	0
10	EDO	D	705	-	3,3,3	0.32	0	2,2,2	0.18	0
18	TRS	C	705	-	7,7,7	0.32	0	9,9,9	0.48	0
9	PEG	C	708	-	6,6,6	0.24	0	5,5,5	0.19	0
9	PEG	A	709	-	6,6,6	0.20	0	5,5,5	0.16	0
10	EDO	D	703	-	3,3,3	0.13	0	2,2,2	0.17	0
12	PGE	A	712	-	9,9,9	0.21	0	8,8,8	0.18	0
10	EDO	C	711	-	3,3,3	0.23	0	2,2,2	0.16	0
10	EDO	C	704	-	3,3,3	0.06	0	2,2,2	0.12	0
10	EDO	C	713	-	3,3,3	0.17	0	2,2,2	0.19	0
9	PEG	A	705	-	6,6,6	0.38	0	5,5,5	0.54	0
8	ZED	C	702	7	22,22,22	0.67	0	24,30,30	0.77	0
11	ACT	A	706	-	3,3,3	1.14	0	3,3,3	0.75	0
12	PGE	D	709	-	9,9,9	0.23	0	8,8,8	0.09	0
16	12P	A	716[A]	-	36,36,36	0.24	0	35,35,35	0.19	0
19	XPE	C	703	-	30,30,30	0.31	0	29,29,29	0.28	0
17	PE8	B	703	-	24,24,24	0.39	0	23,23,23	0.27	0
10	EDO	B	708	-	3,3,3	0.10	0	2,2,2	0.12	0
10	EDO	B	707	-	3,3,3	0.08	0	2,2,2	0.14	0
10	EDO	A	704	-	3,3,3	0.07	0	2,2,2	0.11	0
8	ZED	A	702	7	22,22,22	0.71	0	24,30,30	0.78	1 (4%)

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
10	EDO	B	705	-	-	1/1/1/1	-
9	PEG	B	704	-	-	1/4/4/4	-
10	EDO	C	710	-	-	0/1/1/1	-
18	TRS	B	710	-	-	3/9/9/9	-
9	PEG	D	706	-	-	3/4/4/4	-
9	PEG	C	706	-	-	3/4/4/4	-
10	EDO	C	712	-	-	0/1/1/1	-
9	PEG	B	706	-	-	2/4/4/4	-
10	EDO	A	710	-	-	0/1/1/1	-
10	EDO	A	711	-	-	0/1/1/1	-
8	ZED	D	702	7	-	1/18/30/30	0/2/2/2
8	ZED	B	702	7	-	2/18/30/30	0/2/2/2
16	12P	A	716[B]	-	-	21/34/34/34	-
12	PGE	C	714	-	-	6/7/7/7	-
10	EDO	C	709	-	-	1/1/1/1	-
10	EDO	B	709	-	-	1/1/1/1	-
10	EDO	A	707	-	-	1/1/1/1	-
14	NAG	A	714	1	-	2/6/23/26	0/1/1/1
20	PG4	D	704	-	-	5/10/10/10	-
9	PEG	C	707	-	-	3/4/4/4	-
10	EDO	A	708	-	-	1/1/1/1	-
9	PEG	A	703	-	-	3/4/4/4	-
10	EDO	D	705	-	-	0/1/1/1	-
18	TRS	C	705	-	-	3/9/9/9	-
9	PEG	C	708	-	-	2/4/4/4	-
9	PEG	A	709	-	-	3/4/4/4	-
10	EDO	D	703	-	-	1/1/1/1	-
12	PGE	A	712	-	-	4/7/7/7	-
10	EDO	C	711	-	-	0/1/1/1	-
10	EDO	C	704	-	-	1/1/1/1	-
10	EDO	C	713	-	-	1/1/1/1	-
9	PEG	A	705	-	-	4/4/4/4	-
8	ZED	C	702	7	-	1/18/30/30	0/2/2/2
12	PGE	D	709	-	-	3/7/7/7	-
16	12P	A	716[A]	-	-	20/34/34/34	-
19	XPE	C	703	-	-	14/28/28/28	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	PE8	B	703	-	-	6/22/22/22	-
10	EDO	B	708	-	-	0/1/1/1	-
10	EDO	B	707	-	-	1/1/1/1	-
10	EDO	A	704	-	-	1/1/1/1	-
8	ZED	A	702	7	-	2/18/30/30	0/2/2/2

There are no bond length outliers.

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	B	702	ZED	CZD-CZF-SZ2	-6.77	105.27	114.04
14	A	714	NAG	C1-O5-C5	3.11	116.36	112.19
8	B	702	ZED	CZ9-CZ7-CZ8	3.02	114.52	111.01
8	A	702	ZED	CZD-CZF-SZ2	-2.61	110.66	114.04
14	A	714	NAG	C1-C2-N2	2.22	113.93	110.43

There are no chirality outliers.

5 of 127 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	A	702	ZED	CZC-CZD-CZF-SZ2
8	A	702	ZED	CZE-CZD-CZF-SZ2
8	B	702	ZED	CZC-CZD-CZF-SZ2
8	B	702	ZED	CZE-CZD-CZF-SZ2
14	A	714	NAG	C8-C7-N2-C2

There are no ring outliers.

12 monomers are involved in 29 short contacts:

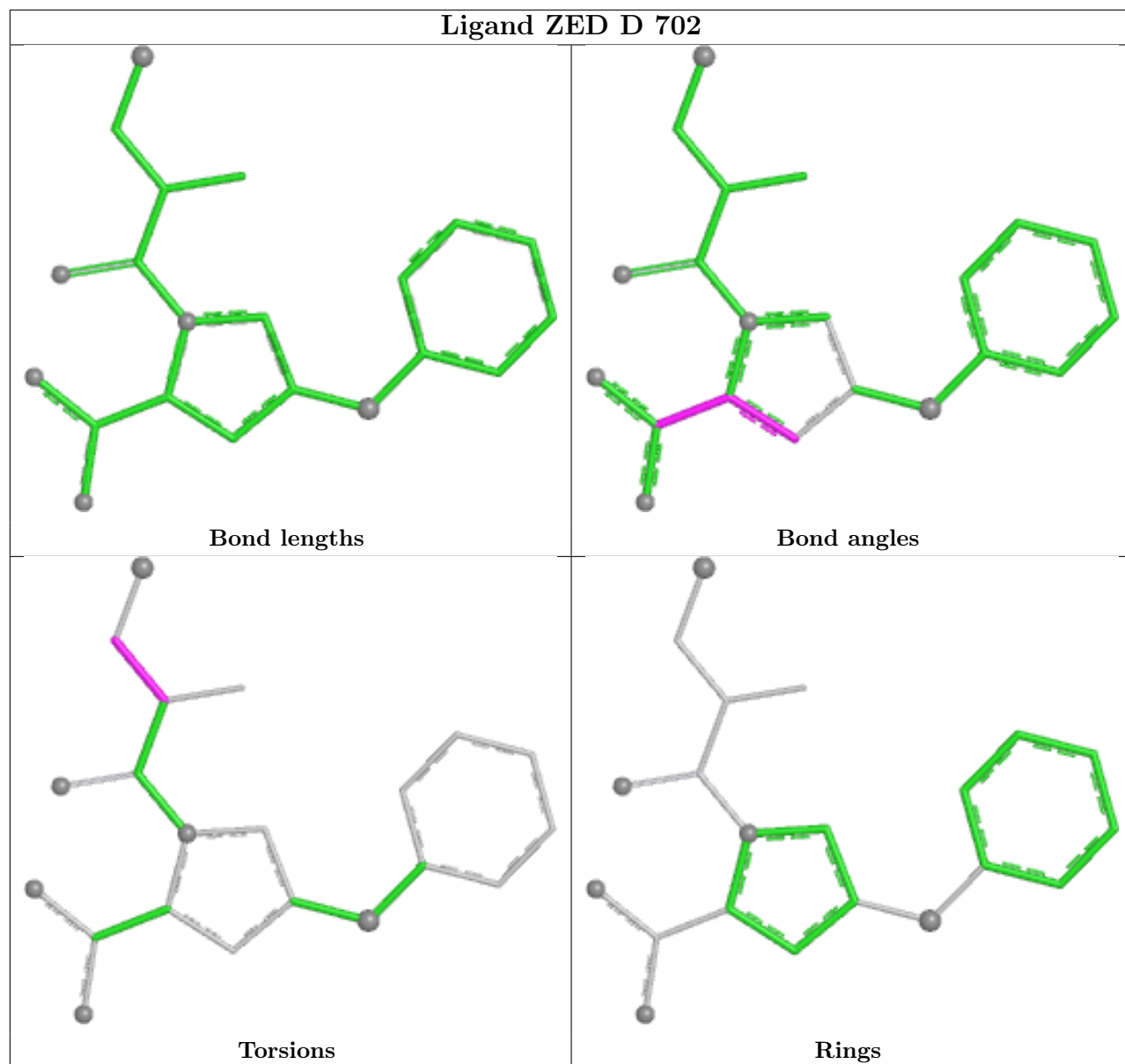
Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	B	704	PEG	1	0
18	B	710	TRS	1	0
9	C	706	PEG	1	0
10	A	711	EDO	2	0
16	A	716[B]	12P	1	0
12	C	714	PGE	5	0
18	C	705	TRS	1	0
9	A	705	PEG	6	0
11	A	706	ACT	1	0
16	A	716[A]	12P	7	0

Continued on next page...

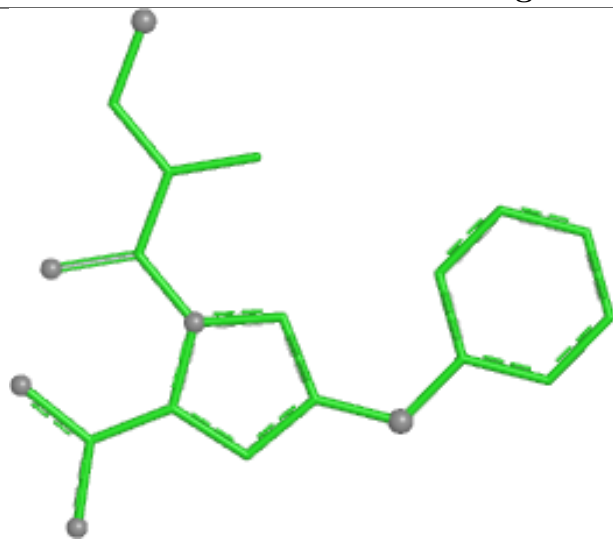
Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
19	C	703	XPE	1	0
17	B	703	PE8	2	0

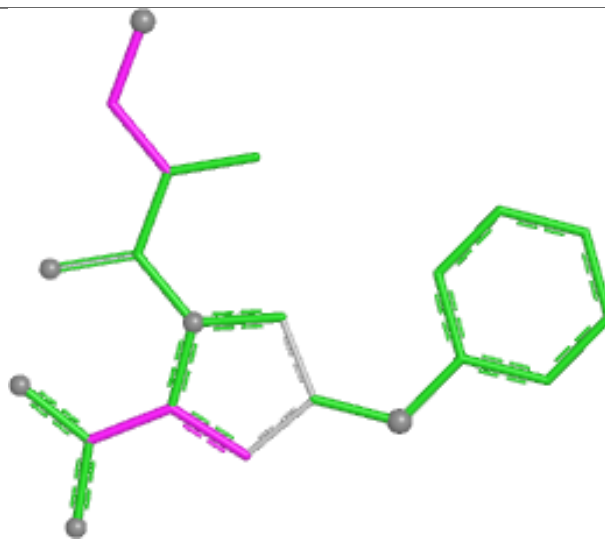
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.



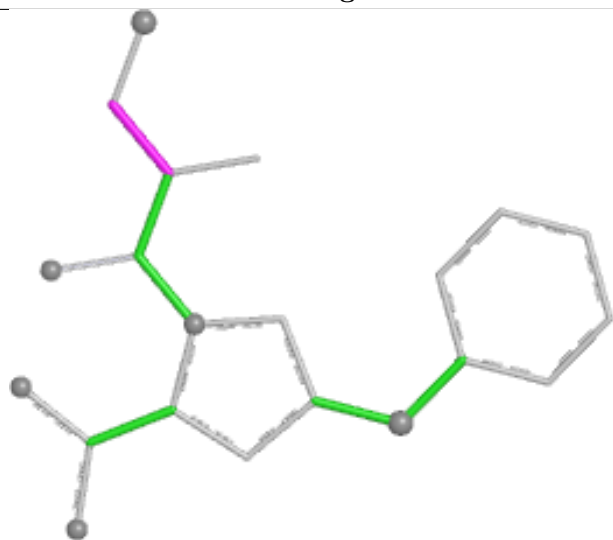
Ligand ZED B 702



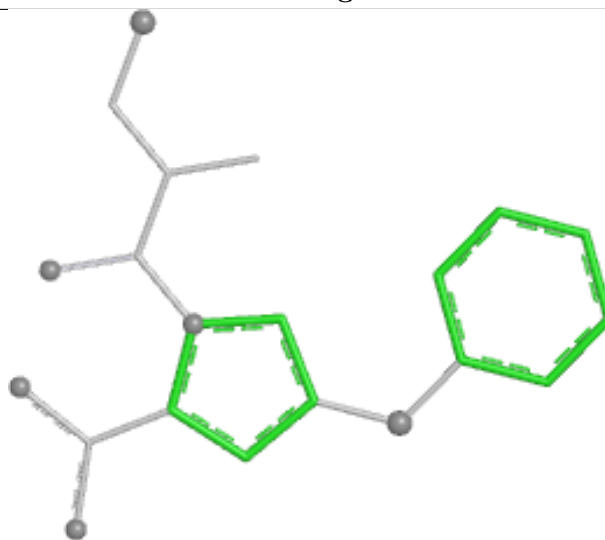
Bond lengths



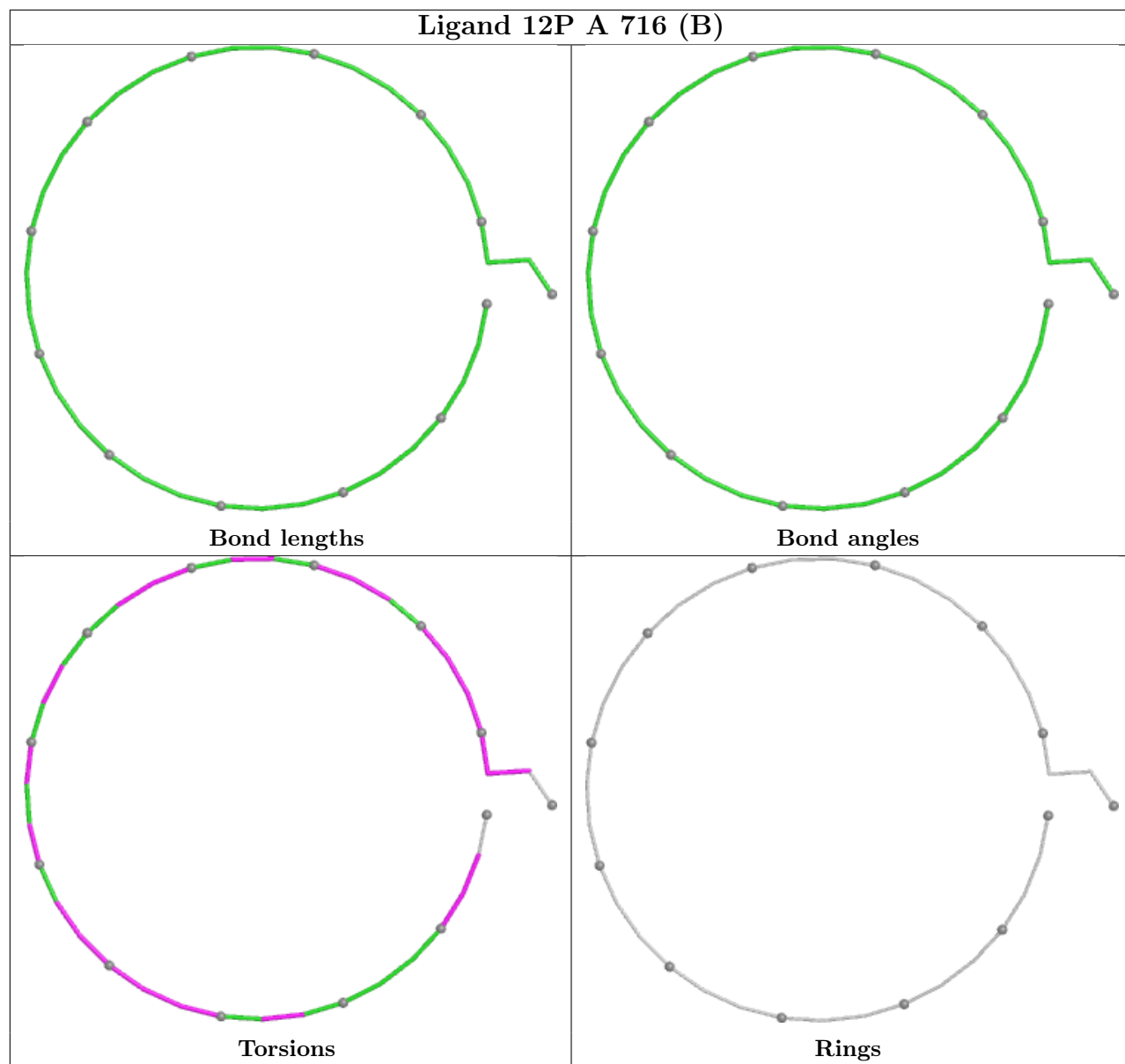
Bond angles

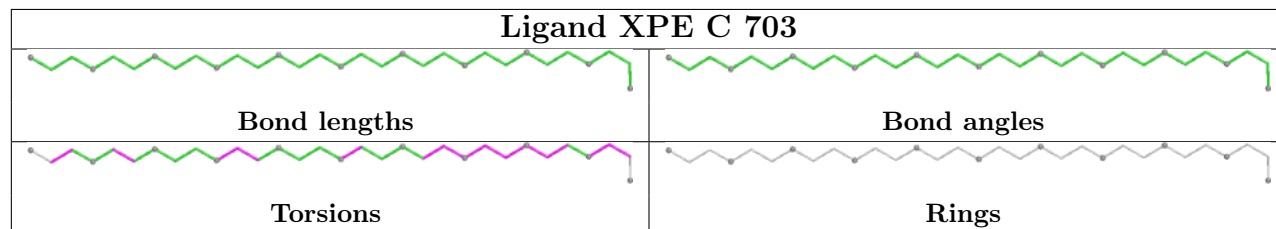
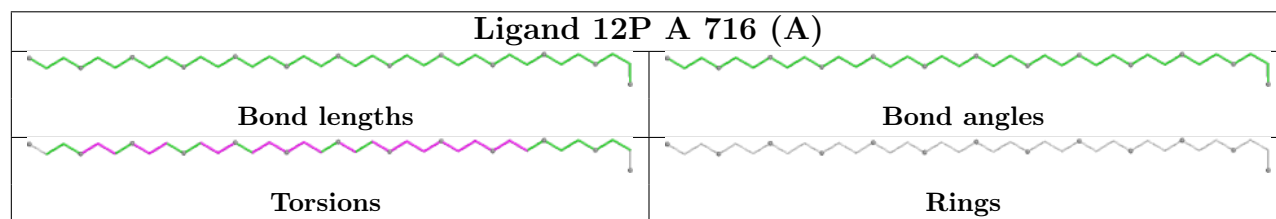
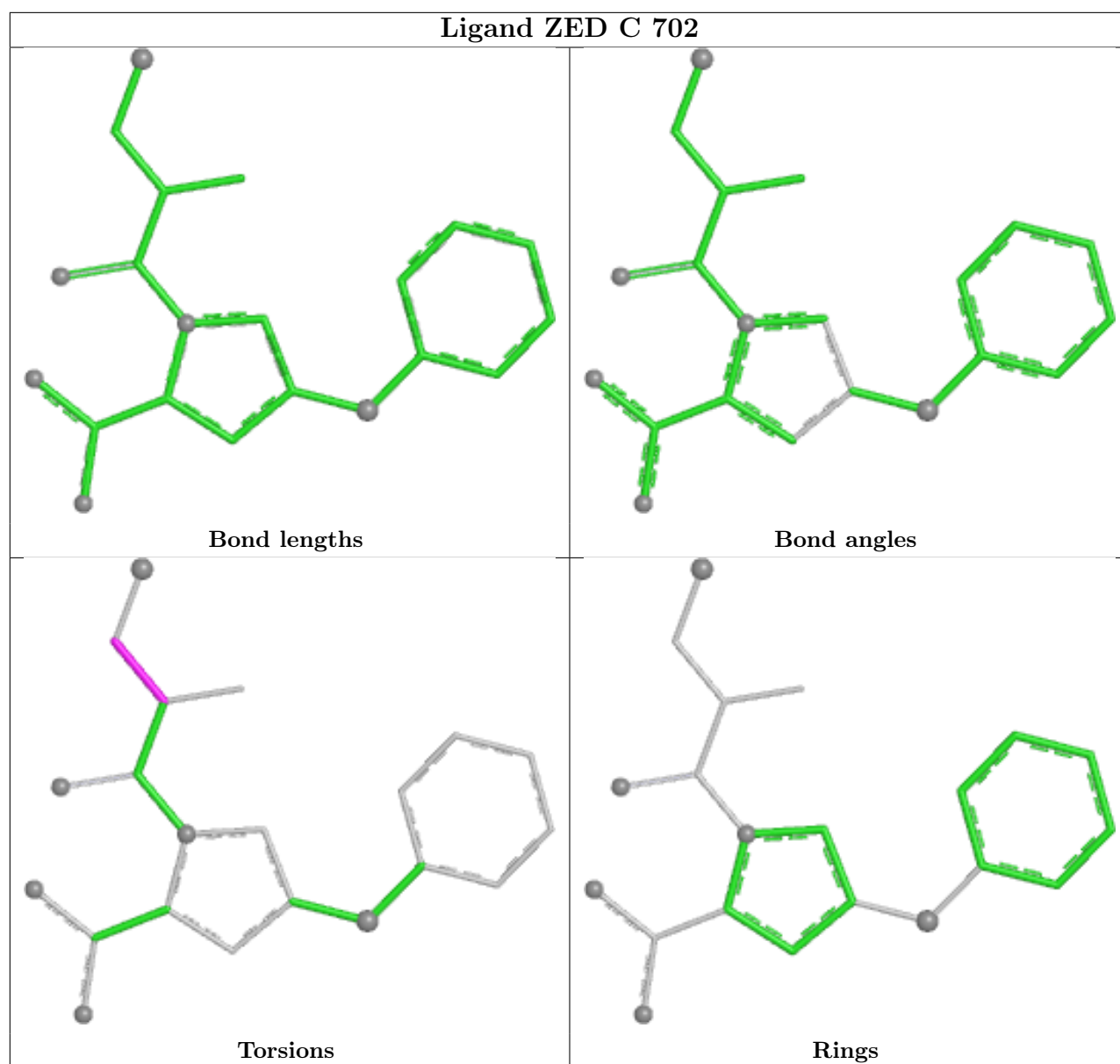


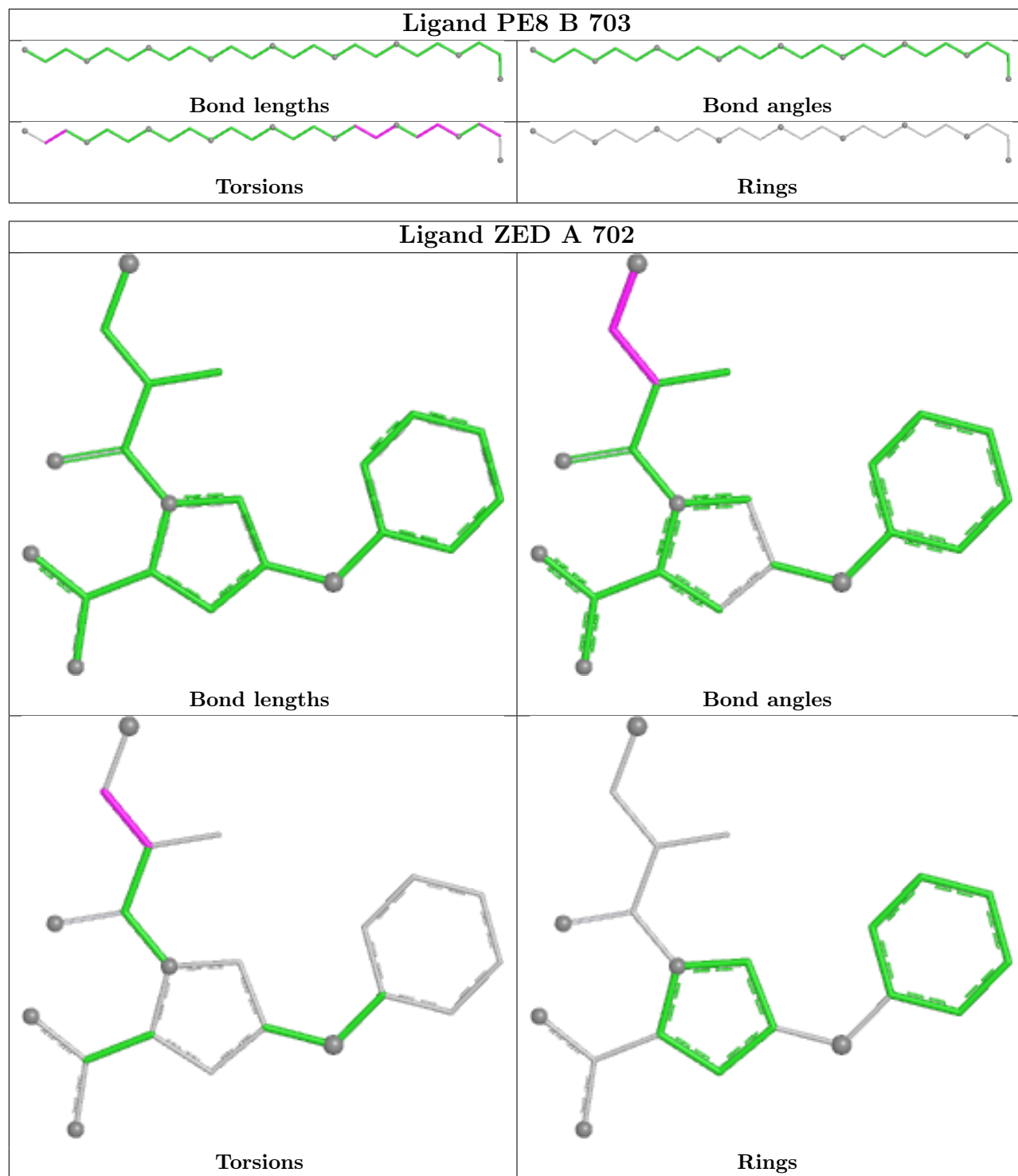
Torsions



Rings







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	603/628 (96%)	0.14	17 (2%) 55 54	12, 28, 48, 76	4 (0%)
1	B	607/628 (96%)	0.16	25 (4%) 41 40	10, 27, 48, 74	7 (1%)
1	C	601/628 (95%)	0.24	10 (1%) 69 68	11, 29, 49, 70	7 (1%)
1	D	611/628 (97%)	0.04	13 (2%) 63 63	9, 25, 44, 74	10 (1%)
All	All	2422/2512 (96%)	0.15	65 (2%) 56 55	9, 28, 48, 76	28 (1%)

The worst 5 of 65 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	414	VAL	6.0
1	D	135	THR	5.0
1	B	135	THR	4.5
1	D	129	LEU	4.4
1	A	130	PRO	4.4

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
2	NAG	K	2	14/15	0.64	0.15	34,42,56,56	0
2	MAN	E	3	11/12	0.65	0.17	79,86,89,89	0

Continued on next page...

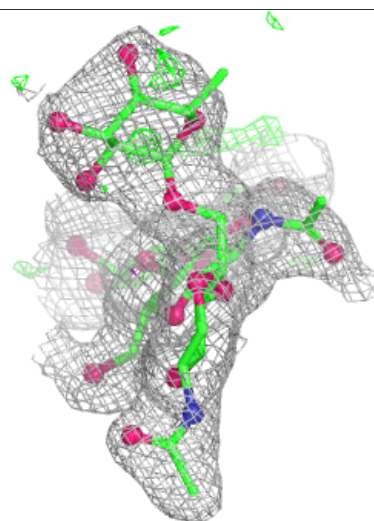
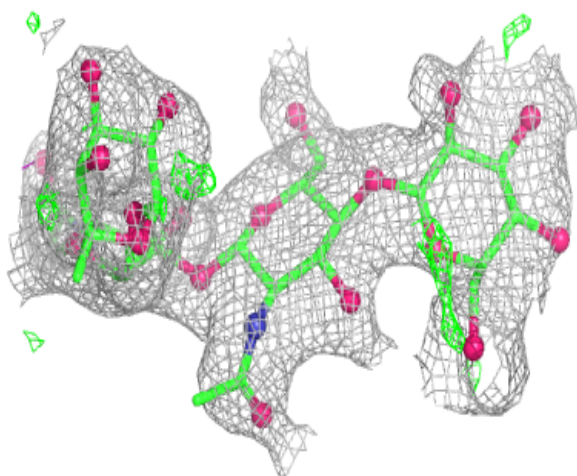
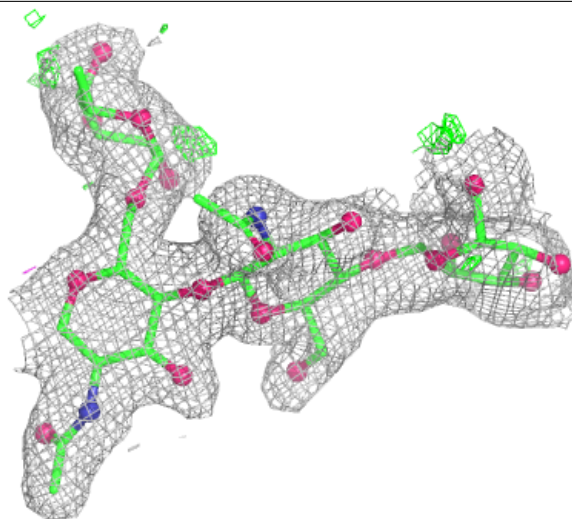
Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	NAG	M	2	14/15	0.79	0.15	46,53,58,61	0
2	NAG	K	1	14/15	0.81	0.13	26,31,40,42	0
2	FUC	E	4	10/11	0.82	0.17	38,43,46,48	10
3	NAG	N	1	14/15	0.82	0.12	34,39,53,53	0
2	MAN	K	3	11/12	-	-	56,64,74,74	0
2	FUC	K	4	10/11	-	-	32,38,41,43	10
3	FUC	H	2	10/11	0.84	0.13	55,63,68,68	0
4	NAG	O	1	14/15	0.85	0.13	29,33,42,54	0
2	MAN	M	3	11/12	-	-	63,69,76,78	0
2	FUC	M	4	10/11	-	-	55,61,63,66	0
3	FUC	N	2	10/11	0.86	0.14	47,54,59,60	0
6	NAG	F	2	14/15	0.87	0.14	57,77,90,93	0
2	NAG	M	1	14/15	0.88	0.11	39,47,54,63	0
6	NAG	G	2	14/15	0.88	0.10	60,81,86,87	0
3	NAG	Q	1	14/15	-	-	32,42,48,49	0
3	FUC	Q	2	10/11	-	-	48,52,54,56	0
6	NAG	G	1	14/15	0.89	0.10	39,50,60,70	0
4	NAG	O	2	14/15	-	-	56,72,80,82	0
4	FUC	O	3	10/11	-	-	41,45,50,53	0
5	NAG	P	1	14/15	-	-	47,54,86,100	0
5	NAG	P	2	14/15	-	-	46,60,63,67	0
5	MAN	P	3	11/12	-	-	66,72,79,79	0
2	NAG	E	2	14/15	0.90	0.12	41,53,64,64	0
3	NAG	H	1	14/15	0.91	0.09	27,38,49,58	0
6	NAG	F	1	14/15	0.93	0.08	39,46,57,64	0
2	NAG	E	1	14/15	0.93	0.09	26,34,42,52	0
6	NAG	R	1	14/15	-	-	31,36,42,53	14
6	NAG	R	2	14/15	-	-	53,59,65,66	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.

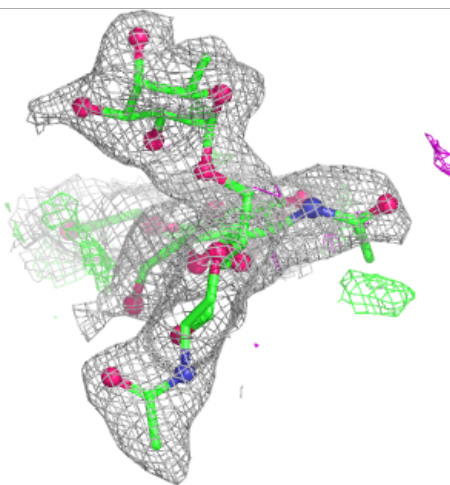
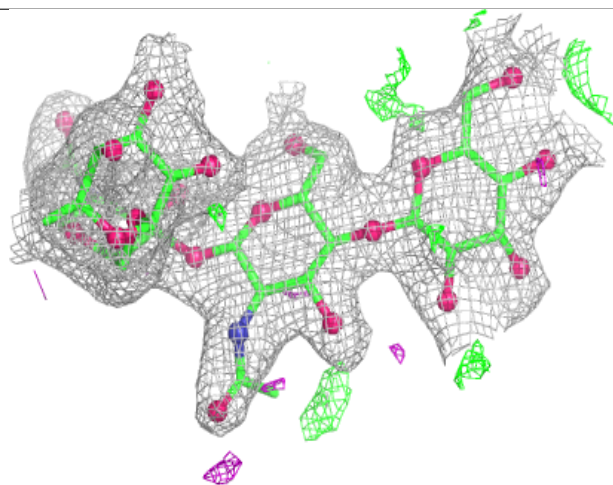
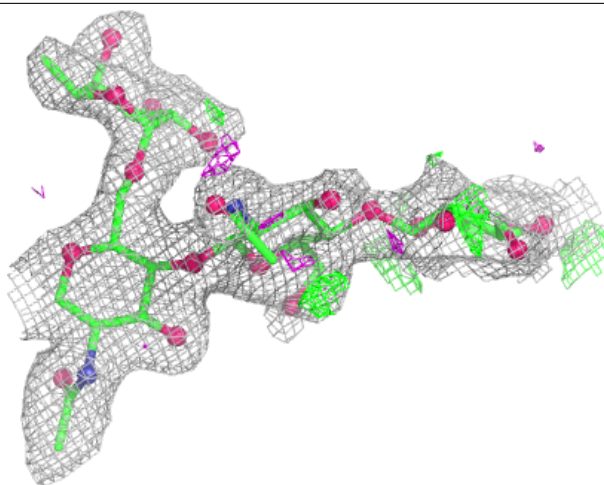
Electron density around Chain E:

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



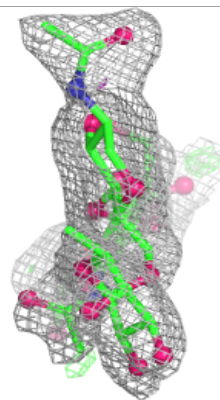
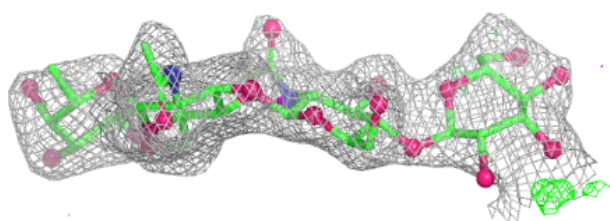
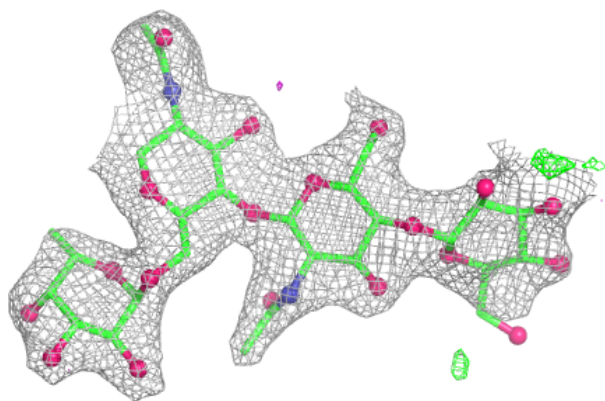
Electron density around Chain K:

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

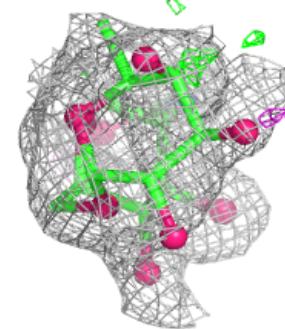
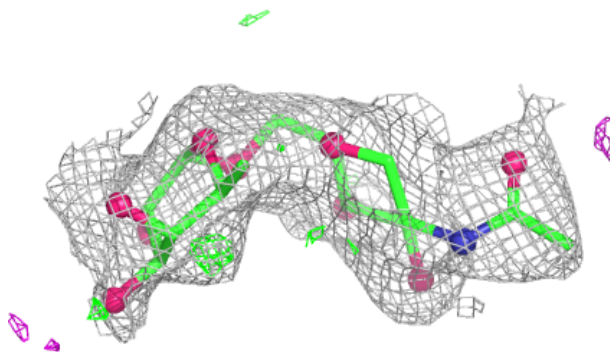
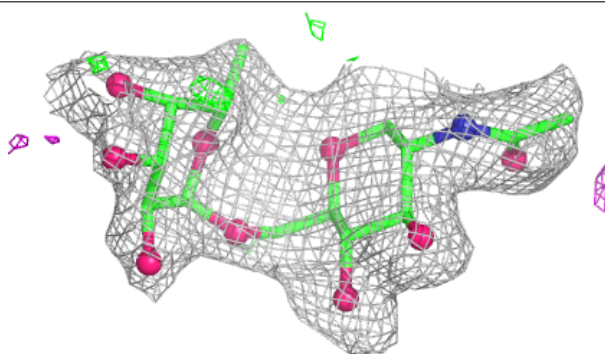


Electron density around Chain M:

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

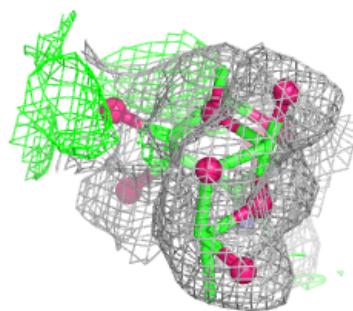
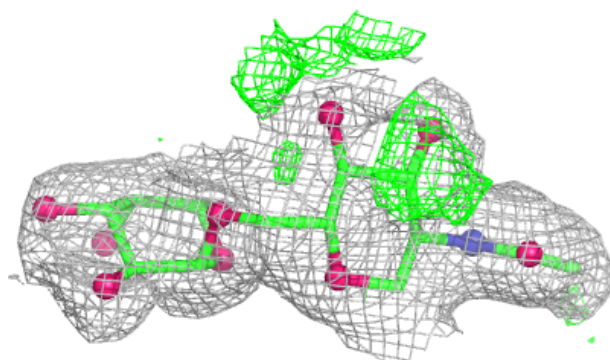
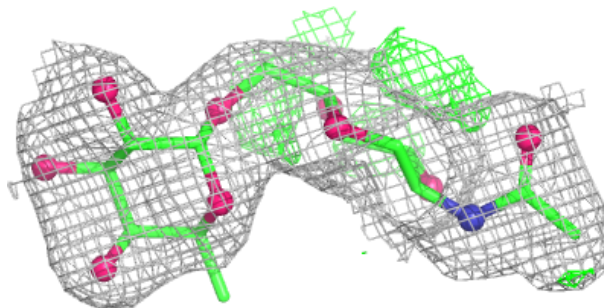
**Electron density around Chain N:**

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

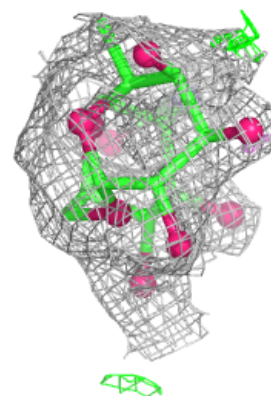
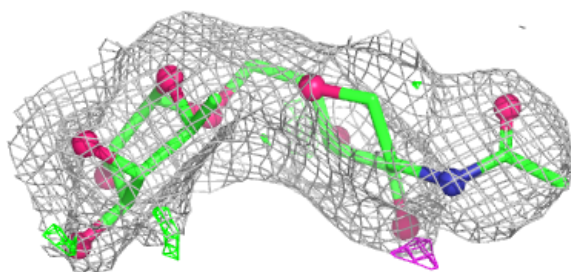
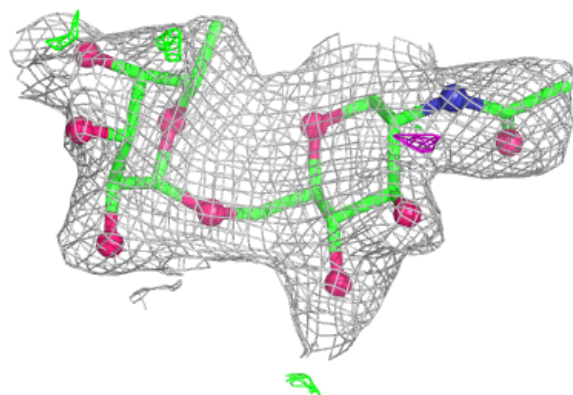


Electron density around Chain H:

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

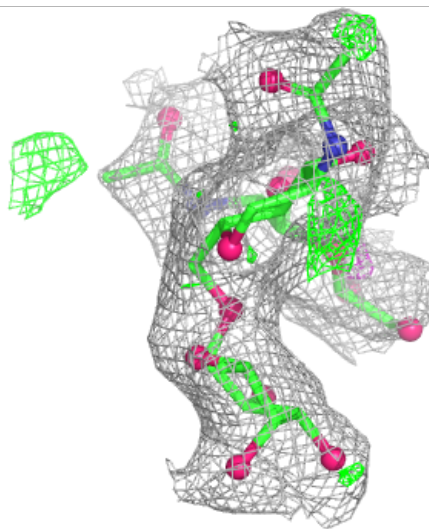
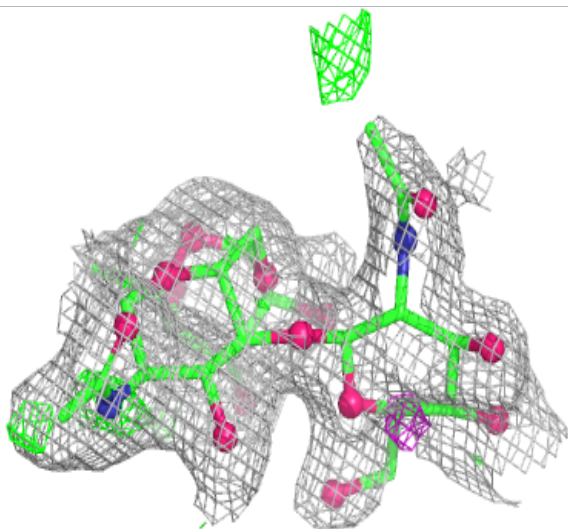
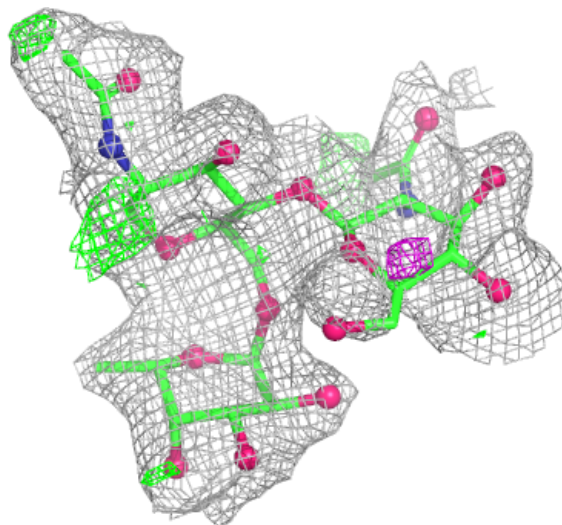
**Electron density around Chain Q:**

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



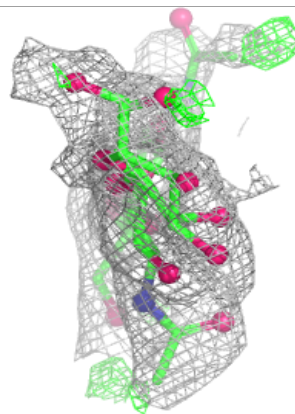
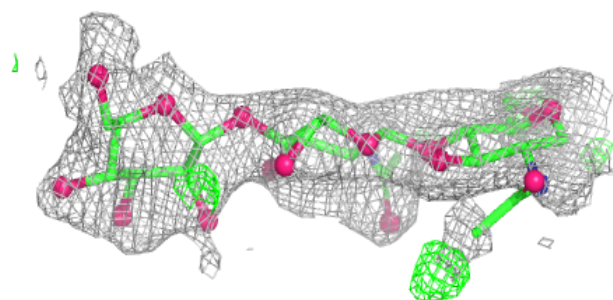
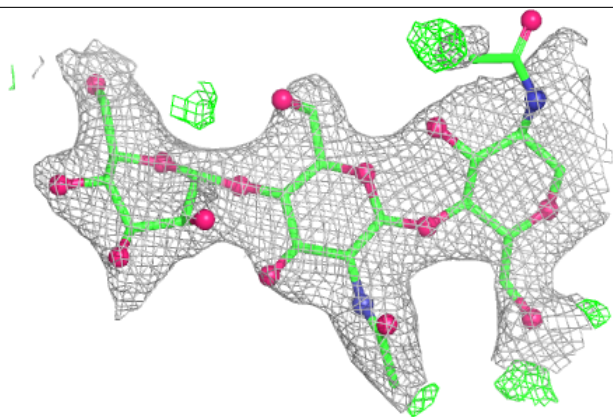
Electron density around Chain O:

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



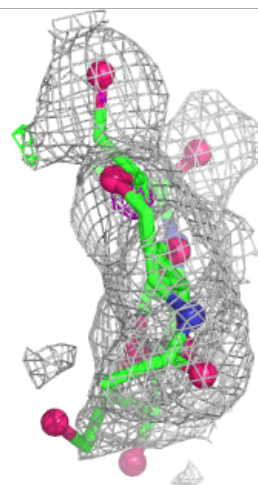
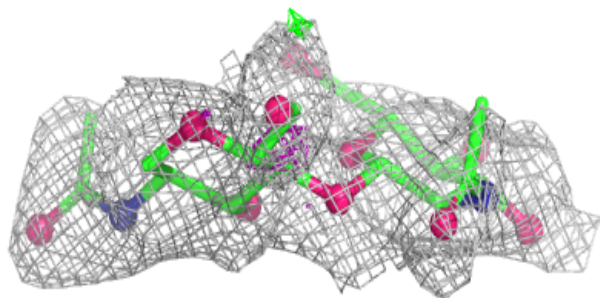
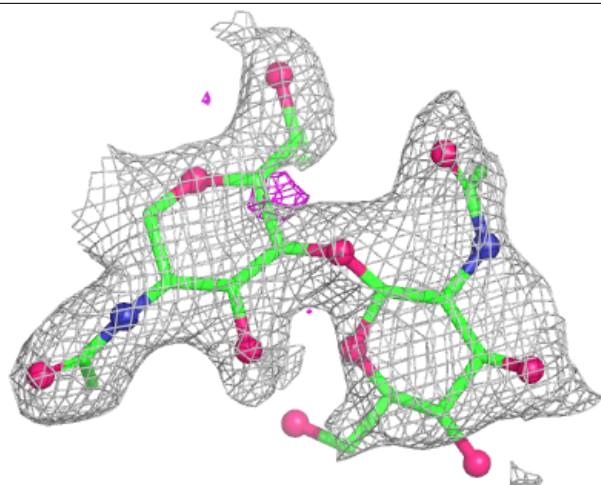
Electron density around Chain P:

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



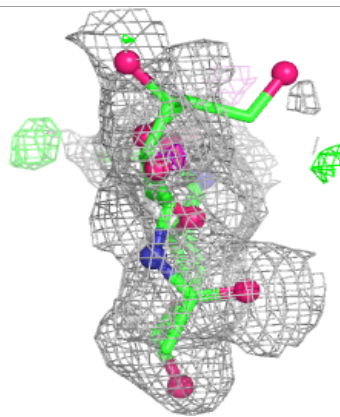
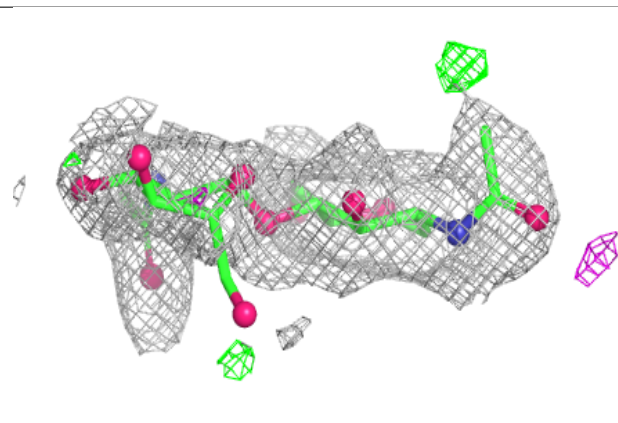
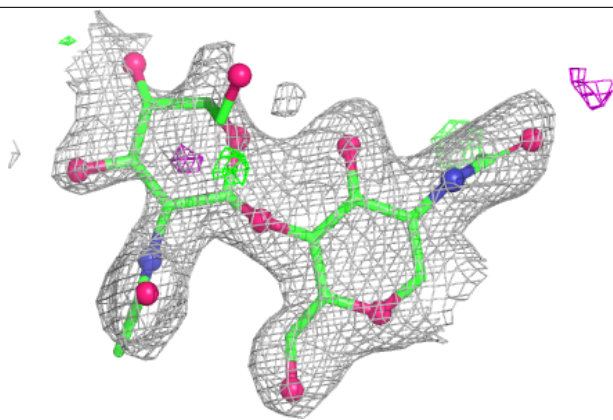
Electron density around Chain F:

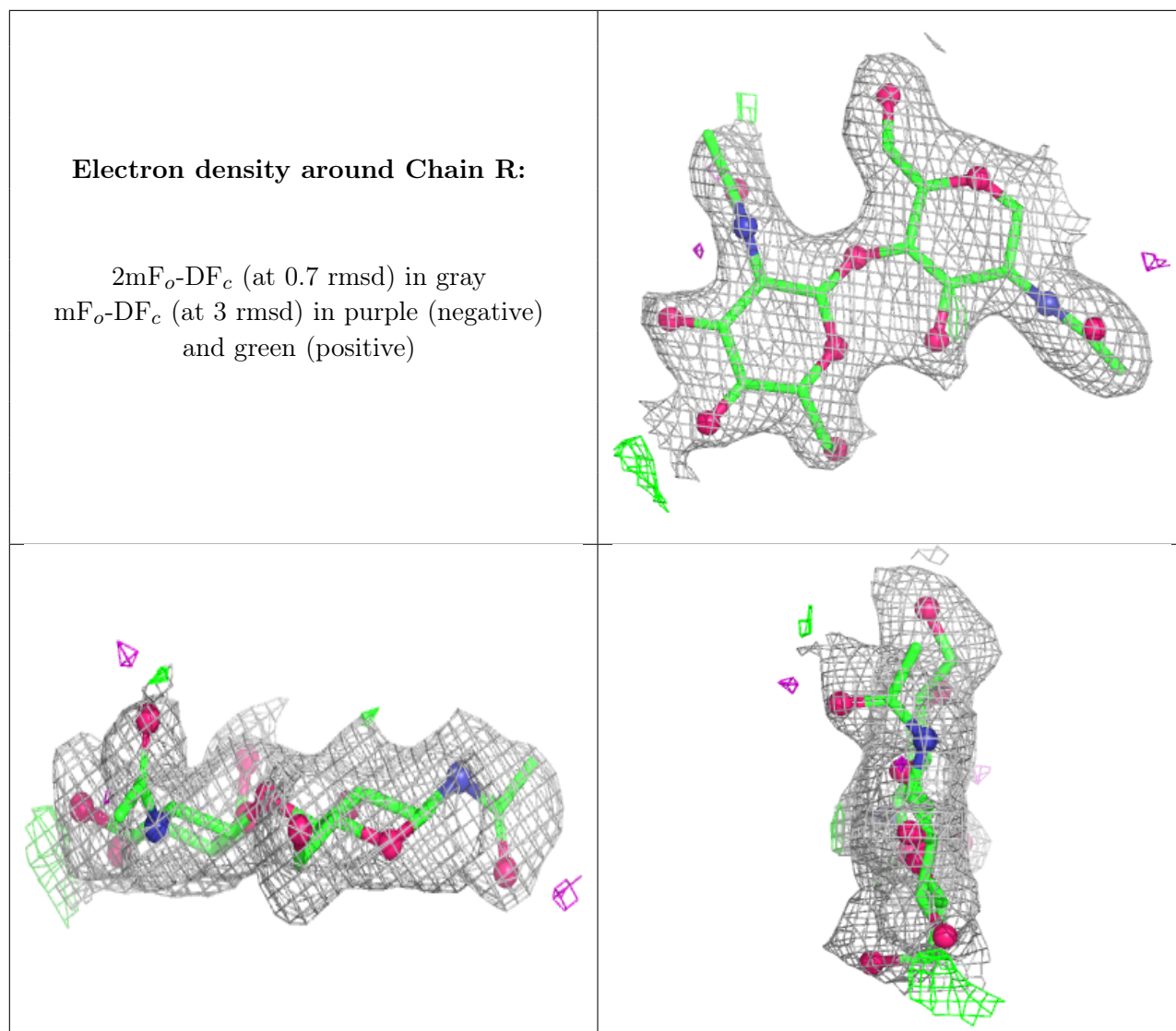
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around Chain G:

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





6.4 Ligands ⓘ

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	C	708	7/7	0.66	0.23	59,69,77,78	0
11	ACT	A	706	4/4	0.69	0.25	65,71,74,77	0
14	NAG	A	714	14/15	0.69	0.17	49,57,65,68	0
10	EDO	A	707	4/4	0.74	0.19	55,55,58,59	0
10	EDO	A	708	4/4	0.74	0.21	58,59,63,65	0
18	TRS	C	705	8/8	0.75	0.20	61,64,68,70	0
9	PEG	B	704	7/7	0.76	0.22	47,58,73,73	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
10	EDO	B	707	4/4	0.77	0.18	68,70,73,74	0
9	PEG	A	705	7/7	0.77	0.26	69,71,76,78	0
10	EDO	C	712	4/4	0.78	0.22	60,60,63,65	0
10	EDO	A	704	4/4	0.79	0.19	48,50,53,53	0
12	PGE	A	712	10/10	0.79	0.23	59,66,78,83	0
10	EDO	C	713	4/4	0.80	0.18	43,51,52,52	0
10	EDO	D	703	4/4	0.80	0.17	46,53,54,56	0
9	PEG	C	707	7/7	0.80	0.19	52,54,55,57	0
9	PEG	C	706	7/7	0.81	0.19	58,60,63,67	0
10	EDO	C	711	4/4	0.81	0.23	52,54,54,58	0
16	12P	A	716[A]	37/37	0.81	0.18	23,31,46,49	37
16	12P	A	716[B]	37/37	0.81	0.18	24,32,50,51	37
9	PEG	A	703	7/7	0.81	0.21	48,55,61,61	0
9	PEG	B	706	7/7	0.83	0.17	62,65,70,72	0
9	PEG	A	709	7/7	0.83	0.17	51,55,60,66	0
10	EDO	B	709	4/4	0.84	0.16	53,55,55,59	0
12	PGE	D	709	10/10	0.84	0.15	51,59,69,72	0
10	EDO	A	710	4/4	0.85	0.15	50,55,56,58	0
10	EDO	A	711	4/4	0.85	0.14	43,45,45,45	0
9	PEG	D	706	7/7	0.85	0.22	46,58,67,68	0
18	TRS	B	710	8/8	0.86	0.15	54,59,68,77	0
20	PG4	D	704	13/13	0.86	0.17	46,58,66,69	0
19	XPE	C	703	31/31	0.87	0.15	45,51,55,56	0
10	EDO	B	705	4/4	0.87	0.18	49,51,51,56	0
10	EDO	C	709	4/4	0.88	0.14	43,44,45,45	0
12	PGE	C	714	10/10	0.89	0.14	48,50,54,56	0
10	EDO	C	710	4/4	0.89	0.13	47,50,52,55	0
10	EDO	D	705	4/4	0.89	0.15	42,44,45,48	0
10	EDO	B	708	4/4	0.90	0.20	50,50,51,55	0
17	PE8	B	703	25/25	0.91	0.12	29,39,49,49	0
10	EDO	C	704	4/4	0.92	0.10	42,43,43,45	0
8	ZED	B	702	21/21	0.93	0.12	23,29,67,68	0
8	ZED	C	702	21/21	0.93	0.10	22,30,44,46	0
8	ZED	A	702	21/21	0.94	0.12	25,28,51,59	0
8	ZED	D	702	21/21	0.95	0.10	21,27,59,64	0
13	CA	B	711	1/1	0.99	0.07	38,38,38,38	0
13	CA	C	715	1/1	0.99	0.06	33,33,33,33	0
13	CA	D	707	1/1	0.99	0.04	28,28,28,28	0
13	CA	A	713	1/1	0.99	0.07	31,31,31,31	0
15	CL	A	715	1/1	0.99	0.05	22,22,22,22	0
15	CL	B	712	1/1	0.99	0.05	20,20,20,20	0
15	CL	D	708	1/1	0.99	0.03	19,19,19,19	0

Continued on next page...

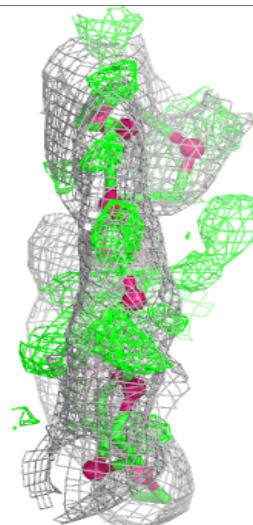
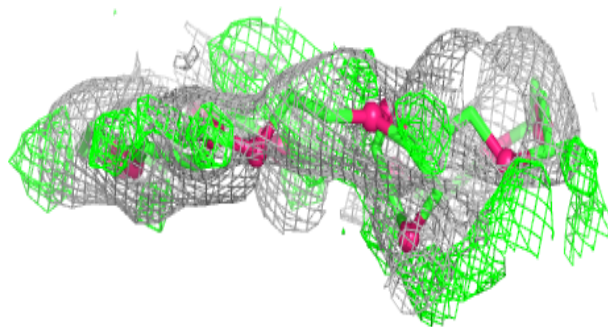
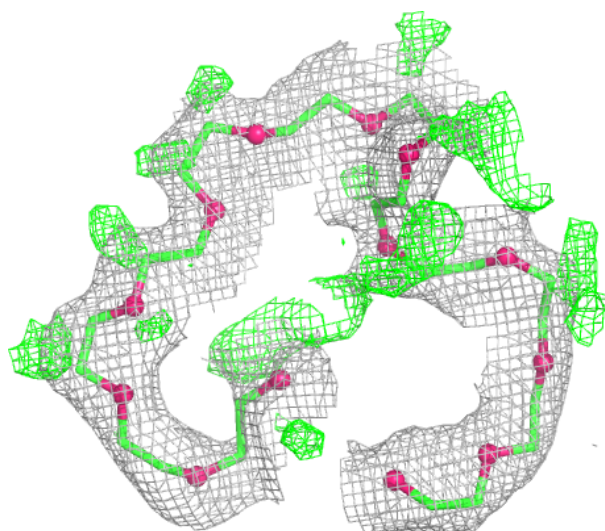
Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
7	ZN	A	701	1/1	1.00	0.01	19,19,19,19	0
15	CL	C	716	1/1	1.00	0.05	23,23,23,23	0
7	ZN	B	701	1/1	1.00	0.01	19,19,19,19	0
7	ZN	C	701	1/1	1.00	0.02	21,21,21,21	0
7	ZN	D	701	1/1	1.00	0.01	18,18,18,18	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.

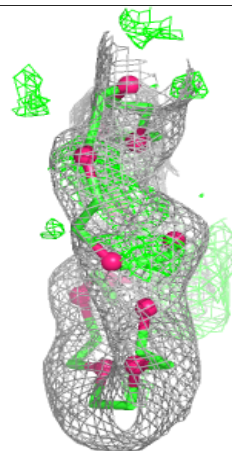
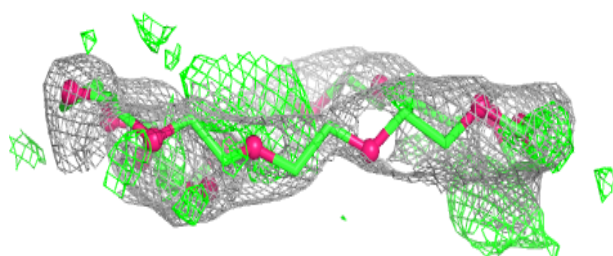
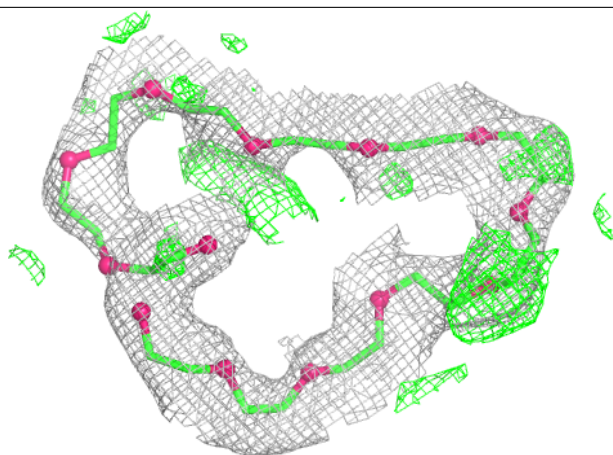
Electron density around 12P A 716 (A):

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



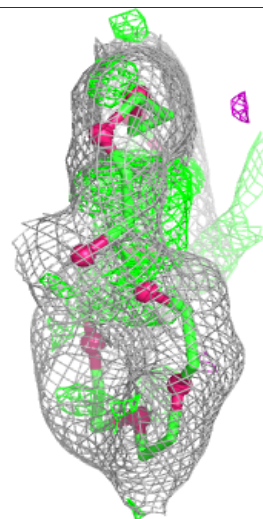
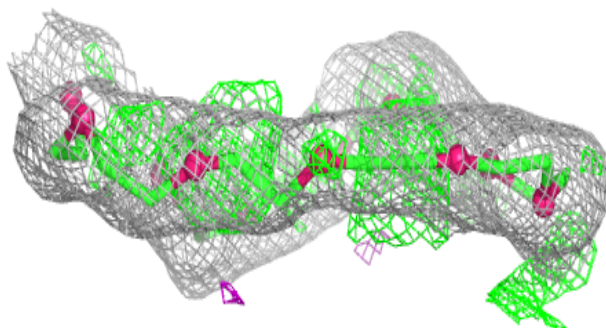
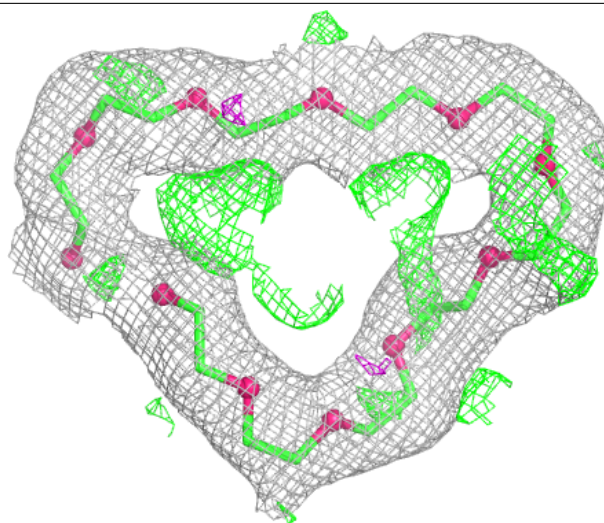
Electron density around 12P A 716 (B):

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



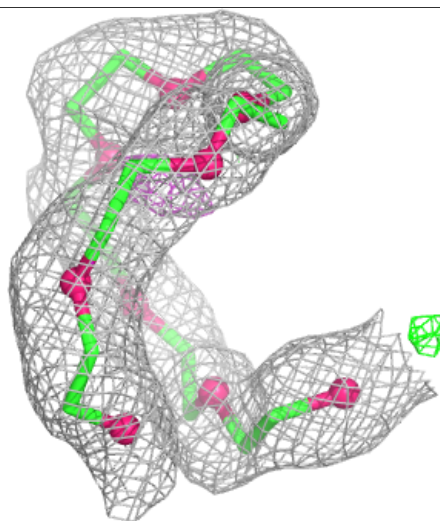
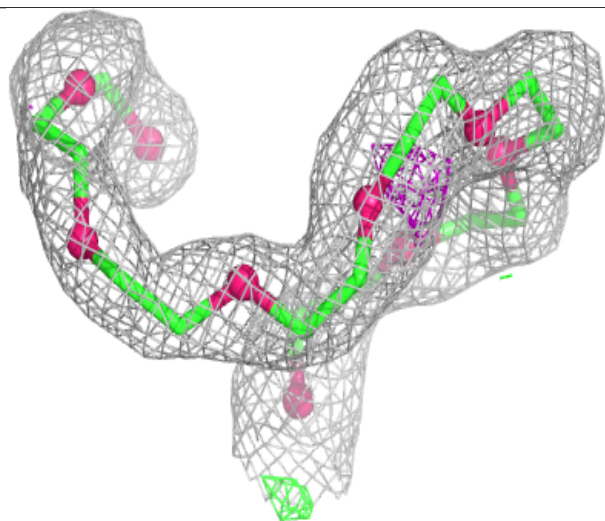
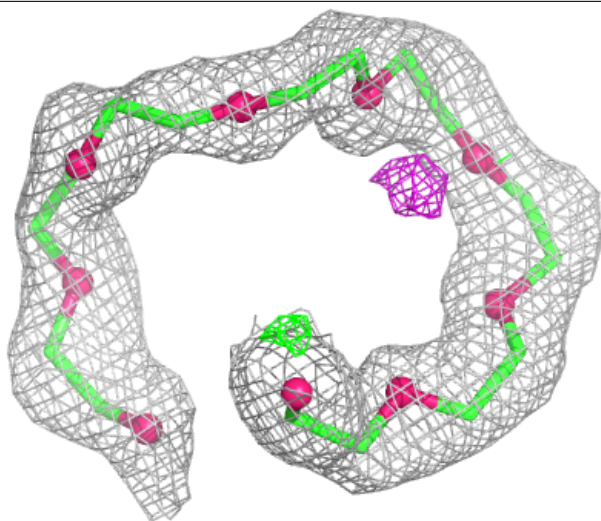
Electron density around XPE C 703:

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



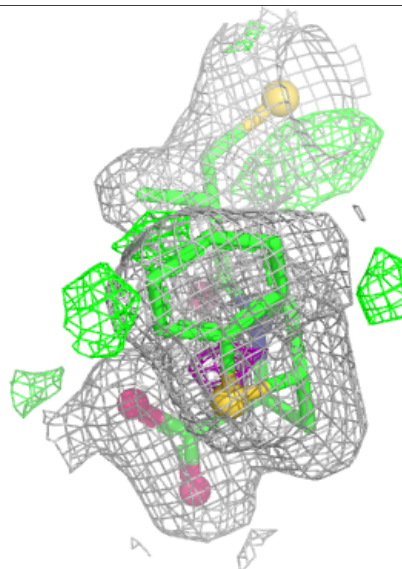
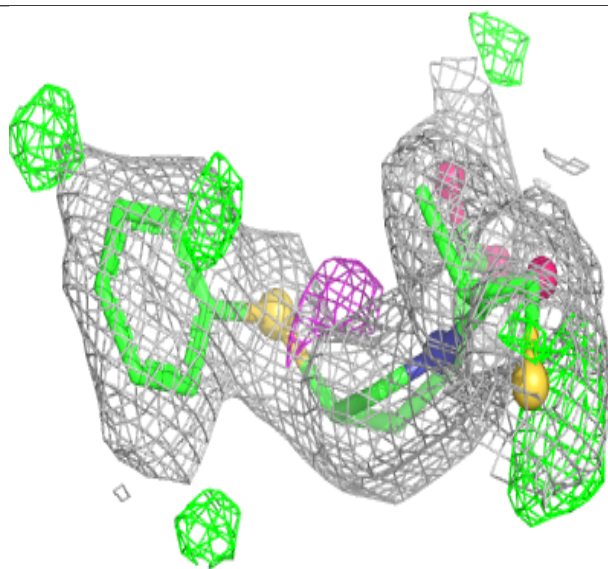
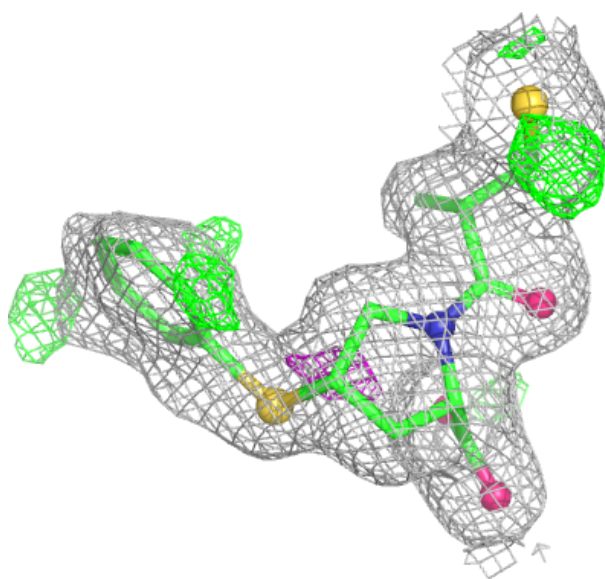
Electron density around PE8 B 703:

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



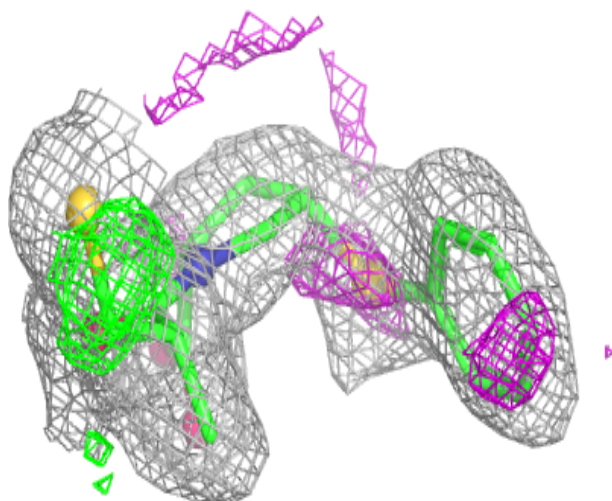
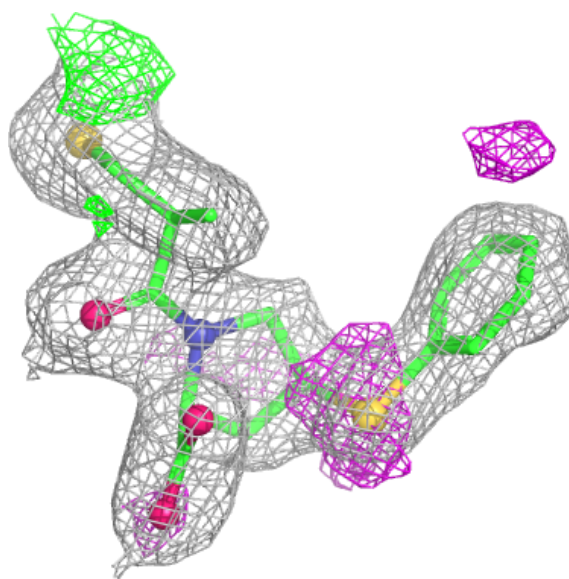
Electron density around ZED B 702:

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



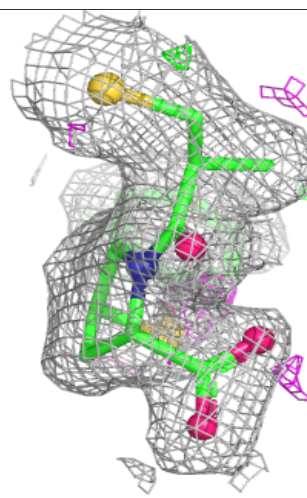
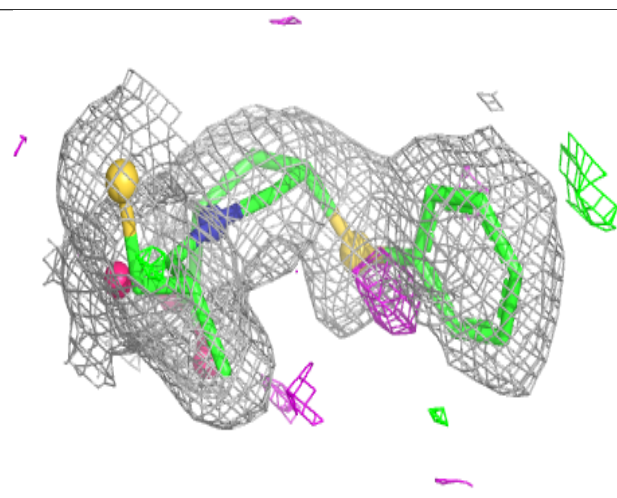
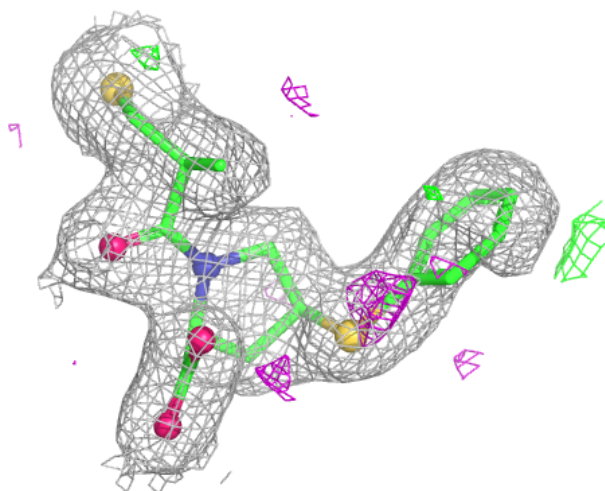
Electron density around ZED C 702:

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



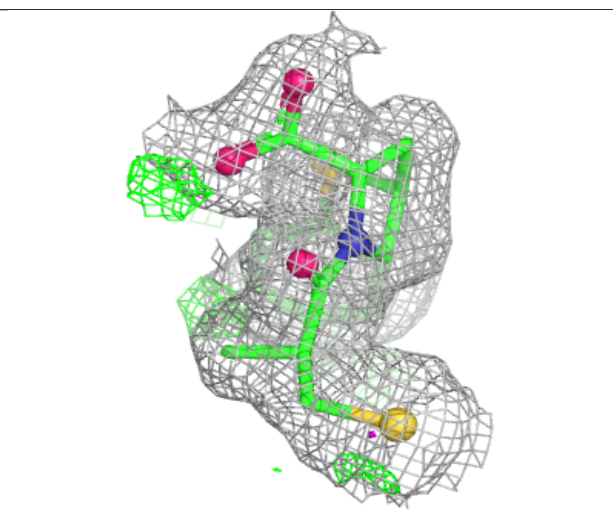
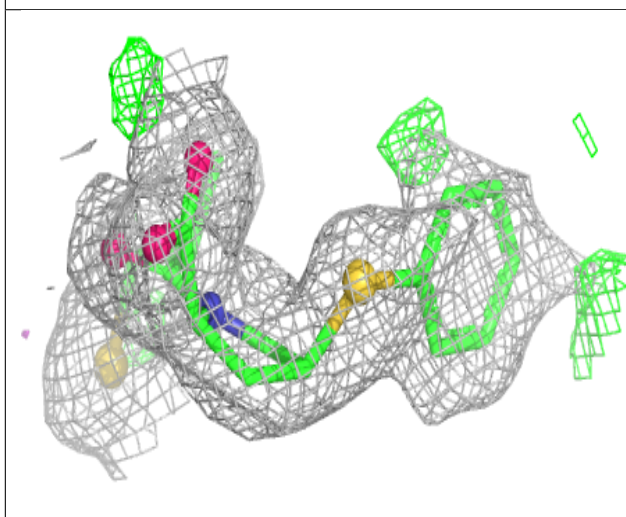
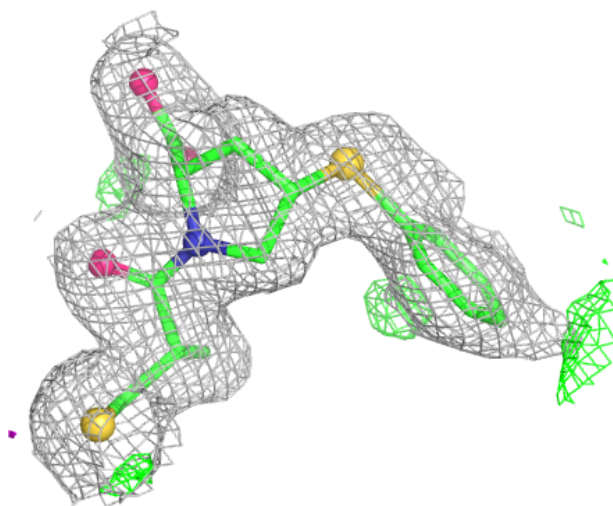
Electron density around ZED A 702:

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



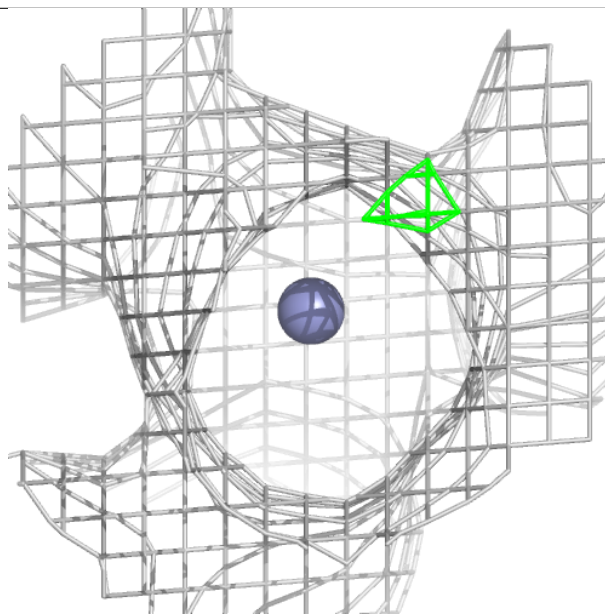
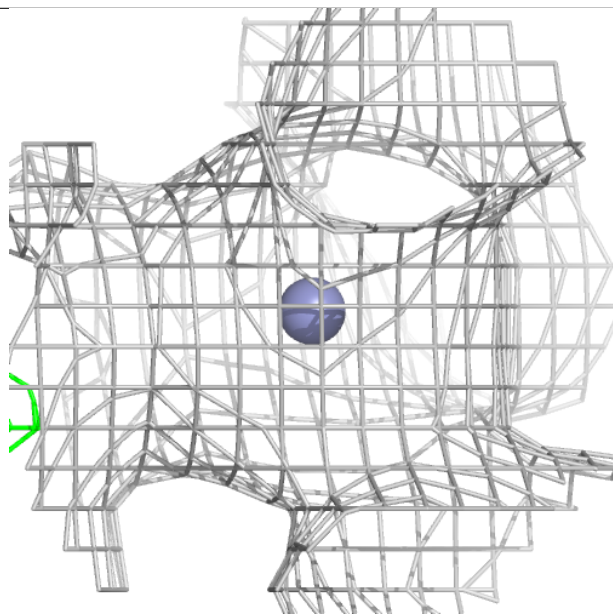
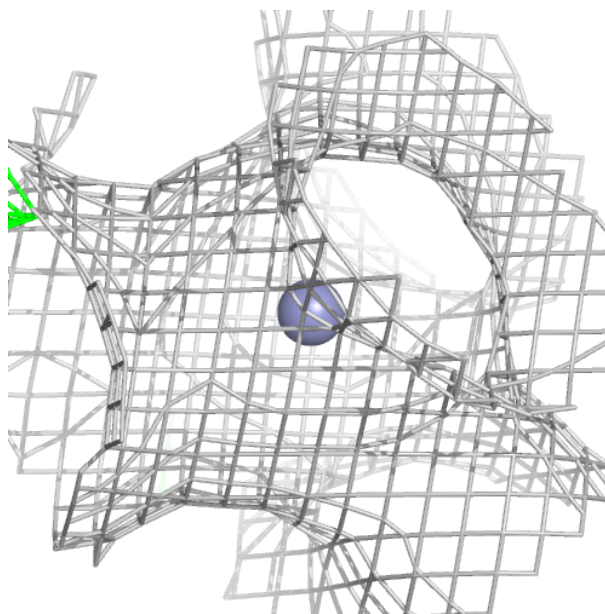
Electron density around ZED D 702:

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



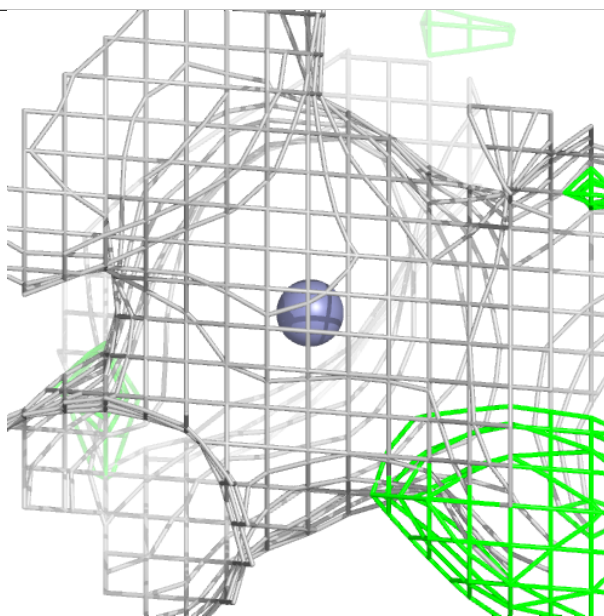
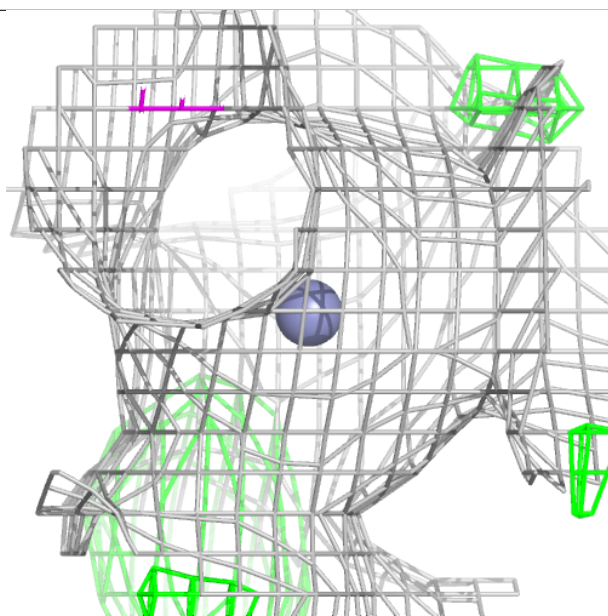
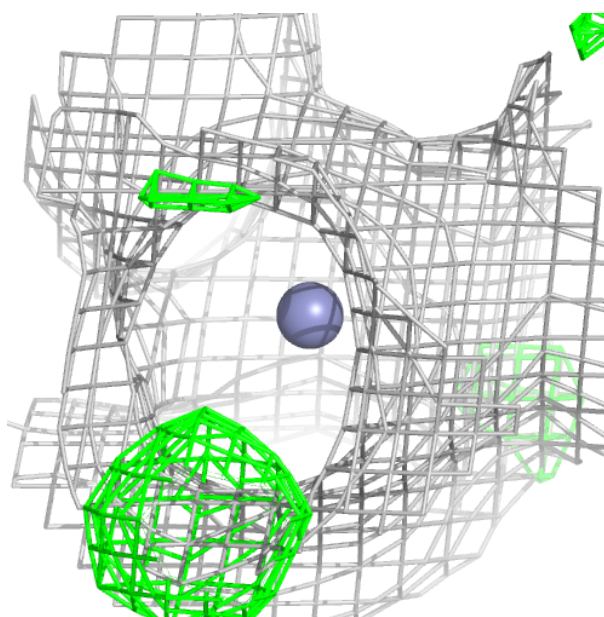
Electron density around ZN A 701:

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



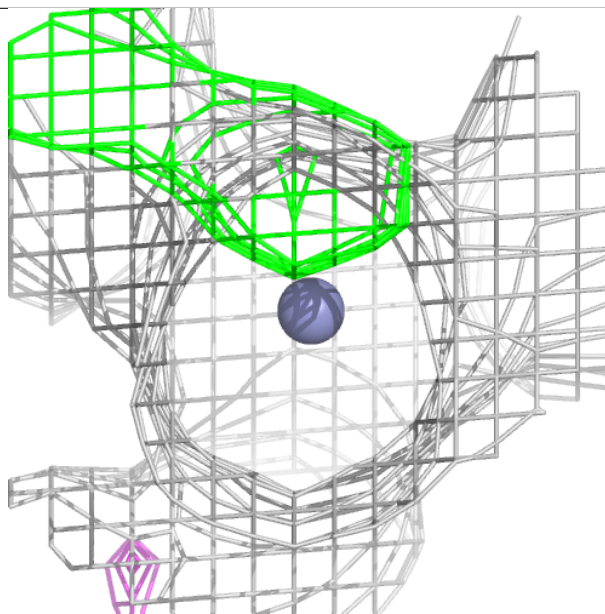
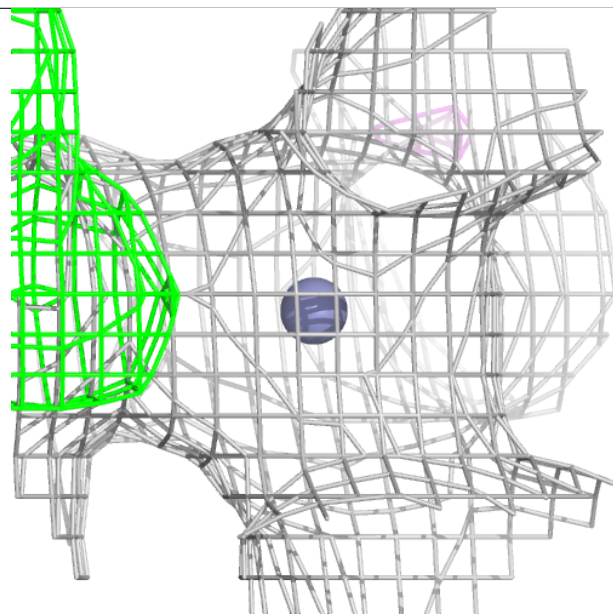
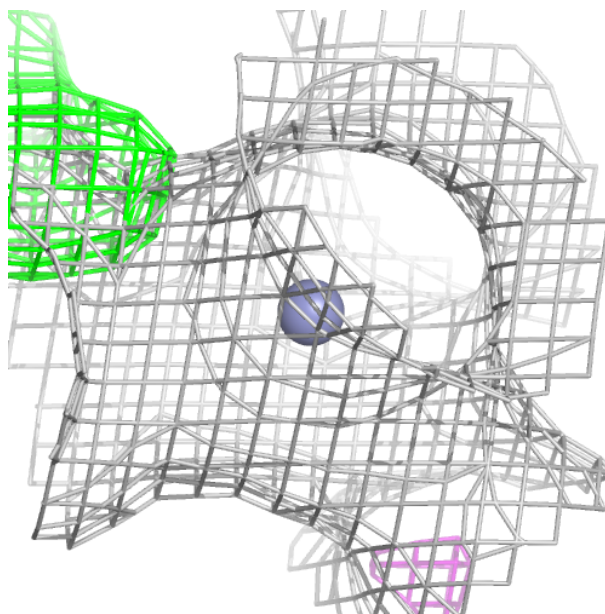
Electron density around ZN B 701:

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



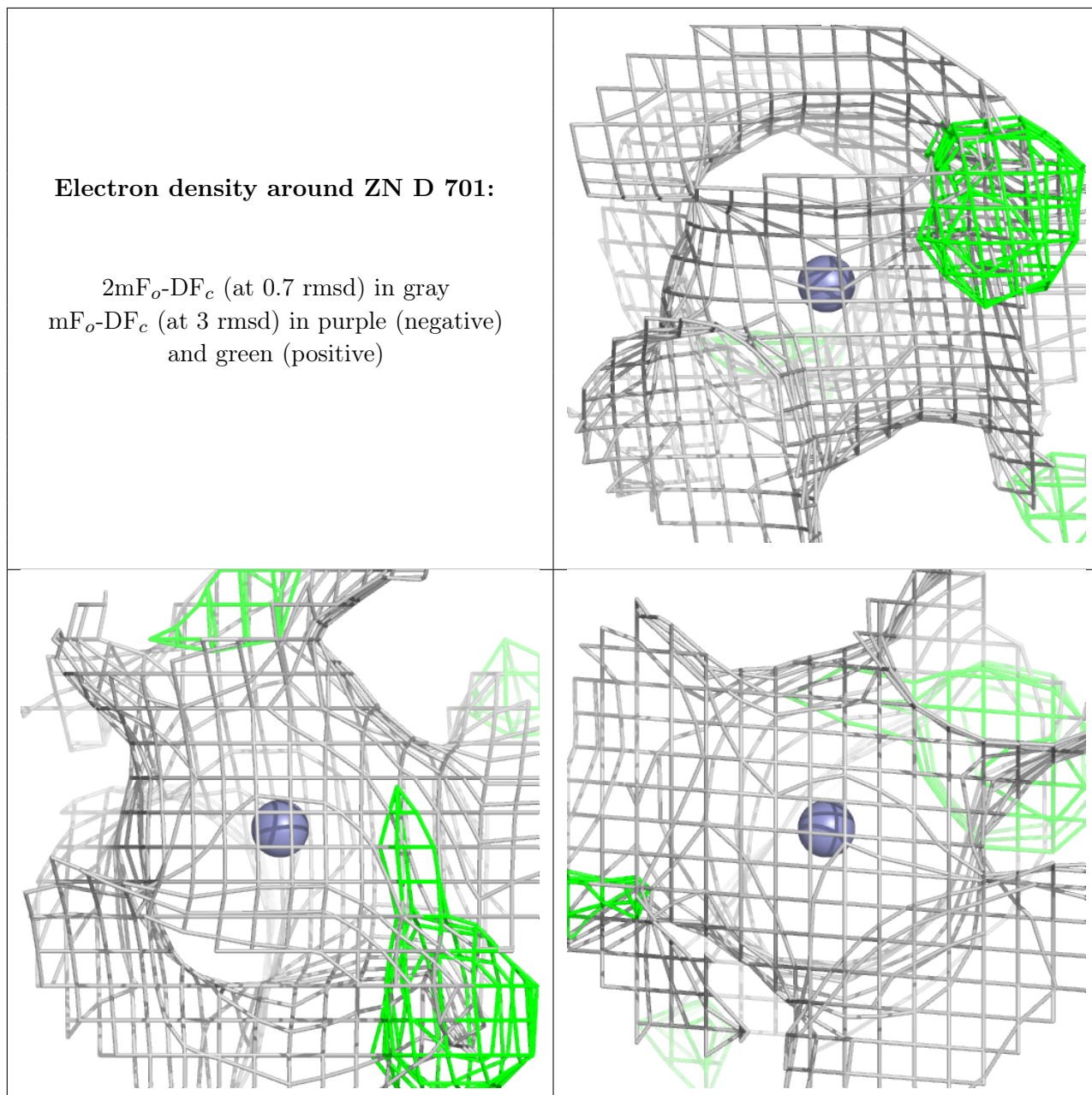
Electron density around ZN C 701:

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



Electron density around ZN D 701:

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



6.5 Other polymers ⓘ

There are no such residues in this entry.