



# Full wwPDB X-ray Structure Validation Report ⓘ

Nov 4, 2025 – 01:15 pm GMT

PDB ID : 9QAM / pdb\_00009qam  
Title : Human angiotensin-1 converting enzyme C-domain in complex with ciprofloxacin  
Authors : Gregory, K.S.; Acharya, K.R.  
Deposited on : 2025-02-28  
Resolution : 1.85 Å(reported)

This is a Full wwPDB X-ray Structure Validation 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	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.46

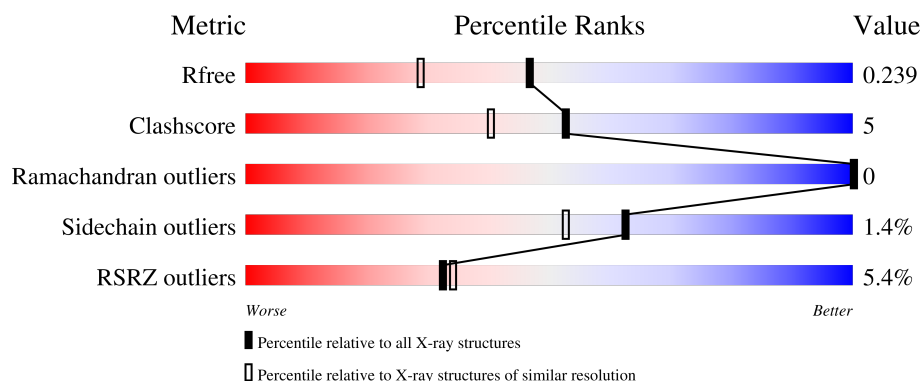
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.85 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	164625	3097 (1.86-1.86)
Clashscore	180529	3359 (1.86-1.86)
Ramachandran outliers	177936	3335 (1.86-1.86)
Sidechain outliers	177891	3335 (1.86-1.86)
RSRZ outliers	164620	3097 (1.86-1.86)

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	578	<div> <div>5%</div> <div> <div></div> <div>85%</div> <div>13%</div> <div>..</div> </div> </div>
2	C	3	<div> <div>100%</div> </div>
3	B	2	<div> <div>50%</div> <div>50%</div> </div>

## 2 Entry composition [i](#)

There are 12 unique types of molecules in this entry. The entry contains 5189 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.

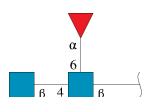
- Molecule 1 is a protein called Angiotensin-converting enzyme, soluble form.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	570	Total	C	N	O	S	0	8	0
			4707	3018	805	860	24			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	64	GLY	GLU	engineered mutation	UNP P12821
A	90	GLN	ASN	engineered mutation	UNP P12821
A	123	GLN	GLU	engineered mutation	UNP P12821
A	155	GLN	ASN	engineered mutation	UNP P12821
A	337	GLN	ASN	engineered mutation	UNP P12821
A	586	GLN	ASN	engineered mutation	UNP P12821

- Molecule 2 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
2	C	3	Total	C	N	O	0	0	0
			38	22	2	14			

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	B	2	Total	C	N	O	0	0	0
			25	14	1	10			

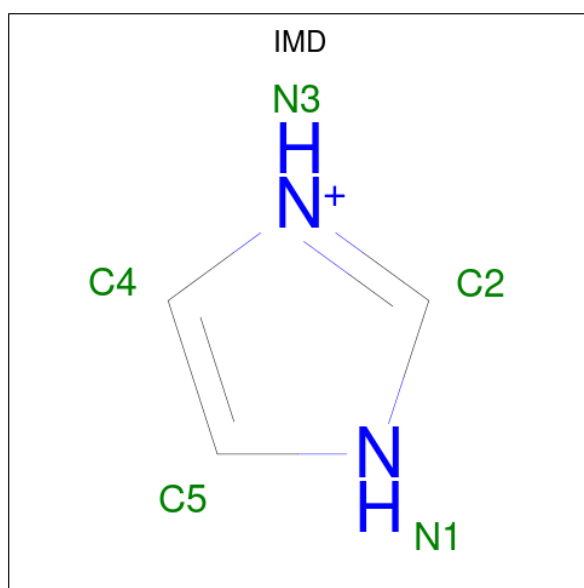
- Molecule 4 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

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

- Molecule 5 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

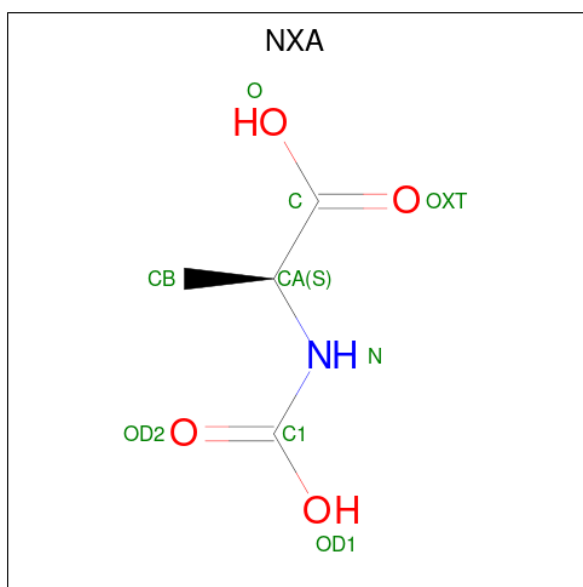
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	2	Total	Cl	0	0
			2	2		

- Molecule 6 is IMIDAZOLE (CCD ID: IMD) (formula: C<sub>3</sub>H<sub>5</sub>N<sub>2</sub>).



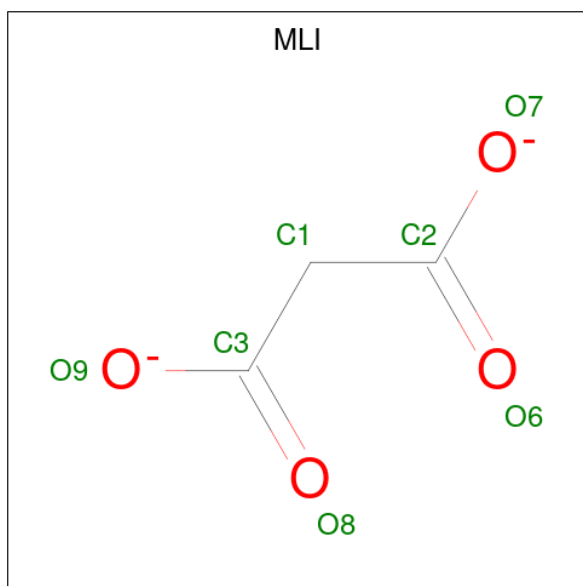
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	N	0	0
			5	3	2		

- Molecule 7 is N-CARBOXYALANINE (CCD ID: NXA) (formula: C<sub>4</sub>H<sub>7</sub>NO<sub>4</sub>).



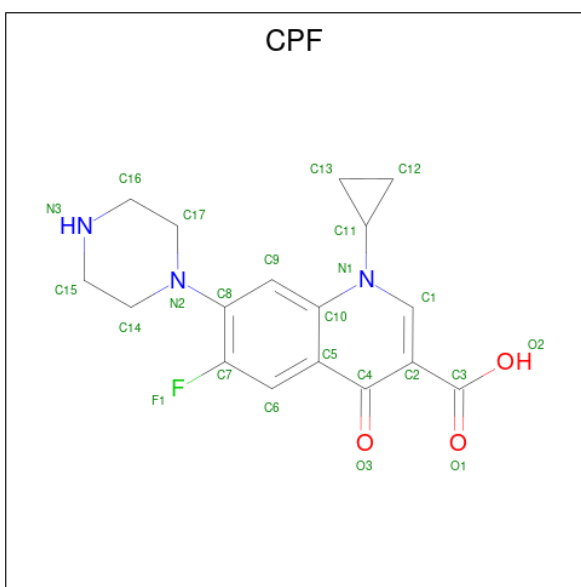
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	A	1	Total	C	N	O	0	0
			9	4	1	4		

- Molecule 8 is MALONATE ION (CCD ID: MLI) (formula:  $C_3H_2O_4$ ).



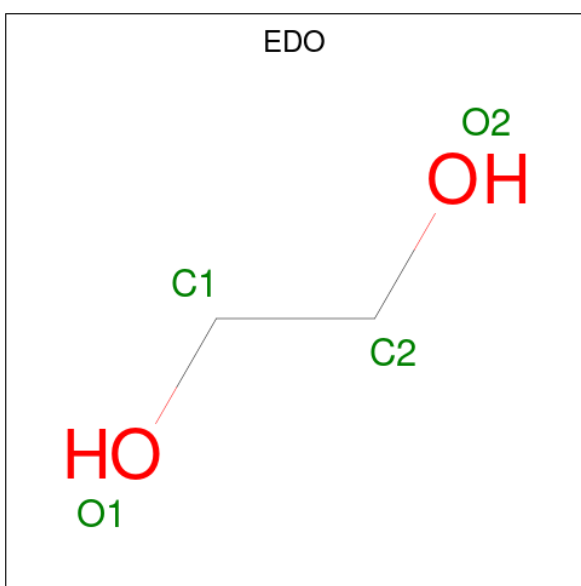
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	A	1	Total	C	O	0	0
			7	3	4		

- Molecule 9 is 1-CYCLOPROPYL-6-FLUORO-4-OXO-7-PIPERAZIN-1-YL-1,4-DIHYDR OQUINOLINE-3-CARBOXYLIC ACID (CCD ID: CPF) (formula:  $C_{17}H_{18}FN_3O_3$ ) (labeled as "Ligand of Interest" by depositor).



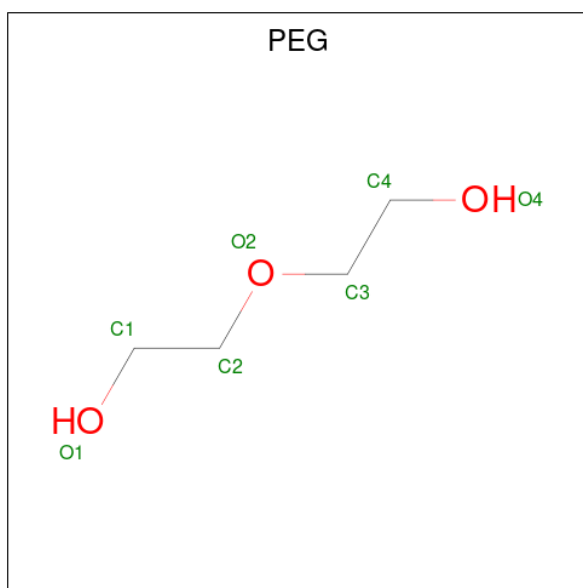
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
9	A	1	Total 24	C 17	F 1	N 3	O 3	0	0
9	A	1	Total 24	C 17	F 1	N 3	O 3	0	0

- Molecule 10 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C<sub>2</sub>H<sub>6</sub>O<sub>2</sub>).



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		

- Molecule 11 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula:  $C_4H_{10}O_3$ ).



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

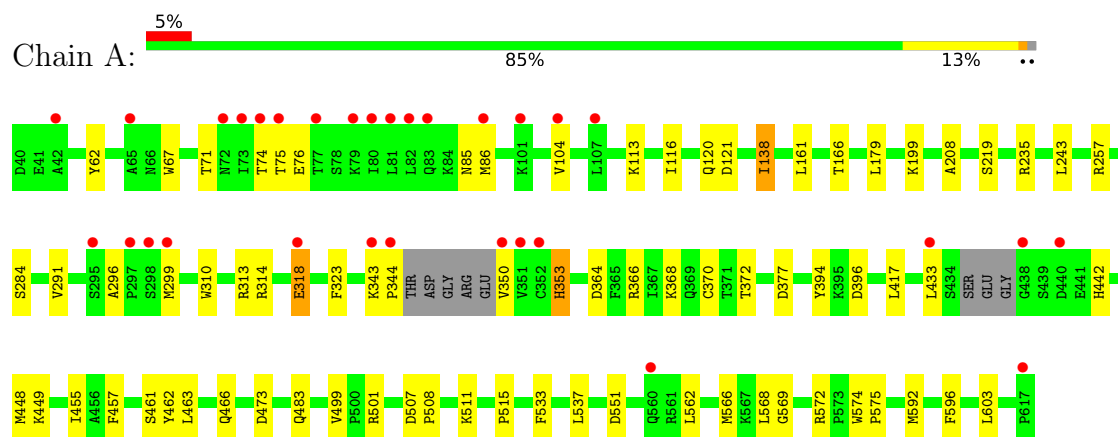
- Molecule 12 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
12	A	332	Total	O	0	0
			332	332		

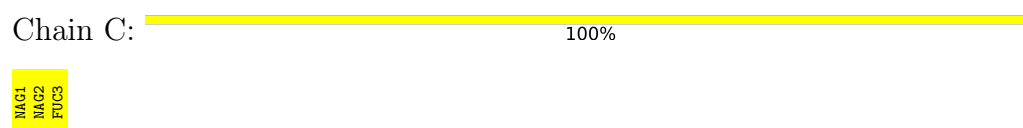
### 3 Residue-property plots [i](#)

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



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





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	60.09Å 85.42Å 135.66Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	72.39 – 1.85 72.28 – 1.85	Depositor EDS
% Data completeness (in resolution range)	100.0 (72.39-1.85) 99.9 (72.28-1.85)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.15 (at 1.84Å)	Xtriage
Refinement program	REFMAC 5.8.0430 (refmacat 0.4.100)	Depositor
R, $R_{free}$	0.199 , 0.227 0.210 , 0.239	Depositor DCC
$R_{free}$ test set	3064 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	25.6	Xtriage
Anisotropy	0.691	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 38.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	5189	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.28% 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

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: FUC, MLI, IMD, NXA, AH2, ZN, CL, PEG, EDO, NAG, CSO, CPF

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	0.62	0/4835	1.12	7/6565 (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

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	473	ASP	CA-CB-CG	6.54	119.14	112.60
1	A	364	ASP	CA-CB-CG	6.20	118.80	112.60
1	A	318	GLU	CB-CG-CD	5.83	122.50	112.60
1	A	291	VAL	N-CA-CB	5.70	119.19	111.21
1	A	551	ASP	CA-CB-CG	5.66	118.26	112.60
1	A	85	ASN	CB-CA-C	-5.39	101.84	110.79
1	A	372	THR	CA-CB-OG1	-5.34	101.59	109.60

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	235	ARG	Sidechain
1	A	313	ARG	Sidechain
1	A	572	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	4707	0	4549	43	0
2	C	38	0	34	1	0
3	B	25	0	13	1	0
4	A	1	0	0	0	0
5	A	2	0	0	0	0
6	A	5	0	5	0	0
7	A	9	0	5	0	0
8	A	7	0	2	0	0
9	A	48	0	34	6	0
10	A	8	0	12	5	0
11	A	7	0	10	0	0
12	A	332	0	0	2	0
All	All	5189	0	4664	47	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

All (47) 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:71:THR:O	1:A:350:VAL:HG12	1.75	0.84
1:A:62:TYR:CE1	9:A:707:CPF:H131	2.22	0.75
1:A:62:TYR:CZ	9:A:707:CPF:H131	2.23	0.74
1:A:219[A]:SER:OG	10:A:710:EDO:O1	2.10	0.68
1:A:62:TYR:CZ	9:A:707:CPF:C13	2.83	0.61
9:A:707:CPF:H121	9:A:707:CPF:H9	1.84	0.59
1:A:116:ILE:O	1:A:120:GLN:HG3	2.05	0.57
1:A:343:LYS:HG3	1:A:344:PRO:HD2	1.87	0.57
1:A:208:ALA:HA	10:A:710:EDO:H21	1.88	0.56
1:A:284:SER:HB2	1:A:449:LYS:HE2	1.88	0.56
9:A:707:CPF:H9	9:A:707:CPF:C12	2.36	0.55
1:A:104:VAL:HG22	1:A:113:LYS:HG3	1.89	0.55
1:A:161:LEU:O	1:A:166:THR:HG23	2.09	0.53
1:A:104:VAL:HG22	1:A:113:LYS:CG	2.41	0.51
1:A:501:ARG:HB2	10:A:709:EDO:H22	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1:NAG:H83	2:C:1:NAG:O3	2.11	0.49
1:A:296:ALA:HB1	1:A:442:HIS:CE1	2.48	0.49
1:A:299:MET:HB2	1:A:433:LEU:HD23	1.95	0.49
1:A:562:LEU:HB3	1:A:566:MET:HE2	1.94	0.48
1:A:462:TYR:O	1:A:466:GLN:HG2	2.15	0.47
1:A:353[B]:HIS:O	1:A:368:LYS:NZ	2.47	0.47
1:A:455:ILE:HD13	1:A:592:MET:HE2	1.98	0.46
1:A:457:PHE:CE2	1:A:461:SER:HB3	2.50	0.46
1:A:533:PHE:O	1:A:537:LEU:HG	2.17	0.45
1:A:574:TRP:N	1:A:575:PRO:CD	2.79	0.45
1:A:396:ASP:OD1	3:B:2:NAG:H82	2.15	0.45
1:A:76:GLU:O	1:A:76:GLU:HG3	2.15	0.45
1:A:86:MET:HA	1:A:86:MET:HE2	1.98	0.45
1:A:257:ARG:NH2	12:A:815:HOH:O	2.49	0.45
1:A:511:LYS:O	1:A:515:PRO:HD2	2.17	0.45
1:A:568:LEU:O	1:A:569:GLY:C	2.60	0.43
1:A:353[A]:HIS:O	1:A:368:LYS:NZ	2.51	0.43
1:A:343:LYS:HB2	1:A:370:CYS:SG	2.58	0.43
1:A:121:ASP:OD1	10:A:710:EDO:H12	2.18	0.43
1:A:507:ASP:N	1:A:508:PRO:CD	2.82	0.43
1:A:62:TYR:CD2	1:A:62:TYR:C	2.97	0.42
9:A:707:CPF:C13	9:A:707:CPF:H9	2.48	0.42
1:A:243:LEU:HD21	1:A:596:PHE:HB3	2.01	0.42
1:A:323:PHE:CZ	1:A:417:LEU:HD22	2.54	0.42
1:A:463:LEU:C	1:A:463:LEU:HD12	2.45	0.42
1:A:353[B]:HIS:CE1	12:A:1031:HOH:O	2.72	0.42
1:A:179:LEU:HD11	1:A:499:VAL:HG23	2.01	0.41
1:A:448:MET:HE1	1:A:603:LEU:HD21	2.03	0.41
1:A:138:ILE:CD1	1:A:199:LYS:HG3	2.50	0.41
1:A:310:TRP:CH2	1:A:318:GLU:HG3	2.56	0.41
1:A:483:GLN:HG3	10:A:709:EDO:H21	2.03	0.40
1:A:67:TRP:CD1	1:A:366:ARG:NH1	2.89	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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	571/578 (99%)	562 (98%)	9 (2%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	504/502 (100%)	496 (98%)	8 (2%)	58	46

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	74	THR
1	A	75	THR
1	A	138	ILE
1	A	314	ARG
1	A	353[A]	HIS
1	A	353[B]	HIS
1	A	377	ASP
1	A	394	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	442	HIS

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue is 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	$\# Z  > 2$
1	CSO	A	496	1	3,6,7	0.75	0	0,6,8	-	-

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
1	CSO	A	496	1	-	0/1/5/7	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.5 Carbohydrates ⓘ

5 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	AH2	B	1	3	11,11,11	1.12	1 (9%)	15,15,15	1.75	4 (26%)
3	NAG	B	2	3	14,14,15	0.44	0	17,19,21	1.00	1 (5%)
2	NAG	C	1	2,1	14,14,15	0.30	0	17,19,21	0.88	0
2	NAG	C	2	2	14,14,15	0.47	0	17,19,21	1.31	1 (5%)
2	FUC	C	3	2	10,10,11	0.32	0	14,14,16	1.03	1 (7%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	AH2	B	1	3	-	2/2/19/19	0/1/1/1
3	NAG	B	2	3	-	2/6/23/26	0/1/1/1
2	NAG	C	1	2,1	-	4/6/23/26	0/1/1/1
2	NAG	C	2	2	-	4/6/23/26	0/1/1/1
2	FUC	C	3	2	-	-	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1	AH2	C2-C3	3.04	1.57	1.52

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	2	NAG	C2-N2-C7	4.02	128.62	122.90
3	B	1	AH2	O3-C3-C2	3.39	116.49	109.99
3	B	1	AH2	C1-C2-C3	3.32	113.75	109.67
3	B	1	AH2	O2-C2-C3	2.64	115.43	110.14
2	C	3	FUC	C1-C2-C3	2.57	112.82	109.67
3	B	2	NAG	C1-C2-N2	2.44	114.65	110.49
3	B	1	AH2	C2-C3-C4	2.13	114.58	110.89

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	1	NAG	C8-C7-N2-C2

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Mol	Chain	Res	Type	Atoms
2	C	1	NAG	O7-C7-N2-C2
3	B	2	NAG	O7-C7-N2-C2
3	B	2	NAG	C8-C7-N2-C2
2	C	2	NAG	O5-C5-C6-O6
2	C	2	NAG	C4-C5-C6-O6
2	C	2	NAG	C8-C7-N2-C2
2	C	2	NAG	O7-C7-N2-C2
3	B	1	AH2	C4-C5-C6-O6
3	B	1	AH2	O5-C5-C6-O6
2	C	1	NAG	C4-C5-C6-O6
2	C	1	NAG	O5-C5-C6-O6

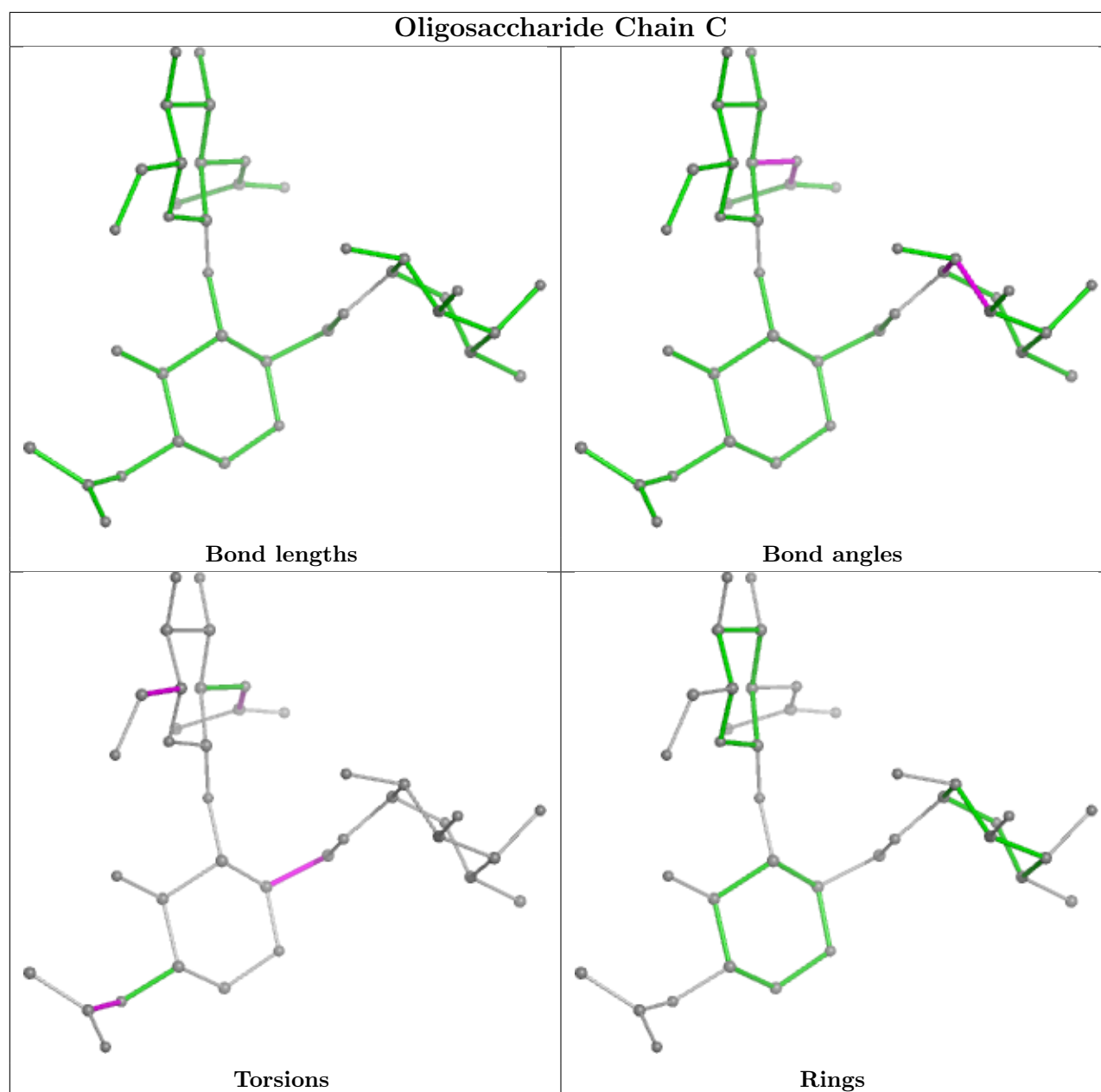
There are no ring outliers.

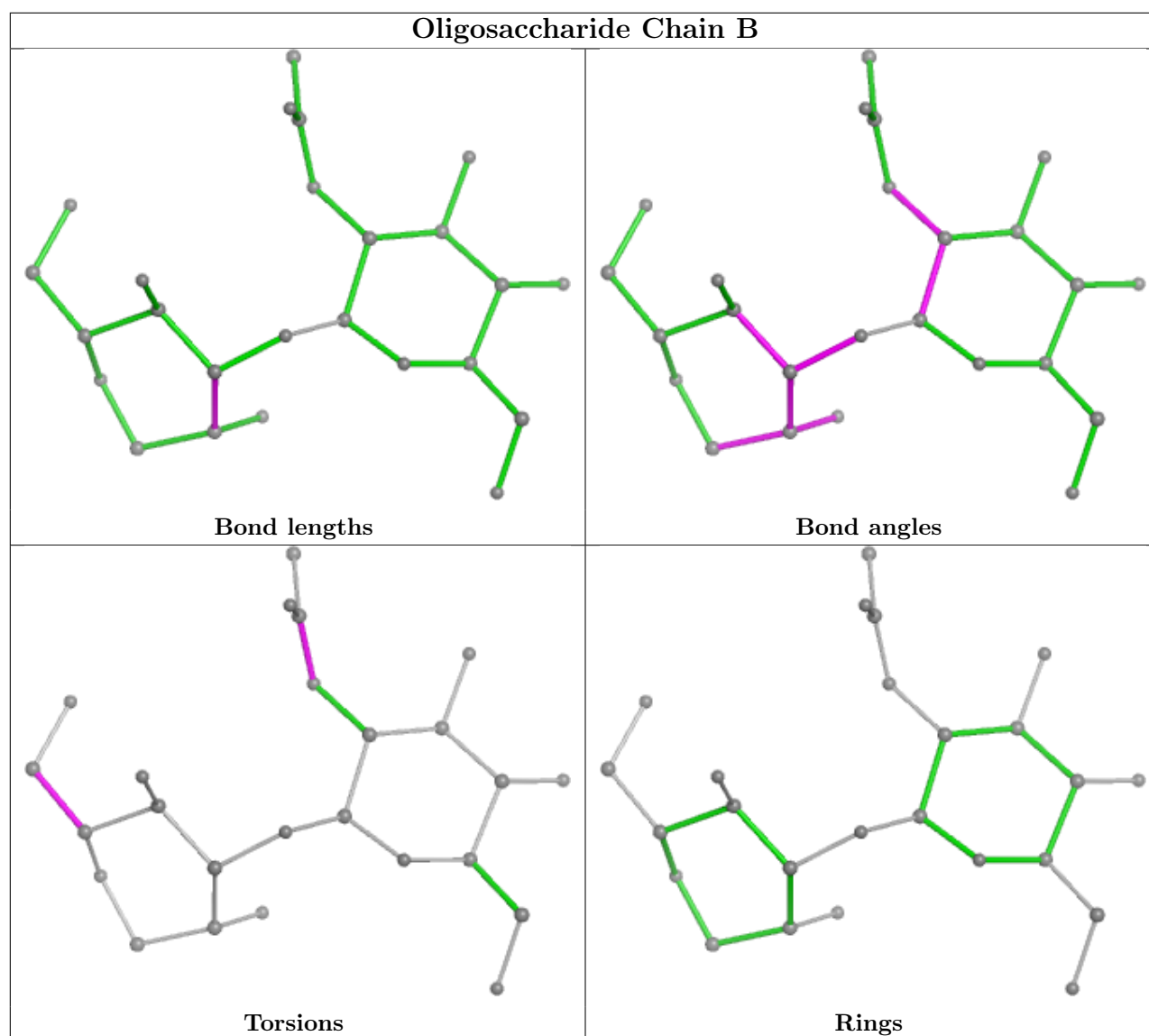
2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	2	NAG	1	0
2	C	1	NAG	1	0

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







## 5.6 Ligand geometry [i](#)

Of 11 ligands modelled in this entry, 3 are monoatomic - leaving 8 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	$\# Z  > 2$
6	IMD	A	704	-	3,5,5	0.29	0	4,5,5	0.68	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
9	CPF	A	708	-	27,27,27	0.91	0	40,40,40	1.13	5 (12%)
8	MLI	A	706	4	6,6,6	1.08	0	7,7,7	1.12	0
11	PEG	A	711	-	6,6,6	0.25	0	5,5,5	0.11	0
10	EDO	A	709	-	3,3,3	0.63	0	2,2,2	0.79	0
9	CPF	A	707	-	27,27,27	0.92	1 (3%)	40,40,40	2.05	10 (25%)
7	NXA	A	705	-	7,8,8	1.52	1 (14%)	8,10,10	0.89	0
10	EDO	A	710	-	3,3,3	0.31	0	2,2,2	0.20	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
6	IMD	A	704	-	-	-	0/1/1/1
9	CPF	A	708	-	-	2/12/22/22	0/4/4/4
8	MLI	A	706	4	-	0/4/4/4	-
11	PEG	A	711	-	-	3/4/4/4	-
10	EDO	A	709	-	-	0/1/1/1	-
9	CPF	A	707	-	-	6/12/22/22	0/4/4/4
7	NXA	A	705	-	-	1/8/8/8	-
10	EDO	A	710	-	-	1/1/1/1	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	A	705	NXA	O-C	-3.36	1.19	1.30
9	A	707	CPF	C9-C8	2.32	1.43	1.39

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	A	707	CPF	C10-N1-C11	7.68	127.97	119.89
9	A	707	CPF	C11-N1-C1	-5.01	112.16	119.73
9	A	707	CPF	C14-N2-C8	3.91	125.53	116.27
9	A	708	CPF	C17-N2-C8	3.55	124.67	116.27
9	A	707	CPF	C9-C10-N1	3.53	123.09	120.53
9	A	707	CPF	O1-C3-C2	-3.26	115.31	122.46
9	A	708	CPF	F1-C7-C8	2.71	120.89	118.42
9	A	707	CPF	F1-C7-C8	2.51	120.71	118.42
9	A	708	CPF	O1-C3-C2	-2.37	117.25	122.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	A	708	CPF	C14-N2-C8	2.32	121.78	116.27
9	A	707	CPF	C12-C11-N1	2.18	122.11	118.84
9	A	707	CPF	C17-N2-C8	2.15	121.38	116.27
9	A	708	CPF	O2-C3-C2	2.15	121.18	115.83
9	A	707	CPF	O2-C3-O1	2.15	128.53	123.61
9	A	707	CPF	C7-C8-N2	2.11	122.98	120.47

There are no chirality outliers.

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	A	707	CPF	C12-C11-N1-C1
9	A	707	CPF	C13-C11-N1-C1
9	A	707	CPF	C12-C11-N1-C10
9	A	708	CPF	C9-C8-N2-C17
9	A	708	CPF	C7-C8-N2-C17
9	A	707	CPF	C13-C11-N1-C10
11	A	711	PEG	O2-C3-C4-O4
9	A	707	CPF	C9-C8-N2-C14
9	A	707	CPF	C7-C8-N2-C14
11	A	711	PEG	C4-C3-O2-C2
10	A	710	EDO	O1-C1-C2-O2
11	A	711	PEG	O1-C1-C2-O2
7	A	705	NXA	OD2-C1-N-CA

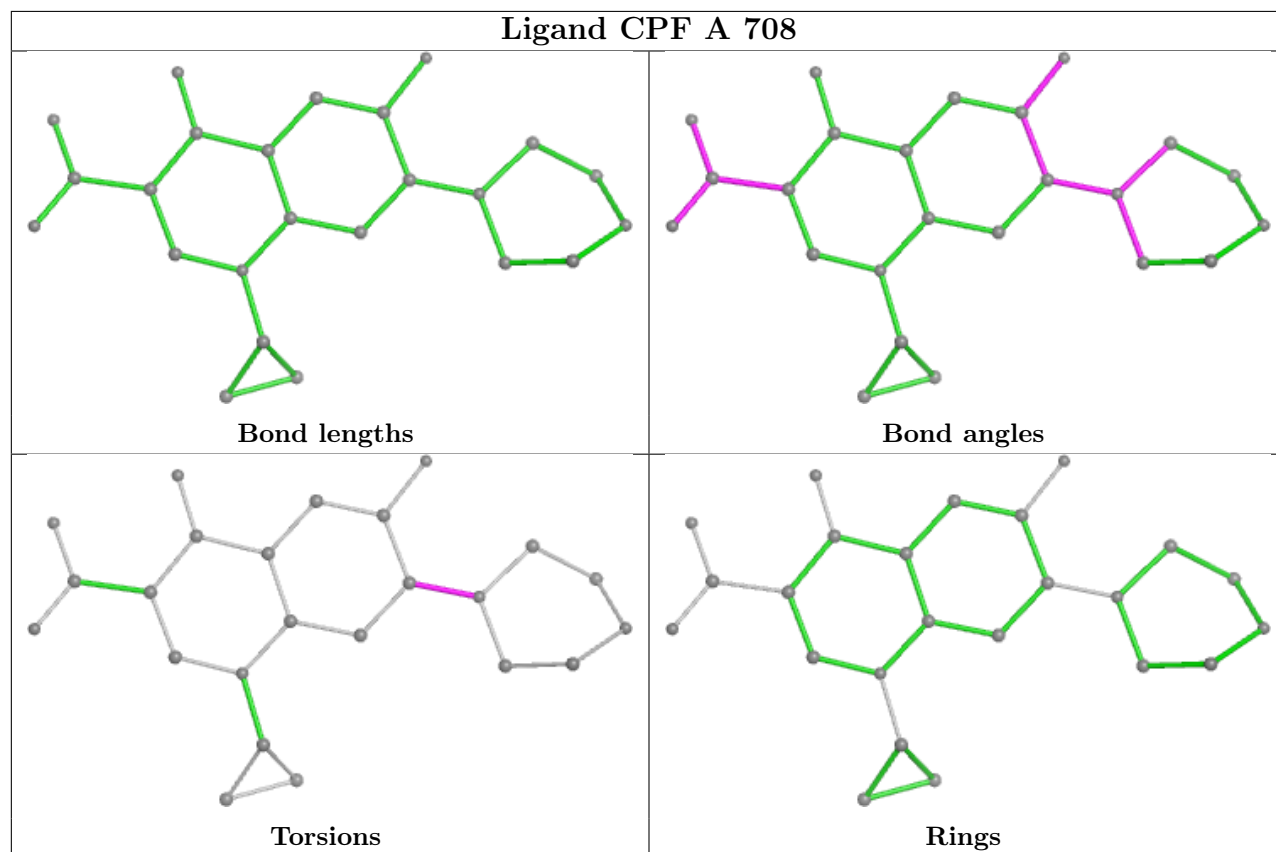
There are no ring outliers.

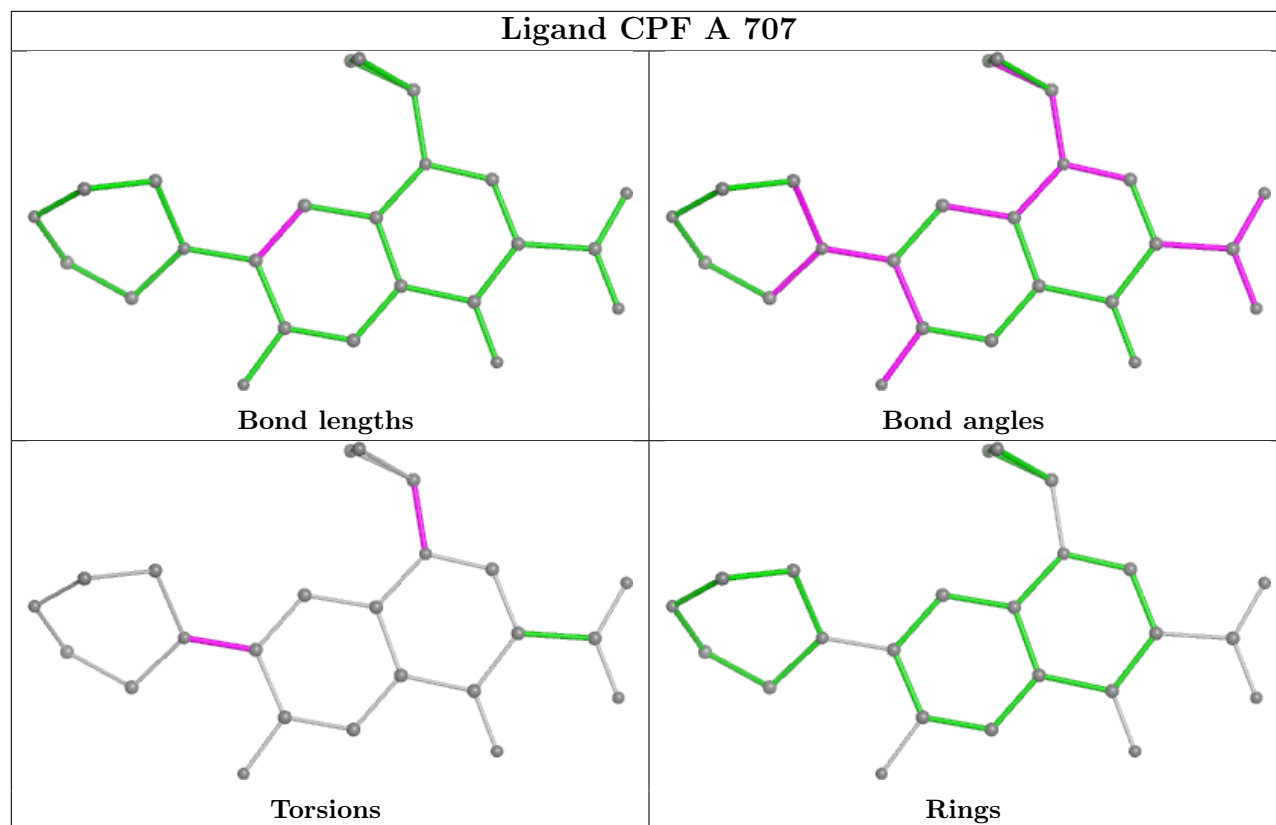
3 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	A	709	EDO	2	0
9	A	707	CPF	6	0
10	A	710	EDO	3	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 ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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	569/578 (98%)	0.32	31 (5%) 32 34	10, 32, 62, 86	8 (1%)

All (31) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	73	ILE	5.8
1	A	344	PRO	5.8
1	A	299	MET	4.8
1	A	82	LEU	3.8
1	A	438	GLY	3.6
1	A	75	THR	3.5
1	A	350	VAL	3.3
1	A	74	THR	3.1
1	A	107	LEU	3.1
1	A	440	ASP	3.1
1	A	104	VAL	3.0
1	A	351	VAL	3.0
1	A	297	PRO	3.0
1	A	77	THR	3.0
1	A	101	LYS	2.9
1	A	560	GLN	2.9
1	A	617	PRO	2.8
1	A	79	LYS	2.8
1	A	86	MET	2.7
1	A	72	ASN	2.7
1	A	295	SER	2.7
1	A	83	GLN	2.5
1	A	80	ILE	2.5
1	A	81	LEU	2.3
1	A	65	ALA	2.2
1	A	42	ALA	2.2
1	A	318	GLU	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	343	LYS	2.2
1	A	298	SER	2.1
1	A	433	LEU	2.1
1	A	352	CYS	2.1

## 6.2 Non-standard residues in protein, DNA, RNA chains [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
1	CSO	A	496	7/8	0.97	0.06	20,21,22,24	0

## 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.

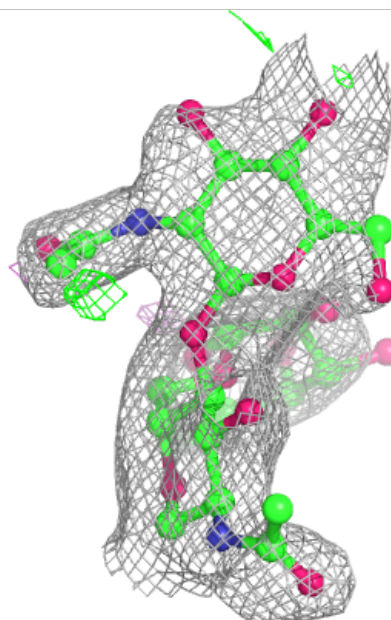
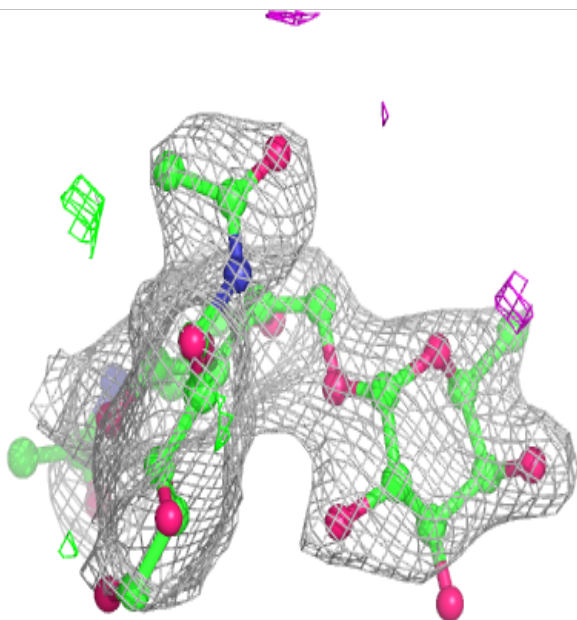
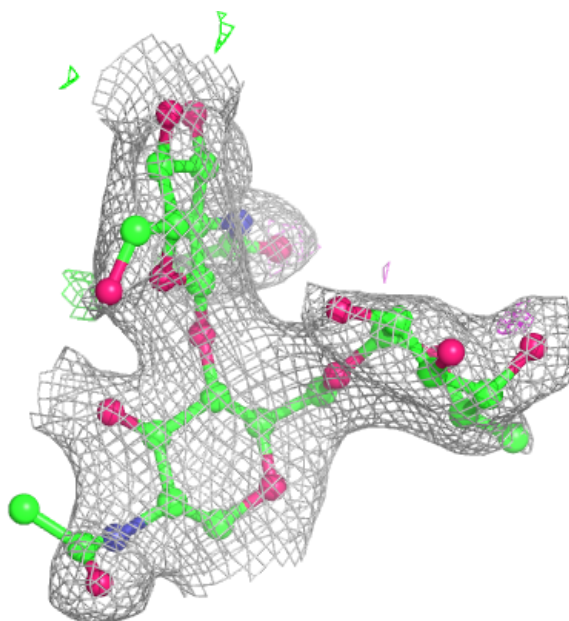
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
2	NAG	C	1	14/15	-	-	49,58,67,68	0
3	NAG	B	2	14/15	0.77	0.16	54,75,87,87	0
2	FUC	C	3	10/11	-	-	49,59,66,74	0
3	AH2	B	1	11/11	-	-	68,74,81,87	0
2	NAG	C	2	14/15	0.78	0.16	52,63,68,68	0

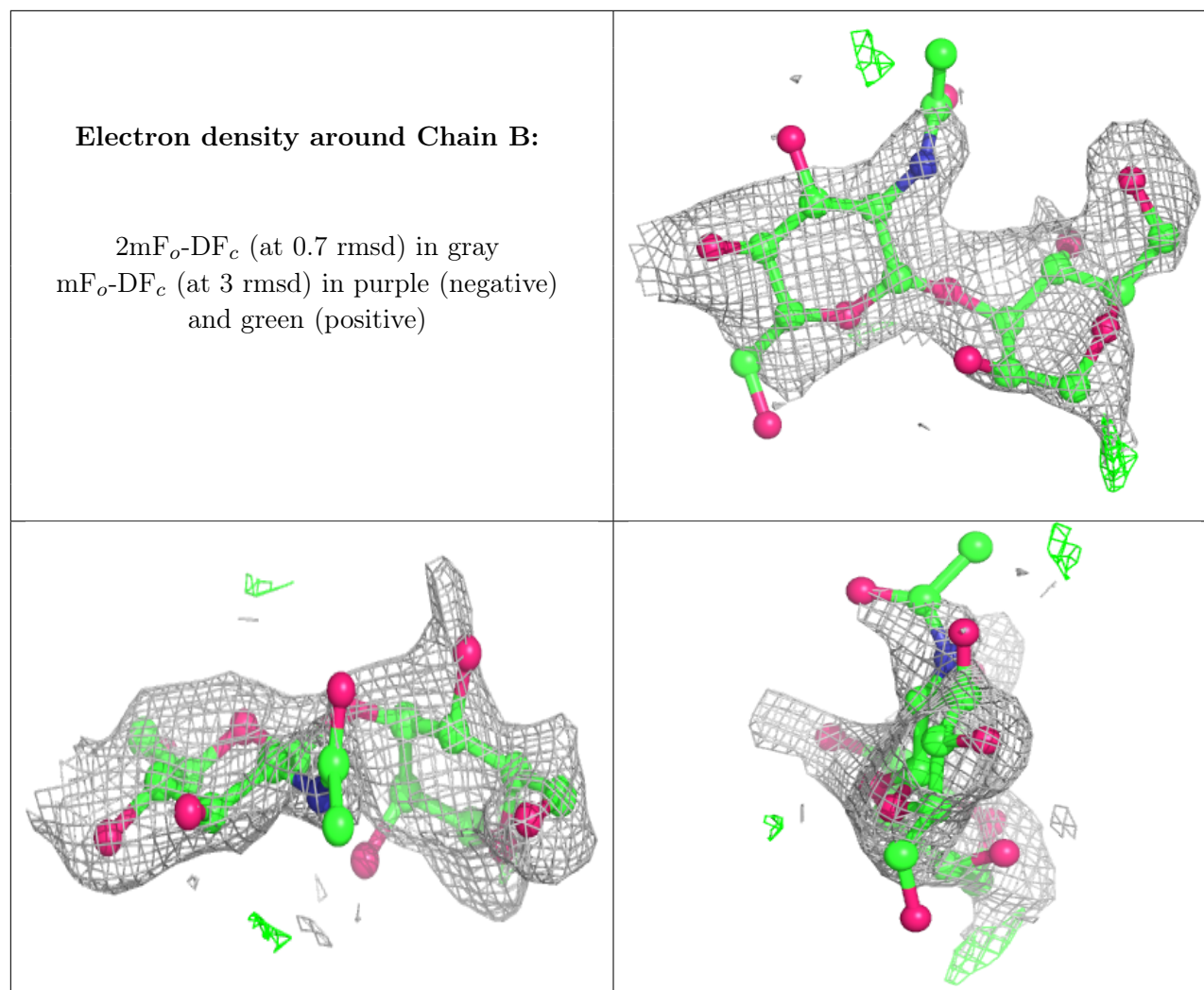
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.



**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)





## 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, 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.

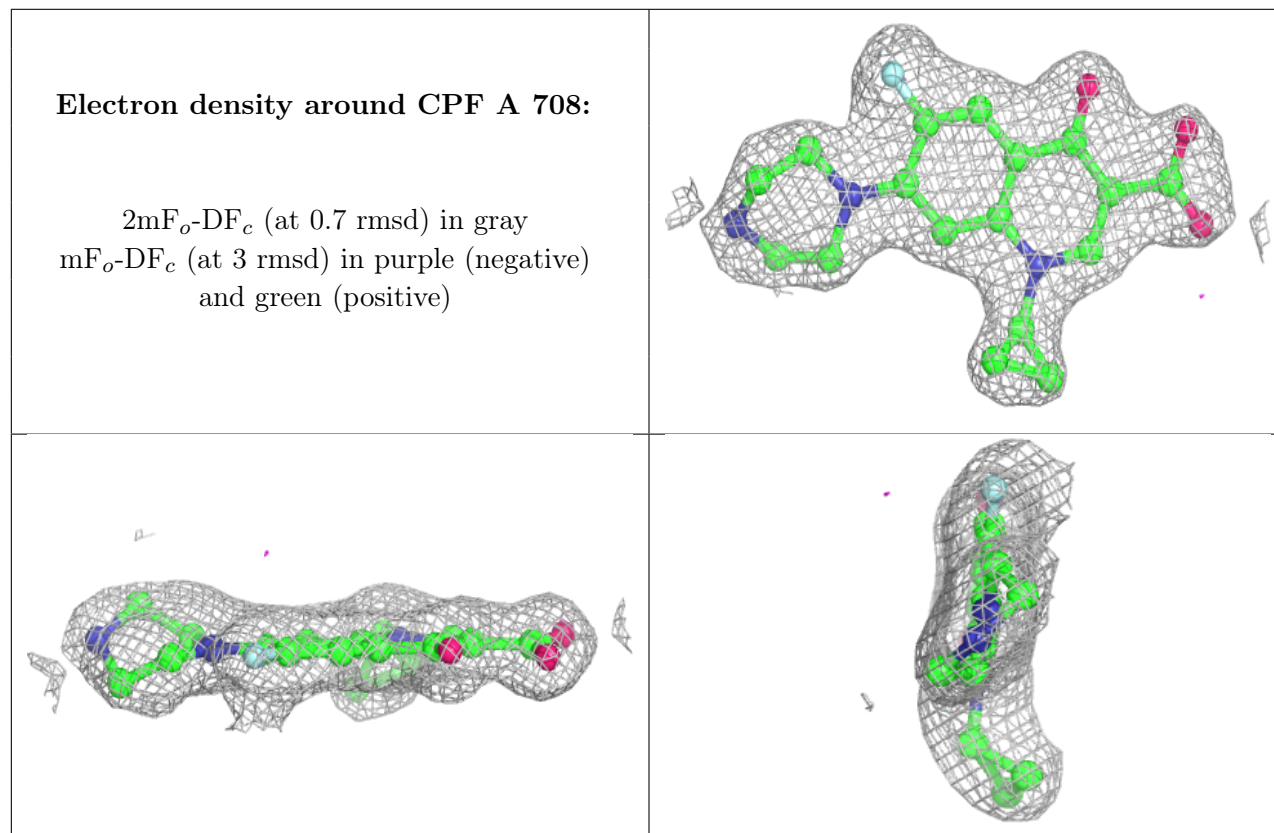
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
10	EDO	A	709	4/4	0.82	0.18	42,48,52,53	0
10	EDO	A	710	4/4	0.86	0.14	32,37,39,42	0
11	PEG	A	711	7/7	0.88	0.14	48,49,55,56	0
7	NXA	A	705	9/9	0.90	0.11	24,32,41,52	0
9	CPF	A	708	24/24	0.91	0.11	43,51,63,67	0
9	CPF	A	707	24/24	0.92	0.10	37,43,51,52	0
8	MLI	A	706	7/7	0.94	0.10	25,33,54,55	0
6	IMD	A	704	5/5	0.95	0.08	34,35,36,38	0
5	CL	A	703	1/1	0.99	0.03	22,22,22,22	0

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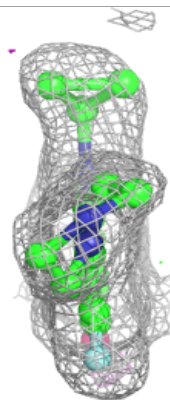
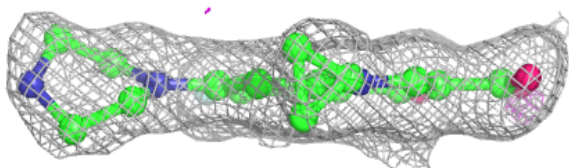
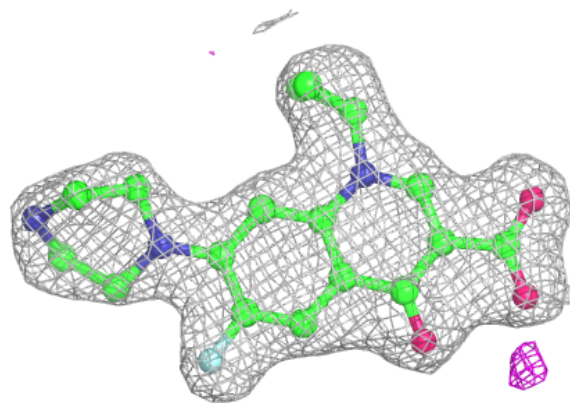
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
5	CL	A	702	1/1	1.00	0.02	21,21,21,21	0
4	ZN	A	701	1/1	1.00	0.05	25,25,25,25	0

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.



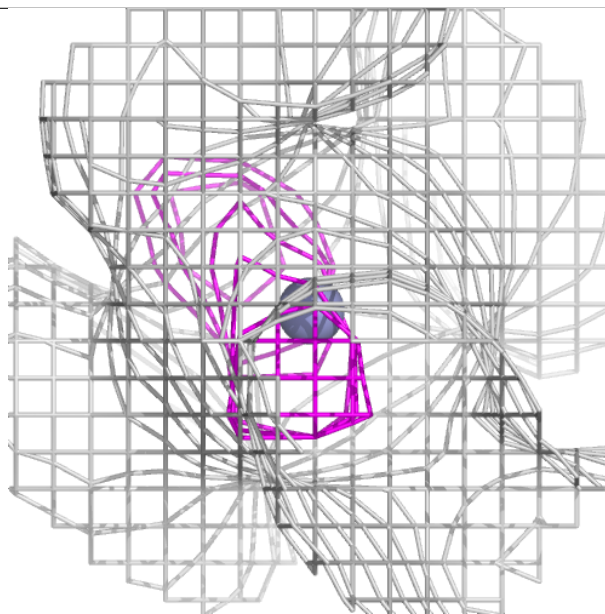
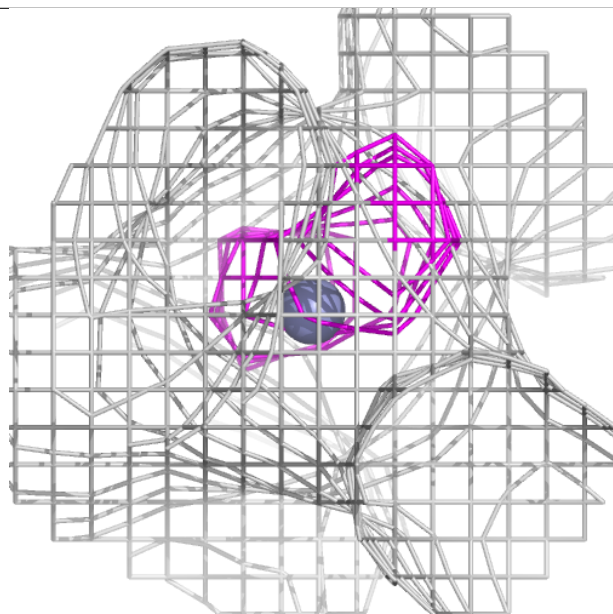
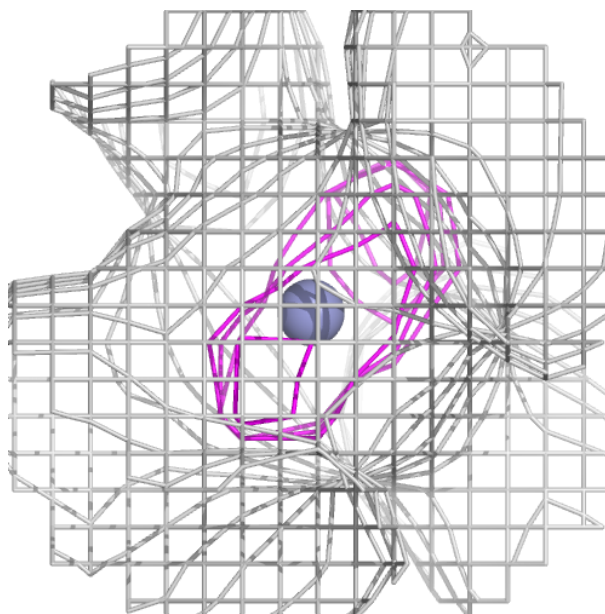
**Electron density around CPF A 707:**

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



**Electron density around ZN A 701:**

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



## 6.5 Other polymers ⓘ

There are no such residues in this entry.