



# wwPDB X-ray Structure Validation Summary Report

Mar 9, 2026 – 08:32 AM UTC

PDB ID : 6TP5 / pdb\_00006tp5  
Title : Crystal structure of human Transmembrane prolyl 4-hydroxylase  
Authors : Myllykoski, M.; Sutinen, A.; Koski, M.K.; Kallio, J.P.; Raasakka, A.; Myllyharju, J.; Wierenga, R.K.; Koivunen, P.  
Deposited on : 2019-12-12  
Resolution : 2.25 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](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

with specific help available everywhere you see the  symbol.

The types of validation reports are described at

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

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

MolProbity : 4-5-2 with Phenix2.0  
Mogul : 2022.3.0, CSD as543be (2022)  
Xtrriage (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

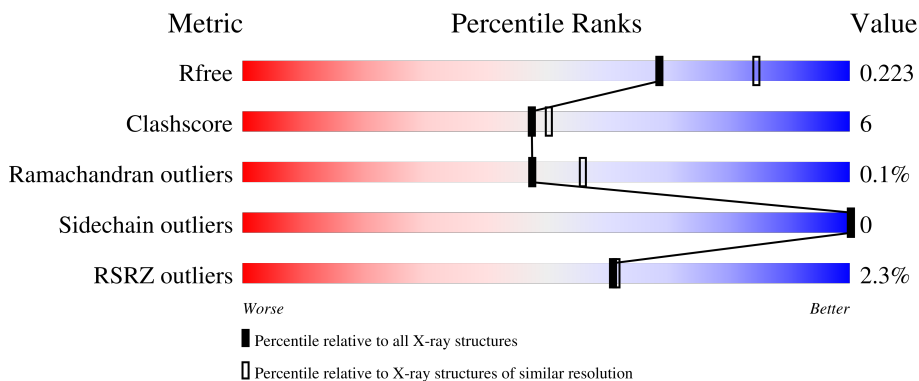
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.25 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	1898 (2.26-2.26)
Clashscore	190562	2005 (2.26-2.26)
Ramachandran outliers	187476	1965 (2.26-2.26)
Sidechain outliers	187428	1966 (2.26-2.26)
RSRZ outliers	180081	1898 (2.26-2.26)

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

Mol	Chain	Length	Quality of chain
1	A	421	 2% 78% 10% 12%
1	B	421	 2% 71% 14% 15%
2	C	2	 50% 50%
2	E	2	 100%
3	D	10	 30% 70%

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Mol	Chain	Length	Quality of chain
4	F	10	 30% 70%

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
8	GLY	A	719	-	X	-	-

## 2 Entry composition [i](#)

There are 11 unique types of molecules in this entry. The entry contains 6394 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 Transmembrane prolyl 4-hydroxylase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	370	2995	1878	544	559	14	0	0	0
1	B	356	2898	1821	529	534	14	0	2	0

There are 14 discrepancies between the modelled and reference sequences:

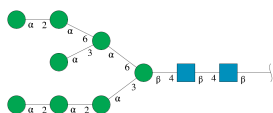
Chain	Residue	Modelled	Actual	Comment	Reference
A	82	HIS	-	expression tag	UNP Q9NXG6
A	83	HIS	-	expression tag	UNP Q9NXG6
A	84	HIS	-	expression tag	UNP Q9NXG6
A	85	HIS	-	expression tag	UNP Q9NXG6
A	86	HIS	-	expression tag	UNP Q9NXG6
A	87	HIS	-	expression tag	UNP Q9NXG6
A	99	VAL	ALA	conflict	UNP Q9NXG6
B	82	HIS	-	expression tag	UNP Q9NXG6
B	83	HIS	-	expression tag	UNP Q9NXG6
B	84	HIS	-	expression tag	UNP Q9NXG6
B	85	HIS	-	expression tag	UNP Q9NXG6
B	86	HIS	-	expression tag	UNP Q9NXG6
B	87	HIS	-	expression tag	UNP Q9NXG6
B	99	VAL	ALA	conflict	UNP Q9NXG6

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



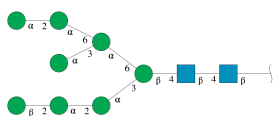
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
2	C	2	28	16	2	10	0	0	0
2	E	2	28	16	2	10	0	0	0

- Molecule 3 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



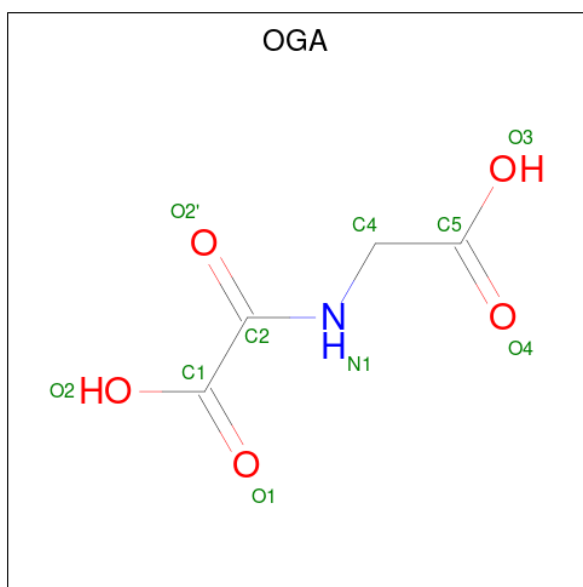
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
3	D	10	116	64	2	50	0	0	0

- Molecule 4 is an oligosaccharide called beta-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]alpha-D-mannopyranose-(1-6)]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
			Total	C	N	O			
4	F	10	116	64	2	50	0	0	0

- Molecule 5 is N-OXALYLGLYCINE (CCD ID: OGA) (formula: C<sub>4</sub>H<sub>5</sub>NO<sub>5</sub>) (labeled as "Ligand of Interest" by depositor).

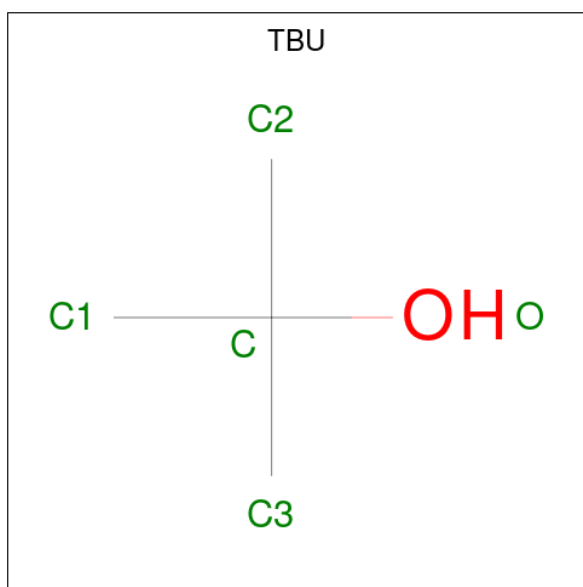


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O	0	0
			10	4	1	5		
5	B	1	Total	C	N	O	0	0
			10	4	1	5		

- Molecule 6 is FE (II) ION (CCD ID: FE2) (formula: Fe) (labeled as "Ligand of Interest" by depositor).

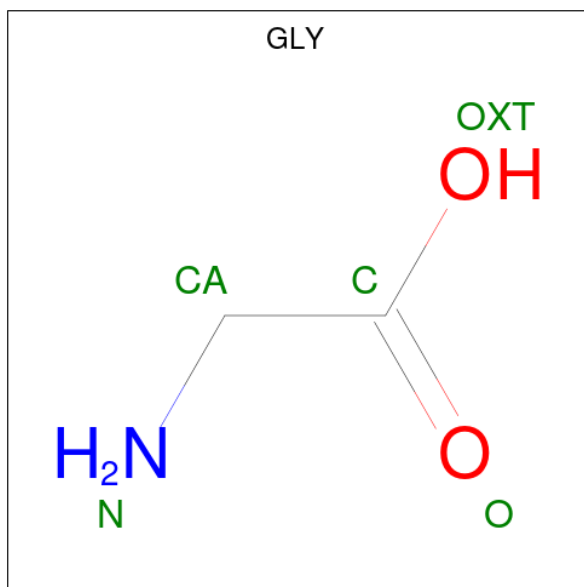
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	1	Total	Fe	0	0
			1	1		
6	B	1	Total	Fe	0	0
			1	1		

- Molecule 7 is TERTIARY-BUTYL ALCOHOL (CCD ID: TBU) (formula: C<sub>4</sub>H<sub>10</sub>O).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total C O 5 4 1	0	0
7	A	1	Total C O 5 4 1	0	0
7	A	1	Total C O 5 4 1	0	0
7	A	1	Total C O 5 4 1	0	0
7	B	1	Total C O 5 4 1	0	0
7	B	1	Total C O 5 4 1	0	0
7	B	1	Total C O 5 4 1	0	0
7	B	1	Total C O 5 4 1	0	0

- Molecule 8 is GLYCINE (CCD ID: GLY) (formula: C<sub>2</sub>H<sub>5</sub>NO<sub>2</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	
8	A	1	Total	C	N	O	0	0
			5	2	1	2		
8	A	1	Total	C	N	O	0	0
			5	2	1	2		

- Molecule 9 is CALCIUM ION (CCD ID: CA) (formula: Ca) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	2	Total	Ca	0	0
			2	2		
9	B	2	Total	Ca	0	0
			2	2		

- Molecule 10 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	2	Total	Cl	0	0
			2	2		

- Molecule 11 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	A	67	Total	O	0	0
			67	67		
11	B	68	Total	O	0	0
			68	68		



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

Chain E:  100%

MAG1  
MAG2

- Molecule 3: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain D:  30% 70%

MAG1  
MAG2  
BMA3  
MAN4  
MAN5  
MAN6  
MAN7  
MAN8  
MAN9  
MAN10

- Molecule 4: beta-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain F:  30% 70%

MAG1  
MAG2  
BMA3  
MAN4  
MAN5  
BMA6  
MAN7  
MAN8  
MAN9  
MAN10

## 4 Data and refinement statistics i

Property	Value	Source
Space group	P 31	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	92.08Å 92.08Å 129.50Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	50.30 – 2.25 50.30 – 2.25	Depositor EDS
% Data completeness (in resolution range)	98.0 (50.30-2.25) 98.0 (50.30-2.25)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	0.98 (at 2.25Å)	Xtrriage
Refinement program	PHENIX 1.15.2_3472	Depositor
R, $R_{free}$	0.181 , 0.221 0.188 , 0.223	Depositor DCC
$R_{free}$ test set	2008 reflections (3.45%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	60.7	Xtrriage
Anisotropy	0.154	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 58.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	0.016 for -h,-k,l 0.042 for h,-h-k,-l 0.032 for -k,-h,-l	Xtrriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	6394	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	87.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.47% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: NAG, BMA, CA, TBU, CL, MAN, FE2, OGA

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	0.21	0/3062	0.42	0/4147
1	B	0.22	0/2964	0.42	0/4014
All	All	0.22	0/6026	0.42	0/8161

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2995	0	2910	31	0
1	B	2898	0	2820	38	0
2	C	28	0	25	0	0
2	E	28	0	25	0	0
3	D	116	0	97	0	0
4	F	116	0	97	0	0
5	A	10	0	3	0	0
5	B	10	0	3	0	0
6	A	1	0	0	0	0
6	B	1	0	0	0	0
7	A	20	0	40	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	B	20	0	40	1	0
8	A	10	0	4	0	0
9	A	2	0	0	0	0
9	B	2	0	0	0	0
10	A	2	0	0	0	0
11	A	67	0	0	0	0
11	B	68	0	0	0	0
All	All	6394	0	6064	69	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 6.

The worst 5 of 69 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)
1:A:222:MET:HE3	7:A:716:TBU:H23	1.67	0.74
1:B:259:LYS:HA	1:B:262:ARG:HB2	1.70	0.72
1:A:340:CYS:HB2	1:A:343:THR:HG22	1.73	0.70
1:B:229:GLU:HG3	7:B:715:TBU:H32	1.75	0.69
1:A:349:GLU:HB3	1:A:351:VAL:HG13	1.76	0.67

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	366/421 (87%)	360 (98%)	6 (2%)	0	100	100
1	B	352/421 (84%)	343 (97%)	8 (2%)	1 (0%)	36	40
All	All	718/842 (85%)	703 (98%)	14 (2%)	1 (0%)	48	56

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	198	ASP

### 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	325/368 (88%)	325 (100%)	0	100	100
1	B	314/368 (85%)	314 (100%)	0	100	100
All	All	639/736 (87%)	639 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 8 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	472	GLN
1	B	455	ASN
1	B	228	GLN
1	B	190	GLN
1	B	288	HIS

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

24 monosaccharides are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and

the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	NAG	C	1	1,2	14,14,15	0.27	0	17,19,21	0.41	0
2	NAG	C	2	2	14,14,15	0.23	0	17,19,21	0.67	1 (5%)
3	NAG	D	1	3,1	14,14,15	0.22	0	17,19,21	0.66	1 (5%)
3	MAN	D	10	3	11,11,12	0.77	0	15,15,17	0.95	2 (13%)
3	NAG	D	2	3	14,14,15	0.32	0	17,19,21	0.43	0
3	BMA	D	3	3	11,11,12	0.61	0	15,15,17	0.68	0
3	MAN	D	4	3	11,11,12	0.92	0	15,15,17	0.94	2 (13%)
3	MAN	D	5	3	11,11,12	0.81	0	15,15,17	0.91	0
3	MAN	D	6	3	11,11,12	0.82	0	15,15,17	0.91	1 (6%)
3	MAN	D	7	3	11,11,12	0.84	0	15,15,17	1.14	1 (6%)
3	MAN	D	8	3	11,11,12	0.75	0	15,15,17	0.98	1 (6%)
3	MAN	D	9	3	11,11,12	0.71	0	15,15,17	0.94	2 (13%)
2	NAG	E	1	1,2	14,14,15	0.38	0	17,19,21	0.49	0
2	NAG	E	2	2	14,14,15	0.24	0	17,19,21	0.48	0
4	NAG	F	1	1,4	14,14,15	0.23	0	17,19,21	0.62	1 (5%)
4	MAN	F	10	4	11,11,12	0.78	0	15,15,17	1.02	1 (6%)
4	NAG	F	2	4	14,14,15	0.27	0	17,19,21	0.42	0
4	BMA	F	3	4	11,11,12	0.60	0	15,15,17	0.74	0
4	MAN	F	4	4	11,11,12	0.94	0	15,15,17	0.95	1 (6%)
4	MAN	F	5	4	11,11,12	0.91	0	15,15,17	1.15	2 (13%)
4	BMA	F	6	4	11,11,12	0.97	0	15,15,17	0.93	1 (6%)
4	MAN	F	7	4	11,11,12	0.72	0	15,15,17	1.05	2 (13%)
4	MAN	F	8	4	11,11,12	0.78	0	15,15,17	0.96	0
4	MAN	F	9	4	11,11,12	0.87	0	15,15,17	0.94	2 (13%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	C	1	1,2	-	1/6/23/26	0/1/1/1
2	NAG	C	2	2	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	D	1	3,1	-	0/6/23/26	0/1/1/1
3	MAN	D	10	3	-	0/2/19/22	0/1/1/1
3	NAG	D	2	3	-	2/6/23/26	0/1/1/1
3	BMA	D	3	3	-	0/2/19/22	0/1/1/1
3	MAN	D	4	3	-	2/2/19/22	0/1/1/1
3	MAN	D	5	3	-	2/2/19/22	0/1/1/1
3	MAN	D	6	3	-	1/2/19/22	0/1/1/1
3	MAN	D	7	3	-	0/2/19/22	0/1/1/1
3	MAN	D	8	3	-	0/2/19/22	0/1/1/1
3	MAN	D	9	3	-	0/2/19/22	0/1/1/1
2	NAG	E	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	E	2	2	-	0/6/23/26	0/1/1/1
4	NAG	F	1	1,4	-	0/6/23/26	0/1/1/1
4	MAN	F	10	4	-	2/2/19/22	0/1/1/1
4	NAG	F	2	4	-	0/6/23/26	0/1/1/1
4	BMA	F	3	4	-	0/2/19/22	0/1/1/1
4	MAN	F	4	4	-	2/2/19/22	0/1/1/1
4	MAN	F	5	4	-	0/2/19/22	0/1/1/1
4	BMA	F	6	4	-	0/2/19/22	0/1/1/1
4	MAN	F	7	4	-	0/2/19/22	0/1/1/1
4	MAN	F	8	4	-	0/2/19/22	0/1/1/1
4	MAN	F	9	4	-	0/2/19/22	0/1/1/1

There are no bond length outliers.

The worst 5 of 21 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	F	5	MAN	O2-C2-C3	-2.80	104.36	110.15
4	F	5	MAN	C1-O5-C5	2.76	115.89	112.19
3	D	7	MAN	C1-O5-C5	2.61	115.68	112.19
4	F	4	MAN	C1-O5-C5	2.42	115.43	112.19
4	F	10	MAN	C1-O5-C5	2.40	115.41	112.19

There are no chirality outliers.

5 of 16 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	2	NAG	C4-C5-C6-O6
3	D	5	MAN	C4-C5-C6-O6
2	C	2	NAG	O5-C5-C6-O6

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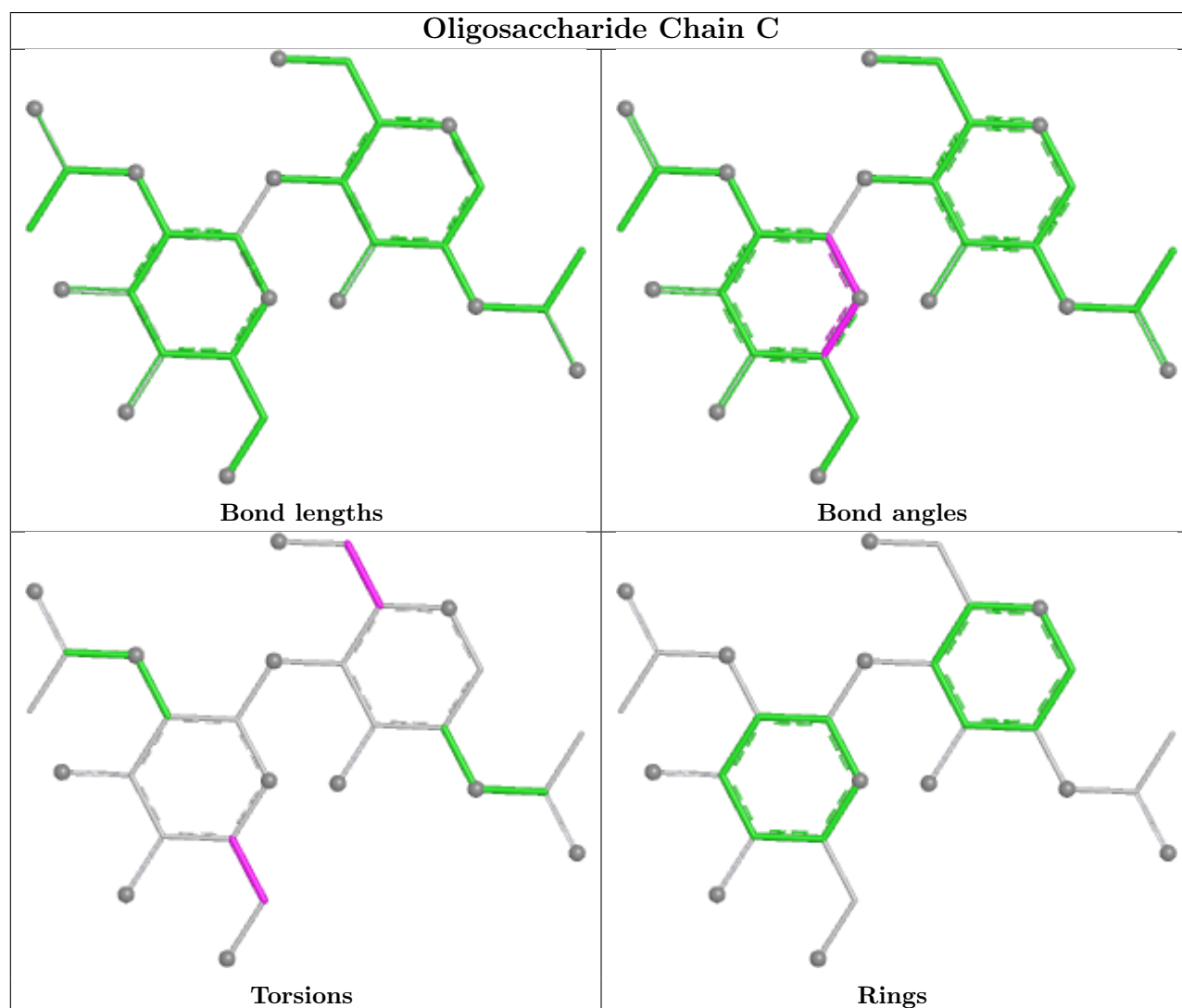
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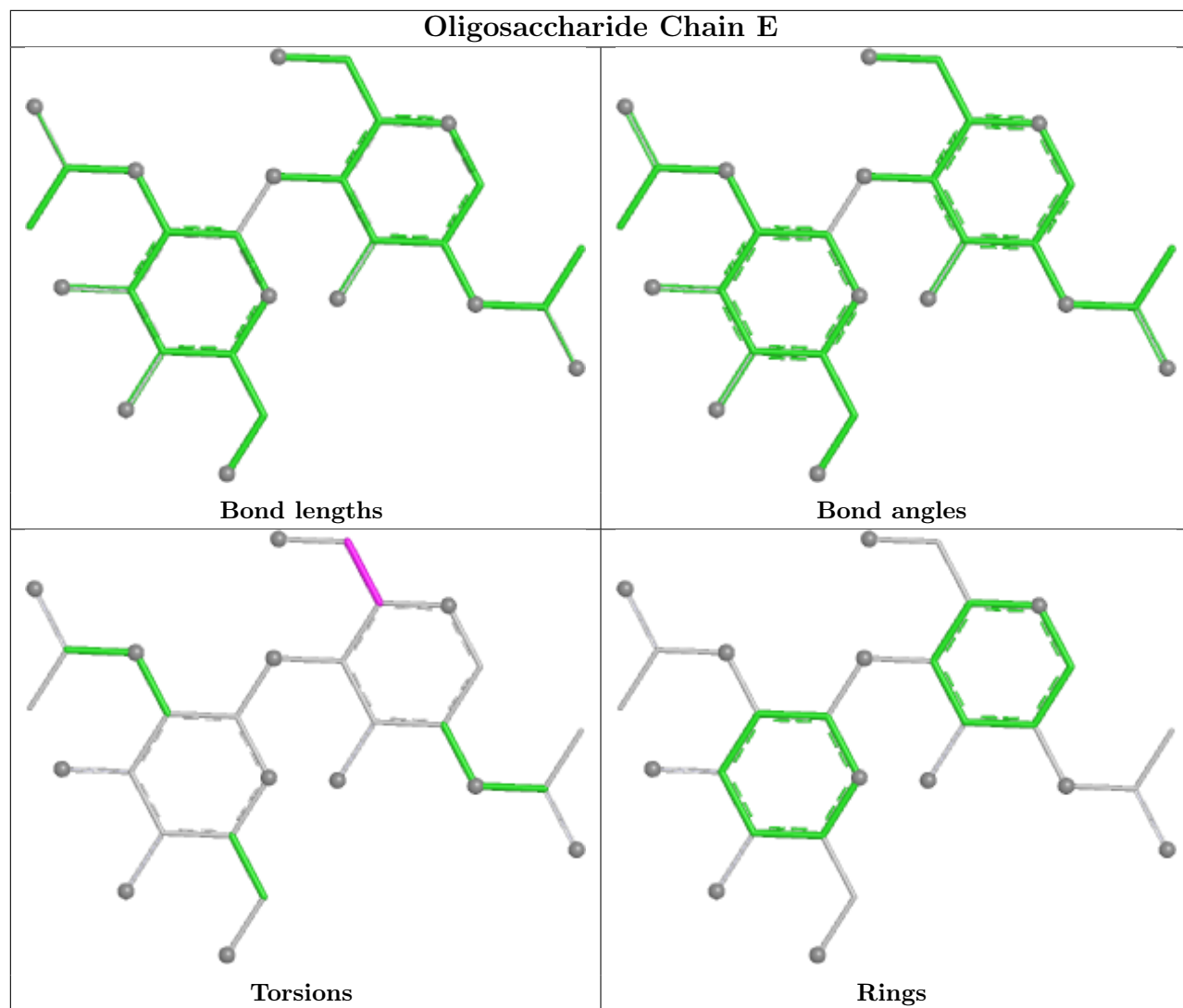
Mol	Chain	Res	Type	Atoms
4	F	4	MAN	O5-C5-C6-O6
4	F	4	MAN	C4-C5-C6-O6

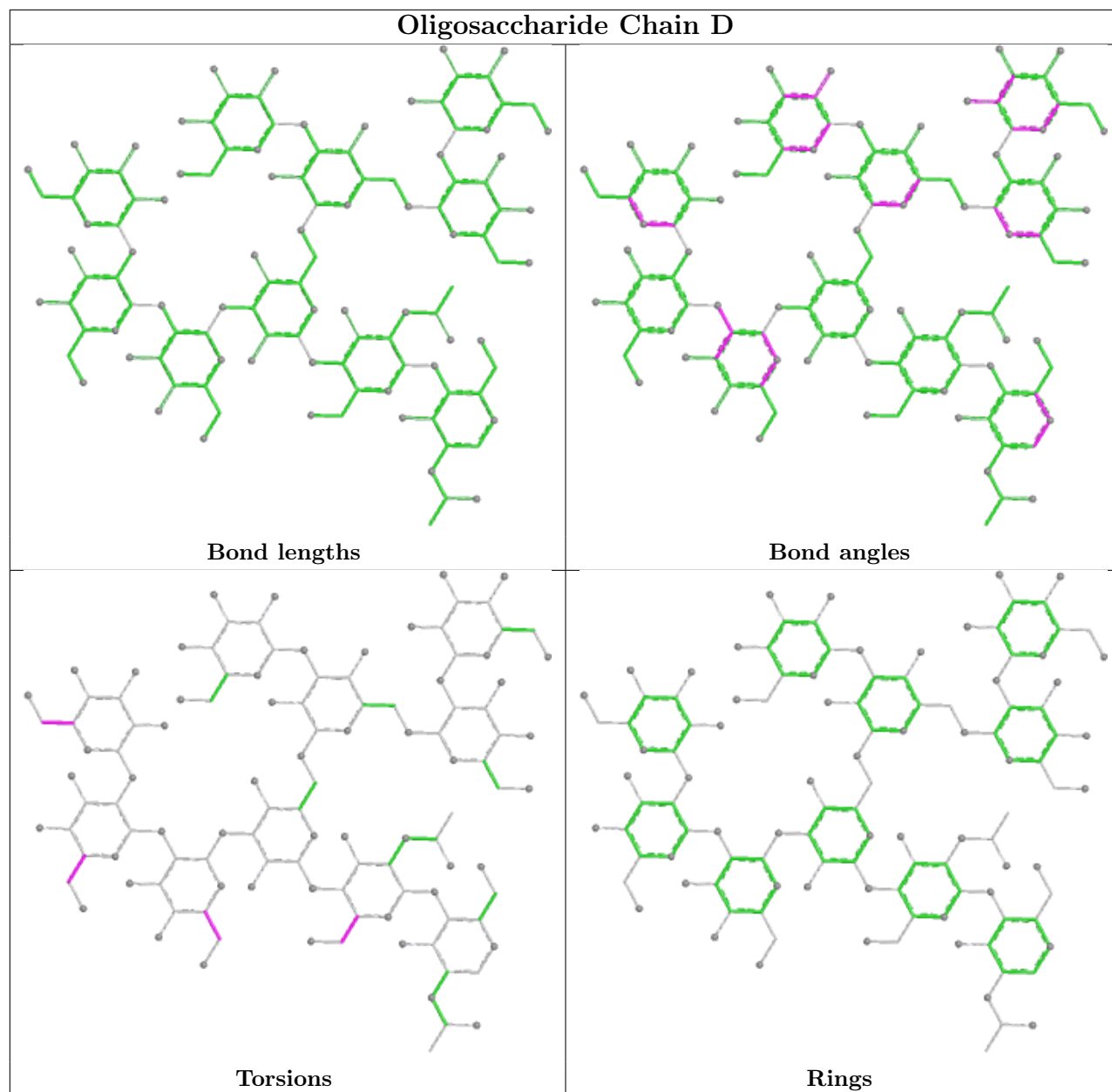
There are no ring outliers.

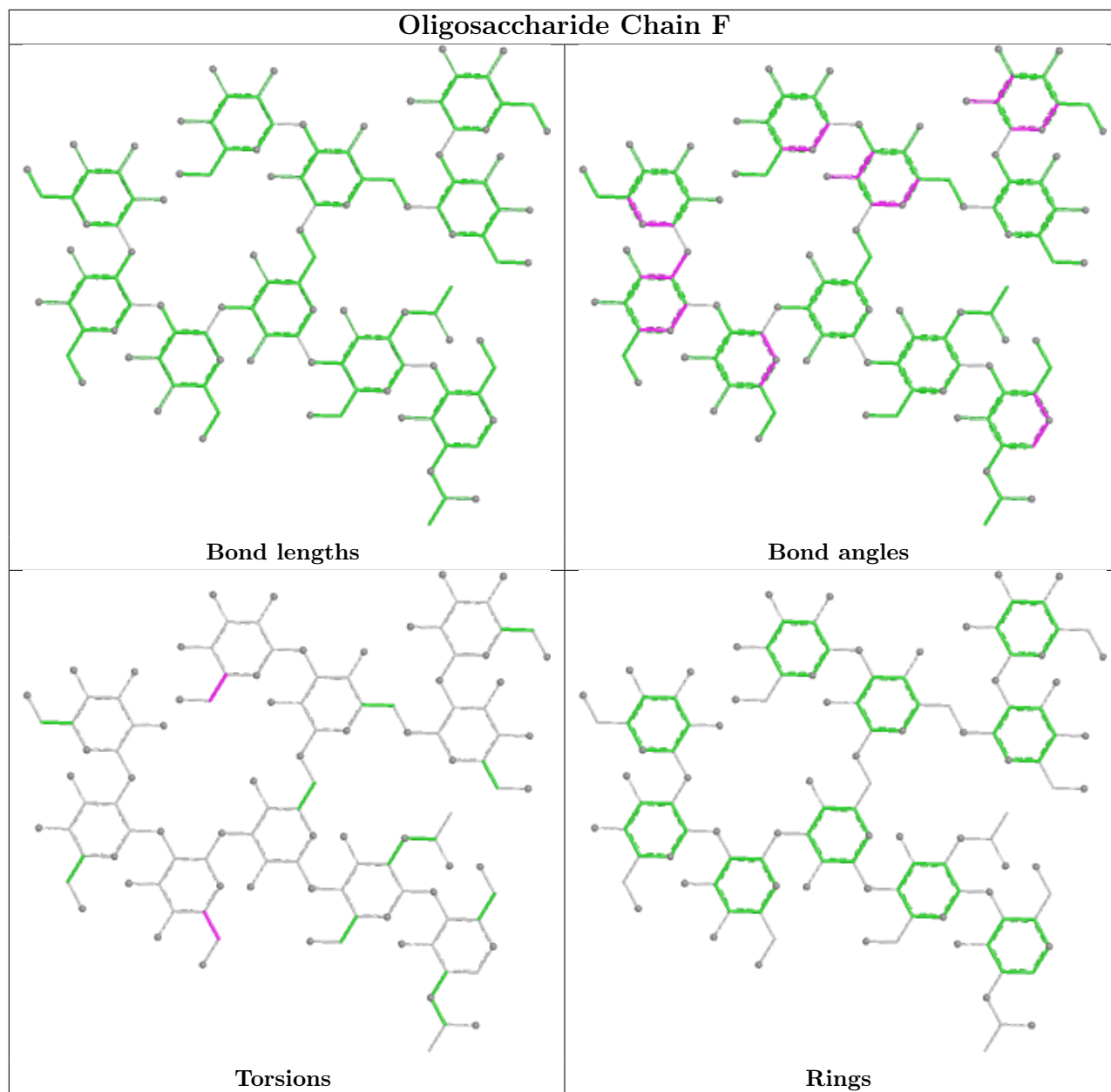
No monomer is involved in short contacts.

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 20 ligands modelled in this entry, 8 are monoatomic - leaving 12 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
7	TBU	A	717	-	4,4,4	0.78	0	6,6,6	0.40	0
7	TBU	B	717	-	4,4,4	0.72	0	6,6,6	0.60	0
8	GLY	A	719	-	4,4,4	1.12	1 (25%)	3,4,4	1.65	1 (33%)
7	TBU	B	716	-	4,4,4	0.75	0	6,6,6	0.46	0
7	TBU	B	718	-	4,4,4	0.79	0	6,6,6	0.41	0
8	GLY	A	720	-	4,4,4	1.17	1 (25%)	3,4,4	1.63	1 (33%)
5	OGA	A	701	6	9,9,9	2.64	2 (22%)	8,11,11	1.37	1 (12%)
7	TBU	A	716	-	4,4,4	0.74	0	6,6,6	0.53	0
5	OGA	B	701	6	9,9,9	2.69	2 (22%)	8,11,11	1.41	1 (12%)
7	TBU	A	718	-	4,4,4	0.76	0	6,6,6	0.46	0
7	TBU	A	703	-	4,4,4	0.79	0	6,6,6	0.53	0
7	TBU	B	715	-	4,4,4	0.78	0	6,6,6	0.44	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
5	OGA	A	701	6	-	5/8/9/9	-
8	GLY	A	719	-	-	2/2/2/2	-
5	OGA	B	701	6	-	5/8/9/9	-
8	GLY	A	720	-	-	0/2/2/2	-

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	701	OGA	C2-N1	7.11	1.45	1.33
5	A	701	OGA	C2-N1	6.86	1.45	1.33
5	A	701	OGA	O2'-C2	-2.46	1.18	1.23
5	B	701	OGA	O2'-C2	-2.33	1.19	1.23
8	A	720	GLY	OXT-C	-2.22	1.23	1.30

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	701	OGA	O3-C5-C4	2.35	121.73	112.81
5	A	701	OGA	O2'-C2-N1	-2.17	119.44	123.35
8	A	719	GLY	OXT-C-O	-2.10	117.93	123.33
8	A	720	GLY	OXT-C-O	-2.07	118.02	123.33

There are no chirality outliers.

5 of 12 torsion outliers are listed below:

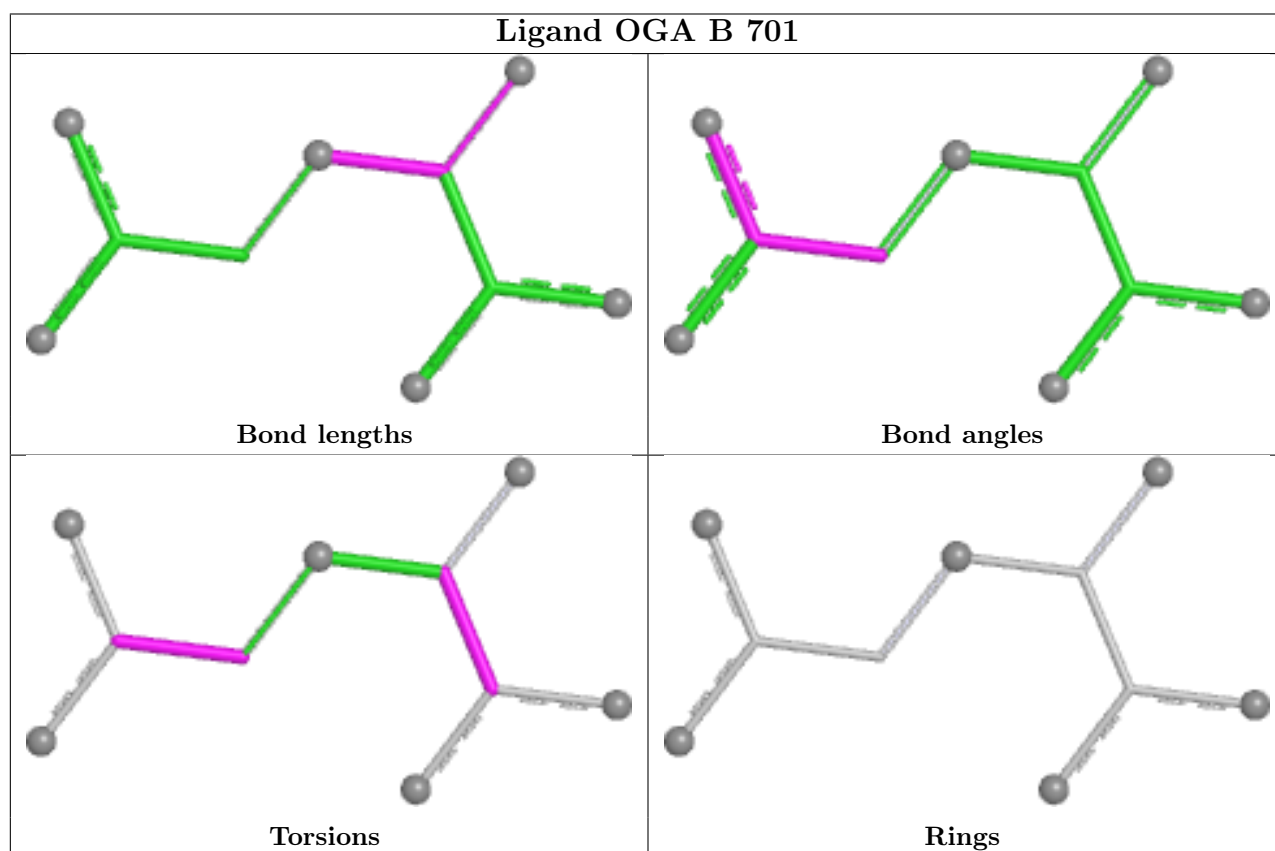
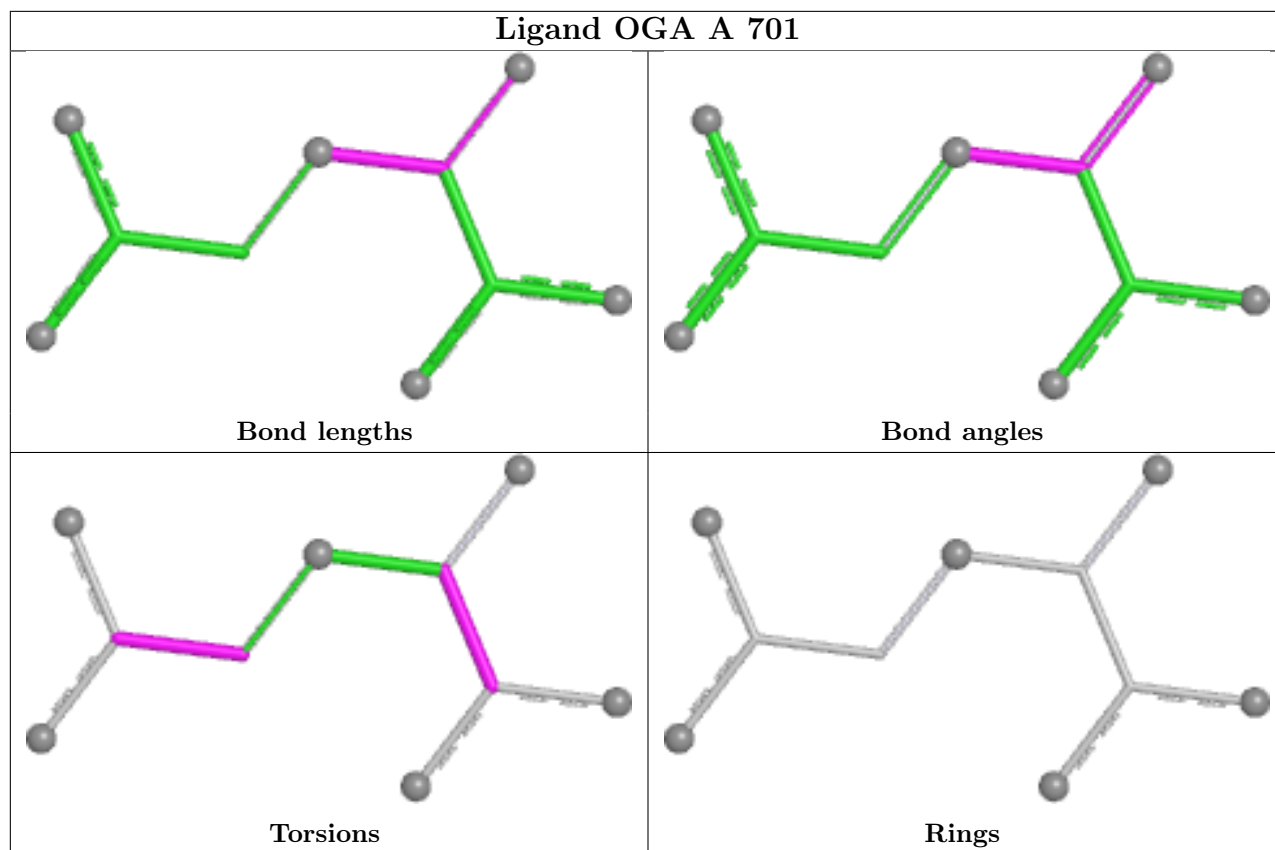
Mol	Chain	Res	Type	Atoms
5	A	701	OGA	O1-C1-C2-O2'
5	A	701	OGA	O1-C1-C2-N1
5	A	701	OGA	O2-C1-C2-O2'
5	B	701	OGA	O1-C1-C2-O2'
5	B	701	OGA	O1-C1-C2-N1

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A	717	TBU	1	0
7	A	716	TBU	1	0
7	B	715	TBU	1	0

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



## 5.7 Other polymers [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, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q < 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	370/421 (87%)	-0.08	7 (1%) 66 67	45, 72, 153, 191	0
1	B	356/421 (84%)	0.15	10 (2%) 55 55	31, 87, 152, 199	2 (0%)
All	All	726/842 (86%)	0.03	17 (2%) 61 61	31, 77, 153, 199	2 (0%)

The worst 5 of 17 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	281[A]	TYR	4.3
1	B	108	LEU	3.4
1	A	345	LEU	3.0
1	B	216	LEU	2.7
1	A	346	VAL	2.5

### 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, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q < 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
3	MAN	D	5	11/12	0.40	0.12	131,159,169,181	0
3	MAN	D	6	11/12	0.49	0.10	147,179,185,188	0
4	BMA	F	6	11/12	0.54	0.09	174,178,183,183	0
2	NAG	C	2	14/15	0.57	0.11	144,155,168,170	0
2	NAG	E	2	14/15	0.62	0.11	127,140,147,150	0

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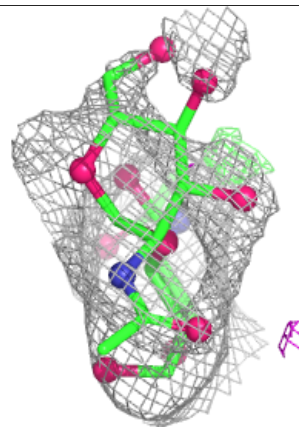
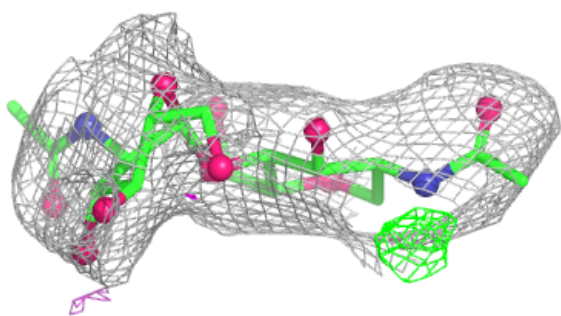
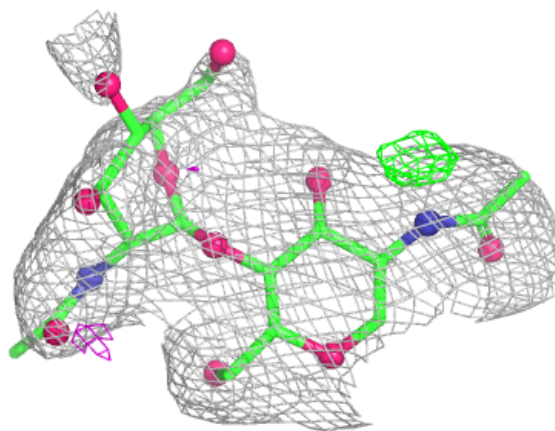
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
4	MAN	F	5	11/12	0.66	0.10	136,146,160,173	0
3	MAN	D	10	11/12	0.68	0.12	123,130,143,144	0
4	MAN	F	10	11/12	0.72	0.14	105,125,144,146	0
3	MAN	D	4	11/12	0.74	0.11	136,146,152,160	0
4	MAN	F	4	11/12	0.78	0.11	109,127,132,139	0
4	MAN	F	9	11/12	0.81	0.14	114,132,135,136	0
3	BMA	D	3	11/12	0.81	0.09	95,108,125,136	0
3	MAN	D	9	11/12	0.82	0.16	111,145,154,157	0
4	MAN	F	7	11/12	0.85	0.09	102,109,117,122	0
4	BMA	F	3	11/12	0.87	0.08	86,113,119,122	0
3	MAN	D	8	11/12	0.88	0.12	120,125,137,145	0
2	NAG	C	1	14/15	0.88	0.08	84,96,120,144	0
4	MAN	F	8	11/12	0.90	0.11	110,115,127,137	0
2	NAG	E	1	14/15	0.90	0.09	83,98,124,132	0
3	MAN	D	7	11/12	0.90	0.08	90,96,112,119	0
4	NAG	F	2	14/15	0.94	0.09	69,80,86,94	0
3	NAG	D	2	14/15	0.95	0.07	69,82,88,103	0
3	NAG	D	1	14/15	0.96	0.08	50,59,65,66	0
4	NAG	F	1	14/15	0.98	0.07	52,56,69,72	0

The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

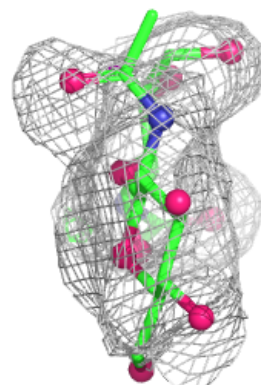
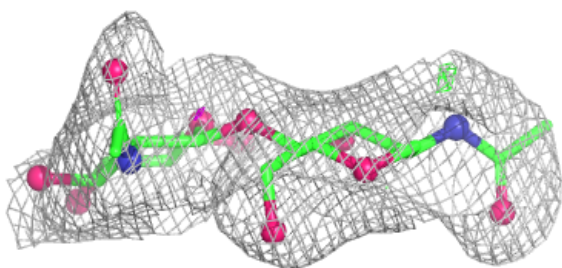
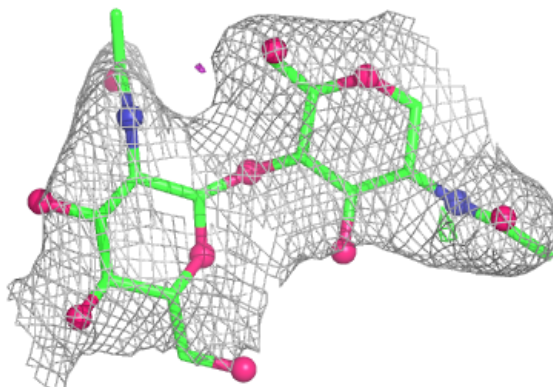
**Electron density around Chain C:**

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



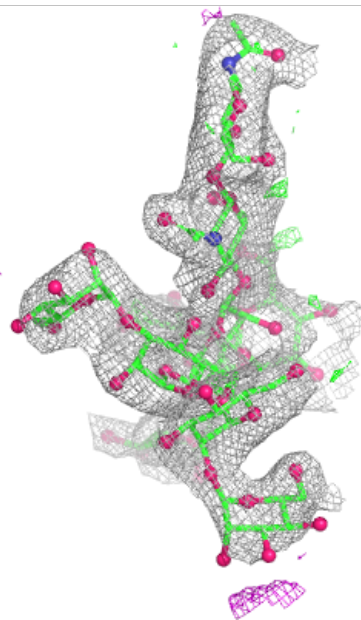
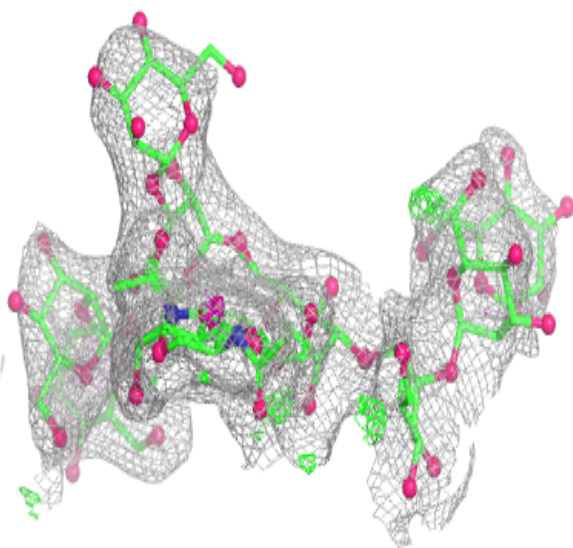
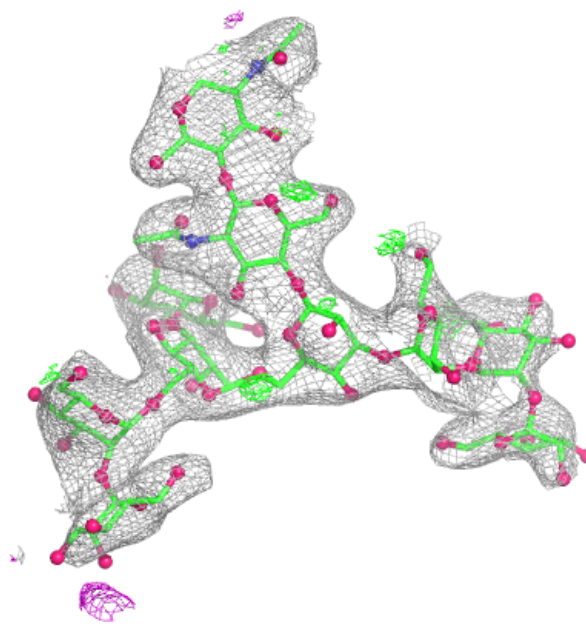
**Electron density around Chain E:**

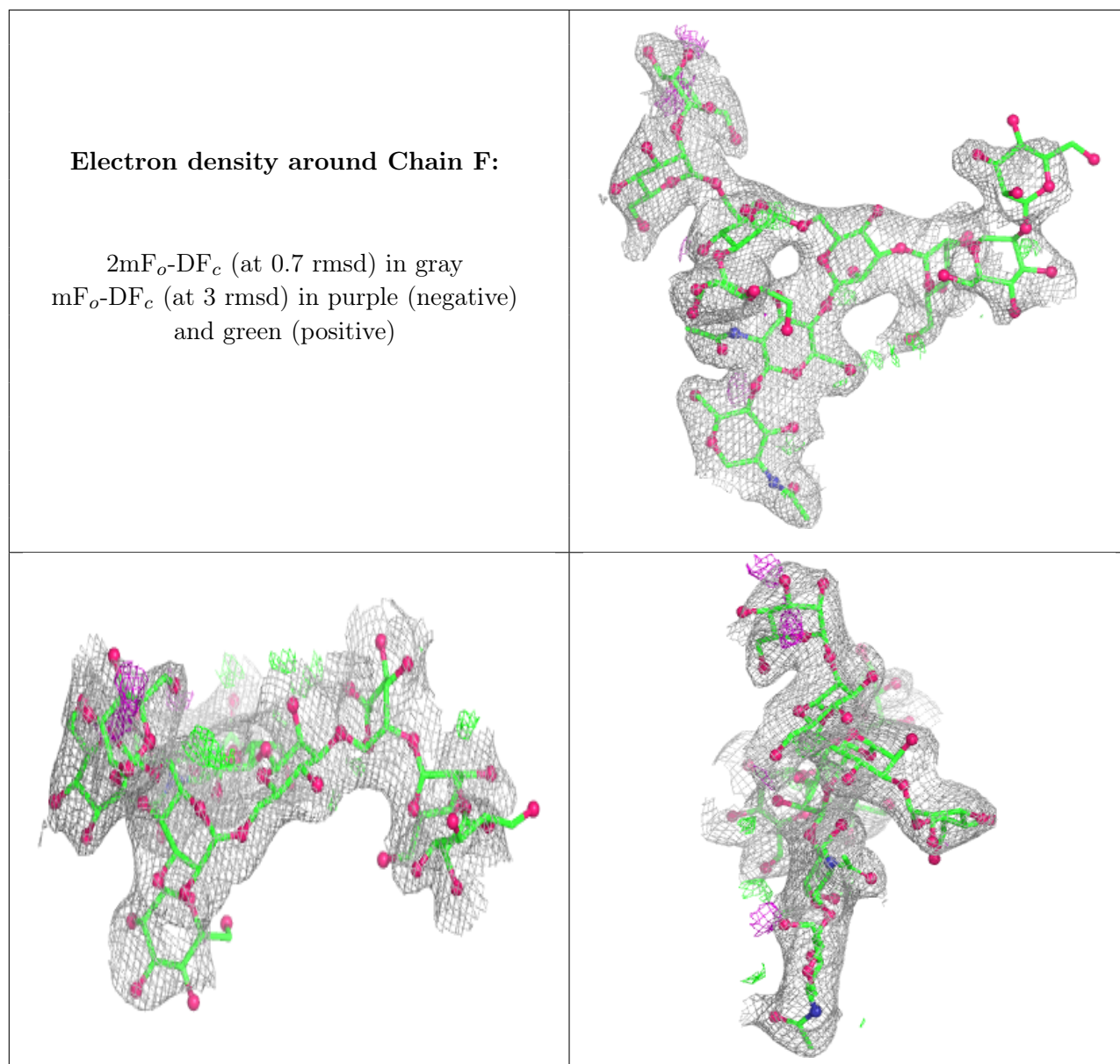
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around Chain D:**

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





## 6.4 Ligands [i](#)

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

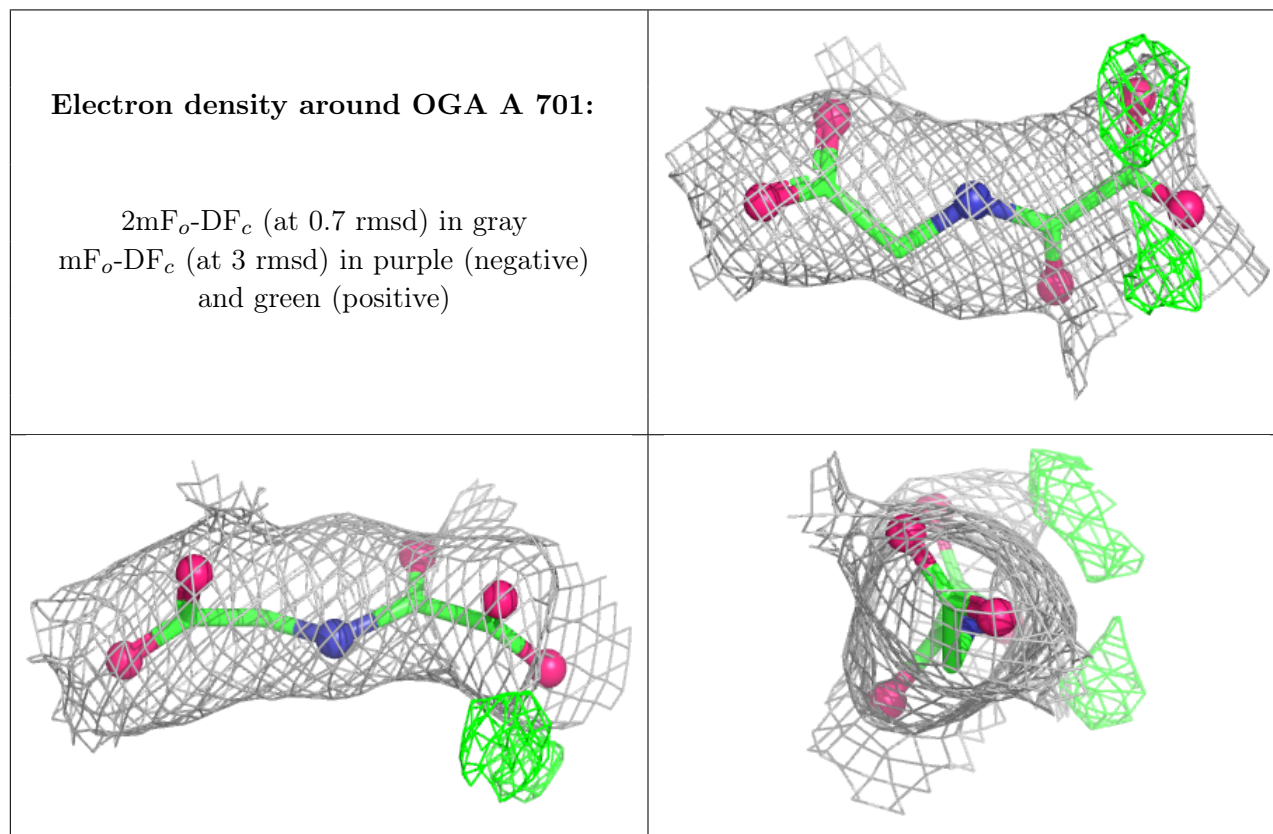
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
8	GLY	A	720	5/5	0.61	0.18	128,137,159,163	0
7	TBU	B	718	5/5	0.85	0.23	85,97,100,101	0
7	TBU	B	715	5/5	0.86	0.34	94,102,103,105	0
7	TBU	A	718	5/5	0.87	0.26	105,106,111,116	0
7	TBU	A	703	5/5	0.88	0.30	86,86,94,95	0

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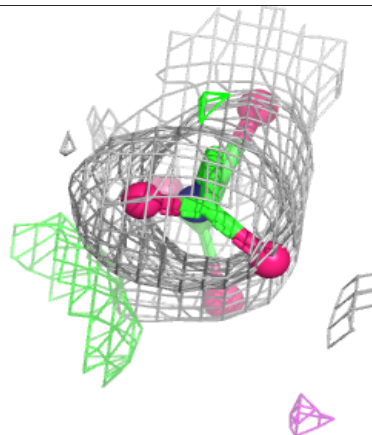
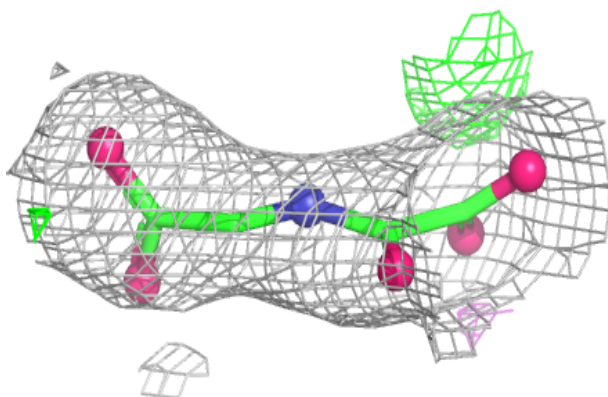
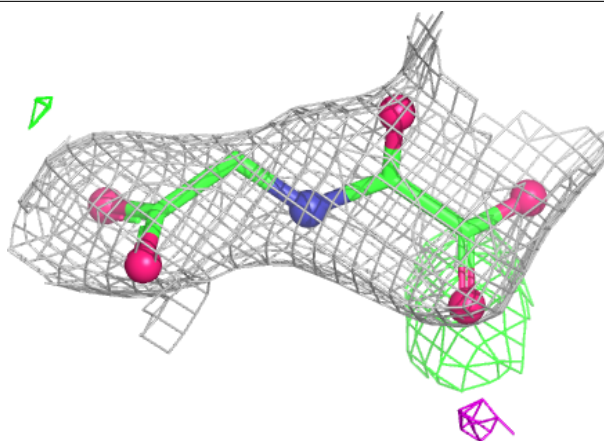
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
7	TBU	B	717	5/5	0.90	0.28	98,101,104,106	0
8	GLY	A	719	5/5	0.91	0.11	95,100,117,119	0
7	TBU	A	717	5/5	0.91	0.18	84,91,103,112	0
10	CL	A	723	1/1	0.91	0.16	102,102,102,102	0
7	TBU	B	716	5/5	0.92	0.25	80,84,95,102	0
7	TBU	A	716	5/5	0.93	0.21	81,85,87,92	0
10	CL	A	724	1/1	0.93	0.13	106,106,106,106	0
5	OGA	A	701	10/10	0.94	0.13	48,82,120,123	0
5	OGA	B	701	10/10	0.94	0.13	54,85,109,111	0
9	CA	B	719	1/1	0.98	0.04	100,100,100,100	0
9	CA	B	720	1/1	0.98	0.04	103,103,103,103	0
6	FE2	A	702	1/1	0.99	0.04	80,80,80,80	0
6	FE2	B	702	1/1	0.99	0.04	85,85,85,85	0
9	CA	A	721	1/1	1.00	0.03	69,69,69,69	0
9	CA	A	722	1/1	1.00	0.03	77,77,77,77	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.



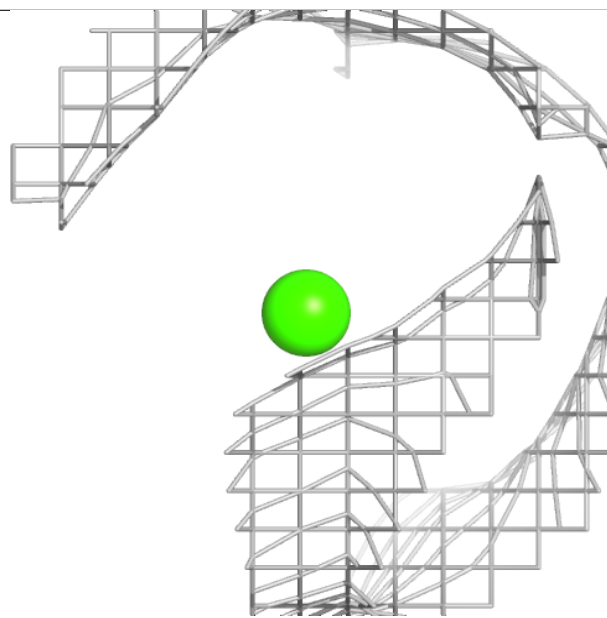
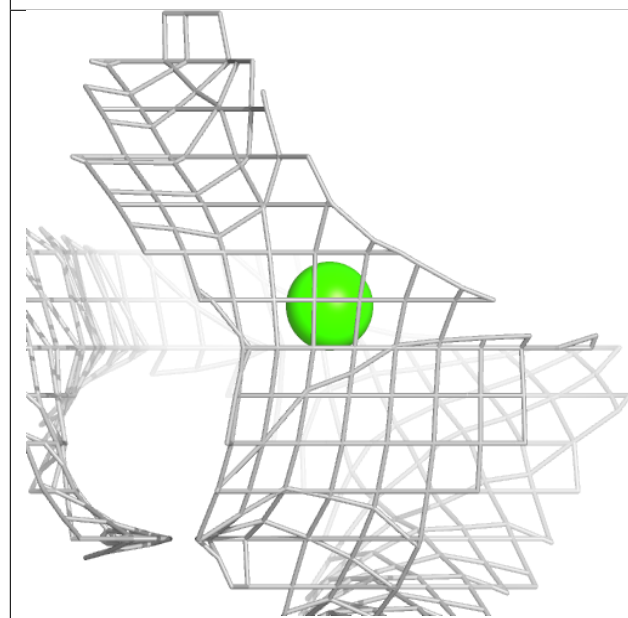
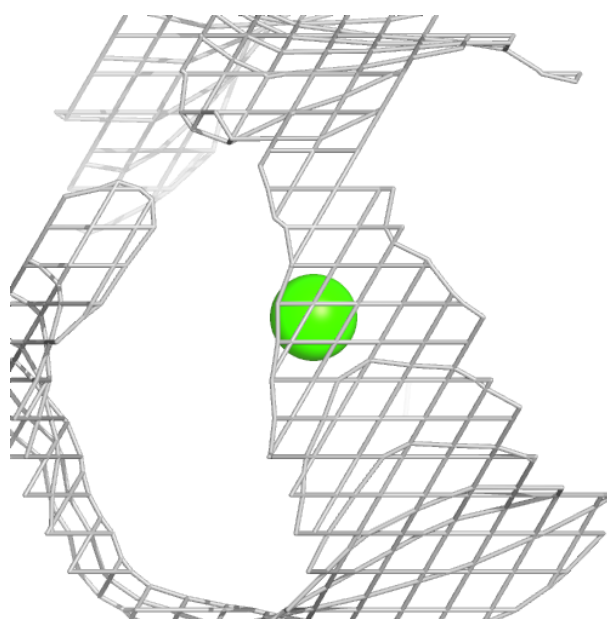
**Electron density around OGA B 701:**

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



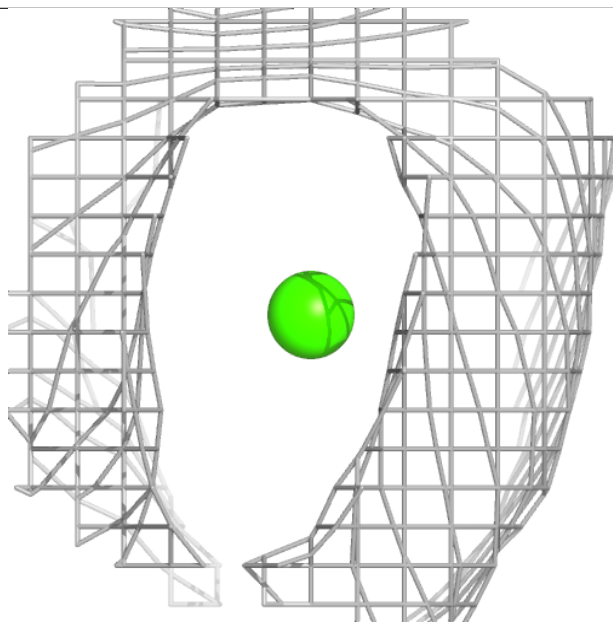
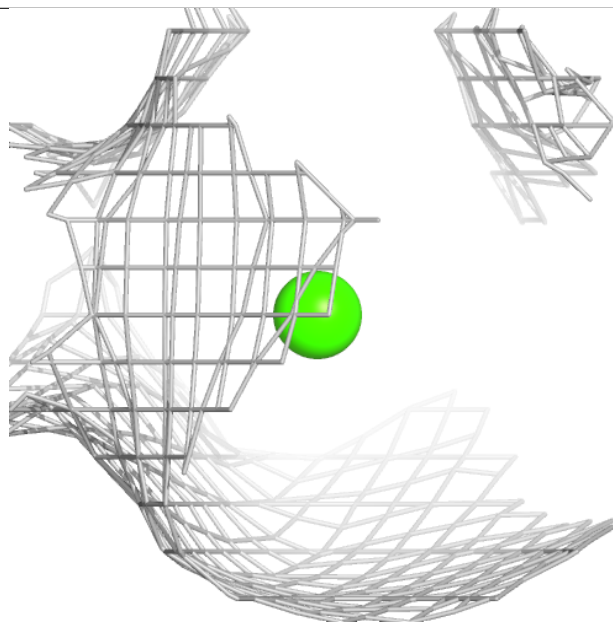
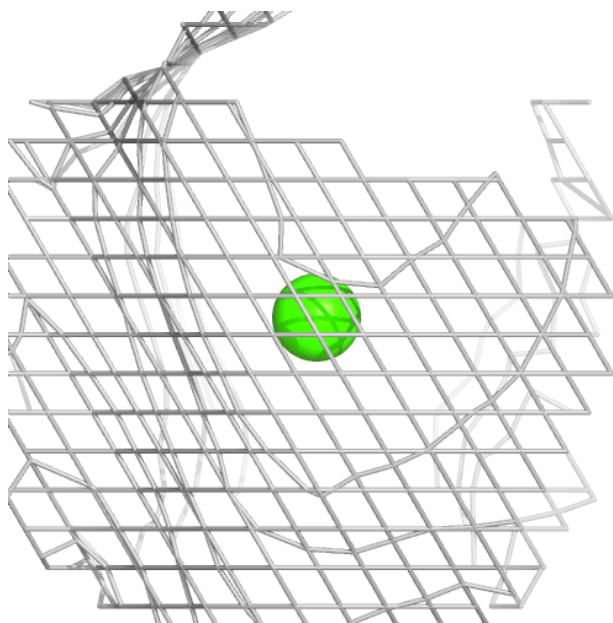
**Electron density around CA B 719:**

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and green (positive)



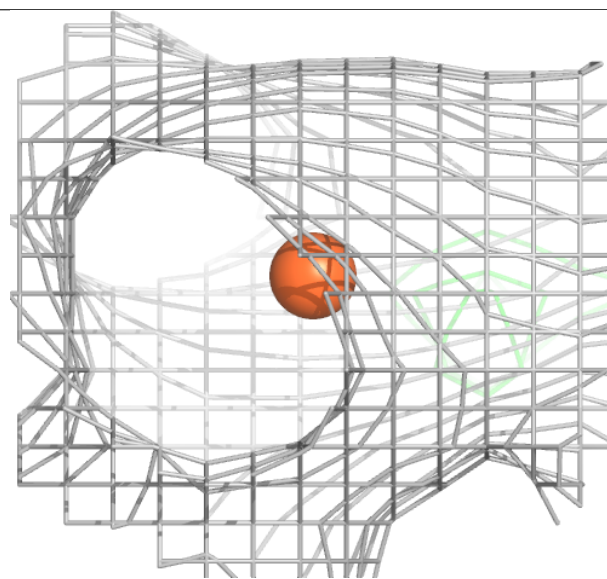
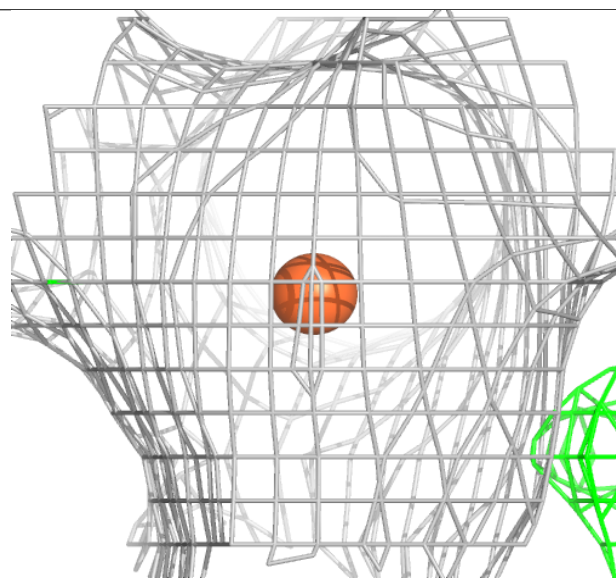
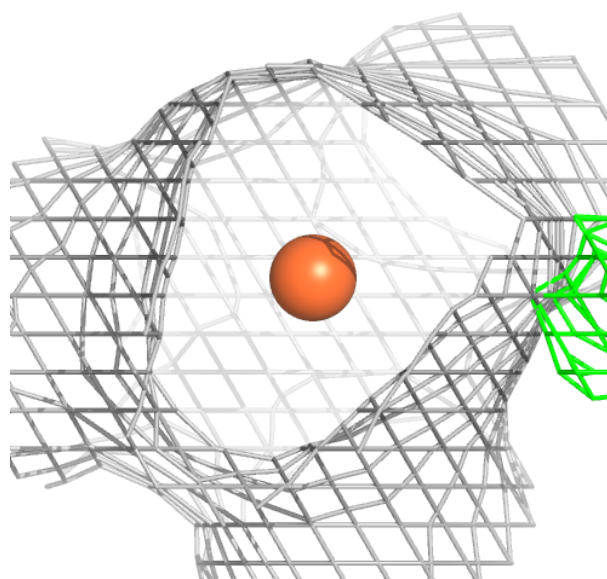
**Electron density around CA B 720:**

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and green (positive)



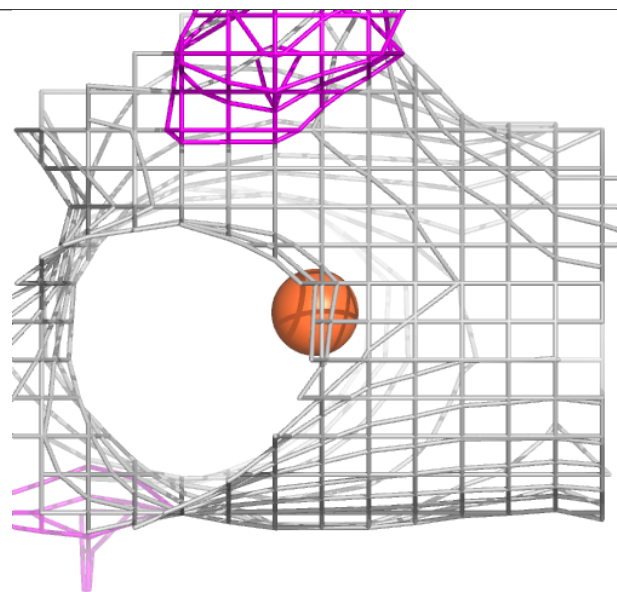
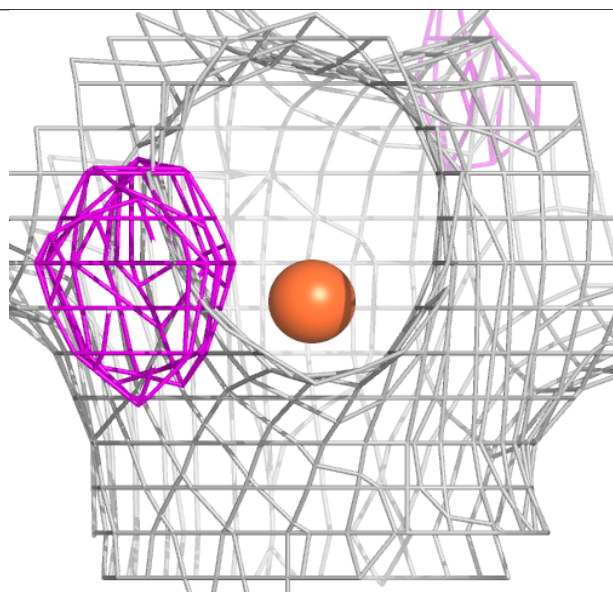
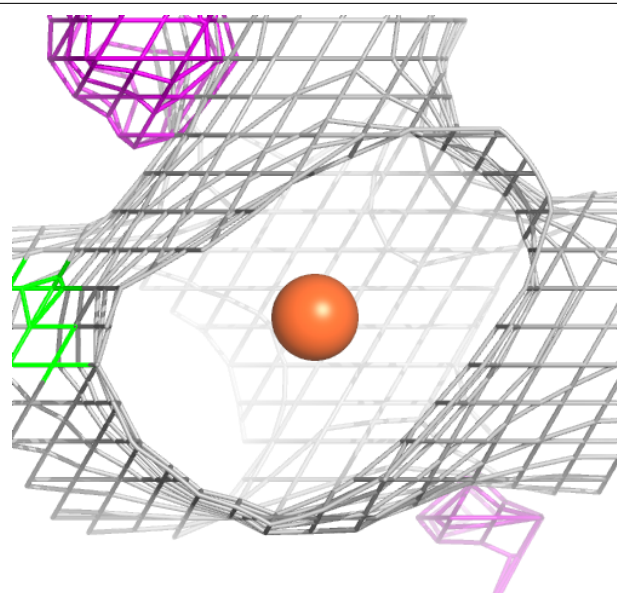
**Electron density around FE2 A 702:**

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and green (positive)



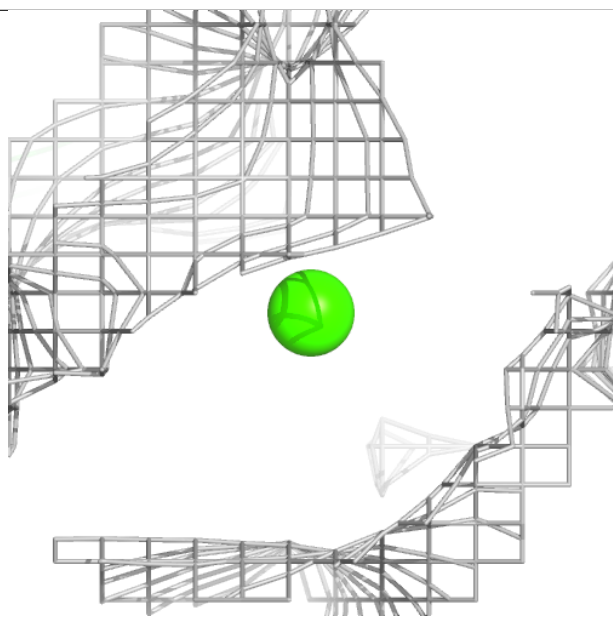
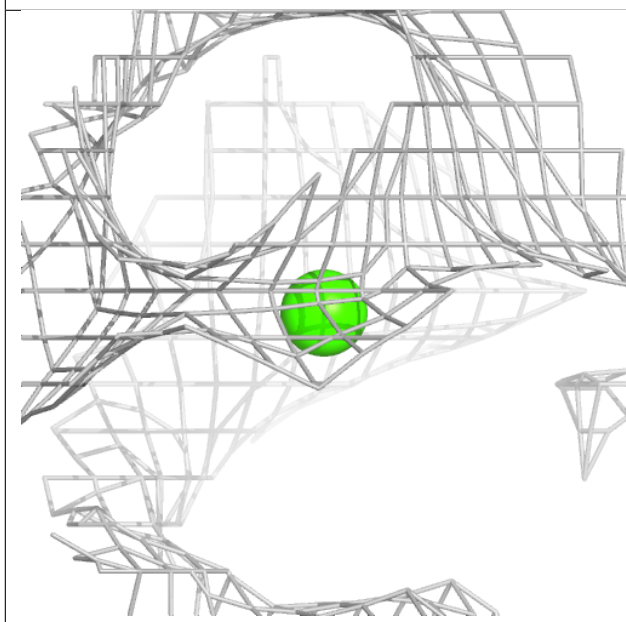
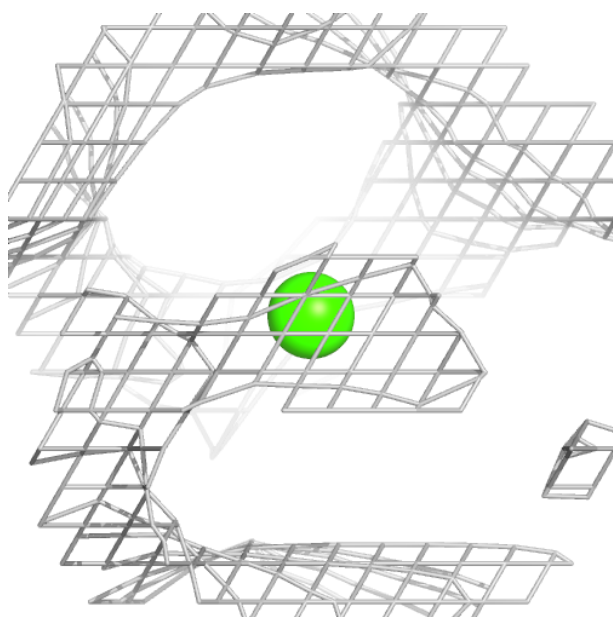
**Electron density around FE2 B 702:**

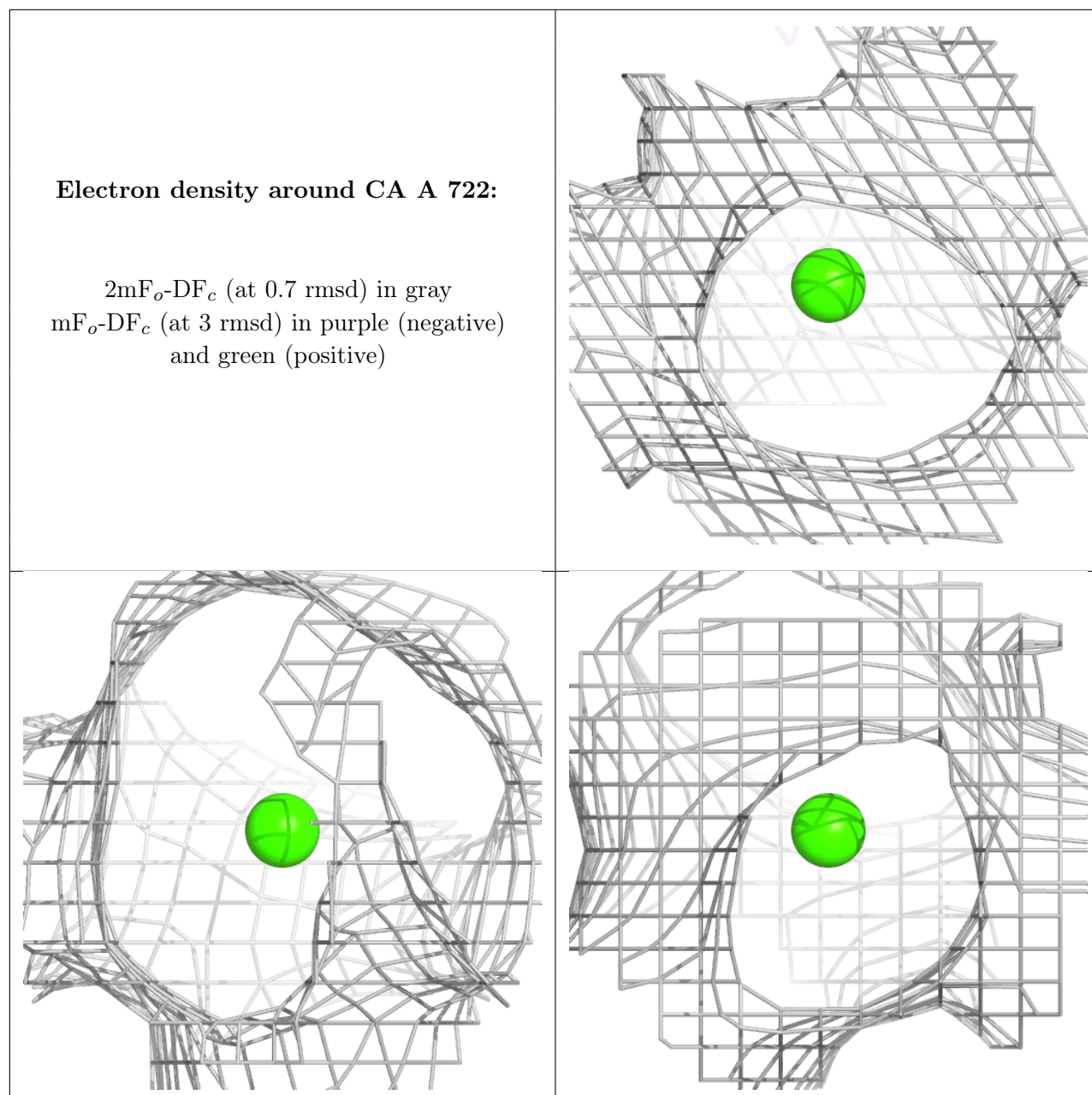
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around CA A 721:**

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





## 6.5 Other polymers [i](#)

There are no such residues in this entry.